# Metropolis-Hastings (continued)

**Algorithm** (Metropolis-Hastings sampling). To construct a **Markov chain** whose **equilibrium distribution** is $p(\theta|y)$, choose a **proposal distribution** $g(\theta^*|\theta_t, y)$, define the **acceptance probability** $\alpha_{MH}(\theta^*|\theta_t, y)$ by (14), and

```
Initialize θ_0; t ← 0
Repeat {
  Sample θ* ~ g(θ|θ_t, y)
  Sample u ~ Uniform(0, 1)
  If u ≤ α_MH(θ*|θ_t, y) then θ_{t+1} ← θ*
    else θ_{t+1} ← θ_t
  t ← (t + 1)
}
```

(15)

When the proposal distribution is **symmetric** in the Metropolis et al. sense, the acceptance probability ratio reduces to $\frac{p(\theta^*|y)}{p(\theta_t|y)}$, which is easy to **motivate intuitively**: whatever the target density is at the current point $\theta_t$, you want to visit points of **higher density more often** and points of **lower density less often**, and it turns out that (14) does this for you in the natural and appropriate way.

As an example of the **MH algorithm in action**, consider a Gaussian model with **known mean** $\mu$ and **unknown variance** $\sigma^2$ applied to the NB10 data in part 2 of the lecture notes.

The **likelihood function** for $\sigma^2$, derived from the sampling model $(Y_i|\sigma^2) \overset{\text{IID}}{\sim} N(\mu, \sigma^2)$ for $i = 1, \ldots, n$, is

$$\begin{aligned} l(\sigma^2|y) &= c \prod_{i=1}^{n} (\sigma^2)^{-\frac{1}{2}} \exp\left[-\frac{(y_i-\mu)^2}{2\sigma^2}\right] \\ &= c\,(\sigma^2)^{-\frac{n}{2}} \exp\left[-\frac{\sum_{i=1}^{n}(y_i-\mu)^2}{2\sigma^2}\right]. \end{aligned} \tag{16}$$

# MH Sampling (continued)

This is recognizable as a member of the **Scaled Inverse** $\chi^2$ family $\chi^{-2}(\nu, s^2)$ (e.g., Gelman, Carlin et al. (2003)) of distributions, which (as we saw in part 2 of the lecture notes) is a **rescaled version** of the Inverse Gamma family chosen so that $s^2$ is an estimate of $\sigma^2$ based upon $\nu$ "observations."

You can now convince yourself that if the **prior** for $\sigma^2$ in this model is taken to be $\chi^{-2}(\nu, s^2)$, then the **posterior** for $\sigma^2$ will also be Scaled Inverse $\chi^2$: with this choice of prior

$$p(\sigma^2|y) = \chi^{-2}\left[\nu + n, \frac{\nu s^2 + \sum_{i=1}^{n}(y_i - \mu)^2}{\nu + n}\right]. \qquad (17)$$

This makes **good intuitive sense**: the **prior estimate** $s^2$ of $\sigma^2$ receives $\nu$ votes and the **sample estimate** $\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \mu)^2$ receives $n$ votes in the **posterior weighted average estimate** $\frac{\nu s^2 + n\widehat{\sigma}^2}{\nu + n}$.

Equation (17) provides a satisfying **closed-form solution** to the Bayesian updating problem in this model (e.g., it's easy to compute posterior moments **analytically**, and you can use numerical integration or well-known approximations to the CDF of the Gamma distribution to compute percentiles).

For **illustration purposes** suppose instead that you want to use **MH sampling** to summarize this posterior.

Then your main **choice** as a user of the algorithm is the specification of the **proposal distribution** (PD) $g\left(\sigma^2|\sigma_t^2, y\right)$.

The goal in choosing the PD is getting a chain that **mixes well** (moves freely and fluidly among all of the possible values of $\theta = \sigma^2$), and nobody has (yet) come up with a **sure-fire strategy** for always succeeding at this task.

Having said that, here are **two basic ideas** that often tend to **promote good mixing**:

# MH Sampling (continued)

(1) Pick a PD that looks like a **somewhat overdispersed version** of the posterior you're trying to sample from (e.g., Tierney (1996)).

Some work is naturally required to overcome the **circularity inherent** in this choice (if I fully knew $p(\theta|y)$ and all of its properties, why would I be using this algorithm in the first place?).

(2) Set up the PD so that the expected value of **where you're going to move to** ($\theta^*$), given that you **accept a move away from where you are now** ($\theta_t$), is to **stay where you are now**: $E_g(\theta^*|\theta_t, y) = \theta_t$.

That way, when you do make a move, there will be an **approximate left-right balance**, so to speak, in the direction you move away from $\theta_t$, which will encourage **rapid exploration of the whole space**.

Using idea (1), a decent choice for the PD in the Gaussian model with unknown variance might well be the **Scaled Inverse $\chi^2$ distribution**: $g\left(\sigma^2|\sigma_t^2, y\right) = \chi^{-2}\left(\nu_*, \sigma_*^2\right)$.

This distribution has **mean** $\frac{\nu_*}{\nu_*-2}\sigma_*^2$ for $\nu_* > 2$.

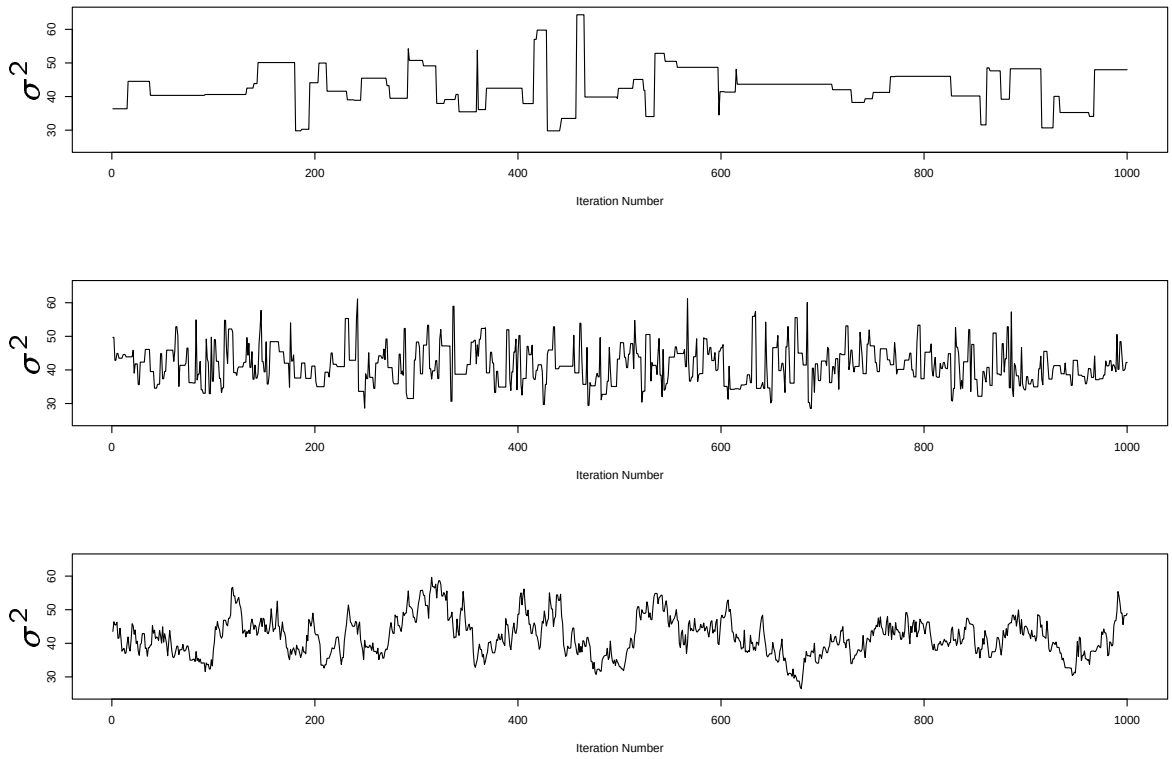
To use idea (2), then, I can **choose** any $\nu_*$ greater than 2 that I want, and as long as I take $\sigma_*^2 = \frac{\nu_*-2}{\nu_*}\sigma_t^2$ that will **center** the PD at $\sigma_t^2$ as desired.

So I'll **use**

$$g\left(\sigma^2|\sigma_t^2, y\right) = \chi^{-2}\left(\nu_*, \frac{\nu_* - 2}{\nu_*}\sigma_t^2\right). \tag{18}$$

This leaves $\nu_*$ as a kind of potential **tuning constant**—the hope is that I can vary $\nu_*$ to improve the **mixing** of the chain.

# MH Sampling (continued)




The above figure (motivated by an analogous plot in Gilks et al. (1996)) presents **time series traces** of some **typical output of the MH sampler** with $\nu_* = (2.5, 20, 500)$.

The **acceptance probabilities** with these values of $\nu_*$ are $(0.07, 0.44, 0.86)$, respectively.

The **SD** of the $\chi^{-2}\left(\nu_*, \frac{\nu_*-2}{\nu_*}\sigma_t^2\right)$ distribution is proportional to $\frac{\nu_*^2}{(\nu_*^2-2)^2\sqrt{\nu_*-4}}$, which decreases as $\nu_*$ increases, and this turns out to be **crucial**: when the proposal distribution SD is too **large** (small $\nu_*$, as in the top panel in the figure), the algorithm tries to make **big jumps** around $\theta$ space (good), but almost all of them get **rejected** (bad), so there are long periods of no movement at all, whereas when the PD SD is too **small** (large $\nu_*$; see the bottom panel of the figure), the algorithm **accepts** most of its proposed moves (good), but they're so tiny that it takes a **long time to fully explore the space** (bad).

# MH Sampling (continued)

Gelman, Roberts, et al. (1995) have shown that in simple problems with **approximately normal target distributions**, the **optimal acceptance rate** for MH samplers like the one illustrated here is about **44%** when the vector of unknowns is one-dimensional, and this can serve as a rough guide: you can **modify the proposal distribution SD** until the acceptance rate is around the Gelman et al. target figure.

The central panel of the figure displays the **best possible MH behavior** in this problem in the family of PDs chosen.

Even with this optimization you can see that the **mixing is not wonderful**, but contemporary computing speeds enable huge numbers of draws to be collected in a short period of time, compensating for the **comparatively slow rate** at which the MH algorithm learns about the posterior distribution of interest.

In this example the unknown quantity $\theta = \sigma^2$ was **real-valued**, but there's nothing in the MH method that requires this; in principle it works equally well when $\theta$ is a **vector of any finite dimension** (look back at the algorithm in (15) to verify this).

Notice, crucially, that to **implement** this algorithm you only need to know how to calculate $p(\theta|y)$ up to a **constant multiple**, since any such constant will **cancel** in computing the acceptance probability (15)—thus you're free to work with **unnormalized versions** of $p(\theta|y)$, which is a **great advantage** in practice.

# MH Sampling (continued)

There's even **more flexibility** in this algorithm than might first appear: it's often possible to identify a set $A$ of **auxiliary variables**—typically these are **latent** (unobserved) quantities—to be sampled along with the parameters, which have the property that they **improve the mixing** of the MCMC output (even though extra time is spent in sampling them).

When the set $(\theta, A)$ of quantities to be sampled is a **vector of length** $k$, there is additional flexibility: you can **block update** all of $(\theta, A)$ at once, or with appropriate modifications of the acceptance probability you can divide $(\theta, A)$ up into **components**, say $(\theta, A) = (\lambda_1, \ldots, \lambda_l)$, and **update the components one at a time** (as Metropolis et al. originally proposed in 1953).

The idea in this **component-by-component** version of the algorithm, which Gilks et al. (1996) call **single-component** MH sampling, is to have $k$ **different** proposal distributions, one for each component of $\theta$.

Each **iteration** of the algorithm (indexed as usual by $t$) has $k$ steps, indexed by $i$; at the beginning of iteration $t$ you **scan** along, updating $\lambda_1$ first, then $\lambda_2$, and so on until you've updated $\lambda_k$, which **concludes** iteration $t$.

Let $\lambda_{t,i}$ stand for the **current state** of component $i$ at the end of iteration $t$, and let $\lambda_{-i}$ stand for the $(\theta, A)$ vector with component $i$ **omitted** (the notation gets awkward here; it can't be helped).

The proposal distribution $g_i(\lambda_i^* | \lambda_{t,i}, \lambda_{t,-i}, y)$ for component $i$ is allowed to **depend** on the most recent versions of all components of $(\theta, A)$; here $\lambda_{t,-i}$ is the **current state** of $\lambda_{-i}$ after step $(i-1)$ of iteration $t$ is finished, so that components 1 through $(i-1)$ have been updated **but not the rest**.

# Gibbs Sampling

The **acceptance probability** for the proposed move to $\lambda_i^*$ that creates the **correct equilibrium distribution** turns out to be

$$\alpha_{MH}(\lambda_i^*|\lambda_{t,-i},\lambda_{t,i},y) = \min\left[1, \frac{p(\lambda_i^*|\lambda_{t,-i},y)\, g_i(\lambda_{t,i}|\lambda_i^*,\lambda_{t,-i},y)}{p(\lambda_{t,i}|\lambda_{t,-i},y)\, g_i(\lambda_i^*|\lambda_{t,i},\lambda_{t,-i},y)}\right]. \tag{19}$$

The distribution $p(\lambda_i|\lambda_{-i},y)$ appearing in (19), which is called the **full conditional** distribution for $\lambda_i$, has a natural interpretation: it represents the posterior distribution for the relevant portion of $(\theta, A)$ **given** $y$ **and the rest of** $(\theta, A)$.

The full conditional distributions act like **building blocks** in constructing the **complete posterior distribution** $p(\theta|y)$, in the sense that **any multivariate distribution is uniquely determined by its set of full conditionals** (Besag (1974)).

An **important special case** of **single-component MH sampling** arises when the **proposal distribution** $g_i(\lambda_i^*|\lambda_{t,i},\lambda_{t,-i},y)$ for component $i$ is chosen to be the **full conditional** $p(\lambda_i^*|\lambda_{t,-i},y)$ for $\lambda_i$: you can see from (19) that when this choice is made a **glorious cancellation** occurs and the **acceptance probability is 1**.

This is **Gibbs sampling**, independently (re)discovered by Geman and Geman (1984): the Gibbs recipe is to **sample from the full conditionals** and **accept all proposed moves**.

Even though it's **just a version of MH**, Gibbs sampling is important enough to merit a **summary** of its own.

**Single-element** Gibbs sampling, in which each real-valued coordinate $(\theta_1,\ldots,\theta_k)$ gets updated in turn, is probably the **most frequent** way Gibbs sampling gets used, so that's what I'll summarize ((20) details Gibbs sampling in the case with **no auxiliary variables** $A$, but the algorithm **works equally well** when $\theta$ is replaced by $(\theta, A)$ in the summary).

# Gibbs Sampling (continued)

**Algorithm** (Single-element Gibbs sampling). To construct a **Markov chain** whose **equilibrium distribution** is $p(\theta|y)$ with $\theta = (\theta_1, \ldots, \theta_k)$,

```
Initialize θ*_{0,1}, ..., θ*_{0,k};  t ← 0
Repeat {
  Sample θ*_{t+1,1} ~ p(θ_1 | y, θ*_{t,2}, θ*_{t,3}, θ*_{t,4}, ..., θ*_{t,k})
  Sample θ*_{t+1,2} ~ p(θ_2 | y, θ*_{t+1,1}, θ*_{t,3}, θ*_{t,4}, ..., θ*_{t,k})
  Sample θ*_{t+1,3} ~ p(θ_3 | y, θ*_{t+1,1}, θ*_{t+1,2}, θ*_{t,4}, ..., θ*_{t,k})
    ⋮          ⋮          ⋮          ⋮          ⋮          ⋮
  Sample θ*_{t+1,k} ~ p(θ_k | y, θ*_{t+1,1}, θ*_{t+1,2}, θ*_{t+1,3}, ..., θ*_{t+1,k-1})
  t ← (t + 1)
}
```

(20)

**Example:** the **NB10 Data**. Recall from the posterior predictive plot toward the end of part 2 of the lecture notes that the Gaussian model for the NB10 data was inadequate: the tails of the data distribution are **too heavy** for the Gaussian.

It was also clear from the normal qqplot that the data are **symmetric**.

This suggests thinking of the NB10 data values $y_i$ as like draws from a $t$ **distribution** with fairly small degrees of freedom $\nu$.

**One way** to write this model is

$$\begin{aligned} (\mu, \sigma^2, \nu) &\sim p(\mu, \sigma^2, \nu) \\ (y_i|\mu, \sigma^2, \nu) &\overset{\text{IID}}{\sim} t_\nu(\mu, \sigma^2), \end{aligned} \tag{21}$$

where $t_\nu(\mu, \sigma^2)$ denotes the **scaled** $t$**-distribution** with mean $\mu$, scale parameter $\sigma^2$, and shape parameter $\nu$.

# Model Expansion

This distribution has variance $\sigma^2\left(\frac{\nu}{\nu-2}\right)$ for $\nu > 2$ (so that shape and scale are mixed up, or **confounded** in $t_\nu(\mu, \sigma^2)$) and may be thought of as the distribution of the quantity $\mu + \sigma\, e$, where $e$ is a draw from the **standard** $t$ distribution that is tabled at the back of all introductory statistics books.

However, a **better way** to think about model (21) is as follows.

It's a fact from **basic distribution theory**, probably of more interest to Bayesians than frequentists, that the $t$ distribution is an

**Inverse Gamma mixture of Gaussians**.

This just means that to generate a $t$ random quantity you can first draw from an Inverse Gamma distribution and then draw from a Gaussian **conditional** on what you got from the Inverse Gamma.

(As noted in **homework 2**, $\lambda \sim \Gamma^{-1}(\alpha, \beta)$ just means that $\lambda^{-1} = \frac{1}{\lambda} \sim \Gamma(\alpha, \beta)$).

In more detail, $(y|\mu, \sigma^2, \nu) \sim t_\nu(\mu, \sigma^2)$ is the same as the **hierarchical model**

$$\begin{aligned} (\lambda|\nu) &\sim \Gamma^{-1}\left(\frac{\nu}{2}, \frac{\nu}{2}\right) \\ (y|\mu, \sigma^2, \lambda) &\sim N\left(\mu, \lambda\,\sigma^2\right). \end{aligned} \tag{22}$$

Putting this together with the **conjugate prior** for $\mu$ and $\sigma^2$ we looked at earlier in the Gaussian model gives the following HM for the NB10 data:

$$\begin{aligned} \nu &\sim p(\nu) \\ \sigma^2 &\sim \text{SI-}\chi^2\left(\nu_0, \sigma_0^2\right) \\ \left(\mu|\sigma^2\right) &\sim N\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right) \\ (\lambda_i|\nu) &\overset{\text{IID}}{\sim} \Gamma^{-1}\left(\frac{\nu}{2}, \frac{\nu}{2}\right) \\ \left(y_i|\mu, \sigma^2, \lambda_i\right) &\overset{\text{indep}}{\sim} N\left(\mu, \lambda_i\,\sigma^2\right). \end{aligned} \tag{23}$$

Remembering also from introductory statistics that the Gaussian distribution is the **limit** of the $t$ family as $\nu \to \infty$, you can see that the idea here has been to **expand** the Gaussian model by embedding it in the richer $t$ family, of which it's a special case with $\nu = \infty$.

# Implementing Gibbs

Model expansion is often the best way to deal with **uncertainty in the modeling process**: when you find deficiencies of the current model, **embed it in a richer class**, with the model expansion in directions suggested by the deficiencies (we'll also see this method in action again later).

**The MCMC Dataset.** Imagine trying to do **Gibbs sampling** on model (21), with the parameter vector $\theta = (\mu, \sigma^2, \nu)$.

Carrying out the iterative program described in (20) above would produce the following **MCMC Dataset**:

| Iteration | Phase | $\mu$ | $\sigma^2$ | $\nu$ |
|---|---|---|---|---|
| 0 | Initializing | $\mu_0$ | $\sigma_0^2$ | $\nu_0$ |
| 1 | Burn-In | $\mu_1(y, \sigma_0^2, \nu_0)$ | $\sigma_1^2(y, \mu_1, \nu_0)$ | $\nu_1(y, \mu_1, \sigma_1^2)$ |
| 2 | Burn-In | $\mu_2(y, \sigma_1^2, \nu_1)$ | $\sigma_2^2(y, \mu_2, \nu_1)$ | $\nu_1(y, \mu_2, \sigma_2^2)$ |
| . | . | . | . | . |
| $b$ | Burn-In | $\mu_b$ | $\sigma_b^2$ | $\nu_b$ |
| $(b+1)$ | Monitoring | $\mu_{b+1}$ | $\sigma_{b+1}^2$ | $\nu_{b+1}$ |
| $(b+2)$ | Monitoring | $\mu_{b+2}$ | $\sigma_{b+2}^2$ | $\nu_{b+2}$ |
| . | . | . | . | . |
| $(b+m)$ | Monitoring | $\mu_{b+m}$ | $\sigma_{b+m}^2$ | $\nu_{b+m}$ |

Looking at iterations 1 and 2 you can see that, in addition to $y$, the sampler makes use **only of parameter values in the current row and the previous row** (this illustrates the Markov character of the samples).

As we've seen above, at the end of the $(b+m)$ iterations, if you want (say) the **marginal posterior** for $\mu$, $p(\mu|y)$, all you have to do is take the $m$ values $\mu_{b+1}, \ldots, \mu_{b+m}$ and summarize them in any ways that interest you: their sample mean is your **simulation estimate** of the posterior mean of $\mu$, their sample histogram (or, better, their **kernel density trace**) is your simulation estimate of $p(\mu|y)$, and so on.

# Practical Issues

**Implementation Details.** (1) How do you figure out the **full conditionals**, and how do you sample from them?

(2) What should you use for **initial values**?

(3) How **large** should $b$ and $m$ be?

(4) More generally, how do you know when the chain has **reached equilibrium**?

Questions (3–4) fall under the heading of **MCMC diagnostics**, which I'll cover a bit later, and I'll address question (2) in the **case studies** below.

**Computing the full conditionals.** For a simple example of working out the full conditional distributions, consider the **conjugate Gaussian model** we looked at earlier:

$$\begin{aligned} \sigma^2 &\sim \text{SI-}\chi^2(\nu_0, \sigma_0^2) \\ (\mu|\sigma^2) &\sim N\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right) \\ (Y_i|\mu,\sigma^2) &\overset{\text{IID}}{\sim} N\left(\mu, \sigma^2\right). \end{aligned} \tag{24}$$

The full conditional distribution for $\mu$ in this model is $p(\mu|\sigma^2, y)$, **considered as a function of $\mu$ for fixed $\sigma^2$ and $y$**—but this is just

$$\begin{aligned} p(\mu|\sigma^2, y) &= \frac{p(\mu, \sigma^2, y)}{p(\sigma^2, y)} \\ &= c\, p(\mu, \sigma^2, y) \\ &= c\, p(\sigma^2)\, p(\mu|\sigma^2)\, p(y|\mu, \sigma^2) \\ &= c \exp\left[-\frac{\kappa_0}{2\sigma^2}(\mu - \mu_0)^2\right] \prod_{i=1}^{n} \exp\left[-\frac{1}{2\sigma^2}(y_i - \mu)^2\right]. \end{aligned} \tag{25}$$

# Full Conditionals

**From this**

$$p(\mu|\sigma^2, y) = c\,\exp\left[-\frac{\kappa_0}{2\sigma^2}(\mu-\mu_0)^2\right]\exp\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\mu)^2\right].$$

**Expanding** out the squares, **collecting** powers of $\mu$, and **completing the square** in $\mu$ gives

$$p(\mu|\sigma^2, y) = c\,\exp\left[-\frac{\kappa_0+n}{2\sigma^2}\left(\mu-\frac{\kappa_0\mu_0+n\bar{y}}{\kappa_0+n}\right)^2\right], \qquad (26)$$

from which it's clear that the **full conditional for $\mu$ in model (24)** is

$$(\mu|\sigma^2, y) \sim N\left(\frac{\kappa_0\mu_0+n\bar{y}}{\kappa_0+n}, \frac{\sigma^2}{\kappa_0+n}\right). \qquad (27)$$

Similarly, the full conditional for $\sigma^2$ in this model, $p(\sigma^2|\mu, y)$, **considered as a function of $\sigma^2$ for fixed $\mu$ and $y$**, is just

$$\begin{aligned} p(\sigma^2|\mu, y) &= \frac{p(\sigma^2, \mu, y)}{p(\mu, y)} \\ &= c\,p(\sigma^2, \mu, y) \qquad (28) \\ &= c\,p(\sigma^2)\,p(\mu|\sigma^2)\,p(y|\mu, \sigma^2) \\ &= c\,\left(\sigma^2\right)^{-(1+\frac{1}{2}\nu_0)}\exp\left(\frac{-\nu_0\,\sigma_0^2}{2\sigma^2}\right)\cdot \\ &\qquad \left(\sigma^2\right)^{-\frac{1}{2}}\exp\left[-\frac{\kappa_0}{2\sigma^2}(\mu-\mu_0)^2\right]\cdot \\ &\qquad \left(\sigma^2\right)^{-\frac{n}{2}}\exp\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\mu)^2\right]. \end{aligned}$$

When this is **simplified** you get

# Full Conditionals (continued)

$$p(\sigma^2|\mu, y) = c\,\left(\sigma^2\right)^{-\left(1+\frac{\nu_0+1+n}{2}\right)}\,\exp\left[-\frac{\nu_0\sigma_0^2 + \kappa_0(\mu-\mu_0)^2 + ns_\mu^2}{2\sigma^2}\right],$$

$$\text{where } s_\mu^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i-\mu)^2.$$

From the **form** of this distribution it becomes clear that

$$(\sigma^2|\mu, y) \sim \text{SI-}\chi^2\left(\nu_0+1+n,\ \frac{\nu_0\sigma_0^2 + \kappa_0(\mu-\mu_0)^2 + ns_\mu^2}{\nu_0+1+n}\right). \tag{29}$$

Thus in **conjugate situations** the full conditional distributions have **conjugate forms**, which are **tedious but straightforward** to compute.

Both the directness and the tedium of this calculation suggest that it should be possible to write a **computer program** to work out the full conditionals for you, and indeed at least **two such programs now exist**:

- `BUGS`, a fairly **general-purpose Gibbs sampling program** produced by David Spiegelhalter and others at the MRC Biostatistics Unit in Cambridge, UK (Spiegelhalter et al., 1997), and
- `MLwiN`, a program that does both **maximum-likelihood** and Bayesian calculations in **hierarchical (multilevel) models** (Rasbash et al. 2000).

`BUGS` runs under **Unix** or **DOS** in a wide variety of hardware configurations, and a `Windows` version called `WinBUGS` is also available; we'll look here at both Unix `BUGS` and `WinBUGS` (together with `MLwiN` if there's time).

`BUGS` and `WinBUGS` are available for **free downloading** at

`www.mrc-bsu.cam.ac.uk/bugs`;

`MLwiN` has a nominal charge and can be downloaded from the web page of the **Multilevel Models Project**,

`multilevel.ioe.ac.uk`

# Why the Metropolis Algorithm Works

Here's a sketch of the crucial part of the **proof**, based on an argument in Gamerman (1997), of the **validity** of the Metropolis algorithm, in the case of a **discrete** (finite or countably infinite) state space $S$ (see chapter 1 in Gilks et al. 1996 for a proof sketch when $S$ is **continuous**).

It will be helpful in looking at the proof sketch to specialize the **Markov chain notation** we've been using so far to the case of discrete state spaces, as follows.

A **stochastic process** $\{\theta_t^*, t \in T\}, T = \{0, 1, \ldots\}$ on a discrete state space $S$ is a **Markov chain** iff

$$P(\theta_{t+1}^* = y | \theta_t^* = x, \theta_{t-1}^* = x_{n-1}, \ldots, \theta_0^* = x_0) = P(\theta_{t+1}^* = y | \theta_t^* = x) \tag{30}$$

for all $t = 0, 1, \ldots$ and $x_0, \ldots, x_{t-1}, x, y \in S$.

In general $P(\theta_{t+1}^* = y | \theta_t^* = x)$ depends on $x, y$, and $t$, but if the probability of transitioning from $x$ to $y$ at time $t$ is **constant** in $t$ things will clearly be simpler; such chains are called **homogeneous** (confusingly, some sources call them **stationary**, but that terminology seems well worth avoiding).

The **random walk** described earlier is obviously a homogeneous Markov chain, and so are any Markov chains generated by the **MH algorithm**; I'll **assume homogeneity** in what follows.

Under **homogeneity** it makes sense to talk about the **transition probability**

$$P(x, y) = P(\theta_{t+1}^* = y | \theta_t^* = x) \quad \text{for all } t, \tag{31}$$

which **satisfies**

$$P(x, y) \geq 0 \text{ for all } x, y \in S \quad \text{and} \quad \sum_{y \in S} P(x, y) = 1 \text{ for all } x \in S. \tag{32}$$

# Metropolis Proof Sketch

When $S$ is discrete a **transition matrix** $P$ can be defined with element $(i, j)$ given by $P(x_i, x_j)$, where $x_i$ is the $i$th element in $S$ according to whatever **numbering convention** you want to use (the second part of (32) implies that the row sums of such a matrix are always 1; this is the defining condition for a **stochastic matrix**).

Suppose the chain is **initialized** at time 0 by making a **draw** from a probability distribution $\pi_0(x) = P(\theta_0^* = x)$ on $S$ (**deterministically** starting it at some point $x_0$ is a special case of this); then the probability distribution $\pi_1(y)$ for where it will be at time 1 is

$$\begin{aligned} \pi_1(y) &= P(\theta_1^* = y) \\ &= \sum_{x \in S} P(\theta_0^* = x, \theta_1^* = y) \\ &= \sum_{x \in S} P(\theta_0^* = x)\, P(\theta_1^* = y | \theta_0^* = x) \\ &= \sum_{x \in S} \pi_0(x)\, P(x, y), \end{aligned} \tag{33}$$

which can be written in **vector** and **matrix** notation as

$$\pi_1 = \pi_0\, P, \tag{34}$$

where $\pi_0$ and $\pi_1$ are regarded as **row vectors**.

Then by the **same reasoning**

$$\pi_2 = \pi_1\, P = (\pi_0\, P)P = \pi_0\, P^2, \tag{35}$$

and **in general**

$$\pi_t = \pi_0\, P^t. \tag{36}$$

For **simple** Markov chains this can be used to work out the **long-run** behavior of the chain as $t \to \infty$, but this becomes **algebraically prohibitive** as the **transition behavior** of the chain increases in **complexity**.