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Topics in Spatial Statistics*

NILS LID HJORT

University of Oslo

HENNING OMRE

Norwegian Institute of Technology

ABSTRACT. An overview is given over a fair range of topics within spatial and spatial–temporal statistics. The theory presented is motivated by and illustrated with actual applications to real world problems. We describe and discuss models for three basic types of spatial processes: continuous random surfaces, mosaic phenomena, and events-against-background processes. Various combinations of these sometimes occur naturally in applications, like Gaussian noise on top of a Markov random field in image restoration problems. Some of these combinations are also discussed. The applications we discuss are drawn from the areas of medical image analysis, pollution monitoring, characterisation of oil reservoirs, estimation of fish and whale stock, forestry surveillance via satellite, statistical meteorology, and symbol recognition.

Key words: Bayesian methods, covariance function, event processes, hidden Markov fields, image restoration, Kriging, marked point processes, Markov random fields, parameter estimation, pseudo-likelihood, quasi-likelihood, semi-Markov random fields, spatial classification, spatial sampling strategy, stochastic simulation

1. Introduction

1.1. What's special about spatial?

Spatial statistical problems call for evaluation by exploratory data analysis, prediction and classification, simulation, and confirmatory statistics, and are accordingly in these respects well within traditional statistics. To pin-point differences, consider a spatial process $\{Y(x): x \in D\}$ with some m-dimensional $Y(x)$ defined over some s-dimensional spatial or spatial–temporal reference region D. We have encountered $s = 2, 3, 4$ in our applications. Traditional statistical dependence between variables may occur in the Y-space, while the spatial reference x allows for dependencies in the reference dimensions. The latter aspect in particular is challenging from a stochastic modelling point of view and usually adds complexity to the sampling and estimation stages. The presence of a reference variable also points to the importance of scale and transformations between different scales.

Spatial phenomena are complicated to understand and model. The objective of a study is often to evaluate characteristics of a single realisation $\{y(x): x \in D\}$, for example, the hydrocarbon present in one particular petroleum reservoir. In this setting the data points $y(x_1), \ldots, y(x_n)$ are "non-repeatable" and the observations may be dependent through their spatial locations. In traditional statistics the underlying assumptions usually include repeatability in the form of (nearly) independent and (nearly) identically distributed observations. In spatial statistics some sort of "pseudo-repeatability" is often obtained by postulating various forms of spatial stationarity. Typical model assumptions could be a constant mean $EY(x) = m$ and/or a stationary covariance function $\operatorname{cov}\{Y(x_1), Y(x_2)\} = C(x_1 - x_2)$. There are parallels to modelling of time series, but spatial problems are often a

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full degree more complicated, due to lack of ordering in the reference space, the fact that border areas of the reference domain often constitute a large proportion of D, and the large variety of sampling options which appear when the dimensionality of D increases. The ergodicity assumption needed in both time series and spatial statistics is much harder to justify in the latter case, since the dependence structure often is strong and D seldomly, with reasonable imagination, can be extended to infinity. Spatial correlation also tends to die out much more slowly than for a dependent one-dimensional process such as time series.

In easier i.i.d.-type problems there is always a Glivenko–Cantelli type theorem which says that one can be ambitious and fit even sophisticated realistic models; the problems are "one-dimensionally" tied to a couple of underlying distributions and nothing else, and the information content of a data set is sufficient to assess intricate features of these. In complex spatial problems, on the other hand, the information content is more thinly spread out in a much larger tapestry of inter-woven problems. Just think of inferring the underlying probabilistic structure of a two-dimensional continuous random function from just observing its values in a finite number of locations for a single realisation!

We have mentioned that sampling of spatial phenomena has several special features. The sampling support B is defined as the domain of the volume over which the sampling is averaged, i.e. $y_B(x_i) = |B|^{-1} \int_B y(x_i - u)\, du$, writing $|B|$ for the volume (or area) of B. A sampling support of zero is in many cases impossible. In petroleum applications, observations in wells are made on about $0.03 \times 0.03 \times 0.05$ m^3, which is of approximate zero support relative to the extent of the reservoir which is typically of size $2500 \times 5000 \times 100$ m^3. Seismically-collected data have a considerable support, however, approximately $100 \times 100 \times 10$ m^3, and this must be accounted for when the two types of data are combined.

Data representativity in the form of a random sampling hypothesis is usually a basic assumption in traditional statistics. Sampling in non-regular regimes is frequent in applications of spatial statistics, however. "Preferential sampling" of some sort frequently occurs in practice, planned or un-planned. One is of course tempted to use available data and knowledge about spatial continuity in order to confirm favourable areas with extreme values of the process. This makes sense from most points of view except from that of traditional statistics. In the petroleum industry one is using seismic data in order to locate the first well in a prospect such that the chances for hitting oil is maximised. The fact that each exploratory well costs about US$ 30 million makes preferential sampling almost mandatory. Consequently one particular challenge of spatial statistics is to correct for preferential sampling when, for example, predicting the total hydrocarbon volume.

The spatial dependence entails that the information content in each sample may vary. In image analysis and remote sensing, where regular sampling occurs, the redundancy in the sometimes enormous data set is usually substantial. The amount of information in the set of observations is often much smaller than what traditionally would have been anticipated.

Measurements of the variable of interest are often expensive or complicated to obtain. Spatial problems frequently involve indirect measurements, like seismic data, in order to improve the spatial coverage of the data. This calls for multivariate spatial models, and often for multivariate calibration methods.

The spatial reference in $\{Y(x): x \in D\}$ provides good opportunities for stochastic modelling. The fact that sampling is scarce and that the spatial dependence complicates the exploratory data analysis renders model verification a very difficult task. When preparing a development plan for a North Sea oil reservoir only about 10^{-8} % of the reservoir volume is directly observable from well data. Geological experience and indirect seismic data are other sources of knowledge, and make the evaluation possible. The verification of the model must often be based on experience.

In typical spatial models with extensive dependence between observations one can only seldomly find explicit closed-form parameter estimators with good efficiency properties. Usually one has to rely on model fitting to the observations through iterative procedures and cross-validation. Note that jackknife and bootstrap procedures are difficult to apply in spatial problems because of the complex dependence structure.

We have so far primarily discussed spatial problems. Problems containing both spatial and temporal elements are considered with increasing interest, however. In problems of this type the samples are often abundant, particularly in the time dimension. This is caused by the increasing use of automatic sensors, and again there are often difficulties stemming from a high degree of data redundancy. The interdependence structure is even more complicated than for spatial problems, and even simple exploratory data analysis may turn out to be very complicated.

1.2. Three ways of applying statistics

Let us return to "general statistics" and its philosophy and use in spatial statistics problems. It seems appropriate and convenient to distinguish between three ways of applying statistical methodology.

(i) *Exploratory statistics* is primarily concerned with the observations $y(x_1), \ldots, y(x_n)$ and their characteristics. When exploring them a minimum of model assumptions is enforced. Usually only some statements about representativity are made, so that data displays and meaningful plots associated with summary statistics can be provided. Exploratory statistics is an important but still underused part of applied statistics. Its uses include generating hypotheses justifying model choices.

(ii) *Predictive statistics* is primarily concerned with prediction and classification of realisations, either because the actual realisation is not observed or because it is observed with noise. An example of the former is spatial interpolation from $y(x_1), \ldots, y(x_n)$ to prediction of $y(x)$ in other positions, perhaps with an uncertainty measure included, and an example of the latter is image restoration. Model assumptions are made only to meet the objective of prediction. In other words, the stochastic model is often constructed more for reasons of pragmatism and convenience than for ambitiously and realistically describing the phenomenon under study. Thus a model could have only vague, intuitive connections to the physical phenomenon. Some clear relations from phenomenon to model are of course preferable, since this eases the justification of the model towards the users, but in the end the quality of the model is judged solely by its predictive success. This viewpoint, whereby statisticians fine-tune parameters of algorithms rather than estimate parameters of models, can of course be adopted also in more traditional frameworks of perhaps one-dimensional independent or nearly independent realisations of some phenomenon, but is, we feel, particularly relevant for complex spatial problems. Model fitting is frequently made by cross-validation based on the available observations. Prediction and classification methods find numerous uses in all sectors of applied statistics.

(iii) *Confirmatory statistics* is mostly occupied with properties of the underlying phenomenon $\{Y(x): x \in D\}$. It requires a stochastic model which in a stronger sense than with predictive statistics truly reflects the key features of the phenomenon, and model parameters must be interpreted in terms of it. The observations $y(x_i)$ are used to express the significance of these parameters. An example is the test for significant correlation between permeability and porosity in sandstone petroleum reservoirs. The quality of this statement is crucially dependent on the validity of the model. Confirmatory statistics are used primarily in such scientific contexts.

The problems addressed in this article will utilise spatial statistics in a predictive setting. Stochastic modelling constitutes a considerable part of the studies presented. This is necessary in order to integrate the different types of available information for the purpose of prediction or classification. Expert experience often constitutes an important source of information, which sometimes invites Bayesian and empirical Bayesian approaches. The Bayesian formalism has proved useful in pragmatic modelling, and since formal testing is seldom performed the disadvantages of the formalism are seldom exposed. Large data volumes with complicated intercorrelation structures and computer intensive solution algorithms are other characteristics.

1.3. Stochastic modelling

Phenomena that vary in space and/or time are frequently observed in nature. The use of stochastic models and statistics in surveying such phenomena has proven useful. Stochastic modelling constitutes the artistic part of the analysis, and some rules of thumb should be kept in mind. The model formulation must be tailored to the question to be answered. Classification of discrete objects, predictions of a continuous surface, and identification of discontinuities require different model formulations. If extensive knowledge about the phenomenon to be evaluated is available it should be used in the modelling. The scale at which the model is valid has to be specified. Consider a porous medium like sandstone; at micro scale a discrete spatial model based on pores and sand grains would be suitable, while on macro scale porosity could be represented by a continuous spatial model. The amount of available data will also influence the modelling. The problem of overfitting is well recognised in statistics, and in spatial–temporal settings the number of parameters is often large and one encounters redundancies in the data. This makes the problem even more crucial. Bayesian approaches with prior qualified guesses on parameter values based on phenomenological information will reduce the problems of overfitting. As previously mentioned, data analysis is often complex and efficient model estimators of known form are rarely available in spatial–temporal settings. Hence the possibilities for model verification and for interpretation of and estimation of parameters should be taken into consideration when choosing the statistical model.

Spatial problems appear with complex interdependence structures, and a large variety of spatial models can be imagined. In this presentation a broad division into three natural main model classes has been made, and this corresponds rougly to the three types of models most frequently encountered in spatial statistics literature. The division is into classes of well-defined mathematical objects, but is mainly motivated by the form of real spatial problems and by the form of the available data sources.

(i) *Models for continuous random surfaces*, say $\{Z(x): x \in D\}$ with $Z(x)$ in some m-dimensional Euclidian space. The model most frequently used is the Gaussian random function model, perhaps after an initial scale-transformation like taking logarithms. It maintains most of the favourable properties from non-spatial models when introducing higher dimensional spatial references. Typical tasks to be carried out include interpolation by estimated conditional expected value $E\{Z(x) \mid z(x_1), \ldots, z(x_n)\}$ and data-conditional simulation of $\{Z_{\text{sim}}(x): x \in D \mid z(x_1), \ldots, z(x_n)\}$.

(ii) *Models for mosaic phenomena*, say $\{L(x): x \in D\}$ with $L(x) \in \{1, \ldots, K\}$. The Markov random fields constitute the most popular class of models, but tesselation techniques are also used. These form an extremely large class of models and only small parts of their potential have been explored. Unfortunately, the nice mathematical properties found in the one-dimensional case are not maintained when higher-

dimensional spatial references are introduced. The lack of ordering causes this. Most applications include stochastic simulations, as a means in itself or as some intermediate block, with the Metropolis algorithm or Gibbs sampler providing ways of generating realisations.

(iii) *Models for events-against-background processes*, say $\{x_1, S_1), \ldots, (x_n, S_n)\}$, in which S_i is a set of attributes assigned to reference location x_i. The models most frequently used are related to the theory of marked point processes. An example could be a simultaneous model for locations and heights of trees in a forest. This model can also be defined in a general manner, but usually only pairwise dependencies of marked points are modelled. Few exact analytical results are available for processes outside the simpler Poisson type ones. Statistical analysis of this type of model is typically carried out through simulation using variations of Ripley–Kelly's spatial birth-and-death algorithm.

1.4. The present article

The material is organised as follows. Section 2 presents a generous list of application examples, sorted into problem areas. The emphasis is on describing problems and modelling ideas, and is not on "solutions". The applications have been chosen from a much longer list of projects we have worked on, with fellow statisticians at the Norwegian Computing Centre and surroundings and with clients. We have strived to represent the most important dimensions in this high-dimensional space of all spatial statistics applications. We have partly been guided by the degree of problem-solving success as criterion but also by the methodologically inclined statistician's view of what constitute interesting models and interesting problems. One of our aims is to show to the statistical community the kind of statistical problems that are currently deemed important to user groups. The application examples presented come from projects that are actually paid for by clients. Judging the usefulness of applied statistical models, methods and expertise by the willingness of users to spend money on them is not an uninteresting yardstick.

Section 3 presents basic methodology, introduces the most useful stochastic models, and discusses ways of analysing them. In particular models for the three main types of phenomena noted above are discussed, as well as a couple of "combinations" where two different models work together. Four of section 2's list of applications are returned to in section 4 for a more complete and more careful treatment, and suggested solutions to the actual real problems are described. Finally section 5 gives some concluding remarks and points to some topics for future work.

This is partly a review of several topics in spatial statistics with a broad range of examples. Some basic references about models in and uses of spatial statistics include Matérn (1960), Yaglom (1962), Matheron (1965), Journel & Huijbregts (1978), Diggle (1983), Ripley (1981, 1988), Stoyan *et al.* (1987), Cressie (1991), and Walden & Guttorp (1992). For the convenience of some readers we point out here what are supposed to be "new contributions", or perhaps only modest new insights into the use of old methods, in our article: the extended "conjugate family" analysis for Bayesian Kriging in section 3.1.3; some new reliable simulation methods for Gaussian surfaces in section 3.1.4; the quasi-likelihood method in section 3.1.5 for estimating covariance function parameters; comparison of maximum likelihood and maximum pseudo-likelihood for Markov chains in section 3.2.2; the semi-Markov type random field models of section 3.2.5; the ways of imposing global constraints on realisations from Markov random fields and marked point processes in sections 3.2 and 3.4 respectively; and generalisations of Geman and Geman

and of Besag methods in image restoration problems with correlated noise, in section 3.4. In addition we hope that the ways by which we approach and solve some of the real world problems in sections 2 and 4 contain some novel ideas in the respective problem areas.

2. Range of applications

In the following a collection of application examples are briefly described. Four of these are returned to in section 4 for a more complete treatment, leading to suggested solutions to the actual real problems.

2.1. *Medical image analysis*

2.1.1. *Tumor identification* (Lundervold *et al.*, 1988)

Identification and classification of tumors in the human brain is obviously a problem of great importance. Magnetic resonance equipment provides the possibility for indirect measurement of various characteristics of the brain with three-dimensional spatial references. The data can be collected without surgery, hence minimising the chance of complications. The observations are indirect and the signal to noise ratio is low. A model based on hidden Markov random field theory with Gaussian noise is often used for segmenting the three-dimensional brain into various pathological units. The pathological units are modelled by requiring $p(X_{ij} = k \mid \text{rest of image})$ to depend upon units in the 5×5 neighbourhood of pixel (i, j) only. Here X_{ij} denotes pathological unit type at pixel (i, j). The noise component is usually of the white noise type, or it may be spatially auto-correlated within some neighbourhood. See sections 3.2 and 3.4. Usually no direct observations will be available, which means that unsupervised classification of the units must be made. Spatial models are required because of the areal extent of the pathological units and the spatially correlated noise.

Experiences with medical image analysis have so far been encouraging, and the methods will hopefully be in commercial use in the near future. From a statistical point of view the traditional Markov random field theory has several shortcomings as a model for the pathological units. The problem surfaces in changes of scale and in parameter estimation, where good estimators for model parameters are hard to construct. Further studies of other models that are more directly suitable for segmentation are needed.

2.1.2. *Identification of heart dysfunction* (Taxt *et al.*, 1990; Storvik & Switzer, 1992)

Heart defects may appear as reduction in pumping capacity, reduced volume pumped, and as decline in elasticity of the heart walls. The dynamic behaviour of the heart can be observed by repeated three-dimensional grey-tone ultra-sound images at 25–35 Hz. The signal-to-noise ratio in each image is normally very poor, hence the time repetitions must be utilised. See section 4.2 for further discussion.

2.1.3. *Noise reduction in nuclear magnetic resonance imaging* (Godtliebsen, 1989)

The common technique for reducing noise in NMR images is to take several measurements on the same slice and then average. This is time-consuming and expensive, and the patients sometimes move during acquisition time, thereby introducing additional noise. Hence a natural challenge is to devise statistical noise reduction algorithms that work on a single slice. One approach is to model the observed image as $y_i = x_i + \varepsilon_i$ in pixel i, where the collection

of x_is come from some Markov random field and the ε_is are independent Gaussian zero mean noise. Studies indicate that the latter assumption is quite acceptable. The Markov random field assumption is less realistic, but can be used to derive image enhancement and image noise reduction techniques. Examples of such methods are in section 3.4. Another method which can be motivated by the model assumptions is to replace observed grey level in a pixel with some weighted average of grey levels over the pixel and neighbouring pixels, with weights determined by the spread of the local data. This can be done in a suitable empirical Bayesian fashion. The study found that sound statistical techniques were able to reduce noise in a single picture with a factor of about three. This particular study was unusual in that a good approximation to the "true scene" was available, taken to be the average of eight consecutive images of the same slice. Accordingly measures of restoration performance could be proposed and compared for different image analysis methods.

2.2. *Pollution monitoring*

2.2.1. *Status of forest* (Strand, 1989)

The decline in the quality of forest may be linked to increased pollution, and the Norwegian authorities have initiated an extensive sampling programme. Sampling takes place in more than 2000 sites in a regular $9 \times 9\,\text{km}^2$ grid over Norway every second year. Each site is $100\,\text{m}^2$ and each tree is located and characteristics such as age, size and top density are sampled. The general environment at each site is also carefully sampled. A spatial regression model is used to analyse the data, see section 3.1. The model is $S(x) = \Sigma_{i=1}^{p} \beta_i f_i(x) + \varepsilon(x)$, where $S(x)$ is some variable representing status of forest and the $f_i(x)$s are known explanatory regressor functions such as elevation, soil quality etc. The residuals $\varepsilon(x)$ are treated as a random function and its regional properties are evaluated in order to find differences due to unexplained factors, which could include air pollution. The data analysis exposes reasonably large regional differences, which at this stage are believed to be linked to pollution level. An extended analysis is planned.

2.2.2. *Air quality* (Halvorsen & Strand, 1987; Høst *et al.*, 1994)

The decline in air quality over Europe is a problem of concern. There are several sources for the pollution, which is transported over long distances. Its solution calls for international cooperation. The European Meteorological Environment Programme has established more than one hundred monitoring stations all over Europe. The air quality is characterised by the volume content of several chemical components, particle density, etc. Sampling is made on a daily basis. Consequently the pollution monitoring can be considered as a time- and space problem, and one approach for evaluation of the problem is further discussed in section 4.4.

2.2.3. *Combining satellite data with field data in pollution monitoring* (Høst *et al.*, 1989)

Some water quality variables from the Hvaler area in Norway have been analysed on the basis of both hard-to-get direct measurements and easy-to-get satellite data. The satellite data are abundant but of course very "indirect", having a small positive correlation with the water quality variables. The challenge is to build a model that makes it possible to integrate these very different data types. On the basis of a validated model a map of the estimated water quality was produced, along with a map of the estimated uncertainty of the estimate.

2.3. Reservoir characterisation

2.3.1. *Seismic depth conversion* (Omre *et al.*, 1989; Abrahamsen *et al.*, 1991; Abrahamsen, 1993)

Petroleum is usually trapped under a geologic horizon having non-permeable characteristics, for example shale. Fortunately, these types of horizons can also be identified from seismic data. The seismic data have good spatial coverage and consist of two-way reflection times down to the horizon. Note that the unit here is time, while the geologists are interested in depth to the horizon. By using depth observations in a small number of wells, seismic reflection time data and basic laws of physics, a model for depth conversion can be constructed. This is further discussed in section 4.1.

2.3.2. *Simulation of facies architecture* (Clemetsen *et al.*, 1989; Hjort *et al.*, 1989; Høiberg *et al.*, 1990, 1992; Omre, 1992; Georgsen & Omre, 1993; Tjelmeland & Holden, 1993)

The petroleum reservoirs in the North Sea appear as heterogeneous in the sense that several units of good and poor quality are packed. The units usually correspond to different rock types of facies. Their packing is according to certain geologic processes. The heterogeneity in the reservoirs has proven to have large impact on the production potential.

The facies architecture is a consequence of the geologic processes, the dynamics of which are partly understood by the geologists. This constitutes the primary base for the modelling. The facies distribution can be observed in the wells, and this provides constraints on the model. Both Markov random fields and marked point processes have been used in modelling the facies architecture, see sections 3.2 and 3.3. The former model postulates that $p(X_{ij} = k \mid \text{all other facies})$ is only dependent upon the neighbourhood facies, with X_{ij} facies type in pixel location (i, j) and $k \in \{1, \ldots, K\}$ facies type. Sometimes there are as many as $K = 12$ facies types on the scene. Simulations of pseudo-reality constrained by some known values of x_{kl} are required. Simulation procedures from recent literature seem to converge very slowly, and exploring their properties is a difficult and time-consuming task. The marked point process traditionally applied has density of the form $f_n(m_1, \ldots, m_n) = \text{const} \exp\{\Sigma_{i=1}^n b(m_i) - \Sigma_{i<j} c(m_i, m_j)\}$, with m_is being the marked points with information on location, size, shape, and facies characteristics. Often global constraints are necessary, and simulated realisations are pushed in the wished-for direction by certain tricks. New model formations of the "semi-Markov" process type have also been studied and seem promising. In order to evaluate the impact of the heterogenity on the production of petroleum, simulations of fluid flow are performed on realisations of the facies architecture.

2.3.3. *Simulation of fractures and faults* (Omre *et al.*, 1992a, b)

The petroleum reservoirs in the North Sea are of sedimentary origin, and they have been changed by considerable tectonic activity. This has forced a complicated fracture and fault pattern on to the reservoirs. The location of large fault zones, i.e. those with offset above 10 m, can be observed on the seismic data. The actual break pattern in the zone has been studied by geologists and is found to consist of swarms of smaller faults. This heterogeneity is important for fluid flow. A more thorough presentation of the problem and model appears in section 4.3.

2.3.4. Interpretation of well log data (Bølviken & Helgeland, 1989; Bølviken *et al.*, 1991; Bølviken, 1993)

The petroleum reservoirs in the North Sea are located at a depth of approximately 3000 m. Wells are drilled to penetrate the reservoir in order to collect information about its characteristics. Few direct observations are available even in the wells. Logging tools are lowered down the well, however, and indirect measurements of radioactivity, acoustic reflection, conductivity etc. are collected every 0.25 m in the reservoir zone. From these data the geologists would like to infer the geologic environment from which the reservoir originates. This entails determining the geologic sequences or sequence of rock types down the wells. The problem can be considered as a spatial segmentation problem based on multivariate data from the log tools.

The model is based on hidden and in fact even on hidden hidden Markov random processes with Gaussian noise, see sections 3.1 and 3.4. There are three ordered stages in the evaluation, say $S \to L \to X$, with sedimentary processes S creating a sequence of lithofacies L which again influence the responses of the logs X. The cornerstone in the model used is that the unobservable part (S, L) has been generated by a Markov process while L can be observed with white Gaussian noise through X. The geological processes make some sequences more probable *a priori* than others, therefore adding a Bayesian dimension to the model. A general model has been constructed and is expected to be widely applicable, but the set of parameters must be estimated for each reservoir.

2.4. Sea resources

2.4.1. Stock of capelin (Hjort & Murray, 1912; Hjort, 1914; Omre & Sølna, 1991a, b)

The fisheries in Norway are important for employment in the western and northern parts of the country and for the national export volume. The fish resources are renewable, but the reproduction cycle varies among the species. For capelin it is approximately four years in the Barent Sea. While capelin is a consumer of low level organisms such as plankton, it is predated by cod in the winter season. The migration of capelin south to the Norwegian coast for spawning in winter causes the contact with cod. Both capelin and cod are of commercial value, hence a multi-species catching strategy is required.

There are surprising amounts of data available. Acoustic data, indirectly observing the echo-sounding reflected by fish with a three-dimensional reference, are abundant. There are trawl samples as well. For several thousand capelin, multi-dimensional observations of age, length, weight, stadium, etc. with space–time references are available each year. For large amounts of cod, stomach content has been analysed with respect to fraction and volume of capelin. Presently only single-species models are operable, and time is the only reference variable. Multi-species models between capelin and cod are being developed, and both time and space references are discussed. It is at present problematic to verify a significant interaction between the two species based on available observations. A reliable space–time model for the species would compensate for some of the time and space variability, and may contribute to a more reliable analysis. Work is in progress on such matters.

2.4.2. Stock of Minke whale (Hjort & Murray, 1912; Schweder *et al.*, 1990; Schweder & Høst, 1991)

Minke whales are considered an endangered species and have been protected by the International Whaling Commission since 1986. The Norwegian authorities have during the last few years performed surveys in order to estimate the size of the stock. "Official

estimates" have been surprisingly low compared to historical catch successes. A serious downward bias is expected in the predictions since these have been based on the assumption of complete sampling in the surveyed areas. Due to the fact that each whale surfaces only about 30 times per hour and that they can be difficult to detect in rough sea, the actual detection success rate for whales passing close to the survey vessel, $g(0)$, is probably significantly smaller than 1.

There are two stochastic elements in the final estimator of the population size. One is the hazard probability $Q(x, r)$, the probability of sighting a whale surfacing at polar coordinates (x, r) relative to the vessel, given that the whale has not been observed before. The parametric form of $Q(x, r)$ is a subject of continued discussion. Its parameters can be estimated from data provided by test surveys where two vessels were run in parallel and covered the same area. The second random element is the surfacing frequency for whales. This has been reproduced by simulation from a spatial Poisson process. From this model the sampling success rate $g(0)$ was found to be approximately 0.5, which means that about one out of two whales were observed. Thus the predicted number of whales is about twice as large as first anticipated.

Methods developed here are partly of a general nature, and aim at being able to integrate very different types of data (viz. "micro" and "macro" data) in a consistent and meaningful framework. They should find applications in other areas as well.

2.5. *Other areas of application*

2.5.1. *Mapping of seabed: spatial sampling strategy to find all shallow areas* (Helgeland *et al.*, 1984)

Let $Z(x)$ be depth to the seabed in geographical location x. Mapping of $Z(x)$ based on point sampling is another problem of spatial interpolation, see section 3.1. Suppose however that it is considered important to find all shallow banks, say where $Z(x)$ is smaller than some level u. Term sets of the type $\{x: Z(x) < u\}$ by Z_u-areas. A question of spatial sampling strategy is therefore: what is a good regime for detecting all Z_u-areas, and what is the probability of not detecting such an area? A solution based on approximate shapes of excursion sets for Gaussian random fields is given in the above reference.

2.5.2. *Automatic recognition of handwritten symbols* (Hjort, 1986; Hjort & Taxt, 1988; Pripp, 1990)

Automatic recognition of printed or handwritten symbols is an established field with several well-explored approaches. Among these are several which are statistical in nature. The usual method comprises two main steps. The first is to extract a feature vector for the symbols, typically of dimension 10 or less. The second is to model the behaviour of feature vectors for each symbol type, and then estimate parameters, perhaps in cheap semi-automatic ways. Finally statistical discriminant anlaysis is used on future symbols.

A more direct approach would be to model the statistical behaviour of the symbols themselves. We have some experience with modelling the boundaries of symbols as random closed curves in the plane, giving rather successful rates of correct classification. This is perhaps not a genuine spatial example since we merely model one-dimensional objects. But the following approach is spatial. Suppose the candidate symbol is digitised to form 0s and 1s on a rectangular grid. Thus a hand-drawn "8" could be digitised on a 20×20 grid and be represented by the resulting collection of 4000 0s and 1s. Then a possibility is to model the mosaic process of 1s on this lattice as a Markov random field, see section 3.2. Each

symbol class (say a hand-written "8") has its own mrf specification of the conditional probability of having a "1" in pixel location (i, j), given the rest of the image. It is of a certain form involving various "award functions" designated by the modeller to encourage or disencourage certain types of local behaviour, and various parameters, some of which may be class-dependent and may vary over the scene. It is sometimes fruitful to impose global constraints too. The mrf parameters can be estimated from data by maximising the product of individual pseudo-likelihoods, see section 3.2. Finally the estimated models are used to construct a classifier.

2.5.3. Meteorology: combining new satellite data with other information sources to improve prognoses (Homleid, 1992)

The Norwegian Institute of Meteorology uses two numerical weather prognosis models for the atmosphere. Input data for such models are observations from ships, radio buoys and sondes, and land-based stations. One is also interested in exploiting satellite data, for example temperature and humidity profiles processed from the TOVS satellite, to build better models for prognosis. Several methods have been tried out but so far the results are not convincingly better. Better ways of combining these very different data sources are currently being explored. The task seems to require (i) simply assessing the current data quality from the satellite, (ii) constructing a successful spatial–temporal statistical model, drawing on both meteorology physics and empirical statistics, (iii) estimating necessary parameters and implementing prognosis formulas, and (iv) evaluating the performance compared to existing methods. Although satellite data obviously add important information to the problem, the improvements in prognosis quality by their inclusion seems to be rather small with the existing prognosis techniques. Research that aims at refining the statistical model formulations, and at a better statistical understanding of why the current improvements are so small, is under way.

3. Theoretical tools

This section presents basic statistical theory that has been developed to solve problems like those listed in section 2. As mentioned above a fruitful division of the various stochastic processes encountered is into continuous random surfaces, finitely-valued or mosaic phenomena, and events-against-background processes. Subsections 1, 2 and 3 study these three basic types. In many problems different data sources may have to be combined, and some combination or other of the three basic model types is called for. Some situations of this sort are discussed in section 3.4.

3.1. Continuous random surfaces

The simplest spatial statistical model capable of describing interesting continuous or near continuous random surfaces is one with some smooth trend surface plus a spatially correlated Gaussian residual process. This model is introduced in section 3.1.1 below. Various aspects of such models are discussed, including theory for spatial interpolation, Bayesian Kriging, simulation, and for estimating parameters in spatial covariance functions.

3.1.1. The basic model

Let $z = z(x)$ be a continuous or nearly continuous surface defined over some domain D of x-values, for example a rectangle in the plane. Suppose $z(x_i)$-data on $z(\cdot)$ are collected in n

distinct locations $x_1, \ldots, x_n$, and that some problem of interest can be phrased in terms of $z(\cdot)$, like that of spatial interpolation. The spatial statistical way of approaching such problems is to view $z(\cdot)$ as a realisation of a stochastic process $Z(\cdot)$. The idea is to translate prior knowledge to a suitable class of models for $Z(\cdot)$, typically viewed as a smooth trend surface plus spatially correlated residual, use data to estimate parameters, and answer the original $z(\cdot)$-question under the model assumption and given all available information. To be specific, suppose that $Z(\cdot)$ is Gaussian with regression type trend surface plus zero mean Gaussian residual, say

$$Z(x) = m(x, \beta) + \varepsilon(x) = \sum_{j=1}^{p} \beta_j f_j(x) + \varepsilon(x). \tag{3.1}$$

Here the $f_j(x)$s are known regressor functions ($f_1(x)$ would typically be the constant 1), the β_js are coefficient parameters, and the covariance function

$$\operatorname{cov}\{Z(x), Z(y)\} = \operatorname{cov}\{\varepsilon(x), \varepsilon(y)\} = \sigma^2 K(x, y) \tag{3.2}$$

describes the variability and the degree of spatial continuity of the residual process. One often postulates shift invariance, so that $K(x, y)$ is of the form $K_0(x - y)$ for appropriate $K_0(\cdot)$ function, and in such cases it is convenient to choose $K(x, x) = K_0(0) = 1$ so that $\operatorname{var} Z(x) = \sigma^2$. The random function is isotropic if in addition $K(x, y)$ only depends on the distance $\|x - y\|$, as in the popular case $K(x, y) = \exp\{-c\|x - y\|\}$.

At this point it is worth noting that the covariance function is only defined when $Z(x)$ has finite variance. A richer class of measures for second order spatial characteristics is the so-called semi-variogram

$$\gamma(x, y) = \tfrac{1}{2} \operatorname{var}\{Z(x) - Z(y)\}, \tag{3.3}$$

which requires only the variances of differences to be finite. When K is shift invariant and $\operatorname{var} Z(x) = \sigma^2 < \infty$ one has $\gamma(x, y) = \sigma^2\{1 - K(x, y)\}$. The idea of and value of requiring finite variances of only certain linear combinations of $Z(\cdot)$ is developed in the theory of intrinsic random functions, see remarks at the end of the following section. The possible choices for semi-variogram functions are linked to the choice of p and $f_j(x)$s together with the requirement of producing non-negative prediction variances; see also remarks below. We have chosen to present most of the general Gaussian random function theory in terms of spatial covariance functions.

3.1.2. Spatial interpolation by universal Kriging, and its precision

Suppose interpolation is called for. Let x be a new location point, and let us follow the programme above. Under the Gaussian assumption

$$\begin{pmatrix} Z(x) \\ Z_{\text{dat}} \end{pmatrix} \sim \mathcal{N}_{n+1}\left\{\begin{pmatrix} f(x)'\beta \\ F\beta \end{pmatrix}, \sigma^2\begin{pmatrix} K(x, x) & k' \\ k & K \end{pmatrix}\right\},$$

in which K is the $n \times n$ matrix of $K(x_i, x_j)$, k and Z_{dat} are the vectors with components respectively $K(x, x_i)$ and $Z(x_i)$, and finally F is the $n \times p$ matrix whose ith row is $f(x_i)' = (f_1(x_i), \ldots, f_p(x_i))$. Hence

$$Z(x) \mid \text{data} \sim \mathcal{N}\{m(x, \beta) + k'K^{-1}(Z_{\text{dat}} - m(\beta)), \sigma^2(K(x, x) - k'K^{-1}k)\},$$

writing $m(\beta)$ for the vector of $m(x_i, \beta)$. Of course $m(\beta) = F\beta$ in the present case, but the notation is meant to suggest its natural generalisation to other regression functions.

Specification and estimation of $K(\cdot, \cdot)$ is discussed in section 3.1.5 below. Suppose for now that a covariance function has been decided on. The natural estimator of β then emerges by minimising $(Z_{\text{dat}} - F\beta)'K^{-1}(Z_{\text{dat}} - F\beta)$. This is the weighted least squares as well as the maximum likelihood principle, when the covariance function is assumed known. The result is

$$\hat{\beta} = HF'K^{-1}Z_{\text{dat}} \quad \text{where } H = (F'K^{-1}F)^{-1},$$

constituting an unbiased estimator with covariance matrix $\sigma^2 H$. The spatial interpolator used in the end is the estimated mean value of $Z(x)$ given the data, that is

$$\hat{Z}(x) = m(x, \hat{\beta}) + k'K^{-1}(Z_{\text{dat}} - m(\hat{\beta})) = f(x)'\hat{\beta} + k'K^{-1}(Z_{\text{dat}} - F\hat{\beta}). \tag{3.4}$$

Note that it is an unbiased predictor in the sense of having $E\{\hat{Z}(x) - Z(x)\} = 0$. The interpolation variance, or prediction error, can be shown to be

$$\begin{aligned}\sigma_{\text{pe}}(x)^2 &= E\{\hat{Z}(x) - Z(x)\}^2 \\ &= \sigma^2[K(x, x) - k'K^{-1}k + (f(x) - F'K^{-1}k)'H(f(x) - F'K^{-1}k)].\end{aligned} \tag{3.5}$$

Note that the mean squared error is computed w.r.t. (the random) $Z(x)$ and not its mean value $f(x)'\beta$, since the intention is to guess $Z(x)$ for the surface under study and not its trend surface. In particular $\sigma_{\text{pe}}(x)^2$ is not the same as $\text{var}\,\hat{Z}(x)$.

The interpolator (3.4) is itself independent of the scale factor σ^2, which however is needed to assess the uncertainty as in (3.5). To estimate σ^2, when some covariance structure $K(\cdot)$ has been decided on, note that $Z_{\text{dat}} - F\hat{\beta}$ has variance matrix $\sigma^2(K - FHF')$, from which it follows that $Q(\hat{\beta}) = (Z_{\text{dat}} - F\hat{\beta})'K^{-1}(Z_{\text{dat}} - F\hat{\beta})$ has mean value equal to σ^2 times the trace of $K^{-1}(K - FHF')$, which is $\text{tr}\,(I_n - HF'K^{-1}F) = \text{tr}\,(I_n - I_p) = n - p$ by the usual tricks. Thus $Q(\hat{\beta})/(n-p)$ is unbiased, even in the present setting with correlated data. The maximum likelihood solution, trusting normality, is $\hat{\sigma}^2 = Q(\hat{\beta})/n$. We should stress that σ^2 and $K(\cdot)$ are defined "together" and should be estimated together. Modelling and estimating $K(\cdot)$ is the harder task, see section 3.1.5 below; σ can be estimated as just described for given $K(\cdot)$. It is also usual in geostatistics to estimate σ^2 by cross-validation techniques, see Davis (1973) and Solow (1990).

Spatial interpolation of a random function with drift can be considered from a somewhat different perspective as well, that of choosing an optimal linear combination, under different assumptions about spatial smoothness. Consider the interpolator $Z^*(x_0) = \Sigma_{i=1}^n c_i Z(x_i)$ at point $x = x_0$, where the weights c_i are to be determined. Unbiasedness, in the sense of $E\{Z^*(x_0) - Z(x_0)\} = 0$, is ensured by the constraints $\Sigma_{i=1}^n c_i f_j(x_i) = f_j(x_0)$ for $j = 1, \ldots, p$. A natural avenue is to minimise the interpolation variance $\text{var}\,\{Z^*(x_0) - Z(x_0)\}$ under these constraints. This may be formulated as minimising $\text{var}\,\Sigma_{i=0}^n c_i Z(x_i)$ under $\Sigma_{i=0}^n c_i f_j(x_i) = 0$, $j = 1, \ldots, p$, where $c_0 = -1$, and the task is solved by the Lagrange technique. The result is in fact $\hat{Z}(x)$ of (3.4), and this Lagrangian way of deriving it is the usual one in the geostatistics tradition. It is called the universal Kriging interpolator, see for example Journel & Huijbregts (1978). Note that the Gaussian assumption, which was used to reach (3.4), is unnecessary in this construction.

One sometimes uses (3.4), in that form or computed by constrained minimisation, with $K(x, y)$ functions that are not genuine non-negative definite covariance functions. The minimum requirements on the K functions for guaranteeing non-negative interpolation variances are that

$$\text{var} \sum_{i=0}^n c_i Z(x_i) = \sum_{i=0}^n \sum_{l=0}^n c_i c_l K(x_i - x_l) = \begin{pmatrix} -1 \\ c \end{pmatrix}' \begin{pmatrix} 1 & k' \\ k & K \end{pmatrix} \begin{pmatrix} -1 \\ c \end{pmatrix} \geq 0$$

for all $x_0, x_1, \ldots, x_n$ and all $c_1, \ldots, c_n$ satisfying the $\Sigma_{i=0}^n c_i f_j(x_i) = 0$ constraints above. It is assumed here that $K(x, y) = K(x - y)$.

Consider cases for which $f_1(x)$ is the constant 1, i.e. the trend surface contains a constant β_1, and $\Sigma_{i=1}^n c_i = 1$ among other constraints. Non-negative interpolation variances are ensured by $c'Kc \geqslant 0$ for all c vectors obeying certain constraints, where K is the matrix of $K(x_i - x_j)$. In terms of the semi-variogram function (3.3) the criterion becomes $c'\Gamma c \leqslant 0$ with constraints on c, where Γ is the matrix of $\gamma(x_i - x_j)$.

Assume in particular that the regressor functions $f_j(x)$ are polynomials in the coordinates of x, of order k or less. The random functions having this property are called "generalised intrinsic functions of order k", and the associated function $K(\cdot)$ is termed a "generalised covariance function of order k". It is clear that this class of generalised covariance functions is larger than the class of simply non-negative definite functions.

By enforcing stronger assumptions on the form of the expected value one can choose among a larger class of generalised covariance functions. This approach to spatial interpolation is widely used in the geostatistics school, see Matheron (1973). It resembles the "integration approach" used in time series analysis, see Box & Jenkins (1976). It can be shown, however, that interpolations based on assumptions of intrinsic random function hypotheses, of any given order k, are equivalent to those obtained from an appropriate universal Kriging with a Gaussian random function model, see Christensen (1990).

Remark 1. A sound implementation is vital here, since inverting large matrices can be slow and unstable if done directly. Rather than using the mathematically and statistically informative (3.4) and (3.5) a good interpolation package would typically use derived formulae from Choleski triangularisation, see for example Ripley (1981, sect. 4.4). □

Remark 2. One valid variogram function, among others, is $\gamma(h) = \sigma^2 h^{2H}$, where $0 \leqslant H < 1$. This family of variogram functions is said to have affine similarity properties and is used to model fractal phenomena, see for example Feder (1988). The H constant is called the Hurst exponent. The Brownian motion process in one dimension is of this type, with $H = 1/2$. □

Remark 3. Note that $\hat{Z}(x_i) = z(x_i)$ and $\sigma^2_{\text{pe}}(x_i) = 0$, that is, the interpolator respects the data points. This is as it should be, since the real interest is interpolation of the actual $z(\cdot)$, rather than its underlying trend surface. In applications of classical non-parametric regression the problem is typically the opposite one of estimating the smooth trend, based on unrelated realisations at different locations. □

Remark 4. In locations x far from all sampled x_is the interpolator is close to the trend estimate $m(x, \hat{\beta})$. □

Remark 5. More robust estimates than the least squares $\hat{\beta}$ could be used as well, without seriously affecting the reasoning or the results. Our arguments can similarly be generalised to cover non-linear models for $m(x, \beta)$, like $\exp(\beta' x)$, without much difficulty. □

Remark 6. The geostatistical Kriging techniques have been extended to cover multivariate cases, see for example the so-called co-Kriging method of Journel & Huijbregts (1978). Another extension is called factorial Kriging, see Sandjivy (1984), consisting in separating a random function into a smoothly varying trend and a correlated residual term. □

Remark 7. The term Kriging was originally used for linear predictors, i.e. linear in the data points $Z(x_i)$. A couple of non-linear predictors have also adopted the Kriging name,

however. Disjunctive Kriging is based on a Hermitean expansion of the bivariate characteristics of the random function, thereby extending the familiar correlation framework, see Matheron (1976). Indicator Kriging is based on a discretisation of the univariate variable into a set of linear combinations of indicator variables, hence providing estimates of the quantiles of the conditional distribution, see Journel (1983) and Isaaks & Srivastava (1989). □

Remark 8. Markovian properties of Gaussian random functions in the one-dimensional case are easily defined and well understood. There are unexpected difficulties with the different possible definitions of Markov-ness in higher dimensions, however, and some of these lead to too restricted classes. See Adler (1981, app) for a review. □

3.1.3. Bayesian Kriging

In some situations there is rather too little data to do interpolation as above with the wished for precision, but there is some prior knowledge about the trend surface. This invites Bayesian and empirical Bayesian considerations. The following treatment partly extends that of Omre (1987) and Omre & Halvorsen (1989). Other relevant references are Pilz (1991) and Le & Zidek (1992).

Let the model be as in (3.1) and (3.2) conditionally on β, and suppose β is given some Gaussian prior distribution, which we parameterise as $\mathcal{N}_p\{\beta_0, \sigma^2 T\}$. For the moment we take σ^2 to be known. The joint distribution of β and data Z_{dat} is easily found to be

$$\begin{pmatrix} \beta \\ Z_{\text{dat}} \end{pmatrix} \sim \mathcal{N}_{p+n}\left\{\begin{pmatrix} \beta_0 \\ F\beta_0 \end{pmatrix}, \sigma^2\begin{pmatrix} T & TF' \\ FT & K + FTF' \end{pmatrix}\right\}.$$

In particular the posterior distribution of β is still normal. After using the convenient matrix identity $(K + FTF')^{-1} = K^{-1} - K^{-1}FG_TF'K^{-1}$, where $G_T = (H^{-1} + T^{-1})^{-1}$, one finds

$$\begin{aligned} \tilde{\beta} &= E\{\beta \mid \text{data}\} = \beta_0 + TF'(K + FTF')^{-1}(Z_{\text{dat}} - F\beta_0) = G_TH^{-1}\hat{\beta} + (I - G_TH^{-1})\beta_0, \\ \text{var}\{\beta \mid \text{data}\} &= \sigma^2\{T - TF'(K + FTF')^{-1}FT\} = \sigma^2(I - G_TH^{-1})T. \end{aligned} \tag{3.6}$$

Note that the Bayes estimator $\tilde{\beta}$ is a combination of the prior guess β_0 and the usual estimate $\hat{\beta}$. Note also that in the case of a flat prior, which corresponds to moving the elements of T so that its eigenvalues tend to infinity, then $G_TH^{-1} \doteq I - HT^{-1}$, in particular G_T tends to H, β tends to $\hat{\beta}$, and var $\{\beta \mid \text{data}\}$ becomes σ^2H.

This is information of value, but the imminent interest is interpolation and its uncertainty. We find

$$\begin{pmatrix} Z(x) \\ Z_{\text{dat}} \end{pmatrix} \sim \mathcal{N}_{n+1}\left\{\begin{pmatrix} f(x)'\beta_0 \\ F\beta_0 \end{pmatrix}, \sigma^2\begin{pmatrix} K(x,x) + f(x)'Tf(x), & (k + FTf(x))' \\ k + FTf(x), & K + FTF' \end{pmatrix}\right\}.$$

Our Bayesian Kriger becomes

$$\begin{aligned} \hat{Z}_B(x) &= E\{Z(x) \mid \text{data}\} = f(x)'\beta_0 + (k + FTf(x))'(K + FTF')^{-1}(Z_{\text{dat}} - F\beta_0) \\ &= f(x)'\tilde{\beta} + k'K^{-1}(Z_{\text{dat}} - F\tilde{\beta}), \end{aligned} \tag{3.7}$$

with associated Bayesian prediction error

$$\begin{aligned} \sigma_{\text{be}}(x)^2 &= E\{\hat{Z}_B(x) - Z(x)^2 \mid \text{data}\} = \text{var}\{Z(x) \mid \text{data}\} \\ &= \sigma^2[K(x,x) + f(x)'Tf(x) - (k + FTf(x))'(K + FTF')^{-1}(k + FTf(x))]. \end{aligned} \tag{3.8}$$

Again there is a natural correspondence for a flat prior, in that the Bayesian interpolator converges to $\hat{Z}(x)$ when the covariance matrix T for the β prior tends to infinity, and $\sigma_{\text{be}}(x)$ tends to $\sigma_{\text{pe}}(x)$. More informatively, calculations show that

$$\hat{Z}_B(x) = \hat{Z}(x) - (f(x) - F'K^{-1}k)'(I - G_T H^{-1})(\hat{\beta} - \beta_0),$$

and $G_T H^{-1}$ is close to $I - HT^{-1}$ when T is large compared to H. This means that in situations where T is large (vague prior information) and/or $\hat{\beta}$ is close to β_0 (good prior guess) the Bayesian and the traditional viewpoints lead to the same quantitative results, regarding interpolator and prediction variance, but with two quite different perspectives. Many statisticians have learned from experience that users very often prefer and relate better to the Bayesian interpretation.

The case of $T = 0$ corresponds to certainty about trend surface $f(x)'\beta = f(x)'\beta_0$, and $\hat{Z}_B(x) = f(x)'\beta_0 + k'K^{-1}(Z_{\text{dat}} - F\beta_0)$ is as in so-called simple Kriging with known trend. The other extreme is when T is very large, corresponding to prior ignorance about β, where $\hat{Z}_B(x)$ becomes as in universal Kriging. There is accordingly a "Bayesian bridge" from simple to universal Kriging.

The Bayesian apparatus becomes more useful and flexible when uncertainty about the scale factor σ^2 is modelled as well. The mathematically simplest Bayesian solution is the following: Suppose the prior distribution for (σ^2, β) is such that $\sigma^2 \sim$ inverse gamma (α, γ) and $\beta \mid \sigma^2 \sim \mathcal{N}_p\{\beta_0, \sigma^2 T\}$, i.e.

$$(\sigma^2, \beta) \sim \text{const}\,(1/\sigma^2)^{\alpha+1} \exp(-\gamma/\sigma^2)\sigma^{-p} \exp\{-\tfrac{1}{2}(\beta - \beta_0)'T^{-1}(\beta - \beta_0)/\sigma^2\}.$$

Then calculations show that (σ^2, β) given data Z_{dat} is exactly of the same type, but with updated parameters:

$$(\sigma^2, \beta) \mid \text{data} \sim \text{inverse gamma}\,(\tilde{\alpha}, \tilde{\gamma}) \times \mathcal{N}_p\{\tilde{\beta}, \sigma^2 G_T\}.$$

Here $\tilde{\alpha} = \alpha + \frac{1}{2}n$ and $\tilde{\gamma} = \gamma + \frac{1}{2}n\hat{\sigma}^2 + \frac{1}{2}(\hat{\beta} - \beta_0)L_T(\hat{\beta} - \beta_0)$, writing $\hat{\sigma}^2 = (Z_{\text{dat}} - F\hat{\beta})'K^{-1}(Z_{\text{dat}} - F_{\hat{\beta}})/n$ for the non-Bayesian estimator and $L_T = T^{-1}G_T H^{-1}$. In particular the Bayesian predictor is as in (3.7) above, and the Bayes estimate of σ^2 is

$$\tilde{\sigma}^2 = E\{\sigma^2 \mid \text{data}\} = \frac{\alpha - 1}{\alpha - 1 + n/2}\sigma_0^2 + \frac{n/2}{\alpha - 1 + n/2}\{\hat{\sigma}^2 + (\hat{\beta} - \beta_0)'L_T(\hat{\beta} - \beta_0)/n\},$$

where $\sigma_0^2 = E\sigma^2 = \gamma/(\alpha - 1)$ is the prior guess value. The Bayesian prediction error is as in (3.8) but with $\tilde{\sigma}^2$ replacing σ^2.

Once more the traditional methods emerge in the limiting case of vague Bayesian ignorance, which here corresponds to $\alpha \to 1$, $\gamma \to 0$, and $T \to \infty$.

3.1.4. *Simulation*

Suppose a simulated realisation $Z_s(\cdot)$ of a fully specified Gaussian random function is needed, perhaps conditioned on some observed values. First of all this means in practice that $Z_s(x)$ is to be simulated on some dense finite lattice of points only. Hence the problem seems simple, since textbooks on multivariate statistics give answers to such questions in terms of simple linear algebra. Such direct methods must involve matrix inversion, perhaps via Cholesky decomposition, and work well on good computers if the dimension of the problem is less than 3000. But in many spatial problems the grid net contains more than 10^6 points, and in such cases smarter simulation algorithms are called for.

One general approach to conditional simulation of the residual process $Z_r(x) = Z(x) - m(x, \beta)$, with associated residual observations $Z_r(x_i) = Z(x_i) - m(x_i, \beta)$ for $i = 1, \ldots, n$, is

by decomposition. Let $Z_r(x) = \hat{Z}_r(x) + \{Z_0(x) - \hat{Z}_0(x)\}$, with $\hat{Z}_r(\cdot)$ the simple Kriging predictor based on the observations, $Z_0(\cdot)$ an arbitrary random function with characteristics identical to $Z_r(x)$, and $\hat{Z}_0(x)$ the simple Kriging predictor based on $Z_0(x_i)$-data. From the orthogonality of $Z_r(\cdot)$ and $\hat{Z}_r(\cdot)$ it is easy to see that the decomposition is correct. Using this trick it suffices to simulate a random function with zero mean and covariance function $K(x, y)$ unconditionally.

The "turning band" procedure of Matheron (1973) provides a general tool for simulating random functions with a specified covariance structure. Several procedures working in the spectral domain are also available, see Ripley (1987, ch. 4).

Spatial and spatial–temporal problems often require simulation on extremely large grid nets, for which the procedures mentioned above will be too slow, even on very fast machines. In Omre *et al.* (1993) some very fast procedures for simulating random functions are presented and evaluated. The procedures use Markov characteristics valid in one dimension and generalise the idea to higher dimensions. The traditional procedures for simulation of fractal processes, see Feder (1988), are in the same spirit. The screening sequential procedure defined in Omre *et al.* (1993) is considerably more reliable than the traditional fractal procedures, however, albeit somewhat slower.

3.1.5. Estimating the covariance function

A point of some importance which has attracted renewed interest recently is that of the specification and estimation of the covariance function K. In the geostatistics tradition the K function has typically been regarded as "given and fixed" once "guessed at", which results in underestimation of interpolation variance, and, sometimes, suboptimal interpolation. Observe that the definition of and the interpretation of K and σ^2 in (3.2) are dependent upon the chosen regression surface model. If one adds a term to a previous regression trend, then K and σ^2 have changed meanings, and σ^2 will in fact tend to be smaller.

Consequences of using incorrect covariance functions have recently been studied by Watkins & Al-Boutiahi (1990) and Stein (1990a, b). Various methods for estimating parameters in such functions have been proposed, and a couple of these and a new one will be mentioned here.

Let us structure the problem somewhat and assume stationarity and isotropy, say $\sigma^2 K(x, y) = \sigma^2 R(\|x - y\|)$, identified by putting $R(0) = 1$, so that σ^2 is the variance of $Z(x)$ and $R(r)$ is the correlation between $Z(x)$ and $Z(y)$ whenever the locations are distance r apart. A non-parametric procedure which can be used with sufficient data is to group together all pairs of points with inter-distance in $(r - \delta, r + \delta)$, say, and estimate the covariance $R(r)$ based on these. This suggestion amounts to

$$\hat{\sigma}^2 \hat{R}(r) = \frac{\sum_{i,j} w(d_{ij})\{z(x_i) - m(x_i, \hat{\beta})\}\{z(x_j) - m(x_j, \hat{\beta})\}}{\sum_{i,j} w(d_{ij})}, \tag{3.9}$$

where the sums are over all $n(n-1)/2$ pairs, and $d_{ij} = \|x_i - x_j\|$ is the inter-distance between locations, but where $w(d)$ is 1 only for $d \in (r - \delta, r + \delta)$ and 0 outside. Somewhat more ambitiously a kernel type weighting of all pairs of data can be proposed. There are some difficulties with the direct use of estimators like (3.9), since one wants to ensure positive-definiteness of the covariance function to be used in Kriging. Therefore (3.9) type estimators are more often used as a means of deciding on some particular parameterised covariance function. Robustness issues are discussed in Omre (1984).

For parametric models $R(r) = R_0(r)$ there is an ongoing dispute over the merits of the mle. Maximising the likelihood over β gives $\hat\beta_\theta = (F'K_\theta^{-1}F)^{-1}F'K_\theta^{-1}Z_{\text{dat}}$, and then over σ gives $\hat\sigma_\theta^2 = Q_\theta/n$, where $Q_\theta = Q_\theta(\hat\beta_\theta) = (Z_{\text{dat}} - F\hat\beta_\theta)'K_\theta^{-1}(Z_{\text{dat}} - F\hat\beta_\theta)$. Here K_θ is the matrix of $R_\theta(d_{ij})$. The resulting profile likelihood must finally be maximised over θ. This amounts to minimising the rather intricate function

$$-\log L(\hat\beta_\theta, \hat\sigma_\theta, \theta) = \tfrac{1}{2}n \log (Q_\theta/n) + \tfrac{1}{2}\log \{\det (K_\theta)\} + \tfrac{1}{2}n. \tag{3.10}$$

There are first of all numerical problems associated with minimising this difficult and possibly multimodal function, and secondly it is not clear that using the maximum likelihood estimator should be a good choice *per se*. See the dispute of Mardia & Marshall (1984), Warnes & Ripley (1987), Ripley (1988, ch. 2), and Mardia & Watkins (1989). Other estimation methods have also been proposed, see Switzer (1984), Stein (1987), and Vecchia (1989). Pseudo-likelihood methods in the manner of Besag (1974) and Jensen & Møller (1991) can also be used.

Let us briefly describe yet another method, the maximum quasi-likelihood procedure of Hjort (1993). This is really a class of methods, and the simplest among them is the following: consider

$$\text{ql}(\beta, \sigma, \theta) = \prod_{i<j} g(z_i, z_j \mid d_{ij}, \beta, \sigma, \theta), \tag{3.11}$$

where the product is over all $N = n(n-1)/2$ pairs of distinct observations, and the g-term is the model-given probability density of $(Z(x_i), Z(x_j))$ for points lying distance d_{ij} apart. Maximising this is easily carried out, as indicated below, without numerical problems. Why is maximising ql a sensible procedure? Suppose $g(z, z' \mid r)$ is the *true* probability density for a pair $(Z(x), Z(x'))$ with inter-distance r. Divide the distance range $[0, \infty)$ into small intervals, and sort for each interval together those pairs in log ql that have inter-distance d_{ij} close to the corresponding distance, say r. An ergodic argument shows that

$$N^{-1}\log \text{ql}(\beta, \sigma, \theta) \doteq \int_0^\infty \left[\int\int g(z, z' \mid r) \log g(z, z' \mid r, \beta, \sigma, \theta)\, dz\, dz'\right] H(dr),$$

in which $H(dr)$ is the distribution of the distance $\|x - x'\|$ between a randomly drawn pair of points. Hence maximising ql aims at finding the parameter values that minimise the particular distance function

$$\Delta[g(\cdot,\cdot \mid \cdot), g(\cdot,\cdot \mid \cdot, \beta, \sigma, \theta)] = \int_0^\infty \Delta_r[g(\cdot,\cdot \mid r),\, g(\cdot,\cdot \mid r, \beta, \sigma, \theta)]\, dH(r),$$

in which the inner distance function between the true density g_r and the modelled density g_r^* for $(Z(x), Z(x'))$ is the Kullback–Leibler one, $\int\int g_r \log \{g_r/g_r^*\}\, dz\, dz'$. In particular the proposed maximum ql method leads to consistent parameter estimates under suitable mild regularity conditions, but we avoid here the precise definition of the asymptotic framework.

Let us see how this works out in the three-parameter model in which $Z(x) \sim \mathcal{N}\{\beta, \sigma^2\}$ and the covariance is $\sigma^2 R_\theta(r)$ for points lying distance r apart. As with the ordinary likelihood method the programme is to maximise w.r.t. β, then over σ, and finally over θ. This leads to the following, where we take the liberty of using the same notation as for the ml case above: let first $\hat\beta_\theta$ minimise

$$Q_\theta(\beta) = \sum_{i<j} \frac{1}{2}\frac{(z_i-\beta)^2 + (z_j-\beta)^2 - 2R_\theta(d_{ij})(z_i-\beta)(z_j-\beta)}{1 - R_\theta(d_{ij})^2},$$

indeed

$$\hat{\beta}_0 = \frac{\sum_{i<j} \frac{(z_i + z_j)/2}{1 + R_0(d_{ij})}}{\sum_{i<j} \frac{1}{1 + R_0(d_{ij})}}.$$

Then let $\hat{\sigma}_0^2 = Q_0(\hat{\beta}_0)/N = Q_0/N$. The remaining task is to minimise

$$-\log \text{ql}\,(\hat{\beta}_0, \hat{\sigma}_0, \theta) = N \log (Q_0/N) + \sum_{i<j} \tfrac{1}{2} \log \{1 - R_0(d_{ij})^2\} + N \tag{3.12}$$

w.r.t. θ, and this is much simpler than minimising (3.10).

There is a connection to the simple non-parametric correlation function estimator (3.9), in that if the particular model which postulates piece-wise constant $R(\cdot)$ is used, then the ql-solution can be shown to be close to (3.9), and the related quasi-likelihood which only uses data pairs with approximate distance r comes even closer.

The virtues of the ql method are that the numerical maximisation problem is much simpler than for the ordinary likelihood method, its relatively wide applicability, that its behaviour is better understood, and that it in fact behaves well. It does not claim to be optimal, and in the asymptotic framework where the region expands to produce nearly independent copies the ml is better. This framework is somewhat inappropriate, however.

Instead of using all pairs one could take the product over all $g(z_i, z_{m(i)} \mid d_i, \beta, \sigma, \theta)$ terms, where $z_{m(i)}$ is nearest neighbour to z_i, with interdistance d_i. Reasoning similar to above shows that this estimation procedure aims at minimising a different distance criterion from true model to parametric approximand, using the $H_0(dr)$ distribution for nearest neighbour distances instead of $H(dr)$ for an arbitrary distance. And there are several related alternative methods. The two procedures above care only about data-pairwise aspects of the model, and would not necessarily be good enough for prediction purposes, for example. One could with some additional efforts use three data points at a time, to fit the empirical three-point-sets distribution to the model. A fuller account is given in Hjort (1993).

The discussion above concerns the basic model of 3.1.1. More sophisticated models are sometimes used when there is enough data, and then appropriate generalisations of the covariance function estimators above are needed. In the growing area of environmental monitoring, for example, there are often abundant time series data in fixed geographical locations, which invites better ways of modelling residual variation. Covariance function modelling and estimation in such frameworks are discussed in Sampson & Guttorp (1992), Loader & Switzer (1992), and Høst *et al.* (1994). See section 4.4.

3.2. Mosaic processes

Here we describe processes that divide the reference space into a set of disjoint segments and assign a label to each segment. The Markov random fields (mrf), defined on regular lattices, are enjoying increasing popularity, though mixed with a widened understanding of the inherent limits and difficulties of the approach. The fundamental simulation scheme called the Metropolis algorithm is explained. Some recently developed amendments and alternative models, including constrained mrfs and semi-mrfs are then discussed. Finally a couple of non-lattice situations are considered.

3.2.1. Markov random fields

We are concerned with stochastic models for the distribution of classes on lattices. One class of such models is the class of mrfs. The following is a brief description of mrfs and some of the statistical properties of such models. We discuss how to estimate parameters of such models, based on an observed "true scene", and describe methods to simulate realisations of mrfs. One needs to be able to simulate both unconditionally and data-conditionally from a specified mrf. Global constraints that one sometimes needs to be able to impose on simulated scenes include preservation of information in some locations and the desire to keep frequencies of some or all classes near specified levels.

For a given lattice system of sites we first need to introduce the notion of a clique. Because of the strong association to image analysis we shall mainly think of the sites as picture elements, or pixels. Assume a system of neighbourhoods has been defined. Then define a clique Q as a set of pixels all of which are neighbours of each other. Note the sociological appropriateness of the term. If "neighbours" means nearest neighbours, not including the diagonal ones, then all cliques are of the type

$$\{(i,j),(i+1,j)\} = \begin{smallmatrix} * & * \end{smallmatrix} \quad \text{or} \quad \{(i,j),(i,j+1)\} = \begin{smallmatrix} * \\ * \end{smallmatrix}.$$

If also diagonal neighbours are included, so that each site has eight neighbours, then there are nine types of cliques:

$$\begin{smallmatrix} & * & & * & * & & * * & & * & & * & & * * \\ * * & & * & & * & & & * & & * * & & * * & \end{smallmatrix} \tag{3.13}$$

The mrf class of probability distributions, or Gibbs processes, are those that satisfy

$$p(\mathbf{x}) = p(x_1,\ldots,x_N) = \text{const} \exp\left[\sum_{i=1}^{N} \alpha_i(x_i) + \sum_{Q} V_Q(x_Q)\right]. \tag{3.14}$$

Here $\mathbf{x} = (x_1,\ldots,x_N)$ is a long vector of class labels, say among $\{1,\ldots,K\}$, in N sites or pixel locations; $V_Q(x_Q) = V_Q(x_{Q,1},\ldots,x_{Q,m(Q)})$ is the "potential" associated with clique Q; $\alpha_i(1),\ldots,\alpha_i(K)$ are class and position dependent parameters that can be tied to the prior probabilities for the various classes; and the sum is over all cliques. One important consequence is that

$$p_i(k \mid \text{rest}) = \Pr\{\text{class} = k \text{ in pixel } i \mid \text{rest}\} = \frac{\exp\{\alpha_i(k) + A_i(k, x_{\partial i})\}}{\sum_{l=1}^{K} \exp\{\alpha_i(l) + A_i(l, x_{\partial i})\}}, \tag{3.15}$$

in which $x_{\partial i}$ is the collection of classes in the neighbouring pixels lying around pixel i. In fact $A_i(k, x_{\partial i}) = \Sigma_{Q:\, i\in Q} V_Q(x_Q; x_i = k)$. This means in particular that $p_i(k \mid \text{rest})$ depends upon only $x_{\partial i}$, i.e.

$$p_i(k \mid \text{rest}) = p_i(k \mid x_{\partial i}). \tag{3.16}$$

This is the Markov property. The probabilities (3.16) are called the local characteristics of the mrf. One could call $A_i(k, x_{\partial i})$ the award function for window $\{i\} \cup \partial i$ around pixel i. The model encourages realisations with high awards.

The remarkable Hammersley–Clifford–Besag theorem identifies processes having the Markov property (3.16) with those having the Gibbs property (3.14), under a positivity condition; see Besag (1974). When faced with the task of constructing a suitable mrf to describe a certain phenomenon it is usually simpler to think "local Markov" in terms of award functions and local characteristics than thinking "global Gibbs" in terms of the potentials.

The following mrf is among the structurally simplest, but has proved useful in image restoration (see section 3.4.3 below) and in other areas: use 3×3 neighbourhoods, and cliques of size two only in (3.13), use class-dependent but position-independent $\alpha_i(x_i) = \alpha(x_i)$, and encourage spatial continuity by putting $V_{(i,j)}(x_i, x_j) = \beta I\{x_i = x_j\}$ in (3.14). This spatial mosaic model has $K + 1$ parameters and local characteristics

$$p_i(k \mid \text{rest}) = \frac{\exp\{\alpha(k) + \beta H_i(k, x_{\partial i})\}}{\sum_{l=1}^{K} \exp\{\alpha(l) + \beta H_i(l, x_{\partial i})\}}, \tag{3.17}$$

in which $H_i(x_i, x_{\partial i})$ is the number of x_i's neighbours that agree with it. The award is a value in $0, \beta, 2\beta, \ldots, 8\beta$.

The mrfs obviously form a very wide class. Including other cliques carefully chosen from larger neighbourhoods and perhaps finer parameterisation than a crude β for each gives one the possibility of including various types of prior knowledge about local structure into the model. In application 2.3.2 described in section 2 we fitted mrfs with $K = 12$ classes that came in four subgroups and 5×5-windows with up to 16 different cliques and up to six different β-parameters, see Hjort *et al.* (1989). In application 2.5.2 similarly complex mrfs have been used to model handwritten numbers, see Pripp (1990). See also the general discussion by Ripley (1992).

Remark 9. It is instructive to compare the 2-D Markov property to the corresponding 1-D one, i.e. for Markov chains $\{x_n\}$. The classical definition of Markov-ness in the chain case is that the distribution of some x_n given the complete past depends on x_{n-1} only. The alternative characterisation that the distribution of x_n given both past and future depends on the nearest neighbours only lends itself much more naturally to higher dimensions. □

3.2.2. *Parameter estimation from a single scene*

Consider for concreteness a mrf with local characteristics of the form (3.17), but with a more general award function structure

$$A_i(x_i, x_{\partial i}) = \beta_1 H_i^{(1)}(x_i, x_{\partial i}) + \cdots + \beta_p H_i^{(p)}(x_i, x_{\partial i}) = \beta' H_i(x_i, x_{\partial i}),$$

for certain parameters $\beta_1, \ldots, \beta_p$ and certain simple functions $H_i^{(j)}(x_i, x_{\partial i})$. The task is to obtain estimates for $\alpha(k)$s and βs (and perhaps further parameters, see section 3.4 below), from a single realisation $\mathbf{x}$ of the assumed mrf process. The $\alpha(k)$s are tied to the prior probabilities in pixel i, but in a rather involved way, because of interaction with the βs.

This is in one way a simply structured exponential model of classical form, say $p(\mathbf{x}) = c(\beta) \exp(\beta' V(\mathbf{x}))$ (having subsumed $\alpha(k)$s in new βs). The maximum likelihood method is seen to be equivalent to solving $V^{(j)}(\mathbf{x}) = \mu^{(j)}(\beta_1, \ldots, \beta_p)$ for $j = 1, \ldots, p$, where $\mu^{(j)}(\beta) = -\partial \log c(\beta)/\partial\beta$ is the expected value of $V^{(j)}(\mathbf{x})$ under the model. These equations cannot be solved directly, due to the formidable normalisation constant $c(\beta)$, defined as a sum of K^N terms. This is the "partition function" of statistical mechanics, and to give an idea of its complexity it suffices to mention that a Nobel Prize was awarded Nils Onsager for just providing an approximation. But ml estimates can be computed after all, through the use of extensive simulations, see the idea sketched in Künsch (1986). Pickard (1987) managed the simplest case of two equally likely classes and a single β parameter. See also Gidas (1991) for a precise and general account.

The alternative maximum pseudo-likelihood method is much simpler to implement, and has become the method of popular choice. It consists of maximising $\text{pl} = \Pi_{i=1}^N p_i(x_i \mid x_{\partial i})$ w.r.t. the parameters of the model. In the case considered

$$\log \text{pl} = \sum_{i=1}^N \left[\alpha(x_i) + \beta' H_i(x_i, x_{\partial i}) - \log \left(\sum_{l=1}^K \exp \{\alpha(l) + \beta' H_i(l, x_{\partial i})\} \right) \right], \tag{3.18}$$

and this function can be maximised numerically w.r.t. the parameters $\beta_1, \ldots, \beta_p$ and the parameters of $\alpha(k)$. To give expressions for partial derivatives, let again $\alpha_i(k)$ terms be subsumed into the H_i functions to form a larger V_i vector, and let $E_i V_i(\cdot, x_{\partial i})$ denote the mean of $V_i(X_i, x_{\partial i})$ conditional on $x_{\partial i}$, so that $X_i = k$ with probability $p_i(k \mid x_{\partial i})$, and let $\text{var}_i\, V_i(\cdot, x_{\partial i})$ be the accompanying variance matrix. Then

$$\frac{\partial \log \text{pl}}{\partial \beta_j} = \sum_{i=1}^N \{V_i^{(j)}(x_i, x_{\partial i}) - E_i V_i^{(j)}(\cdot, x_{\partial i})\},$$

$$\frac{\partial^2 \log \text{pl}}{\partial \beta_j \, \partial \beta_m} = -\sum_{i=1}^N \{\text{var}_i\, V_i(\cdot, x_{\partial i})\}_{j,m},$$

which shows that log pl is concave and well-behaved as a function of β.

A natural first step is to employ parameter-free prior probabilities $\exp\{\alpha(k)\} = \pi(k)$, for example position-independent ones and taken from some "prior scene", so that log pl needs to be maximised only w.r.t. $\beta_1, \ldots, \beta_p$. The maximisation could if necessary go on in an iterational manner. If $\alpha(k)$ is treated as an unknown parameter then $\partial \log \text{pl}/\partial\alpha(k) = 0$ leads to the natural equation $\pi_k(\mathbf{x}) = (1/N) \sum_{i=1}^N I\{x_i = k\} = (1/N) \sum_{i=1}^N p_i(k \mid x_{\partial i})$. In application 2.3.2 we have also had occasion to use and fit mrfs with non-linear exponents. All in all parameter estimation using maximum pseudo-likelihood requires some reliable maximisation algorithms, along with a flexibly structured environment to handle such data structures, but is not a major obstacle.

Remark 10. Why does pseudo-likelihood work? And is it clear that ordinary maximum likelihood works, if arduously carried through? Again it is instructive to consider the one-dimensional case of Markov chains. Suppose data $\{x_a : a = 0, \ldots, n\}$ are observed from some stationary process and are to be fitted to some parametric first-order Markov chain model $\Pr\{X_{a+1} = j \mid X_a = i\} = p_\beta(j \mid i)$. Let $p_\beta(i) = \Pr\{X_a = i\}$ be the accompanying marginal distribution, which is the equilibrium distribution. The ml procedure and the pl procedure maximise respectively

$$L(\beta) = \prod_{a=1}^n p_\beta(x_a \mid x_{a-1}) = \prod_{i,j} p_\beta(j \mid i)^{N(i,j)}$$

and

$$\text{pl}\,(\beta) = \prod_{a=1}^{N-1} p_\beta(x_a \mid x_{a-1}, x_{a+1}) = \prod_{i,j,k} p_\beta(j \mid i, k)^{N(i,j,k)}$$

in self-explanatory notation.

To examine the aims of ml and pl let us merely postulate that the true underlying model for the chain is some stationary distribution with $\Pr\{X_a = i, X_{a+1} = j\} = p(i,j) = p(i)p(j \mid i)$ and $\Pr\{X_a = i, X_{a+1} = j, X_{a+2} = k\} = p(i,j,k)$. By ergodic arguments $N(i,j)/n$ and $N(i,j,k)/n$ tend to $p(i,j)$ and $p(i,j,k)$ in probability. Hence

$$\frac{1}{n} \log L(\beta) \xrightarrow{p} \lambda_1(\beta) = \sum_{i,j} p(i,j) \log p_\beta(j \mid i) = \sum_i p(i) \sum_j p(j \mid i) \log p_\beta(j \mid i)$$

and

$$\frac{1}{n}\log \mathrm{pl}\,(\beta) \xrightarrow{p} \lambda_{\mathrm{pl}}(\beta) = \sum_{i,j,k} p(i,j,k)\log p_\beta(j \mid i,k)$$

$$= \sum_{i,k} p(i,\cdot,k) \sum_j p(j \mid i,k)\log p_\beta(j \mid i,k),$$

in which $p(i,\cdot,k)$ is the sum of $p(i,j,k)$ over all j. It follows that ml and pl in general aim at different "least false" or "most appropriate" parameter values. The ml procedure aims at and will be consistent for the parameter value β_0 which is least false according to the distance measure

$$\mathrm{dist}_1\{\text{truth, model}\} = \sum_i p(i) \sum_j p(j \mid i)\log\frac{p(j \mid i)}{p_\beta(j \mid i)},$$

a weighted sum of Kullback–Leibler distances between true and modelled transition probabilities. The pl procedure, on the other hand, aims at and is consistent for the second parameter value β_1 that minimises the different distance measure

$$\mathrm{dist}_{\mathrm{pl}}\{\text{truth, model}\} = \sum_{i,k} p(i,\cdot,k) \sum_j p(j \mid i,k)\log\frac{p(j \mid i,k)}{p_\beta(j \mid i,k)},$$

another weighted sum of Kullback–Leibler distances, this time between true and modelled local characteristics $\Pr\{X_a = j \mid X_{a-1} = i, X_{a+1} = k\}$. On may also study limit distributions in this framework. The ml is somewhat better on the model's home turf.

This discussion is pertinent considering our proclaimed view that models should be fitted and "adapted" but not necessarily trusted. □

3.2.3. *Unconditional simulation*

The task considered is that of simulating realisations of a specified mrf. This amounts to simulating from a discrete probability distribution $p(\mathbf{x})$, see (3.14), on an enormous but finite space, the set S of all K^N possible combinations of classes on the given lattice. In application 2.3.2 mentioned in section 2 we worked with $K = 12$ classes and for example $N = 200 \times 100$ sites or pixels in the scene, which leads to enormous numbers of size $10^{20.000}$ and the like for the number of different scenes. Numbers become mind-boggling in 3-D! Ordinarily methods can of course not cope with this kind of magnitude of the problem.

The simulation tricks to be used employ (MC^2) Markov Chain Monte Carlo methods. Assume that a huge transition matrix for a Markov chain with state space S has elements $m(\mathbf{x}, \mathbf{x}')$ that satisfy the reversibility criterion

$$p(\mathbf{x})m(\mathbf{x}, \mathbf{x}') = p(\mathbf{x}')m(\mathbf{x}', \mathbf{x}) \tag{3.19}$$

for all possible scenes, in which $p(\mathbf{x})$ is the mrf distribution given in (3.14). Then one can show that $p(\cdot)$ is the equilibrium distribution for the Markov chain. To sample from $p(\cdot)$, therefore, one might choose a convenient transition matrix with elements $m(\cdot,\cdot)$ obeying (3.19), and then run it until equilibrium seems to have settled in.

There are several possibilities of choice of $m(\cdot,\cdot)$. A convenient class of such can be described as follows. Choose first a symmetric transition matrix with elements $q(\mathbf{x}, \mathbf{x}')$ that are mostly equal to zero. Assume the simulation chain has come to scene $\mathbf{x} = (x_1, \ldots, x_N)$. Select a potential new scene $\mathbf{x}'(x'_1, \ldots, x'_N)$ from $q(\mathbf{x}, \cdot)$, and move from $\mathbf{x}$ to $\mathbf{x}'$ with

probability $\min\{1, p(\mathbf{x}')/p(\mathbf{x})\}$, otherwise remain at $\mathbf{x}$. This is the Metropolis algorithm, or perhaps "the class of Metropolis algorithms". One can check that (3.19) holds. The basic idea behind this simulation trick seems to be due to Metropolis (see Metropolis *et al.* (1953), and Hastings (1970) and Ripley (1987, ch. 4) for more statistical accounts).

It remains to specify $q(\cdot,\cdot)$, and again several options are available. One possibility is to have $q(\mathbf{x}, \mathbf{x}')$ positive only if $\mathbf{x}$ and $\mathbf{x}'$ differ at a single site. If this site is i, and $\mathbf{x} = (x_1, \ldots, k, \ldots, x_N)$ and $\mathbf{x}' = (x_1, \ldots, l, \ldots, x_N)$, then

$$\frac{p(\mathbf{x}')}{p(\mathbf{x})} = \frac{p_i(l \mid \text{rest})}{p_i(k \mid \text{rest})} = \frac{\exp\{\alpha_i(l) + A_i(l, x_{\partial i})\}}{\exp\{\alpha_i(k) + A_i(k, x_{\partial i})\}},$$

see (3.15). One feasible simulation method, for generating a single realisation $\mathbf{x}$, is therefore as follows. Start out with some initial scene, for example with class labels simulated independently in different pixels, from the prior probabilities $\pi_i(k)$. Carry out complete iteration cycles until apparent equilibrium, where one iteration cycle means a full scan over the scene. And when such a scan visits site i, choose class label l randomly, and let x_i change from its current label k to l with probability $\min\{1, p_i(l \mid \text{rest})/p_i(k \mid \text{rest})\}$.

Among several other convenient methods the so-called Gibbs sampler is perhaps the most popular. It consists of running complete iteration cycles until convergence, as above, with the following schedule for changing class labels during a full scan. If the current tth generation scene is $\mathbf{x}_t = (x_{1,t}, \ldots, x_{N,t})$, choose a random class label $x_{i,t+1} = k$ for site i according to the local probabilities $p_i(k \mid \mathbf{x}_t - \{i\}) = p_i(k \mid \text{rest}_t)$. Only empirical evidence can be given for preferring one simulation scheme to another. The "current folklore", in this hectic but still young field of stochastic simulation, seems to favour the Gibbs sampler. Some references are Geman & Geman (1984), Gidas (1985), Ripley (1987), and Tjelmeland & Holden (1993).

3.2.4. *Constrained simulation*

A pleasing facet of the mrf simulation scheme is that one can condition on known class values in some locations. Just go on running the Markov simulation chain as in the previous subsection, for example the Gibbs sampler, but with the class labels fixed at their known values, at all sites where such labels are known.

In some situations realisations of the mrf are only close to reality if the areas covered by each class are somewhat close to prior conceptions. It is therefore important to be able to constrain simulated realisations of a mrf to have class proportions equal to or close to specified values. This is not an easy problem, and some confusion surrounds the few methods that have been proposed in the literature. One possibility is a spin exchange method due to Flinn, see Hjort *et al.* (1989) for a brief review. Another and in many ways more promising avenue is to consider a new stochastic model with probability distribution

$$p_\sigma(\mathbf{x}) = p_\sigma(x_1, \ldots, x_N) = \text{const}\; p(x_1, \ldots, x_N) \exp\{-\sigma \Delta(x_1, \ldots, x_N)\}, \tag{3.20}$$

in which $\Delta(x_1, \ldots, x_N) = \Sigma_{k=1}^K (N_k/N - \pi_k^0)^2$ is a measure of discrepancy between the class frequencies of the scene $\mathbf{x}$ and the specified class frequencies. It is for each given σ possible to simulate from $p_\sigma(\cdot)$, by methods similar to those outlined above, even though this random field is not any longer a mrf w.r.t. the neighbourhood system. The idea is then to let σ slowly increase as the Markov simulation chain moves on. The result is that the observed class proportions are forced towards the prescribed π_k^0s.

Let us elaborate this point. The local characteristics of the new model are of the form

$$p_\sigma(x_i = k \mid \text{rest}) = \frac{p_\sigma(x_1, \ldots, k, \ldots, x_N)}{\sum_{l=1}^{K} p_\sigma(x_1, \ldots, l, \ldots, x_N)}$$
$$= \frac{\exp[\alpha_i(k) + A_i(k, x_{\partial i}) - \sigma\Delta(x_1, \ldots, k, \ldots, x_N)]}{\sum_{l=1}^{K} \exp[\alpha_i(l) + A_i(l, x_{\partial i}) - \sigma\Delta(x_1, \ldots, l, \ldots, x_N)]}.$$

This expression is generally valid for any given Δ-function of discrepancy between observed and ideal characteristics of the scene $\mathbf{x} = (x_1, \ldots, x_N)$. With the present Δ-function further simplification is possible, see Hjort *et al.* (1989), and it is not difficult to use the Gibbs sampler, as follows. Complete iteration cycles of simulated scenes are run until apparent equilibrium, where one cycle is a full scan over the scene. During one such scan, suppose the current scene is $\mathbf{x} = (x_1, \ldots, k_0, \ldots, x_N)$. Then move from k_0 to k with probability $p_\sigma(x_i = k \mid \text{rest})$.

Remark 11. This approach is useful also for other $\Delta(\mathbf{x})$-measures of discrepancy between observed and specified characteristics of the scene. It has been used in various forms in projects we have worked on, also for marked point processes (see sections 3.3 and 4.3). It was also proposed in a remark by Green (1986) in the context of mrfs for image restoration. □

3.2.5. Semi-mrf and other mosaic processes

Yes, there are others, and the mrfs have perhaps had too much attention during the last few years. Let us here briefly mention some other approaches for modelling mosaic type phenomena.

There are attempts at making the ordinary mrfs less crucially dependent on the given grid, or given resolution. See Nicholls & Petrou (1993) for ideas and experiments on renormalisation group transformation methods. In some applications the boundaries between class patches are approximately linear, and the resulting mosaic image is polygonal. A natural approach is therefore to model the boundaries themselves, and perhaps model class labels separately afterwards. Switzer (1965) gives a class of Poisson line models, which has been used by Owen (1984) and Hjort (1985a) in image reconstruction problems, cf. section 3.4.2 below. The Switzer process has a Markov property along line transects, but is not spatially Markovian; the distribution of lines and class labels in the interior of a convex bounded region given what is outside the region is not determined by knowledge of lines and class labels on the boundary. A more complex process which has this spatial Markov property has been introduced by Arak & Surgailis (1989). Clifford & Middleton (1989) outline mathematical properties of its potential use in image reconstruction, where there are problems of simulating from the posterior distribution. See also Arak *et al.* (1994). There is also a differently motivated approach based on coverage processes, covered by Hall (1988). Yet another method involves tesellations, Voronoi cells, etc., see Ripley (1981, ch. 4).

Let us finally describe a semi-mrf approach that aims at combining some of the convenient featues of the mrf methods with some larger-scale modifications. A realisation $\mathbf{x}$ on a lattice defines "bodies", maximally connected sets of sites that belong to the same class. There are several possibilities for making this intuitive notion mathematically precise; see Holden & Tjelmeland (1990) for one definition that is even valid in 3-D. The idea is that users often know something about the typical sizes and forms and directions of bodies, at least for some

of the classes. If bodies of sites from class 2 tend to be elliptical, for example, one can try to specify distributions of the angle and the axis lengths, and then build a model that is locally a mrf but encourages such bodies to take place, using a more complicated version of (3.20). One would also want to be able to gear such a model towards respecting certain borders on the scene, or towards respecting prior information of the type "bodies from class 3 very rarely touch bodies from class 4". The challenge is to build a sufficiently general and flexible model that can do this and which makes it possible to simulate realisations. This rather ambitious scheme is carried out in Holden & Tjelmeland (1990) and in Tjelmeland & Holden (1993), using models of the form

$$p(\mathbf{x}) = \text{const}\, p_0(\mathbf{x}) \exp\left\{\sum_{b=1}^{B} \gamma_b W_{\text{class}(B_b)}(B_b, f(B_b)) - \sum_{d=1}^{D} \sigma_d \Delta_d(\mathbf{x})\right\},$$

where $p_0(\mathbf{x})$ is some ordinary mrf, perhaps with 5×5 windows, the B_bs are bodies with features $f(B_b)$ such as size and form, the Ws are award functions that encourage bodies to meet certain specifications, and the Δ_ds are certain discrepancy functions. This model has been used to build a programme system that produces simulations of reservoir architecture and reservoir properties for oil companies; see the references mentioned.

3.3. Event processes

Here we briefly review some theory for spatial point processes. To solve problems associated with applications described in sections 2.3.3, 2.3.4 and 2.4.2, for example, one typically needs to model both location of points and associated "marks". This is one of the combinations of processes we treat in section 3.4. It will be seen that natural and simple models sometimes are easy to construct, but that parameter estimation and model verification typically become difficult tasks. Simulation based inference and use becomes important.

3.3.1. Spatial point processes

How can we model the geographical positions of a collection of points, or small objects, in a given region? The simplest possibility is a Poisson process with constant intensity λ, say, which postulates that the number of points falling in disjoint regions are independent and Poisson distributed with parameters equal to λ times the areas of the regions. A wider class of models emerges by allowing the intensity to vary, perhaps even stochastically. Many important phenomena are not well modelled by even such varying-intensity or doubly stochastic Poisson processes, however. A typical feature is that the smallest inter-point distances are not as small as they would be under Poisson-ness.

A rich class of models for point patterns is the pairwise interaction processes, with density (Radon–Nikodym derivative) $f(\{x_1, \ldots, x_n\}) = \text{const}\, \Pi_{i=1}^{n} g(x_i) \Pi_{i<j} h(\|x_i - x_j\|)$ w.r.t. the Poisson point process (with unit intensity, say). Here $g(x)$ is some non-negative function of geographical position, often taken to be constant; $h(r)$ is some non-negative function of the distance r between points, usually bounded by 1; and the integration constant is unwieldy. One is usually content to study models for fixed number of points n, where the pairwise interaction model says

$$f_n(x_1, \ldots, x_n) = \text{const} \prod_{i=1}^{n} g(x_i) \prod_{i<j} h(\|x_i - x_j\|).$$

There are some measure-theoretic details to work through here; see Lotwick & Silverman (1981) and Baddeley & Møller (1989) for good accounts. Typical examples include

$$h(r) = \begin{cases} \gamma & \text{if } r < \rho, \\ 1 & \text{if } r \geqslant \rho, \end{cases}$$

which gives the so-called Strauss model, and other simple functions that in some way climb from 0 (or from some extra parameter ε) to 1 when r runs from 0 to ρ. The special case $\gamma = 0$ is possible in the Strauss model, and corresponds to a Poisson process which is never allowed to have points closer to each other than ρ; this is also called a hard core process with hard core distance ρ.

With these choices for $h(\cdot)$ there is an upper limit after which no interaction occurs, and the product above is only over all neighbour pairs, where being neighbours means $\|x_i - x_j\| < \rho$. This invites Markov connections. Indeed the random collection $X = \{x_1, \ldots, x_n\}$ has a spatial Markov property, see Baddeley & Møller (1989). General references for modelling spatial point patterns include Ripley (1977, 1981, 1988, 1989a, b) and Stoyan *et al.* (1987). Some geological applications are described in Omre (1992).

3.3.2. *How to simulate*

An operational definition of "understanding a model" is that one should be able to simulate realisations from it. For the Strauss model with $\gamma = 0$, for example, one could conceivably generate points from the Poisson model (which for fixed n means simulating from the uniform distribution in the region considered) and only keep those realisations that have smallest distance at least ρ. This can be seriously inefficient, and better methods are called for.

What seems now to be the best way is that of the spatial birth-and-death processes introduced for this task by Ripley (1977) and Ripley & Kelly (1977). The scheme is (usually) to delete one of the n points at random and then add back another one, with probability

$$\Pr\{\text{add } x_n \mid x_1, \ldots, x_{n-1}\} = \frac{f_n(x_1, \ldots, x_n)}{f_{n-1}(x_1, \ldots, x_{n-1})} = g(x_n) \prod_{i=1}^{n-1} h(\|x_i - x_n\|)$$

assigned to position x_n. The point is that this birth-and-death process has a unique equilibrium distribution which is exactly the point process with density f. Note that the probability above only depends on the new point and its neighbours, in case of a h-function with finite range. The simulation is usually carried out using some appropriate rejection sampling scheme. Cleverness in doing this is often essential for the algorithm to work fast enough.

3.3.3. *How to read a point pattern*

There is a need to summarise the main features of a given picture of point locations. One can think of a "first order" summary picture, where the intensity of points per unit area is estimated in some smoothing fashion. This part is related to the $g(x)$-function of section 3.3.1. When the intensity can reasonably be assumed to be homogeneous over a region one needs a suitable "second order" summary. The method of choice here has become Ripley's K or L functions. The $K(t)$ function is a measure related to the covariance between the number of points falling in two areas, and under ideal Poisson conditions $K(t) = \pi t^2$. This is the motivation for studying $L(t) = \{K(t)/\pi\}^{1/2}$ instead. We refer to Ripley (1981, 1988) and to Stoyan *et al.* (1987) for proper definitions and constructions of estimators that in various ways take edge effects into account. These summary curves can be used to detect non-Poisson behaviour, to suggest other models, and to estimate parameters in such.

If the "points" have associated areas, for example, then other summary characteristics are needed as well. Ripley (1986; 1988, ch. 6) surveys several such based on morphology and

Serra calculus. See also 3.4.8 below for more general processes that combine point locations with "marks".

3.3.4. *Estimating parameters*

Even a simple-looking model like the Strauss model with $g = 1$ is notoriously difficult to estimate from data. Maximum likelihood estimation is difficult because of the intractable integration constant, but can be carried out through simulation procedures. One Monte Carlo method is described in Ripley (1988, ch. 4), and the rudiments of a general stochastic approximation method are presented in Moyeed & Baddeley (1991), following an idea of Künsch. Versions of pseudo-likelihood methods are studied in Grabarnik & Särkkä (1992), Särkkä (1993), and in Jensen & Møller (1991). Another method via conditioning of Palm probabilities has been developed by Takacs & Fiksel; see Fiksel (1988) and Grabarnik & Särkkä (1992), who point out connections to pseudo-likelihood again. Non-parametric estimation of the $h(r)$ function is very difficult to do with reasonable precision, and is perhaps only feasible with very large sample sizes. It can nevertheless be carried out, see Diggle *et al.* (1987), and be used as a data analytic summary. Goodness of fit is considered in Diggle (1979).

3.4. *Combinations*

In this final subsection a couple of naturally occurring cross-situations are discussed, in which Gaussian random functions, mosaic processes, and event processes appear in combination.

3.4.1. *Hidden Markov fields and image restoration*

The following situation occurs naturally in image analysis applications. There is an underlying true image $\mathbf{x}$ with value x_i in pixel i, but corrupting noise is present and $y_i = x_i + \varepsilon_i$ is observed instead. More generally there could be a vector y_i carrying information about the true x_i, for example in the form of $y_i \mid x_i \sim \mathcal{N}_d\{\mu(x_i), \Sigma(x_i)\}$.

In some situations there is a low number of possible values for x_i, say $1, \ldots, K$, which suggests using mosaic models of the type discussed in 3.2 for this "hidden truth". Thus the land cover classes in a remote sensing application could be modelled as a mrf with an appropriate neighbourhood structure. In other situations there is a larger number of possible x_i-values, and the $\mathbf{x}$ process could be viewed as a discretisation of a continuous random function. The noise is typically assumed to be Gaussian and independent from pixel to pixel given the $\mathbf{x}$ labels. In applications we have worked with involving fine-resolution multichannel satellite data, the measurements from the same underlying class have indeed been quite Gaussian, but have exhibited strong autocorrelation. In many other situations the independent white noise assumption has proven quite realistic.

Let us consider the case of a hidden mosaic process $\mathbf{x}$ with independent Gaussian observations $\mathbf{y}$ on top of it, say $y_i \mid \{x_i = k\} \sim f(y_i \mid x_i) = \mathcal{N}_d\{\mu(k), \Sigma\}$ for definiteness. The restoration problem is to estimate the full image $\mathbf{x}$ from the observed $\mathbf{y}$. This can be viewed as a spatial classification task. The simplest solution is to carry out ordinary discriminant analysis for each pixel, that is, use as $\hat{x}_i$ the class label k that maximises $\pi(k)f(y_i \mid k)$, where $\pi(1), \ldots, \pi(K)$ are the prior probabilities for the K classes. Of course the parameters $\mu(1), \ldots, \mu(K)$, Σ must have been estimated from some initial training stage. In some applications the class densities have large pairwise interdistances and this simple non-contextual method is sufficient. In other applications it is not, and contextual methods can offer significant improvements. We discuss two major approaches below, the "local modelling"

developed by Hjort & Mohn (1984, 1987) and others and the mrf based one developed by Geman & Geman (1984), Besag (1986) and others. Other approaches are mentioned in section 3.4.4.

3.4.2. An approach based on neighbourhood models

Let us see where basic statistical decision theory leads us in the present spatial context. Assume that the loss incurred when we assign label $\hat{x}_i$ to pixel i, whose true label is x_i, is of the type

$$L(x_i, \hat{x}_i) = \begin{cases} 0 & \text{if } \hat{x}_i = x_i \text{ (correct decision),} \\ 1 & \text{if } \hat{x}_i \neq x_i \text{ and } \hat{x}_i \in \{1, \ldots, K\} \text{ (wrong decision),} \\ t & \text{if } \hat{x}_i = D \text{ (being in doubt),} \end{cases} \tag{3.21}$$

in which t is a threshold between 0 and 1. Thus the possibility of being in doubt and state nothing about x_i is reserved, having in mind, for example, mixed pixels in some remote sensing application. Now, if the total measure of consequence is the average of the individual loss-contributions, i.e. the misclassification rate plus t times the doubt rate, then the optimal rule becomes

$$\hat{x}_i = \begin{cases} k & \text{if } k \text{ maximises } P_i\{k \mid \mathbf{y}\}, \text{ and this maximum exceeds } 1 - t; \\ D & \text{if } P_i\{k \mid \mathbf{y}\} \leq 1 - t \text{ for each } k. \end{cases} \tag{3.22}$$

Two points to note here are that all the data in principle are conditioned on in the posterior probabilities $P_i\{k \mid \mathbf{y}\}$, and that the rule classifies one pixel at a time.

In practice one has to limit oneself to a small subset $y_{N(i)}$, containing at least y_i, of all the data. If $y_{N(i)}$ is chosen to consist of y_i and its four immediate neighbours, for example, then the natural approximation to (3.22) is the rule that maximises

$$P_i\{k \mid y_{N(i)}\} = \text{const } \pi(k) f(y_{N(i)} \mid c_i = k)$$

$$= \text{const } \pi(k) \sum_{a,b,c,d} g(a, b, c, d \mid k)\, h(y_{N(i)} \mid k, a, b, c, d). \tag{3.23}$$

Here the two basic stochastic elements of the problem enter in a natural and illuminating way: $g(a, b, c, d \mid k)$ is the conditional probability of getting class configurations a, b, c, d given class k in the centre pixel, and is tied to the $\mathbf{x}$ process. And $h(y_{N(i)} \mid k, a, b, c, d)$ is the simultaneous density for the five vectors in question, given that the underlying classes are k, a, b, c, d. The summation in (3.23) is, in general, over all K^4 configurations. The rule based on (3.23) is an approximation to (3.22), but we emphasise that it also enjoys a natural optimality property by itself, namely that of achieving lowest expected average loss among all rules using the neighbour information $y_{N(i)}$ for the ith decision.

For each specification of global, simultaneous models for the processes $\mathbf{x}$ and for $\mathbf{y}$ given $\mathbf{x}$ formulae for g and h above can in principle be derived, after which we have a contextual classification algorithm. It is not really necessary for us to derive g and h from fully given, simultaneous probability distributions, however; we may if we wish forget the full scene and come up with realistic local models for the pixel neighbourhood alone, i.e. model g and h above directly. Even if some proposed local g-model should turn out to be inconsistent with a full model for $\mathbf{x}$, say, we are allowed to view it merely as a convenient approximation to the complex schemes Nature employs when she distributes class labels over the scene.

Another typical feature in these problems is also illustrated in formula (3.23): the models we use must not only be realistic and fitable, but also feasible in the sense of not needing too much computing time. A satellite scene can contain about a million pixels, and a rule that needs to sum K^4 terms for each class before it can decide on a class label for a pixel will be useless in most cases. Accordingly we should look for clever approximations and/or for convenient model choices that lead to reduced and simplified expressions. One such clever version of the general (3.23) is the following: suppose that y_i-vectors given the underlying classes are independent, and let $g(a, b, c, d \mid k) = p(a \mid k)p(b \mid k)p(c \mid k)p(d \mid k)$, where the $p(a \mid k)$s are neighbour transition probabilities (which must be estimated). The Markov mesh model for classes on a lattice studied by Pickard (1977) has in fact this multiplicative property. Then (3.23) simplifies to

$$P_i\{k \mid y_{N(i)}\} = \text{const}\, \pi(k) f(y_i \mid k) T_k(y_{i1}) \cdots T_k(y_{i4}), \quad T_k(y) = \sum_{m=1}^{K} p(m \mid k) f(y \mid m), \tag{3.24}$$

where the y_{ij}s stem from the four neighbour pixels. This produces the classification rule reached by Hjort & Mohn (1984), Haslett (1985), and others, from somewhat different perspectives.

Hjort & Mohn (1985) obtained a natural generalisation of this rule to the case where spatial autocorrelation between y_is is allowed for. Specifically,

$$P_i\{k \mid y_{N(i)}\} = \text{const}\, \pi(k) f(y_i \mid k) U_k(y_i, y_{i1}) \cdots U_k(y_i, y_{i4}), \tag{3.25}$$

where the U-functions are appropriate generalisations of the T-functions appearing in (3.24). They also provide evidence that such autocorrelation is prominently present with high resolution satellite data and ought to be taken into account. Hjort & Mohn (1984) and Sæbø *et al.* (1985) consider other variations on theme (3.23) as well.

The reasoning above applies equally well to larger neighbourhoods than the cross, but exact expressions based on the appropriate generalisation of (3.23) quickly become long and untractable. Again we feel that the statistician should not be afraid of constructing pragmatic approximations, even if they should lead him outside the safe ground of exact expressions under exact models. For the 3×3 pixel box with eight neighbours, for example, we may use a formula similar to (3.24), with four more terms entering the product, involving transition probabilities for diagonal neighbours, say $q(\cdot \mid k)$, which can be expressed in terms of the one-step neighbour transition probabilities $p(\cdot \mid \cdot)$s. This produces a valid classification algorithm with good error rate properties, although it, in fact, cannot be deduced from a bona fide global model for the classes.

A natural question is how much gain there is in being (more) sophisticated and cpu-consuming, by including neighbours at all, and by including say eight neighbours instead of only four. Hjort (1985a) studies one particular eight-neighbour method of the type (3.23), by an appropriate generalisation of a four-neighbour method due to Owen (1984). Exact formulae for error rates cannot be obtained, but they can be expressed via probabilities for events involving nine or fewer independent normal variates (univariate, even if the y_is are multivariate), and can as such be evaluated by computer simulation. (In this way we do not have to simulate the scenes or portions of the scene itself.) Some numerical information is presented in Hjort & Mohn (1987), and indicates first of all that using context can lead to appreciably increased accuracy, and secondly that using larger neighbourhoods usually will be worth the extra trouble and cpu-time. This is also supported by experience from simulation studies, see for example Hjort *et al.* (1987).

3.4.3. Markov random field approaches

The loss function (3.21) is local in nature, and corresponds essentially to viewing pixel-wise error rate as the basic quality measure. A radically different suggestion is the global loss measure

$$L(\mathbf{x}, \hat{\mathbf{x}}) = \begin{cases} 0 & \text{if } \textit{every} \text{ pixel is correctly classified;} \\ 1 & \text{if one or more pixels are misclassified.} \end{cases} \tag{3.26}$$

The optimal rule in this case becomes: find $\hat{\mathbf{x}} = (\hat{x}_1, \ldots, \hat{x}_N)$ to maximise the posterior probability

$$p(\mathbf{x} \mid \mathbf{y}) = \text{const}\, p(\mathbf{x}) f(\mathbf{y} \mid \mathbf{x}).$$

This requires first of all full model specifications for $\mathbf{x}$ and $\mathbf{y}$ (as opposed to only "local models"). Secondly, it may appear practically impossible to find this maximum *a posteriori* probability scene, because of the enormous number K^N of different possibilities to search through. But modern ideas from numerical–probabilistical optimisation made it possible for both Geman & Geman (1984) and Besag (1986), in two important papers, to give satisfactory solutions, for the broad family of mrf prior distributions studied in section 3.2.

Consider for illustration the simplest type of mrf (3.17), with a single β parameter in addition to class-parameters $\alpha(k)$. Assume also that the y_is are conditionally independent. Then

$$\begin{aligned} p(\mathbf{x} \mid \mathbf{y}) &= \text{const}\, p(\mathbf{x}) f(\mathbf{y} \mid \mathbf{x}) \\ &= \text{const}\, \exp\left[\sum_{i=1}^{N} \{\alpha(x_i) + \log f(y_i \mid x_i)\} + \beta \sum_{i<j} I\{x_i = x_j\} \right]. \end{aligned}$$

Accordingly $\mathbf{x}$ given data is again a mrf, only with updated $\alpha(x_i)$s. Geman & Geman (1984) discuss a "statistical cooling" technique from combinatorial optimisation for coming at least close to the maximum *a posteriori* picture, which is the optimal solution w.r.t. loss function (3.26). It is computationally demanding and requires several hundred iterative scans over the full scene. See Marroquin *et al.* (1987) for considerations about massive parallel processors and speed, and for applications of mrfs to computer vision. Besag (1986), on the other hand, has proposed a much simpler computational scheme that in effect, in a coordinate-ascent way, goes for a local maximum of the posterior distribution. The intuitively plausible idea is to start with an initial estimate $\bar{\mathbf{x}}$ for the scene, and then update $\bar{\mathbf{x}}$ to a perhaps better $\hat{\mathbf{x}}$ by finding $\hat{x}_i = k$ to maximise

$$p_i(x_i = k \mid \mathbf{y}, \hat{\mathbf{x}}_{S-i}) = \text{const}\, \exp\left[\alpha(k) + \beta H_i(k, \bar{x}_{\partial i})\right] f(y_i \mid k), \tag{3.27}$$

with notation as in (3.17). Note that this is like ordinary discriminant analysis but with neighbour-influenced "prior" probabilities $\pi(k) = \text{const}\, \exp\left[\alpha(k) + \beta H_i(k, \bar{x}_{\partial i})\right]$. In this way the full scene is swept over, in some order, and we have a new, updated estimate $\hat{\mathbf{x}}$. The process is iterated until convergence; usually 6–10 times suffice. The starting point is ordinarily that corresponding to $\beta = 0$, i.e. the non-contextual, but the "iterated conditional modes" method could equally well use a contextual classification as its starting point. It has been argued that smaller values of β should be used for the first couple of iterations.

It is our experience from high resolution satellite data that realistic models must allow positive spatial correlation for y_i-vectors given the scene. A simple model that serves to illustrate the general principle and the wider potential of the mrf approach is the following:

$$f(\mathbf{y} \mid \mathbf{x}) = \text{const} \exp\left\{-\tfrac{1}{2}\sum_i (y_i - \mu(x_i))' \Sigma^{-1}(y_i - \mu(x_i)) - \sum_{i<j} \gamma_{ij}(y_i - \mu(x_i))' \Sigma^{-1}(y_j - \mu(x_j))\right\},$$

in which $\gamma_{ij} = \frac{1}{2}\gamma$ when i and j are immediate (first order) neighbours and zero otherwise. This is a Gaussian mrf, or conditional autoregressive scheme, with corresponding local characteristics

$$y_i \mid \mathbf{x}, \mathbf{y}_{S-i} \sim N\{\mu(x_i) + \gamma(\bar{y}_{\partial i} - \bar{\mu}_{\partial i}), \Sigma\}, \tag{3.28}$$

writing $\bar{y}_{\partial i}$ for the average of the four immediate y_j neighbours to y_i and similarly $\bar{\mu}_{\partial i}$ for the average of the four accompanying $\mu(x_j)$s. It is easily seen that $\mathbf{x}$ given $\mathbf{y}$ again is a mrf. An appropriately modified version of the Geman and Geman method is capable of coming close to the simultaneous optimisation of $p(\mathbf{x} \mid \mathbf{y})$, which is seen to mean maximising

$$\sum_i [\alpha(x_i) - \tfrac{1}{2}(y_i - \mu(x_i))'\Sigma^{-1}(y_i - \mu(x_i))] + \sum_{i<j} [\beta I\{x_i = x_j\} + \tfrac{1}{2}\gamma(y_i - \mu(x_i))'\Sigma^{-1}(y_j - \mu(x_j))],$$

where the second sum is over all pairs of neighbours. The natural generalisation of Besag's method to the present spatial correlation model is simpler, and amounts to maximising for each i, and for the current estimate $\bar{\mathbf{x}}$ of the rest of the scene,

$$p_i(x_i = k \mid \mathbf{y}, \bar{\mathbf{x}}_{S-i}) = \text{const} \exp[\alpha(k) + \beta H_i(k, \bar{x}_{\partial i})] f(y_i \mid k, \bar{\mathbf{x}}_{S-i}, \mathbf{y}_{S-i}). \tag{3.29}$$

Thus the conditional mode step again acts like discriminant analysis, but this time with both neighbour-corrected prior probability and neighbour-corrected class density.

3.4.4. *Other approaches to classification*

Let us briefly touch upon some other spatial classification techniques. Underlying the previous methods are the loss functions (3.21) and (3.26). A simple intermediate loss function that is less crude than (3.21) but nevertheless has a "contextual element" is L = number of misclassified 2×2 blocks of pixels. The optimal rule becomes one of simultaneously classifying four pixels, by maximising the posterior probability given data over the K^4 possible outcomes. Hjort (1987) has worked out simple rules of this type based on a geometric probability model for classes, under which only $6K^2 - 5K$ of the possible configurations have positive probability. This geometrical model used the Switzer process for Poisson lines mentioned in section 3.2.5.

Relaxation procedures is a term used for algorithms that iteratively adjust posterior probabilities based on estimated or known spatial relationships among the class labels. Some of these use wider and wider neighbourhoods as the iterations go on. They are perhaps best understood in terms of connections to mrf models, and to analysis of incomplete data, see Kay & Titterington (1986) and Fiskum (1986), and section 4.2 below.

Other references of interest include Switzer & Green (1984) and Switzer & Ingebritsen (1986) on min/max autocorrelation factors that aim to separate noise from signal; Conradsen & Nielsen (1987), studying the benefits of using texture-type features derived from neighbourhoods; Green & Titterington (1987) who study recursive procedures under an interesting model for sequences of images; Esbensen & Geladi (1989) where soft bi-linear modelling is used; Greig *et al.* (1989) who obtain and demonstrate an exact maximum *a posteriori* image algorithm for the two class case; Owen (1989), where the smoothing parameters of Besag

type methods are studied; and Taxt & Bølviken (1991), where new restoration algorithms are motivated through an analogy with quantum physics.

3.4.5. *Predicting a continuous variable*

In several remote sensing applications one is as interested in estimating a ground parameter as in classifying pixels into ground classes. Imaging that z_i is such a variable of interest, associated with ground surface element i. In a water quality application of MSS- and LANDSAT-satellite data we have worked on there are in fact several z_is of interest: the amount of plankton in sea element i, along with turbidity, water transparency, and other measures of water quality. In an application to forestry surveillance the total tree mass volume for each 20 m × 20 m element on the ground was of interest. With luck these z_is are correlated with the remotely sensed y_i-vectors, and predictions based on these can be made. Examples of this sort abound in the remote sensing literature, and make it clear that many important surveillance tasks can now be carried out with the help of remote sensing, in proper combination with ground truth measurements from land stations.

Let us for convenience still use y_i to denote the vector of pertinent observations at pixel i, for example spectral data, possibly transformed, and possibly supplemented with other available covariates thought to be useful for the prediction of z_i. (In the water quality application, the component of y_i are two chromaticity indices supplemented with topographic information.) Let us also keep z_i one-dimensional (extensions are straightfoward). A useful mathematical assumption, used as a vehicle for producing good prediction procedures, is

$$\begin{pmatrix} z_i \\ y_i \end{pmatrix} \mid (x_i = k) \sim \mathcal{N}_{d+1}\left\{\begin{pmatrix} \nu_k \\ \mu_k \end{pmatrix}, \begin{pmatrix} \tau_k^2 & \omega_k' \\ \omega_k & \Sigma \end{pmatrix}\right\}.$$

Thus z_i in pixel i is viewed as a realisation of a random variable. The natural predictor, if we know that the pixel in question is of ground type k, is

$$\bar{z}_i(k) = E\{z_i \mid y_i, x_i = k\} = \nu_k + \omega_k' \Sigma^{-1}(y_i - \mu_k), \tag{3.30}$$

and the conditional variance $\sigma(k)^2 = \tau_k^2 - \omega_k' \Sigma^{-1} \omega_k$ can be used to construct prediction intervals for z_i. Without knowledge of the pixel's class one might weight these with the posterior probabilities $P_i\{k \mid y_i\}$ to form a (non-contextual) predictor.

There are several ways to incorporate spatial context in the method. One strategy that uses a spatial model for a continuous residual function is explained and illustrated in Høst *et al.* (1989). Let us now examine some other contextual alternatives that use spatial models for the underlying classes.

3.4.6. *Predictors constructed from neighbourhood models*

Hjort & Mohn (1987) derived prediction rules with variance measures for this framework. Assume that z_is given y and x are independent, with $z_i \mid (y_i, x_i) \sim f(z_i \mid y_i, x_i)$, a normal with mean $\hat{z}_i(x_i)$ and variance $\sigma(x_i)^2$. The predictors take the form

$$\hat{z}_i = E\{z_i \mid y_{N(i)}\} = \sum_{k=1}^{K} P_i\{k \mid y_{N(i)}\}\hat{z}_i(k).$$

One readily shows that z_i given data $y_{N(i)}$, i.e. the information from pixel i and its neighbours, is distributed as a mixture of the densities $f(z_i \mid y_i, x_i)$ with $P_i\{k \mid y_{N(i)}\}$ as weights. Accordingly

$$\text{var}\{z_i \mid y_{N(i)}\} = \sum_{k=1}^{K} P_i\{k \mid y_{N(i)}\}\{\sigma(k)^2 + (z_i(k) - \hat{z}_i)^2\},$$

which is of use when confidence intervals are called for. Observe that if a contextual classification is carried out using the local modelling method then the extra computational burden needed to compute predictors and standard deviations is mild.

3.4.7. Markov random field methods

Assume that $\mathbf{x}$ is a mrf with distribution (3.14), that $\mathbf{y}$ given $\mathbf{x}$ is a Gaussian mrf with local characteristics (3.28), and that z_is are conditionally independent as above. Then one can show that $(\mathbf{y}, \mathbf{z})$ has a simultaneous mrf distribution given $\mathbf{x}$, and that $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ is a simultaneous mrf. The most important fact is that the unobserved processes $(\mathbf{x}, \mathbf{z})$ given the data $\mathbf{y}$, the Bayesian posterior distribution, is yet another mrf, with local characteristics

$$(x_i, z_i) \mid (\mathbf{y}, \mathbf{x}_{S-i}, \mathbf{z}_{S-i}) \sim \text{const} \exp\{\alpha(x_i) + \beta H_i(x_i, x_{\partial i})\} f(y_i \mid \mathbf{x}, \mathbf{y}_{S-i}) f(z_i \mid y_i, x_i), \tag{3.31}$$

cf. (3.17) and (3.28). This generalises the result (3.29).

Besag's method of taking iterative conditional modes can be generalised to the present state of affairs, with both $\mathbf{x}$ and $\mathbf{z}$ to be estimated from the image data $\mathbf{y}$. This is done in Hjort & Mohn (1987, sect. 4). The best method depends on the specific loss function used. When the loss function is $I\{\hat{\mathbf{x}} \neq \mathbf{x}\}$ plus average squared prediction error then the Bayes solution is as follows: first use the usual Besag method (in this case, as explained around (3.29)) to arrive at the scene estimate $\hat{\mathbf{x}}$. Then compute

$$\hat{z}_i = E\{z_i \mid \mathbf{y}, \hat{\mathbf{x}}_{S-i}, \mathbf{z}_{S-i}\} = \frac{\sum_{k=1}^{K} \exp\{\alpha(k) + \beta H_i(k, \hat{x}_{\partial i})\} f(y_i \mid k, \hat{\mathbf{x}}_{S-i}, \mathbf{y}_{S-i}) \hat{z}_i(k)}{\sum_{k=1}^{K} \exp\{\alpha(k) + \beta H_i(k, \hat{x}_{\partial i})\} f(y_i \mid k, \hat{\mathbf{x}}_{S-i}, \mathbf{y}_{S-i})}.$$

Note that the autocorrelation parameter γ enters via $f(y_i \mid \mathbf{x}, \mathbf{y}_{S-i})$.

In this case $\hat{z}_i$ emerged as an explicit function of the finally classified scene $\hat{\mathbf{x}}$. This is because we assumed conditional independence of z_is given $\mathbf{x}$ and $\mathbf{y}$. In models where z_is must be taken interdependent, given scene and y-data, a simultaneous, iterational updating of $\mathbf{x}$ and $\mathbf{z}$ may be called for. An example is given in Hjort & Mohn (1987, sect. 4).

3.4.8. Marked point processes

Suppose there is a mark or set of attributes z_i associated with each point x_i of a spatial point process. An example with a 4-dimensional mark for each point is described in section 4.3 below. If the marks live in a mark space $\mathscr{Z}$ then the process with outcomes (x_i, z_i) is just a spatial point process in some appropriate $\mathscr{X} \times \mathscr{Z}$, so the most important parts of the theory presented in section 3.3 carry over to marked point processes. In particular, simulation of realisations can be carried out using a spatial birth and death process. The hardest and most vital task is often simply that of building a good model, with distance functions and pairwise interaction functions, that produces realistic outcomes. A general reference with theory and example is Stoyan *et al.* (1987).

3.4.9. Estimation problems

There are challenging estimation problems associated with several of the models described. Hjort (1985b) and Hjort & Mohn (1987) develop estimation methods for many of the image models mentioned in section 3.4.2. In particular they describe methods that utilise unclassified

vectors via estimation of mixture distributions. Besag (1986) proposes an iteration scheme to restore an image and simultaneously estimate the parameters of the mrf model used for $\mathbf{x}$, used in section 3.4.3, assuming the y_is to be conditionally independent. This scheme is somewhat biased and inconsistent, as pointed out along with a remedy in Hjort & Mohn (1987). Lakshmanan & Derin (1989) describe a simulated annealing method that stops at regular intervals to estimate the mrf parameters. Veijanen (1990) gives another method for imperfectly observed mrfs and proves consistency. A deep treatment for maximum pseudo-likelihood estimation with hidden mrfs is given by Comets & Gidas (1992). Georgsen & Omre (1993) consider estimation in a model that combines fibre processes with a Gaussian random function.

4. Some worked-through examples of applications

4.1. *Depth conversion of seismic data* (Omre & Halvorsen, 1989; see also Abrahamsen *et al.*, 1991 and Abrahamsen, 1993)

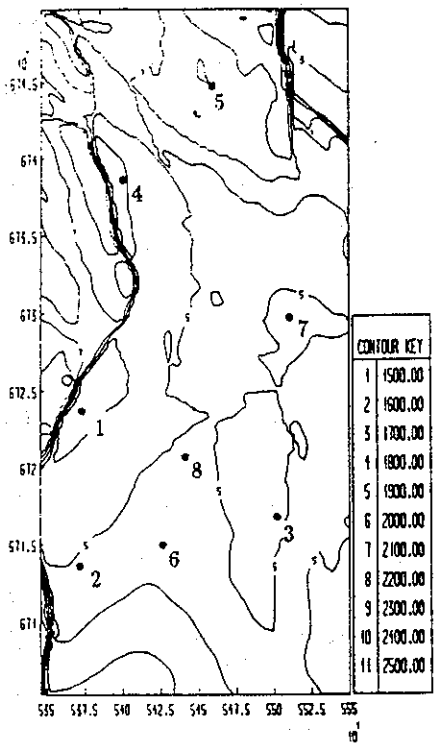
The petroleum reservoirs in the North Sea are located at a depth of approximately 3000 m and have an areal extent of typically 3.0×5.0 km^2. In the reservoir the hydrocarbons tend to migrate upwards in the structures until they are trapped under a syncline of non-permeable geologic layers, usually shale-rich horizons. The mapping of these horizons is important both for exploration purposes and for prediction of hydrocarbon volume *in situ*.

Fortunately these non-permeable horizons tend to have properties very different from the porous reservoir, and can be identified from seismic data. Seismic data can be collected in an inexpensive way from ships, and vast amounts with good areal coverage are usually available. The seismic reflection signal has geographical reference horizontally and reflection time reference vertically. After seismic cleaning, which is a discipline in itself, a relatively reliable seismic reflection time surface $\{t(x): x \in D\}$ is obtained, see Fig. 1. The challenge is to convert this into a map of depths to the horizon $\{z(x): x \in D\}$. This could of course be done by simply multiplying reflection time and signal velocity. The fact that the signal velocity varies considerably, both vertically and laterally, complicates this.

Two other sources of information are available for the depth conversion. The first is the knowledge of the geophysicists. The areal extent of some of these horizons is often huge and covers other reservoirs. Hence experience from other areas of the North Sea is relevant. In addition the physical understanding of packing of reservoir rock provides some constraints on the vertical velocity profile. Secondly, exact depth observations $z(x_1), \ldots, z(x_n)$ are available in certain well positions, see Fig. 1. The fact that the four first wells are the most shallow ones indicates preferential drilling and non-representative positioning of the observations in the design space. Note, however, that the seismic reflections have a support of 100×100 m^2 of the horizon while the support of well observations is 0.2×0.2 m^2. Hence the former must be considered as weakly smoothed.

The example is from a study of a huge offshore gas field in the North Sea. A set of parameters, intended to be as realistic as possible, were defined in cooperation with geophysicists in a Norwegian oil company. The sensitivity to the influence of the prior knowledge was evaluated. The changes in the predictions over time, i.e. as a function of the available wells, were also studied. The stochastic model used for merging the various pieces of information in this study is of the form

$$Z(x) = V(x)t(x) + \varepsilon(x) = \left(\beta_1 + \beta_2 t(x) + \beta_3 \frac{x_1 - x_{1,\min}}{x_{1,\max} - x_{1,\min}}\right) t(x) + \varepsilon(x), \tag{4.1}$$



well id.	depth
1	1584.1
2	1770.3
3	1715.4
4	1586.5
5	2062.8
6	1846.7
7	1836.0
8	1784.6

Fig. 1. Map of seismic reflection times and list of depths observed in the wells.

where $\varepsilon(x)$ is a continuous residual surface, compensating for the smoothing in the seismic signal, with correlation structure $\sigma^2 K(\|x-y\|)$. In other words, the signal velocity increases with depth according to the increase in reflection time and there exists a lateral trend in the West–East or x_1-direction. Geophysical knowledge is included through carefully assessed prior distributions on $\beta_1, \beta_2, \beta_3$. The model is accordingly within the Bayesian Kriging framework as discussed in section 3.1.3. The spatial covariance function used is

$$K(r) = \begin{cases} 1 - \frac{3}{2}\frac{r}{2800} + \frac{1}{2}\left(\frac{r}{2800}\right)^3 & \text{if } 0 \leqslant r \leqslant 2800, \\ 0 & \text{if } r \geqslant 2800, \end{cases}$$

where r is the distance from x to y, and the σ parameter was estimated to be 200.0 m. This estimate was based on estimates in comparable reservoirs with numerous wells and on understanding of the physics of seismic reflections. The prior distribution was assessed in cooperation with experienced geophysicists, and is as follows:

$$\beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} \sim \mathcal{N}_3\left\{\begin{bmatrix} 0.600 \\ 0.0002 \\ 0.070 \end{bmatrix}, \tau^2 \begin{bmatrix} (0.055)^2 & 0 & 0 \\ 0 & (0.0001)^2 & 0 \\ 0 & 0 & (0.022)^2 \end{bmatrix}\right\}. \tag{4.2}$$

The 0.055, 0.0001, 0.022 values were the actual prior standard deviation parameters used, but the scale parameter τ was also included and varied in order to evaluate the sensitivity to the choice of prior distribution; see also the relevant discussion in Omre & Halvorsen (1989).

For τ equal to zero the coefficients β are fully specified and the underlying trend surface can be subtracted. This corresponds to what is termed simple Kriging in geostatistical