STSCI 4780
Conditional distributions & Gibbs sampling

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Agenda

1. **Joint from conditionals**
2. **Gibbs sampling**
3. **Appendix: Proof of the Hammersley-Clifford theorem**

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.

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*

Hammersley-Clifford theorem

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*?

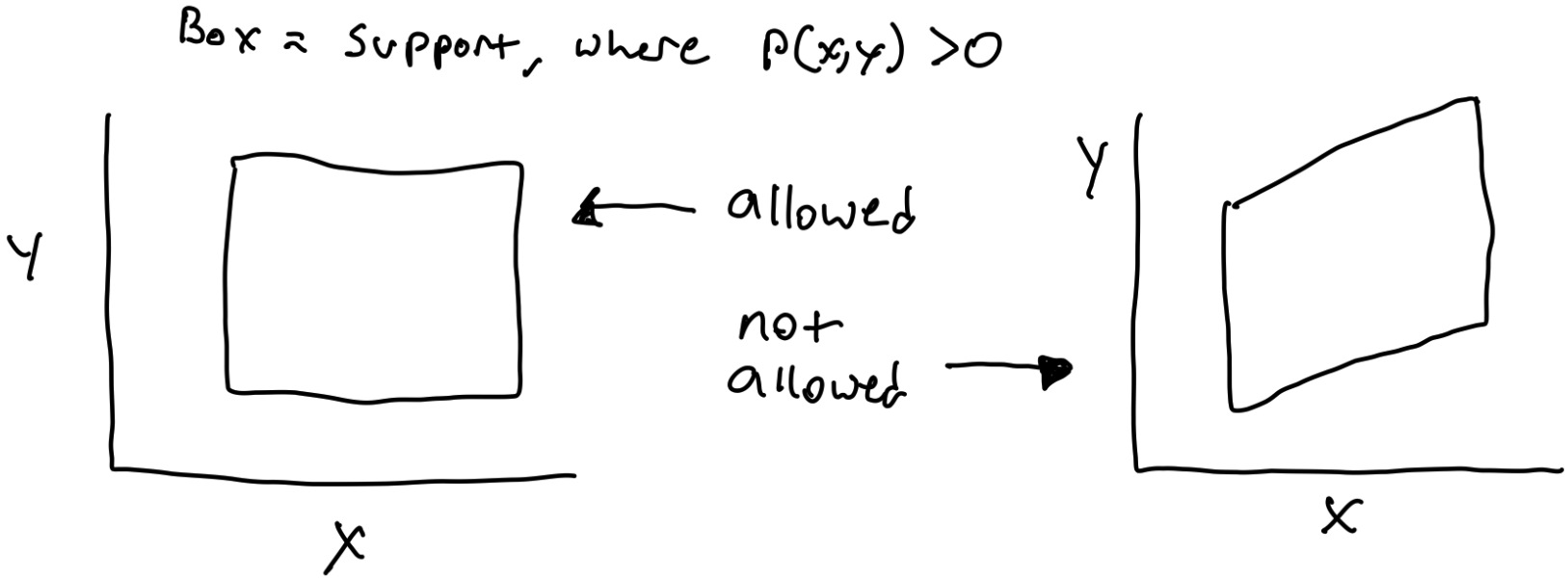
The Hammersley-Clifford theorem addresses this:

Knowing all the conditionals
uniquely determines the joint

There is a *positivity condition* on the joint dist'n: support of joint = cartesian product of supports of marginals (i.e., the range y can't depend on x, and vice versa)

(See appendix for proof of a special case.)

About the H-C positivity condition:



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

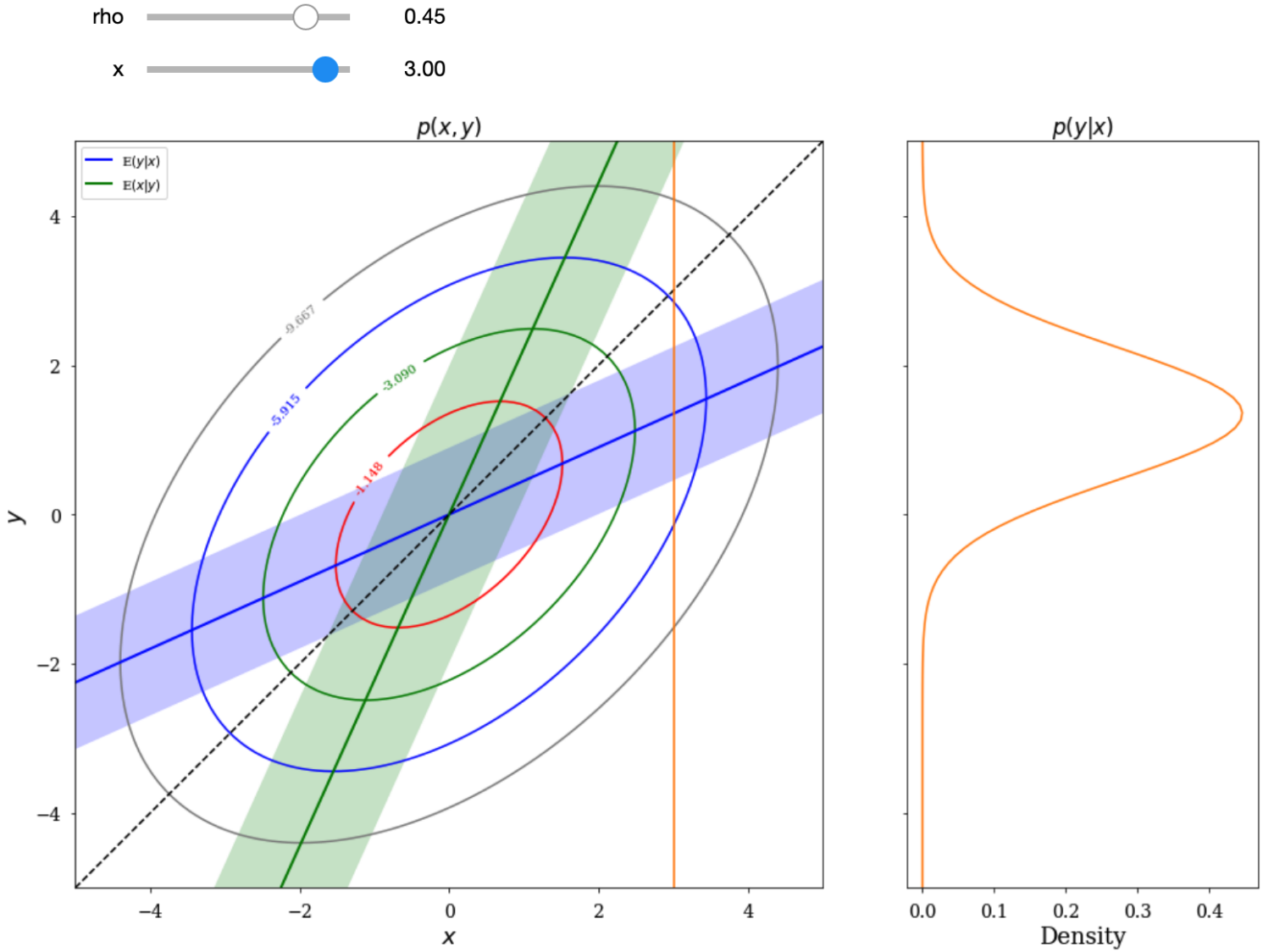
$$p(x|y, z) = \frac{p(x, y, z)}{p(y, z)}$$

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
(illustrated on next slide)

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

Slice along y of BVN(x,y)



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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* $c_{12}(x; y) = p(x|y)$, leaving y unchanged (setting $y' = y$); then

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

The acceptance ratio is

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

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

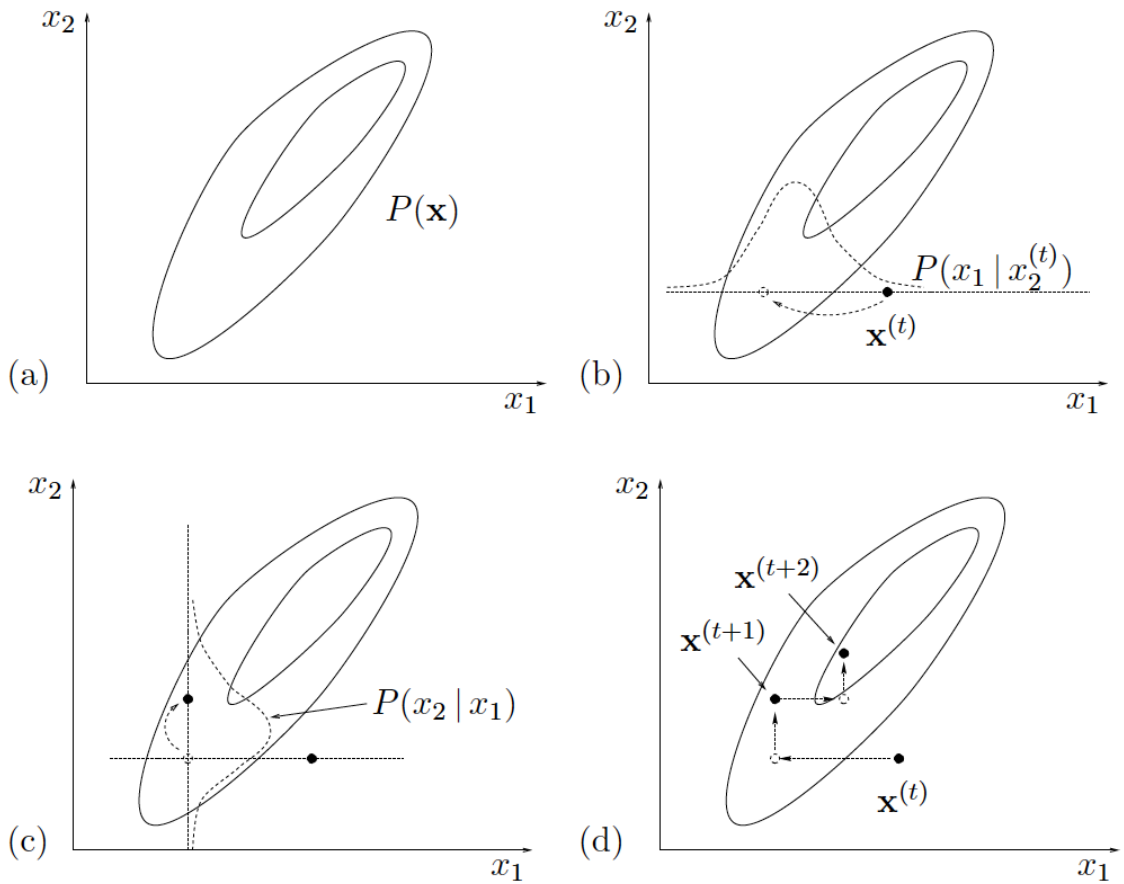
$$\begin{aligned} r(x', y'|x, y) &= \frac{p(x', y')}{p(x, y)} \times \frac{c_{12}(x; y')\delta(y - y')}{c_{12}(x'; y)\delta(y' - y)} \\ &= \frac{p(x', y)}{p(x, y)} \times \frac{c_{12}(x; y)}{c_{12}(x'; y)} \\ &= \frac{p(y)c_{12}(x'; y)}{p(y)c_{12}(x; y)} \times \frac{c_{12}(x; y)}{c_{12}(x'; y)} \\ &=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

We always accept a proposal from a full conditional!

If we only propose x updates, the chain is reducible (we don't explore y at all!) $\rightarrow$ 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 $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)$:

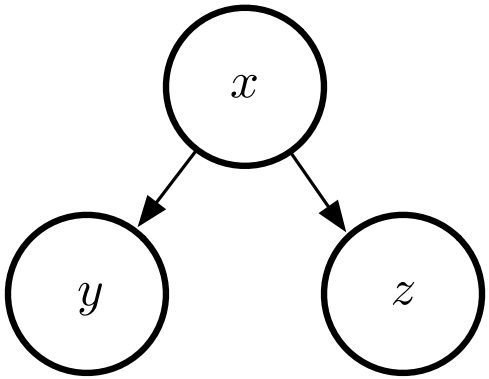
$$p(\theta_i | \boldsymbol{\theta}_{-i}) = \frac{p(\theta_1, \ldots, \theta_p)}{p(\theta_1, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_p)}$$

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)

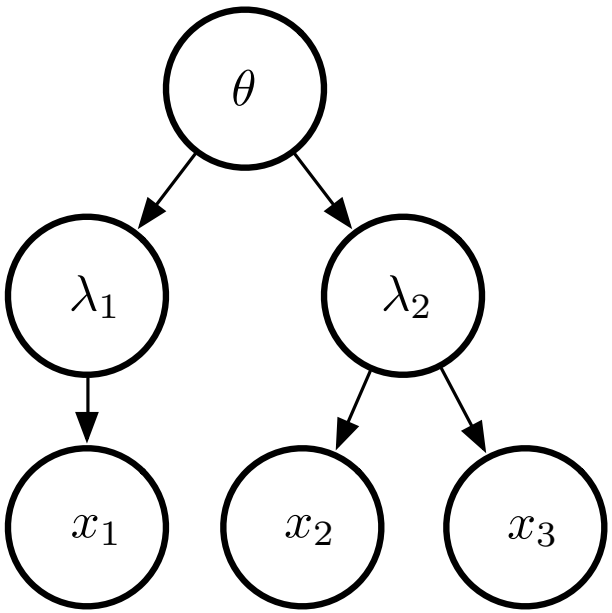
- Write the joint PDF, ignoring any constants of proportionality
- Drop any factors that don't depend on θ_i
- If possible, identify the remaining function as the kernel for a well-studied PDF with a known sampling algorithm; otherwise sample θ_i using accept/reject, Metropolis, etc.

For graphical models, the DAG can guide identification of full conditionals—for each node, its full conditions is the PDF for that node times the PDFs for the nodes it points to (the node's variable will appear in those PDFs)



$$p(x, y, z) = p(x)p(y|x)p(z|x)$$

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



$$p(\theta, \lambda, x) = p(\theta)\, p(\lambda_1|\theta)\, p(\lambda_2|\theta) \times p(x_1|\lambda_1)p(x_2|\lambda_2)p(x_3|\lambda_2)$$

$$p(\lambda_2|\ldots) \propto p(\lambda_2|\theta)\, p(x_2|\lambda_2)\, p(x_3|\lambda_2)$$

$$p(x_1|\ldots) = p(x_1|\lambda_1)$$

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Hammersley-Clifford theorem (special case)

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,

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

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:

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

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

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

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):

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