Explaining the Gibbs Sampler

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Computer-intensive algorithms, such as the Gibbs sampler, have become increasingly popular statistical tools, both in applied and theoretical work. The properties of such algorithms, however, may sometimes not be obvious. Here we give a simple explanation of how and why the Gibbs sampler works. We analytically establish its properties in a simple case and provide insight for more complicated cases. There are also a number of examples.

KEY WORDS: Data augmentation; Markov chains; Monte Carlo methods; Resampling techniques.

1. INTRODUCTION

The continuing availability of inexpensive, high-speed computing has already reshaped many approaches to statistics. Much work has been done on algorithmic approaches (such as the EM algorithm; Dempster, Laird, and Rubin 1977), or resampling techniques (such as the bootstrap; Efron 1982). Here we focus on a different type of computer-intensive statistical method, the Gibbs sampler.

The Gibbs sampler enjoyed an initial surge of popularity starting with the paper of Geman and Geman (1984), who studied image-processing models. The roots of the method, however, can be traced back to at least Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller (1953), with further development by Hastings (1970). More recently, Gelfand and Smith (1990) generated new interest in the Gibbs sampler by revealing its potential in a wide variety of conventional statistical problems.

The Gibbs sampler is a technique for generating random variables from a (marginal) distribution indirectly, without having to calculate the density. Although straightforward to describe, the mechanism that drives this scheme may seem mysterious. The purpose of this article is to demystify the workings of these algorithms by exploring simple cases. In such cases, it is easy to see that Gibbs sampling is based only on elementary properties of Markov chains.

Through the use of techniques like the Gibbs sampler, we are able to avoid difficult calculations, replacing them instead with a sequence of easier calculations. These methodologies have had a wide impact on practical problems, as discussed in Section 6. Although most applications of the Gibbs sampler have been in Bayesian models, it is also extremely useful in classical (likelihood) calculations [see Tanner (1991) for many examples]. Furthermore, these calculational methodologies have also had an impact on theory. By freeing statisticians from dealing with complicated calculations, the statistical aspects of a problem can become the main focus. This point is wonderfully illustrated by Smith and Gelfand (1992).

In the next section we describe and illustrate the application of the Gibbs sampler in bivariate situations. Section 3 is a detailed development of the underlying theory, given in the simple case of a 2×2 table with multinomial sampling. From this detailed development, the theory underlying general situations is more easily understood, and is also outlined. Section 4 elaborates the role of the Gibbs sampler in relating conditional and marginal distributions and illustrates some higher dimensional generalizations. Section 5 describes many of the implementation issues surrounding the Gibbs sampler, and Section 6 contains a discussion and describes many applications.

2. ILLUSTRATING THE GIBBS SAMPLER

Suppose we are given a joint density $f(x, y_1, \ldots, y_p)$, and are interested in obtaining characteristics of the marginal density

$$f(x) = \int \cdots \int f(x, y_1, \ldots, y_p)\, dy_1 \cdots dy_p, \quad (2.1)$$

such as the mean or variance. Perhaps the most natural and straightforward approach would be to calculate $f(x)$ and use it to obtain the desired characteristic. However, there are many cases where the integrations in (2.1) are extremely difficult to perform, either analytically or numerically. In such cases the Gibbs sampler provides an alternative method for obtaining $f(x)$.

Rather than compute or approximate $f(x)$ directly, the Gibbs sampler allows us effectively to generate a sample $X_1, \ldots, X_m \sim f(x)$ *without requiring* $f(x)$. By simulating a large enough sample, the mean, variance, or any other characteristic of $f(x)$ can be calculated to the desired degree of accuracy.

It is important to realize that, in effect, the end result of any calculations, although based on simulations, are the population quantities. For example, to calculate the mean of $f(x)$, we could use $(1/m)\sum_{i=1}^{m} X_i$, and the fact that

$$\lim_{m\to\infty} \frac{1}{m} \sum_{i=1}^{m} X_i = \int_{-\infty}^{\infty} xf(x)\, dx = EX. \quad (2.2)$$

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Thus, by taking m large enough, any population characteristic, even the density itself, can be obtained to any degree of accuracy.

To understand the workings of the Gibbs sampler, we first explore it in the two-variable case. Starting with a pair of random variables (X, Y), the Gibbs sampler generates a sample from $f(x)$ by sampling instead from the conditional distributions $f(x \mid y)$ and $f(y \mid x)$, distributions that are often known in statistical models. This is done by generating a "Gibbs sequence" of random variables

$$Y_0', X_0', Y_1', X_1', Y_2', X_2', \ldots, Y_k', X_k'. \quad (2.3)$$

The initial value $Y_0' = y_0'$ is specified, and the rest of (2.3) is obtained iteratively by alternately generating values from

$$X_j' \sim f(x \mid Y_j' = y_j')$$
$$Y_{j+1}' \sim f(y \mid X_j' = x_j'). \quad (2.4)$$

We refer to this generation of (2.3) as Gibbs sampling. It turns out that under reasonably general conditions, the distribution of X_k' converges to $f(x)$ (the true marginal of X) as $k \to \infty$. Thus, for k large enough, the final observation in (2.3), namely $X_k' = x_k'$, is effectively a sample point from $f(x)$.

The convergence (in distribution) of the Gibbs sequence (2.3) can be exploited in a variety of ways to obtain an approximate sample from $f(x)$. For example, Gelfand and Smith (1990) suggest generating m independent Gibbs sequences of length k, and then using the final value of X_k' from each sequence. If k is chosen large enough, this yields an approximate iid sample from $f(x)$. Methods for choosing such k, as well as alternative approaches to extracting information from the Gibbs sequence, are discussed in Section 5. For the sake of clarity and consistency, we have used only the preceding approach in all of the illustrative examples that follow.

Example 1. For the following joint distribution of X and Y,

$$f(x, y) \propto \binom{n}{x} y^{x+\alpha-1}(1-y)^{n-x+\beta-1},$$
$$x = 0, 1, \ldots, n \quad 0 \le y \le 1, \quad (2.5)$$

suppose we are interested in calculating some characteristics of the marginal distribution $f(x)$ of X. The Gibbs sampler allows us to generate a sample from this marginal as follows. From (2.5) it follows (suppressing the overall dependence on n, α, and β) that

$$f(x \mid y) \text{ is Binomial } (n, y) \quad (2.6a)$$
$$f(y \mid x) \text{ is Beta } (x + \alpha, n - x + \beta). \quad (2.6b)$$

If we now apply the iterative scheme (2.4) to the distributions (2.6), we can generate a sample $X_1, X_2, \ldots, X_m$ from $f(x)$ and use this sample to estimate any desired characteristic.

As the reader may have already noticed, Gibbs sampling is actually not needed in this example, since $f(x)$ can be obtained analytically from (2.5) as

$$f(x) = \binom{n}{x} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{\Gamma(x+\alpha)\Gamma(n-x+\beta)}{\Gamma(\alpha+\beta+n)},$$
$$x = 0, 1, \ldots, n, \quad (2.7)$$

the beta-binomial distribution. Here, characteristics of $f(x)$ can be directly obtained from (2.7), either analytically or by generating a sample from the marginal and not fussing with the conditional distributions. However, this simple situation is useful for illustrative purposes. Figure 1 displays histograms of two samples $x_1, \ldots, x_m$ of size $m = 500$ from the beta-binomial distribution of (2.7) with $n = 16$, $\alpha = 2$, and $\beta = 4$.

The two histograms are very similar, giving credence to the claim that the Gibbs scheme for random variable generation is indeed generating variables from the marginal distribution.

One feature brought out by Example 1 is that the Gibbs sampler is really not needed in any bivariate situation where the joint distribution $f(x, y)$ can be calculated, since $f(x) = f(x, y)/f(y \mid x)$. However, as the next example shows, Gibbs sampling may be indispensable in situations where $f(x, y)$, $f(x)$, or $f(y)$ cannot be calculated.

Example 2. Suppose X and Y have conditional distributions that are exponential distributions restricted to the interval $(0, B)$, that is,

$$f(x \mid y) \propto ye^{-yx}, \quad 0 < x < B < \infty \quad (2.8a)$$
$$f(y \mid x) \propto xe^{-xy}, \quad 0 < y < B < \infty, \quad (2.8b)$$

where B is a known positive constant. The restriction to the interval $(0, B)$ ensures that the marginal $f(x)$ exists. Although the form of this marginal is not easily calculable, by applying the Gibbs sampler to the conditionals in (2.8) any characteristic of $f(x)$ can be obtained.

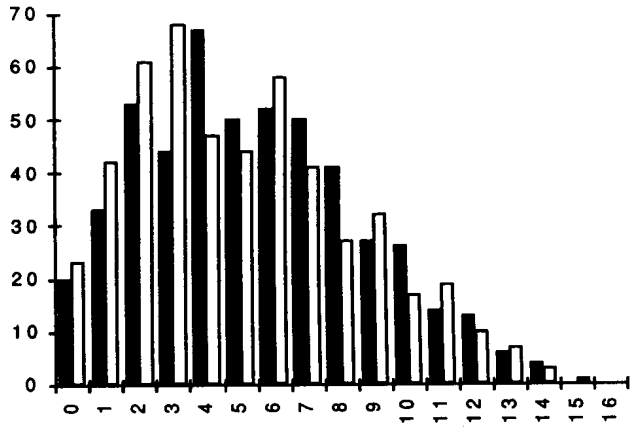

Figure 1. Comparison of Two Histograms of Samples of Size $m = 500$ From the Beta-Binomial Distribution With $n = 16$, $\alpha = 2$, and $\beta = 4$. The black histogram sample was obtained using Gibbs sampling with $k = 10$. The white histogram sample was generated directly from the beta-binomial distribution.

In Figure 2 we display a histogram of a sample of size $m = 500$ from $f(x)$ obtained by using the final values from Gibbs sequences of length $k = 15$.

In Section 4 we see that if B is not finite, then the densities in (2.8) are not a valid pair of conditional densities in the sense that there is no joint density $f(x, y)$ to which they correspond, and the Gibbs sequence fails to converge.

Gibbs sampling can be used to estimate the density itself by averaging the final conditional densities from each Gibbs sequence. From (2.3), just as the values $X_k' = x_k'$ yield a realization of $X_1, \cdots, X_m \sim f(x)$, the values $Y_k' = y_k'$ yield a realization of $Y_1, \cdots, Y_m \sim f(y)$. Moreover, the average of the conditional densities $f(x \mid Y_k' = y_k')$ will be a close approximation to $f(x)$, and we can estimate $f(x)$ with

$$\hat{f}(x) = \frac{1}{m} \sum_{i=1}^{m} f(x \mid y_i), \tag{2.9}$$

where $y_1, \cdots, y_m$ is the sequence of realized values of final Y observations from each Gibbs sequence. The theory behind the calculation in (2.9) is that the expected value of the conditional density is

$$E[f(x \mid Y)] = \int f(x \mid y) f(y)\, dy = f(x), \tag{2.10}$$

a calculation mimicked by (2.9), since $y_1, \cdots, y_m$ approximate a sample from $f(y)$. For the densities in (2.8), this estimate of $f(x)$ is shown in Figure 2.

Example 1 (continued): The density estimate methodology of (2.9) can also be used in discrete distributions, which we illustrate for the beta-binomial of Example 1. Using the observations generated to construct Figure 1, we can, analogous to (2.9), estimate the marginal probabilities of X using

$$\hat{P}(X = x) = \frac{1}{m} \sum_{i=1}^{m} P(X = x \mid Y_i = y_i). \tag{2.11}$$

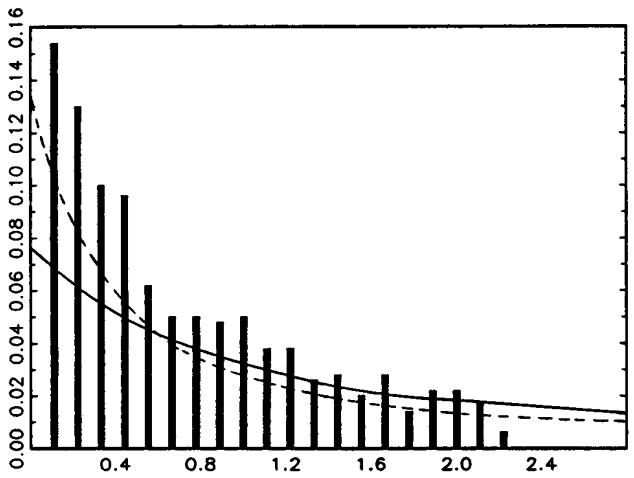

Figure 2. Histogram for x of a Sample of Size m = 500 From the Pair of Conditional Distributions in (2.8), With B = 5, Obtained Using Gibbs Sampling With k = 15 Along With an Estimate of the Marginal Density Obtained From Equation (2.9) (solid line). The dashed line is the true marginal density, as explained in Section 4.1.

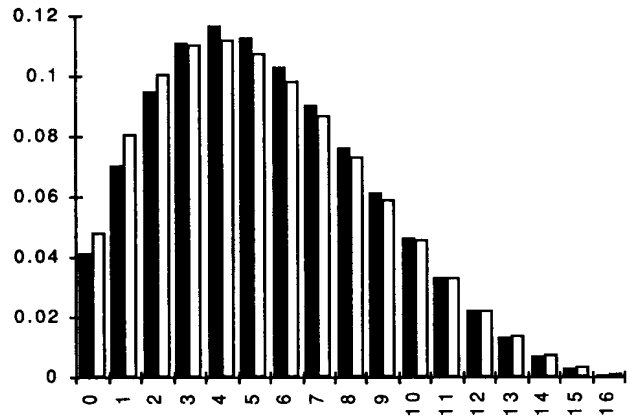

Figure 3. Comparison of Two Probability Histograms of the Beta-Binomial Distribution With n = 16, α = 2, and β = 4. The black histogram represents estimates of the marginal distribution of X using Equation (2.11), based on a sample of Size m = 500 from the pair of conditional distributions in (2.6). The Gibbs sequence had length k = 10. The white histogram represents the exact beta-binomial probabilities.

Figure 3 displays these probability estimates overlayed with the exact beta-binomial probabilities for comparison.

The density estimates (2.9) and (2.11) illustrate an important aspect of using the Gibbs sampler to evaluate characteristics of $f(x)$. The quantities $f(x \mid y_1), \cdots, f(x \mid y_m)$, calculated using the simulated values $y_1, \cdots, y_m$, carry more information about $f(x)$ than $x_1, \cdots, x_m$ alone, and will yield better estimates. For example, an estimate of the mean of $f(x)$ is $(1/m)\ \Sigma_{i=1}^{m}\ x_i$, but a better estimate is $(1/m)\ \Sigma_{i=1}^{m}\ E(X \mid y_i)$, as long as these conditional expectations are obtainable. The intuition behind this feature is the Rao-Blackwell theorem (illustrated by Gelfand and Smith 1990), and established analytically by Liu, Wong, and Kong (1991).

3. A SIMPLE CONVERGENCE PROOF

It is not immediately obvious that a random variable with distribution $f(x)$ can be produced by the Gibbs sequence of (2.3) or that the sequence even converges. That this is so relies on the Markovian nature of the iterations, which we now develop in detail for the simple case of a 2×2 table with multinomial sampling.

Suppose X and Y are each (marginally) Bernoulli random variables with joint distribution

		X = 0	X = 1
Y	0	p_1	p_2
	1	p_3	p_4

$$p_i \geq 0, p_1 + p_2 + p_3 + p_4 = 1,$$

or, in terms of the joint probability function,

$$\begin{bmatrix} f_{x,y}(0,0) & f_{x,y}(1,0) \\ f_{x,y}(0,1) & f_{x,y}(1,1) \end{bmatrix} = \begin{bmatrix} p_1 & p_2 \\ p_3 & p_4 \end{bmatrix}.$$

For this distribution, the marginal distribution of x is given by

$$f_x = [f_x(0) \quad f_x(1)] = [p_1 + p_3 \quad p_2 + p_4], \quad (3.1)$$

a Bernoulli distribution with success probability $p_2 + p_4$.

The conditional distributions of $X \mid Y = y$ and $Y \mid X = x$ are straightforward to calculate. For example the distribution of $X \mid Y = 1$ is Bernoulli with success probability $p_4/(p_3 + p_4)$. All of the conditional probabilities can be expressed in two matrices,

$$A_{y|x} = \begin{bmatrix} \frac{p_1}{p_1 + p_3} & \frac{p_3}{p_1 + p_3} \\ \frac{p_2}{p_2 + p_4} & \frac{p_4}{p_2 + p_4} \end{bmatrix}$$

and

$$A_{x|y} = \begin{bmatrix} \frac{p_1}{p_1 + p_2} & \frac{p_2}{p_1 + p_2} \\ \frac{p_3}{p_3 + p_4} & \frac{p_4}{p_3 + p_4} \end{bmatrix},$$

where $A_{y|x}$ has the conditional probabilities of Y given $X = x$, and $A_{y|x}$ has the conditional probabilities of X given $Y = y$.

The iterative sampling scheme applied to this distribution yields (2.3) as a sequence of 0's and 1's. The matrices $A_{x|y}$ and $A_{y|x}$ may be thought of as transition matrices giving the probabilities of getting to x states from y states and vice versa, that is, $P(X = x \mid Y = y)$ = probability of going from state y to state x.

If we are only interested in generating the marginal distribution of X, we are mainly concerned with the X' sequence from (2.3). To go from $X_0' \to X_1'$ we have to go through Y_1', so the iteration sequence is $X_0' \to Y_1' \to X_1'$, and $X_0' \to X_1'$ forms a Markov chain with transition probability

$$P(X_1' = x_1 \mid X_0' = x_0) = \sum_y P(X_1' = x_1 \mid Y_1' = y) \times P(Y_1' = y \mid X_0' = x_0). \quad (3.2)$$

The transition probability matrix of the X' sequence, $A_{x|x}$, is given by

$$A_{x|x} = A_{y|x}A_{x|y},$$

and now we can easily calculate the probability distribution of any X_k' in the sequence. That is, the transition matrix that gives $P(X_k' = x_k \mid X_0' = x_0)$ is $(A_{x|x})^k$. Furthermore, if we write

$$f_k = [f_k(0) \quad f_k(1)]$$

to denote the marginal probability distribution of X_k', then for any k,

$$f_k = f_0A_{x|x}^k = (f_0A_{x|x}^{k-1})A_{x|x} = f_{k-1}A_{x|x}. \quad (3.3)$$

It is well known (see, for example, Hoel, Port, and Stone 1972), that as long as all the entries of $A_{x|x}$ are positive, then (3.3) implies that for any initial probability f_0, as $k \to \infty$, f_k converges to the unique distribution f that is a *stationary point* of (3.3), and satisfies

$$fA_{x|x} = f. \quad (3.4)$$

Thus, if the Gibbs sequence converges, the f that satisfies (3.4) must be the marginal distribution of X. Intuitively, there is nowhere else for this iteration to go; in the long run we will get X's in the proportion dictated by the marginal distribution. However, it is straightforward to check that (3.4) is satisfied by f_x of (3.1), that is,

$$f_xA_{x|x} = f_xA_{y|x}A_{x|y} = f_x.$$

As $k \to \infty$, the distribution of X_k' gets closer to f_x, so if we stop the iteration scheme (2.3) at a large enough value of k, we can assume that the distribution of X_k' is approximately f_x. Moreover, the larger the value of k, the better the approximation. This topic is discussed further in Section 5.

The algebra for the 2×2 case immediately works for any $n \times m$ joint distribution of X's and Y's. We can analogously define the $n \times n$ transition matrix $A_{x|x}$ whose stationary distribution will be the marginal distribution of X. If either (or both) of X and Y are continuous, then the finite dimensional arguments will not work. However, with suitable assumptions, all of the theory still goes through, so the Gibbs sampler still produces a sample from the marginal distribution of X. Equation (3.2) would now represent the conditional density of X_1' given X_0', and could be written

$$f_{X_1'|X_0'}(x_1 \mid x_0) = \int f_{X_1'|Y_1'}(x_1 \mid y)f_{Y_1'|X_0'}(y \mid x_0)\, dy.$$

(Sometimes it is helpful to use subscripts to denote the density.) Then, step by step, we could write the conditional densities of $X_2'|X_0'$, $X_3'|X_0'$, $X_4'|X_0'$, $\cdots$. Similar to the k-step transition matrix $(A_{x|x})^k$, we derive an "infinite transition matrix" with entries that satisfy the relationship

$$f_{X_k'|X_0'}(x \mid x_0) = \int f_{X_k'|X_{k-1}'}(x \mid t)f_{X_{k-1}'|X_0'}(t \mid x_0)\, dt, \quad (3.5)$$

which is the continuous version of (3.3). The density $f_{X_k'|X_{k-1}'}$ represents a one-step transition, and the other two densities play the role of f_k and f_{k-1}. As $k \to \infty$, it again follows that the stationary point of (3.5) is the marginal density of X, the density to which $f_{X_k'|X_{k-1}'}$ converges.

4. CONDITIONALS DETERMINE MARGINALS

Gibbs sampling can be thought of as a practical implementation of the fact that knowledge of the conditional distributions is sufficient to determine a joint distribution (if it exists!). In the bivariate case, the derivation of the marginal from the conditionals is fairly straightforward. Complexities in the multivariate case, however, make these connections more obscure. We

begin with some illustrations in the bivariate case and then investigate higher dimensional cases.

4.1 The Bivariate Case

Suppose that, for two random variables X and Y, we know the conditional densities $f_{X|Y}(x \mid y)$ and $f_{Y|X}(y \mid x)$. We can determine the marginal density of X, $f_X(x)$, and hence the joint density of X and Y, through the following argument. By definition,

$$f_X(x) = \int f_{XY}(x, y)\, dy,$$

where $f_{XY}(x, y)$ is the (unknown) joint density. Now using the fact that $f_{XY}(x, y) = f_{X|Y}(x \mid y)f_Y(y)$, we have

$$f_X(x) = \int f_{X|Y}(x \mid y)f_Y(y)\, dy,$$

and if we similarly substitute for $f_Y(y)$, we have

$$\begin{aligned} f_X(x) &= \int f_{X|Y}(x \mid y) \int f_{Y|X}(y \mid t)f_X(t)\, dt\, dy \\ &= \int \left[\int f_{X|Y}(x \mid y)f_{Y|X}(y \mid t)\, dy \right] f_X(t)\, dt \\ &= \int h(x, t)f_X(t)\, dt, \end{aligned} \tag{4.1}$$

where $h(x, t) = [\int f_{X|Y}(x \mid y)f_{Y|X}(y \mid t)\, dy]$. Equation (4.1) defines a *fixed point integral equation* for which $f_X(x)$ is a solution. The fact that it is a unique solution is explained by Gelfand and Smith (1990).

Equation (4.1) is the limiting form of the Gibbs iteration scheme, illustrating how sampling from conditionals produces a marginal distribution. As $k \to \infty$ in (3.5),

$$f_{X_k|X_0}(x \mid x_0) \to f_X(x)$$

and

$$f_{X_k|X_{k-1}}(x \mid t) \to h(x, t), \tag{4.2}$$

and thus (4.1) is the limiting form of (3.5).

Although the joint distribution of X and Y determines all of the conditionals and marginals, it is not always the case that a set of proper conditional distributions will determine a proper marginal distribution (and hence a proper joint distribution). The next example shows this.

Example 2 (continued): Suppose that $B = \infty$ in (2.8), so that X and Y have the conditional densities

$$f(x \mid y) = ye^{-yx}, \quad 0 < x < \infty \tag{4.3a}$$

$$f(y \mid x) = xe^{-xy}, \quad 0 < y < \infty. \tag{4.3b}$$

Applying (4.1), the marginal distribution of X is the solution to

$$\begin{aligned} f_X(x) &= \left[\int ye^{-yx}te^{-ty}\, dy \right] f_X(t)\, dt \\ &= \int \left[\frac{t}{(x + t)^2} \right] f_X(t)\, dt. \end{aligned} \tag{4.4}$$

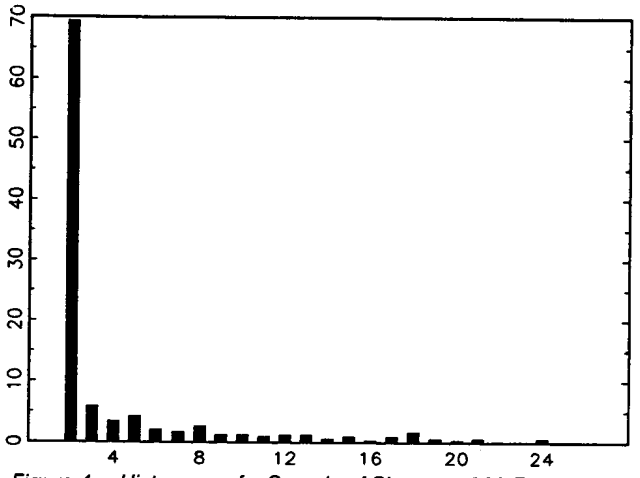

Figure 4. Histogram of a Sample of Size m = 500 From the Pair of Conditional Distributions in (4.3), Obtained Using Gibbs Sampling With k = 10.

Substituting $f_X(t) = 1/t$ into (4.4) yields

$$\frac{1}{x} = \int \left[\frac{t}{(x + t)^2} \right] \frac{1}{t}\, dt,$$

solving (4.4). Although this is a solution, $1/x$ is not a density function. When the Gibbs sampler is applied to the conditional densities in (4.3), convergence breaks down. It does not give an approximation to $1/x$, in fact, we do not get a sample of random variables from a marginal distribution. A histogram of such random variables is given in Figure 4, which vaguely mimics a graph of $f(x) = 1/x$.

It was pointed out by Trevor Sweeting (personal communication) that Equation (4.1) can be solved using the truncated exponential densities in (2.8). Evaluating the constant in the conditional densities gives $f(x|y) = ye^{-yx}/(1 - e^{-By})$, $0 < x < B$, with a similar expression for $f(y|x)$. Substituting these functions into (4.1) yields the solution $f(x) \propto (1 - e^{-Bx})/x$. This density (properly normalized) is the dashed line in Figure 2.

The Gibbs sampler fails when $B = \infty$ above because $\int f_X(x)dx = \infty$, and there is no convergence as described in (4.2). In a sense, we can say that a sufficient condition for the convergence in (4.2) to occur is that $f_X(x)$ is a proper density, that is $\int f_X(x)dx < \infty$. One way to guarantee this is to restrict the conditional densities to lie in a compact interval, as was done in (2.8). General convergence conditions needed for the Gibbs sampler (and other algorithms) are explored in detail by Schervish and Carlin (1990), and rates of convergence are also discussed by Roberts and Polson (1990).

4.2 More Than Two Variables

As the number of variables in a problem increase, the relationship between conditionals, marginals, and joint distributions becomes more complex. For example, the relationship conditional × marginal = joint does not hold for all of the conditionals and marginals. This means that there are many ways to set up a fixed-point equation like (4.1), and it is possible to use different sets of conditional distributions to calculate the

marginal of interest. Such methodologies are part of the general techniques of *substitution sampling* (see Gelfand and Smith 1990, for an explanation). Here we merely illustrate two versions of this technique.

In the case of two variables, all substitution sampling algorithms are the same. The three variable case, however, is sufficiently complex to illustrate the differences between algorithms, yet sufficiently simple to allow us to write things out in detail. Generalizing to cases of more than three variables is reasonably straightforward.

Suppose we would like to calculate the marginal distribution $f_X(x)$ in a problem with random variables X, Y, and Z. A fixed-point integral equation like (4.1) can be derived if we consider the pair (Y, Z) as a single random variable. We have

$$f_X(x) = \int \left[\iint f_{X|YZ}(x \mid y, z) f_{YZ|X}(y, z \mid t)\, dy\, dz \right] f_X(t)\, dt, \quad (4.5)$$

analogous to (4.1). Cycling between $f_{X|YZ}$ and $f_{YZ|X}$ would again result in a sequence of random variables converging in distribution to $f_X(x)$. This is the idea behind the Data Augmentation Algorithm of Tanner and Wong (1987). By sampling iteratively from $f_{X|YZ}$ and $f_{YZ|X}$, they show how to obtain successively better approximations to $f_X(x)$.

In contrast, the Gibbs sampler would sample iteratively from $f_{X|YZ}$, $f_{Y|XZ}$, and $f_{Z|XY}$. That is, the jth iteration would be

$$\begin{aligned} X_j' &\sim f(x \mid Y_j' = y_j', Z_j' = z_j') \\ Y_{j+1}' &\sim f(y \mid X_j' = x_j', Z_j' = z_j') \\ Z_{j+1}' &\sim f(z \mid X_j' = x_j', Y_{j+1}' = y_{j+1}'). \end{aligned} \quad (4.6)$$

The iteration scheme of (4.6) produces a Gibbs sequence

$$Y_0', Z_0', X_0', Y_1', Z_1', X_1', Y_2', Z_2', X_2', \ldots, \quad (4.7)$$

with the property that, for large k, $X_k' = x_k'$ is effectively a sample point from $f(x)$. Although it is not immediately evident, the iteration in (4.6) will also solve the fixed-point equation (4.5). In fact, a defining characteristic of the Gibbs sampler is that it always uses the full set of univariate conditionals to define the iteration. Besag (1974) established that this set is sufficient to determine the joint (and any marginal) distribution, and hence can be used to solve (4.5).

As an example of a three-variable Gibbs problem, we look at a generalization of the distribution examined in Example 1.

Example 3. In the distribution (2.5), we now let n be the realization of a Poisson random variable with mean λ, yielding the joint distribution

$$f(x, y, n) \propto \binom{n}{x} y^{x+\alpha-1}(1-y)^{n x+\beta-1} e^{-\lambda} \frac{\lambda^n}{n!},$$

$$x = 0, 1, \ldots, n,\ 0 \le y \le 1,\ n = 1, 2, \ldots. \quad (4.8)$$

Again, suppose we are interested in the marginal distribution of X. Unlike Example 1, here we cannot calculate the marginal distribution of X in closed form.

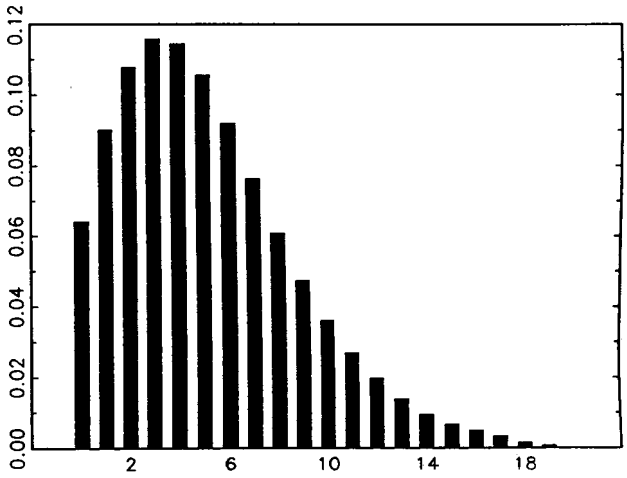

Figure 5. Estimates of Probabilities of the Marginal Distribution of X Using Equation (2.11), Based on a Sample of Size m = 500 From the Three Conditional Distributions in (4.9) With λ = 16, α = 2, and β = 4. The Gibbs sequences had length k = 10.

However, from (4.8) it is reasonably straightforward to calculate the three conditional densities. Suppressing dependence on λ, α, and β,

$$\begin{aligned} &f(x \mid y, n) \text{ is binomial } (n, y) \\ &f(y \mid x, n) \text{ is beta } (x + \alpha, n - x + \beta) \\ &f(n \mid x, y) \propto e^{-(1-y)\lambda} \frac{[(1-y)\lambda]^{n-x}}{(n-x)!}, \\ &\qquad n = x, x+1, \cdots. \end{aligned} \quad (4.9)$$

If we now apply the iterative scheme (4.6) to the distributions in (4.9), we can generate a sequence $X_1, X_2, \ldots, X_m$ from $f(x)$ and use this sequence to estimate the desired characteristic. The density estimate of $P(X = x)$, using Equation (2.11) can also be constructed. This is done and is given in Figure 5. This figure can be compared to Figure 3, but here there is a longer right tail from the Poisson variability.

The model (4.9) can have practical applications. For example, conditional on n and y, let x represent the number of successful hatchings from n insect eggs, where each egg has success probability y. Both n and y fluctuate across insects, which is modeled in their respective distributions, and the resulting marginal distribution of X is a typical number of successful hatchings among all insects.

5. EXTRACTING INFORMATION FROM GIBBS SEQUENCE

Some of the more important issues in Gibbs sampling surround the implementation and comparison of the various approaches to extracting information from the Gibbs sequence in (2.3). These issues are currently a topic of much debate and research.

5.1 Detecting Convergence

As illustrated in Section 3, the Gibbs sampler generates a Markov chain of random variables which converge to the distribution of interest $f(x)$. Many of the

popular approaches to extracting information from the Gibbs sequence exploit this property by selecting some large value for k, and then treating any X_j' for $j \geq k$ as a sample from $f(x)$. The problem then becomes that of choosing the appropriate value of k.

A general strategy for choosing such k is to monitor the convergence of some aspect of the Gibbs sequence. For example, Gelfand and Smith (1990) and Gelfand, Hills, Racine-Poor, and Smith (1990) suggest monitoring density estimates from m independent Gibbs sequences, and choosing k to be the first point at which these densities appear to be the same under a "felt-tip pen test." Tanner (1991) suggests monitoring a sequence of weights that measure the discrepancy between the sampled and the desired distribution. Geweke (in press) suggests monitoring based on time series considerations. Unfortunately, such monitoring approaches are not foolproof, illustrated by Gelman and Rubin (1991). An alternative may be to choose k based on theoretical considerations, as in Raftery and Banfield (1990). M.T. Wells (personal communication) has suggested a connection between selecting k and the cooling parameter in simulated annealing.

5.2 Approaches to Sampling the Gibbs Sequence

A natural alternative to sampling the kth or final value from many independent repetitions of the Gibbs sequence, as we did in Section 2, is to generate one long Gibbs sequence and then extract every rth observation (see Geyer, in press). For r large enough, this would also yield an approximate iid sample from $f(x)$. An advantage of this approach is that it lessens the dependence on initial values. A potential disadvantage is that the Gibbs sequence may stay in a small subset of the sample space for a long time (see Gelman and Rubin 1991).

For large, computationally expensive problems, a less wasteful approach to exploiting the Gibbs sequence is to use all realizations of X_j' for $j \leq k$, as in George and McCulloch (1991). Although the resulting data will be dependent, it will still be the case that the empirical distribution of X_j' converges to $f(x)$. Note that from this point of view one can see that the "efficiency of the Gibbs sampler" is determined by the rate of this convergence. Intuitively, this convergence rate will be fastest when X_j' moves rapidly through the sample space, a characteristic that may be thought of as mixing. Variations on these and other approaches to exploiting the Gibbs sequence have been suggested by Gelman and Rubin (1991), Geyer (in press), Muller (1991), Ritter and Tanner (1990), and Tierney (1991).

6. DISCUSSION

Both the Gibbs sampler and the Data Augmentation Algorithm have found widespread use in practical problems and can be used by either the Bayesian or classical statistician. For the Bayesian, the Gibbs sampler is mainly used to generate posterior distributions, whereas for the classical statistician a major use is for calculation of the likelihood function and characteristics of likelihood estimators.

Although the theory behind Gibbs sampling is taken from Markov chain theory, there is also a connection to "incomplete data" theory, such as that which forms the basis of the EM algorithm. Indeed, both Gibbs sampling and the EM algorithm seem to share common underlying structure. The recent book by Tanner (1991) provides explanations of all these algorithms and gives many illustrative examples.

The usefulness of the Gibbs sampler increases greatly as the dimension of a problem increases. This is because the Gibbs sampler allows us to avoid calculating integrals like (2.1), which can be prohibitively difficult in high dimensions. Moreover, calculations of the high dimensional integral can be replaced by a series of one-dimensional random variable generations, as in (4.6). Such generations can in many cases be accomplished efficiently (see Devroye 1986; Gilks and Wild 1992; Ripley 1987).

The ultimate value of the Gibbs sampler lies in its practical potential. Now that the groundwork has been laid in the pioneering papers of Geman and Geman (1984), Tanner and Wong (1987), and Gelfand and Smith (1990), research using the Gibbs sampler is exploding. A partial (and incomplete) list includes applications to generalized linear models [Dellaportas and Smith (1990), who implement the Gilks and Wild methodology, and Zeger and Rizaul Karim (1991)]; to mixture models (Diebolt and Robert 1990; Robert 1990; to evaluating computing algorithms (Eddy and Schervish 1990); to general normal data models (Gelfand, Hill, and Lee 1992); to DNA sequence modeling (Churchill and Casella 1991; Geyer and Thompson, in press); to applications in HIV modeling (Lange, Carlin, and Gelfand 1990); to outlier problems (Verdinelli and Wasserman 1990); to logistic regression (Albert and Chib 1991); to supermarket scanner data modeling (Blattberg and George 1991); to constrained parameter estimation (Gelfand et al. 1992); and to capture–recapture modeling (George and Robert 1991).

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