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Stochastic geometry models in image analysis and spatial statistics

M.N.M. van Lieshout

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PREFACE

This monograph is a revision of my dissertation at the Vrije Universiteit Amsterdam which was completed in 1994. Many thanks are due to my promotor A J Baddeley and co-promotor J Oosterhoff for their support.

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M N M van Lieshout

Coventry February 1995

Table of Contents

1	Intr	roduction	11
2	Ma	ximum likelihood object recognition	17
	2.1	Object recognition	17
	2.2	Noise models	19
	2.3	Maximum likelihood estimation	22
		2.3.1 Connection with mathematical morphology	23
		2.3.2 Relation to pre-processing	24
	2.4	Iterative methods for MLE	27
		2.4.1 Add-and-delete algorithms	27
		2.4.2 General add-delete-shift algorithms	28
	2.5	Relation to Hough transform	30
	2.6	Example	32
3	Ma	rkov spatial processes	35
	3.1	Survey of Markov spatial models	35
		3.1.1 Objects	35
		3.1.2 Markov object processes	36
		3.1.3 Nearest-neighbour Markov object processes	39
	3.2	Area-interaction processes	42
		3.2.1 Definition of the process	42
		3.2.2 Limiting cases	46
		3.2.3 Markov property	47
	3.3	Stationary area-interaction process	50

	3.4	İnferei	1ce	52
		3.4.1	Sufficient statistics, exponential families	52
		3.4.2	Maximum likelihood	52
		3.4.3	Takacs-Fiksel	53
		3.4.4	Approximation by lattice processes	54
		3.4.5	Pseudolikelihood estimation	56
4	Bav	esian d	bject recognition	59
-	4 1	Gener		59
	1.1	4.1.1	Prior models	60
	4.2	Iterati	ve algorithms	62
	1.2	4.2.1	Examples	63
		4 2 2	Belation to Hough transform	64
		4.2.3	Parameter estimation	65
	4.3	Perfor	mance evaluation	69
		4.3.1	Beconstructions	69
		4.3.2	Typical behaviour	71
		4.3.3	Initial state influence	73
		4.3.4	Noise influence	74
	4.4	Fixed	temperature sampling	75
		4.4.1	Construction	76
	4.5	Conve	rgence of inhomogeneous Markov processes	82
		4.5.1	Definitions	82
		4.5.2	Limit theorems	84
	4.6	Object	recognition by stochastic annealing	87
		4.6.1	The summability condition	87
		4.6.2	The Dobrushin condition	88
		4.6.3	Example	91
		4.6.4	Remarks and extensions	94
	4.7	Impler	nentation and computational complexity	96
		4.7.1	Sampling	97
		4.7.2	Multiresolution techniques	98
5	Spat	tial clu	stering	103
-	5.1	Introd	uction	103
	5.2	Cluste	r processes	105
		5.2.1	General	105
		5.2.2	Inhomogeneous Poisson models	106
	5.3	Maxin	um likelihood estimation	109
	5.4	The B	ayesian approach	111
		5.4.1	Deterministic algorithms	111
		5.4.2	Stochastic algorithms	112

 5.5 Example. 5.5.1 Model. 5.5.2 Analysis 5.6 Offspring Assignment. 5.6.1 Overview. 5.6.2 The Metropolis step 5.6.3 The Gibbs step 5.6.4 Convergence 5.6.5 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection Markov properties of cluster processes 6.1 Setup 6.1.1 Markov point processes 6.2 Statement of results 	115 116 118 123				
 5.5 Example	115116118123102				
5.5.1 Model 5.5.2 Analysis 5.6 Offspring Assignment 5.6.1 Overview 5.6.2 The Metropolis step 5.6.3 The Gibbs step 5.6.4 Convergence 5.6.5 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results	116 118 123				
 5.5.2 Analysis	118 123				
 5.6 Offspring Assignment	123				
5.6.1 Overview 5.6.2 The Metropolis step 5.6.3 The Gibbs step 5.6.4 Convergence 5.6.5 Relations to other methods 5.6.6 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs	109				
5.6.2 The Metropolis step 5.6.3 The Gibbs step 5.6.4 Convergence 5.6.5 Relations to other methods 5.6.6 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs	123				
5.6.3 The Gibbs step 5.6.4 Convergence 5.6.5 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection Markov properties of cluster processes 6.1 Setup 6.1.1 Markov point processes 6.2 Statement of results	124				
5.6.4 Convergence 5.6.5 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results	126				
5.6.5 Relations to other methods 5.7 Other applications 5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection 5.7.2 High-level edge detection 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs	127				
 5.7 Other applications	128				
5.7.1 Fitting curves to point patterns 5.7.2 High-level edge detection 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results	130				
5.7.2 High-level edge detection Markov properties of cluster processes 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs	130				
Markov properties of cluster processes 6.1 Setup 6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs	130				
 6.1 Setup	133				
6.1.1 Markov point processes 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs	133				
 6.1.2 Cluster processes 6.2 Statement of results 6.3 Proofs 	134				
6.2 Statement of results	125				
6.3 Proofs	100				
	135 136				
REFERENCES					
APPENDIX					

Chapter 1 Introduction

The pioneering work by Geman & Geman [42] and Besag [16] stimulated a surge of interest in statistical approaches to image analysis. Until recently, most attention has been given to segmentation or classification tasks, i.e. dividing an image into relatively homogeneous regions of different type. Following [16, 42], a Bayesian approach is usually taken in which a Markov random field model is used as a prior distribution to impose smoothness on segmentations. Computational problems due to the high dimensionality of images are overcome by iterative algorithms relying only on the local characteristics of the probabilistic model. An efficient deterministic technique to find a locally optimal segmentation is Besag's Iterated Conditional Mode (ICM) algorithm. Realisations of the posterior distribution can be obtained by a Gibbs sampler, and a simulated annealing schedule to approximate a globally optimal classification can be designed [42].

The goal of this monograph is to argue that the (continuous) Markov or Gibbs processes studied in stochastic geometry, spatial statistics and statistical physics [11, 101, 104, 105, 107] provide a rich collection of models usable in a broad range of problems involving the higher-level interpretation of spatial and image data.

Object recognition is the task of interpreting a noisy image to identify certain geometrical features. An object recognition algorithm must decide whether there are any objects of a specified kind in the scene, and if so, determine the number of objects and their locations, shapes, sizes and spatial relationship. The image data are noisy and sometimes blurred. There is a wide field of applications, including industrial robot vision, document reading, interpretation of medical scans [20], automated cytology [86], classification of astronomical features [87, 108] and identification of grain structures in materials science.

It is increasingly acknowledged that discrete Markov random fields (MRFs) are not the appropriate prior models to use in object recognition. This is partly because geometrical shapes with smooth boundaries are unlikely to arise as realisations of a discrete MRF; but more importantly because the *procedures* that result from applying a discrete MRF model do not combine information 'globally' to identify geometrical shape.

This issue is familiar from the computer vision literature as the distinction between 'low-level' and 'high-level' vision. Low-level tasks such as segmentation, classification and tomographic reconstruction call for local (pixel neighbourhood) operations, converting the input image into another raster image. In high-level tasks such as object recognition and scene analysis we have to interpret the image globally, reducing it to a compact description (e.g. a vector graphics representation) of the scene.

Here we study the problem of detecting an unknown number of objects of (usually simple) shape in an unknown spatial arrangement, possibly overlapping each other. This requires a prior stochastic model for the spatial arrangement of the objects. We propose to use the Markov object processes [11, 107] which have a simple mathematical form, and for which there is a natural analogue of the Gibbs sampler (a spatial birth-anddeath process [11, 88, 101]). Thus, analogues of the ICM and simulated annealing algorithms can be developed. Also, some existing techniques in computer vision turn out to be equivalent to maximum likelihood methods. The use of Markov point process models was also proposed by Ripley and coauthors [87, 106, 108].

Alternative approaches have been described in recent studies [28, 86, 87, 108] on recognising the shape of an interesting object (hand, galaxy, mitochondrion). The shape is described by a flexible template, typically a polygon, with edge lengths and angles governed by a joint prior distribution, typically a Markov chain.

We claim that the general framework described above is flexible enough to be easily adaptable to various other tasks in high-level vision and spatial statistics, for instance the clustering of (image) features. As in object recognition, these problems involve the extraction of an underlying pattern from a given set of data (that is not necessarily in image form). Applications include large-scale edge detection [91], the identification of cluster centres in a point pattern [13, 19, 23, 96], but also the analysis of geological faults in relation to earthquakes or the reconstruction of ancient roads using archaeological finds [117].

Stochastic geometry is helpful in providing both the (conditional) cluster models for the data and, as in object recognition, a prior Markov process. We discuss sampling techniques that simultaneously partition the data into groups and find the centres of clustering. A connection with the classical k-means algorithm (see also [23]) is established and we note that under obvious conditions the nearest parent approximation [70, 71] is in fact a maximum likelihood estimator.

As argued above, Markov spatial models provide useful prior distributions in image analysis, but they are equally interesting in their own right. Until recently attention has focused mostly on pairwise interaction models. These provide a flexible class for negative association between neighbouring objects but they do not seem to be able to model clustered patterns and Møller [89] has argued that nearest-neighbour Markov models [11] are better suited to this task.

In support of this claim, we show that many cluster processes with bounded non-empty clusters fall within the class of nearest-neighbour Markov point processes. In particular, any Poisson cluster process with uniformly bounded clusters is Markov with respect to the connected component relation [11, p. 106]. If a Markov or nearest-neighbour Markov point process is used as the parent process in a cluster model and the clusters are uniformly bounded and almost surely nonempty, then the cluster process is again nearest-neighbour Markov. These results suggest that nearest-neighbour Markov processes may be suitable multiple-generation cluster models [66] and help to explain why statistical inference for Poisson cluster processes based on interpoint distances [78] bears so close a resemblance to that for Markov point processes.

On the other hand, the simpler Markov models [107] also allow clustered patterns if interactions between more than two points or objects are permitted. We discuss a model that can exhibit both clustering [125] and inhibition according to the value of a single parameter. The model has interactions of arbitrary high order and is closely related to the empty space function.

Much of the research presented in this tract was performed in collaboration with others. Chapter 2 is based on A.J. Baddeley and M.N.M. van Lieshout. ICM for object recognition. In *Computational Statistics*, Y. Dodge and J. Whittaker (Eds). Volume 2, pp. 271–286. Heidelberg-New York: Physica/Springer, 1992.

A.J. Baddeley and M.N.M. van Lieshout. Object recognition using Markov spatial processes. In *Proceedings 11th IAPR International Conference on Pattern Recognition* pp. B 136– 139. Los Alamitos: IEEE Computer Society Press, 1992.

The model in Chapter 3 is reported in

A.J. Baddeley and M.N.M. van Lieshout. Area-interaction point processes. CWI Report BS-R9318, November 1993. To appear in Annals of the Institute of Statistical Mathematics.

The deterministic algorithms in Chapter 4 can be found in

A.J. Baddeley and M.N.M. van Lieshout. ICM for object recognition. In *Computational Statistics*, Y. Dodge and J. Whittaker (Eds). Volume 2, pp. 271–286. Heidelberg-New York: Physica/Springer, 1992.

while the stochastic annealing approach is in

M.N.M. van Lieshout. Stochastic annealing for nearest-neighbour point processes with application to object recognition. Advances in Applied Probability 26, pp. 281–300, 1994.

See also [75, 5, 76, 3, 8].

The application in spatial statistics is based on

A.J. Baddeley and M.N.M. van Lieshout. Stochastic geometry models in high-level vision. K.V. Mardia and G.K. Kanji (Eds.) Statistics and images Volume 1. Advances in Applied Statistics, a supplement to Journal of Applied Statistics 20, pp. 231-256, 1993.

and the author's part in ongoing research

A.B. Lawson, M.N.M. van Lieshout and A.J. Baddeley. Markov chain Monte Carlo methods for spatial cluster processes. Finally, the last chapter is a revision of

A.J. Baddeley, M.N.M. van Lieshout and J. Møller. Markov properties of cluster processes. Research Report 278, Department of Theoretical Statistics, University of Aarhus, 1994. Submitted for publication.

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Chapter 2

Maximum likelihood object recognition

Object recognition can be formulated as a parameter estimation problem by direct analogy with the formulation of segmentation and classification [16, 40, 42] and in keeping with the general setup of Grenander [49, 50, 51]. In this Chapter we define the object recognition problem, develop a simple maximum likelihood treatment, and show that this is very similar to some existing techniques in computer vision.

2.1. OBJECT RECOGNITION

Object recognition techniques are surveyed in [36, 99, 109]. They can be divided into methods such as region growing which detect an object of unspecified shape and size by characterising it as a region of homogeneous pixel intensity (etc.), and template matching methods which compare the data image with a translated and rotated copy of a reference shape and locate the optimal match [109]. Here we follow the template matching approach.

Suppose the experimental data consist of an image $\mathbf{y} = (y_t ; t \in T)$ where the 'image space' T is an arbitrary finite set. Apart from the usual two-dimensional rectangular grids, T could be a pair of grids (carrying left and right stereo images), a temporal sequence, etc. The observed value y_t at pixel $t \in T$ ranges over a set V that is arbitrary. Examples include $\{0, 1\}$ for binary images, $\{0, 1, \ldots, 255\}$ for 8-bit digitised grey level images or IR. The class U of possible objects is an arbitrary set ('object space'). Typical examples would be the class of all polygons in \mathbb{R}^2 or all convex polyhedra in \mathbb{R}^3 . However U need not be a class of subsets of \mathbb{R}^d since the specification of an object may also include properties like colour or surface texture. Section 3.1.1 discusses this further. Here we assume only that each object $u \in U$ determines a subset $R(u) \subseteq T$ of image space 'occupied' by the object.

An object configuration is simply a finite set of objects

$$\mathbf{x} = \{x_1, \cdots, x_n\}$$

where $x_i \in U$, $i = 1, \dots, n$, $n \ge 0$. The objects may be in any spatial relation to each other; the number of objects is variable and may be zero.

The goal then is to extract the unobserved underlying pattern \mathbf{x} from a given data image \mathbf{y} .

A standard numerical criterion for the degree of match between x and y is the *Hough transform*, originally proposed by Hough [57] to detect straight lines in binary images [12, 24, 35, 65, 114]. A recent survey is [60]. The Hough transform is a real valued function of the object parameter vector u defined by

$$H_{\mathbf{y}}(u) = \sum_{t \in R(u)} y_t , u \in U$$
(2.1.1)

where \mathbf{y} is the data image. This is often interpreted as a vote-counting operation: each pixel t votes with strength y_t for all the objects that contain that pixel. Objects are located typically by finding local maxima of the matching criterion, or by accepting all template positions where the match exceeds a threshold value.

An alternative approach using mathematical morphology is to perform an erosion with respect to the template. For example if y is a binary image and Y is the set of white pixels define the generalised erosion [112, 113] of Y by

$$E_R(Y) = \{u : R(u) \subseteq Y\} = \{u : y_t = 1 \text{ for all } t \in R(u)\}$$
(2.1.2)

i.e. accept only those objects u for which every pixel in the template R(u) is white. On a discrete image lattice, the erosion is the set of parameters u where the Hough transform attains its maximum possible value.

2.2. Noise models

In the likelihood approach to image analysis the observed image \mathbf{y} depends on the true object configuration \mathbf{x} through a known conditional probability density $f(\mathbf{y} \mid \mathbf{x})$. This density describes the 'forward problem' of image formation and includes both the deterministic influence of \mathbf{x} and the stochastic noise inherent in observing \mathbf{y} .

Following custom, we assume that the data pixel values y_t are conditionally independent given $X = \mathbf{x}$. This embraces additive and multiplicative random noise as well as Poisson distributed counts and more general exponential family models. Without loss of generality the conditional distributions of individual pixel values belong to a family of distributions with densities $\{g(\cdot \mid \theta) : \theta \in \Theta\}$ indexed by a parameter space Θ .

Definition 1 An independent noise model is a stochastic model for Y given $X = \mathbf{x}$, which assumes pixel values y_t are conditionally independent given \mathbf{x} , with joint probability density

$$f(\mathbf{y} \mid \mathbf{x}) = \prod_{t \in T} g(y_t \mid \theta^{(\mathbf{x})}(t))$$
(2.2.3)

where $\{g(\cdot \mid \theta) : \theta \in \Theta\}$ is a family of probability densities on V and $\theta^{(\mathbf{x})}(t)$ is the parameter value of the conditional distribution of y_t given **x**. Then $\theta^{(\mathbf{x})}(\cdot)$ is a Θ -valued image, deterministically derived from **x**, which we call the signal.

Note that no assertions are made about the way objects interact and that the model does not imply that the pixel values are (unconditionally) independent.

A simple example is the signal

$$\theta^{(\mathbf{x})}(t) = \begin{cases} \theta_1 & \text{if } t \in S(\mathbf{x}) \\ \theta_0 & \text{otherwise} \end{cases}$$
(2.2.4)

where θ_1 , θ_0 are known parameters (foreground and background signal values) and $S(\mathbf{x})$ is the silhouette

$$S(\mathbf{x}) = \bigcup_{i=1}^{n} R(x_i)$$

formed by taking the union of all objects in the configuration. In other words, under this simple model, each of the objects in the configuration \mathbf{x} is 'painted' onto the scene, and independent random pixel noise is superimposed on the result.

We call this a *blur-free* independent noise model. It may seem oversimplified; yet we shall show that several standard techniques in computer vision are equivalent to assuming this model.

The following are examples of independent noise models. Strictly speaking, they represent a whole family of models; members are obtained by varying the signal function.

Model 1: additive Gaussian white noise

 y_t is normally distributed with mean $\mu = \theta^{(\mathbf{x})}(t) \in \mathbb{R}$ and fixed variance $\sigma^2 > 0$:

$$g(y_t \mid \mu) = (2\pi\sigma^2)^{-1/2} e^{-(y_t - \mu)^2/(2\sigma^2)}$$

Model 2: additive Laplacian noise

 y_t is double exponentially distributed with mean $\mu = \theta^{(\mathbf{x})}(t) \in \mathbb{R}$ and fixed dispersion parameter $\lambda > 0$:

$$g(y_t \mid \mu) = \frac{\lambda}{2} e^{-\lambda |y_t - \mu|}.$$

Model 3: binary image

 y_t has a Bernoulli distribution with success probability $\theta^{(\mathbf{x})}(t)$:

$$g(y_t \mid \theta) = \theta^{y_t} (1 - \theta)^{(1 - y_t)}.$$

Special cases are a) salt-and-pepper noise where

$$\theta^{(\mathbf{x})}(t) = \begin{cases} 1-p & \text{if } t \in S(\mathbf{x}) \\ p & \text{else} \end{cases}$$

and **b**) **pepper noise** where:

$$\theta^{(\mathbf{x})}(t) = \begin{cases} 1 & \text{if } t \in S(\mathbf{x}) \\ p & \text{else} \end{cases}$$

Here 0 is fixed.

Model 4: Poisson counts

 y_t is integer valued and Poisson distributed with mean $\mu = \theta^{(\mathbf{x})}(t) \in \mathbb{R}^+$:

$$g(y_t \mid \mu) = e^{-\mu} \frac{\mu^{y_t}}{y_t!}.$$

.

Model 1 is widely used in image analysis. In Models 3a and 3b the silhouette is converted to a binary image and noise introduced by randomly flipping pixel values with probability p. In Model 3a all pixels are subject to change, while in Model 3b only background pixels are flipped. Model 4 is the usual model in emission tomography where a patient is injected with a radioactive isotope and emitted particles are recorded in a system of detectors placed around the patient.

2.3. MAXIMUM LIKELIHOOD ESTIMATION

Given observation of \mathbf{y} , the likelihood of a configuration \mathbf{x} is defined to be $\ell(\mathbf{x}; \mathbf{y}) = f(\mathbf{y} \mid \mathbf{x})$, and we seek 'the' maximum likelihood estimate of \mathbf{x}

$$\widehat{\mathbf{x}} = \operatorname{argmax}_{\mathbf{x}} f(\mathbf{y} \mid \mathbf{x}) \tag{2.3.5}$$

which may be nonexistent or nonunique. Specifically, note that for any blur-free model the likelihood depends on \mathbf{x} only through its silhouette $S(\mathbf{x})$, so configurations with the same silhouette cannot be distinguished in likelihood.

Since the log-likelihood is a sum of individual pixel error terms

$$L(\mathbf{x} ; \mathbf{y}) = \log f(\mathbf{y} \mid \mathbf{x}) = \sum_{t \in T} \log g(y_t \mid \theta^{(\mathbf{x})}(t)),$$

maximum likelihood estimation is equivalent to regression of \mathbf{y} on the class of signals $\theta^{(\mathbf{x})}(\cdot)$ for all possible \mathbf{x} , with pixelwise loss function $-\log g(y_t \mid \cdot)$.

Lemma 1 An MLE for Model 1 is a solution of the least squares regression of y on the class of functions

$$\left\{\theta^{(\mathbf{x})}(t): \mathbf{x} = \{x_1, \ldots, x_n\}, x_i \in U, n \ge 0\right\}.$$

In Model 2 any MLE solves a least absolute deviation regression on the same class.

Proof: Writing |T| for the area or number of pixels in T, the loglikelihood is

$$L(\mathbf{x} ; \mathbf{y}) = -\frac{1}{2} |T| \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{t \in T} (y_t - \theta^{(\mathbf{x})}(t))^2$$

for Model 1 and

$$L(\mathbf{x} ; \mathbf{y}) = |T| \log \frac{\lambda}{2} - \lambda \sum_{t \in T} |y_t - \theta^{(\mathbf{x})}(t)|$$

for Model $\mathbf 2$.

Typically, the equation (2.3.5) cannot be solved directly. This is clearly true for the regression above, because of the combinatorial and geometric complexity of the functions $\theta^{(\mathbf{x})}(t)$. We will return to this problem below.

Lemma 2 For Model 3a with 0 , the ML equations are

 $\hat{\mathbf{x}} = argmin_{\mathbf{x}} |S(\mathbf{x}) \bigtriangleup Y|$

where \triangle denotes the symmetric set difference ('exclusive-or') and $Y = \{t \in T : y_t = 1\}$ is the set of white pixels.

Proof:

$$L(\mathbf{x} ; \mathbf{y}) = |S(\mathbf{x}) \setminus Y| \log p + |S(\mathbf{x}) \cap Y| \log(1-p)$$

+ |Y \ S(\mathbf{x})| \log p + (|T| - |Y \cup S(\mathbf{x})|) \log(1-p)
= |T| \log(1-p) + |S(\mathbf{x}) \triangle Y| \log \frac{p}{1-p}

and for p < 1/2 the coefficient of $|S(\mathbf{x}) \Delta Y|$ is negative.

Squared error and L^1 error have been proposed as optimality criteria for object recognition in their own right but we see here that they are special cases of the maximum likelihood approach. These results confirm recent arguments in the literature [79, 81] in favour of using L^1 filtering, except when the noise is Gaussian.

2.3.1 Connection with mathematical morphology

The following result shows that standard morphological operators solve the ML equations (2.3.5) for a simple noise model.

Lemma 3 A maximum likelihood estimator for Model 3b is the generalised erosion (2.1.2)

$$\hat{\mathbf{x}}_{\max} = E_R(Y) = \{ u \in U : R(u) \subseteq Y \} .$$

where $Y = \{t \in T : y_t = 1\}$. This is the largest solution of the ML equations; the other solutions are the subsets $\hat{\mathbf{x}} \subseteq \hat{\mathbf{x}}_{\max}$ with the same silhouette,

$$S(\hat{\mathbf{x}}) = S(\hat{\mathbf{x}}_{\max}).$$

Proof: The density is nonzero only if $S(\mathbf{x}) \subseteq Y$ and in this case equals

$$f(\mathbf{y}|\mathbf{x}) = \prod_{t \in T \setminus S(\mathbf{x})} p^{y_t} (1-p)^{(1-y_t)}.$$

The log likelihood is then

$$L(\mathbf{x} ; \mathbf{y}) = |Y \setminus S(\mathbf{x})| \log p + (|T| - |Y|) \log(1 - p)$$

= $|T| \log(1 - p) + |Y| \log \frac{p}{1 - p} - |S(\mathbf{x})| \log p$

and the result follows.

The 'classical' erosion operator \ominus [112] is the special case where $U = T \subset \mathbb{R}^2$ and R(u) = u + R is the translation over u of a fixed subset $R \subseteq T$. Then

$$\hat{\mathbf{x}}_{\max} = Y \ominus \hat{R} := \{ u : (u+R) \subseteq Y \}.$$
(2.3.6)

Thus the erosion operator is the MLE for a simple translation model; its corresponding silhouette is the *opening* of Y by R [112].

The dual of (2.3.6) is the *dilation* \oplus

$$Y \oplus \check{R} := \{u : (u+R) \cap Y \neq \emptyset\}$$
$$= \{u : (u+R) \not\subseteq Y^c\}$$
$$= (Y^c \oplus \check{R})^c$$

(see [112]), generalised straightforwardly to

$$D_R(Y) = \{ u \in U : R(u) \cap Y \neq \emptyset \}.$$

Hence by exchanging foreground and background, i.e. taking $\theta^{(\mathbf{x})}(t) = 1 - p$ for $t \in S(\mathbf{x})$ and 0 otherwise, one obtains a similar result for the dilation: a maximum likelihood estimator is a subset of the generalised dilation $D_R(Y)$ of Y.

2.3.2 Relation to pre-processing

It is also interesting to note that popular 'pre-processing' techniques, such as change of scale, thresholding or gamma correction, amount to simply modifying the noise model. If the pixel values y_t are subjected to an invertible, differentiable transformation ('anamorphosis' in morphology parlance) $y'_t = \phi(y_t)$ then the model (2.2.3) is transformed into another model of the same type with g replaced by another density g'

$$f(\mathbf{y}' \mid \mathbf{x}) = \prod_{t \in T} g'(y'_t \mid \theta^{(\mathbf{x})}(t))$$

where

$$g'(y'_t \mid \theta^{(\mathbf{x})}(t)) = g(\phi^{-1}(y'_t) \mid \theta^{(\mathbf{x})}(t)) \ J(y'_t);$$

 $J(y'_t)$ being 1 for grey level data, and $\left|\frac{d}{dz}\phi^{-1}(y'_t)\right|$ in the absolutely continuous case. In particular, for exponential families the transformed data is again an exponential family.

This is also true for transformations such as 'clipping' pixel values to an interval [a, b]

$$\operatorname{clip}(s, a, b) = \begin{cases} a & \text{if } s < a \\ s & \text{if } a \leq s \leq b \\ b & \text{if } s > b \end{cases}$$

Treating clipped pixel data as if they arise from additive Gaussian noise is equivalent to assuming additive two-sided exponential noise with signal (= mean) values $\theta_0 = a$, $\theta_1 = b$.

Lemma 4 For Model 2 with $\theta^{(\mathbf{x})}(t)$ defined by (2.2.4) with $\theta_0 < \theta_1$

$$L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) =$$
$$2\lambda \left\{ \sum_{t \in R(u) \setminus S(\mathbf{x})} y'_t - \frac{\theta_1 + \theta_0}{2} |R(u) \setminus S(\mathbf{x})| \right\}$$

where $y'_t = \operatorname{clip}(y_t, \theta_0, \theta_1)$.

Proof: Observe that (with a < b)

$$\begin{split} |s-b| - |s-a| &= 1\{s < a\}(b-a) + 1\{s > b\}(a-b) \\ &+ 1\{a \le s \le b\}(a+b-2s) \\ &= a+b-2s+1\{s < a\}(-2a+2s) \\ &+ 1\{s > b\}(-2b+2s) \\ &= a+b-2\text{clip}(s,a,b). \end{split}$$

Hence

$$L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) =$$

$$= -\lambda \sum_{t \in R(u) \setminus S(\mathbf{x})} \{ |y_t - \theta_1| - |y_t - \theta_0| \}$$
$$= -\lambda \sum_{t \in R(u) \setminus S(\mathbf{x})} \{ \theta_0 + \theta_1 - 2\operatorname{clip}(y_t, \theta_0, \theta_1) \}$$
$$= 2\lambda \left\{ \sum_{t \in R(u) \setminus S(\mathbf{x})} y'_t - \frac{\theta_1 + \theta_0}{2} |R(u) \setminus S(\mathbf{x})| \right\}$$

,

and the result follows.

These remarks do not hold for more complex pre-processing operations such as neighbourhood filtering, which interfere with the dependence structure of (2.2.3).

2.4. Iterative methods for MLE

It is usually impossible to solve the ML estimating equations (2.3.5) directly, and one has to resort to iterative approximation methods.

2.4.1 Add-and-delete algorithms

The simplest form of iterative adjustment is to add or delete objects one-at-a-time. If the current configuration is \mathbf{x} then we consider adding a new object $u \notin \mathbf{x}$, yielding configuration $\mathbf{x} \cup \{u\}$, if the log likelihood ratio

$$L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) = \log \frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x})}$$
(2.4.7)

is sufficiently large or deleting an existing object $u \in \mathbf{x}$ yielding $\mathbf{x} \setminus \{u\}$ if

$$L(\mathbf{x} \setminus \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) = \log \frac{f(\mathbf{y} \mid \mathbf{x} \setminus \{u\})}{f(\mathbf{y} \mid \mathbf{x})}$$
(2.4.8)

is sufficiently large. Two variations of this scheme are to visit the possible objects u sequentially (assuming U is discretised) applying the above rules at each step, or to scan the whole of U to find the object u whose addition or deletion would most increase the likelihood.

Algorithm 1 (Coordinatewise optimisation) Initialise $\mathbf{x}^{(0)} = \emptyset$ or some other chosen initial state. When the current reconstruction is $\mathbf{x}^{(k-1)}$, visit every $u \in U$ sequentially in a predetermined order. If $u \notin \mathbf{x}^{(k-1)}$ and $L(\mathbf{x}^{(k-1)} \cup \{u\}; \mathbf{y}) - L(\mathbf{x}^{(k-1)}; \mathbf{y}) \ge w$, where $w \ge 0$ is a fixed threshold, then add u to the configuration, yielding $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} \cup$ $\{u\}$. If $u = x_i \in \mathbf{x}^{(k-1)}$ and $L(\mathbf{x}^{(k-1)} \setminus \{x_i\}; \mathbf{y}) - L(\mathbf{x}^{(k-1)}; \mathbf{y}) \ge w$, then delete x_i yielding $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} \setminus \{x_i\}$. Update recursively until one complete scan of the image yields no changes.

Algorithm 2 (Steepest ascent) Initialise $\mathbf{x}^{(0)} = \emptyset$ or some other chosen initial state. Given $\mathbf{x}^{(k-1)}$, determine

$$a = \max_{x_i \in \mathbf{x}^{(k-1)}} \left\{ L(\mathbf{x}^{(k-1)} \setminus \{x_i\} ; \mathbf{y}) - L(\mathbf{x}^{(k-1)} ; \mathbf{y}) \right\}$$

and

$$b = \sup_{u \in U} \left\{ L(\mathbf{x}^{(k-1)} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x}^{(k-1)} ; \mathbf{y}) \right\}.$$

If $\max\{a, b\} < w$, then stop. Otherwise, if $b \ge a$, add the corresponding object, while if a > b, delete the corresponding object.

These algorithms bear a very strong resemblance to Besag's ICM algorithm [16] except for the lack of a prior distribution. The analogy will be explored in Chapter 4.

Clearly these algorithms increase the likelihood at each step,

$$f(\mathbf{y} \mid \mathbf{x}^{(k+1)}) \ge f(\mathbf{y} \mid \mathbf{x}^{(k)}).$$

As there are only a finite number of possible configurations, convergence of $f(\mathbf{y} | \mathbf{x}^{(k)})$ is guaranteed and (if w = 0) we reach a local maximum of the likelihood function. At worst there is cycling between images of equal likelihood. However the algorithms do not necessarily yield the global maximum likelihood solution, and the local maximum obtained will depend on the initial configuration $\mathbf{x}^{(0)}$ and for Algorithm 1 on the scanning order as well. We should therefore choose a sensible initial state, such as the empty list \emptyset , or the set of local maxima of

$$rac{f(\mathbf{y} \mid \{u\})}{f(\mathbf{y} \mid \emptyset)}$$

wherever this ratio is larger than 1.

Complications arise if the model $f(\mathbf{y} \mid \mathbf{x})$ contains unknown parameters. We will return to this problem in Section 4.2.3.

2.4.2 General add-delete-shift algorithms

Another form of iterative adjustment is to change an existing object slightly by translation, rotation or expansion. The aim is to obtain methods that are more robust against imprecise information contained in the initial estimate. Another advantage is that convergence may be faster, as throwing away an incorrect object and replacing it by the right one can then be carried out in one single step.

Write

$$M(\mathbf{x}, x_i, u) = (\mathbf{x} \cup \{u\}) \setminus \{x_i\}$$

for the configuration obtained from \mathbf{x} by moving the element $x_i \in \mathbf{x}$ to a new position u. Let $Q(\mathbf{x}, x_i)$ be the set of all object points u for which this operation is permitted. Typically u will be required to be close to x_i but not equal to any x_j , say $Q(\mathbf{x}, x_i) = N(x_i) \setminus \mathbf{x}$ where $N(x_i)$ is some neighbourhood of x_i . Then the criterion for a move from $x_i \in \mathbf{x}$ is

$$\max_{u \in Q(\mathbf{x}, x_i)} \left\{ L(M(\mathbf{x}^{(k-1)}, x_i, u) ; \mathbf{y}) - L(\mathbf{x}^{(k-1)} ; \mathbf{y}) \right\}$$
(2.4.9)

and the analogues of Algorithms 1 and 2 are as follows.

Algorithm 3 (Coordinatewise optimisation with shifts)

Assuming that the parameter space is finite, visit every $u \in U$ sequentially. Consider every possible transition involving u and select the maximum from (2.4.7), (2.4.8) and (2.4.9). If this maximum log likelihood ratio is larger than a given threshold w, update the reconstruction accordingly.

Algorithm 4 (Steepest ascent with shifts) Consider all possible transitions from the current state x and take that transition that has the maximum log likelihood ratio exceeding threshold w.

The convergence properties are similar to Algorithms 1-2. Here, however, a 'local maximum' of the likelihood is a state \mathbf{x} such that no neighbouring configuration $\mathbf{x} \cup \{u\}$ or $\mathbf{x} \setminus \{x_i\}$ or $M(\mathbf{x}, x_i, u)$ has larger likelihood. This is a more stringent definition than for the previous algorithms, and one expects the results to be better.

2.5. Relation to Hough transform

The Hough transform (2.1.1) is very similar to the log likelihood ratio (2.4.7) for a blur-free model:

$$L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) = \sum_{R(u) \setminus S(\mathbf{x})} z_t$$
(2.5.10)

where $z_t = \log g(y_t|\theta_1) - \log g(y_t|\theta_0)$ is the difference in goodness-offit at pixel t. Note that pixels can also cast fractional or negative votes, a modification that has been suggested ad hoc by several authors [12, 27, 122, 124] and [22, 26] respectively. In fact, (2.5.10) is identical to the (generalised) Hough transform of image \mathbf{z} when the new object u does not overlap any existing object $x_i \in \mathbf{x}$. For example, the Hough transform is the log likelihood ratio for comparing $\{u\}$, the scene consisting of a single object, against the empty scene \emptyset [58]. When objects do overlap, the likelihood ratio (2.5.10) is a generalisation of the Hough transform, with domain of summation 'masked' by the silhouette of the current configuration. Equivalently (2.5.10) is the Hough transform of the masked image $w_t^{(\mathbf{x})} = z_t \mathbf{1}\{t \notin S(\mathbf{x})\}$.

The similarity between (2.1.1) and (2.5.10) is even stronger since z_t is linear in y_t for many exponential noise models. For additive Gaussian noise

$$z_t = \frac{\theta_1 - \theta_0}{\sigma^2} \left(y_t - \frac{\theta_0 + \theta_1}{2} \right)$$

and for Poisson noise

$$z_t = y_t \log \frac{\theta_1}{\theta_0} - (\theta_1 - \theta_0).$$

The likelihood ratio is then of the form

$$L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) = a \sum_{R(u) \setminus S(\mathbf{x})} y_t - b|R(u) \setminus S(\mathbf{x})|.(2.5.11)$$

In particular when u does not overlap \mathbf{x} this is a linear adjustment of the Hough transform of \mathbf{y} . More generally, let g be an exponential family of the form

$$g(y_t \mid \theta) = \exp \left[A(\theta) + B(y_t) + C(\theta)D(y_t)\right]$$

for some real-valued functions A, B, C and D. Then (2.5.11) holds if y_t is replaced by $D(y_t)$. The generalisation to vector-valued functions is straightforward.

Apart from illuminating the meaning of the Hough transform, these results show how to correctly interpret values of the Hough transform when the objects do not have equal area, e.g. in the presence of edge effects. For Gaussian or Poisson additive noise (say), the likelihood ratio is positive when the average value of y_t over $R(u) \setminus S(\mathbf{x})$ exceeds a critical value. The latter is simply the Neyman-Pearson critical value for classifying a single observation y_t as foreground or background ($\theta \in$ $\{\theta_0, \theta_1\}$).

For the general 'blurred' model (2.2.3) the likelihood ratio equals

$$\sum_{t \in Z(\mathbf{x},u)} h(y_t, \theta^{(\mathbf{x})}(t), \theta^{(\mathbf{x} \cup \{u\})}(t))$$
(2.5.12)

and thus is again similar to the Hough transform, where

$$h(y_t, \theta, \theta') = \log \frac{g(y_t| heta')}{g(y_t| heta)}$$

is as before the difference in goodness-of-fit at pixel t and

$$Z(\mathbf{x}, u) = \{t : \theta^{(\mathbf{x})}(t) \neq \theta^{(\mathbf{x} \cup \{u\})}(t)\}$$
(2.5.13)

is the set of pixels where the signal is affected by the addition of object u.

The log likelihood ratio for a transition from \mathbf{x} to $M(\mathbf{x}, x_i, u)$ (Algorithms 3 and 4) can be represented as

$$[L(\mathbf{z} \cup \{u\} ; \mathbf{y}) - L(\mathbf{z} ; \mathbf{y})] - [L(\mathbf{z} \cup \{x_i\} ; \mathbf{y}) - L(\mathbf{z} ; \mathbf{y})]$$

where $\mathbf{z} = \mathbf{x} \setminus \{x_i\}$. This is a difference of two values of the generalised Hough transform (2.5.12) for the configuration with x_i deleted. In particular it depends only on data pixels within a region $Z(\mathbf{z}, u) \cup Z(\mathbf{z}, x_i)$.

2.6. EXAMPLE

Figure 2.1 shows a scanned 128×128 image ('pellets') taken from the Brodatz texture album [21]. This is a relatively easy dataset for object recognition but helps to illustrate the approach.

We treat the pellets as discs of fixed radius 4 pixels but with blurred boundaries. The grey-level histogram has two distinct peaks at value 8 and 172, suggesting that we can regard the background and foreground signal as roughly constant at these values. Assuming additive Gaussian noise, its variance was estimated by thresholding the image and taking the sample variance, giving an estimate of 83.1. Blurring was modelled by assuming that the original blur-free signal was subjected to a 3×3 averaging (linear) filter with relative weights 4 for the central pixel, 2 for horizontal and vertical neighbours and 1 for diagonal neighbours.

Figure 2.2 shows an approximate MLE computed by steepest ascent (Algorithm 2) from an empty initial configuration at threshold w = 0. Pellets are correctly identified but there is 'multiple response', i.e. the MLE sometimes contains clusters of objects around the position of each 'true' object.



Figure 2.1: Pellets image taken from [21], digitised on a 128×128 square grid.



Figure 2.2: Approximate maximum likelihood reconstruction by steepest ascent of the pellets texture at threshold w = 0 from an empty initial state.

Chapter 3 Markov spatial processes

The first Section of this Chapter is an overview with some adaptations of the theory of random processes of geometrical objects [117] with emphasis on Markov object processes [107, 11]. These provide a flexible class of models for inhibition and we propose to use them as priors in the object recognition problem discussed in Chapter 2. In Sections 3.2 and 3.3 we introduce a Markov point process proposed by Baddeley and Van Lieshout [9] that exhibits both clustered and ordered pattern according to the value of a parameter. It has infinite order interactions and is related to the empty space function F as the Strauss model is to Ripley's K-function. Statistical inference for this model is studied in Section 3.4.

3.1. SURVEY OF MARKOV SPATIAL MODELS

3.1.1 Objects

The 'objects' featuring in stochastic geometry range from simple geometrical figures (points, lines, discs) through plane polygons and convex compact sets to completely general closed sets. A given class of objects U is treated as a space in its own right, so that objects are regarded as points in U.

At one extreme, simple geometrical figures can be specified by the values of a few parameters (giving location, orientation etc.) so that U is isomorphic to a subset of \mathbb{R}^d . For example a disc in \mathbb{R}^2 can be specified by its centre (x, y) and radius r so that $U = \mathbb{R}^2 \times \mathbb{R}^+$. At

the other extreme, the space \mathcal{F} of all closed subsets of \mathbb{R}^d can be made into a locally compact, second countable Hausdorff space (l.c.s. space) so that a random closed set can be defined as a random element of \mathcal{F} [84].

It is often useful to represent an object as a 'marked point', i.e. a pair (s, m) consisting of a point $s \in \mathbb{R}^d$ and a 'mark' $m \in \mathcal{M}$, where \mathcal{M} is an arbitrary l.c.s. space. The point s fixes the location of the object and the mark m contains all other information such as size and shape. A disc in \mathbb{R}^2 can be regarded as a point (x, y) marked by a radius r. Objects with additional properties such as colour and surface texture can be represented as marked points by choosing an appropriate mark space \mathcal{M} . For example a grey-scale surface texture can be formalised as an upper-semicontinuous function $\mathbb{R}^d \to \mathbb{R}^+$, and the space of all such functions is l.c.s.

3.1.2 Markov object processes

Let U be the class of objects. As before, a configuration is a finite set $\mathbf{x} = \{x_1, \ldots, x_n\}$ of objects $x_i \in U$. Writing Ω for the set of all configurations, a random process of objects is a random element of Ω , or equivalently, a point process on U consisting of a finite number of 'points' with probability 1.

The basic reference model is the *Poisson object process* in U with intensity μ , where μ is a finite non-atomic measure on U. Under this model the total number of objects has a Poisson distribution with mean $\mu(U)$; given that exactly n objects are present, they are independent and identically distributed in U with probability distribution proportional to μ , i.e. $\mathbb{P}(x_i \in B) = Q(B) = \mu(B)/\mu(U)$ for $B \subseteq U$.

Further details can be consulted in [117].

Our interest is in constructing non-Poisson spatial processes exhibiting dependence between neighbouring objects. To do this we shall specify the probability density of the new process with respect to the Poisson process (thereby restricting attention to processes that are absolutely continuous with respect to the Poisson). The density is a measurable and integrable function $p: \Omega \rightarrow [0, \infty)$. For the new process, the distribution of the total number of objects is

$$\mathbb{P}(N=n)=\frac{e^{-\mu(U)}}{n!}\int_U\cdots\int_U p(\{x_1,\ldots,x_n\})\ d\mu(x_1)\ldots d\mu(x_n).$$

Writing $q_n = \mathbb{P}(N = n)$, given N = n, the *n* random objects have joint probability density

$$p_n(x_1,\ldots,x_n) = e^{-\mu(U)} \mu(U)^n p(\{x_1,\ldots,x_n\}) / (n! q_n)$$
with respect to the distribution of n i.i.d. objects in U with distribution Q.

Provisionally define two objects u, v to be 'neighbours' if their induced sets (cf. Section § 2.1) overlap,

$$u \sim v \quad \Leftrightarrow \quad R(u) \cap R(v) \neq \emptyset.$$
 (3.1.1)

This can be replaced by any symmetric $(u \sim v \text{ iff } v \sim u)$, reflexive relation between elements of U. The *neighbourhood* N(A) of a set $A \subseteq U$ is the set of all points in U neighbouring a point in A:

$$N(A) = \{ u \in U : u \sim a \text{ for some } a \in A \}.$$

The simplest kind of spatial interaction is that which forbids objects to overlap. Consider a Poisson process of objects in T conditioned on the event that no pair of objects is overlapping. Its density with respect to the original Poisson process is simply

$$p(\mathbf{x}) = \begin{cases} 0 & \text{if } x_i \sim x_j \text{ for some } i \neq j \\ \alpha & \text{otherwise} \end{cases}$$
(3.1.2)

where $\alpha > 0$ is the normalising constant (= reciprocal of the probability that Poisson process has no overlapping objects). Call this a *hard object process* by analogy with the better-known hard core point process.

Next consider a pairwise interaction

$$p(\mathbf{x}) = \alpha \beta^{n(\mathbf{x})} \prod_{x_i \sim x_j} g(x_i, x_j)$$
(3.1.3)

where $\alpha, \beta > 0$ are constants, $n(\mathbf{x})$ is the number of points in \mathbf{x} , and $g: U \times U \to [0, \infty)$. The product is over all pairs of neighbouring objects $x_i \sim x_j$ with i < j.

If $g \equiv 1$ then (3.1.3) is simply a Poisson process with intensity measure $\beta \mu$; if $g \equiv 0$ it is the hard object process (3.1.2). If the (measurable) function $g \leq 1$, the process is *purely inhibitory*.

The special case $g \equiv \gamma$ for a constant $0 < \gamma < 1$ is called a *Strauss* object process and the density can be written

$$p(\mathbf{x}) = \alpha \beta^{n(\mathbf{x})} \gamma^{s(\mathbf{x})}$$
(3.1.4)

where

$$s(\mathbf{x}) = \sum_{i < j} \mathbb{1}\{x_i \sim x_j\}$$

is the number of pairs of neighbouring objects (e.g. number of overlaps) in the configuration. This process exhibits 'repulsion' or 'inhibition' between objects, since $s(\mathbf{x})$ tends to be smaller than under the Poisson model. The density (3.1.4) is typically not integrable for $\gamma > 1$.

Just as discrete Markov random fields are closely connected with statistical physics, pairwise interaction processes (3.1.3) also occur as models of interacting particle systems. The negative log probability density of a particular configuration \mathbf{x} can be interpreted as its physical 'energy': it is the sum of a ground potential $\log \alpha$, a potential $\log \beta$ for the presence of each object x_i , and an interaction potential $\log g(u, v)$ between each pair of neighbouring objects u, v.

The density (3.1.3) bears a close resemblance to the distribution of a discrete Markov random field with pairwise interaction. However, the number of terms appearing in the product in (3.1.3) depends on the realisation **x**. Some configurations have more interaction than others.

Note that if $u \in U, u \notin \mathbf{x}$ with $p(\mathbf{x}) > 0$, the ratio

$$\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} = \beta \prod_{x_i \sim u} g(u, x_i)$$
(3.1.5)

depends only on u and on the neighbours of u in x. This important property signifies that all interaction is 'local'. In the statistical physics interpretation, $-\log p(\mathbf{x} \cup \{u\}) + \log p(\mathbf{x})$ is the energy required to add a new point u to an existing configuration x. In probabilistic terms $p(\mathbf{x} \cup \{u\})/p(\mathbf{x})$ is the Papangelou conditional intensity $\lambda(u; \mathbf{x})$ at u given the rest of the pattern x on $U \setminus \{u\}$, see [25]. Roughly speaking, $\lambda(u; \mathbf{x})du$ is the conditional probability of a point in the infinitesimal region du centred at u given the configuration agrees with x outside this region.

Following are definitions and results of Ripley and Kelly [107] trivially generalised to random object processes [11, Section 3]. Let \sim be any symmetric, reflexive relation on U.

Definition 2 A random object process X with density p is called a Markov object process with respect to \sim if for all $\mathbf{x} \in \Omega$

- (a) $p(\mathbf{x}) > 0$ implies $p(\mathbf{y}) > 0$ for all $\mathbf{y} \subseteq \mathbf{x}$;
- (b) if p(x) > 0, then

$$\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} \tag{3.1.6}$$

depends only on u and $N(\{u\}) \cap \mathbf{x} = \{x_i \in \mathbf{x} : u \sim x_i\}.$

The term 'Markov' is justified by the following spatial Markov property. Let A be a measurable subset of U. Then the conditional distribution of $X \cap A$ given $X \cap A^c$ depends only on X in the neighbourhood $N(A) \cap A^c = \{u \in A^c : u \sim a \text{ for some } a \in A\}$:

$$\mathcal{L}(X \cap A \mid X \cap A^c) = \mathcal{L}(X \cap A \mid X \cap N(A) \cap A^c).$$

Define a configuration $\mathbf{x} \in \Omega$ to be a *clique* if all members of \mathbf{x} are neighbours $(x_i \sim x_j \text{ for all } i \neq j)$. Configurations of 0 or 1 objects are cliques. Then the Ripley-Kelly analogue of the Hammersley-Clifford theorem [107] states that a process with density $p: \Omega \to [0, \infty)$ is Markov iff

$$p(\mathbf{x}) = \prod_{\text{cliques } \mathbf{y} \subseteq \mathbf{x}} q(\mathbf{y})$$
(3.1.7)

for all $\mathbf{x} \in \Omega$, where the product is restricted to *cliques* $\mathbf{y} \subseteq \mathbf{x}$, and $q: \Omega \to [0, \infty)$ is an (arbitrary) function.

To conclude this Section, consider the following area-interaction process

$$p(\mathbf{x}) = \alpha \beta^{n(\mathbf{x})} \gamma^{-|S(\mathbf{x})|}$$
(3.1.8)

with parameters $\beta > 0$, $\gamma > 0$ and normalising constant $\alpha > 0$. As usual $|S(\mathbf{x})|$ is the area (or pixel count) of the silhouette. This is a *Markov* overlapping object model (i.e. Markov with respect to (3.1.1)) with interactions of infinite order. For $\gamma < 1$, configurations with relatively few overlapping objects are favoured, for $\gamma = 1$ it is a Poisson process and for $\gamma > 1$ the model encourages clustered patterns. This model is interesting in its own right and will be discussed in greater detail in Sections 3.2 and 3.4.

3.1.3 Nearest-neighbour Markov object processes

A further extension due to Baddeley and Møller [11] is to allow interaction behaviour to depend on the realisation of the process. For example, in a one-dimensional renewal process, each point can be said to interact with its nearest neighbours to the left and right, regardless of how far distant these neighbours may be. In two dimensions we would like to construct point processes exhibiting interaction between those pairs of points that are neighbours with respect to the Voronoi (Dirichlet) tessellation generated by the point pattern.

Assume that for each configuration \mathbf{x} we have a symmetric reflexive relation $\underset{\mathbf{x}}{\sim}$ defined on \mathbf{x} . We might prefer to think of this as a finite graph whose vertices are the objects $x_i \in \mathbf{x}$.

Consider the following *pairwise interaction model* (cf. (3.1.3))

$$p(\mathbf{x}) = lpha eta^{n(\mathbf{x})} \prod_{i < j; x_i \stackrel{\sim}{\mathbf{x}} x_j} g(x_i, x_j).$$

Any generalisation of Definition 2 should at least embrace p. However

$$\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} = \beta \prod_{\substack{x_i \in \mathcal{X} \cup \{u\}^u}} g(x_i, u) \frac{\prod_{x_i \in \mathcal{X} \cup \{u\}} x_j g(x_i, x_j)}{\prod_{x_i \in \mathcal{X}^x_j} g(x_i, x_j)}$$

The extra factor arises, since $\underset{\mathbf{x}}{\sim}$ is depending on the pattern \mathbf{x} . If $\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})}$ is to depend on 'local' information only, conditions must be imposed on $\underset{\mathbf{x}}{\sim}$.

The following definitions and results are taken from [11] to which we refer for further details. Define the x-neighbourhood of a subset $z \subseteq x$ as

$$N(\mathbf{z} \mid \mathbf{x}) = \left\{ \xi \in \mathbf{x} : \xi \underset{\mathbf{x}}{\sim} \eta \text{ for some } \eta \in \mathbf{z} \right\}.$$

Let $\mathbf{y} \subseteq \mathbf{z} \in \Omega$ and $u, v \in U$ with $u, v \notin \mathbf{z}$. Then require

(C1) $\chi(\mathbf{y} \mid \mathbf{z}) \neq \chi(\mathbf{y} \mid \mathbf{z} \cup \{u\})$ implies $\mathbf{y} \subseteq N(\{u\} \mid \mathbf{z} \cup \{u\})$;

(C2) if $u \not\sim_{\mathbf{x}} v$ where $\mathbf{x} = \mathbf{z} \cup \{u\} \cup \{v\}$ then

$$\chi(\mathbf{y} \mid \mathbf{z} \cup \{u\}) + \chi(\mathbf{y} \mid \mathbf{z} \cup \{v\}) = \chi(\mathbf{y} \mid \mathbf{z}) + \chi(\mathbf{y} \mid \mathbf{x}).$$

where χ is the clique indicator function.

Examples of relations satisfying these conditions are

- x_i ~ x_j iff x_i ~ x_j where ~ is any symmetric, reflexive relation on U (i.e. not depending on the configuration x);
- for points or marked points in \mathbb{R}^2 , $x_i \underset{\mathbf{x}}{\sim} x_j$ iff x_i, x_j are joined by an edge of the Delaunay triangulation generated by \mathbf{x} ;
- for compact sets in \mathbb{R}^d , $x_i \underset{\mathbf{x}}{\sim} x_j$ iff x_i and x_j belong to the same connected component of the union of the objects.

The proofs can be found in [11, Appendix].

Definition 3 A random object process with density p is called a nearestneighbour Markov object process (nnMp) with respect to $\{\underset{\mathbf{x}}{\sim} : \mathbf{x} \in \Omega\}$ if, for all \mathbf{x} with $p(\mathbf{x}) > 0$

- $p(\mathbf{y}) > 0$ for all $\mathbf{y} \subseteq \mathbf{x}$;
- the ratio $\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})}$ depends only on u, on $N(\{u\} \mid \mathbf{x} \cup \{u\}) \cap \mathbf{x} = \{x_i \in \mathbf{x} : x_i \sim u\}$ and on the relations $\approx, \sim \mathbf{x} \in \mathbf{x} : \mathbf{x}_i \sim u\}$ restricted to $N(\{u\} \mid \mathbf{x} \cup \{u\}) \cap \mathbf{x}$.

A subset $\mathbf{y} \subseteq \mathbf{x}$ is a *clique in* \mathbf{x} if all members of \mathbf{y} are \mathbf{x} -neighbours of one another $(u \underset{\mathbf{x}}{\sim} v \text{ for all } u, v \in \mathbf{y})$.

A generalised Hammersley-Clifford theorem holds [11]: a process with density p is nnMp iff

$$p(\mathbf{x}) = \begin{cases} \prod_{\text{cliques } \mathbf{y} \subseteq \mathbf{x}} q(\mathbf{y}) & \text{if } q(\mathbf{y}) > 0 \text{ for all } \mathbf{y} \subseteq \mathbf{x} \\ 0 & \text{otherwise} \end{cases}$$
(3.1.9)

where $q: \Omega \to \mathbb{R}_+$ satisfies certain regularity conditions ((I1)–(I2) of [11]).

Kendall [64] proved a spatial Markov property for nnMps.

3.2. Area-interaction processes

Pairwise interaction Markov processes (3.1.3) have been studied intensively. They provide a flexible class for modelling inhibition patterns and can be interpreted quite easily using the Hammersley-Clifford representation (3.1.7). However, they do not seem to be able to produce clustered patterns in sufficient variety. The original clustering model of Strauss [118] turned out [63] to be non-integrable for parameter values $\gamma > 1$ corresponding to the desired clustering; Gates and Westcott [39] showed that partly-attractive potentials may violate a stability condition, implying that they produce extremely clustered patterns with high probability; and recent simulation experiments by Møller [89] suggest that the behaviour of the Strauss model with fixed *n* undergoes an abrupt transition from 'Poisson-like' patterns to tightly clustered patterns rather than exhibiting intermediate, moderately clustered patterns.

The area-interaction model (3.1.8) in contrast is a Markov model that can yield both moderately clustered and moderately ordered patterns.

It has interactions of infinite order, and is similar in form to the pairwise interaction Strauss model (3.1.4). Both densities reduce to a Poisson process when $\gamma = 1$, and exhibit ordered patterns for $0 < \gamma < 1$; in contrast to the Strauss model, (3.1.8) is well-defined for all values of $\gamma > 0$ and produces clustering when $\gamma > 1$. The attractive case was proposed by Widom and Rowlinson [125] as the 'penetrable sphere model' for spherical molecules in the study of liquid-vapour phase transitions.

3.2.1 Definition of the process

As usual for Gibbs point processes we treat separately the cases of a finite point process (say, points in a bounded region $A \subseteq \mathbb{R}^d$) and a stationary point process on \mathbb{R}^d . The formal construction of finite Gibbs point processes is described in [25, p. 121 ff] or [100].

As before, let U be a locally compact complete separable metric space (typically \mathbb{R}^d or a compact subset). The space of all possible realisations \mathbf{x} shall be identified with the space N^f of all integer-valued measures on U which have finite total mass and are simple (do not have atoms of mass exceeding 1). Write $n(\mathbf{x})$ for the total number of points and \mathbf{x}_B for \mathbf{x} restricted to $B \subseteq U$. The σ -algebra \mathcal{N}^f on N^f is the Borel σ -algebra of the weak topology, i.e. \mathcal{N}^f is the smallest σ -algebra with respect to which the evaluation $\mathbf{x} \mapsto n(\mathbf{x}_B)$ is measurable for every (bounded) Borel set $B \subseteq U$.

Given a totally finite, non-atomic measure μ on U, construct the Poisson process of intensity μ as in Section 3.1.2 (typically μ is the restriction of Lebesgue measure to a compact window $A \subseteq \mathbb{R}^d$, yielding the unit

rate Poisson process restricted to A). Let π be its probability distribution on (N^f, \mathcal{N}^f) . Then we construct (Gibbs) point processes by specifying their density with respect to π .

Definition 4 ("Standard case") The area-interaction process in a compact region $A \subseteq \mathbb{R}^d$ is the process with density

$$p(\mathbf{x}) = \alpha \,\beta^{n(\mathbf{x})} \,\gamma^{-m(S_r(\mathbf{x}))} \tag{3.2.10}$$

with respect to the unit rate Poisson process on A, where $\beta, \gamma, r > 0$ are parameters and α is the normalising constant. Here m is Lebesgue measure and

$$S_r(\mathbf{x}) = \bigcup_{i=1}^n B(x_i, r)$$

is the union of spheres or discs of radius r centred at the points of the realisation, $B(x_i, r) = \left\{ a \in \mathbb{R}^d : ||a - x_i|| \le r \right\}.$

For $\gamma = 1$ this of course reduces to a Poisson process with intensity measure $\beta\mu$. It is intuitively clear that for $0 < \gamma < 1$ the pattern will tend to be 'ordered' and for $\gamma > 1$ 'clustered'. The clustered model was introduced by Widom and Rowlinson [125]. See also [56, 110, 111].

It is often more convenient to use the parameter $\eta = \gamma^{-\pi r^2}$, since the addition of one point *a* to the configuration **x** alters $p(\mathbf{x})$ by a factor ranging from β to $\beta\eta$.

Various modifications are of interest, for example, one may wish to replace $S_r(\mathbf{x})$ by $A \cap S_r(\mathbf{x})$, or to allow the radii of the discs $B(x_i, r)$ to vary across the region [68]. More generally, the discs $B(x_i, r)$ can be replaced by compact sets $Z(x_i)$ depending on x_i . We assume that the mapping Z onto the space \mathcal{K} of all compact subsets is continuous with respect to the myopic topology [84, p. 12] generated by $\{K \in \mathcal{K} : K \cap F = \emptyset\}$ for all closed $F \subseteq U$ and $\{K \in \mathcal{K} : K \cap G \neq \emptyset\}$ for all open subsets $G \subseteq U$.

Definition 5 ("General case") Let ν be a totally finite, regular Borel measure on U and Z : $U \rightarrow \mathcal{K}$ a myopically continuous function [84, p. 12], assigning to each point $u \in U$ a set $Z(u) \subseteq U$ in the space of all compact subsets \mathcal{K} . Then the general area-interaction process is defined to have density

$$p(\mathbf{x}) = \alpha \,\beta^{n(\mathbf{x})} \,\gamma^{-\nu(S(\mathbf{x}))} \tag{3.2.11}$$

with respect to π (the distribution of the finite Poisson process with intensity μ), where $S(\mathbf{x})$ is the compact set $\bigcup_{i=1}^{n} Z(x_i)$.

In a parametric statistical model the measure ν and the definition of $Z(\cdot)$ might also be allowed to depend on the parameter θ . Other generalisations are possible, for instance

$$p(\mathbf{x}) = a(\theta) \prod_{i=1}^{n} b(x_i; \theta) \exp\left(-\int_A f(d(\mathbf{x}, u)) \, du\right)$$

where $d(\mathbf{x}, u) = \min_i ||x_i - u||$ and $f : [0, \infty] \to (-\infty, \infty]$. The model we will discuss in this Section is a special case, analogous to the Strauss process.

Lemma 5 The density (3.2.11) is measurable and integrable for all values of $\beta, \gamma > 0$.

Proof: Let t > 0 and consider $V = \{ \mathbf{x} \in N^f : \nu(S(\mathbf{x})) < t \}$. We show that V is open in the weak topology.

Choose $\mathbf{x} \in V$. Since ν is regular, there is an open set $G \subseteq U$ containing $S(\mathbf{x})$ such that $\nu(G) < t$ too. Consider $W = \{\mathbf{y} \in N^f : S(\mathbf{y}) \subseteq G\}$; we have $\mathbf{y} \in W$ iff \mathbf{y} has no points in $H = \{u \in U : Z(u) \cap G^c \neq \emptyset\}$. Now H is closed in U since $u \mapsto Z(u)$ is myopically continuous and the class of all compact sets intersecting a given closed set is closed in the myopic topology on \mathcal{K} . Moreover, $W = \{\mathbf{y} \in N^f : n(\mathbf{y} \cap H) = 0\}$ is open in the weak topology. To see this, note that for any $\mathbf{y} \in W$, the open ball in the Prohorov metric [25, p. 622] with radius $\epsilon < \min\{d(\mathbf{y}, H), 1\}$ centred at \mathbf{y} is an open environment of \mathbf{y} contained in W. Thus, W is an open environment of \mathbf{x} contained in V and, since \mathbf{x} was arbitrary, V is weakly open.

In fact this shows that $\mathbf{x} \mapsto \nu(S(\mathbf{x}))$ is weakly upper semicontinuous. It follows that the map $g : N^f \to [0,\infty)$ defined by $\mathbf{x} \mapsto \exp[-\nu(S(\mathbf{x})) \log \gamma]$ is weakly upper semicontinuous for $\gamma \in (0,1)$ and lower semicontinuous for $\gamma > 1$. Hence g is measurable. By definition of the weak topology, $\mathbf{x} \mapsto \beta^{n(\mathbf{x})}$ is measurable, and hence the density (3.2.11) is measurable.

To check integrability, observe that

$$0 \le \nu(S(\mathbf{x})) \le \nu(U) < \infty \tag{3.2.12}$$

Now the function $f(\mathbf{x}) = \beta^{n(\mathbf{x})}$ is integrable, yielding the Poisson process with intensity measure $\beta\mu$. Hence (3.2.11) is dominated by an integrable function, hence integrable.

In fact (3.2.12) establishes a slightly stronger result.

Lemma 6 The distribution $P_{\beta,\gamma}$ of the general area interaction process is uniformly absolutely continuous with respect to the distribution of the Poisson process π^{β} with intensity $\beta\mu$, that is its Radon-Nikodym derivative is uniformly bounded.

In particular, the general area-interaction process satisfies the linear stability condition in [39]. Explicit bounds on the density $\alpha \gamma^{-\nu(S(\mathbf{x}))}$ with respect to a Poisson process of intensity $\beta \mu$ are

$$\min\left\{\gamma^{\nu(U)}, \gamma^{-\nu(U)}\right\} \le f \le \max\left\{\gamma^{\nu(U)}, \gamma^{-\nu(U)}\right\}.$$

This suggests that the 'singularity' (highly clustered behaviour) of the Strauss model is unlikely.

As usual, the normalising constant α is difficult to compute, since

 $\alpha^{-1} = \mathbb{E}\beta^{n(X)}\gamma^{-\nu(S(X))}$

where the expectation is with respect to the reference Poisson process; this entails computing the moment generating function of $\nu(S(X))$, or equivalently, the vacancy distribution in the coverage problem [53]. A notable exception is the 1-dimensional penetrable sphere model [125].

Area-interaction seems a plausible model for some biological processes. For example the points x_i may represent plants or animals which consume food within a radius r of their current location. The total area of accessible food is then $S_r(\mathbf{x})$, and the herd will tend to maximise this area, so an area-interaction model with $\gamma < 1$ is plausible. Alternatively assume that the animals or plants are hunted by a predator which appears at a random position and catches any prey within a distance r. Then $S_r(\mathbf{x})$ is the area of vulnerability, and the herd as a whole should tend to minimise this [55] so an area-interaction model with $\gamma > 1$ is plausible. Area-interaction processes with $\gamma > 1$ are also used as a model for liquid-vapour equilibrium in chemical physics.

The process can be derived from Poisson processes.

Lemma 7 Let X, Y be independent Poisson processes in A with intensity measures $\beta\mu$ and $|\log \gamma|\nu$ respectively. If $\gamma > 1$ then the conditional distribution of X given $\{Y \cap S(X) = \emptyset\}$ is an area-interaction process with parameter γ . If $\gamma < 1$ then the conditional distribution of X given $\{Y \subseteq S(X)\}$ is an area-interaction process with parameter γ .

Proof: If $\gamma > 1$

$$\mathbb{P}(Y \cap S(X) = \emptyset | X) = e^{-\nu(S(X)) \log \gamma} = \gamma^{-\nu(S(X))}$$

hence the conditional distribution of X given $Y \cap S(X) = \emptyset$ has a density proportional to the right hand side. Similarly if $\gamma < 1$

$$\mathbb{P}(Y \subseteq S(X)|X) = \mathbb{P}(Y \cap (A \setminus S(X)) = \emptyset)$$

= $e^{\nu(A \setminus S(X)) \log \gamma} = \gamma^{\nu(A)} \gamma^{-\nu(S(X))}.$

3.2.2 Limiting cases

Here we study the convergence of the area-interaction process as $\gamma \to 0, \infty$.

Let $\nu^* = \max_{\mathbf{x}} \nu(S(\mathbf{x}))$, typically the measure of the observation window or its (generalised) dilation and

$$H = \{\mathbf{x} : \nu(S(\mathbf{x})) = \nu^*\}.$$

Further, write π^{β} for the distribution of the Poisson process of rate β in U and finally, in the standard case, denote

$$HC = \left\{ \mathbf{x} : \ m(S(\mathbf{x})) = n(\mathbf{x})\pi r^2 \right\}$$

for the set of configurations respecting a hard core distance r.

Lemma 8 Let $P_{\beta,\gamma}$ be the distribution of the area interaction process with density (3.2.11).

If $\gamma \to 0$ with β fixed, then $P_{\beta,\gamma}$ converges to a uniform process on H, i.e. $P_{\beta,\gamma}(E) \to \pi^{\beta}(E \cap H)/\pi^{\beta}(H)$.

In the standard case, if $\gamma \to 0$ and $\beta \to 0$ so that $\beta \gamma^{-\pi r^2} \to \zeta \in (0, \infty)$, then $P_{\beta,\gamma}(E)$ converges to $P(E) = \pi^{\zeta}(E \cap HC)/\pi^{\zeta}(HC)$, a hard core process.

If $\gamma \to \infty$ with $\beta < \infty$ fixed, then $P_{\beta,\gamma}$ converges to a process that is empty with probability 1.

Proof: First consider $\gamma \to 0$. Then $\int \gamma^{\nu^* - \nu(S(\mathbf{x}))} d\pi^{\beta}(\mathbf{x}) \to \pi^{\beta}(H)$, hence

$$p_{\beta,\gamma}(\mathbf{x}) = \frac{\gamma^{\nu^* - \nu(S(\mathbf{x}))}}{\int \gamma^{\nu^* - \nu(S(\mathbf{x}))} d\pi^{\beta}(\mathbf{x})} \to \frac{\mathbf{1}\{\mathbf{x} \in H\}}{\pi^{\beta}(H)}$$

from which the first assertion follows. To prove the second assertion, note that for $m(S_r(\mathbf{x})) < n(\mathbf{x})\pi r^2$, $\gamma^{n(\mathbf{x})\pi r^2 - m(S_r(\mathbf{x}))} \to 0$. Hence

$$p_{\beta,\gamma}(\mathbf{x}) \rightarrow \frac{\zeta^{n(\mathbf{x})} \mathbf{1}\{\mathbf{x} \in HC\}}{\int_{HC} \zeta^{n(\mathbf{x})} d\pi^{1}(\mathbf{x})}.$$

The third statement follows similarly, by noting that the density converges pointwise to zero unless the pattern is empty. \Box

3.2.3 Markov property

Define two points $a, b \in U$ to be neighbours whenever $Z(a) \cap Z(b) \neq \emptyset$. In the standard case $a \sim b$ iff $||a - b|| \leq 2r$.

Lemma 9 The area-interaction process (3.2.11) is a Markov point process with respect to (3.1.1) in the sense of Ripley and Kelly [107].

Proof: The likelihood ratio

$$\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} = \beta \gamma^{-\nu(Z(u) \setminus S(\mathbf{x}))}$$
(3.2.13)

is computable in terms of u and $\{x_i : x_i \sim u\}$, since

$$Z(u) \setminus S(\mathbf{x}) = Z(u) \cap \left[\bigcup_{i} Z(x_i)\right]^c$$
$$= Z(u) \cap \left[\bigcup_{x_i \sim u} Z(x_i)\right]^c$$

Hence (3.2.11) defines a Markov point process with respect to \sim .

The Ripley-Kelly analogue of the Hammersley-Clifford theorem (3.1.7) then implies that the density p can be written as a product of clique interaction terms

$$p(\mathbf{x}) = \prod_{\mathbf{y} \subseteq \mathbf{x}} q(\mathbf{y})$$

where $q(\mathbf{y}) = 1$ unless $y_i \sim y_j$ for all elements of \mathbf{y} . To compute the interaction terms explicitly, invoke the inclusion-exclusion formula:

$$\nu(S(\mathbf{x})) = \sum_{i=1}^{n} \nu(Z(x_i)) - \sum_{i < j} \nu(Z(x_i) \cap Z(x_j)) + \cdots + (-1)^{n+1} \nu\left(\bigcap_{i=1}^{n} Z(x_i)\right)$$

which gives

$$q(\emptyset) = \alpha$$

$$q(\{a\}) = \beta \gamma^{-\nu(Z(a))}$$

$$q(\{y_1, \dots, y_k\}) = \gamma^{(-1)^k \nu(\bigcap_{i=1}^k Z(y_i))}, \ k \ge 2.$$
(3.2.14)

That is, the process exhibits interactions of infinite order.

The process satisfies a spatial Markov property (cf. [64, 107]). Define the dilation of a set $E \subseteq U$ by

$$D_Z(E) = \{ u \in U : \exists e \in E \text{ such that } Z(u) \cap Z(e) \neq \emptyset \}. \quad (3.2.15)$$

In the standard case this becomes the classical dilation of mathematical morphology

$$D_Z(E) = \left\{ u \in \mathbb{R}^d : d(u, E) \le 2r \right\}$$
(3.2.16)

where $d(u, E) = \inf \{ ||u - v|| : v \in E \}$. Then the spatial Markov property states that the restriction of the process to E is conditionally independent of the restriction to $D_Z(E)^c$ given the information in $D_Z(E) \setminus E$.

Figure 3.1 shows simulated realisations of (3.2.10). The number of points was fixed and the alternating birth/death technique of [102] used. This method entails alternating deletion of a random point and addition of a new point u to the current configuration \mathbf{x} from a probability density proportional to $p(\mathbf{x} \cup \{u\})$. The latter step can be implemented using rejection sampling, since the birth ratio (3.1.6) is dominated by a known constant by virtue of (3.2.12). In practice this will be a good bound for γ close to 1.



Figure 3.1: Simulated realisations of an area-interaction process conditional on n = 100 points, with r = 5 in a window of size 256×256 . Left: ordered pattern, $\gamma = 0.9711$, $\gamma^{-25\pi} = 10$; Right: clustered pattern, $\gamma = 1.02975$, $\gamma^{-25\pi} = 0.1$.

3.3. STATIONARY AREA-INTERACTION PROCESS

Here we use the methods of Preston [100] to check that the area interaction model (standard case) can be considered as the restriction to a bounded sampling window of a stationary point process on the whole of \mathbb{R}^{d} .

Let N be the space of all locally finite counting measures (i.e. integervalued Radon measures) on \mathbb{R}^d with the vague topology, and \mathcal{N} its Borel σ -algebra; that is, \mathcal{N} is the smallest σ -algebra making $\mathbf{x} \mapsto n(\mathbf{x}_B)$ measurable for all bounded Borel sets B.

Write C for the class of all bounded Borel sets in \mathbb{R}^d . For every $B \in C$ let N_B be the subspace of those $\mathbf{x} \in N$ contained in B (i.e. putting no mass outside B), $\mathcal{N}_B \subseteq \mathcal{N}$ the induced σ -algebra on N and π_B^β the distribution on (N, \mathcal{N}) of the homogeneous Poisson process of rate β on B. Note that any $\mathbf{x} \in N$ can be decomposed as $\mathbf{x} = \mathbf{x}_B \cup \mathbf{x}_{B^c}$. Define $f^B : N \to [0, \infty)$ by

$$f^B(\mathbf{x}) = \alpha_B(\mathbf{x}_{B^c}) \ \gamma^{-m(S_r(\mathbf{x}) \cap B_{\oplus r})}$$
(3.3.17)

where $S_r(\mathbf{x}) = \bigcup_{x_i \in \mathbf{x}} B(x_i, r)$, $B_{\oplus r} = B \oplus B(0, r)$ and $\alpha_B(\mathbf{x}_{B^c})$ is the normalising constant

$$\alpha_B(\mathbf{x}_{B^c})^{-1} = \int_{N_B} \gamma^{-m(S_r(\mathbf{y} \cup \mathbf{x}_{B^c}) \cap B_{\oplus r})} d\pi_B^\beta(\mathbf{y}).$$

To check that this is well-defined, observe that

$$S_r(\mathbf{x}) \cap B_{\oplus r} = S_r(\mathbf{x}_{B_{\oplus 2r}}) \cap B_{\oplus r}$$

so that $\mathbf{x} \mapsto m(S_r(\mathbf{x}) \cap B_{\oplus r})$ is measurable with respect to $\mathcal{N}_{B_{\oplus 2r}}$ and a fortiori with respect to \mathcal{N} . It is clearly integrable. Hence, by Fubini's theorem, $\alpha_B(\cdot)^{-1}$ is $\mathcal{N}_{B_{\oplus 2r}\setminus B}$ -measurable. Since α_B is uniformly bounded away from zero, α^{-1} is also measurable. Thus, (3.3.17) is \mathcal{N} measurable and integrable, and we may define for $\mathbf{x} \in \mathcal{N}, F \in \mathcal{N}$

$$\kappa_B(\mathbf{x}, F) = \int_{N_B} \mathbf{1}_F(\mathbf{x}_{B^c} \cup \mathbf{y}) f^B(\mathbf{x}_{B^c} \cup \mathbf{y}) \, d\pi_B^\beta(\mathbf{y}). \tag{3.3.18}$$

Theorem 10 There exists a stationary point process X on \mathbb{R}^d such that

$$\mathbb{P}(X \in F \mid X_{B^c}) = \kappa_B(X, F) \quad a.s$$

for all $B \in C$ and $F \in N$. That is, (3.3.18) is a specification without forbidden states [100, p. 12] and the distribution of X is a stationary Gibbs state with this specification. The corresponding potential $V : N^f \to \mathbb{R}$,

$$V(\mathbf{x}) = (-\log \gamma) m(S_r(\mathbf{x}))$$

is stable [100, p. 96].

Note that this result does not exclude the possibility that the Gibbs state is not unique, i.e. there may be 'phase transition' [100, p. 46]. **Proof:** First we prove consistency condition (6.10) of [100, p. 91]. For any bounded Borel sets $A \subseteq B$

$$\frac{f^B(\mathbf{x})}{f^A(\mathbf{x})} = \frac{\alpha_B(\mathbf{x}_{B^c})}{\alpha_A(\mathbf{x}_{A^c})} \gamma^{-m(S_r(\mathbf{x}_{A^c}) \cap B_{\oplus r} \setminus A_{\oplus r})}.$$

On the other hand

$$\int_{\mathbf{N}_{\mathbf{A}}} \mathbf{f}^{\mathbf{B}}(\mathbf{x}_{\mathbf{A}^{c}} \cup \mathbf{y}) \ \mathrm{d}\pi^{\beta}_{\mathbf{A}}(\mathbf{y}) = \alpha_{\mathbf{B}}(\mathbf{x}_{\mathbf{B}^{c}}) \ \int_{\mathbf{N}_{\mathbf{A}}} \gamma^{-\mathbf{m}(\mathbf{S}_{\mathbf{r}}(\mathbf{x}_{\mathbf{A}^{c}} \cup \mathbf{y}) \cap \mathbf{B}_{\oplus \mathbf{r}})} \ \mathrm{d}\pi^{\beta}_{\mathbf{A}}(\mathbf{y}).$$

Since $m(S_r(\mathbf{x}_{A^c} \cup \mathbf{y}) \cap B_{\oplus r}) = m(S_r(\mathbf{x}_{A^c} \cup \mathbf{y}) \cap A_{\oplus r}) + m(S_r(\mathbf{x}_{A^c}) \cap B_{\oplus r} \setminus A_{\oplus r}), \int_{N_A} f^B(\mathbf{x}_{A^c} \cup \mathbf{y}) d\pi^{\beta}_A(\mathbf{y}) = f^B(\mathbf{x})/f^A(\mathbf{x}).$ It follows [100, pp. 90–91] that $\{\kappa_B : B \in \mathcal{C}\}$ is a specification in the sense of [100, p. 12].

Now we check the conditions of Theorem 4.3 of [100, p. 58]. Condition (3.6) of [100, p. 35] is trivially satisfied. Arguments similar to those used to derive Lemma 6 above yield that for any $K \in \mathcal{K}$ the family $\{\pi_K(\mathbf{y}, \cdot)\}_{\mathbf{y}\in N}$ considered as a class of measures on (N, \mathcal{N}_K) is uniformly absolutely continuous with respect to π_K^β ; hence Preston's condition (3.11) [100, p. 41] holds, which implies his (3.10). It remains to check (3.8) of [100, p. 35]. Let \mathcal{K} be the class of all compact subsets of \mathbb{R}^d ; then we claim that

for any $B \in \mathcal{C}$ and $F \in \mathcal{N}_K$ where $K \in \mathcal{K}$, there exists $L \in \mathcal{K}$ such that $\kappa_B(\cdot, F)$ is measurable with respect to \mathcal{N}_L .

To check this, choose L to contain $K \cup B_{\oplus 2r}$ and observe that $1_F(\mathbf{x}_{B^c} \cup \mathbf{y})$ and $f^B(\mathbf{x}_B^c \cup \mathbf{y})$ are measurable with respect to $\mathcal{N}_L \otimes \mathcal{N}_B$, then apply Fubini's theorem. This proves the claim, which implies Preston's (3.8) and hence the conditions of his Theorem 4.3.

It is easy to see that V is the unique canonical potential corresponding to the densities f^B (cf. [100, p. 92]). Since $0 \le m(S_r(\mathbf{x})) \le \pi r^2 n(\mathbf{x})$, V is stable.

3.4. INFERENCE

This Section surveys parameter estimation techniques. We also derive a new identity from the Nguyen–Zessin formula that can be computed quite generally as an index for clustering and for estimating model parameters.

3.4.1 Sufficient statistics, exponential families

Consider a family of standard area-interaction processes (3.2.10) indexed by a parameter $\theta = (\beta, \gamma)$, with r and $A \subseteq \mathbb{R}^d$ fixed. This is an exponential family with canonical sufficient statistic

$$T(\mathbf{x}) = (n(\mathbf{x}), M(\mathbf{x}, \cdot))$$

where

$$M(\mathbf{x},r) = m(S_r(\mathbf{x})) = m(\bigcup_{i=1}^n B(x_i,r)).$$

Modifying this slightly we obtain a connection with the 'empty space statistic' $F(t) = \mathbb{P}(X \cap B(0, t) \neq \emptyset)$ [31, 103]. Define

$$\widehat{F(r)} = \frac{m(A_{(-r)} \cap (\bigcup_{i=1}^{n} B(x_i, r)))}{m(A_{(-r)})}$$
(3.4.19)

where

$$A_{(-t)} = \{a \in A : B(a,t) \subseteq A\}.$$

This is the 'border method' [104, p. 25] or 'reduced sample' estimator [4] of the empty space function.

Lemma 11 $(n(\mathbf{x}), \hat{F})$ is a sufficient statistic for the area-interaction process (3.2.11) with parameters (β, γ) when Z(u) = B(u, r) and the measure ν is Lebesgue measure restricted to $A_{(-r)}$.

The canonical parameter is $-\log \gamma$ but we prefer to use γ to maintain the comparison with the Strauss process.

3.4.2 Maximum likelihood

As usual for Markov point processes, the likelihood (3.2.11) is easy to compute except for a normalising constant α that is not known analytically. Maximum likelihood estimation therefore rests on numerical or Monte Carlo approximations of α [93, 94, 95, 98] or recursive approximation methods [90]. For a more detailed review see [33, 45] or [104]. We will not explore this further here, except to note that the maximum likelihood estimating equations are as usual

$$n(\mathbf{x}) = \mathbb{E}_{\beta,\gamma} n(X) \tag{3.4.20}$$

$$\nu(S(\mathbf{x})) = \mathbb{E}_{\beta,\gamma}\nu(S(X)) \tag{3.4.21}$$

where **x** is the observed pattern and X is a random pattern with density (3.2.11). For the model conditioned on $n(\mathbf{x}) = n$ the ML estimating equation is analogous to (3.4.21) with β absent.

3.4.3 Takacs-Fiksel

The Takacs-Fiksel estimation method exploits the Nguyen–Zessin identity [92]

$$\lambda \mathbb{E}_{a}^{!} f(X) = \mathbb{E}[\lambda(a; X) f(X)]$$
(3.4.22)

holding for any bounded measurable non-negative function $f: N \to \mathbb{R}_+$ and any stationary Gibbs process X on \mathbb{R}^d with finite intensity λ , see [46, 47, 67, 85, 62] or [104, p. 54–55], [33, §2.4]. The expectation on the left hand side of (3.4.22) is with respect to the reduced Palm distribution of X at $a \in \mathbb{R}^d$, that is the conditional distribution of the *rest* of the process given that there is a point at a; $\lambda(a; \mathbf{x})$ is the Papangelou conditional intensity of X at a (cf. Section §3.1.2). Thus (3.4.22) states that the reduced Palm distribution of X at a is equivalent to the $\lambda(a; X)$ -weighted distribution of X.

A Takacs-Fiksel method [37, 38, 120, 121] is then to choose suitable functions and to estimate both sides in the above formula. The resulting set of equations is solved, yielding estimates for the parameters of the model. The idea was originally suggested by Takacs [120, 121] for a particular case and generalised by Fiksel [37, 38]. A variant using only nearest neighbour measurements was developed by Tomppo [123].

For a Gibbs process the conditional intensity can be computed in terms of likelihood ratios [62]. For the standard area-interaction process

$$\lambda(a;\mathbf{x}) = \beta \gamma^{-m(B(a,r) \setminus S_r(\mathbf{x}))}$$

for $a \notin \mathbf{x}$; this depends only on $\mathbf{x}_{B(a,2r)}$. One interesting instance of (3.4.22) is

$$f(\mathbf{x}) = \frac{\mathbf{1}\{\mathbf{x} \cap B(0,s) = \emptyset\}}{\lambda(0;\mathbf{x})}$$

using 0 as an arbitrary point of \mathbb{R}^d (cf. [117, (5.5.18), p. 159]). Then $\mathbb{E}[\lambda(0; X) \ f(X)] = 1 - F(s)$ where $F(s) = \mathbb{P}(X \cap B(0, s) \neq \emptyset)$ is the

empty space function of X. Now if s > 2r,

$$\begin{split} \lambda \mathbb{E}_{0}^{!} f(X) &= \lambda \int \mathbf{1} \{ X \cap B(0,s) = \emptyset \} \beta^{-1} \gamma^{m(B(0,r) \setminus S_{r}(X))} dP_{0}^{!}(X) \\ &= \lambda \int \mathbf{1} \{ X \cap B(0,s) = \emptyset \} \beta^{-1} \gamma^{m(B(0,r))} dP_{0}^{!}(\mathbf{x}) \\ &= \lambda \beta^{-1} \gamma^{\pi r^{2}} [1 - G(s)] \end{split}$$

where $G(s) = \mathbb{P}_0^!(X \cap B(0, s) \neq \emptyset)$ is the nearest neighbour distance distribution function of X. Equivalently

$$J(s) = \frac{1 - G(s)}{1 - F(s)} = \frac{\beta \gamma^{-\pi r^2}}{\lambda}.$$
(3.4.23)

for all s > 2r.

Thus parameter estimates for the area-interaction process can be extracted directly from the standard statistics F and G. Similar identities hold for any (Markov) model with finite range of interaction. The ratio can be computed in many cases, when F and G separately cannot, and the graph provides an estimate for the interaction range. For further development of this idea see [78].

Identity (3.4.23) also provides a further description of the typical pattern generated by the model; F and G are used in spatial statistics as measures of clustering versus regularity, with $1 - F(t) = 1 - G(t) = \exp\{-\lambda \pi t^2\}$ and hence $(1 - G)/(1 - F) \equiv 1$ in the case of a Poisson process. Clustering is sometimes characterised by elevated G and lowered F; regularity by elevated F and lowered G [31]. Hence (1 - G)/(1 - F) < 1for clustering and > 1 for regularity.

3.4.4 Approximation by lattice processes

Besag, Milne and Zachary [18] proved that any purely inhibitory (or hard core) pairwise interaction point process is the weak limit of a sequence of lattice processes, and remark [18, p. 214] this is also true of general Gibbs point processes, again of purely inhibitory type. Here we extend the result to the area-interaction model, which is *not* inhibitory.

Consider a partition $\{C_1, \ldots, C_m\}$ of the observation window A and choose representatives $\xi_i \in C_i$. Denote the area of C_i by $A_i > 0$ and the set of all representatives by Ξ . We shall construct a $\{0, 1\}$ -valued stochastic process $\mathbf{n} = \{n_i : i = 1, \ldots, m\}$ which is auto-logistic,

$$\frac{\mathbb{P}(n_i = 1 \mid n_j, j \neq i)}{\mathbb{P}(n_i = 0 \mid n_j, j \neq i)} = \mu_i(C_i)$$
(3.4.24)

where

$$\mu_i(C_i) = A_i \prod q(\xi_i \cup \mathbf{y})^{\eta(\mathbf{y})};$$

the product ranges over all (possibly empty) subsets of $\Xi \setminus \{\xi_i\}$, the set function q is the clique interaction function (3.2.14) and $\eta(\mathbf{y}) = \prod_{\xi_j \in \mathbf{y}} n_j$ is either 0 or 1.

Given a realisation of **n**, construct a realisation **x** of a point process X such that if $n_i = 0$ then $\mathbf{x} \cap C_i$ is empty, while if $n_i = 1$ then $\mathbf{x} \cap C_i$ consists of one point uniformly distributed in C_i independently of other points.

Lemma 12 The conditional distributions (3.4.24) specify a distribution for **n** and

$$\frac{\mathbf{P}(\mathbf{n})}{\mathbf{P}(\mathbf{0})} = \prod_i A_i^{n_i} \prod_{\emptyset \neq \mathbf{y} \subseteq \Xi} q(\mathbf{y})^{\eta(\mathbf{y})}.$$

The point process X is absolutely continuous with respect to a unit rate Poisson process on A, with density

 $f(\mathbf{x}) = f(\emptyset) \prod_{\emptyset \neq \mathbf{y} \subseteq \Xi} q(\mathbf{y})^{\eta_{\mathbf{X}}(\mathbf{y})}.$

Here $\eta_{\mathbf{x}}(\mathbf{y}) = \prod n(\mathbf{x} \cap C_j)$ and the product ranges over all j such that $\xi_j \in \mathbf{y}$.

Proof: Use Besag's factorisation theorem [14, p. 195].

Theorem 13 Consider a sequence of partitions $C_r = \{C_{r,1}, \ldots, C_{r,m(r)}\}$ such that $\max_i \dim(C_{r,i}) \to 0$. Then the corresponding point process $\mathbf{x}^{(r)}$ converges weakly and in total variation to the area-interaction process $p(\cdot)$.

Proof: Let f_r be the density of $\mathbf{x}^{(r)}$. For fixed \mathbf{x}

$$\frac{f_r(\mathbf{x})}{f_r(\emptyset)} \to \prod_{\emptyset \neq \mathbf{y} \subseteq \mathbf{x}} q(\mathbf{y}) = \beta^{n(\mathbf{x})} \ \gamma^{-\nu(S(\mathbf{x}))} = \frac{1}{\alpha} \ p(\mathbf{x})$$

since all cells ultimately contain at most one point, and q is continuous in all its arguments. By dominated convergence,

$$\frac{1}{f_r(\emptyset)} = \int \frac{f_r(\mathbf{x})}{f_r(\emptyset)} \, d\pi(\mathbf{x}) \to \int \frac{1}{\alpha} \, p(\mathbf{x}) \, d\pi(\mathbf{x}) = \frac{1}{\alpha};$$

thus,

$$f_r(\mathbf{x}) = \frac{f_r(\mathbf{x})}{f_r(\emptyset)} f_r(\emptyset) \to p(\mathbf{x})$$

pointwise and the theorem is proved.

3.4.5 Pseudolikelihood estimation

Because of the lattice approximation, the model parameters can be estimated by pseudolikelihood [15, 18, 61]. Using the notation of Section 3.4.4, the pseudolikelihood for partition $\{C_i\}_{i=1}^m$ is

$$PL(\theta) = \prod_{\mathbf{x} \cap C_i \neq \emptyset} \mathbb{P}(n_i = 1 \mid n_j, j \neq i)$$

$$\cdot \prod_{\mathbf{x} \cap C_i = \emptyset} \{1 - \mathbb{P}(n_i = 1 \mid n_j, j \neq i)\}.$$

Since

$$\mathbb{P}(n_i = 1 \mid n_j, j \neq i) = \frac{A_i \lambda(\xi_i; \mathbf{x})}{1 + A_i \lambda(\xi_i; \mathbf{x})}$$

where $\lambda(\cdot; \mathbf{x})$ is the Papangelou conditional intensity, we have

$$\lim_{A_i \to 0} \frac{1}{A_i} \mathbb{P}(n_i = 1 \mid n_j, j \neq i) = \lambda(\xi_i; \mathbf{x})$$

or $\mathbb{P}(n_i = 1 \mid n_j, j \neq i) \approx A_i \lambda(\xi_i; \mathbf{x})$. Therefore, for small A_i ,

$$\log PL(\theta) - n(\mathbf{x}) \log A_i = \sum_{\mathbf{x} \cap C_i \neq \emptyset} \log \left\{ \frac{1}{A_i} \mathbb{P}(n_i = 1 \mid n_j, j \neq i) \right\}$$
$$+ \sum_{\mathbf{x} \cap C_i = \emptyset} \log \left\{ 1 - \mathbb{P}(n_i = 1 \mid n_j, j \neq i) \right\}$$
$$\approx \sum_{\mathbf{x} \cap C_i \neq \emptyset} \log \lambda(\xi_i; \mathbf{x}) - \sum_{\mathbf{x} \cap C_i = \emptyset} A_i \lambda(\xi_i; \mathbf{x})$$
$$\approx \sum_{\xi \in \mathbf{x}} \log \lambda(\xi; \mathbf{x}) - \int_A \lambda(\xi; \mathbf{x}) \, d\xi.$$

In the limit, the pseudolikelihood equations are

$$PL(\beta,\gamma;\mathbf{x}) = \exp\left\{-\int_{A}\lambda(u;\mathbf{x})du\right\} \prod_{i=1}^{n}\lambda(x_{i};\mathbf{x}).$$
(3.4.25)

For the area-interaction model (3.2.10)

$$\lambda(u;\mathbf{x}) = \frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x} \setminus \{u\})} = \beta \ \gamma^{-m(B(u,r) \setminus S_r(\mathbf{x} \setminus \{u\}))}.$$

Writing $t(u) = m(B(u, r) \setminus S_r(\mathbf{x} \setminus \{u\}))$ the maximum pseudolikelihood estimates of β and γ are the solutions of

$$n = \beta \int_{A} \gamma^{-t(u)} du \qquad (3.4.26)$$

$$\sum_{i=1}^{n} t(x_i) = \beta \int_A t(u) \gamma^{-t(u)} du$$
 (3.4.27)

Note that these have exactly the same form as the pseudolikelihood equations for the Strauss model [104, p. 53]; in that case -t(u) is the number of points in **x** with $0 < ||u - x_i|| \le r$.

For inhibitory pairwise interaction models it is known that pseudolikelihood estimation is a special case of the Takacs-Fiksel method when the interaction radius r is fixed [33, Section 2.4], [104, p. 54] or [115, Section 4]. The same is true for the area-interaction model.

Theorem 14 For a stationary area-interaction process, the pseudolikelihood equations (3.4.26) and (3.4.27) are special cases of the Takacs-Fiksel method.

Proof: Take f to be either of

$$\begin{aligned} f_{\beta}(\mathbf{x}) &= \beta^{-1}, \\ f_{\gamma}(\mathbf{x}) &= -\gamma^{-1}m(B(0,r)\setminus S_r(\mathbf{x}\setminus\{0\})). \end{aligned}$$

These are the partial derivatives of $\log \lambda(0; \mathbf{x})$ with respect to β and γ . When $f = f_{\beta}$ an unbiased estimator for the left hand side of (3.4.22) is

$$\frac{n}{m(A)}\frac{1}{\beta}$$

and, by stationarity, an unbiased estimator of the right hand side is

$$\frac{1}{m(A)}\int_A \frac{1}{\beta} \beta \gamma^{-t(u)} du.$$

When $f = f_{\gamma}$, the average over the observed events

$$\frac{n}{m(A)} \frac{1}{n} \sum_{i=1}^{n} \frac{-t(x_i)}{\gamma}$$

is an unbiased estimator of the left hand side of (3.4.27) by the Campbell-Mecke formula [117, p. 113], while an unbiased estimator for the right hand side is the window mean

$$rac{1}{m(A)}\int_A rac{-t(u)}{\gamma}eta\gamma^{-t(u)}\;du.$$

These reduce to (3.4.26) - (3.4.27).

Chapter 4 Bayesian object recognition

This Chapter develops a Bayesian approach to object recognition. We describe iterative optimisation schemes related to Besag's ICM [16] and discuss how spatial birth-and-death processes can be used for sampling and stochastic annealing [42]. The relative merits of the methods are investigated by means of a simple synthetic example.

4.1. GENERAL

A strong motivation for adopting a Bayesian approach to object recognition is that the MLE tends to contain clusters of almost identical objects, i.e. there is 'multiple response' to each true object, as noted in Section 2.6. This is related to the fact that the Hough transform has rather flat peaks around the correct object positions. Multiple response is undesirable if it is important to correctly determine the number of objects, and if it is believed that objects do not lie extremely close to one another. For instance in document reading it is known in advance that characters usually do not overlap. A standard approach in computer vision is to select one object per peak of the Hough transform; but this is very similar to a Bayesian approach using a prior model which assigns low probability to configurations in which objects are close to one another.

Natural prior models $p(\mathbf{x})$ belong to the class of nearest-neighbour Markov object processes described in Chapter 3. Given observation of image \mathbf{y} , the posterior probability density for scene \mathbf{x} is then

$$p(\mathbf{x} \mid \mathbf{y}) \propto f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}). \tag{4.1.1}$$

The posterior distribution is often a nearest-neighbour object process too, though possibly with respect to a different neighbour relation. Specifically, for the overlapping objects relation (3.1.1) and a blur-free independent noise model with $g(\cdot | \cdot) > 0$, the posterior distribution is Markov with respect to (3.1.1) as well.

A Maximum A Posteriori (MAP) estimator of the true configuration solves

$$\tilde{\mathbf{x}} = \operatorname{argmax}_{\mathbf{x}} p(\mathbf{x} \mid \mathbf{y}) = \operatorname{argmax}_{\mathbf{x}} f(\mathbf{y} \mid \mathbf{x}) p(\mathbf{x}).$$

$$(4.1.2)$$

Again, the optimisation is over the space Ω of all object configurations. In decision theoretic terms, this corresponds to imposing a 0-1 loss function, according to whether the recognition is perfect or imperfect. Assuming $p(\cdot) > 0$ rewrite (4.1.2) as

$$\tilde{\mathbf{x}} = \operatorname{argmax}_{\mathbf{x}} \left[\log f(\mathbf{y} \mid \mathbf{x}) + \log p(\mathbf{x}) \right].$$
(4.1.3)

Because of this expression, $\tilde{\mathbf{x}}$ is also called a *penalised maximum likelihood estimator*. The factor $\log f(\mathbf{y} | \mathbf{x})$ is interpreted as a measure of goodness of fit to the data, and $-\log p(\mathbf{x})$ as a penalty for the complexity of the configuration \mathbf{x} . Typically, $p(\cdot)$ assigns low weight to configurations with many similar objects. Alternatively, P.J. Green noted that (4.1.3) can be interpreted as an optimisation of Euler-Lagrange type.

4.1.1 Prior models

A simple prior is the Strauss process (3.1.4) which results in a penalty of $-\log\beta$ for the presence of each object $x_i \in \mathbf{x}$ and a penalty of $-\log\gamma$ for each pair of neighbouring objects (e.g. overlapping objects). Modifications which might be useful in this application are

$$p(\mathbf{x}) = \alpha \prod_{i=1}^{n} \beta^{|R(x_i)|} \prod_{i < j} \gamma^{|R(x_i) \cap R(x_j)|}$$
(4.1.4)

and, for marked objects, to allow the interaction terms to depend on the marks.

Regarding the choice of parameter values, note that if the raster is made finer (say, quadrupling the number of pixels) then the log likelihood typically increases by the same factor. This suggests that to maintain the balance between f and p in (4.1.2)–(4.1.3) the parameters $\log \beta$ and $\log \gamma$ of a Strauss model should also be multiplied by this factor. Models such as (4.1.4) with interactions expressed in terms of pixel counts, do not require such adjustment.

Since the area-interaction model (3.1.8)

$$p(\mathbf{x}) = \alpha \beta^{n(\mathbf{x})} \gamma^{-|S(\mathbf{x})|}$$

is also defined through pixel counts, the same remark holds. To enforce inhibition, choose $\gamma < 1$. Then, with the number of objects fixed, the silhouette area $|S(\mathbf{x})|$ is maximal if there is as little overlap as possible.

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4.2. **ITERATIVE ALGORITHMS**

Iterative methods are needed in order to find the MAP estimator (4.1.2). As in Section 2.4 we consider algorithms which add or delete objects one at a time. The log likelihood ratio criterion is now replaced by a log posterior probability ratio.

Algorithm 5 Apply Algorithms 1, 2, 3 or 4 with $f(\mathbf{y} | \mathbf{x})$ replaced by the posterior probability $p(\mathbf{x} | \mathbf{y})$. Thus we iteratively add object u to list \mathbf{x} iff

$$\log \frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) \ p(\mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} \geq w,$$

delete existing object x_i iff

$$\log \frac{f(\mathbf{y} \mid \mathbf{x} \setminus \{x_i\}) \ p(\mathbf{x} \setminus \{x_i\})}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} \ge w$$

and if shifts are permitted, we shift $x_i \in \mathbf{x}$ to u iff $u \in Q(\mathbf{x}, x_i)$ and

$$\log \frac{f(\mathbf{y} \mid M(\mathbf{x}, x_i, u)) \ p(M(\mathbf{x}, x_i, u))}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} \ge w$$

where $w \ge 0$ is a chosen threshold.

The convergence properties of Algorithms 1–4 remain valid for this new objective function. An alternative description of Algorithm 5 is that the static threshold value used in the likelihood ratio algorithms is replaced by one that depends on the current reconstruction and on a smoothing parameter.

Algorithm 5 is a close analogue of Besag's ICM algorithm [16]. If the object space U is finite, consider labelling each $u_i \in U$ with value

$$v_j = \left\{ egin{array}{cc} 1 & ext{if } u_j \in \mathbf{x} \ 0 & ext{else} \end{array}
ight. .$$

The ICM approach would be to visit each object sequentially and update its label in the light of current estimates for the other objects: when the labelling is \hat{v} , the label of the current object u_j is updated to

$$\operatorname{argmax} \mathbb{P}(V_j = k \mid \mathbf{y}, (\hat{v}_i)_{i \neq j}).$$

But this is clearly equivalent to comparing

 $f(\mathbf{y} \mid \hat{\mathbf{x}} \setminus \{u_j\}) \ p(\hat{\mathbf{x}} \setminus \{u_j\})$

against

$$f(\mathbf{y} \mid (\hat{\mathbf{x}} \setminus \{u_j\}) \cup \{u_j\}) \ p((\hat{\mathbf{x}} \setminus \{u_j\}) \cup \{u_j\})$$

where $\hat{\mathbf{x}}$ is the current object list; and this is Algorithm 5 (w = 0).

Algorithm 2 is a simple variant of ICM, at least in the discrete case. This algorithm is also defined when U is 'continuous' (any l.s.c. space) but the interpretation is more complex. We add a new object u at the position where the Papangelou conditional intensity of the posterior distribution, given the current configuration \mathbf{x} on $U \setminus \{u\}$, is maximal, provided this is greater than e^w (relative to the reference measure μ).

4.2.1 Examples

Figure 4.1 shows the result of steepest ascent ICM for the pellet texture of Section 2.6. The prior was a Strauss process of overlapping discs (3.1.4) with $\log \beta = \log \gamma = -1000$.



Figure 4.1: MAP reconstruction of the Brodatz pellets texture by steepest ascent from an empty initial state (w = 0) using a Strauss prior with $\log \beta = \log \gamma = -1000$.

As another example, consider a noise corrupted image of a scene consisting of rectangles of various sizes (Figure 4.2). The object space is four-dimensional; any rectangle can be described by the coordinates of its upper left and lower right corner. The forward model is blur-free Gaussian white noise. Because the object size is variable, MLE solutions cannot distinguish between one large rectangle and a union of several small ones having the same silhouette. Therefore we introduce a



Figure 4.2: Realisation from a Gaussian blur-free independent noise model with $\sigma = 10$, $\theta_1 = 150$ and $\theta_0 = 100$, digitised on a 128×116 grid.

penalty $-\log \beta = 5.0$ on addition of an object and obtain a (non-unique) steepest ascent reconstruction given in Figure 4.3 (top). Fine tuning is possible by allowing the corners to move one pixel in every direction. The result is shown in Figure 4.3 (middle).

Note that the posterior distribution cannot distinguish between an equal number of objects having the same silhouette. If it is desirable to have as many overlap as possible, a penalty $-\log \gamma = 5.0$ on every pair of overlapping objects can be introduced, resulting in Figure 4.3 (bottom), or for every pixel in the intersection (resolving uncertainty in the two objects in the top centre of the image).

4.2.2 Relation to Hough transform

In many cases, computing the posterior log likelihood ratio is a local operation, related to the Hough transform. For example, taking the Strauss prior (3.1.4), $g(\cdot|\cdot) > 0$ and a blur-free signal,

$$\log \frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) \ p(\mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} = \log \beta + r(u; \mathbf{x}) \log \gamma + \sum_{R(u) \setminus S(\mathbf{x})} z_t$$

where $r(u; \mathbf{x}) = s(\mathbf{x} \cup \{u\}) - s(\mathbf{x})$ is the number of neighbours of u in \mathbf{x} and $z_t = \log g(y_t|\theta_1) - g(y_t|\theta_0)$ (cf. Section 2.5). The new term in γ is a penalty against adding an object in the vicinity of existing objects. For the area-interaction prior (3.1.8) the term involving γ is replaced by $-|R(u) \setminus S(\mathbf{x})| \log \gamma$ so that we again obtain something very similar to the Hough transform.

In general, for any independent noise model (2.2.3) with $g(\cdot|\cdot) > 0$, and any nearest neighbour Markov object prior (Definition 3), the pos-

64

terior log likelihood ratio depends only on data pixels in the update zone $Z(\mathbf{x}, u)$ and on the configuration (and relations) in the restricted neighbourhood $\mathbf{x} \cap N(u \mid \mathbf{x} \cup \{u\})$ of the added object.

4.2.3 Parameter estimation

Until now we assumed that the model parameters were known exactly. However, in realistic situations unknown physical variables have to be taken into account. In some applications where many similar images are available, these can be used for parameter estimation. In the absence of training data, estimation and recognition of objects must be carried out simultaneously.

Maximum likelihood can be applied to obtain estimates. This is feasible for many noise models; in particular for independent noise models the method is straightforward. The prior distribution, however, involves a normalising constant which cannot be evaluated, making maximum likelihood estimation intractable. An alternative, more efficient method is maximum pseudolikelihood estimation [14, 15, 61], which maximises the product of conditional densities. This product does not involve the normalising constant and is easy to compute for Markov processes. However, it is not a genuine likelihood, except in the case of spatially independent objects. (See also Section 3.4.5).

For the superficially similar case of image segmentation using Markov random fields, Besag [16] proposed the following procedure. Unknown parameters in f and p are denoted by ϕ and ψ respectively.

Algorithm 6

- 1. obtain an initial estimate $\hat{\mathbf{x}}$ of the true pattern, with guesses for ϕ and ψ if necessary;
- 2. estimate ϕ by maximising $f(\mathbf{y} \mid \hat{\mathbf{x}}; \phi)$; optionally, estimate ψ by the maximum pseudolikelihood method;
- **3.** carry out a single step of the reconstruction algorithm based on the current estimates $\hat{\mathbf{x}}$, $\hat{\phi}$ and $\hat{\psi}$, leading to a new estimate $\hat{\mathbf{x}}$, and return to step 2.

An alternative, fully Bayesian approach is to specify a prior distribution for each model parameter and replace step 2 above by sampling from the posterior distributions.

As an illustration, Figure 4.4 displays a digitised piece of music, reproduced with kind permission of R. van den Boomgaard. The data was scanned by P. Tax (University of Amsterdam). Here we will focus on finding the locations of notes. To a good approximation their shape is







Figure 4.3: Steepest ascent reconstructions for the data in Figure 4.2 at threshold w = 0 using a Strauss prior. The initial state is empty. Top: only births and deaths, $\log \beta = -5$ and $\log \gamma = 0$. Middle: translations over 1 pixel in every direction, $\log \beta = -5$ and $\log \gamma = 0$. Bottom: translations over 1 pixel in every direction, $\log \beta = -5$ and $\log \gamma = -5$.

elliptical, the major axis making a 30 degree angle with the horizontal coordinate axis. As the shape is assumed to be constant, the parameter space and image space coincide, i.e. this is a translation model.



Figure 4.4: Binary image of a small piece of music digitised on a 250×65 grid.

For the noise distribution a salt-and-pepper model was chosen, with unknown error fraction p. As it is known in advance that notes cannot overlap each other, a suitable choice for the prior distribution is a hard core object process (3.1.2).

A steepest ascent reconstruction, starting from an empty list, for the data in Figure 4.4 is given in Figure 4.5. Here, w = 0 and $\log \beta = -50$. The noise error fraction p is estimated during iteration by its maximum likelihood estimator

$$\hat{p} = \frac{|S(\mathbf{x})\Delta Y|}{|T|}.$$

Recall that Y is the set of pixels with value 1 and Δ denotes the symmetric set difference. To facilitate interpretation the data image was masked by the reconstruction and vice versa.



Figure 4.5: Steepest ascent reconstruction (white) 'masked' by the data. The initial configuration is empty, w = 0 and the prior distribution is hard core with $\log \beta = -50$.

The scene contains not only notes, but also other features such as horizontal and vertical lines, thick bars etc. However, their contribution to the Hough transform is small in comparison to real notes, due to the fact that negative pixel votes serve to compensate the positive contributions. In other words, the objects R(u) are large enough to accumulate strong evidence in the Hough transform and to suppress noise. By setting the penalty $-\log\beta$ for addition of a new object high enough, only desired objects are detected.

It is interesting to note that the parts in the image are strongly connected. Vertical line segments are usually linked with the basic notes (except to separate measures) and might be joined by bars. Once the basic ellipses have been found, one could add an extra stage to look for line segments and then bars, thus building a hierarchical method for automatic music reading. We do not pursue this issue further.

4.3. PERFORMANCE EVALUATION

In this Section we study in detail a simple synthetic example in which a pattern of discs of fixed radius (parameterised by the centre coordinates) has been observed after addition of Gaussian noise (Figure 4.6). As the true scene is known, it is possible to compare algorithms by computing numeric performance measures.





Figure 4.6: Binary silhouette scene of discs with radius 4 and realisation from Gaussian model with $\sigma = 50$, $\theta_1 = 150$ and $\theta_0 = 100$, digitised on a 98 × 98 square grid.

4.3.1 Reconstructions

Figure 4.7 shows maximum likelihood reconstructions obtained by the coordinatewise optimisation algorithm (Algorithms 1 and 3) taking threshold value w = 0. The pixels were scanned in row major order and for the initial state we took the local maxima of

$$\log rac{f(\mathbf{y} \mid \{u\})}{f(\mathbf{y} \mid \emptyset)}$$

where the expression was non-negative. Furthermore, Algorithm 3 allowed translations over one pixel in every direction. Note the multiple response, especially where discs overlap each other.

The reconstructions obtained using steepest ascent (Algorithms 2 and 4) with empty initial state and threshold value w = 0 are given in figure 4.8. In this case it seems important to stop short of convergence. Typically, when all the objects that are really present have been detected, the method keeps adding spurious ones. This can be counteracted by taking a higher threshold value. In the present example choosing w = 6 will result in the 'best' reconstruction shown in Figure 4.9.

Algorithm 5 is illustrated in Figure 4.10 for coordinatewise optimisation. Again, the pixels were scanned in row major order choosing the



Figure 4.7: MLE reconstructions using coordinatewise ascent with the local extrema of the Hough transform as initial state. Left: only births and deaths; right: births, deaths and translation.



Figure 4.8: MLE reconstructions using steepest ascent with the empty list as initial state. Left: only births and deaths; right: births, deaths and translation.



Figure 4.9: 'Best' intermediate MLE reconstruction using steepest ascent with the empty list as initial state (both Algorithms 2 and 4).

local extrema of the Hough transform as initial configuration. A Strauss prior model was used with parameters $\beta = .0025$ and $\gamma = .25$. In the steepest ascent case fewer spurious discs are added. Indeed the final result is the 'best' one for this particular example (Figure 4.11). Overall, MAP gives a clear improvement over MLE, successfully combating multiple response.

4.3.2 Typical behaviour

In the discussion below, we define one 'step' of each algorithm as a complete scan through the discretised parameter space. The number of 'transitions' (additions or deletions of objects) per scan may vary:



Figure 4.10: MAP reconstructions using coordinatewise ascent with the local extrema of the Hough transform as initial state. The prior distribution is a Strauss model with $\beta = .0025$ and $\gamma = .25$. Left: only births and deaths; right: births, deaths and translations.



Figure 4.11: MAP reconstructions using steepest ascent with the empty list as initial state. The prior distribution is a Strauss model with $\beta = .0025$ and $\gamma = .25$. Left: only births and deaths; right: births, deaths and translations.

steepest ascent (and some sampling techniques) generate one transition per scan, while coordinatewise optimisation yields a variable number depending on the data, the current reconstruction and the scanning order. 'Steps' are roughly proportional to total computer time, although this ignores the possibility of parallelism: steepest ascent could be implemented in parallel computation, but coordinatewise optimisation is inherently sequential.

The performance of an algorithm is measured by computing the log likelihood $L(\mathbf{x}^{(k)}; \mathbf{y})$ itself and two 'external' measures of fidelity, Pratt's figure of merit [1]

$$\frac{1}{\max\{n(\mathbf{x}), n(\mathbf{x}^{(k)})\}} \sum_{x'_i \in \mathbf{x}^{(k)}} \frac{1}{1 + \frac{1}{9}d(x'_i, \mathbf{x})}$$

and Baddeley's Δ_2 metric [2]

$$\left\{\frac{1}{n(T)}\sum_{t\in T}\left(d(t,\mathbf{x})-d(t,\mathbf{x}^{(k)})\right)^2\right\}^{1/2}.$$

With a slight abuse of notation, the same symbol d is used to denote the distance from either a lattice or a configuration member to a given pattern. It can be justified by noting that in this particular example image space and object space coincide.

We computed the Δ_2 distance and the figure of merit for the reconstruction $\mathbf{x}^{(k)}$ at each iteration. Figure .1 graphs the performance of coordinatewise optimisation starting with the local extrema of the Hough transform. Pixels were scanned in row major order. Again MAP shows
a clear improvement over the MLE in terms of the external performance measures. Note that for Bayesian algorithms the log likelihood graph need not be monotone, as these methods aim at increasing the *posterior* likelihood.

For the steepest ascent algorithms the behaviour is qualitatively different, see Figure .2. While coordinatewise optimisation needs only a few scans through the image, steepest ascent from an empty initial image requires at least as many scans as there are objects in the image. New objects are added one-by-one, gradually improving the reconstruction quality, until all objects are detected; then the reconstructions deteriorate. This method can however yield more accurate reconstructions than coordinatewise optimisation algorithms, especially in the non-Bayesian case.

A widely used technique for object recognition is to compute the Hough transform and find its local extrema. In noisy images this procedure performs badly, as can be seen from the graphs in Figure .1 where the y intercept is the performance of the Hough extrema operator.

4.3.3 Initial state influence

Tables 1–12 show performance measures for the eight possible algorithms using various initial states.

First restrict attention to the methods based only upon addition and deletion. Using initial configurations other than the empty list does not change the overall pattern described above. Coordinatewise optimisation converges in a few steps; steepest ascent slowly improves the reconstruction by removing incorrect objects and replacing them by the right ones. MAP shows less sensitivity to the initial state than does MLE.

Not surprisingly, the best reconstructions were obtained when initialising with the true image, but a perfect match is not guaranteed. This reflects the fact that the truth is not necessarily a solution of the MAP equations.

One proposal is to use the local extrema of the Hough transform as the initial state. This appears sensible for the coordinatewise optimisation algorithms but not for steepest ascent. In most cases better reconstructions could be obtained with an empty image as initial state.

The same remarks hold if the initial state is a translation of the true state. A possible explanation is that extra effort is required to throw away incorrect estimates and replace them with better ones.

In summary, for the add-delete algorithms, it is best as a rule of thumb to use the empty list as a starting state for the steepest ascent algorithms, unless additional information about the objects to be detected is available. This is especially so since time is wasted in throwing away incorrect objects. Another advantage is that no preprocessing (e.g. computing the Hough transform) of the data is required.

Turning now to the add-delete-shift algorithms, we note that these exhibit less sensitivity to the choice of initial state. Another advantage is that the number of scans needed for steepest ascent decreases, as it is no longer necessary to throw away spurious objects first and then replace them by better ones. This is illustrated in Figure .2 where it must be noted that the plot for Algorithm 2 is cut off, as 71 transitions were needed. The graphs for the refined algorithms are smoother than those for the techniques based upon addition and deletion only, and the levels at convergence are better. The Bayesian method with only births and deaths is unable to reposition many discs, as the posterior log likelihood ratios are too small. When using Algorithm 2 more discs are thrown away and readded at their proper positions, but many more scans through the image are required.

4.3.4 Noise influence

It is also of interest to investigate the influence of signal-to-noise ratio. We generated ten independent realisations of Model 1 for several values of σ^2 . Reconstructions were obtained and the average quality calculated for Algorithms 1–5. The results are depicted in Figure .3.

As could be expected, the reconstructions become poorer when more noise is added. Due to the extra term penalising undesirable configurations, the MAP solutions are less sensitive to the noise variance than ML estimates. Steepest ascent is more robust than coordinatewise optimisation.

4.4. FIXED TEMPERATURE SAMPLING

The natural analogue of the Gibbs sampler in this context is a spatial birth-and-death process [101, 88]. This is a continuous time, pure jump Markov process, whose states are configurations $\mathbf{x} \in \Omega$, and for which the only transitions are the birth of a new object (instantaneous transition from \mathbf{x} to $\mathbf{x} \cup \{u\}$) or the death of an existing one (transition from \mathbf{x} to $\mathbf{x} \cup \{u\}$) or the death of an existing one (transition from \mathbf{x} to $\mathbf{x} \setminus \{x_i\}$). Formally, write \mathcal{B} for the (Borel) σ -algebra on U and let $D(\cdot, \cdot) : \Omega \times U \to [0, \infty)$ be a measurable function and $B(\cdot, \cdot) : \Omega \times \mathcal{B} \to [0, \infty)$ a finite kernel, i.e. $B(\mathbf{x}, \cdot)$ is a finite measure on (U, \mathcal{B}) and $B(\cdot, F)$ is a measurable function on Ω . These are called the *death rate* and *birth rate*. The reason is clear from the following. Given the state \mathbf{x} at time t,

- the probability of a death $\mathbf{x} \to \mathbf{x} \setminus \{x_i\}$ during a time interval $(t, t+h), h \to 0$, is $D(\mathbf{x} \setminus \{x_i\}, x_i)h + o(h)$;
- the probability of a birth $\mathbf{x} \to \mathbf{x} \cup \{u\}$ during time (t, t+h), where u lies in a given measurable subset $F \subseteq U$, is $B(\mathbf{x}, F)h + o(h)$;
- the probability of more than one transition during (t, t+h) is o(h).

We will assume that $B(\mathbf{x}, \cdot)$ has a density $b(\mathbf{x}, \cdot)$ with respect to μ on U, so that intuitively $b(\mathbf{x}, u)$ is the transition rate for a birth $\mathbf{x} \to \mathbf{x} \cup \{u\}$. Write

$$B(\mathbf{x}) = \int_U b(\mathbf{x}, u) \ d\mu(u)$$

for the total birth rate, and similarly define

$$D(\mathbf{x}) = \sum_{x_i \in \mathbf{x}} D(\mathbf{x} \setminus \{x_i\}, x_i).$$

To avoid explosion, i.e. an infinite number of transitions occurring in finite time, the rates have to satisfy certain assumptions. Preston [101, Prop. 5.1, Thm. 7.1] gave sufficient conditions under which there exists a unique spatial birth-and-death process with given rates solving Kolmogorov's backward equations

$$\frac{d}{dt} \mathbb{P}(X_t \in A | X_0 = \mathbf{x}) = -[B(\mathbf{x}) + D(\mathbf{x})] \mathbb{P}(X_t \in A | X_0 = \mathbf{x}) + \int_{\Omega} \mathbb{P}(X_t \in A | X_0 = \mathbf{z}) R(\mathbf{x}, d\mathbf{z})$$

with $R(\mathbf{x}, A) = B(\mathbf{x}, \{u \in U : \mathbf{x} \cup \{u\} \in A\}) + \sum_{x_i \in \mathbf{x}} 1\{\mathbf{x} \setminus \{x_i\} \in A\}$ $D(\mathbf{x} \setminus \{x_i\}, x_i)$ the total rate from pattern \mathbf{x} into a measurable subset $A \subseteq \Omega$. For a given process $(X_t)_t$ he also found conditions for the existence of a unique invariant probability measure and convergence in distribution (i.e. convergence of $\mathbb{P}(X_t \in F | X_0 = \mathbf{x})$). **Theorem 15** For each n = 0, 1, ... define $\kappa_n = \sup_{n(\mathbf{x})=n} B(\mathbf{x})$ and $\delta_n = \inf_{n(\mathbf{x})=n} D(\mathbf{x})$. Assume $\delta_n > 0$ for all $n \ge 1$. If either (a) $\kappa_n = 0$ for all sufficiently large $n \ge 0$, or (b) $\kappa_n > 0$ for all $n \ge 0$ and both the following hold:

$$\sum_{n=1}^{\infty} \frac{\kappa_0 \cdots \kappa_{n-1}}{\delta_1 \cdots \delta_n} < \infty$$
$$\sum_{n=1}^{\infty} \frac{\delta_1 \cdots \delta_n}{\kappa_1 \cdots \kappa_n} = \infty$$

then there exists a unique spatial birth-and-death process for which $B(\cdot, \cdot)$ and $D(\cdot, \cdot)$ are the transition rates; this process has a unique equilibrium distribution to which it converges in distribution from any initial state.

A slightly stronger result given by Møller [88] includes the case $\kappa_0 = 0$, $\kappa_n > 0$ for all $n \ge 1$ and both $\sum_{n=2}^{\infty} \frac{\kappa_1 \cdots \kappa_{n-1}}{\delta_1 \cdots \delta_n} < \infty$ and $\sum_{n=1}^{\infty} \frac{\delta_1 \cdots \delta_n}{\kappa_1 \cdots \kappa_n} = \infty$, still assuming all δ_n positive for $n \ge 1$.

4.4.1 Construction

Suppose we want to sample from the temperature modified posterior distribution

$$p_H(\mathbf{x} \mid \mathbf{y}) \propto \{ f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}) \}^{1/H} \,. \tag{4.4.5}$$

The purpose of introducing a temperature parameter is to sharpen peaks in posterior probability. For small H > 0, configurations with large posterior density are favoured, while others are suppressed. Indeed, if object space U is discretised $p_H(\cdot | \mathbf{y})$ converges pointwise to a uniform distribution on the set of MAP solutions as H tends to zero.

Consider any blur-free independent noise model (2.2.3) with $g(\cdot|\cdot) > 0$ and a nearest-neighbour Markov object prior. The former assumption is needed so that the class $K = \{\mathbf{x} : f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}) > 0\}$ is hereditary. For some fixed $k \in [0, 1]$ set

$$b_H(\mathbf{x}, u) = \begin{cases} \left(\frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) \ p(\mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})}\right)^{k/H} & \text{if } \mathbf{x} \in K\\ 0 & \text{if } \mathbf{x} \notin K \end{cases}$$
(4.4.6)

for $u \notin \mathbf{x}$ and death rate

$$D_H(\mathbf{x} \setminus \{x_i\}, x_i) = \begin{cases} \left(\frac{f(\mathbf{y} \mid \mathbf{x}) p(\mathbf{x})}{f(\mathbf{y} \mid \mathbf{x} \setminus \{x_i\}) p(\mathbf{x} \setminus \{x_i\})}\right)^{\frac{k-1}{H}} & \text{if } \mathbf{x} \in K\\ \delta'_n(\mathbf{x})/n(\mathbf{x}) & \text{if } \mathbf{x} \notin K \end{cases} (4.4.7)$$

Here $\delta'_n = \inf \{ \sum_{x_i \in \mathbf{X}} D_H(\mathbf{x} \setminus \{x_i\}, x_i) \mid f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}) > 0, \ n(\mathbf{x}) = n \}$. By convention, the infimum of the empty set equals ∞ . Note that by this definition $\delta'_n = \delta_n$, where δ_n is defined as in Theorem 15. The boundary cases k = 0 ('constant birth rate') and k = 1 ('constant death rate') are well-known in spatial statistics, to obtain realisations of a point process. It is widely argued (e.g. [102]) that the constant death rate procedure should be preferred, as under the constant birth rate process there is a high probability that a newly-added object will have a large death rate and thus be rapidly deleted again.

For a nearest-neighbour Markov prior the above expressions are typically easy to evaluate, since the normalising constant α is eliminated. Moreover the 'detailed balance' equations

$$b_H(\mathbf{x}, u) \ p_H(\mathbf{x} \mid \mathbf{y}) = D_H(\mathbf{x}, u) \ p_H(\mathbf{x} \cup \{u\} \mid \mathbf{y})$$

$$(4.4.8)$$

are satisfied whenever $f(\mathbf{y} | \mathbf{x} \cup \{u\}) p(\mathbf{x} \cup \{u\}) > 0$. Intuitively, under the equilibrium distribution $p_H(\cdot | \mathbf{y})$ transitions from \mathbf{x} into $\mathbf{x} \cup \{u\}$ are exactly matched by transitions from $\mathbf{x} \cup \{u\}$ into \mathbf{x} . Given a spatial birth-and-death process with rates satisfying (4.4.8), Ripley [102] remarked that the process is necessarily time reversible and $p_H(\cdot|\mathbf{y})$ is the density of its unique invariant probability measure. For each application, however, one should verify that the process just described is well-defined. For instance the following corollary of Theorem 15 holds.

Corollary 16 Let y and H > 0 be fixed. For any blur-free independent noise model with $g(\cdot|\cdot) > 0$, and any nearest-neighbour Markov object process $p(\cdot)$ with uniformly bounded likelihood ratios

$$\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} \le \beta < \infty$$

there exists a unique spatial birth-and-death process for which (4.4.6)and (4.4.7) are the transition rates. The process has unique equilibrium distribution $p_H(\cdot | \mathbf{y})$ and it converges in distribution to $p_H(\cdot | \mathbf{y})$ from any initial state.

Proof: We will prove the following properties:

- 1. $\delta_n > 0$, for $n \ge 1$;
- 2. if $\kappa_{n_0} = 0$ for some $n_0 \ge 1$, then $\kappa_n = 0 \ \forall n \ge n_0$;
- 3. if $\kappa_n > 0$ for all *n*, then condition (b) of Theorem 15 holds.

Property 1: Use the representation of the log likelihood ratio as a generalised Hough transform (2.1.1). Since T is finite, we have upper and lower bounds on the goodness of fit, say $|h(y_t, \theta_0, \theta_1)| \leq a$ for all t. Hence

$$|L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y})| \le a \ n(R(u)) \le a \ n(T)$$

where *n* denotes the number of pixels. For $p(\cdot)$ we have by assumption $\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} \leq \beta$. If $p(\mathbf{x}) > 0$ this implies that

$$D_{H}(\mathbf{x} \setminus \{u\}, u) = \left(\frac{f(\mathbf{y} \mid \mathbf{x})}{f(\mathbf{y} \mid \mathbf{x} \setminus \{u\})} \frac{p(\mathbf{x})}{p(\mathbf{x} \setminus \{u\})}\right)^{\frac{k-1}{H}}$$
$$\geq \exp\left[\frac{k-1}{H}\left(|L(\mathbf{x} \setminus \{u\}; \mathbf{y}) - L(\mathbf{x}; \mathbf{y})| + \log\beta\right)\right]$$
$$\geq \exp\left[\frac{k-1}{H}\left(a \ n(T) + \log\beta\right)\right] =: \delta > 0.$$

Suppose $p(\mathbf{x}) = 0$. If $p(\mathbf{z}) = 0$ for all \mathbf{z} with $n(\mathbf{z}) = n(\mathbf{x})$, then $D_H(\mathbf{x} \setminus \{u\}, u) = \infty \ge \delta$. Otherwise $n(\mathbf{x}) D_H(\mathbf{x} \setminus \{u\}, u) = \inf \{D_H(\mathbf{z}) \mid n(\mathbf{z}) = n(\mathbf{x}), p(\mathbf{z}) > 0\}$. By the above argument, $D_H(\mathbf{z} \setminus \{z_i\}, z_i) \ge \delta$ for all such \mathbf{z} and $z_i \in \mathbf{z}$. Hence $D_H(\mathbf{z}) \ge \delta n(\mathbf{x})$ and $D_H(\mathbf{x} \setminus \{u\}, u) \ge \delta$. Therefore $D_H(\mathbf{x}) \ge \delta n(\mathbf{x})$ for all patterns \mathbf{x} , and hence $\delta_n \ge \delta n > 0$ for $n \ge 1$.

Property 2: Use the fact that $K = \{\mathbf{x} : f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}) > 0\}$ is hereditary.

Property 3: The birth rates are also bounded. For $p(\mathbf{x}) > 0$

$$b_H(\mathbf{x}, u) = \left(\frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x})} \frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})}\right)^{k/H}$$

$$\leq \exp\left[\frac{k}{H} (a \ n(T) + \log \beta)\right]$$

$$=: \ \kappa > 0.$$

For $p(\mathbf{x}) = 0$, again $b_H(\mathbf{x}, u) = 0 \le \kappa$. Hence $B_H(\mathbf{x}) \le \kappa \mu(U)$ and so $\kappa_n \le \kappa \mu(U)$.

Using these bounds, one obtains

$$\frac{\kappa_0 \cdots \kappa_{n-1}}{\delta_1 \cdots \delta_n} \le \frac{\kappa^n \ \mu(U)^n}{n! \ \delta^n}$$

Since $\mu(U)$ is finite by assumption, the first assertion follows. Similarly

$$\frac{\delta_1 \cdots \delta_n}{\kappa_1 \cdots \kappa_n} \ge \frac{n! \, \delta^n}{\kappa^n \, \mu(U)^n}$$

which does not converge to zero as $n \to \infty$. The Corollary is proved if we combine these properties with Theorem 15.

If the state space is discretised, the situation is easier. Recall that any Markov chain on a finite state space is uniquely defined by its transition rates and if for an irreducible Markov chain with rates R(i, j), $i \neq j$, π is a probability measure satisfying the detailed balance equations

$$R(i,j) \ \pi(i) = R(j,i) \ \pi(j) \tag{4.4.9}$$

then the chain is time reversible and has unique limit distribution π (see for instance [97, pp. 277–278]). Hence, if $f(\mathbf{y} | \mathbf{x}) > 0$ for all \mathbf{x} the class K is hereditary, due to the Markov property of $p(\cdot)$. It follows that the birth-and-death process defined above restricted to K is irreducible.

To simulate the birth-and-death process we generate the successive states $X^{(k)}$ and the sojourn times $T^{(k)}$ as follows. Given $X^{(k)} = \mathbf{x}^{(k)}$, $T^{(k)}$ is exponentially distributed with mean $1/(D_H(\mathbf{x}^{(k)}) + B_H(\mathbf{x}^{(k)}))$, independent of other sojourn times and of past states. The next state transition is a death with probability $D_H(\mathbf{x}^{(k)})/(D_H(\mathbf{x}^{(k)}) + B_H(\mathbf{x}^{(k)}))$, obtained by deleting one of the existing points x_i with probability

$$\frac{D_H(\mathbf{x}^{(k)} \setminus \{x_i\}, x_i)}{D_H(\mathbf{x}^{(k)})}.$$

Otherwise the transition is a birth generated by choosing one of the points $u \notin \mathbf{x}^{(k)}$ with probability density

$$\frac{b_H(\mathbf{x}^{(k)}, u)}{B_H(\mathbf{x}^{(k)})}$$

with respect to μ and adding u to the state.

Algorithm 7 (Fixed temperature sampling) Run the process described above for a 'large' time period C and take $\mathbf{x}^{(L)}$ where

$$L = \min\{k = 0, 1, 2, \dots | \sum_{i=0}^{k} t^{(i)} > C\}.$$

For a discussion of the rate of convergence see [88].

Figure 4.12 shows a single realisation from the posterior distribution for the pellets texture of Section 2.6 using the same Strauss prior as for Figure 4.1. The realisation was obtained by running the constant death rate process described above Algorithm 7.

The main advantage of sampling techniques compared to deterministic methods is the ability to estimate any functional of the (modified) posterior distribution by taking a sufficient number of independent realisations. Examples of useful functionals are: the distribution (mean, variance) of the number of objects; the probability that there is no object in a given subregion of the image; the distribution of the distance from a given reference point to the nearest object and the first-order intensity [117]. In the discrete case the first-order intensity at u is simply the (posterior) probability that u belongs to \mathbf{x} . It can be regarded as an alternative to the Hough transform. The posterior intensity is given in Figure 4.13.

Clearly, other sampling techniques [44] could be used as well. However, at small temperatures, those based on (standard) rejection sampling may have unacceptably long waiting times.



Figure 4.12: Realisation from the posterior distribution for the Brodatz pellets texture sampled at time 1. The prior distribution is a Strauss process with $\log \beta = \log \gamma = -1000$.



Figure 4.13: Posterior intensity estimated over 10 time units for the Brodatz pellets texture. The prior distribution is a Strauss process with $\log \beta = \log \gamma = -1000$.

4.5. Convergence of inhomogeneous Markov processes

Given a family of well-defined spatial birth-and-death processes indexed by temperature parameter H, each converging in distribution to the corresponding $p_H(\cdot | \mathbf{y})$, stochastic annealing involves an inhomogeneous Markov process with H gradually dropping to zero. To find an annealing schedule that ensures convergence to a mode of the posterior distribution, some results on inhomogeneous Markov processes are needed. The discrete time case has been studied in [52, 126].

4.5.1 Definitions

Let μ and ν be probability measures on a common measurable space (S, A). Their *total variation distance* is defined as the maximal difference in mass on measurable subsets $A \in A$

$$\|\mu - \nu\| = \sup_{A \in \mathcal{A}} |\mu(A) - \nu(A)|.$$

If $|\mathcal{S}| < \infty$

$$\|\mu - \nu\| = \frac{1}{2} \sum_{i \in S} |\mu(i) - \nu(i)|.$$

Similarly in the continuous case, if both μ and ν are absolutely continuous with respect to some measure m with Radon-Nikodym derivatives f_{μ} and f_{ν} ,

$$\|\mu - \nu\| = \frac{1}{2} \int_{\mathcal{S}} |f_{\mu}(s) - f_{\nu}(s)| dm(s).$$

Definition 6 For a transition probability function (stochastic matrix) $P(\cdot, \cdot)$ on (S, A), **Dobrushin's contraction coefficient** c(P) is defined by

$$c(P) = \sup_{x,y \in \mathcal{S}} \| P(x, \cdot) - P(y, \cdot) \|.$$

We list some properties that will be used in the sequel (see Dobrushin [34, Section 3]).

Lemma 17 Let Λ be the set of all probability measures on (S, A). Then for all transition probability functions P and Q and for all $\mu, \nu \in \Lambda$ the following hold

(i) $c(P) \leq 1;$

(ii)
$$c(P) = \sup_{\mu \neq \nu \in \Lambda} \frac{\|\mu P - \nu P\|}{\|\mu - \nu\|};$$

(iii) $\|\mu P - \nu P\| \le c(P) \|\mu - \nu\|;$

(iv) $c(PQ) \leq c(P) c(Q)$.

For completeness, the proof is given below. Much can be found in [34].

Proof: Property (i) is trivial;

To prove (ii) first note that, since $\|\delta_x - \delta_y\| = 1$ for all $x \neq y$,

$$c(P) = \sup_{x \neq y} \frac{\|\delta_x P - \delta_y P\|}{\|\delta_x - \delta_y\|}$$

$$\leq \sup_{\nu \neq \mu \in \Lambda} \frac{\|\mu P - \nu P\|}{\|\mu - \nu\|}.$$

For the reverse inequality, choose $\nu, \mu \in \Lambda$ and consider 'the' Jordan-Hahn decomposition [54] of S with respect to $\mu - \nu$, i.e. find a disjoint measurable partition A^+, A^- such that

$$(\mu - \nu)(A) \ge 0 \quad \forall A^+ \supseteq A \in \mathcal{A},$$

 $(\mu - \nu)(A) \le 0 \quad \forall A^- \supseteq A \in \mathcal{A}.$

Then $\|\mu - \nu\| = (\mu - \nu)(A^+) \lor (\nu - \mu)(A^-)$ and since $(\mu - \nu)(A^+ \cup A^-) = 0$,

$$\|\mu - \nu\| = (\mu - \nu)(A^+) = (\nu - \mu)(A^-).$$

Setting $\tau(A) := \inf_{y \in S} P(y, A)$, for all $x \in S$

$$P(x, A) - \tau(A) \le \sup_{x,y,A} |P(x, A) - P(y, A)| = c(P).$$

Consider the case $\mu P(A) \ge \nu P(A)$. The other case is similar. Then

$$\begin{split} \mu P(A) &- \nu P(A) = \int_{\mathcal{S}} P(x, A)(\mu - \nu)(dx) \\ &= \int_{A^{+}} P(x, A)(\mu - \nu)(dx) + \int_{A^{-}} P(x, A)(\mu - \nu)(dx) \\ &\leq \int_{A^{+}} P(x, A)(\mu - \nu)(dx) + \int_{A^{-}} \tau(A)(\mu - \nu)(dx) \\ &= \int_{A^{+}} (P(x, A) - \tau(A)) (\mu - \nu)(dx) \\ &\leq c(P) (\mu - \nu)(A^{+}) = c(P) \|\mu - \nu\|. \end{split}$$

Therefore

$$\|\mu P - \nu P\| = \sup_{A \in \mathcal{A}} |\mu P(A) - \nu P(A)| \le c(P) \|\mu - \nu\|$$

and hence

$$\sup_{\nu \neq \mu \in \Lambda} \frac{\|\mu P - \nu P\|}{\|\mu - \nu\|} \le c(P)$$

which proves (ii). Property (iii) is an easy consequence of property (ii); for (iv) note that

$$\begin{aligned} \|(PQ)(x,\cdot) - (PQ)(y,\cdot)\| &= \|P(x,\cdot)Q - P(y,\cdot)Q\| \\ &\leq c(Q) \|P(x,\cdot) - P(y,\cdot)\|. \end{aligned}$$

Therefore

$$c(PQ) = \sup_{x,y} \|PQ(x,\cdot) - PQ(y,\cdot)\|$$

$$\leq c(Q) \sup_{x,y} \|P(x,\cdot) - P(y,\cdot)\|$$

$$= c(P) c(Q).$$

4.5.2 Limit theorems

The main theorem of this Section states sufficient conditions under which a sequence of Markov processes converges in total variation to a welldefined limit.

Recall that the transition semi-group $(Q_t)_{t\geq 0}$ of a Markov process $(Y_t)_{t\geq 0}$ in continuous time is the semi-group of probability kernels representing its conditional distributions,

$$Q_t(y,F) = \mathbb{P}(Y_t \in F \mid Y_0 = y).$$

Theorem 18 Let $(X_t)_{t\geq 0}$ be a non-stationary Markov process on a measurable space (S, \mathcal{A}) , defined by a sequence of transition semi-groups $(Q_n)_{n\in\mathbb{N}}$. The process follows the transition rules Q_n in the time period $[t_n, t_{n+1})$, that is

$$\mathbb{P}(X_s \in F \mid X_r = y) = (Q_n)_{s-r}(y, F)$$

for $t_n \leq r < s < t_{n+1}$. Here $t_n \nearrow \infty$ as $n \to \infty$. Assume that for each $n \in \mathbb{N}$, Q_n has an invariant measure μ_n , i.e.

$$\int_{\mathcal{S}} (Q_n)_t(x,F) \ d\mu_n(x) = \mu_n(F)$$

for all $F \in A$ and $t \ge 0$. Assume moreover that the following hold

(C)
$$\sum_{n=1}^{\infty} \|\mu_n - \mu_{n+1}\| < \infty$$

(D)
$$c(P_{tt'}) \to 0 \text{ as } t' \to \infty \text{ for all } t \ge 0$$

where $P_{tt'}(x, F) = \mathbb{P}(X_{t'} \in F \mid X_t = x)$. Then $\mu_{\infty} = \lim \mu_n$ exists and $\nu P_{0t} \rightarrow \mu_{\infty}$ in total variation as $t \rightarrow \infty$, uniformly in the initial distribution ν .

Proof: Condition (C) implies that (μ_n) is a Cauchy sequence in $\|\cdot\|$ and hence converges in total variation to μ_{∞} , say. Define $n(t) = \sup \{n : t_n \leq t\}$ choose $0 \leq t < t_{n(t)+1} < t' < \infty$. Then

$$\mu_{\infty} P_{tt'} - \mu_{\infty} = (\mu_{\infty} - \mu_{n(t)}) P_{tt'} + \mu_{n(t)} P_{tt'} - \mu_{\infty}$$

= $(\mu_{\infty} - \mu_{n(t)}) P_{tt'} + \mu_{n(t)} P_{tt_{n(t)+1}} P_{t_{n(t)+1}t'} - \mu_{\infty}$

Since $\mu_{n(t)}$ is an invariant measure one sees that

$$\begin{split} \mu_{\infty} P_{tt'} - \mu_{\infty} &= (\mu_{\infty} - \mu_{n(t)}) P_{tt'} + \mu_{n(t)} P_{t_{n(t)+1}t'} - \mu_{\infty} \\ &= (\mu_{\infty} - \mu_{n(t)}) P_{tt'} + \sum_{k=n(t)}^{n(t')-1} (\mu_k - \mu_{k+1}) P_{t_{k+1}t'} \\ &+ \mu_{n(t')} - \mu_{\infty}. \end{split}$$

Hence

$$\begin{aligned} \|\mu_{\infty}P_{tt'} - \mu_{\infty}\| &\leq \left\|\mu_{\infty} - \mu_{n(t)}\right\| c(P_{tt'}) \\ &+ \sum_{k=n(t)}^{n(t')-1} \|\mu_{k} - \mu_{k+1}\| c(P_{t_{k+1}t'}) + \left\|\mu_{n(t')} - \mu_{\infty}\right\| \\ &\leq 2 \sup_{k \geq n(t)} \|\mu_{k} - \mu_{\infty}\| + \sum_{k=n(t)}^{\infty} \|\mu_{k} - \mu_{k+1}\| \\ &\to 0 \ (t \to \infty). \end{aligned}$$

Let $\epsilon > 0$. Choose t such that $\|\mu_{\infty}P_{tt'} - \mu_{\infty}\| < \epsilon/2$ for all $t' > t_{n(t)+1}$. Next observe that

$$\begin{aligned} \|\nu P_{0t'} - \mu_{\infty}\| &= \|(\nu P_{0t} - \mu_{\infty}) P_{tt'} + \mu_{\infty} P_{tt'} - \mu_{\infty}\| \\ &\leq \|\nu P_{0t} - \mu_{\infty}\| c(P_{tt'}) + \|\mu_{\infty} P_{tt'} - \mu_{\infty}\| \\ &\leq c(P_{tt'}) + \|\mu_{\infty} P_{tt'} - \mu_{\infty}\|. \end{aligned}$$

Use condition (D) to choose t' such that $c(P_{tt'}) < \epsilon/4$. Summarising, we obtain

$$\|\nu P_{0t} - \mu_{\infty}\| \to 0$$
 uniformly in $\nu \ (t \to \infty)$.

A sufficient condition for (D) is given by the next result. It is easier to work with, since only stationary Markov chains have to be considered.

Lemma 19 Use the same notation as in the previous Theorem. If $c(P_{t_nt_{n+1}}) \leq 1 - 1/n$ for all $n \geq 2$, the Dobrushin condition (D) holds.

Proof: Write $P_n = P_{t_n t_{n+1}}$. Then

$$-\log c(P_n) \ge 1 - c(P_n) \ge \frac{1}{n}.$$

Thus

$$-\sum_{n=2}^{\infty} \log c(P_n) \ge \sum_{n=2}^{\infty} \frac{1}{n} = \infty$$

or equivalently

$$\prod_{n=2}^N c(P_n) \to 0 \ (N \to \infty).$$

Fix t. Then for $t' > t_{n(t)+2}$

$$\begin{aligned} c(P_{tt'}) &= c(P_{tt_{n(t)+1}}P_{t_{n(t)+1}t_{n(t)+2}}\cdots P_{t_{n(t')}t'}) \\ &\leq c(P_{tt_{n(t)+1}}) \left[\prod_{i=n(t)+1}^{n(t')-1} c(P_i)\right] c(P_{t_{n(t')}t'}) \\ &\leq \prod_{i=n(t)+1}^{n(t')-1} c(P_i) \to 0 \ (t' \to \infty). \end{aligned}$$

.

4.6. OBJECT RECOGNITION BY STOCHASTIC ANNEALING

An alternative method for solving the MAP equations (4.1.2) can be based on the results of Section 4.5. Assuming the conditions of Corollary 16, for each fixed H we can construct a spatial birth-and-death process with equilibrium distribution $p_H(\cdot | \mathbf{y})$. Our proposal therefore is to use a stochastic annealing algorithm that simulates these processes consecutively with H gradually dropping to zero. In contrast to ICM, if the temperature H decreases sufficiently slowly, stochastic annealing results in a global maximum.

In the superficially similar context of image segmentation, a simulated annealing algorithm was developed by Geman and Geman [42]. However, the Markov processes involved are rather different. Since in segmentation problems both object and image space are finite pixel grids, a discrete time Markov chain changing each pixel label in turn suffices.

4.6.1 The summability condition

First we consider the summability condition (C) in Theorem 18.

Lemma 20 For fixed data y, let $H_n \searrow 0$ $(n \to \infty)$ and consider the sequence of H_n -modified posterior distributions with densities

$$p_{H_n}(\mathbf{x} \mid \mathbf{y}) \propto \{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})\}^{1/H_n}$$

with respect to the reference measure π on Ω (law of Poisson process or counting measure in the discretised case). Assume that $\pi(\mathcal{M}) > 0$, where \mathcal{M} denotes the set of solutions to the MAP equations (4.1.2). Then the sequence p_{H_n} converges in total variation to a uniform distribution on \mathcal{M} . Moreover the sequence satisfies condition (C).

Proof: Since $\pi(\mathcal{M}) > 0, \exists \mathbf{x}^{\#}$ attaining the maximum. Denote

$$l_n(\mathbf{x}) = \left(\frac{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})}{f(\mathbf{y} \mid \mathbf{x}^{\#}) \ p(\mathbf{x}^{\#})}\right)^{1/H_n}, \quad Z_n = \int_{\Omega} l_n(\mathbf{x}) d\pi(\mathbf{x})$$

It is easily seen that $l_n(\mathbf{x}) \to 1\{\mathbf{x} \in \mathcal{M}\}, (n \to \infty)$, and

$$\lim_{n \to \infty} Z_n = \int_{\Omega} \lim_{n \to \infty} l_n(\mathbf{x}) d\pi(\mathbf{x}) = \int_{\Omega} 1\{\mathbf{x} \in \mathcal{M}\} d\pi(\mathbf{x}) = \pi(\mathcal{M})$$

by the dominated convergence theorem. Moreover, $Z_n \downarrow \pi(\mathcal{M})$, $\sup Z_n = Z_1 \leq \pi(\Omega) < \infty$.

To prove condition (C), suppress the dependence on \mathbf{x} and consider

$$\frac{l_n}{Z_n} - \frac{l_{n+1}}{Z_{n+1}} \bigg| = (Z_n Z_{n+1})^{-1} | l_n Z_{n+1} - l_{n+1} Z_n |$$

$$\leq (Z_n Z_{n+1})^{-1} \{ l_{n+1} | Z_{n+1} - Z_n | + Z_{n+1} | l_{n+1} - l_n | \}$$

$$\leq \frac{1}{\pi(\mathcal{M})^2} \{ Z_{n+1}(l_n - l_{n+1}) + l_{n+1}(Z_n - Z_{n+1}) \}$$

$$\leq \frac{\pi(\Omega)}{\pi(\mathcal{M})^2} \{ l_n - l_{n+1} + Z_n - Z_{n+1} \}$$

Therefore

$$\begin{split} &\sum_{n=1}^{N-1} \int_{\Omega} \left| \frac{l_n(\mathbf{x})}{Z_n} - \frac{l_{n+1}(\mathbf{x})}{Z_{n+1}} \right| d\pi(\mathbf{x}) \leq \\ &\leq \sum_{n=1}^{N-1} \frac{\pi(\Omega)}{\pi(\mathcal{M})^2} \int_{\Omega} \left\{ l_n(\mathbf{x}) - l_{n+1}(\mathbf{x}) + Z_n - Z_{n+1} \right\} d\pi(\mathbf{x}) \\ &= \frac{\pi(\Omega)}{\pi(\mathcal{M})^2} \int_{\Omega} \sum_{n=1}^{N-1} \left\{ l_n(\mathbf{x}) - l_{n+1}(\mathbf{x}) + Z_n - Z_{n+1} \right\} d\pi(\mathbf{x}) \\ &= \frac{\pi(\Omega)}{\pi(\mathcal{M})^2} \int_{\Omega} \left\{ l_1(\mathbf{x}) - l_N(\mathbf{x}) + Z_1 - Z_N \right\} d\pi(\mathbf{x}) \\ &= \frac{\pi(\Omega)}{\pi(\mathcal{M})^2} \left(1 + \pi(\Omega) \right) \left(Z_1 - Z_N \right) \end{split}$$

Letting $N \to \infty$ the right hand side converges to $\frac{\pi(\Omega)}{\pi(\mathcal{M})^2} (1 + \pi(\Omega)) (Z_1 - \pi(\mathcal{M})) < \infty$.

A more restricted version, $\pi_n \propto \exp[-f/H_n]$ for a bounded, measurable function f was proved in Theorem 3.3.a of [52]. The assumption $\pi(\mathcal{M}) > 0$ is needed; if $\pi(\mathcal{M}) = 0$ the sequence of modified posterior distributions will not converge in total variation (cf. [52, Theorem 3.3.b]).

4.6.2 The Dobrushin condition

From now on let f be a blur-free independent noise model with $g(\cdot|\cdot) > 0$. Again, let $H_n \searrow 0$ and consider the family $(X^{(n)})_{n \in \mathbb{N}}$ of spatial birthand-death processes on $K = \{\mathbf{x} : f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}) > 0\}$ defined by (4.4.6) and (4.4.7). As K is closed and irreducible, the processes are well-defined and converge to the unique limit $p_H(\cdot \mid \mathbf{y})$ (see Section 4.4).

Recall the following result by Møller [88], a generalisation of earlier work by Lotwick and Silverman [80].

Theorem 21 Let X_t be a spatial birth-and-death process and define κ_n , δ_n as in Theorem 15. Assume moreover that $\delta_n > 0$ for all $n \ge 1$ and $\kappa_n = 0$ for all $n > n_0$ (condition (a)). Then for all fixed $t_0 > 0$

$$\sup_{\mathbf{x},\mathbf{y}} \|P_t(\mathbf{x},\cdot) - P_t(\mathbf{y},\cdot)\| \le 2 \left(1 - K(t_0)\right)^{\frac{t}{t_0} - 1}$$

for all $t > t_0$. The supremum is taken over all initial states \mathbf{x}, \mathbf{y} containing at most n_0 objects.

Here

$$\tilde{\delta}_m = \min_{i,j:i+j=m} \delta_i + \delta_j; \ \tilde{\kappa}_m = \max_{i,j:i+j=m} \kappa_i + \kappa_j; \ \tilde{\alpha}_m = \tilde{\delta}_m + \tilde{\kappa}_m;$$

$$K_1(j,t) = \left[1 - e^{-\tilde{\alpha}_j t}\right] \ \frac{\tilde{\delta}_j}{\tilde{\alpha}_j}; \ K_0(n,t_0) = \prod_{j=1}^n K_1(j,\frac{t_0}{n});$$

$$K(t_0) = \min_{n \le n_0} K_0(n,t_0).$$
(4.6.10)

Therefore, by Lemma 19 we can construct an annealing schedule satisfying condition (D) by requiring

$$2(1 - K(t_0))^{\frac{t}{t_0} - 1} \le 1 - \frac{1}{n}$$

or equivalently

$$t \ge t_0 \left(1 + \frac{\log(\frac{1}{2} (1 - \frac{1}{n}))}{\log(1 - K(t_0))} \right).$$
(4.6.11)

Under the assumption in Lemma 20, condition (C) also holds and by Theorem 18 the sequence of birth-and-death processes constructed this way converges in total variation to a uniform distribution on the set of global maxima of the posterior distribution, regardless of the initial state.

The proof of Theorem 21 is instructive and needed for the generalisations discussed below.

Proof: (Lotwick & Silverman, Møller)

Let X_t and Y_t be two independent spatial birth-and-death processes and assume that the number of objects is bounded by n_0 . The initial distributions are λ , an arbitrary probability measure concentrated on configurations with at most n_0 points and the equilibrium measure ν respectively. Write $Z_t = (X_t, Y_t)$. Since state (0,0) is discrete, coupling applies. Define

$$U_t = \begin{cases} X_t, & t < \tau \\ Y_t, & t \ge \tau \end{cases}$$

where $\tau = \inf \{t > 0 : X_t = Y_t = 0\}.$

Then τ is a stopping time and $U_t \stackrel{d}{=} X_t$. Hence for every measurable A,

$$\begin{aligned} \mathbb{P}_{\lambda}(X_t \in A) - \nu(A) &= \mathbb{P}_{\lambda}(U_t \in A) - \nu(A) \\ &= \mathbb{P}_{\lambda}(X_t \in A \; ; \; t < \tau) + \mathbb{P}_{\lambda}(Y_t \in A \; ; \; t \ge \tau) - \nu(A) \\ &\leq \mathbb{P}_{\lambda}(X_t \in A \; ; \; t < \tau) + \mathbb{P}_{\lambda}(Y_t \in A) - \nu(A) \\ &= \mathbb{P}_{\lambda}(X_t \in A \; ; \; t < \tau) \le \mathbb{P}(t < \tau). \end{aligned}$$

Similarly

$$\nu(A) - \mathbb{P}_{\lambda}(X_t \in A) = \nu(A) - \mathbb{P}_{\lambda}(U_t \in A)$$
$$= \nu(A) - \mathbb{P}_{\lambda}(X_t \in A \; ; \; t < \tau) - \mathbb{P}_{\lambda}(Y_t \in A \; ; \; t \ge \tau)$$
$$= \mathbb{P}_{\lambda}(Y_t \in A \; ; \; t < \tau) - \mathbb{P}_{\lambda}(X_t \in A \; ; \; t < \tau)$$
$$\leq \mathbb{P}_{\lambda}(Y_t \in A \; ; \; t < \tau) \le \mathbb{P}_{\lambda}(t < \tau).$$

Thus

$$\|\nu - \mathbb{P}_{\lambda}(X_t \in \cdot)\| \le \mathbb{P}_{\lambda}(t < \tau). \tag{4.6.12}$$

To find a bound on $\mathbb{P}_{\lambda}(t < \tau)$, again assume that X_t and Y_t are independent birth-and-death processes and fix an initial state $Z_0 = (\mathbf{x}, \mathbf{y})$ containing m and n objects respectively. Then $\mathbb{P}($ first transition in Zoccurs before time t and is a death $|Z_0| \ge K_1(m+n, t)$. To see this, set

$$f(x,y) = [1 - e^{-x-y}] \frac{y}{x+y}$$

where $x = (B_H(\mathbf{x}) + B_H(\mathbf{y})) \ t \ge 0$ and $y = (D_H(\mathbf{x}) + D_H(\mathbf{y})) \ t > 0$. The partial derivatives of f are

$$\begin{split} &\frac{\partial f}{\partial x}(x,y) = \frac{y}{(x+y)^2} \; [(1+x+y)e^{-x-y} - 1]; \\ &\frac{\partial f}{\partial y}(x,y) = \frac{y}{x+y} \; e^{-x-y} + \frac{x}{(x+y)^2} \; (1-e^{-x-y}) > 0. \end{split}$$

Set $g(z) = (1+z)e^{-z} - 1$ on $(0, \infty)$. Since $g'(z) = -ze^{-z} < 0$, $\frac{\partial f}{\partial x}(x, y) < 0$. Therefore a lower bound can be obtained by taking x as large and y as small as possible. It follows that

$$\mathbb{P}(\tau \leq t_0 \mid Z_0) \geq$$

 $\mathbb{P}(\text{ first } m + n \text{ transitions occur before } t_0 \text{ and all are deaths } | Z_0) \geq 1$

 $\mathbb{P}(\text{ first } m+n \text{ sojourn times are all } \leq \frac{t_0}{m+n}$

and all these transitions are deaths $|Z_0| \ge K_0(m+n, t_0)$.

Since the number of objects is bounded above by n_0 , $K(t_0) = \min_{n \le n_0} K_0(n, t_0) > 0$ and $\mathbb{P}(\tau \le t_0) \ge K(t_0)$ for all initial distributions. In fact,

$$\mathbb{P}(\tau > kt_0) \le (1 - K(t_0))^k$$

for all $k \in \mathbb{N}$.

The proof is by induction. For k = 1 the assertion has been proved already and we may assume the statement is correct for some $k \in \mathbb{N}$. Then

$$\mathbb{P}(\tau > (k+1)t_0) = \int \mathbb{P}(Z_t \neq (0,0) \text{ in } (t_0, (k+1)t_0) \mid Z_{t_0} = z)$$

$$\mathbb{P}(Z_t \neq (0,0) \text{ before } t_0 \text{ and } Z_{t_0} \in dz)$$

$$\leq (1 - K(t_0))^k \int \mathbb{P}(Z_t \neq (0,0) \text{ before } t_0 \text{ and } Z_{t_0} \in dz)$$

$$= (1 - K(t_0))^k \mathbb{P}(Z_t \neq (0,0) \text{ before } t_0) \leq (1 - K(t_0))^{k+1}$$

which completes the induction argument.

Now, for arbitrary $t > t_0$,

$$\mathbb{P}(\tau > t) \le \mathbb{P}(\tau > \lfloor \frac{t}{t_0} \rfloor t_0) \le (1 - K(t_0))^{\lfloor \frac{t}{t_0} \rfloor} \le (1 - K(t_0))^{\frac{t}{t_0} - 1}.$$

Using (4.6.12), Theorem 21 is proved.

4.6.3 Example

Consider the synthetic example studied in Section 4.3. We will use the same parameter values here, to enable comparison.

In practice, the theoretical temperature schedule (4.6.11) is too slow and one resorts to 'feasible' schemes. Here we chose a geometric cooling of rate 1/2 and initial temperature H = 4.0. The log posterior likelihood as a function of time is given in Figure .4; Figure .5 graphs the number of objects against time. Finally a typical reconstruction sampled at H = .25 is given in Figure 4.14. The constant death rate method was used throughout. In contrast to ICM, stochastic annealing results in a global maximum, regardless of the initial state. Experiments with several initial states are in accordance with the theory in that similar reconstructions were obtained. One has to be careful though, since a too fast cooling schedule was used. For a discussion on the implications of such ad hoc choices, see [48].



Figure 4.14: Sample taken at time 25 for a geometric cooling schedule starting at H = 4.0 of rate .5 (left) and from the posterior distribution after 2.0 time units (right) for a Strauss prior with $\beta = .0025$ and $\gamma = .25$

A good compromise between ICM and stochastic annealing is to sample at a fixed 'low' temperature (see also [41]). A reconstruction obtained by running the constant death rate procedure at H = 1 is given in Figure 4.14. Using constant birth rate instead was found to behave worse. The latter method tends to add an unlikely object and immediately deletes it again. This confirms experience reported in the literature ([88, 102]).

Estimates of the posterior intensity (Figure 4.15) suggest that the posterior distribution is rather peaked and can be used as an approximation to MAP estimation, apart from being interesting in its own right.

Typical runs of the constant death rate method are illustrated in Figure .6, where the Δ_2 distance [2] to the 'true' pattern is graphed against time. Starting from an empty scene, objects are immediately added to form a plausible reconstruction followed by deletion and immediate readding of one of the objects. Note that the results obtained this way are comparable to steepest ascent reconstructions.

For the Brodatz pellet texture of Figure 2.1, the results of simulated annealing are very similar to those of posterior sampling (Figure 4.12), as could be expected from Figure 4.13.



Figure 4.15: Posterior intensity at temperature 4.0, 1.0 and .25 (from top to bottom).

4.6.4 Remarks and extensions

Generalisations to diffusing objects are possible. In the finite case $|U| < \infty$, write

 $M(\mathbf{x}, x_i, u)$

for the configuration obtained from \mathbf{x} by replacing x_i by u. The set of $u \in U$ for which this operation is allowed is denoted by $Q(\mathbf{x}, x_i)$. Typically it consists of unoccupied objects close but not identical to x_i .

Suppose the diffusion rates are also powers of the log likelihood ratios

$$c_H(\mathbf{x}, x_i, u) = \left\{ \frac{f(\mathbf{y} \mid M(\mathbf{x}, x_i, u)) \ p(M(\mathbf{x}, x_i, u))}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} \right\}^{k/H}.$$
 (4.6.13)

If detailed balance is required to hold as well, necessarily $k = \frac{1}{2}$.

Writing $C_H(\mathbf{x})$ for the total diffusion rate out of state \mathbf{x} , the expected sojourn time $\frac{1}{B_H(\mathbf{x})+C_H(\mathbf{x})+D_H(\mathbf{x})}$ is less than $1/(B_H(\mathbf{x})+D_H(\mathbf{x}))$, the expected waiting time for the process with only births and deaths. New positions with a large increase in posterior likelihood are favoured.

The following additional notation is needed.

$$\gamma_i = \max_{n(\mathbf{x})=i} C_H(\mathbf{x}); \ \tilde{\gamma}_m = \max_{i,j:i+j=m} \gamma_i + \gamma_j; \ \tilde{\alpha}_m = \tilde{\delta}_m + \tilde{\kappa}_m + \tilde{\gamma}_m$$

and K_1, K_0, K as in (4.6.10).

Lemma 22 The Markov chain on K with rates given by (4.4.6), (4.4.7) and (4.6.13) is irreducible and satisfies the detailed balance equations. It is time reversible and has unique equilibrium distribution $p_H(\cdot|\mathbf{y})$. Moreover for all fixed $t_0 > 0$

$$\max_{\mathbf{x},\mathbf{y}} || P_t(\mathbf{x},\cdot) - P_t(\mathbf{y},\cdot) || \le 2 (1 - K(t_0))^{\frac{L}{t_0} - 1}$$

for all $t > t_0$.

Proof: Every configuration \mathbf{x} can be reached from every other configuration \mathbf{z} by first deleting all points in $\mathbf{x} \setminus \mathbf{z}$ and then adding $\mathbf{z} \setminus \mathbf{x}$, since all birth and death rates are strictly positive. Thus the Markov chain is irreducible. Since the detailed balance equations hold by construction, the first part of the result follows. The second part can be derived by coupling arguments similar to those in the proof of Theorem 21. The only change is that we now have to prove that $\mathbb{P}($ the first transition in Z occurs before time t and is a death $|Z_0\rangle =$

$$\begin{bmatrix} 1 - \exp\left\{-\left(B_H(\mathbf{x}) + B_H(\mathbf{y}) + C_H(\mathbf{x}) + C_H(\mathbf{y}) + D_H(\mathbf{x}) + D_H(\mathbf{y})\right)t\right\} \end{bmatrix} \\ \frac{D_H(\mathbf{x}) + D_H(\mathbf{y})}{B_H(\mathbf{x}) + B_H(\mathbf{y}) + C_H(\mathbf{x}) + C_H(\mathbf{y}) + D_H(\mathbf{x}) + D_H(\mathbf{y})} \ge K_1(m+n,t). \text{ To see this, let} \\ f(x,y,z) = \left[1 - e^{-(x+y+z)}\right] \frac{z}{x+y+z}. \text{ The partial derivatives are}$$

. . . .

$$\begin{aligned} \frac{\partial f}{\partial x}(x,y,z) &= \frac{z}{(x+y+z)^2} \left[(x+y+z+1) \ e^{-(x+y+z)} - 1 \right];\\ \frac{\partial f}{\partial y}(x,y,z) &= \frac{z}{(x+y+z)^2} \left[(x+y+z+1) \ e^{-(x+y+z)} - 1 \right]; \end{aligned}$$

and

$$\frac{\partial f}{\partial z}(x,y,z) = e^{-(x+y+z)}\frac{z}{x+y+z} + \left[1 - e^{-(x+y+z)}\right]\frac{x+y}{(x+y+z)^2}.$$

Since $\frac{\partial f}{\partial x}(x, y, z) < 0$, $\frac{\partial f}{\partial y}(x, y, z) < 0$ and $\frac{\partial f}{\partial z}(x, y, z) > 0$, the statement follows.

In the continuous case, n objects can perform a diffusion on U^n

$$d\mathbf{x}_t = \nabla \log p_H(\mathbf{x} \mid \mathbf{y}) \ dt + \sqrt{2H} \ dB_t$$

at least if $p_H(\cdot | \mathbf{y})$ is strictly positive and infinitely differentiable [102, p. 178]. Here B_t denotes Brownian motion. See also [43, 86].

4.7. IMPLEMENTATION AND COMPUTATIONAL COMPLEXITY

The building blocks of Algorithms 1-7 are the forward log likelihood ratios (2.4.7), (2.4.8) and (2.4.9) and the prior log likelihood ratios (3.1.5). The former is a function of the object parameter u, that is closely related to the Hough transform and involves only pixels in a relatively small zone $Z(\mathbf{x}, u)$ determined by u and the current pattern \mathbf{x} (cf. (2.5.12), Section 2.5). Focusing on blur-free models, the (generalised) Hough transform (2.5.10) depends on the data image only through

$$z_t = h(y_t, \theta_0, \theta_1) = \log \frac{g(y_t \mid \theta_1)}{g(y_t \mid \theta_0)}$$

which can therefore be 'precomputed' in the initialisation step (in general, the data image is directly involved). Moreover, after adding or deleting a particular point u the log likelihood ratio (2.5.10) requires updating only for v in the region

$$V(u) = \{ v \in U : R(v) \cap R(u) \neq \emptyset \}.$$

For example, in a translation model with $U = T = \mathbb{R}^d$ and $R(u) = R_0 + u$ this is the central symmetrisation $V(u) = R_0 \oplus \check{R}_0 + u$.

For a nearest-neighbour Markov prior, the latter component is 'local' too and depends only on those objects in the current reconstruction that are neighbours of u (cf. Section 3.1.3).

Computations are carried out on a logarithmic scale to avoid overflow. In fixed-temperature sampling or stochastic annealing, write a_H for the log birth rate (cf. formulas (4.4.6) and (4.4.7)),

$$a_H(\mathbf{x}, u) = \frac{k}{H} \left(L(\mathbf{x} \cup \{u\} ; \mathbf{y}) - L(\mathbf{x} ; \mathbf{y}) + \log \frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} \right).$$

One could first find

$$m(\mathbf{x}) = \max_{u} a_H(\mathbf{x}, u)$$

and then digitise to compute

$$B_H(\mathbf{x}) = e^{m(\mathbf{x})} \sum_j \exp\left[a_H(\mathbf{x}, u_j) - m(\mathbf{x})\right]$$

where the exponential terms lie between 0 and 1. The conditional likelihood of a birth at u is computable from the same summands

$$rac{b_H(\mathbf{x},u)}{B_H(\mathbf{x})} = \exp\left[a_H(\mathbf{x},u) - m(\mathbf{x})
ight] \exp\left[m(\mathbf{x}) - \log B_H(\mathbf{x})
ight].$$

The death rates can be dealt with similarly.

We implemented the simulations and reconstructions in C++ (AT&T, [119]) using the CLIP library [116] for manipulating the image data. The C++ language is well suited, since it allows the user to define separate classes for each of the mathematical entities; changes in one class do not affect any other class. Here the model components are template shapes, object configurations, signal function, noise model and prior distribution. For each of these we defined a C++ class maintaining the relevant parameter settings, performing update operations and computing the likelihood ratios. Computations were carried out in single precision arithmetic; using double precision resulted in slightly different reconstructions.

4.7.1 Sampling

In fixed temperature sampling or stochastic annealing $(k \neq 1)$, the computational effort is mainly in sampling from $b_H(\mathbf{x}, \cdot)/B_H(\mathbf{x})$. Since the birth rate $b_H(\mathbf{x}, u)$ is an exponential function of the Hough transform (2.5.12), it tends to have sharp peaks as a function of u when H is small or when \mathbf{x} is suboptimal. There is then a high probability that the next transition will add a new object u at one of the locations that is close to maximal for $b_H(\mathbf{x}, u)$. This implies that rejection sampling methods that generate a putative new object uniformly become impractical. Many proposals would be rejected and the waiting times would be unacceptably long. This suggests using an algorithm which incorporates a search operation over U.

One simple algorithm of this kind is to find the global maximum of birth rate $b^* = \max_u b'_H(\mathbf{x}, u)$, then locate all objects u satisfying $b_H(\mathbf{x}, u) \ge ab^*$ where a < 1, or larger than a given threshold value. Making a list of all such candidates we proceed as if these are the only objects in U, computing the total birth rate of the candidates and performing rejection sampling. After each transition the list of candidates has to be recomputed. This algorithm is an approximation to the desired birth-and-death process: larger values of a increase the speed but decrease accuracy of the approximation.

An exact algorithm can be obtained by incorporating a rejection sampling step. Denote the threshold on the birth rates defined above by $w_H(\mathbf{x})$ and, for $u \notin \mathbf{x}$, set

$$g_H(\mathbf{x}, u) = \begin{cases} b_H(\mathbf{x}, u) & \text{if } b_H(\mathbf{x}, u) \ge w_H(\mathbf{x}); \\ w_H(\mathbf{x}) & \text{else.} \end{cases}$$

Writing $G_H(\mathbf{x})$ for the integral of g_H , we generate a sequence $(X^{(k)}, T^{(k)})$ of states and sojourn times as follows.

Algorithm 8 An initial state $\mathbf{x}^{(0)}$ is given. For each k = 0, 1, 2, ... compute $D = D_H(\mathbf{x}^{(k)})$, $G = G_H(\mathbf{x}^{(k)})$ and set $T^{(k)} = 0$.

- Add an exponentially distributed time to $T^{(k)}$ with mean 1/(D+G);
- with probability $\frac{D}{D+G}$ generate a death $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} \setminus x_I$ by deleting one of the points in $\mathbf{x}^{(k)}$ at random according to distribution $D_H(\cdot, \cdot)$ and stop;
- else sample a point u from $g_H(\mathbf{x}^{(k)}, u)/G$; with probability $\frac{b_H(\mathbf{x}^{(k)}, u)}{g_H(\mathbf{x}^{(k)}, u)}$ accept a birth $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} \cup \{u\}$ and stop; otherwise repeat the whole procedure.

It is important to note that the method does not require computation of the total birth rate.

To see the validity of the algorithm above, note that we generate a (1-dimensional) Poisson process of putative events with rate D+G. The acceptance probability p of an event is

$$rac{D}{D+G}+rac{G}{D+G}\int_Urac{b_H(\mathbf{x},u)}{g_H(\mathbf{x},u)}\;rac{g_H(\mathbf{x},u)}{G}\;d\mu(u)=rac{D+B_H(\mathbf{x})}{D+G}$$

Due to the thinning property of Poisson processes [25, p. 241] the sojourn time is exponentially distributed with mean $1/(B_H(\mathbf{x}) + D_H(\mathbf{x}))$. Next, consider the transition rate for the addition of an object u to pattern \mathbf{x} :

$$\sum_{k=0}^{\infty} (1-p)^k \frac{G}{D+G} \frac{b_H(\mathbf{x},u)}{g_H(\mathbf{x},u)} \frac{g_H(\mathbf{x},u)}{G}$$
$$= \frac{1}{D+G} b_H(\mathbf{x},u) \sum_{k=0}^{\infty} (1-p)^k = \frac{b_H(\mathbf{x},u)}{D_H(\mathbf{x}) + B_H(\mathbf{x})}.$$

The death rates can be treated similarly.

4.7.2 Multiresolution techniques

Whatever strategy is adopted, there will be problems with the 'curse of dimension', i.e. as the dimension of the object space U increases, the cost of searching U increases exponentially. This problem is wellknown in the context of Hough transforms; it is often named as the major limitation on their performance, and multiresolution strategies are usually recommended.

We propose using the following multiresolution algorithm. For each 'resolution level' m = 0, 1, ..., M conceptually divide object space U into a partition $\mathcal{U}_m = \{U_{1,m}, \ldots, U_{k_m,m}\}$ such that each partition is a

refinement of the previous one: $U_{i,m} = \bigcup_j U_{\ell_j,m+1}$ for all i, m. 'Conceptually' means that the subdivision of a block U_{im} into smaller blocks is only carried out when needed. The standard example is the quad-tree in which the unit square is divided into $2^m \times 2^m$ smaller squares at stage m.

Interpret each partition \mathcal{U}_m as a class of 'large objects' in T by defining for any $V \subseteq U$

$$R(V) = \bigcup_{u \in V} R(u)$$

(or $\bigcup_{u \in V} Z(\mathbf{x}, u)$ in the blurred case).

Define a Hough transform on \mathcal{U}_m

$$H_{\mathbf{w}}^{(m)}(V) = \sum_{t \in R(V)} w_t, \quad V \in \mathcal{U}_m$$

where **w** is any image. This provides an upper bound for the Hough transform on U, provided $w_t \ge 0$:

$$H_{\mathbf{w}}^{(m)}(V) \ge \max_{u \in V} H_{\mathbf{w}}(u).$$

Furthermore the Hough transform at level m is an upper bound for the Hough transform at level m + 1

$$H_{\mathbf{w}}^{(m)}(U_{im}) \ge \max_{U_{j,m+1} \subset U_{im}} H_{\mathbf{w}}^{(m+1)}(U_{j,m+1}).$$
(4.7.14)

Suppose we can find an image \mathbf{w} , possibly depending on \mathbf{x} , such that

$$w_t \geq \max_{u \in U} h(y_t, \theta^{(\mathbf{x})}(t), \theta^{(\mathbf{x} \cup \{u\})}(t))$$

where h is as in (2.5.12). For example in the blur-free case we can take

$$w_t = 1\{t \notin S(\mathbf{x})\} \ (h(y_t, \theta_0, \theta_1))^+$$

where $a^+ = \max\{a, 0\}$. Assuming the conditions of Corollary 16 hold, we obtain a decreasing sequence of upper bounds on the birth rates of the stochastic annealing procedure:

$$b(\mathbf{x}, u) \le b^{(M)}(\mathbf{x}, U_{i_M, M}) \le \dots \le b^{(0)}(\mathbf{x}, U_{i_0, 0})$$
 (4.7.15)

where $u \in U_{i_M,M} \subset \ldots \subset U_{i_0,0}$ and

$$b^{(m)}(\mathbf{x}, V) = \left[\beta \exp\{H_{\mathbf{w}}^{(m)}(V)\}\right]^{1/H}$$

with β as in Corollary 16. The maximum birth rate, and the set of locations where the birth rate is near to maximum, can then be determined by searching the multiresolution space dynamically in the usual way. This method bears many resemblances to the adaptive Hough transform [59].

An application of this technique is shown in Figure 4.16. This is a synthetic example modelled on the problem of identifying linear features such as long crystals and fission tracks in micrographs of minerals. The objects are line segments of variable length, so that the object space U is 4-dimensional, making simple search methods computationally expensive.



Figure 4.16: Synthetic 256×256 image of blurred line segments degraded by additive Gaussian noise with $\sigma^2 = 9$ (left). Reconstruction by steepest ascent using a Strauss prior with $\beta = .002$ and $\gamma = 0.25$ (right). The initial configuration is empty and w = 0.

The signal is assumed to be a function of the distance $d(t, \mathbf{x})$ from t to $S(\mathbf{x})$, in this case linear decay

$$\theta^{(\mathbf{x})}(t) = \begin{cases} \theta_1 + \frac{d(t,\mathbf{x})}{c} (\theta_0 - \theta_1) & \text{for } d(t,\mathbf{x}) \le c; \\ \theta_0 & \text{otherwise.} \end{cases}$$

Figure 4.16 is a simulation of this model with (arbitrary) line segments of length ranging between 60 and 70, foreground brightness 100, background brightness 254, decay radius c = 4 pixel units, and additive Gaussian noise with variance 9.0.

The choice of parametrisation is important for the computational cost of the multiresolution algorithm. We choose to parametrise segments by their length ℓ , orientation ρ , and the coordinates (d, t) of the midpoint of the segment after rotation $by -\rho$, so that d is the distance from the (arbitrary) origin O to the infinite line L containing the segment, and t is the distance from the midpoint of the segment to the foot of the perpendicular OL.

It is interesting to note that this is the standard parametrisation of lines in \mathbb{R}^2 in stochastic geometry, where this choice is dictated by properties of the 'invariant' measure for random lines. One may speculate that stochastic geometry can help suggest the right parametrisation for the Hough transform for other classes of geometrical objects, and in general, suggest the right way to formulate many problems in image analysis.

Our multiresolution algorithm splits U at level 0 into blocks of roughly constant (ρ, d) with a tolerance of 1 degree in ρ and 1 pixel unit in d. That is, we group together all those segments which lie (approximately) along a given infinite line of orientation ρ and distance d from the origin. The objects R(V) at level 0 are thickened lines, whose Hough transform is relatively easy to compute.

We introduce a neighbourhood structure by defining two line segments to be neighbours $u \sim v$ iff their dilations by a ball of decay radius have a non-empty intersection. The prior model is a Strauss process with $\beta = 0.002$ and $\gamma = 0.25$. We applied the multiresolution algorithm with upper bounds (4.7.15) computed from $w_t = \frac{1}{2\sigma^2} (y_t - \theta^{(\mathbf{x})}(t))^2$. Note that the choice of parametrisation also means that the bounds (4.7.15) at level 0 are rather tight. The result of steepest ascent is given in Figure 4.16.

Chapter 5 Spatial clustering

This Chapter studies the high-level task of clustering image features. A clustering algorithm must decide whether the data can be partitioned into meaningful groups and locate the group centres. This can be formulated within the same general framework discussed at length in Chapter 4, but note that the data is now a list of features instead of a digital image. Hence, both the data and the unknown centres can be modelled conveniently as a point process. Here, we study in detail the special case of spatial point patterns, and indicate how the framework can be tailored to other applications.

5.1. INTRODUCTION

There are many similarities between object recognition (Chapter 4) and the problem of detecting clusters in a spatial pattern. In both problems, the goal is to extract an underlying pattern from a set of data that can be a digital image, a point pattern in Euclidean space or the output of an edge detector. In particular, the formal framework is the same and the techniques presented in Chapter 4 carry over with some adaptations.

The localisation of cluster centres is of interest in many areas of applications, for instance in forestry where seedlings tend to scatter around mature trees. While methods to test whether a spatial pattern is clustered (as opposed to 'random') abound in the spatial statistics literature, see eg [31], these do not allow the estimation of cluster centre location or cluster membership. Other types of techniques test for the presence of a cluster at a *fixed* location. For instance, the Geographical Analysis Machine by Openshaw et al. [96] is a grid based procedure using Monte Carlo testing in each disc centred at a grid point. The method is computer intensive, suffers from multiple response and has unknown power. It was improved by Besag and Newell [19]. Their method centres around observations rather than grid points and is less computer intensive, but remains admittedly rather ad hoc.

An early work that does attempt to locate centres of clustering is Baudin [13]. He derived a formula for the posterior intensity of a Neyman-Scott cluster process. However, it was found too complicated for practical application.

Here we present a stochastic model in keeping with the general framework described in Chapter 4 and introduce a Markov prior to combat overestimation of the number of clusters and to improve robustness. These ideas in connection with object recognition were proposed by Baddeley and Van Lieshout [8]. Independently, a Gibbs sampler technique for detection of cluster centres in a Cox process was developed by Lawson [69, 70, 71, 73]. The presentation here is based on [8] and the author's contribution to ongoing research with A.J. Baddeley and A.B. Lawson.

5.2. Cluster processes

The data consist of a finite set of points $\mathbf{y} = \{y_1, \ldots, y_m\} \subseteq T, m \ge 1$, where $T \subseteq \mathbb{R}^2$ (say) is the window of observation and it is required to determine the locations of an unspecified number of cluster centres $x_1, \ldots, x_n \in U$. In other words, both \mathbf{x} and \mathbf{y} are modelled as a realisation of a point process, albeit not necessarily on the same space. Typical applications include the analysis of spatial pattern in the occurrence of rare diseases and the estimation of the positions of ancestors of the current generation of trees in a wood.

5.2.1 General

The analogue of the conditional independence assumption in Section 2.2 is that conditional on $X = \mathbf{x}$, the observed point process Y is a superposition of independent finite point processes Z_{x_i} of 'daughters' associated with each 'parent' $x_i \in X$:

 $Y = \bigcup_{x_i \in X} Z_{x_i}.$

We take a likelihood approach by restricting ourselves to processes that are absolutely continuous. Thus, the distribution of each daughter pattern Z_{x_i} is specified by its density $g(\cdot | x_i)$ with respect to the distribution π of a Poisson point process on T with a finite, non-atomic intensity measure μ (as reviewed in Chapter 3). If $g(\cdot | \cdot) : \Omega \times U$ is jointly measurable in its arguments, the cluster process is well-defined [25, p. 236].

In many applications, the daughter processes Z_{x_i} are identically distributed up to translation .

$$Z_{x_i} \stackrel{D}{=} Z_0 + x_i,$$

in which case

$$g(\mathbf{z} \mid x_i) = g(\mathbf{z} - x_i \mid 0).$$

The interested reader can consult [25, 31] or [117] for further details.

The distribution of the total offspring is found by superposition, and can be expressed in terms of the component densities $g(\cdot | \cdot)$ as follows.

Lemma 23 For independent clustering, the forward density with respect to π is

$$f(\mathbf{y} \mid \mathbf{x}) = e^{\mu(T)} \sum_{\phi} \prod_{i=1}^{n(\mathbf{x})} \left[g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i) e^{-\mu(T)} \right].$$
(5.2.1)

Here $g(\cdot | u)$ denotes the (jointly measurable) Radon-Nikodym density of daughter process Z_u . The sum is over all ordered partitions $\phi : \{1, \ldots, n(\mathbf{y})\} \rightarrow \{1, \ldots, n(\mathbf{x})\}$, assigning a parent to each observation and for every $I \subseteq \{1, \ldots, n(\mathbf{y})\}$, $\mathbf{y}_I = \{y_i : i \in I\}$.

Proof: Set $m = n(\mathbf{y})$ and use the Janossy densities $j_m(\cdot | \mathbf{x})$ [25, p. 122] which can be interpreted as the conditional intensity of having exactly m events, one in each of m infinitesimal regions centred at y_i . Hence

$$j_m(\mathbf{y} \mid \mathbf{x}) = e^{-\mu(T)} f(\mathbf{y} \mid \mathbf{x})$$

On the other hand, by partitioning in groups belonging to the same parent

$$j_m(\mathbf{y} \mid \mathbf{x}) = \sum_{\phi} \prod_{i=1}^{n(\mathbf{x})} \left[g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i) e^{-\mu(T)} \right].$$

Therefore

$$e^{-\mu(T)}f(\mathbf{y} \mid \mathbf{x}) = \sum_{\phi} \prod_{i=1}^{n(\mathbf{x})} \left[g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i) \ e^{-\mu(T)} \right].$$

and the assertion follows.

5.2.2 Inhomogeneous Poisson models

A class of models that is fairly general, yet amenable to calculations, is that of *inhomogeneous Poisson processes* [117] (also called *general Poisson processes* [25]). Under this model, each Z_{ξ} is a Poisson process on T with intensity function $h(\cdot | \xi)$; thus ξ gives birth to a Poisson number of daughters with mean $\int_T h(t | \xi) d\mu(t)$ and given m daughters, these are independent and identically distributed with density

$$\frac{h(\cdot \mid \xi)}{\int_T h(t \mid \xi) \, d\mu(t)}$$

(with respect to μ) on T. The class of Poisson processes is closed under independent superposition, hence the total offspring is a Poisson process with intensity

$$\lambda(t \mid \mathbf{x}) = \sum_{i=1}^{n(\mathbf{x})} h(t \mid x_i)$$
(5.2.2)

and has a simple density, given in Definition 7 below. If moreover the daughter distributions are identical up to translation, $\lambda(\cdot | \mathbf{x})$ simplifies to

$$\lambda(t \mid \mathbf{x}) = \sum_{i=1}^{n(\mathbf{x})} h(t - x_i).$$
(5.2.3)

Definition 7 An independent inhomogeneous Poisson cluster process is a point process on T having conditional density

$$f(\mathbf{y} \mid \mathbf{x}) = \exp\left[\int_T (1 - \lambda(t \mid \mathbf{x})) d\mu(t)\right] \prod_{j=1}^m \lambda(y_j \mid \mathbf{x}).$$
(5.2.4)

with respect to the reference Poisson process π . Here, the intensity function $\lambda(t \mid \mathbf{x}) = \sum_{i=1}^{n(\mathbf{x})} h(t \mid x_i)$ for measurable, integrable functions $h(\cdot \mid x_i): T \to [0, \infty)$.

Summarising, the total number of offspring n(Y) is Poisson distributed with mean $\int_T \lambda(t \mid \mathbf{x}) d\mu(t)$ and conditionally on n(Y) = m the joint density is

$$f_m(\mathbf{y} \mid \mathbf{x}) = \frac{\prod_{j=1}^m \lambda(y_j \mid \mathbf{x})}{\left(\int_T \lambda(t \mid \mathbf{x}) \, d\mu(t)\right)^m}$$
(5.2.5)

with respect to μ^m .

It can be verified that (5.2.4) is in accordance with Lemma 23 by noting that

$$\prod_{j=1}^{m} \left[\sum_{i=1}^{n} h(y_j \mid x_i) \right] = \sum_{\phi} \left[\prod_{j=1}^{m} h(y_j \mid x_{\phi(j)}) \right]$$
(5.2.6)

where the sum is over all ordered partitions $\phi : \{1, \ldots, n(\mathbf{y})\} \rightarrow \{1, \ldots, n(\mathbf{x})\}$.

The forward distribution (5.2.4) depends on the underlying pattern \mathbf{x} only through the intensity function $\lambda(\cdot | \mathbf{x})$. Therefore λ takes over the role of the signal function in object recognition.

If the parents follow a Poisson process, the unconditional distribution of Y is that of a *Neyman-Scott process*; allowing an arbitrary parent distribution, Y is *Cox*. Kingman [66] has argued that Cox processes are a natural framework in which to model the spatial pattern of a population of reproducing individuals. See also [10] or Chapter 6.

We conclude this Section with a few examples. The *Matérn process* [83] assumes that daughters are uniformly distributed in a disc of some fixed radius r around the cluster centre,

$$h(t - x_i) = \frac{\mu}{\pi r^2} \mathbb{1}\{||t - x_i|| \le r\}.$$
(5.2.7)

If the uniform distribution is replaced by a radially symmetric Gaussian distribution

$$h(t - x_i) = \frac{\mu}{2\pi\sigma^2} e^{-||t - x_i||^2/2\sigma^2}$$
(5.2.8)

we obtain a *modified Thomas process*. Strictly speaking, the original models both assume a Poisson process for the parents, but with a slight abuse of language we will use these names for any parent distribution. Although these examples are isotropic, directional effects can be modelled as easily.

In an epidemiological context, information on population density is often taken into account as a modulating function $k(\cdot)$, estimated non-parametrically from census data [32, 72]. Thus

$$\lambda(t \mid \mathbf{x}) = k(t) \sum_{i=1}^{n} h(t \mid x_i).$$
(5.2.9)

Background noise can be added by superposition of a (stationary) Poisson process, adding one extra term to the expression (5.2.2).

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108
5.3. MAXIMUM LIKELIHOOD ESTIMATION

Given observation of a point pattern \mathbf{y} , the unknown pattern of cluster centres \mathbf{x} is regarded as the parameter to be estimated. Thus the maximum likelihood equations are

 $\hat{\mathbf{x}} = \operatorname{argmax}_{\mathbf{x}} f(\mathbf{y} \mid \mathbf{x})$

where the optimisation is over all realisations $\mathbf{x} \in \Omega$. Again, these equations do not necessarily allow a (unique) solution.

Lemma 24 For an independent inhomogeneous Poisson cluster model (5.2.4) the maximum likelihood equations are

$$\hat{\mathbf{x}} = \operatorname{argmax}_{\mathbf{x}} \left[\sum_{j=1}^{m} \log \lambda(y_j \mid \mathbf{x}) - \int_T \lambda(t \mid \mathbf{x}) \, d\mu(t) \right].$$
(5.3.10)

Proof: The log likelihood is

$$L(\mathbf{x} ; \mathbf{y}) = \sum_{j=1}^{m} \log \lambda(y_j \mid \mathbf{x}) + \int_T (1 - \lambda(t \mid \mathbf{x})) \, d\mu(t)$$

hence the maximum likelihood equations are (5.3.10).

Since for any Poisson process the Papangelou conditional intensity is equal to the unconditional intensity

$$\lambda(t \; ; \; \mathbf{y} \mid \mathbf{x}) = \frac{f(\mathbf{y} \cup \{t\} \mid \mathbf{x})}{f(\mathbf{y} \mid \mathbf{x})} = \lambda(t \mid \mathbf{x})$$

the maximum likelihood and pseudolikelihood equations (cf. Section 3.4.5) coincide.

Solving the maximum likelihood equations is equivalent to solving a regression problem. The result should be compared to Lemma 1.

Lemma 25 An MLE for Model (5.2.4) is a solution of the regression of \mathbf{y} on the class of intensity functions $\{\lambda(\cdot \mid \mathbf{x}) : \mathbf{x} \in \Omega\}$ with pointwise loss

$$rac{1}{m}\int_T\lambda(t\mid \mathbf{x})d\mu(t) - \log\lambda(y_j\mid \mathbf{x})$$

Proof: Immediate from (5.3.10).

A simple illustration is given in the result below.

Lemma 26 For the Matérn cluster process (Model (5.2.7))

$$\hat{\mathbf{x}} = argmax \left[\sum_{j=1}^{m} \log n(\mathbf{x} \cap B(y_j, r)) - \frac{\mu}{\pi r^2} \sum_{i=1}^{n(\mathbf{x})} \mu(T \cap B(x_i, r)) \right]$$

Here B(u,r) denotes the closed ball with radius r centred at u and the maximum is taken over $\Omega(\mathbf{y}) = \{\mathbf{x} \in \Omega : \mathbf{x} \cap B(y_j, r) \neq \emptyset \text{ for all } y_j \in \mathbf{y}\}.$

Proof: Note that the likelihood is positive only for $\mathbf{x} \in \Omega(\mathbf{y})$. In that case the log likelihood is well-defined,

$$L(\mathbf{x} ; \mathbf{y}) - \mu(T) = \sum_{j=1}^{m} \log \left[\frac{\mu}{\pi r^2} n(\{i : \|x_i - y_j\| \le r\} \right]$$

$$- \frac{\mu}{\pi r^2} \sum_{i=1}^{n(\mathbf{x})} \int_T 1\{\|t - x_i\| \le r\} d\mu(t)$$

$$= m \log \frac{\mu}{\pi r^2} + \sum_{j=1}^{m} \log n(\mathbf{x} \cap B(y_j, r))$$

$$- \frac{\mu}{\pi r^2} \sum_{i=1}^{n(\mathbf{x})} \mu(T \cap B(x_i, r)).$$

	-

5.4. THE BAYESIAN APPROACH

Generally a maximum likelihood estimator $\hat{\mathbf{x}}$ of \mathbf{x} may run into difficulties similar to those encountered in the context of object recognition. If h is smooth and almost flat near its maximum, and the data pattern is 'dense', the maximum likelihood estimate tends to contain multiple responses to each true cluster. This is precisely what we wish to avoid.

To see where multiple response occurs, first consider a 'blur-free' inhomogeneous Poisson model with intensity function

$$\lambda(t \mid \mathbf{x}) = \lambda \ \mathbf{1}\{t \in S(\mathbf{x})\},\$$

where $S(\mathbf{x}) = \bigcup B(x_i, r)$ denotes the 'silhouette' of pattern \mathbf{x} . This model cannot distinguish between configurations with the same silhouette (compare this to the situation in Chapter 2). As another example consider the Matérn model and assume a single isolated disc. Now add a parent to this configuration close to the true centre, such that all daughters are in the overlap. This will be more likely if

$m \log 2 > \mu$

or equivalently $m > 1.4 \mu$ (see Lemma 26). Since the variance in the number of points is μ , this will happen frequently. If discs are overlapping, some points contribute a factor log 1.5 instead of log 2 and the effect is even stronger. Background scatter noise or incorrect parameter estimates may also cause multiple response.

As in Chapter 4 we introduce a nearest-neighbour Markov model to penalise scenes containing too many parents close together. Writing $p(\cdot)$ for the density with respect to a Poisson process with intensity measure ν (say), the MAP equations are formally given by (4.1.2)

 $\tilde{\mathbf{x}} = \operatorname{argmax} f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}).$

Note that f is the density of a point process instead of a pixel-based random field. Generally, the MAP equations cannot be solved explicitly due to the high dimensionality of the space.

Throughout the remainder of this Section assume the inhomogeneous Poisson model (5.2.2).

5.4.1 Deterministic algorithms

The algorithms of Chapter 4 can be modified for use in this context. Typically, the observation window is 2-dimensional, and can easily be discretised and scanned.

Iterative updating is based on repeatedly performing additions, deletions and possibly shifts (cf. Algorithms 3–4), based on their posterior likelihood ratios. The (forward) likelihood ratios for the general model (5.2.1) can be rather intractable, but for the Cox model (5.2.4) they simplify to

$$\frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x})} = e^{-H(u)} \prod_{j=1}^{m} \left[1 + \frac{h(y_j \mid u)}{\sum_{i=1}^{n} h(y_j \mid x_i)} \right]$$
(5.4.11)

and

$$\frac{f(\mathbf{y} \mid \mathbf{x} \setminus \{x_i\})}{f(\mathbf{y} \mid \mathbf{x})} = e^{H(x_i)} \prod_{j=1}^m \left[1 - \frac{h(y_j \mid x_i)}{\sum_{k=1}^n h(y_j \mid x_k)} \right]$$
(5.4.12)

If shifts are permitted,

$$\frac{f(\mathbf{y} \mid M(\mathbf{x}, x_i, u))}{f(\mathbf{y} \mid \mathbf{x})} = e^{H(x_i) - H(u)} \prod_{j=1}^{m} \left[1 + \frac{h(y_j \mid u) - h(y_j \mid x_i)}{\sum_{k=1}^{n} h(y_j \mid x_k)} \right]$$
(5.4.13)

where, as in Chapter 2, $M(\mathbf{x}, x_i, u)$ denotes the configuration $(\mathbf{x} \cup \{u\}) \setminus \{x_i\}$ obtained by replacing $x_i \in \mathbf{x}$ by u and $H(u) = \int_T h(t \mid u)) d\mu(t)$. The ratio (5.4.11) is comparable to the Hough transform, in the sense that each point y_j votes with variable strength for a cluster centre at u.

The prior likelihood ratios are easy to compute if p is a nearestneighbour Markov point process (Definition 3).

Algorithm 9 Apply any of Algorithms 1-4 for the transition criteria (5.4.11), (5.4.12) and (5.4.13) above.

5.4.2 Stochastic algorithms

The posterior distribution for the parent pattern is too complicated to sample directly. Instead we construct a spatial birth-and-death process as in Section 4.4. An important feature is that the cluster models described in Section 5.2 all assume at least one parent, and the empty configuration $\mathbf{x} = \emptyset$ has zero posterior probability when $\mathbf{y} \neq \emptyset$. This causes difficulty, since the class $K = \{\mathbf{x} : f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x}) > 0\}$ ought to be *hereditary*. A similar remark holds for zero-likelihood configurations, as found e.g. in the Matérn cluster process (Model (5.2.7)) which assigns zero posterior density to any configuration \mathbf{x} that does not place at least one parent point within a distance r of each data point.

To overcome these problems we propose to introduce a background stationary Poisson noise process with (small) intensity ϵ . The resulting superposition is still an inhomogeneous Poisson process for any parent configuration. An alternative in the absence of other zero-likelihood configurations is to set $f(\mathbf{y} \mid \boldsymbol{\emptyset}) = \epsilon^m \exp[\mu(T)(1-\epsilon)]$.

Recalling the definition of temperature modified posterior distributions

$$p_H(\mathbf{x} \mid \mathbf{y}) \propto \{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})\}^H,$$

we want to construct a spatial birth-and-death process with rates given in (4.4.6) and (4.4.7) converging weakly to $p_H(\cdot | \mathbf{y})$.

Lemma 27 Let y and H > 0 be fixed and assume an independent inhomogeneous Poisson cluster model superimposed on a background Poisson process of constant rate ϵ . Moreover let the prior model be a nearest-neighbour Markov process $p(\cdot)$ with uniformly bounded likelihood ratios

$$\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} \le \beta < \infty$$

If $0 \leq h(\cdot | \cdot) \leq h^* < \infty$, then there exists a unique spatial birth-anddeath process for which (4.4.6) and (4.4.7) are the transition rates. The process has unique equilibrium distribution $p_H(\cdot | \mathbf{y})$ and it converges in distribution to $p_H(\cdot | \mathbf{y})$ from any initial state.

Proof: If p(x) > 0, $b_H(x, u) =$

$$\begin{split} & \left(\prod_{j=1}^{m} \left[1 + \frac{h(y_j \mid u)}{\lambda(y_j \mid \mathbf{x})}\right] \exp\left[-\int_T h(t \mid u) \ d\mu(t)\right] \frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})}\right)^{k/H} \\ & \leq \left(1 + \frac{h^*}{\epsilon}\right)^{mk/H} \beta^{k/H} =: \kappa > 0 \end{split}$$

and $D_H(\mathbf{x} \setminus \{u\}, u) =$

$$\begin{split} &\left(\prod_{j=1}^{m}\left[1+\frac{h(y_{j}\mid u)}{\lambda(y_{j}\mid \mathbf{x}\setminus\{u\})}\right]\exp\left[-\int_{T}h(t\mid u)\ d\mu(t)\right]\ \frac{p(\mathbf{x})}{p(\mathbf{x}\setminus\{u\})}\right)^{\frac{k-1}{H}}\\ &\geq \left(1+\frac{h^{*}}{\epsilon}\right)^{\frac{m(k-1)}{H}}\beta^{(k-1)/H}=:\delta>0. \end{split}$$

Once these bounds have been obtained, the proof follows the lines of the proof of Lemma 15. $\hfill \Box$

Having specified a family of well-defined Markov processes with equilibrium distribution $p_H(\cdot | \mathbf{y})$, H > 0, the theory developed in Sections 4.5 to 4.7 applies. In particular, a simulated annealing algorithm can be developed to approximate a MAP-reconstruction of the parent process. Furthermore, functionals of the posterior distribution such as the distribution of the number of cluster centres, the probability that there is no cluster in a particular region, and the first-order intensity of cluster locations can be estimated.

Parameters in f and p can be estimated in advance or during iteration. Alternatively, one can specify a Gibbs sampler but note that this approach requires a set of prior distributions, one for each parameter.

In [70] a somewhat different Gibbs sampler approach was taken for a Neyman-Scott model conditioned on the number of observations. Here $n(\mathbf{x})$ and \mathbf{x} were treated separately, using rather severe approximations [71].

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5.5. Example

Figure 5.1 shows the locations of 62 redwood seedlings in a square of side approximately 23 m. The data was extracted by Ripley [102] from a larger data set in Strauss [118]. The K-function for this data is given in [102] and suggests aggregation. As noted by Strauss this is caused by the presence of stumps known to exist in the plot, but whose position has not been recorded.



Figure 5.1: Positions of 62 redwood seedlings in a unit square (Ripley 1977).

Previous analyses of this data set include Strauss' who fitted a model later criticised by Kelly and Ripley [63]. Ripley [102] rejected the Poisson hypothesis and remarked that there appears to be both clustering and inhibition between clusters. Diggle [31] fitted a Poisson cluster process of Thomas type and reported least squares estimates (25.6, .042) for the parent intensity and the standard deviation of daughter-parent distances. A goodness of fit test showed adequate fit, but from a biological point of view, a mean number of 26 stumps is implausible. In [30], Diggle fitted a Poisson cluster process of Matérn type with similar results (radius .098).

None of the above have looked at cluster centre location. This was first studied by Lawson [70] who fitted a Poisson Thomas cluster process and reported 16 parents.

5.5.1 Model

Following [31, 70] we assume the number of daughters per parent is Poisson and seedlings follow a radially symmetric Gaussian distribution around their ancestor. In contrast to the aforementioned work, a Strauss prior (3.1.4) with strict inhibition ($0 < \gamma < 1$) is introduced.

Lemma 28 Maximum likelihood estimators for Model (5.2.8) solve the following set of equations.

$$\hat{\mu} = m / \int_T \frac{1}{2\pi\hat{\sigma}^2} \sum_{i=1}^n \exp\left[-\frac{1}{2\hat{\sigma}^2} ||t - x_i||^2\right] d\mu(t)$$

and

$$\frac{1}{m} \sum_{j=1}^{m} \left(\frac{\sum_{i=1}^{n} \exp\left[-\frac{1}{2\hat{\sigma}^2} ||y_j - x_i||^2\right] ||y_j - x_i||^2}{\sum_{i=1}^{n} \exp\left[-\frac{1}{2\hat{\sigma}^2} ||y_j - x_i||^2\right]} \right) = \frac{\int_T \sum_{i=1}^{n} \exp\left[-\frac{1}{2\hat{\sigma}^2} ||t - x_i||^2\right] ||t - x_i||^2 d\mu(t)}{\int_T \sum_{i=1}^{n} \exp\left[-\frac{1}{2\hat{\sigma}^2} ||t - x_i||^2\right] d\mu(t)}.$$

Proof: The score functions are

$$\frac{\partial}{\partial \mu} L(\mathbf{x} ; \mathbf{y}) = \frac{m}{\mu} - \int_T \frac{1}{2\pi\sigma^2} \sum_{i=1}^n \exp\left[-\frac{1}{2\sigma^2} ||t - x_i||^2\right] d\mu(t)$$

and

$$\begin{split} \frac{\partial}{\partial \sigma^2} L(\mathbf{x} \; ; \; \mathbf{y}) \;\; &=\;\; \sum_{j=1}^m \frac{1}{\lambda(y_j \mid \mathbf{x})} \sum_{i=1}^n h(y_j - x_i) \left[-\frac{1}{\sigma^2} + \frac{||y_j - x_i||^2}{2\sigma^4} \right] \\ &-\;\; \int_T \sum_{i=1}^n h(t - x_i) \left[\frac{-1}{\sigma^2} + \frac{||t - x_i||^2}{2\sigma^4} \right] \, d\mu(t) \\ &=\;\; \frac{-m}{\sigma^2} + \frac{1}{2\sigma^4} \sum_{j=1}^m \frac{\sum_{i=1}^n h(y_j - x_i) \, ||y_j - x_i||^2}{\sum_{i=1}^n h(y_j - x_i)} \\ &+\;\; \frac{1}{\sigma^2} \int_T \sum_{i=1}^n h(t - x_i) d\mu(t) \\ &-\;\; \frac{1}{2\sigma^4} \int_T \sum_{i=1}^n h(t - x_i) \, ||t - x_i||^2 \, d\mu(t). \end{split}$$

Equating to zero completes the proof.

The pseudolikelihood estimators for the Strauss model are well-known [104, Chapter 4, page 53], see also (3.4.26)–(3.4.27) and subsequent remarks.

In the Lemma above, no background noise process was taken into account since doing so would lead to an intractable set of equations. However, in the simulations below we did include a Poisson noise process with intensity parameter ϵ set to a small constant. Then, since $h \leq \frac{\mu}{2\pi\sigma^2}$ and $\frac{p(\mathbf{x} \cup \{u\})}{p(\mathbf{x})} \leq \beta$, Lemma 15 applies.

5.5.2 Analysis

We analysed the redwood data using a Strauss prior with interaction distance .084 [31] and $\log \beta = \log \gamma = -10$. Throughout, a constant death rate spatial birth-and-death process was used.

Setting the initial parameter values to $\mu = 7$, $\sigma = .042$ and an empty list of cluster centres, we ran the birth-and-death process for 2 time units and found maximum likelihood estimates $\mu = 6.5$ and $\sigma = .05$. For these values, a sample taken after 2 time units is shown in Figure 5.2 and the posterior intensity estimated over 50 time units in Figure 5.3. For reasons of clarity, here *black* corresponds to high values.



Figure 5.2: Realisation from the posterior distribution taken after 2 time units (black), for a Thomas model with $\mu = 6.5$, $\sigma = .05$ and a Strauss prior with $\log \beta = \log \gamma = -10$, r = .084. The data is displayed in grey.



Figure 5.3: Posterior intensity of redwood seedlings (Ripley) estimated over 50 time units, for a Thomas model with $\mu = 6.5$, $\sigma = .05$ and a Strauss prior with $\log \beta = \log \gamma = -10$, r = .084.

Surprisingly, although the redwood data as extracted by Ripley [102] appear frequently in the spatial statistics literature, to the best of our knowledge the full data set [118] has not been reanalysed before. Thus we scanned region II of [118, Figure 1, p. 474], the roughly triangular area containing almost all the redwood stumps (Figure 5.4). The point coordinates in the range from 0 to 200 are listed in the Appendix.

Again assuming a Thomas type cluster model with a Strauss prior, we computed the posterior intensity for the same (rescaled) model parameters used to obtain Figures 5.2 and 5.3. An estimate based on running a constant death rate Markov process (4.4.6)-(4.4.7) for 50 time units is displayed in Figure 5.5; a typical realisation sampled at time 2 is shown in Figure 5.6.



Figure 5.4: Positions of 123 redwood seedlings in a subset of the unit square (Strauss 1975).

Note that the results agree on the intersection of Figure 5.1 and Figure 5.4 and provide a plausible description of the clustered pattern. In particular, the Markov prior successfully combats the 'overestimation' (from a biological point of view) of the number of cluster centres.



Figure 5.5: Posterior intensity of redwood seedlings in region II (Strauss) estimated over 50 time units, for a Thomas model with $\mu = 6.5$, $\sigma = .025$ and a Strauss prior with $\log \beta = \log \gamma = -10$, r = .042.



Figure 5.6: Realisation from the posterior distribution taken after 2 time units (black), for a Thomas model with $\mu = 6.5$, $\sigma = .025$ and a Strauss prior with $\log \beta = \log \gamma = -10$, r = .042. The data is displayed in grey.

5.6. Offspring Assignment

A cluster model can conveniently be interpreted as a marked point process $\mathbf{w} = \{(x_1, Z_{x_1}), \ldots, (x_n), Z_{x_n})\}$ of parents $\{x_1, \ldots, x_n\}$ marked by their offspring Z_{x_i} , $i = 1, \ldots, n$ (see Section 5.2.1). So far, we concentrated on estimating the parent configuration \mathbf{x} . It is the purpose of this Section to study the joint distribution of parents and their offspring (conditional on the data), thus enabling us to label observations by the cluster they belong to.

5.6.1 Overview

The task described above resembles approaches to finite mixture models [23, 29] dealing with assigning independent realisations to a component density. The indicators specifying which component density a given data point is drawn from are treated as missing data. A variant of the EM algorithm or Gibbs sampler then augments the observations by estimating or sampling these missing variables.

The basic difference with the current problem is that the number of densities in a mixture model is fixed and known, while our problem entails recovering a point pattern with a variable number of points. This distinction is quite crucial, as it implies the impossibility to build a Gibbs sampler, alternatingly sampling the marks (or centers) given data and centers (or marks) [29].

Here, we propose a two-step algorithm for sampling $p(\mathbf{w} | \mathbf{y})$ that combines a Metropolis-Hastings step for the parents with a Gibbs step drawing from the conditional distribution of the marks. The basic idea is that, when a new parent configuration \mathbf{x}' is generated from the current $\mathbf{x} = \{x_1, \ldots, x_n\}$ and marks $\mathbf{Z}_{\mathbf{x}} = (Z_{x_i})_{i=1}^n$, \mathbf{x}' does not have to conform to $\mathbf{Z}_{\mathbf{x}}$ (eg. \mathbf{x}' could have one point fewer than \mathbf{x}). We then update the marks to $\mathbf{Z}'_{\mathbf{x}'}$ and require conformity with \mathbf{x}' , allowing empty sets of offspring.

Algorithm 10 Given an initial parent configuration \mathbf{x} , a labelling $\mathbf{Z}_{\mathbf{x}} = (Z_{x_i})_{i=1}^{n(\mathbf{x})}$ and data \mathbf{y} , alternate between a Metropolis-Hastings and a Gibbs step as follows.

- 1. given $\mathbf{w} = \{(x_1, Z_{x_1}), \dots, (x_n, Z_{x_n})\}$ and \mathbf{y} , perform a Metropolis-Hastings step for \mathbf{x} only, independent of the marks $\mathbf{Z}_{\mathbf{x}}$, yielding the new configuration \mathbf{x}' ;
- 2. given \mathbf{x}' , \mathbf{y} reallocate the offspring by a Gibbs step, sampling $\mathbf{Z}'_{\mathbf{x}'}$ from the conditional distribution $\mathbb{P}(\mathbf{Z}'_{\mathbf{x}'} \mid \mathbf{x}', \mathbf{y})$. Replace \mathbf{x} by \mathbf{x}' , $\mathbf{Z}_{\mathbf{x}}$ by $\mathbf{Z}'_{\mathbf{x}'}$ and return to step 1.

An assignment of data to clusters can be interpreted as an *ordered* partition of the data (cf. Lemma 23). If one considers *unordered* partitions instead, a Gibbs sampler can be developed. Intuitively, these unordered partition elements correspond to 'sibling sets' generated by a common, if unspecified, parent. Then, by allowing parents not having any offspring at all, the number of cluster centres can be changed, but the conditional distributions involved are rather awkward.

Offspring labelling can be combined with density estimation to assess the goodness-of-fit of the cluster distribution. Assuming Model (5.2.3), given a label assignment $\phi : \mathbf{y} \to \mathbf{x}$ which maps y_j onto its parent, one has a set of vector differences $y_j - \phi(y_j)$ to which a density can be fitted. Comparison with the model h is an indication of its validity.

5.6.2 The Metropolis step

The Metropolis-Hastings sampling method [44] uses a discrete time Markov process whose transition kernel is a mixture of two transition kernels

$$Q(F \mid \mathbf{x}) = (1 - p) Q_0(F \mid \mathbf{x}) + p Q_1(F \mid \mathbf{x}), \ 0 \le p \le 1.$$

The first kernel governs transitions between configurations consisting of the same number of points, the second kernel controls births and deaths. Both adopt the Metropolis-Hastings strategy of generating a proposal state and accepting it with a probability based on the likelihood ratio of the desired equilibrium distribution $p(\cdot | \mathbf{y})$.

Specifically, for $\mathbf{x} \neq \emptyset$, Q_0 selects a current point $x_i \in \mathbf{x}$ with equal probability (say), a new point $u \in U$ from a probability density $c(\mathbf{x}, x_i, u)$ concentrated on $\{u : f(\mathbf{y} \mid M(\mathbf{x}, x_i, u)) \ p(M(\mathbf{x}, x_i, u)) > 0\}$, with the property that $c(\mathbf{x}, x_i, u) > 0$ if and only if $c(M(\mathbf{x}, x_i, u), u, x_i) > 0$. A change from \mathbf{x} to $\mathbf{x}' = M(\mathbf{x}, x_i, u)$ is accepted with probability

$$A_0(\mathbf{x}'|\mathbf{x}) = \min\left\{1, \frac{p(\mathbf{x}'|\mathbf{y})c(\mathbf{x}', u, x_i)}{p(\mathbf{x}|\mathbf{y})c(\mathbf{x}, x_i, u)}\right\}.$$
(5.6.14)

Note that Q_0 is concentrated on $K_n = \{\mathbf{x} : n(\mathbf{x}) = n; f(\mathbf{y} | \mathbf{x}) p(\mathbf{x}) > 0\}$. The proposal kernel of Q_1 is concentrated on $K_{n-1} \cup K_{n+1}$ (or K_1 if n = 0) and constructed as follows.

• with probability $q(\mathbf{x})$ generate a new point u from a density $b(\mathbf{x}, u)$ with respect to ν ; accept with probability

$$A_1(\mathbf{x} \cup \{u\} | \mathbf{x}) = \min\{1, r(\mathbf{x}, u)\}$$

if $f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) p(\mathbf{x} \cup \{u\}) > 0$ and 0 otherwise;

• otherwise (with probability $1 - q(\mathbf{x})$) delete a point $x_i \in \mathbf{x}$ with probability $D(\mathbf{x} \setminus \{x_i\}, x_i)$ (or if n = 0 do nothing); accept with probability

$$A_1(\mathbf{x} \setminus \{x_i\} | \mathbf{x}) = \min\{1, 1/r(\mathbf{x} \setminus \{x_i\}, x_i)\}$$

if $f(\mathbf{y} \mid \mathbf{x}) p(\mathbf{x}) > 0$ and 0 otherwise.

Here, if $f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) p(\mathbf{x} \cup \{u\}) > 0$

$$r(\mathbf{x}, u) = \frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) \ p(\mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} \ \frac{1 - q(\mathbf{x} \cup \{u\})}{q(\mathbf{x})} \ \frac{D(\mathbf{x}, u)}{b(\mathbf{x}, u)}.$$

By construction, the detailed balance equations are satisfied.

We shall assume that $p(\cdot | \mathbf{y})$ is hereditary (or modified to be hereditary, see the discussion in Section 5.4.2). Moreover for any configuration \mathbf{x} and any $u \in U$ such that $f(\mathbf{y} | \mathbf{x} \cup \{u\}) p(\mathbf{x} \cup \{u\}) > 0$

$$D(\mathbf{x}, u) > 0, b(\mathbf{x}, u) > 0, q(\mathbf{x} \cup \{u\}) < 1 \text{ and } q(\mathbf{x}) > 0.$$
 (5.6.15)

Of course this leaves us with many choices for $b(\cdot, \cdot)$, $c(\cdot, \cdot, \cdot)$, $D(\cdot, \cdot)$, and $q(\cdot)$. One of the simplest is

$$q(\cdot) \equiv \frac{1}{2}, \ b(\cdot, \cdot) = c(\cdot, \cdot, \cdot) \equiv \frac{1}{\nu(U)}, \ \text{ and } D(\mathbf{x}, \cdot) \equiv \frac{1}{n(\mathbf{x}) + 1}$$

with acceptance probabilities

$$A_1(\mathbf{x}'|\mathbf{x}) = \min\left\{1, \nu(U)^{n(\mathbf{x}')-n(\mathbf{x})} \frac{f(\mathbf{y} \mid \mathbf{x}') \ p(\mathbf{x}')n(\mathbf{x})!}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})n(\mathbf{x}')!}\right\}$$

and A_0 as in (5.6.14).

However this may tend to generate too many proposals with low acceptance probabilities. A more rapid algorithm may be obtained by generating the new point in the shift part Q_0 uniformly within some neighbourhood $D(x_i)$ of the deleted point x_i (or more generally, from some symmetric probability density $c(\mathbf{x}, x_i, u) = c(x_i - u)$). To maintain detailed balance, we require symmetry: $u \in D(v)$ if and only if $v \in D(u)$. See [93, 95].

Another possibility resembling spatial birth-and-death processes (cf. Section 4.4) is to set $D(\mathbf{x}, \cdot) \equiv \frac{1}{n(\mathbf{x})+1}$ as before and

$$b(\mathbf{x}, u) = \frac{f(\mathbf{y} \mid \mathbf{x} \cup \{u\}) \ p(\mathbf{x} \cup \{u\})}{f(\mathbf{y} \mid \mathbf{x}) \ p(\mathbf{x})} \frac{1}{B(\mathbf{x})}, q(\mathbf{x}) = \frac{B(\mathbf{x})}{n(\mathbf{x}) + B(\mathbf{x})},$$

where

$$B(\mathbf{x}) = \int_U \frac{p(\mathbf{x} \cup \{u\} \mid \mathbf{y})}{p(\mathbf{x} \mid \mathbf{y})} \, d\nu(u).$$

Then

$$r(\mathbf{x}, u) = \frac{B(\mathbf{x}) + n(\mathbf{x})}{B(\mathbf{x} \cup \{u\}) + n(\mathbf{x} \cup \{u\})}$$

5.6.3 The Gibbs step

Regarding the Gibbs step in Algorithm 10, we now proceed to derive the conditional distributions of marks given \mathbf{x} .

Theorem 29 Given a parent configuration \mathbf{x} and a data pattern \mathbf{y} , for any $Z_{\mathbf{x}_i}$, $i = 1, \ldots, n = n(\mathbf{x})$ forming a partition of \mathbf{y}

$$\mathbb{P}((Z_{x_i})_{i=1}^n \mid \mathbf{x}, \mathbf{y}) = \frac{\prod_{i=1}^n g(Z_{x_i} \mid x_i)}{\sum_{\phi} \prod_{i=1}^n g(y_{\phi^{-1}(i)} \mid x_i)},$$

provided there exists at least one $\mathbf{Z}_{\mathbf{x}}$ for which this expression is strictly positive.

Proof: Assume that $\mathbf{Z}_{\mathbf{x}}$ and \mathbf{y} are compatible and write $m = n(\mathbf{y})$. Then we can identify the marks with a function $\phi : \{1, \ldots, m\} \rightarrow \{1, \ldots, n\}$. The Janossy densities with respect to $(\nu \times \pi)^n$

$$j_n(\{(x_1, Z_{x_1}), \dots, (x_n, Z_{x_n})\}) = e^{-\nu(U)} p(\{x_1, \dots, x_n\}) \prod_{i=1}^n g(Z_{x_i} \mid x_i)$$

can be rewritten in terms of \mathbf{x} , \mathbf{y} and ϕ as

$$l_n(\mathbf{x}, \mathbf{y}, \phi) = e^{-\nu(U)} p(\{x_1, \dots, x_n\}) \prod_{i=1}^n g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i)$$

with respect to $(\nu \times \pi)^n$ or equivalently by the family

$$l_{nm}(\mathbf{x}, \mathbf{y}, \phi) = e^{-\nu(U)} p(\{x_1, \dots, x_n\}) \prod_{i=1}^n \left[g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i) e^{-\mu(T)} \right]$$

with respect to $\nu^n \mu^m$. Therefore

$$\mathbb{P}((Z_{x_i})_{i=1}^n \mid \mathbf{x}, \mathbf{y}) = \frac{l_{nm}(\mathbf{x}, \mathbf{y}, \phi)}{e^{-\mu(T)} f(\mathbf{y} \mid \mathbf{x}) e^{-\nu(U)} p(\mathbf{x})}$$
$$= \frac{\prod_{i=1}^n \left[g(Z_{x_i} \mid x_i) e^{-\mu(T)} \right]}{\sum_{\psi} \prod_{i=1}^n \left[g(\mathbf{y}_{\psi^{-1}(i)} \mid x_i) e^{-\mu(T)} \right]}.$$

The last equality follows from Lemma 23.

The class of independent inhomogeneous Poisson cluster models is of special interest. Superposition of an independent Poisson noise process is covered, by noting that noise can be interpreted as offspring from an imaginary (fixed) parent.

Corollary 30 For Model (5.2.2), $\mathbf{y} = \bigcup_{i=1}^{n} Z_{x_i}$ and $n = n(\mathbf{x})$

$$\mathbb{P}((Z_{x_i})_{i=1}^n \mid \mathbf{x}, \mathbf{y}) = \frac{\prod_{i=1}^n \prod_{t \in Z_{x_i}} h(t \mid x_i)}{\prod_{j=1}^m (\sum_i h(y_j \mid x_i))}$$
(5.6.16)

assuming at least one Z exists for which (5.6.16) is strictly positive.

Proof: Apply the previous theorem and formula (5.2.6).

Rephrasing (5.6.16) in terms of a labelling ϕ , it follows that the labels attributing each data point to a cluster centre are independent, with probabilities

$$\frac{h(y_j \mid x_{\phi(j)})}{\sum_i h(y_j \mid x_i)}.$$

Hence, simulation of the mark process is easy.

5.6.4 Convergence

Returning to Algorithm 10, note that since

 $f(\mathbf{w}|\mathbf{y}) = p(\mathbf{x}|\mathbf{y})\mathbb{P}(\mathbf{Z}_{\mathbf{x}}|\mathbf{x},\mathbf{y}),$

the detailed balance equations for Algorithm 10 reduce to the detailed balance equations of a Metropolis-Hastings algorithm for the marginal parent process and hence are satisfied whenever (5.6.15) hold. In that case, applying the arguments in [44, Section 4] yields that the process is irreducible (with respect to $f(\mathbf{w} | \mathbf{y})$) and positive Harris recurrent. Hence, if the chain is aperiodic (e.g. when p < 1 or $q(\emptyset) < 1$), Algorithm 10 converges in total variation and ergodically to $f(\mathbf{w} | \mathbf{y})$. It follows that sample path averages of any absolutely integrable functional converge almost surely to its expectation under the limit distribution. In particular, we can consider functionals such as the probability that two data points are offspring of the same parent, or the distribution function of displacements from the parent.

Geyer & Møller [44] also establish a central limit theorem under additional conditions.

5.6.5 Relations to other methods

Corollary 30 can be used as a justification for the *nearest-parent classifier* proposed by Lawson [70]. Given a set of sites $\mathbf{y} = \{y_1, \ldots, y_m\}$ and a set of parents $\mathbf{x} = \{x_1, \ldots, x_n\}$, suppose the task is to assign to each y_j a label $\phi(j) \in \{1, \ldots, n\}$ corresponding to centre $x_{\phi(j)}$. In Model (5.2.2) the labels are independent and hence a maximum likelihood classifier is

$$\hat{\phi}(j) = \operatorname{argmax}_{i=1,\dots,n} h(y_j \mid x_i). \tag{5.6.17}$$

If we superimpose a background Poisson process, whenever the maximum is less than ϵ , y_j is considered to be noise.

Lemma 31 For Model (5.2.3), if $h(\cdot)$ is isotropic (i.e. h(t) is a function of ||t|| only) and decreasing in the norm of its argument, the maximum likelihood classifier (5.6.17) is the nearest parent classifier.

Proof: Immediate from (5.6.17).

As remarked above, conditionally on the number of parents, sibling information can be incorporated as missing auxiliary variables in a Gibbs

sampling algorithm [17, 29]. The distribution of offspring labels given data and parents is derived in Theorem 29. The conditional density of parents given the labelled data is treated below.

Theorem 32 For any labelling $\phi : \{1, \ldots, n(\mathbf{y})\} \to \{1, \ldots, n\}$, the conditional density of the n cluster centres with respect to ν^n is

$$p_n(\mathbf{x} \mid \phi, \mathbf{y}) = \frac{p(\mathbf{x}) \prod_{i=1}^n g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i)}{\int_{U^n} p(\mathbf{x}) \prod_{i=1}^n g(\mathbf{y}_{\phi^{-1}(i)} \mid x_i) d\nu(x_1) \dots d\nu(x_n)}.$$

Proof: Since Janossy densities are not ordered, and ν^n is we have

$$p_{n}(\mathbf{x} \mid \phi, \mathbf{y}) = \frac{1}{n!} \frac{l_{nm}(\mathbf{x}, \mathbf{y}, \phi)}{\frac{1}{n!} \int_{U^{n}} l_{nm}(\mathbf{x}, \mathbf{y}, \phi) d\nu(x_{1}) \dots d\nu(x_{n})}$$
$$= \frac{\frac{1}{n!} e^{-\nu(U)} p(\mathbf{x}) \prod_{i=1}^{n} \left[g(\mathbf{y}_{\phi^{-1}(i)} \mid x_{i}) e^{-\mu(T)} \right]}{\frac{1}{n!} e^{-\nu(U)} \int_{U^{n}} p(\mathbf{x}) \prod_{i=1}^{n} \left[g(\mathbf{y}_{\phi^{-1}(i)} \mid x_{i}) e^{-\mu(T)} \right] d\nu(x_{1}) \dots d\nu(x_{n})}$$

(using the notation in the proof of Theorem 29) and the theorem follows. \Box

In particular, if the prior model is a Poisson process with intensity function $\lambda(\cdot)$, the centres x_i are independent with density

$$\frac{\lambda(x_i) \ g(Z_i \mid x_i)}{\int_U \lambda(u) \ g(Z_i \mid u) \ d\nu(u)}$$

determined by their offspring Z_i .

Summarising, the Gibbs sampling algorithm runs as follows.

- given a current parent configuration \mathbf{x} assign a labelling ϕ with probability $\mathbb{P}(\phi \mid \mathbf{x}, \mathbf{y})$;
- given a current labelling $\phi : \{1, \ldots, m\} \to \{1, \ldots, n\}$ sample n parent positions from $p_n(\mathbf{x} \mid \phi, \mathbf{y})$.

In the context of finite mixture models, a similar Gibbs sampler was introduced by Diebolt and Robert [29]. Celeux and Govaert [23] developed a stochastic EM (SEM) algorithm, alternating sampling the missing labels with maximum likelihood parameter estimation. All above techniques can be thought of as stochastic versions of the classical *k-means algorithm*, a deterministic method that iteratively assigns labels by means of the nearest parent classifier (Lemma 31) and then recomputes the parent positions as the centres of gravity of the current clusters.

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5.7. OTHER APPLICATIONS

We will briefly consider two other examples of identifying clusters in spatial patterns [8]: fitting lines to point patterns and high-level edge detection.

5.7.1 Fitting curves to point patterns

In our first example, the data again consist of a point pattern $\mathbf{y} = \{y_1, \ldots, y_m\} \subseteq T$ with $T \subseteq \mathbb{R}^2$ bounded, but the points are believed to lie close to a curve or curves, possibly not contiguous, and the objective is to estimate the curves. An example is the image analysis task of joining a dot pattern into a curvilinear boundary. An application to spatial statistics is the identification of ancient roads or trade routes given information about the location of archaeological finds such as pottery or coins [117, p. 139], or the analysis of earthquake occurrences in relation to geographical fault patterns (Ogata, personal communication).

Let the curves be parametrised by a small number of real parameters and let U be the corresponding parameter space. The true curve pattern is then a configuration $\mathbf{x} = \{x_1, \ldots, x_n\} \subseteq U$. Again we can assume an independent cluster model in which each curve x_i gives rise to a point pattern Z_{x_i} and these daughter patterns are conditionally independent given \mathbf{x} .

It is no longer appropriate to assume that the daughter patterns Z_{x_i} are equivalent up to translation, since e.g. the expected number of points may well depend on the length of the curve. However we can assume $Z_{(x_i)}$ is Poisson with intensity $h(\cdot | x_i)$, so that the observed point pattern is again a Cox process [117, p. 138]. Particular cases of interest would be the analogues of the Matérn and Thomas models in which distance to the cluster centre is replaced by distance to the nearest point on the cluster curve.

The treatment of this problem is formally equivalent to that in the previous Sections, the only difference being that the cluster parents now belong to a general family of objects U instead of T. The general techniques of Section 5.4 apply.

5.7.2 High-level edge detection

Our final example is the high-level vision problem of identifying large scale edges in a scene using the output of a low-level edge detector. The 'data' \mathbf{y} consist of a pattern of line segments and the objective is to cluster them around a small number of larger line segments [91].

Let W denote the set of possible outputs of the low-level edge detector. For example these may be line segments restricted to have unit length (= 1 pixel width) and orientation which is a multiple of 45 degrees. As usual U denotes the space of objects we are looking for, which in this case are also line segments, but have unrestricted length and orientation.

Model **y** as a superposition of conditionally independent line segment processes Z_{x_i} associated with each true line segment x_i . Again it is not reasonable to suppose that all clusters are identically distributed up to translation, but we may assume they are all Poisson so that **y** is a Cox line segment process. Typically the expected number of line segments in Z_{x_i} will depend on the length of x_i .

The MLE and MAP estimators of \mathbf{x} can then be determined using the techniques we have described above.

The possible benefits of a prior model for \mathbf{x} include the ability to encourage long lines and continuity between lines, and to penalise lines that cross one another.

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Chapter 6 Markov properties of cluster processes

The goal of this Chapter (a revision of Baddeley, Van Lieshout and Møller [10]) is to establish a theoretical link between Markov processes and cluster models. We prove that a Poisson cluster process with uniformly bounded clusters is a nearest-neighbour Markov point process with respect to the connected component relation introduced by Baddeley and Møller [11]; moreover, if a (fixed range) Markov or nearest-neighbour Markov point process is used as the parent process for a cluster process, and the clusters are uniformly bounded and a.s. nonempty, then the cluster process is 'again nearest-neighbour Markov. These results convincingly support Møller's claim [89] that nearest-neighbour Markov processes provide a rich class of models for (moderate) spatial clustering. The former result may also be helpful in understanding why statistical theory (as developed in Van Lieshout and Baddeley [78]) for Poisson cluster processes so closely resembles that for Markov point processes.

6.1. Setup

We consider finite, simple point processes X on a locally compact, complete separable metric space U (typically \mathbb{R}^d or a compact subset). The metric is denoted d and the set of all configurations is identified with the space N^f of all simple, totally finite counting measures on U. For more details see Sections 3.1.2 and 3.2.1.

Let μ be a finite, non-atomic Borel measure on U. We will restrict attention to processes whose distributions are absolutely continuous with

respect to the law π of a Poisson process on U with finite intensity measure μ and denote the density by f.

Recall that f is called *hereditary* [107] if

$$f(\mathbf{x}) > 0$$
 implies $f(\mathbf{z}) > 0$ for all $\mathbf{z} \subseteq \mathbf{x}$. (6.1.1)

We say that f is hereditary excluding \emptyset if (6.1.1) holds except when $\mathbf{z} = \emptyset$.

6.1.1 Markov point processes

We are interested in Markov point processes [107] (cf. Definition 2) with respect to the following relation. Define $u, v \in U$ to be *r*-close if $0 < d(u, v) \leq r$ where d is the metric of U and write $u \sim v$.

We also consider nearest-neighbour Markov point processes (compare to Definition 3) with respect to the following realisation dependent relation.

Definition 8 For each $\mathbf{x} \in N^f$, define the connected component relation [11] between points of \mathbf{x} by

$$x_i \sim x_j$$
 iff $x_i \sim z_1 \sim \cdots \sim z_n \sim x_j$ for some $z_1, \ldots, z_n \in \mathbf{x}$

In other words, two points of \mathbf{x} are related under $\underset{\mathbf{x}}{\sim}$ if they are in the same connected component of the finite graph whose edges connect every pair of *r*-close points in \mathbf{x} .

The Hammersley-Clifford theorem (3.1.9) [11, Theorem 4.13] specialises to the following result.

Lemma 33 A point process X is nearest-neighbour Markov with respect to the connected component relation \sim iff

$$f(\mathbf{x}) = \prod_{\text{cliques } \mathbf{z} \subseteq \mathbf{x}} \varphi(\mathbf{z})$$
(6.1.2)

where $\varphi(\cdot) \ge 0$ is such that whenever \mathbf{z} is a $\approx -clique$ with $\varphi(\mathbf{z}) > 0$ then $\varphi(\mathbf{w}) > 0$ for all $\mathbf{w} \subseteq \mathbf{z}$.

Equivalently, X is nearest-neighbour Markov w.r.t. \sim iff

$$f(\mathbf{x}) = f(\emptyset) \prod_{k=1}^{K} \Phi(x_{D_k})$$
(6.1.3)

where x_{D_1}, \ldots, x_{D_K} are the connected components of \mathbf{x} and $\Phi(\cdot) \geq 0$ is such that if \mathbf{x} is a $\underset{\mathbf{x}}{\sim}$ -clique and $\mathbf{z} \subseteq \mathbf{x}$ is a $\underset{\mathbf{z}}{\sim}$ -clique then $\Phi(\mathbf{x}) > 0$ implies $\Phi(\mathbf{z}) > 0$.

6.1.2 Cluster processes

In the remainder of this Chapter we will consider the independent clustering model described in Section 5.2, in which each point ξ in an unobserved parent process X gives rise to a finite point process Z_{ξ} of daughters. The data model Y is the superposition

$$Y = \bigcup_{x_i \in X} Z_{x_i}.$$

Interpreted as a marked point process $\{(x_1, Z_{x_1}), \ldots, (x_n, Z_{x_n})\}$, we assume that the marks Z_{x_i} are independent. For convenience we will sometimes consider densities with respect to $\rho = e^{\mu(U)}\pi$. Writing Q_{ξ} for the distribution of offspring of a parent at point ξ , we assume henceforth that

- (A) Q_{ξ} is absolutely continuous with respect to ρ with density $q_{\xi} = g(\cdot | \xi) e^{-\mu(U)}$; equivalently, Q_{ξ} is absolutely continuous with respect to π with density $g(\cdot | \xi)$;
- (B) $(\xi, \mathbf{z}) \mapsto q_{\xi}(\mathbf{z})$ is Borel measurable $U \times N^f \to \mathbb{R}_+$;
- (C) (uniform boundedness) $Z_{\xi} \subseteq B(\xi, R)$ a.s. for some R > 0;
- (D) q_{ξ} is hereditary excluding \emptyset .

Here $B(\xi, R)$ denotes the closed ball in the metric d with centre ξ and radius R.

Lemma 34 The cluster process described above is absolutely continuous with respect to π with Radon-Nikodym derivative

$$f(\mathbf{y}) = \mathbb{E}\left(e^{\mu(U)} \sum_{C_1,\dots,C_n(\mathbf{x})} \prod_{i=1}^{n(\mathbf{x})} q_{x_i}(\mathbf{y}_{C_i})\right)$$
(6.1.4)

where \mathbb{E} denotes expectation with respect to the distribution of X, and the sum is over all ordered partitions of $\mathbf{y} = \{y_1, \ldots, y_m\}$ into n subconfigurations $\mathbf{y}_{C_1}, \ldots, \mathbf{y}_{C_n}$ (allowing empty sets).

Proof: Conditionally given $X = \mathbf{x}$, the density with respect to π is

$$f(\mathbf{y} \mid \mathbf{x}) = e^{\mu(U)} \sum_{C_1, \dots, C_n} \prod_{i=1}^n q_{x_i}(\mathbf{y}_{C_i})$$

by Lemma 23. Here the sum is over all ordered partitions of \mathbf{y} into $n = n(\mathbf{x})$ clusters, allowing empty sets. The result follows by integrating over \mathbf{x} .

6.2. STATEMENT OF RESULTS

Theorem 35 Let X be a unit rate Poisson point process on U and Y a cluster process with parent process X and clusters satisfying the assumptions (A)-(D) of Section 6.1.2. Then Y is a nearest-neighbour Markov point process with respect to the connected component relation at distance 2R.

Any Poisson process with finite intensity measure λ can be treated in the same way by replacing the reference measure μ by $\lambda\mu$.

Consider the special case in which the offspring of each parent are Poisson. In \mathbb{R}^d , say, consider a parent process on a compact subset B and let μ be Lebesgue measure restricted to the dilated set $B_{\oplus R} = B \oplus B(0, R)$. Assume that a parent at ξ has a Poisson number of offspring with mean ω , positioned i.i.d. with probability density $h(y_i - \xi)$ with respect to μ where h is supported on B(0, R). For $\mathbf{y} \neq \emptyset$, the density is

$$f(\mathbf{y}) = \sum_{n=1}^{\infty} \left\{ \frac{e^{\mu(B_{\oplus R} \setminus B)} \omega^m e^{-\omega n}}{n!} \int_B \cdots \int_B \prod_{j=1}^m \left(\sum_{i=1}^n h(y_j - x_i) \right) d\mu(x_1) \dots d\mu(x_n) \right\}.$$

This is easily (or via the proof of Theorem 35) factorised as

$$f(\mathbf{y}) = e^{\mu(B_{\oplus R})} \omega^m e^{-m\omega} e^{-\beta} \left[\sum_{C_1, \dots, C_k} e^{\omega(m-k)} J(\mathbf{y}_{C_1}) \dots J(\mathbf{y}_{C_k}) \right],$$

$$\cdot \qquad (6.2.5)$$

where $\beta = (1 - e^{-\omega}) \mu(B)$, the sum is over all *unordered* partitions of **y** into disjoint *non-empty* subconfigurations, and

$$J(\mathbf{y}_{C}) = \int_{B} \prod_{y_{j} \in \mathbf{y}_{C}} h(y_{j} - \xi) d\mu(\xi).$$
 (6.2.6)

Since $J(\mathbf{y}_C) = 0$ unless \mathbf{y}_C is a \mathbf{y}_C -clique, the only nonzero terms in (6.2.5) are those for partitions which are refinements of the partition of \mathbf{x} into connected components. Thus (6.2.5) factorises into terms associated with each connected component. According to (6.1.2) the process is nearest-neighbour Markov, provided the positivity condition stated below (6.1.2) is satisfied.

A special case is the Matérn cluster process in which $h \equiv \text{constant}$ on B(0, R): then we have

$$J(\mathbf{y}_C) = \mu\left(\bigcap_{y_j \in \mathbf{y}_C} B(y_j, R) \cap B\right)$$

i.e. $J(\mathbf{y}_C)$ is the volume occupied within B by the intersection of the balls of radius R centred at the points of \mathbf{y}_C . In this case the positivity condition is clearly satisfied, so that the Matérn cluster process is nearest-neighbour Markov.

In Theorem 35, nearest-neighbour Markov cannot be replaced by Markov in the sense of Ripley and Kelly.

Counterexample 1 A Neyman-Scott process with uniformly bounded clusters in general is not a Markov point process at any fixed range $s < \infty$.

For, consider a configuration of three points y_1, y_2, y_3 such that $||y_1 - y_2|| < \min\{s, 2R\}, ||y_2 - y_3|| < \min\{s, 2R\},$ but $||y_1 - y_3|| > \max\{s, 2R\}$. If f were a Markov function at range s then

$$f(\{y_1, y_2, y_3\})f(\{y_2\}) = f(\{y_1, y_2\})f(\{y_2, y_3\}).$$

Substituting (6.2.5) gives

$$[1 + e^{\omega}J(y_1, y_2) + e^{\omega}J(y_2, y_3)] = [1 + e^{\omega}J(y_1, y_2)] [1 + e^{\omega}J(y_2, y_3)]$$

If we assume that $J(y_i, y_j) > 0$ whenever $||y_i - y_j|| < 2R$ (e.g. the Matérn model), this is clearly a contradiction. Hence f is not a Markov density in the Ripley-Kelly sense.

Next we turn to non-Poisson parent processes. The simplest generalisation is to take a Ripley-Kelly Markov parent process. However, in general, the cluster process constructed as in Section 6.1.2 is not nearestneighbour Markov.

Heuristically, this is because parents without offspring can cause interaction by merging of disjoint \sim -cliques. If we require each parent to have at least one daughter, the cluster process is nearest-neighbour Markov.

Theorem 36 Let X be a Markov point process at range r and Y the associated cluster process satisfying (A)-(D) of Section 6.1.2. If moreover

(E) the clusters are nonempty a.s.

then Y is a nearest-neighbour Markov point process for the connected component relation at range 2R + r.

It is clear from the proof that the same result holds when the parent process is nearest-neighbour Markov. This suggests that a population of reproducing individuals can be modelled by the mechanism in Theorem 36. See also [66].

Theorem 37 Let X be a nearest-neighbour Markov point process at range r and Y the associated cluster process satisfying (A)-(D) of Section 6.1.2. If moreover

(E) the clusters are nonempty a.s.

then Y is a nearest-neighbour Markov point process for the connected component relation at range 2R + r.

Proof: The following adaptation in the proof of Theorem 36 is needed. Let $\epsilon : \{1, \ldots, m\} \to \{1, \ldots, n\}$ be a surjective mapping such that $d(y_j - x_{\epsilon(j)}) \leq R$ for all j. Suppose $\mathbf{z} \subseteq \mathbf{x}$ is a connected component with respect to $\underset{\mathbf{x}}{\sim}$ at range r such that $\epsilon^{-1}(\mathbf{z}) = \mathbf{w} \subseteq \mathbf{y}$. Then \mathbf{w} is a connected component in \mathbf{y} at range 2R + r. To see this, choose any $w_1, w_2 \in \mathbf{w}$. There exists a \mathbf{x} -connecting path between the ϵ images $z_1, z_2 \in \mathbf{z}$, say

 $z_1 \sim x_{i_1} \sim \cdots \sim x_{i_m} \sim z_2.$

As ϵ is surjective, x_{i_j} is the image of some $y_{k_j} \in \mathbf{y}$. Now apply the triangle inequality to obtain

$$d(w_1 - y_{k_1}) \le d(w_1 - z_1) + d(z_1 - x_{i_1}) + d(x_{i_1} - y_{k_1})$$
$$\le R + r + R = 2R + r.$$

Continuing in this manner proves the claim.

Corollary 38 Let X be a (nearest-neighbour) Markov point process at range r and Y the associated cluster process obtained by translating each $x_i \in X$ independently, where the displacements are absolutely continuous with respect to μ with density supported in B(0, R). Then Y is a nearest-neighbour Markov point process for the connected component relation at range 2R + r.

Proof: Apply Theorem 36 or Theorem 37.

6.3. Proofs

In this Section we give the proofs of the main results.

Proof: (Lemma 33)

Suppose that (6.1.2) holds. Let $\mathbf{x} \in N^f$, $\xi \in U$ and let $\mathbf{x}_{D_1}, \ldots, \mathbf{x}_{D_K}$ and $\mathbf{w} \cup \{\xi\}$ denote the connected components of $\mathbf{x} \cup \{\xi\}$. Then, if $\mathbf{x}_{D_{K+1}}, \ldots, \mathbf{x}_{D_L}$ are the connected components of \mathbf{w} , we have that \mathbf{x}_{D_1} , \ldots, \mathbf{x}_{D_L} are the connected components of \mathbf{x} , and

$$f(\mathbf{x} \cup \{\xi\}) = \varphi(\emptyset) \left[\prod_{i=1}^{K} \prod_{\emptyset \neq \mathbf{z} \subseteq \mathbf{x}_{D_i}} \varphi(\mathbf{z}) \right] \prod_{\emptyset \neq \mathbf{z} \subseteq \mathbf{w} \cup \{\xi\}} \varphi(\mathbf{z})$$

while

$$f(\mathbf{x}) = \varphi(\emptyset) \left[\prod_{i=1}^{K} \prod_{\emptyset \neq \mathbf{z} \subseteq \mathbf{x}_{D_i}} \varphi(\mathbf{z}) \right] \prod_{j=K+1}^{L} \prod_{\emptyset \neq \mathbf{z} \subseteq \mathbf{x}_{D_j}} \varphi(\mathbf{z}).$$

Hence $f(\mathbf{x} \cup \{\xi\}) > 0$ implies $f(\mathbf{x}) > 0$ (as $\mathbf{z} \subseteq \mathbf{x}_{D_j}$ for j > K implies that $\mathbf{z} \subseteq \mathbf{w}$) and $f(\mathbf{x} \cup \{\xi\})/f(\mathbf{x})$ satisfies the conditions of Definition 3. Thus X is nearest-neighbour Markov with respect to the connected component relation.

Conversely, suppose X is nearest-neighbour Markov. By the analogue of the Hammersley-Clifford theorem [11, Theorem 4.13],

$$f(\mathbf{x}) = \prod_{\mathbf{y} \subseteq \mathbf{x}} \varphi(\mathbf{y})^{\chi(\mathbf{y}|\mathbf{x})} \qquad (\text{taking } 0^0 = 0)$$
(6.3.7)

where $\chi(\mathbf{y} \mid \mathbf{x}) = 1$ if \mathbf{y} is a $\underset{\mathbf{x}}{\sim}$ -clique and 0 otherwise; and $\varphi: N^f \to \mathbb{R}_+$ satisfies

- (I1) $\varphi(\mathbf{x}) > 0$ implies $\varphi(\mathbf{y}) > 0$ for all $\mathbf{y} \subseteq \mathbf{x}$
- (I2) $\varphi(\mathbf{x}) > 0$ and $\varphi(N(\{\xi\} \mid \mathbf{x} \cup \{\xi\})) > 0$ imply $\varphi(\mathbf{x} \cup \{\xi\}) > 0$

where $N(\{\xi\} \mid \mathbf{x} \cup \{\xi\})$ denotes the neighbourhood of ξ in $\mathbf{x} \cup \{\xi\}$ (see Section 3.1.3). Note that, in the case of the connected component relation, $\xi \sim_{\mathbf{y}} \eta$ implies $\xi \sim_{\mathbf{x}} \eta$ for $\mathbf{x} \supseteq \mathbf{y}$, so that $\chi(\mathbf{y} \mid \mathbf{y}) = 1$ implies $\chi(\mathbf{y} \mid \mathbf{x})$ for any $\mathbf{x} \supseteq \mathbf{y}$.

To prove that (6.3.7) reduces to (6.1.2) we need to show that, if $\varphi(\mathbf{y}) > 0$ for all $\mathbf{y} \subseteq \mathbf{x}$ with $\chi(\mathbf{y} \mid \mathbf{x}) = 1$, then $\varphi(\mathbf{y}) > 0$ for all $\mathbf{y} \subseteq \mathbf{x}$.

To prove this, suppose $\mathbf{v}, \mathbf{w} \subseteq \mathbf{x}$ are disjoint connected subconfigurations of \mathbf{x} . If $\xi \in \mathbf{v}$ then $N(\{\xi\} \mid \mathbf{w} \cup \{\xi\}) = \{\xi\}$. By assumption $\varphi(\{\xi\}) > 0, \ \varphi(\mathbf{w}) > 0$ so (I2) gives $\varphi(\mathbf{w} \cup \{\xi\}) > 0$. Similarly, if $\{\xi, \eta\} \subseteq \mathbf{v}$ with $\eta \sim \xi$ then $N(\{\eta\} \mid \mathbf{w} \cup \{\xi, \eta\}) = \{\xi, \eta\}$, and by assumption $\varphi(\{\xi, \eta\}) > 0$, so (I2) gives $\varphi(\mathbf{w} \cup \{\xi, \eta\}) = \{\xi, \eta\}$, and by asthis way we obtain that $\varphi(\mathbf{y}) > 0$ for all $\mathbf{y} \subseteq \mathbf{x}$. Hence if X is nearest-neighbour Markov then its density is of the form (6.1.2) where φ satisfies (I1) and hence the condition stated in the Lemma.

Proof: (Theorem 35) By (6.1.4), the density $f(\mathbf{y})$ of $\mathbf{y} \neq \emptyset$ with respect to π is

$$\sum_{n=1}^{\infty} \frac{e^{-\mu(U)}}{n!} \int_{U} \cdots \int_{U} e^{\mu(U)} \sum_{C_1, \dots, C_n} \prod_{i=1}^n q_{x_i}(\mathbf{y}_{C_i}) d\mu(x_1) \cdots d\mu(x_n)$$
$$= \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{C_1, \dots, C_n} \prod_{i=1}^n \int_{U} q_{\xi}(\mathbf{y}_{C_i}) d\mu(\xi); \qquad (6.3.8)$$

here the inner sum is over all ordered partitions of \mathbf{y} into n disjoint, possibly empty, sets. For $\mathbf{y} = \emptyset$,

$$f(\emptyset) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\int_{U} q_{\xi}(\emptyset) \, d\mu(\xi) \right]^{n}$$
(6.3.9)

$$= e^{\mu(U)-\beta}$$
 (6.3.10)

if we define $\beta = \int_U (1 - q_{\xi}(\emptyset)) d\mu(\xi)$. Note that since the parent process is Poisson, the number of non-empty clusters is Poisson distributed with mean β .

Now $q_{\xi}(\mathbf{z}) = 0$ whenever $\mathbf{z} \not\subseteq B(\xi, R)$; hence if $q_{\xi}(\mathbf{z}) \neq 0$ then all pairs of points in \mathbf{z} are closer than 2R apart, i.e. \mathbf{z} is a clique with respect to the finite range relation with distance 2R. Hence the integral in (6.3.8) is nonzero only when the partition consists of 2R-cliques.

For $\mathbf{y} \neq \emptyset$, let $\mathbf{y}_{D_1}, \ldots, \mathbf{y}_{D_{k_m}}$ be the connected components of \mathbf{y} for the relation \sim with range 2*R*. Then the integral in (6.3.8) is nonzero only when the partition is a refinement of D_1, \ldots, D_{k_m} . Let C_1, \ldots, C_k be an *unordered* partition refining D_1, \ldots, D_{k_m} , consisting of *non-empty* sets. This contributes a term

$$\alpha \prod_{i=1}^k \int_U q_{\xi}(\mathbf{y}_{C_i}) \, d\mu(\xi)$$

to the density. Since $\int_U q_{\xi}(\emptyset) \ d\mu(\xi) = \mu(U) - \beta$, the coefficient α is

$$\sum_{n=k}^{\infty} \frac{1}{n!} (\mu(U) - \beta)^{n-k} n(n-1) \cdots (n-k+1) = e^{\mu(U) - \beta}.$$

The class of all partitions that are refinements of D_1, \ldots, D_{k_m} is the Cartesian product of the sets of partitions of each D_i . Hence, for $\mathbf{y} \neq \emptyset$,

$$f(\mathbf{y}) = e^{\mu(U) - \beta} \prod_{i=1}^{k_m} \Phi(\mathbf{y}_{D_i})$$
(6.3.11)

where

$$\Phi(\mathbf{z}) = \sum_{k \ge 1} \sum_{\mathbf{z}_{C_1}, \dots, \mathbf{z}_{C_k}} \prod_{j=1}^k \int_U q_{\xi}(\mathbf{z}_{C_j}) \, d\mu(\xi)$$
(6.3.12)

where $\mathbf{z}_{C_1}, \ldots, \mathbf{z}_{C_k}$ range over all unordered partitions of \mathbf{z} into nonempty subconfigurations.

Since the offspring densities q_{ξ} are hereditary excluding \emptyset , clearly Φ is hereditary excluding \emptyset , and hence f is hereditary. According to (6.1.2) the density (6.3.11) is nearest-neighbour Markov with respect to the connected component relation at range 2R.

Proof: (Theorem 36)

The density $p(\mathbf{x})$ can be factorised as in (6.1.2).

By (6.1.4), the density of **y** with respect to π is

$$f(\mathbf{y}) = e^{\mu(U)} \int_{N^f} p(\mathbf{x}) \sum_{C_1, \dots, C_n(\mathbf{x})} \prod_{i=1}^{n(\mathbf{x})} q_{x_i}(\mathbf{y}_{C_i}) d\pi(\mathbf{x})$$

where the inner sum ranges over all ordered partitions of \mathbf{y} into disjoint, possibly empty subconfigurations.

First note that by assumption $q_{\xi}(\emptyset) = 0$, hence the integrand can be rewritten as

$$p(\mathbf{x}) \sum_{\epsilon} \prod_{i=1}^{n} q_{x_i}(\mathbf{y}_{\epsilon^{-1}(i)})$$
(6.3.13)

where ϵ ranges over all surjective mappings of the points of **y** onto the points of **x**, identified with mappings from $\{1, \ldots, m\}$ onto $\{1, \ldots, n\}$.

We can restrict attention to those ϵ such that

$$d(y_j - x_{\epsilon(j)}) \le R \qquad \text{for all } j \tag{6.3.14}$$

since all other terms are zero. For such ϵ , if $\mathbf{z} \subseteq \mathbf{x}$ is an *r*-clique and $\epsilon^{-1}(\mathbf{z}) = \mathbf{w} \subseteq \mathbf{y}$, then \mathbf{w} must be a 2R + r-clique. To see this, take $y_i, y_j \in \mathbf{w}$ and apply the triangle inequality:

$$d(y_i - y_j) \leq d(y_i - x_{\epsilon(i)}) + d(x_{\epsilon(i)} - x_{\epsilon(j)}) + d(x_{\epsilon(j)} - y_j)$$

$$\leq R + r + R.$$

Let $\mathbf{y}_{D_1}, \ldots, \mathbf{y}_{D_{k_m}}$ be the connected components of \mathbf{y} at distance 2R + r. Then we can rewrite (6.3.13) as

$$\prod_{\substack{\text{cliques } \mathbf{z} \subseteq \mathbf{x}}} \varphi(\mathbf{z}) \sum_{\epsilon} \prod_{i=1}^{n} q_{x_i}(\mathbf{y}_{\epsilon^{-1}(i)}) =$$

$$\sum_{\epsilon} \left[\prod_{i=1}^{n} q_{x_i}(\mathbf{y}_{\epsilon^{-1}(i)}) \prod_{k=1}^{k_m} \prod_{\substack{\text{cliques } \mathbf{z} \subseteq \mathbf{x}:\epsilon^{-1}(\mathbf{z}) \subseteq D_k}} \varphi(\mathbf{z}) \right] =$$

$$\sum_{\epsilon} \prod_{k=1}^{k_m} \left[\prod_{i:\epsilon^{-1}(i) \subseteq D_k} q_{x_i}(\mathbf{y}_{\epsilon^{-1}(i)}) \prod_{\substack{\text{cliques } \mathbf{z} \subseteq \mathbf{x}:\epsilon^{-1}(\mathbf{z}) \subseteq D_k}} \varphi(\mathbf{z}) \right]. (6.3.15)$$

Any ϵ of the type described above can be represented as a family of surjective mappings

 $\epsilon_k: D_k \to D'_k = \{i \mid d(x_i, y_j) \le R \text{ for some } j \in D_i\}$

automatically satisfying the norm condition (6.3.14). Note that $\mathbf{x}_{D'_k}$ form a disjoint partition of \mathbf{x} . Thus (6.3.15) is

$$\prod_{k=1}^{k_m} \sum_{\epsilon_k} \left[\prod_{i \in D'_k} q_{x_i}(\mathbf{y}_{\epsilon_k^{-1}(i)}) \prod_{\text{cliques } \mathbf{z} \subseteq \mathbf{x}_{D'_k}} \varphi(\mathbf{z}) \right].$$

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Integrating over **x** and exploiting the form of π yields $f(\mathbf{y}) =$

$$e^{\mu(U)} \prod_{k=1}^{k_m} \int_{N^f(\mathbf{y}_{D_k} \oplus R)} \sum_{\epsilon_k} \prod_{i=1}^{n(\mathbf{v})} q_{v_i}(\mathbf{y}_{\epsilon_k^{-1}(i)}) \prod_{\text{cliques } \mathbf{z} \subseteq \mathbf{v}} \varphi(\mathbf{z}) \ d\pi_k(\mathbf{v})$$

where we write π_k for the Poisson process on the corresponding exponential space $N^f(\mathbf{y}_{D_k} \oplus R)$. Thus, f factorises as required by (6.1.2). The hereditary property follows as in the proof of the previous Theorem.

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Appendix

Delta distance

Initial pattern	MLE	MAP
	(coordinatewise)	(coordinatewise)
empty	.546	.404
true	.230	.099
shifted	.367	.335
Hough extrema	.314	.170

Table .1: Delta distance between the true pattern and the reconstruction obtained using coordinatewise ascent. The only transitions are births and deaths.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.210	.140
true	.235	.099
shifted	.260	.291
Hough extrema	.213	.182

Table .2: Delta distance between the true pattern and the reconstruction obtained using steepest ascent. The only transitions are births and deaths.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.093	.140
true	.000	.000
shifted	.192	.291
Hough extrema	.178	.182

Table .3: Optimal delta distance between the true pattern and intermediate reconstructions using steepest ascent. The only transitions are births and deaths.

Initial pattern	MLE	MAP
	(coordinatewise)	(coordinatewise)
empty	.528	.207
true	.236	.132
shifted	.344	.132
Hough extrema	.335	.132

Table .4: Delta distance between the true pattern and the reconstruction obtained using coordinatewise ascent. The transitions are births, deaths and translations.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.205	.132
true	.205	.132
shifted	.210	.132
Hough extrema	.220	.132

Table .5: Delta distance between the true pattern and the reconstruction obtained using steepest ascent. The transitions are births, deaths and translations.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.093	.132
true	.000	.000
shifted	.049	.099
Hough extrema	.187	.132

Table .6: Optimal delta distance between the true pattern and intermediate reconstructions using steepest ascent. The transitions are births, deaths and translations.

Figure of merit

Initial pattern	MLE	MAP
	(coordinatewise)	(coordinatewise)
empty	.627	.733
true	.883	.960
shifted	.794	.815
Hough extrema	.802	.929

Table .7: Figure of merit between the true pattern and the reconstruction obtained using coordinatewise ascent. The only transitions are births and deaths.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.900	.944
true	.879	.960
shifted	.865	.859
Hough extrema	.890	.926

Table .8: Figure of merit between the true pattern and the reconstruction obtained using steepest ascent. The only transitions are births and deaths.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.985	.944
true	1.00	1.00
shifted	.906	.860
Hough extrema	.907	.931

Table .9: Optimal figure of merit between the true pattern and intermediate reconstructions using steepest ascent. The only transitions are births and deaths.

Initial pattern	MLE	MAP
	(coordinatewise)	(coordinatewise)
empty	.632	.908
true	.881	.948
shifted	.809	.948
Hough extrema	.787	.948

Table .10: Figure of merit between the true pattern and the reconstruction obtained using coordinatewise ascent. The transitions are births, deaths and translations.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.902	.948
true	.902	.948
shifted	.900	.948
Hough extrema	.890	.948

Table .11: Figure of merit between the true pattern and the reconstruction obtained using steepest ascent. The transitions are births, deaths and translations.

Initial pattern	MLE	MAP
	(steepest ascent)	(steepest ascent)
empty	.985	.948
true	1.00	1.00
shifted	.993	.960
Hough extrema	.906	.948

Table .12: Optimal figure of merit between the true pattern and intermediate reconstructions using steepest ascent. The transitions are births, deaths and translations.



Figure .1: Reconstruction quality at successive steps of coordinatewise ascent with the local maxima of the conditional Hough transform as initial state.





number of iterations



Figure .2: Reconstruction quality for the successive reconstructions obtained using steepest ascent starting with a diagonally translated copy of the true configuration.



Figure .3: Average reconstruction quality for 10 independent realisations at different noise levels. Top: coordinatewise ascent; bottom: steepest ascent.



Figure .4: Log posterior likelihood against time for a geometric cooling schedule starting at H = 4.0 of rate .5 and a Strauss prior with $\beta = .0025$ and $\gamma = .25$



Figure .5: Number of objects against time for a geometric cooling schedule starting at H = 4.0 of rate .5 and a Strauss prior with $\beta = .0025$ and $\gamma = .25$



Figure .6: Delta-2 distance between reconstructed and true pattern as a function of time. The cutoff value is 4.

Coo	rdinates of points	in region II of Strauss'	$redwood \ data$
167	5	170	5
144	6	174	7
144	8	146	11
13	12	145	14
125	17	161	17
37	18	144	18
150	19	154	19
160	19	52	20
143	20	152	21
155	22	33	23
137	23	133	24
144	24	33	25
141	25	138	26
137	27	134	28
36	30	82	32
98	36	83	42
30	45	49	45
46	46	57	46
63	48	65	49
67	51	54	52
59	54	129	54
147	54	18	56
127	56	66	57
121	58	49	59
123	59	126	59
52	60	49	61
60	61	122	61
127	61	51	62
54	62	98	64
110	70	44	74
60	76	46	79
109	79	107	80
41	81	40	85
84	89	98	96
85	107	42	109
51	109	85	109
90	109	48	111
91	111	53	112
80	113	51	114
78	115	89	115
80	116	85	118

89	119	70	123
72	125	71	127
67	128	62	132
69	132	65	133
67	134	21	137
22	137	23	139
28	144	28	146
23	149	25	152
22	153	22	154
54	156	15	157
17	157	20	157
60	157	16	159
54	159	58	161
54	162	50	16
30	169	47	172
53	172	51	175
26	177	46	177
50	178	25	179
36	181	39	181
30	182	32	183
42	183		

Index

 L^p optimisation, 23 area-interaction process, 39, 42, 61 Bayesian approach, 59, 111 clique, 39, 41, 134 cluster process, 105, 133, 135 clustered pattern, 42, 54 configuration, 18, 59, 107, 123 connected component relation, 40, 134 coordinatewise optimisation, 27, 29, 62 Cox process, 107 curve fitting, 130 detailed balance, 77, 125, 127 diffusion, 94 dilation, 24, 48 Dobrushin's contraction coefficient, 82,88 edge detection, 130 empty space statistic, 52 erosion, 18, 24

finite mixture model, 123, 129 fixed temperature sampling, 79, 97, 112 forward density, 19, 106 Gibbs sampler, 114, 123, 129 Hammersley-Clifford theorem, 39, 41, 47, 134 hard core process, 37 hereditary, 38, 41, 76, 112, 125, 134 Hough transform, 18, 30, 59, 64, 96 ICM algorithm, 28, 62 image space, 17 independent noise model, 19, 60, 64 inference, 52 inhibition, 42, 54, 59, 111 inhomogeneous Poisson process, 106, 127 intensity function, 107 interaction, 37, 47 iterative optimisation, 27, 62, 111 k-means algorithm, 129

lattice process, 54 likelihood approach, 19, 105 likelihood ratio, 27, 62, 112 Markov object process, 38, 59 Markov point process, 47, 111, 134, 137, 138 mathematical morphology, 18, 23 Matérn process, 107, 110 maximum a posteriori estimation, 60, 87, 111 maximum likelihood estimation, 22, 27, 52, 109 maximum pseudolikelihood estimation, 56, 65, 109 Metropolis-Hastings algorithm, 124 modified Thomas process, 108 multiple response, 59, 104, 111 multiresolution, 98 nearest neighbour distance, 54

nearest-neighbour Markov object process, 39, 59 nearest-neighbour Markov point process, 111, 134, 136, 138 nearest-parent classifier, 128 Neyman-Scott process, 107, 137 object recognition, 17, 59, 87

object recognition, 17, 39, 87 object space, 18, 35 offspring assignment, 123

pairwise interaction, 37–39 Papangelou conditional intensity, 38, 53, 56, 63, 109 phase transition, 51 Poisson object process, 36 posterior distribution, 59, 76, 111 pre-processing, 24

regression, 22, 109

segmentation, 11

signal, 19 silhouette, 19, 39, 111 spatial birth-and-death process, 75, 76, 87, 112 spatial clustering, 103 spatial point process, 35, 103 stationary area-interaction process, 50 steepest ascent, 27, 29, 62 stochastic annealing, 87, 113 stochastic EM algorithm, 129 Strauss object process, 37, 60 Strauss process, 42, 57 sufficient statistic, 52

Takacs-Fiksel method, 53, 57 temperature, 76, 87, 112 template matching, 17 total variation, 82, 85, 127

Voronoi tessellation, 39

CWI TRACTS

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