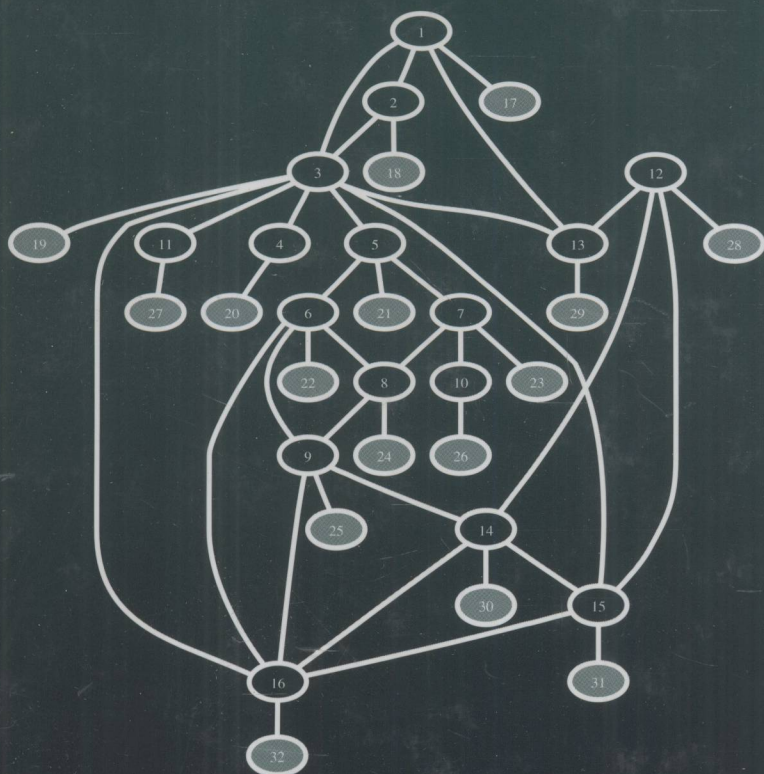


Gaussian Markov Random Fields

Theory and Applications



Håvard Rue
Leonhard Held

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TO MONA AND ULRIKE

Preface

This monograph describes Gaussian Markov random fields (GMRFs) and some of its applications in statistics. At first sight, this seems to be a rather specialized topic, as the wider class of Markov random fields is probably known only to researchers in spatial statistics and image analysis. However, GMRFs have applications far beyond these two areas, for example in structural time-series analysis, analysis of longitudinal and survival data, spatiotemporal statistics, graphical models, and semi-parametric statistics.

Despite the wide range of application, there is a unified framework for both representing, understanding and computing with GMRFs using the graph formulation. Our main motivation to write this monograph is to provide the first comprehensive account of the main properties of GMRFs, to emphasize the strong connection between GMRFs and numerical methods for sparse matrices, and to outline various applications of GMRFs for statistical inference.

Complex hierarchical models are at the core of modern statistics, and GMRFs play a central role in this framework to describe the spatial and temporal dynamics of nature and real systems. Statistical inference in hierarchical models, however, can typically only be done using simulation, in particular through Markov chain Monte Carlo (MCMC) methods. Thus we emphasize computational issues, which allow us to construct fast and reliable algorithms for (Bayesian) inference in hierarchical models with GMRF components. We emphasize the concept of *blocking*, i.e., updating all or nearly all of the parameters jointly, which we believe to be perhaps the only way to overcome problems with convergence and mixing of ordinary MCMC algorithms. We hope that the reader will share our enthusiasm and that the examples provided in this book will stimulate further research in this area.

The book can be loosely categorized as follows. We begin in Chapter 1 by introducing GMRFs through two simple examples, an autoregressive model in time and a conditional autoregressive model in space. We then briefly discuss numerical methods for sparse matrices, and why they are important for simulation-based inference in GMRF models. We illustrate this through a simple hierarchical model. We finally describe various areas where GMRFs are used in statistics.

Chapter 2 is the main theoretical chapter, describing the most important results for GMRFs. It starts by introducing the necessary notation and describing the central concept of conditional independence. GMRFs are then defined and studied in detail. Efficient direct simulation from a GMRF is described using numerical techniques for sparse matrices. A numerical case study illustrates the performance of the algorithms in different scenarios. Finally, two optional sections follow: The first describes the theory of *stationary* GMRFs, where circulant and block circulant matrices become important. Lastly we discuss the problem on how to parameterize the precision matrix, the inverse covariance matrix, of a GMRF without destroying positive definiteness.

In Chapter 3 we give a detailed discussion of intrinsic GMRFs (IGMRFs). IGMRFs do have precision matrices which are no longer of full rank. They are of central importance in Bayesian hierarchical models, where they are often used as a nonstationary prior distribution for dependent parameters in space or in time. A key concept to understanding IGMRFs is the conditional distribution of a proper GMRF under linear constraints. We then describe IGMRFs of various kinds, on the line, the lattice, the torus, and on irregular graphs. A final optional section is devoted to the representation of integrated Wiener process priors as IGMRFs.

In Chapter 4 we discuss various applications of GMRFs for hierarchical modeling. We outline how to use MCMC algorithms in hierarchical models with GMRF components. We start with some general comments regarding MCMC via blocking. We then discuss models with normal observations, auxiliary variable models for probit and logistic regression and nonnormal regression models, all with latent GMRF components. The GMRFs may have a temporal or a spatial component, or they relate to particular covariate effects in a semiparametric regression framework.

Finally, in Chapter 5 we first describe how GMRFs can be used to approximate so-called *Gaussian fields*, i.e., normal distributed random vectors where the covariance matrix rather than its inverse, the precision matrix, is specified. The final section in Chapter 5 is devoted to the problem of how to construct improved and non-GMRF approximations to hidden GMRFs.

Appendices A and B describe the distributions we use and the implementation of the algorithms in the public-domain library **GMRFlib**.

Chapters 2 and 3 are fairly self-contained and do not require much prior knowledge from the reader, except for some familiarity with probability theory and linear algebra. Chapters 4 and 5 assume that the reader is experienced in the area of Bayesian hierarchical models and their statistical analysis via MCMC, perhaps at the level of standard textbooks such as Carlin and Louis (1996), Gilks et al. (1996), Robert

PREFACE

and Casella (1999), or Gelman et al. (2004).

This monograph can be read chronologically. Sections marked with a ‘★’ indicate more advanced material which can be skipped at first reading. We might ask too much of some readers patience in Chapter 2 and 3, which are motivated from the various applications of GMRFs for hierarchical modeling in Chapter 4. It might therefore be useful to skim through Chapter 4 before reading Chapter 2 and 3 in detail.

This book was conceived in the spring of 2003 but the main body of work was done in the first half of 2004. We are indebted to Julian Besag, who read his seminal paper on Markov random fields (Besag, 1974) 30 years ago to the Royal Statistical Society, his seminal contributions to this field since then, and for introducing LH to MRFs in 1995/1996 during a visit to the University of Washington. We also appreciate his comments on the initial draft and sending us a copy of Mondal and Besag (2004).

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We look forward to returning to everyday life and enjoying our families, Kristine and Mona, Valentina and Ulrike. Thank you for your patience!

HÅVARD RUE
LEONHARD HELD

Trondheim
Munich
Summer 2004

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Introduction

1.1 Background

This monograph considers *Gaussian Markov random fields* (GMRFs) covering both theory and applications. A GMRF is really a simple construct: It is just a (finite-dimensional) random vector following a multivariate normal (or Gaussian) distribution. However, we will be concerned with more restrictive versions where the GMRF satisfies additional *conditional independence* assumptions, hence the term *Markov*.

Conditional independence is a powerful concept. Let $\mathbf{x} = (x_1, x_2, x_3)^T$ be a random vector, then x_1 and x_2 are conditionally independent given x_3 if, for known value of x_3 , discovering x_2 tells you nothing new about the distribution of x_1 . Under this condition the joint density $\pi(\mathbf{x})$ must have the representation

$$\pi(\mathbf{x}) = \pi(x_1 | x_3) \pi(x_2 | x_3) \pi(x_3),$$

which is a simplification of a general representation

$$\pi(\mathbf{x}) = \pi(x_1 | x_2, x_3) \pi(x_2 | x_3) \pi(x_3).$$

The conditional independence property implies that $\pi(x_1 | x_2, x_3)$ is simplified to $\pi(x_1 | x_3)$, which is easier to understand, to represent, and to interpret.

1.1.1 An introductory example

As a simple example of a GMRF, consider an autoregressive process of order 1 with standard normal errors, which is often expressed as

$$x_t = \phi x_{t-1} + \epsilon_t, \quad \epsilon_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1), \quad |\phi| < 1 \quad (1.1)$$

where the index t represents time. Assumptions about conditional independence are not stated explicitly here, but show up more clearly if we express (1.1) in the conditional form

$$x_t | x_1, \dots, x_{t-1} \sim \mathcal{N}(\phi x_{t-1}, 1) \quad (1.2)$$

for $t = 2, \dots, n$. In this model x_s and x_t with $1 \leq s < t \leq n$ are conditionally independent given $\{x_{s+1}, \dots, x_{t-1}\}$ if $t - s > 1$.

In addition to (1.2), let us now assume that the marginal distribution of x_1 is normal with mean zero and variance $1/(1 - \phi^2)$, which is simply the stationary distribution of this process. Then the joint density of \mathbf{x} is

$$\begin{aligned}\pi(\mathbf{x}) &= \pi(x_1) \pi(x_2 | x_1) \cdots \pi(x_n | x_{n-1}) \\ &= \frac{1}{(2\pi)^{n/2}} |\mathbf{Q}|^{1/2} \exp\left(-\frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x}\right),\end{aligned}\tag{1.3}$$

where the *precision matrix* \mathbf{Q} is the tridiagonal matrix

$$\mathbf{Q} = \begin{pmatrix} 1 & -\phi & & & & \\ -\phi & 1 + \phi^2 & -\phi & & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\phi & 1 + \phi^2 & -\phi \\ & & & & -\phi & 1 \end{pmatrix}$$

with zero entries outside the diagonal and first off-diagonals. The conditional independence assumptions impose certain restrictions on the precision matrix. The tridiagonal form is due to the fact that x_i and x_j are conditionally independent for $|i - j| > 1$, given the rest. This also holds in general for any GMRF: If $Q_{ij} = 0$ for $i \neq j$, then x_i and x_j are conditionally independent given the other variables $\{x_k : k \neq i \text{ and } k \neq j\}$ and vice versa. The sparse structure of \mathbf{Q} prepares the ground for fast computations of GMRFs to which we return in Section 1.2.1.

The simple relationship between conditional independence and the zero structure of the precision matrix is not evident in the covariance matrix $\mathbf{\Sigma} = \mathbf{Q}^{-1}$, which is a (completely) dense matrix with entries

$$\sigma_{ij} = \frac{1}{1 - \phi^2} \phi^{|i-j|}.$$

For example, for $n = 7$,

$$\mathbf{\Sigma} = \frac{1}{1 - \phi^2} \begin{pmatrix} 1 & \phi & \phi^2 & \phi^3 & \phi^4 & \phi^5 & \phi^6 \\ \phi & 1 & \phi & \phi^2 & \phi^3 & \phi^4 & \phi^5 \\ \phi^2 & \phi & 1 & \phi & \phi^2 & \phi^3 & \phi^4 \\ \phi^3 & \phi^2 & \phi & 1 & \phi & \phi^2 & \phi^3 \\ \phi^4 & \phi^3 & \phi^2 & \phi & 1 & \phi & \phi^2 \\ \phi^5 & \phi^4 & \phi^3 & \phi^2 & \phi & 1 & \phi \\ \phi^6 & \phi^5 & \phi^4 & \phi^3 & \phi^2 & \phi & 1 \end{pmatrix}.$$

It is therefore difficult to derive conditional independence properties from the structure of $\mathbf{\Sigma}$. Clearly, the entries in $\mathbf{\Sigma}$ only give (direct) information about the *marginal* dependence structure, not the conditional one. For

example, in the autoregressive model, x_s and x_t are *marginally dependent* for any finite s and t as long as $\phi \neq 0$.

Simplifications due to conditional independence do not only appear for the *directed* conditional distributions as in (1.2), but also for the *undirected* conditional distributions, often called *full conditionals* $\{\pi(x_t|\mathbf{x}_{-t})\}$, where \mathbf{x}_{-t} denotes all elements in \mathbf{x} but x_t . In the autoregressive example,

$$x_t | \mathbf{x}_{-t} \sim \begin{cases} \mathcal{N}(\phi x_{t+1}, 1) & t = 1, \\ \mathcal{N}\left(\frac{\phi}{1+\phi^2}(x_{t-1} + x_{t+1}), \frac{1}{1+\phi^2}\right) & 1 < t < n, \\ \mathcal{N}(\phi x_{n-1}, 1) & t = n, \end{cases} \quad (1.4)$$

so x_t depends in general both on x_{t-1} and x_{t+1} . Equation (1.4) is important as it allows for an alternative specification of the first-order autoregressive models through the full conditionals $\pi(x_t|\mathbf{x}_{-t})$ for $t = 1, \dots, n$. In fact, by starting with these full conditionals, we obtain an alternative and completely equivalent representation of this model with the same joint density for \mathbf{x} . This is not so obvious as for the directed conditional distributions (1.2), where the joint density is simply the product of the densities corresponding to (1.2) for $t = 2, \dots, n$ times the (marginal) density of x_1 .

1.1.2 Conditional autoregressions

We now make the discussion more general, leaving autoregressive models. Let \mathbf{x} be associated with observations or some property of points or regions in the spatial domain. For example, x_i could be the value of pixel i in an image, the height of tile i in a tessellation or the relative risk for some disease in the i th district. Now there is no natural ordering of the indices and (1.3) is no longer useful to specify the joint density of \mathbf{x} . A common approach is then to specify the joint density of a zero mean GMRF implicitly by specifying each of the n full conditionals

$$x_i | \mathbf{x}_{-i} \sim \mathcal{N}\left(\sum_{j:j \neq i} \beta_{ij} x_j, \kappa_i^{-1}\right), \quad (1.5)$$

which was pioneered by Besag (1974, 1975). These models are also known by the name *conditional autoregressions*, abbreviated as *CAR* models. There is also an alternative and more restrictive approach to CAR models, the so-called *simultaneous autoregressions* (SAR), which we will not discuss specifically. This approach dates back to Whittle (1954), see for example, Cressie (1993) for further details.

The n full conditionals (1.5) must satisfy some consistency conditions to ensure that a joint normal density exists with these full conditionals.

These reduces to require that $\mathbf{Q} = (Q_{ij})$ with elements

$$Q_{ij} = \begin{cases} \kappa_i & i = j \\ -\kappa_i \beta_{ij} & i \neq j, \end{cases}$$

is symmetric and positive definite. Symmetry is ensured by $\kappa_i \beta_{ij} = \kappa_j \beta_{ji}$ for all $i \neq j$, while positive definiteness requires $\kappa_i > 0$ for all $i = 1, \dots, n$, but imposes further (and often quite complicated) constraints on the β_{ij} 's. A common (perhaps too common!) approach to ensure positive definiteness is to require that \mathbf{Q} is *diagonal dominant*, which means that, in each row (or column) of \mathbf{Q} , the diagonal entry is larger than the sum of the absolute off-diagonal entries. This is a sufficient but not necessary condition for positive definiteness.

The conditional independence properties of this GMRF can now be found by simply checking if Q_{ij} is zero or not. If $Q_{ij} = 0$ then x_i and x_j are conditionally independent given the rest, and if $Q_{ij} \neq 0$ then they are conditionally dependent. It is useful to represent these findings using an *undirected graph* with nodes $\{1, \dots, n\}$ and an edge between node i and $j \neq i$ if and only if $Q_{ij} \neq 0$. We then say that \mathbf{x} is a GMRF with respect to this graph. The neighbors to node i are all nodes $j \neq i$ with $\beta_{ij} \neq 0$, hence all nodes on which the full conditional (1.5) depends. Going back to the autoregressive model (1.4), the neighbors of i are $\{i-1, i+1\}$ for $i = 2, \dots, n-1$, and $\{2\}$ and $\{n-1\}$ of node 1 and n , respectively.

In general the neighbors of i are often those that are, in one way or the other, in the 'proximity' of node i . The common approach is first to specify the graph by choosing a suitable set of neighbors to each node, and then to choose β_{ij} for each pair $i \sim j$ of neighboring nodes i and j .

Figure 1.1 displays two such graphs, (a) a linear graph corresponding to (1.2) with $n = 50$ and (b) the graph corresponding to the 16 states of Germany where two states are neighbors if they share a common border. The graph in (b) is not drawn to mimic the map of Germany but only to visualize the graph itself. The number of neighbors in (b) varies between 2 and 9.

Figure 1.2 displays a graph constructed similarly to Figure 1.1(b), but which now corresponds to the 366 regions in Sardinia. The neighborhood structure is now slightly more complex and the number of neighbors varies between 1 and 13 with a median of 5. This is a typical (but simple) graph for applications of GMRF models.

The case where \mathbf{Q} is symmetric and positive semidefinite is of particular interest. This class is known under the name *intrinsic conditional autoregressions* or *intrinsic GMRFs* (IGMRFs). The density of \mathbf{x} is then improper but, by construction, \mathbf{x} defines a proper distribution on a specific lower-dimensional space. For example, if each row (or column) of \mathbf{Q} sums up to zero, then \mathbf{Q} has rank $n-1$ and the (improper) density