STSCI 4780
Conditional distributions & Gibbs sampling

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Agenda

1. **Joint from conditionals**

2. Gibbs sampling

Joint distribution from conditionals?

The symmetric parameterization of the BVN has 5 parameters:

- Marginal means: μ_x, μ_y
- Marginal standard deviations: σ_x, σ_y
- Correlation coefficient: ρ

If we fix $(\mu_x, \sigma_x, \mu_y, \sigma_y)$ and vary ρ, we generate a family of distributions with *identical marginals but different joint distributions*

Specifying marginals does not *uniquely determine the joint*

Specifying one marginal and its associated conditional does give the joint:

$$\begin{aligned} p(x, y) &= p(x)\, p(y|x) \\ &= p(y)\, p(x|y) \end{aligned}$$

What about *specifying the two conditionals*?

Hammersly-Clifford theorem

We'll be evaluating joint, marginal, and conditional distributions for multiple choices of (x, y), so we introduce notation distinguishing the various functions (instead of using $p()$ for everything):

$$
\begin{aligned}
f(x, y) &\equiv p(x, y) \\
m_1(x) &\equiv p(x) = \int \mathrm{d}y\, p(x, y) \\
m_2(y) &\equiv p(y) = \int \mathrm{d}x\, p(x, y) \\
c_{12}(x; y) &\equiv p(x|y) \\
c_{21}(y; x) &\equiv p(y|x)
\end{aligned}
$$

From the product rule, for any choice of a, b,

$$\begin{aligned} f(a,b) &= m_1(a)\, c_{21}(b;a) \\ \to m_1(a) &= \frac{f(a,b)}{c_{21}(b;a)},\ \text{for } \textit{any } b \\ \text{similarly } m_2(b) &= \frac{f(a,b)}{c_{12}(a;b)},\ \text{for } \textit{any } a \end{aligned}$$

Now use the product rule for $p(x, y)$, replacing marginals:

$$\begin{aligned} f(x,y) &= m_1(x)\, c_{21}(y;x) \\ &= \frac{f(x,b)}{c_{21}(b;x)}\, c_{21}(y;x),\ \text{for any } b \\ &= \frac{m_2(b) c_{12}(x;b)}{c_{21}(b;x)}\, c_{21}(y;x) \\ &= f(a,b) \frac{c_{12}(x;b)}{c_{12}(a;b)}\, \frac{c_{21}(y;x)}{c_{21}(b;x)} \end{aligned}$$

for any choice (a, b) (requires a *positivity condition*: support of joint = cartesian product of supports of marginals)

$$f(x, y) = f(a, b) \, \frac{c_{12}(x; b)}{c_{12}(a; b)} \, \frac{c_{21}(y; x)}{c_{21}(b; x)}$$

Here $f(a, b)$ is independent of (x, y), playing the role of a normalization constant for the remaining (x, y)-dependent factors

$$\int \mathrm{d}x \int \mathrm{d}y \; f(x, y) = f(a, b) \; \int \mathrm{d}x \int \mathrm{d}y \; \frac{c_{12}(x; b)}{c_{12}(a; b)} \, \frac{c_{21}(y; x)}{c_{21}(b; x)} = 1$$

Knowing all the conditionals
uniquely determines the joint

A slightly trickier approach gives a simpler result. Pick up from here:

$$f(x, y) = m_2(b)\frac{c_{12}(x; b)}{c_{21}(b; x)}\, c_{21}(y; x)$$

Bring the fraction to the other side, and integrate over b:

$$\begin{aligned}\int \mathrm{d}b\, f(x, y)\frac{c_{21}(b; x)}{c_{12}(x; b)} &= \int \mathrm{d}b\, m_2(b)\, c_{21}(y; x)\\ f(x, y)\int \mathrm{d}b\, \frac{c_{21}(b; x)}{c_{12}(x; b)} &= c_{21}(y; x)\end{aligned}$$

$$\Rightarrow \quad f(x, y) = \frac{c_{21}(y; x)}{\int \mathrm{d}b\, \frac{c_{21}(b;x)}{c_{12}(x;b)}}$$

Alternatively, starting with the $m_2 \times c_{12}$ factorization,

$$f(x, y) = \frac{c_{12}(x; y)}{\int \mathrm{d}a\, \frac{c_{12}(a;y)}{c_{21}(y;a)}}$$

Uses of this result (and its generalizations):

- Pseudo-likelihood methods
- Complex graphical models—Markov random fields
- *Gibbs sampling*: Using conditionals to build a MH proposal distribution

Agenda

1. Joint from conditionals

2. **Gibbs sampling**

Variable-at-time sampling

Motivation: We have fast algorithms to directly sample from many standard 1-D distributions, and good tools for sampling from non-standard 1-D distributions (e.g., inverse CDF, accept-reject). Can we build multivariate samplers by some kind of composition of 1-D samplers for the individual variables?

BVN example: We can draw an (x, y) pair using a marginal-conditional factorization, e.g.,

$$p(x, y) = p(x)\, p(y|x) \quad = \mathrm{Norm}(x|\mu_x, \sigma_x) \times \mathrm{Norm}(y|\beta_0 + \beta_1 x, \tilde{\sigma}_y)$$

Each of these is a univariate normal, for which we have fast direct samplers.

But this requires having the marginal $p(x) = \int \mathrm{d}y\, p(x, y)$ available. In Bayesian inference problems, we have the joint (prior $\times$ likelihood), but single-variable marginals generally aren't available.

Full conditionals

Full conditionals (conditionals for a subset of parameters given *all* of the others) are more readily available than marginals

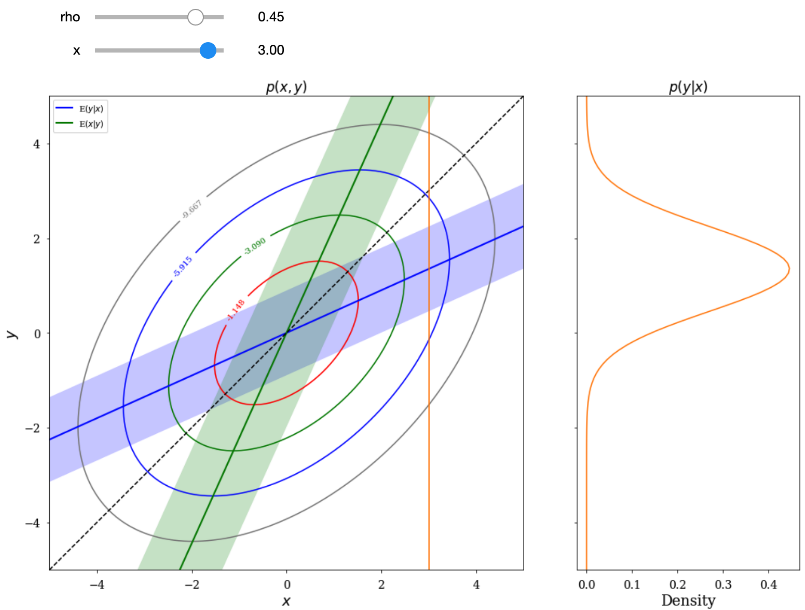
E.g., write $p(x, y, z) = p(y, z)\, p(x|y, z)$, so

$$p(x|y, z) = \frac{p(x, y, z)}{p(y, z)}$$

As a function of x, the RHS is proportional to the joint PDF, with $p(y, z)$ being a normalization constant

A full conditional is proportional to a "slice" of the joint

Moreover, for graphical models, full conditionals are often straightforward to compute, because conditional independence simplifies the conditioning (reduces the number of relevant variables) — see below



rho
0.45
x
3.00
$p(x, y)$
E(y|x)
E(x|y)
-9.667
-5.915
-3.090
-1.148
y
x
$p(y|x)$
Density

Gibbs sampling

Consider the MH algorithm for sampling from a 2-D distribution, $p(x, y)$, with proposal distribution $k(x', y'|x, y)$ for proposing a candidate new state (x', y') when the current state is (x, y)

The acceptance probability is $\alpha(x', y'|x, y) = \min[r(x', y'|x, y), 1]$ with

$$r(x', y'|x, y) = \frac{p(x', y')}{p(x, y)} \times \frac{k(x, y|x', y')}{k(x', y'|x, y)}$$

Suppose we update only x, by *sampling from the full conditional* $c_{12}(x; y) = p(x|y)$,

$$k(x', y'|x, y) = c_{12}(x'; y)\delta(y' - y)$$

The acceptance ratio is

$$r(x', y'|x, y) \quad = \quad \frac{p(x', y')}{p(x, y)} \times \frac{c_{12}(x; y')\delta(y - y')}{c_{12}(x'; y)\delta(y' - y)}$$

Accounting for $y' = y$ and using the product rule (being a bit cavalier with δs!),

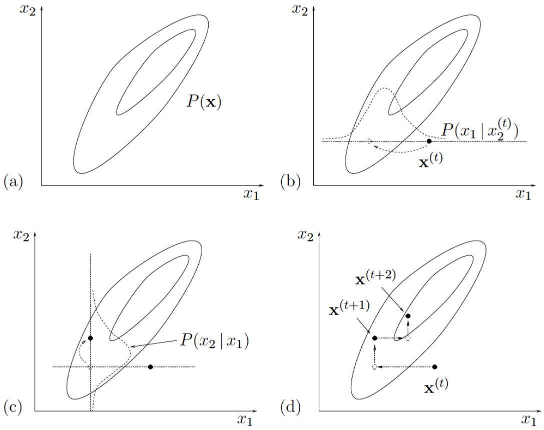
$$
\begin{aligned}
r(x', y'|x, y) &= \frac{p(x', y')}{p(x, y)} \times \frac{c_{12}(x; y')\delta(y - y')}{c_{12}(x'; y)\delta(y' - y)} \\
&= \frac{p(x', y)}{p(x, y)} \times \frac{c_{12}(x; y)}{c_{12}(x'; y)} \\
&= \frac{p(y)c_{12}(x'; y)}{p(y)c_{12}(x; y)} \times \frac{c_{12}(x; y)}{c_{12}(x'; y)} \\
&= 1
\end{aligned}
$$

We always accept a proposal from a full conditional!

If we only propose x updates, the chain is reducible $\rightarrow$ need to do one of these:

- **Random scan:** Randomly pick which parameter to update at each step
- **Cyclic scan:** Cycle through all parameters in a fixed order

This also works for *blocks* of parameters in many-parameter problems



(a) The joint density $P(\mathbf{x})$ from which samples are required. (b) Starting from a state $\mathbf{x}^{(t)}$, x_1 is sampled from the conditional density $P(x_1 \mid x_2^{(t)})$. (c) A sample is then made from the conditional density $P(x_2 \mid x_1)$. (d) A couple of iterations of Gibbs sampling.

MacKay (2003)

Finding full conditionals

For $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)$:

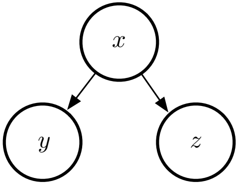
$$p(\theta_i|\boldsymbol{\theta}_{-i}) = \frac{p(\theta_1, \ldots, \theta_p)}{p(\theta_1, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_p)}$$

Denominator doesn't depend on θ_i: The full conditional PDF for θ_i is just the *joint PDF*, considered only as a function of θ_i (and appropriately normalized)

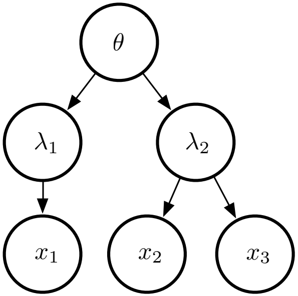
For each parameter θ_i (or block of parameters)

- Write the joint PDF, ignoring any constants of proportionality
- Drop any factors that don't depend on θ_i
- Try to identify the remaining function as the kernel for a known PDF (some numerical methods relax this, e.g., using 1-D accept-reject)

For graphical models, the DAG can guide identification of full conditionals—just use the factors from nodes that connect to the variable



$$p(x, y, z) = p(x)p(y|x)p(z|x)$$
$$p(z|x, y) = \frac{p(x, y, z)}{p(x, y)} = p(z|x)$$



$$\begin{aligned} p(\theta, \lambda, x) &= p(\theta)\, p(\lambda_1|\theta)\, p(\lambda_2|\theta) \\ &\qquad \times p(x_1|\lambda_1)p(x_2|\lambda_2)p(x_3|\lambda_2) \\ p(\lambda_2|\ldots) &\propto p(\lambda_2|\theta)\, p(x_2|\lambda_2)\, p(x_3|\lambda_2) \\ p(x_1|\ldots) &= p(x_1|\lambda_1) \end{aligned}$$