Now suppose we move from a maximum likelihood approach to a full Bayesian treatment in which we wish to sample from the posterior distribution over the parameter vector $\boldsymbol{\theta}$. In principle, we would like to draw samples from the joint posterior $p(\boldsymbol{\theta}, \mathbf{Z}|\mathbf{X})$, but we shall suppose that this is computationally difficult. Suppose further that it is relatively straightforward to sample from the complete-data parameter posterior $p(\boldsymbol{\theta}|\mathbf{Z}, \mathbf{X})$. This inspires the *data augmentation* algorithm, which alternates between two steps known as the I-step (imputation step, analogous to an E step) and the P-step (posterior step, analogous to an M step).

IP Algorithm

I-step. We wish to sample from $p(\mathbf{Z}|\mathbf{X})$ but we cannot do this directly. We therefore note the relation

$$p(\mathbf{Z}|\mathbf{X}) = \int p(\mathbf{Z}|\boldsymbol{\theta}, \mathbf{X}) p(\boldsymbol{\theta}|\mathbf{X}) \, \mathrm{d}\boldsymbol{\theta} \tag{11.30}$$

and hence for $l = 1, \ldots, L$ we first draw a sample $\boldsymbol{\theta}^{(l)}$ from the current estimate for $p(\boldsymbol{\theta}|\mathbf{X})$, and then use this to draw a sample $\mathbf{Z}^{(l)}$ from $p(\mathbf{Z}|\boldsymbol{\theta}^{(l)}, \mathbf{X})$.

P-step. Given the relation

$$p(\boldsymbol{\theta}|\mathbf{X}) = \int p(\boldsymbol{\theta}|\mathbf{Z}, \mathbf{X}) p(\mathbf{Z}|\mathbf{X}) \, \mathrm{d}\mathbf{Z} \tag{11.31}$$

we use the samples $\{\mathbf{Z}^{(l)}\}$ obtained from the I-step to compute a revised estimate of the posterior distribution over $\boldsymbol{\theta}$ given by

$$p(\boldsymbol{\theta}|\mathbf{X}) \simeq \frac{1}{L} \sum_{l=1}^{L} p(\boldsymbol{\theta}|\mathbf{Z}^{(l)}, \mathbf{X}). \tag{11.32}$$

By assumption, it will be feasible to sample from this approximation in the I-step.

Note that we are making a (somewhat artificial) distinction between parameters $\boldsymbol{\theta}$ and hidden variables $\mathbf{Z}$. From now on, we blur this distinction and focus simply on the problem of drawing samples from a given posterior distribution.

11.2. Markov Chain Monte Carlo

In the previous section, we discussed the rejection sampling and importance sampling strategies for evaluating expectations of functions, and we saw that they suffer from severe limitations particularly in spaces of high dimensionality. We therefore turn in this section to a very general and powerful framework called Markov chain Monte Carlo (MCMC), which allows sampling from a large class of distributions,

and which scales well with the dimensionality of the sample space. Markov chain Monte Carlo methods have their origins in physics (Metropolis and Ulam, 1949), and it was only towards the end of the 1980s that they started to have a significant impact in the field of statistics.

As with rejection and importance sampling, we again sample from a proposal distribution. This time, however, we maintain a record of the current state $\mathbf{z}^{(\tau)}$, and the proposal distribution $q(\mathbf{z}|\mathbf{z}^{(\tau)})$ depends on this current state, and so the sequence of samples $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots$ forms a Markov chain. Again, if we write $p(\mathbf{z}) = \widetilde{p}(\mathbf{z})/Z_p$, we will assume that $\widetilde{p}(\mathbf{z})$ can readily be evaluated for any given value of $\mathbf{z}$, although the value of Z_p may be unknown. The proposal distribution itself is chosen to be sufficiently simple that it is straightforward to draw samples from it directly. At each cycle of the algorithm, we generate a candidate sample $\mathbf{z}^\star$ from the proposal distribution and then accept the sample according to an appropriate criterion.

Section 11.2.1

In the basic *Metropolis* algorithm (Metropolis *et al.*, 1953), we assume that the proposal distribution is symmetric, that is $q(\mathbf{z}_A|\mathbf{z}_B) = q(\mathbf{z}_B|\mathbf{z}_A)$ for all values of $\mathbf{z}_A$ and $\mathbf{z}_B$. The candidate sample is then accepted with probability

$$A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\widetilde{p}(\mathbf{z}^\star)}{\widetilde{p}(\mathbf{z}^{(\tau)})}\right). \tag{11.33}$$

This can be achieved by choosing a random number u with uniform distribution over the unit interval $(0, 1)$ and then accepting the sample if $A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) > u$. Note that if the step from $\mathbf{z}^{(\tau)}$ to $\mathbf{z}^\star$ causes an increase in the value of $p(\mathbf{z})$, then the candidate point is certain to be kept.

If the candidate sample is accepted, then $\mathbf{z}^{(\tau+1)} = \mathbf{z}^\star$, otherwise the candidate point $\mathbf{z}^\star$ is discarded, $\mathbf{z}^{(\tau+1)}$ is set to $\mathbf{z}^{(\tau)}$ and another candidate sample is drawn from the distribution $q(\mathbf{z}|\mathbf{z}^{(\tau+1)})$. This is in contrast to rejection sampling, where rejected samples are simply discarded. In the Metropolis algorithm when a candidate point is rejected, the previous sample is included instead in the final list of samples, leading to multiple copies of samples. Of course, in a practical implementation, only a single copy of each retained sample would be kept, along with an integer weighting factor recording how many times that state appears. As we shall see, as long as $q(\mathbf{z}_A|\mathbf{z}_B)$ is positive for any values of $\mathbf{z}_A$ and $\mathbf{z}_B$ (this is a sufficient but not necessary condition), the distribution of $\mathbf{z}^{(\tau)}$ tends to $p(\mathbf{z})$ as $\tau \to \infty$. It should be emphasized, however, that the sequence $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots$ is not a set of independent samples from $p(\mathbf{z})$ because successive samples are highly correlated. If we wish to obtain independent samples, then we can discard most of the sequence and just retain every M^{th} sample. For M sufficiently large, the retained samples will for all practical purposes be independent. Figure 11.9 shows a simple illustrative example of sampling from a two-dimensional Gaussian distribution using the Metropolis algorithm in which the proposal distribution is an isotropic Gaussian.

Further insight into the nature of Markov chain Monte Carlo algorithms can be gleaned by looking at the properties of a specific example, namely a simple random

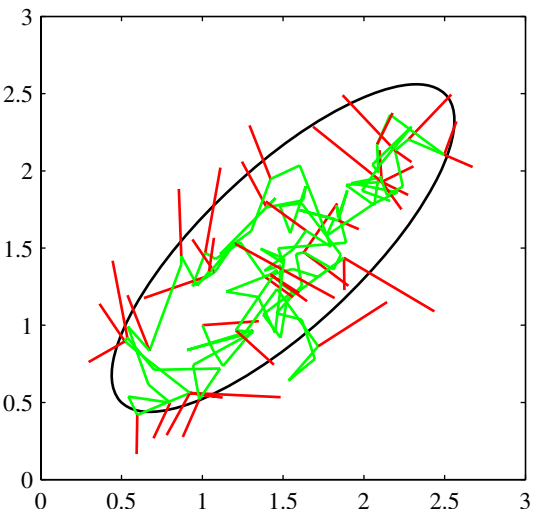


Figure 11.9 A simple illustration using Metropolis algorithm to sample from a Gaussian distribution whose one standard-deviation contour is shown by the ellipse. The proposal distribution is an isotropic Gaussian distribution whose standard deviation is 0.2. Steps that are accepted are shown as green lines, and rejected steps are shown in red. A total of 150 candidate samples are generated, of which 43 are rejected.

walk. Consider a state space z consisting of the integers, with probabilities

$$p(z^{(\tau+1)} = z^{(\tau)}) = 0.5 \tag{11.34}$$

$$p(z^{(\tau+1)} = z^{(\tau)} + 1) = 0.25 \tag{11.35}$$

$$p(z^{(\tau+1)} = z^{(\tau)} - 1) = 0.25 \tag{11.36}$$

where $z^{(\tau)}$ denotes the state at step τ. If the initial state is $z^{(1)} = 0$, then by symmetry the expected state at time τ will also be zero $\mathbb{E}[z^{(\tau)}] = 0$, and similarly it is easily seen that $\mathbb{E}[(z^{(\tau)})^2] = \tau/2$. Thus after τ steps, the random walk has only travelled a distance that on average is proportional to the square root of τ. This square root dependence is typical of random walk behaviour and shows that random walks are very inefficient in exploring the state space. As we shall see, a central goal in designing Markov chain Monte Carlo methods is to avoid random walk behaviour.

Exercise 11.10

11.2.1 Markov chains

Before discussing Markov chain Monte Carlo methods in more detail, it is useful to study some general properties of Markov chains in more detail. In particular, we ask under what circumstances will a Markov chain converge to the desired distribution. A first-order Markov chain is defined to be a series of random variables $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(M)}$ such that the following conditional independence property holds for $m \in \{1, \ldots, M-1\}$

$$p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}) = p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)}). \tag{11.37}$$

This of course can be represented as a directed graph in the form of a chain, an example of which is shown in Figure 8.38. We can then specify the Markov chain by giving the probability distribution for the initial variable $p(\mathbf{z}^{(0)})$ together with the

conditional probabilities for subsequent variables in the form of *transition probabilities* $T_m(\mathbf{z}^{(m)}, \mathbf{z}^{(m+1)}) \equiv p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)})$. A Markov chain is called *homogeneous* if the transition probabilities are the same for all m.

The marginal probability for a particular variable can be expressed in terms of the marginal probability for the previous variable in the chain in the form

$$p(\mathbf{z}^{(m+1)}) = \sum_{\mathbf{z}^{(m)}} p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)})p(\mathbf{z}^{(m)}). \tag{11.38}$$

A distribution is said to be invariant, or stationary, with respect to a Markov chain if each step in the chain leaves that distribution invariant. Thus, for a homogeneous Markov chain with transition probabilities $T(\mathbf{z}', \mathbf{z})$, the distribution $p^\star(\mathbf{z})$ is invariant if

$$p^\star(\mathbf{z}) = \sum_{\mathbf{z}'} T(\mathbf{z}', \mathbf{z})p^\star(\mathbf{z}'). \tag{11.39}$$

Note that a given Markov chain may have more than one invariant distribution. For instance, if the transition probabilities are given by the identity transformation, then any distribution will be invariant.

A sufficient (but not necessary) condition for ensuring that the required distribution $p(\mathbf{z})$ is invariant is to choose the transition probabilities to satisfy the property of *detailed balance*, defined by

$$p^\star(\mathbf{z})T(\mathbf{z}, \mathbf{z}') = p^\star(\mathbf{z}')T(\mathbf{z}', \mathbf{z}) \tag{11.40}$$

for the particular distribution $p^\star(\mathbf{z})$. It is easily seen that a transition probability that satisfies detailed balance with respect to a particular distribution will leave that distribution invariant, because

$$\sum_{\mathbf{z}'} p^\star(\mathbf{z}')T(\mathbf{z}', \mathbf{z}) = \sum_{\mathbf{z}'} p^\star(\mathbf{z})T(\mathbf{z}, \mathbf{z}') = p^\star(\mathbf{z}) \sum_{\mathbf{z}'} p(\mathbf{z}'|\mathbf{z}) = p^\star(\mathbf{z}). \tag{11.41}$$

A Markov chain that respects detailed balance is said to be *reversible*.

Our goal is to use Markov chains to sample from a given distribution. We can achieve this if we set up a Markov chain such that the desired distribution is invariant. However, we must also require that for $m \to \infty$, the distribution $p(\mathbf{z}^{(m)})$ converges to the required invariant distribution $p^\star(\mathbf{z})$, irrespective of the choice of initial distribution $p(\mathbf{z}^{(0)})$. This property is called *ergodicity*, and the invariant distribution is then called the *equilibrium* distribution. Clearly, an ergodic Markov chain can have only one equilibrium distribution. It can be shown that a homogeneous Markov chain will be ergodic, subject only to weak restrictions on the invariant distribution and the transition probabilities (Neal, 1993).

In practice we often construct the transition probabilities from a set of 'base' transitions $B_1, \ldots, B_K$. This can be achieved through a mixture distribution of the form

$$T(\mathbf{z}', \mathbf{z}) = \sum_{k=1}^{K} \alpha_k B_k(\mathbf{z}', \mathbf{z}) \tag{11.42}$$

for some set of mixing coefficients $\alpha_1, \ldots, \alpha_K$ satisfying $\alpha_k \geqslant 0$ and $\sum_k \alpha_k = 1$. Alternatively, the base transitions may be combined through successive application, so that

$$T(\mathbf{z}', \mathbf{z}) = \sum_{\mathbf{z}_1} \ldots \sum_{\mathbf{z}_{n-1}} B_1(\mathbf{z}', \mathbf{z}_1) \ldots B_{K-1}(\mathbf{z}_{K-2}, \mathbf{z}_{K-1}) B_K(\mathbf{z}_{K-1}, \mathbf{z}). \quad (11.43)$$

If a distribution is invariant with respect to each of the base transitions, then obviously it will also be invariant with respect to either of the $T(\mathbf{z}', \mathbf{z})$ given by (11.42) or (11.43). For the case of the mixture (11.42), if each of the base transitions satisfies detailed balance, then the mixture transition T will also satisfy detailed balance. This does not hold for the transition probability constructed using (11.43), although by symmetrizing the order of application of the base transitions, in the form $B_1, B_2, \ldots, B_K, B_K, \ldots, B_2, B_1$, detailed balance can be restored. A common example of the use of composite transition probabilities is where each base transition changes only a subset of the variables.

11.2.2 The Metropolis-Hastings algorithm

Earlier we introduced the basic Metropolis algorithm, without actually demonstrating that it samples from the required distribution. Before giving a proof, we first discuss a generalization, known as the *Metropolis-Hastings* algorithm (Hastings, 1970), to the case where the proposal distribution is no longer a symmetric function of its arguments. In particular at step τ of the algorithm, in which the current state is $\mathbf{z}^{(\tau)}$, we draw a sample $\mathbf{z}^\star$ from the distribution $q_k(\mathbf{z}|\mathbf{z}^{(\tau)})$ and then accept it with probability $A_k(\mathbf{z}^\star, \mathbf{z}_\tau)$ where

$$A_k(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\widetilde{p}(\mathbf{z}^\star) q_k(\mathbf{z}^{(\tau)}|\mathbf{z}^\star)}{\widetilde{p}(\mathbf{z}^{(\tau)}) q_k(\mathbf{z}^\star|\mathbf{z}^{(\tau)})}\right). \quad (11.44)$$

Here k labels the members of the set of possible transitions being considered. Again, the evaluation of the acceptance criterion does not require knowledge of the normalizing constant Z_p in the probability distribution $p(\mathbf{z}) = \widetilde{p}(\mathbf{z})/Z_p$. For a symmetric proposal distribution the Metropolis-Hastings criterion (11.44) reduces to the standard Metropolis criterion given by (11.33).

We can show that $p(\mathbf{z})$ is an invariant distribution of the Markov chain defined by the Metropolis-Hastings algorithm by showing that detailed balance, defined by (11.40), is satisfied. Using (11.44) we have

$$\begin{aligned} p(\mathbf{z}) q_k(\mathbf{z}|\mathbf{z}') A_k(\mathbf{z}', \mathbf{z}) &= \min\left(p(\mathbf{z}) q_k(\mathbf{z}|\mathbf{z}'), p(\mathbf{z}') q_k(\mathbf{z}'|\mathbf{z})\right) \\ &= \min\left(p(\mathbf{z}') q_k(\mathbf{z}'|\mathbf{z}), p(\mathbf{z}) q_k(\mathbf{z}|\mathbf{z}')\right) \\ &= p(\mathbf{z}') q_k(\mathbf{z}'|\mathbf{z}) A_k(\mathbf{z}, \mathbf{z}') \end{aligned} \quad (11.45)$$

as required.

The specific choice of proposal distribution can have a marked effect on the performance of the algorithm. For continuous state spaces, a common choice is a Gaussian centred on the current state, leading to an important trade-off in determining the variance parameter of this distribution. If the variance is small, then the

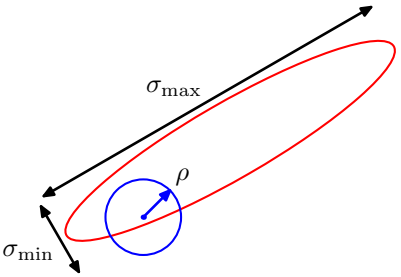


Figure 11.10 Schematic illustration of the use of an isotropic Gaussian proposal distribution (blue circle) to sample from a correlated multivariate Gaussian distribution (red ellipse) having very different standard deviations in different directions, using the Metropolis-Hastings algorithm. In order to keep the rejection rate low, the scale ρ of the proposal distribution should be on the order of the smallest standard deviation $\sigma_{\min}$, which leads to random walk behaviour in which the number of steps separating states that are approximately independent is of order $(\sigma_{\max}/\sigma_{\min})^2$ where $\sigma_{\max}$ is the largest standard deviation.

proportion of accepted transitions will be high, but progress through the state space takes the form of a slow random walk leading to long correlation times. However, if the variance parameter is large, then the rejection rate will be high because, in the kind of complex problems we are considering, many of the proposed steps will be to states for which the probability $p(\mathbf{z})$ is low. Consider a multivariate distribution $p(\mathbf{z})$ having strong correlations between the components of $\mathbf{z}$, as illustrated in Figure 11.10. The scale ρ of the proposal distribution should be as large as possible without incurring high rejection rates. This suggests that ρ should be of the same order as the smallest length scale $\sigma_{\min}$. The system then explores the distribution along the more extended direction by means of a random walk, and so the number of steps to arrive at a state that is more or less independent of the original state is of order $(\sigma_{\max}/\sigma_{\min})^2$. In fact in two dimensions, the increase in rejection rate as ρ increases is offset by the larger steps sizes of those transitions that are accepted, and more generally for a multivariate Gaussian the number of steps required to obtain independent samples scales like $(\sigma_{\max}/\sigma_2)^2$ where σ_2 is the second-smallest standard deviation (Neal, 1993). These details aside, it remains the case that if the length scales over which the distributions vary are very different in different directions, then the Metropolis Hastings algorithm can have very slow convergence.

11.3. Gibbs Sampling

Gibbs sampling (Geman and Geman, 1984) is a simple and widely applicable Markov chain Monte Carlo algorithm and can be seen as a special case of the Metropolis-Hastings algorithm.

Consider the distribution $p(\mathbf{z}) = p(z_1, \ldots, z_M)$ from which we wish to sample, and suppose that we have chosen some initial state for the Markov chain. Each step of the Gibbs sampling procedure involves replacing the value of one of the variables by a value drawn from the distribution of that variable conditioned on the values of the remaining variables. Thus we replace z_i by a value drawn from the distribution $p(z_i|\mathbf{z}_{\setminus i})$, where z_i denotes the i^{th} component of $\mathbf{z}$, and $\mathbf{z}_{\setminus i}$ denotes $z_1, \ldots, z_M$ but with z_i omitted. This procedure is repeated either by cycling through the variables

in some particular order or by choosing the variable to be updated at each step at random from some distribution.

For example, suppose we have a distribution $p(z_1, z_2, z_3)$ over three variables, and at step τ of the algorithm we have selected values $z_1^{(\tau)}$, $z_2^{(\tau)}$ and $z_3^{(\tau)}$. We first replace $z_1^{(\tau)}$ by a new value $z_1^{(\tau+1)}$ obtained by sampling from the conditional distribution

$$p(z_1|z_2^{(\tau)}, z_3^{(\tau)}). \tag{11.46}$$

Next we replace $z_2^{(\tau)}$ by a value $z_2^{(\tau+1)}$ obtained by sampling from the conditional distribution

$$p(z_2|z_1^{(\tau+1)}, z_3^{(\tau)}) \tag{11.47}$$

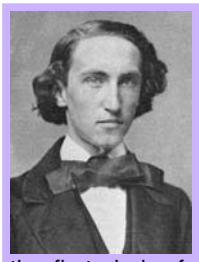
so that the new value for z_1 is used straight away in subsequent sampling steps. Then we update z_3 with a sample $z_3^{(\tau+1)}$ drawn from

$$p(z_3|z_1^{(\tau+1)}, z_2^{(\tau+1)}) \tag{11.48}$$

and so on, cycling through the three variables in turn.

Gibbs Sampling

1. Initialize $\{z_i : i = 1, \ldots, M\}$
2. For $\tau = 1, \ldots, T$:
   - Sample $z_1^{(\tau+1)} \sim p(z_1|z_2^{(\tau)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$.
   - Sample $z_2^{(\tau+1)} \sim p(z_2|z_1^{(\tau+1)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$.
   - $\vdots$
   - Sample $z_j^{(\tau+1)} \sim p(z_j|z_1^{(\tau+1)}, \ldots, z_{j-1}^{(\tau+1)}, z_{j+1}^{(\tau)}, \ldots, z_M^{(\tau)})$.
   - $\vdots$
   - Sample $z_M^{(\tau+1)} \sim p(z_M|z_1^{(\tau+1)}, z_2^{(\tau+1)}, \ldots, z_{M-1}^{(\tau+1)})$.



Josiah Willard Gibbs
1839–1903

Gibbs spent almost his entire life living in a house built by his father in New Haven, Connecticut. In 1863, Gibbs was granted the first PhD in engineering in the United States, and in 1871 he was appointed to the first chair of mathematical physics in the United States at Yale, a post for which he received no salary because at the time he had no publications. He developed the field of vector analysis and made contributions to crystallography and planetary orbits. His most famous work, entitled *On the Equilibrium of Heterogeneous Substances*, laid the foundations for the science of physical chemistry.

To show that this procedure samples from the required distribution, we first of all note that the distribution $p(\mathbf{z})$ is an invariant of each of the Gibbs sampling steps individually and hence of the whole Markov chain. This follows from the fact that when we sample from $p(z_i|\{\mathbf{z}_{\setminus i})$, the marginal distribution $p(\mathbf{z}_{\setminus i})$ is clearly invariant because the value of $\mathbf{z}_{\setminus i}$ is unchanged. Also, each step by definition samples from the correct conditional distribution $p(z_i|\mathbf{z}_{\setminus i})$. Because these conditional and marginal distributions together specify the joint distribution, we see that the joint distribution is itself invariant.

The second requirement to be satisfied in order that the Gibbs sampling procedure samples from the correct distribution is that it be ergodic. A sufficient condition for ergodicity is that none of the conditional distributions be anywhere zero. If this is the case, then any point in z space can be reached from any other point in a finite number of steps involving one update of each of the component variables. If this requirement is not satisfied, so that some of the conditional distributions have zeros, then ergodicity, if it applies, must be proven explicitly.

The distribution of initial states must also be specified in order to complete the algorithm, although samples drawn after many iterations will effectively become independent of this distribution. Of course, successive samples from the Markov chain will be highly correlated, and so to obtain samples that are nearly independent it will be necessary to subsample the sequence.

We can obtain the Gibbs sampling procedure as a particular instance of the Metropolis-Hastings algorithm as follows. Consider a Metropolis-Hastings sampling step involving the variable z_k in which the remaining variables $\mathbf{z}_{\setminus k}$ remain fixed, and for which the transition probability from $\mathbf{z}$ to $\mathbf{z}^\star$ is given by $q_k(\mathbf{z}^\star|\mathbf{z}) = p(z_k^\star|\mathbf{z}_{\setminus k})$. We note that $\mathbf{z}_{\setminus k}^\star = \mathbf{z}_{\setminus k}$ because these components are unchanged by the sampling step. Also, $p(\mathbf{z}) = p(z_k|\mathbf{z}_{\setminus k})p(\mathbf{z}_{\setminus k})$. Thus the factor that determines the acceptance probability in the Metropolis-Hastings (11.44) is given by

$$A(\mathbf{z}^\star, \mathbf{z}) = \frac{p(\mathbf{z}^\star)q_k(\mathbf{z}|\mathbf{z}^\star)}{p(\mathbf{z})q_k(\mathbf{z}^\star|\mathbf{z})} = \frac{p(z_k^\star|\mathbf{z}_{\setminus k}^\star)p(\mathbf{z}_{\setminus k}^\star)p(z_k|\mathbf{z}_{\setminus k}^\star)}{p(z_k|\mathbf{z}_{\setminus k})p(\mathbf{z}_{\setminus k})p(z_k^\star|\mathbf{z}_{\setminus k})} = 1 \tag{11.49}$$

where we have used $\mathbf{z}_{\setminus k}^\star = \mathbf{z}_{\setminus k}$. Thus the Metropolis-Hastings steps are always accepted.

As with the Metropolis algorithm, we can gain some insight into the behaviour of Gibbs sampling by investigating its application to a Gaussian distribution. Consider a correlated Gaussian in two variables, as illustrated in Figure 11.11, having conditional distributions of width l and marginal distributions of width L. The typical step size is governed by the conditional distributions and will be of order l. Because the state evolves according to a random walk, the number of steps needed to obtain independent samples from the distribution will be of order $(L/l)^2$. Of course if the Gaussian distribution were uncorrelated, then the Gibbs sampling procedure would be optimally efficient. For this simple problem, we could rotate the coordinate system in order to decorrelate the variables. However, in practical applications it will generally be infeasible to find such transformations.

One approach to reducing random walk behaviour in Gibbs sampling is called *over-relaxation* (Adler, 1981). In its original form, this applies to problems for which

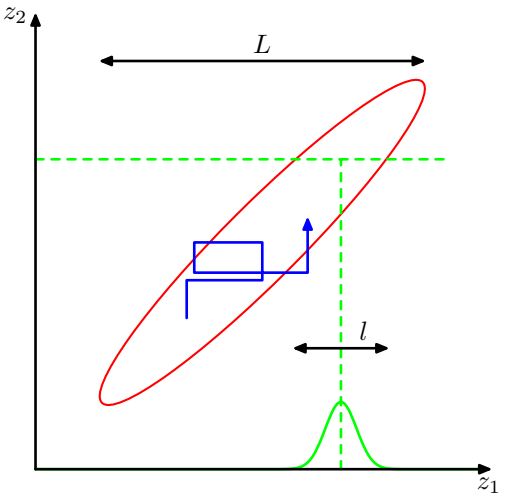


Figure 11.11 Illustration of Gibbs sampling by alternate updates of two variables whose distribution is a correlated Gaussian. The step size is governed by the standard deviation of the conditional distribution (green curve), and is $O(l)$, leading to slow progress in the direction of elongation of the joint distribution (red ellipse). The number of steps needed to obtain an independent sample from the distribution is $O((L/l)^2)$.

the conditional distributions are Gaussian, which represents a more general class of distributions than the multivariate Gaussian because, for example, the non-Gaussian distribution $p(z, y) \propto \exp(-z^2y^2)$ has Gaussian conditional distributions. At each step of the Gibbs sampling algorithm, the conditional distribution for a particular component z_i has some mean μ_i and some variance σ_i^2. In the over-relaxation framework, the value of z_i is replaced with

$$z_i' = \mu_i + \alpha(z_i - \mu_i) + \sigma_i(1 - \alpha_i^2)^{1/2}\nu \tag{11.50}$$

where ν is a Gaussian random variable with zero mean and unit variance, and α is a parameter such that $-1 < \alpha < 1$. For $\alpha = 0$, the method is equivalent to standard Gibbs sampling, and for $\alpha < 0$ the step is biased to the opposite side of the mean. This step leaves the desired distribution invariant because if z_i has mean μ_i and variance σ_i^2, then so too does z_i'. The effect of over-relaxation is to encourage directed motion through state space when the variables are highly correlated. The framework of *ordered over-relaxation* (Neal, 1999) generalizes this approach to non-Gaussian distributions.

The practical applicability of Gibbs sampling depends on the ease with which samples can be drawn from the conditional distributions $p(z_k|\mathbf{z}_{\setminus k})$. In the case of probability distributions specified using graphical models, the conditional distributions for individual nodes depend only on the variables in the corresponding Markov blankets, as illustrated in Figure 11.12. For directed graphs, a wide choice of conditional distributions for the individual nodes conditioned on their parents will lead to conditional distributions for Gibbs sampling that are log concave. The adaptive rejection sampling methods discussed in Section 11.1.3 therefore provide a framework for Monte Carlo sampling from directed graphs with broad applicability.

If the graph is constructed using distributions from the exponential family, and if the parent-child relationships preserve conjugacy, then the full conditional distributions arising in Gibbs sampling will have the same functional form as the orig-

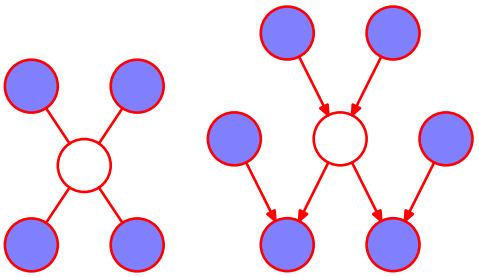


Figure 11.12 The Gibbs sampling method requires samples to be drawn from the conditional distribution of a variable conditioned on the remaining variables. For graphical models, this conditional distribution is a function only of the states of the nodes in the Markov blanket. For an undirected graph this comprises the set of neighbours, as shown on the left, while for a directed graph the Markov blanket comprises the parents, the children, and the co-parents, as shown on the right.

inal conditional distributions (conditioned on the parents) defining each node, and so standard sampling techniques can be employed. In general, the full conditional distributions will be of a complex form that does not permit the use of standard sampling algorithms. However, if these conditionals are log concave, then sampling can be done efficiently using adaptive rejection sampling (assuming the corresponding variable is a scalar).

If, at each stage of the Gibbs sampling algorithm, instead of drawing a sample from the corresponding conditional distribution, we make a point estimate of the variable given by the maximum of the conditional distribution, then we obtain the iterated conditional modes (ICM) algorithm discussed in Section 8.3.3. Thus ICM can be seen as a greedy approximation to Gibbs sampling.

Because the basic Gibbs sampling technique considers one variable at a time, there are strong dependencies between successive samples. At the opposite extreme, if we could draw samples directly from the joint distribution (an operation that we are supposing is intractable), then successive samples would be independent. We can hope to improve on the simple Gibbs sampler by adopting an intermediate strategy in which we sample successively from groups of variables rather than individual variables. This is achieved in the *blocking Gibbs* sampling algorithm by choosing blocks of variables, not necessarily disjoint, and then sampling jointly from the variables in each block in turn, conditioned on the remaining variables (Jensen *et al.*, 1995).

11.4. Slice Sampling

We have seen that one of the difficulties with the Metropolis algorithm is the sensitivity to step size. If this is too small, the result is slow decorrelation due to random walk behaviour, whereas if it is too large the result is inefficiency due to a high rejection rate. The technique of *slice sampling* (Neal, 2003) provides an adaptive step size that is automatically adjusted to match the characteristics of the distribution. Again it requires that we are able to evaluate the unnormalized distribution $\widetilde{p}(\mathbf{z})$.

Consider first the univariate case. Slice sampling involves augmenting z with an additional variable u and then drawing samples from the joint (z, u) space. We shall see another example of this approach when we discuss hybrid Monte Carlo in Section 11.5. The goal is to sample uniformly from the area under the distribution

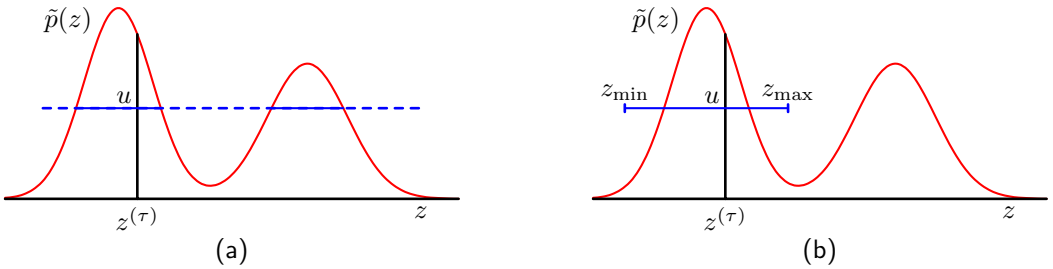


Figure 11.13 Illustration of slice sampling. (a) For a given value $z^{(\tau)}$, a value of u is chosen uniformly in the region $0 \leqslant u \leqslant \widetilde{p}(z^{(\tau)})$, which then defines a 'slice' through the distribution, shown by the solid horizontal lines. (b) Because it is infeasible to sample directly from a slice, a new sample of z is drawn from a region $z_{\min} \leqslant z \leqslant z_{\max}$, which contains the previous value $z^{(\tau)}$.

given by

$$\widehat{p}(z,u) = \begin{cases} 1/Z_p & \text{if } 0 \leqslant u \leqslant \widetilde{p}(z) \\ 0 & \text{otherwise} \end{cases} \tag{11.51}$$

where $Z_p = \int \widetilde{p}(z)\,\mathrm{d}z$. The marginal distribution over z is given by

$$\int \widehat{p}(z,u)\,\mathrm{d}u = \int_0^{\widetilde{p}(z)} \frac{1}{Z_p}\,\mathrm{d}u = \frac{\widetilde{p}(z)}{Z_p} = p(z) \tag{11.52}$$

and so we can sample from $p(z)$ by sampling from $\widehat{p}(z,u)$ and then ignoring the u values. This can be achieved by alternately sampling z and u. Given the value of z we evaluate $\widetilde{p}(z)$ and then sample u uniformly in the range $0 \leqslant u \leqslant \widetilde{p}(z)$, which is straightforward. Then we fix u and sample z uniformly from the 'slice' through the distribution defined by $\{z : \widetilde{p}(z) > u\}$. This is illustrated in Figure 11.13(a).

In practice, it can be difficult to sample directly from a slice through the distribution and so instead we define a sampling scheme that leaves the uniform distribution under $\widehat{p}(z,u)$ invariant, which can be achieved by ensuring that detailed balance is satisfied. Suppose the current value of z is denoted $z^{(\tau)}$ and that we have obtained a corresponding sample u. The next value of z is obtained by considering a region $z_{\min} \leqslant z \leqslant z_{\max}$ that contains $z^{(\tau)}$. It is in the choice of this region that the adaptation to the characteristic length scales of the distribution takes place. We want the region to encompass as much of the slice as possible so as to allow large moves in z space while having as little as possible of this region lying outside the slice, because this makes the sampling less efficient.

One approach to the choice of region involves starting with a region containing $z^{(\tau)}$ having some width w and then testing each of the end points to see if they lie within the slice. If either end point does not, then the region is extended in that direction by increments of value w until the end point lies outside the region. A candidate value z' is then chosen uniformly from this region, and if it lies within the slice, then it forms $z^{(\tau+1)}$. If it lies outside the slice, then the region is shrunk such that z' forms an end point and such that the region still contains $z^{(\tau)}$. Then another