Lecture 4 Basics of Bayesian Inference

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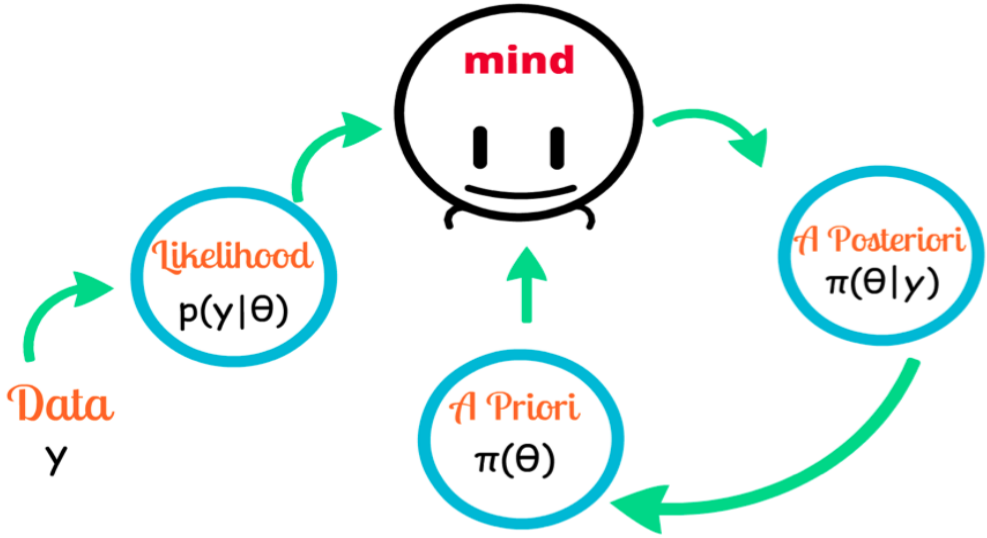
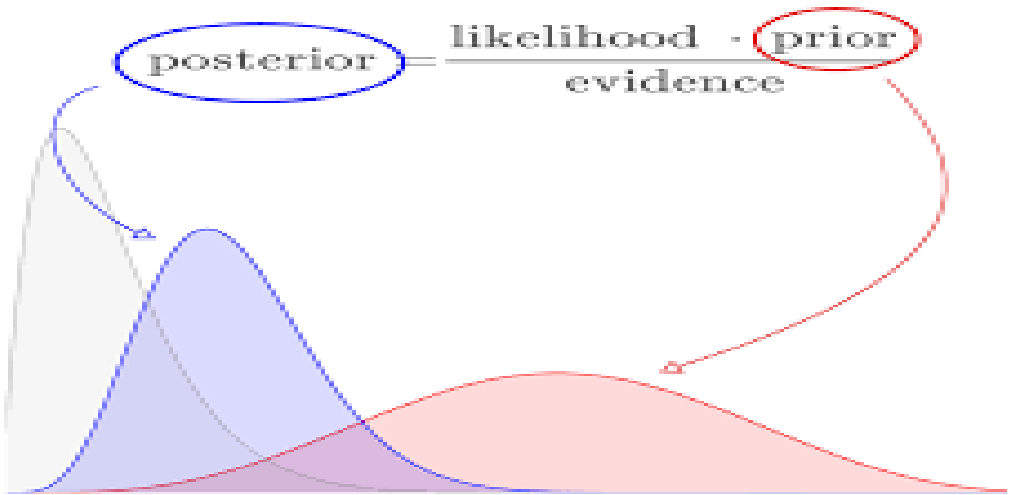
What is Bayesian statistics?



What is Bayesian statistics?



Why do we use Bayesian statistics?

- Probability is subjective: to quantify people's belief of something.
- Bayesian approach provides a coherent framework for combining complex data models and external knowledge or expert opinion.
- It comes with natural uncertainty quantification.
- It enables complex hierarchical models.
- Modern computers make it practical for computation.
- ...

Bayes' theorem

- For two events, A and B, *Bayes' theorem* can be simply presented as follows:

$$P(B|A) = \frac{P(B)P(A|B)}{P(A)}$$

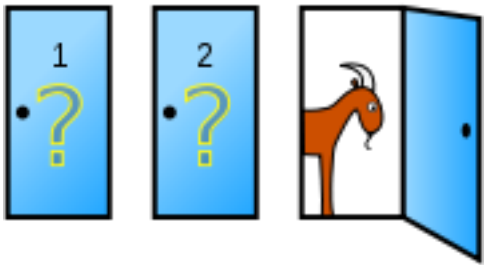
- Also, recall that if $B = (B_1, B_2, ..., B_n)$ are a set of events that partition the sample space, Ω, using the law of total probability, we have:

$$\begin{aligned} P(A) &= P(A|B_1)P(B_1) + ... + P(A|B_n)P(B_n) \\ P(B_i|A) &= \frac{P(B_i)P(A|B_i)}{\sum_{i'}^{n} P(B_{i'})P(A|B_{i'})} \end{aligned}$$

- This simple formula which is known as *Bayes' theorem* is the basis of Bayesian analysis. (However, using this theorem does not automatically make you a Bayesian!)

Monty Hall problem

- The problem is based on a TV game show hosted by Monty Hall. In this show, contestants have the chance to win cars. Before each show, a car is put behind one of three closed doors. The other two doors have goats behind them. The contestant is asked to choose one of the three doors. Then, Monty Hall then opens one of the other two doors, which he knows does not have a car behind it. After that, the contestant can choose to switch the the remaining unopened door, or stay with his original selection. The question is: should he switch?



Bayesian hierarchical modeling

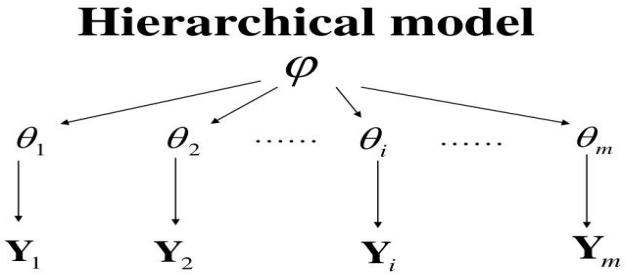
- Given observed data $\mathrm{y} = (y_1, \cdots, y_n)$, we specify the *likelihood* model $f(\mathrm{y}|\boldsymbol{\theta})$ for a vector of unknown parameter $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_k)$.
- In Bayesian statistics, we assue $\boldsymbol{\theta}$ is also a random quantity sampled from a *prior* distribution $\pi(\boldsymbol{\theta}|\boldsymbol{\varphi})$, where $\boldsymbol{\varphi}$ is a vector of *hyperparameters*.
- If $\boldsymbol{\varphi}$ is known, inference concerning $\boldsymbol{\theta}$ is based on its *posterior* distribution

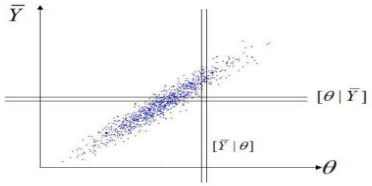
$$p(\boldsymbol{\theta}|\mathrm{y}, \boldsymbol{\varphi}) = \frac{p(\mathrm{y}, \boldsymbol{\theta}|\boldsymbol{\varphi})}{p(\mathrm{y}|\boldsymbol{\varphi})} = \frac{f(\mathrm{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta}|\boldsymbol{\varphi})}{\int f(\mathrm{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta}|\boldsymbol{\varphi})d\boldsymbol{\theta}} \tag{1}$$

- In practice, $\boldsymbol{\varphi}$ is unknown and given another prior distribution called *hyperprior*, denoted as $h(\boldsymbol{\varphi})$. Then we reduce

$$p(\boldsymbol{\theta}|\mathrm{y}) = \frac{p(\mathrm{y}, \boldsymbol{\theta})}{p(\mathrm{y})} = \frac{\int f(\mathrm{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta}|\boldsymbol{\varphi})h(\boldsymbol{\varphi})d\boldsymbol{\varphi}}{\int f(\mathrm{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta}|\boldsymbol{\varphi})h(\boldsymbol{\varphi})d\boldsymbol{\theta}d\boldsymbol{\varphi}} \tag{2}$$

Bayesian hierarchical modeling





Bayesian Linear regression models

- Consider the following liner regression model:

$$y|X, \beta, \sigma^2 \sim N(X\beta, \sigma^2 I_n)$$

- y is a column vector of n outcome observations, X is an $n \times (p+1)$ matrix of predictors with its first column being all 1's.
- β is a column vector with $p+1$ elements $(\beta_0, \beta_1, ..., \beta_p)$ where β_0 is the intercept and β_j is the effect of the j^{th} predictor x_j on y.
- In Bayesian analysis, a common prior for parameters are

$$\beta|\mu_0, \Lambda_0 \sim N_{p+1}(\mu_0, \Lambda_0)$$

where $\mu_0 = (\mu_{00}, \mu_{01}, ..., \mu_{0p})$ typically set to zero (unless we believe otherwise), and $\Lambda_0 = \mathrm{diag}(\tau_0^2, \tau_1^2, ..., \tau_p^2)$ should be sufficiently broad.

Bayesian Linear regression models

- The posterior distributions of β has the following closed form:

$$\begin{aligned} \beta|X,y,\sigma^2 &\sim N(\mu_n,\Lambda_n) \\ \mu_n &= (x_*'\Sigma_*^{-1}x_*)^{-1}x_*'\Sigma_*^{-1}y_* \\ \Lambda_n &= (x_*'\Sigma_*^{-1}x_*)^{-1} \\ x_* &= \begin{pmatrix} X \\ I_{p+1} \end{pmatrix} \qquad y_* = \begin{pmatrix} y \\ \mu_0 \end{pmatrix} \qquad \Sigma_* = \begin{pmatrix} \sigma^2 I_n & 0 \\ 0 & \Lambda_0 \end{pmatrix} \end{aligned}$$

- Looking at it this way, the prior plays the role of extra data with $x_{\beta=I_{p+1}}$, $y_\beta = \mu_0$ and the covariance Λ_0.
- That's why Bayesian models do not break down when $p > n$.

Bayesian Linear regression models

- Let's take a closer look at the maximum a posterior (MAP)

$$\begin{aligned}\mu_n &= (x_*'\Sigma_*^{-1}x_*)^{-1}x_*'\Sigma_*^{-1}y_* \\ &= (\sigma^{-2}X'X + \Lambda_0^{-1})^{-1}(\sigma^{-2}X'y + \Lambda_0^{-1}\mu_0)\end{aligned}$$

- Let $\mu_0 = 0$, $\sigma^2\Lambda_0^{-1} = \lambda I$, then we have

$$\mu_n = \hat{\beta}^{\text{ridge}} = (X'X + \lambda I)^{-1}X'y$$

- This is exactly the solution to ridge regression!
- If we do not have any informative priors, we can instead assume $p(\beta|x) \propto 1$.
- For β this is equivalent (in limit) to taking all $\tau_j^2 \to \infty$.
- The posterior distribution therefore becomes

$$\begin{aligned}\beta|y,\sigma^2 &\sim N(\hat{\beta}, V_\beta\sigma^2) \\ \hat{\beta} &= (X'X)^{-1}X'y, \qquad V_\beta = (X'X)^{-1}\end{aligned}$$

- $\hat{\beta}$ is exactly the OLS solution!

Bayesian Linear regression models

- Note, we have

$$\begin{aligned} y|X,\beta,\sigma^2 &\sim N(X\beta,\sigma^2 I_n) \\ \beta|\mu_0,\Lambda_0 &\sim N_{p+1}(\mu_0,\Lambda_0) \end{aligned}$$

- Then a priori, we actually assume

$$y|X,\sigma^2 \sim N(\mu_0, X\Lambda_0 X^T + \sigma^2 I_n) \tag{3}$$

- This can be viewed as a realization of Gaussian process $y(x) \sim \mathcal{GP}(\mu, \mathcal{C})$, with the following linear covariance

$$C_{ij} = \mathrm{Cov}(y_i, y_j) = \sum_{k=0}^{p} x_{ik} x_{jk} \tau_k^2 + \sigma^2 \delta_{ij} \tag{4}$$

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Bayesian Inference

- Point estimation:
  1. posterior mean: $\hat{\theta} = \mathrm{E}[\theta|\mathrm{y}]$
  2. posterior median: $\hat{\theta} : F(\hat{\theta}|\mathrm{y}) = \Pr(\theta \leq \hat{\theta}|\mathrm{y}) = 0.5$
  3. posterior mode: $\hat{\theta} : p(\hat{\theta}|\mathrm{y}) = \sup_\theta p(\theta|\mathrm{y})$
- Interval estimation: (q_L, q_U) is a $100 \times (1-\alpha)\%$ *credible* set (or *Bayesian confidence interval*) for θ if $\Pr(q_L < \theta < q_U|\mathrm{y}) = 1-\alpha$.
  1. When the posterior $\theta|\mathrm{y}$ is (nearly) symmetric, then

$$\int_{-\infty}^{q_L} p(\theta|\mathrm{y})d\theta = \int_{q_U}^{\infty} p(\theta|\mathrm{y})d\theta = \alpha/2 \tag{5}$$

  2. *highest posterior density* (HPD) constitutes θ having posterior density as large as possible such that

$$1-\alpha \leq \Pr(C|\mathrm{y}) = \int_C p(\theta|\mathrm{y})d\theta \tag{6}$$

Hypothesis testing and model choice

- Hypothesis testing is less straightforward. We consider model choice instead.
- Model choice essentially requires specification of the *utility* for a model.
- What are choices of the utility? For what purpose? Explanation? Prediction?
- In the following, we introduce *Deviance Information Criterion (DIC)* and *continuous rank probability score (CRPS)* and other related concepts.

Bayes factor

- Given two models M_1 (H_0) and M_2 (H_A). Associated are two parameter vectors $\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$, with priors $\pi_i(\boldsymbol{\theta}_i)$ for $i = 1, 2$ respectively. The marginal distributions of Y are:

$$p(\mathrm{y}|M_i) = \inf f(\mathrm{y}|\boldsymbol{\theta}_i, M_i)\pi_i(\boldsymbol{\theta}_i)d\boldsymbol{\theta}_i, \quad i = 1, 2 \tag{7}$$

- Then the *Bayes factor (BF)*, is the ratio of the posterior odds of the M_1 to the prior odds of M_1, given by Bayes' Theorem as

$$\mathrm{BF} = \frac{\Pr(M_1|\mathrm{y})/\Pr(M_2|\mathrm{y})}{\Pr(M_1)/\Pr(M_2)} = \frac{p(\mathrm{y}|M_1)}{p(\mathrm{y}|M_2)} \tag{8}$$

- This reduces to likelihood ratio for simple-simple model comparison $M_i : \boldsymbol{\theta} = \boldsymbol{\theta}_i$: $\mathrm{BF} = \frac{f(\mathrm{y}|\boldsymbol{\theta}_1)}{f(\mathrm{y}|\boldsymbol{\theta}_2)}$

Information Criteria

- *Bayesian Information Criterion (BIC)*

$$\Delta\mathrm{BIC} = W - (p_2 - p_1)\log n \tag{9}$$

where p_i is the number of parameters in model M_i, $i = 1, 2$ and the usual likelihood ratio test statistic $W = -2\log\left[\frac{\sup_{M_1} f(\mathrm{y}|\boldsymbol{\theta})}{\sup_{M_2} f(\mathrm{y}|\boldsymbol{\theta})}\right]$.

- Schwarz (1978) showed that for nonhierarchical (two-stage) models, $\mathrm{BIC} \sim -2\log \mathrm{BF}$ for large n.
- *Akaike Information Criterion (AIC)*

$$\Delta\mathrm{AIC} = W - 2\log n \tag{10}$$

- Both AIC and BIC are penalized likelihood ratio model choice criteria; BIC criticizes difference in model dimension more strongly than AIC does.

Information Criteria

- Spiegelhalter et al. (2002) propose a generalization of the AIC for hierarchical (3 or more level) models based on the posterior distribution of the *deviance* statistic,

$$D(\boldsymbol{\theta}) = -2 \log f(\mathrm{y}|\boldsymbol{\theta}) + 2 \log h(\mathrm{y}) \tag{11}$$

  where $f(\mathrm{y}|\boldsymbol{\theta})$ is the likelihood and $h(\mathrm{y})$ is some standardizing function of data.
- The *complexity* of a model is measured by the effective number of the following parameter p_D

$$p_D = \mathrm{E}_{\theta|y}[D(\theta)] - D(\mathrm{E}_{\theta|y}[\boldsymbol{\theta}]) = \bar{D} - D(\bar{\boldsymbol{\theta}}) \tag{12}$$

- *Deviance Information Criterion (DIC)*

$$\mathrm{DIC} = \bar{D} + p_D = 2\bar{D} - D(\bar{\boldsymbol{\theta}}) \tag{13}$$

Predictive Criteria

- Gelfand and Ghosh (1998) propose the *posterior predictive loss* (performance) approach. It focuses on prediction with regard to replicates of the observed data, $Y_{\ell,rep}, \ell = 1, \cdots, n$.
- The selected models are those that perform well under a so-called *balanced loss* function that penalizes actions both for departure from observed values ("fit") and for departure from what we expect the replicate to be ("smoothness").

$$\begin{aligned} D_k &= \frac{k}{k+1} G + P \\ G &= \sum_{\ell=1} Tn(\mu_\ell - y_{\ell,obs})^2, \quad P = \sum_{\ell=1} \sigma_\ell^2 \end{aligned} \tag{14}$$

where $\mu_\ell = \mathrm{E}[Y_{\ell,rep}|\mathrm{y}]$ and $\sigma_\ell^2 = \mathrm{Var}[Y_{\ell,rep}|\mathrm{y}]$ can be calculated by

$$p(y_{\ell,rep}|\mathrm{y}) = \int p(y_{\ell,rep}|\boldsymbol{\theta}_i) p(\boldsymbol{\theta}_i|\mathrm{y}) d\boldsymbol{\theta}_i \tag{15}$$

Predictive Criteria

- For prediction task, one can partition the dataset into a fitting (or learning) set and a validation or "hold out" set ($20-30\%$). Then apply the criterion to the hold out data after fitting the model to the fitting dataset.
- Gneiting and Raftery (2007) propose the *continuous rank probability score* (CRPS) measure

$$\mathrm{CRPS}(F, y) = \int_{-\infty}^{\infty} (F(u) - 1(u \geq y))^2 du \tag{16}$$

where F is the predictive distribution and y is the observed value.

- Gneiting and Raftery (2007) present a convenient alternative form

$$\mathrm{CRPS}(F, y) = \frac{1}{2}\mathrm{E}_F|Y - Y'| = \mathrm{E}_F|Y - y| \tag{17}$$

where Y and Y' are independent replicates from F. With samples from F, we have immediate Monte Carlo integrations.

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The Metropolis-Hastings algorithm

- Suppose that we are interested in sampling from a distribution π. We known the density of π up to a constant, i.e., $cf(x)$.
- We can construct a Markov chain with a transition probability (a.k.a, *proposal distribution*) $g(x, y)$.
- Now follow these steps
  1. Given our current state $X^{(n)} = x$, we propose a new state $Y^{(n+1)} = y$ according to the transition probability (for example, if we chose $N(x, 1)$, we sample from a normal centered at x with variance 1).
  2. Calculated the acceptance probability

$$a(x, y) = \min(1, \frac{f(y)g(y, x)}{f(x)g(x, y)})$$

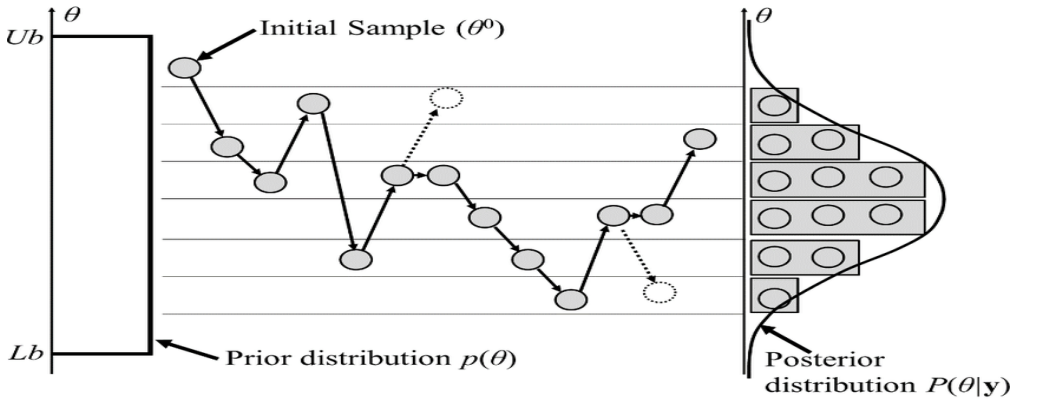
  3. Accept the proposed state y as the new state with probability $a(x, y)$ or remain at state x. That is, sample $u \sim Unif(0, 1)$ and set

$$X^{(n+1)} = \begin{cases} y & u < a(x, y) \\ x & \text{otherwise} \end{cases}$$

Markov Chain Monte Carlo

This is different from optimization!

- The goal for MCMC is to construct a Markov chain with transition kernel $P(\boldsymbol{\theta}_n, \boldsymbol{\theta}_{n+1})$ such that it converges to the target distribution $\pi(\cdot)$ in the sense that $\lim_{n\to\infty} P^n(\boldsymbol{\theta}_0, A) = \pi(A)$ for any measurable set $A \subset \Omega$, regardless of initial point $\boldsymbol{\theta}_0$.



Decomposing the parameter space

- At iteration i, given our current state $(x_1^{(i)}, x_2^{(i)}, ..., x_d^{(i)})$ we follow these steps:
  1. Sample $Y_1^{(i+1)} = y_1$ from the univariate proposal distribution $g_1(x_1^{(i)}, y_1)$
  2. Accept this new value and set $x_1^{(i+1)} = y_1$ with probability

$$a(x_1^{(i)}, y_1) = \min\left[1, \frac{p(y_1, x_2^{(i)}, ..., x_d^{(i)})}{p(x_1^{(i)}, x_2^{(i)}, ..., x_d^{(i)})}\right]$$

     or reject it and set $x_1^{(i+1)} = x_1^{(i)}$
  3. Now sample $Y_2^{(i+1)} = y_2$ from the univariate proposal distribution $g_2(x_2^{(i)}, y_2)$.
  4. Accept this new value for x_2 with probability

$$a(x_2^{(i)}, y_2) = \min\left[1, \frac{p(x_1^{(i+1)}, y_2, ..., x_d^{(i)})}{p(x_1^{(i+1)}, x_2^{(i)}, ..., x_d^{(i)})}\right]$$

     or reject it and set $x_1^{(i+1)} = x_1^{(i)}$
  5. Continue to update all d components.

Gibbs sampler

- When we have conditional conjugacy, i.e. $P(\theta_j|y,\theta_{-j})$ has a closed form, we have the following Gibbs sampler
- At iteration i, given our current state $(x_1^{(i)}, x_2^{(i)}, ..., x_d^{(i)})$ we cycle through the components one at a time:
  - Sample $x_1^{(i+1)}$ from the conditional distribution $P(x_1|x_2^{(i)}, x_3^{(i)}, ..., x_d^{(i)})$
  - Sample $x_2^{(i+1)}$ from the conditional distribution $P(x_2|x_1^{(i+1)}, x_3^{(i)}, ..., x_d^{(i)})$
  - $\vdots$
  - Sample $x_j^{(i+1)}$ from the conditional distribution $P(x_j|x_1^{(i+1)}, ..., x_{j-1}^{(i+1)}, x_{j+1}^{(i)}, ..., x_d^{(i)})$
  - $\vdots$
  - Sample $x_d^{(i+1)}$ from the conditional distribution $P(x_d|x_1^{(i+1)}, x_2^{(i+1)}, ..., x_{d-1}^{(i+1)})$

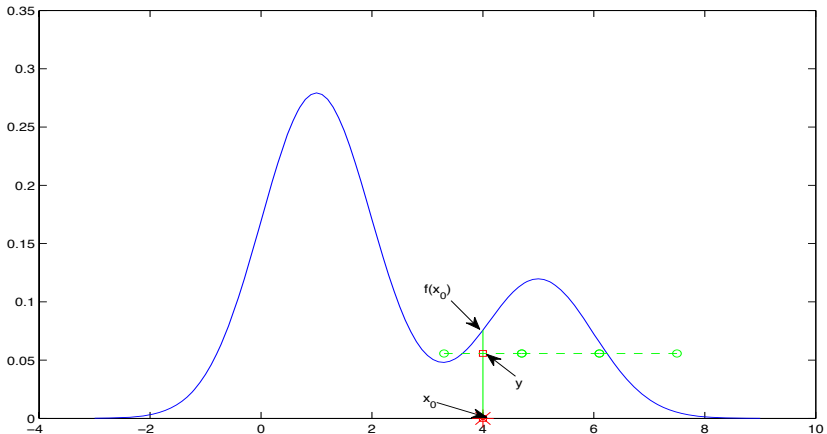
Gibbs sampler

- Note that we are not just proposing anymore, we are directly sampling.
- Or you can look at it as a proposal that will be accepted with probability 1.
- Looking at it this way, the Gibbs sampler is a special case of the Metropolis-Hastings algorithm (note that the transition distribution is not symmetric)

$$\begin{aligned} a(x_j^{(i)}, x_j^{(i+1)}) &= \min\left[1, \frac{p(x_j^{(i+1)}, x_{-j}^{(i)})p(x_j^{(i)}|x_{-j}^{(i)})}{p(x_j^{(i)}, x_{-j}^{(i)})p(x_j^{(i+1)}|x_{-j}^{(i)})}\right] \\ &= \min\left[1, \frac{p(x_j^{(i+1)}|x_{-j}^{(i)})p(x_{-j}^{(i)})p(x_j^{(i)}|x_{-j}^{(i)})}{p(x_j^{(i)}|x_{-j}^{(i)})p(x_{-j}^{(i)})p(x_j^{(i+1)}|x_{-j}^{(i)})}\right] \\ &= 1 \end{aligned}$$

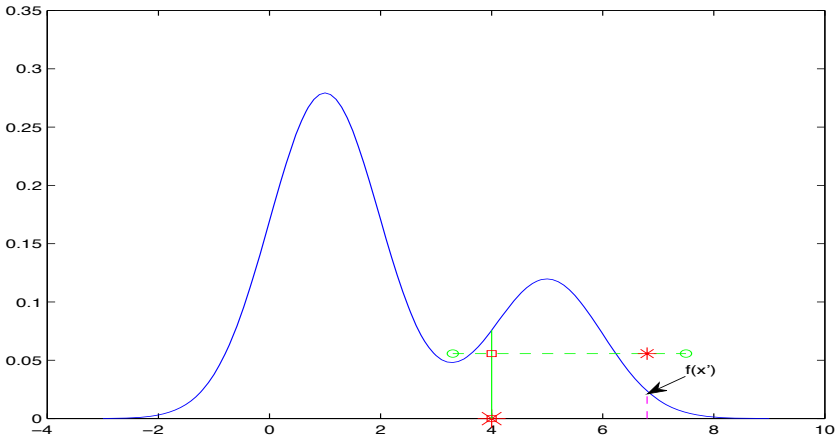
Slice sampling

- Sampling $y \sim \text{Uniform}(0, f(x_0))$ and stepping out (of size w) until we reach points outside the area under the density.



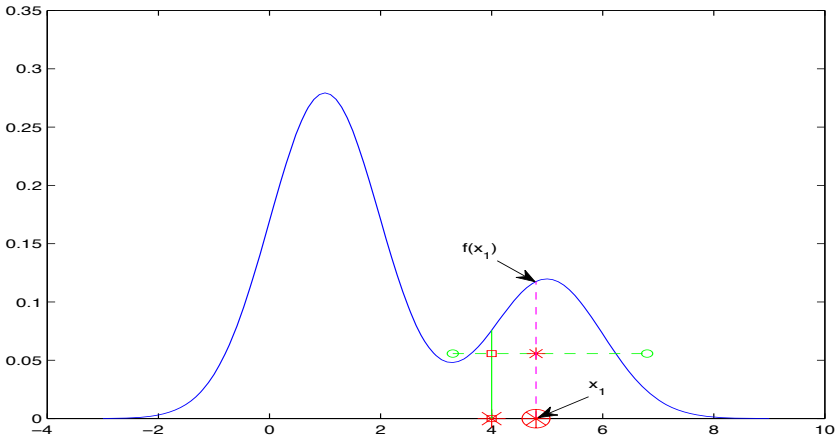
Slice sampling

- Shrinkage of interval to a point, x', which is sampled (uniformly) from the interval but it has $f(x') < y$.



Slice sampling

- Continuing shrinkage until we reach a point x_1 such that $y < f(x_1)$. We accept x_1 as our new sample.



Slice sampling

- The following figure (provided in Neal, 2003), shows the stepping out procedure to create an interval $[L, R]$ around our current point x_0, with $y \sim \text{Uniform}(0, f(x_0))$.

Input: f = function proportional to the density
x_0 = the current point
y = the vertical level defining the slice
w = estimate of the typical size of a slice
m = integer limiting the size of a slice to mw

Output: (L, R) = the interval found

$U \sim \text{Uniform}(0, 1)$
$L \leftarrow x_0 - w * U$
$R \leftarrow L + w$
$V \sim \text{Uniform}(0, 1)$
$J \leftarrow \text{Floor}(m * V)$
$K \leftarrow (m - 1) - J$

repeat while $J > 0$ and $y < f(L)$:
  $L \leftarrow L - w$
  $J \leftarrow J - 1$

repeat while $K > 0$ and $y < f(R)$:
  $R \leftarrow R + w$
  $K \leftarrow K - 1$

Figure: The stepping out procedure to create interval $[L, R]$ around x_0.

Slice sampling

- The following figure (provided in Neal, 2003) shows how we can sample a new point from the interval $[L, R]$ around x_0.

Input: f = function proportional to the density
x_0 = the current point
y = the vertical level defining the slice
(L, R) = the interval to sample from
Output: x_1 = the new point

$\bar{L} \leftarrow L, \quad \bar{R} \leftarrow R$

Repeat:
  $U \sim \text{Uniform}(0, 1)$
  $x_1 \leftarrow \bar{L} + U * (\bar{R} - \bar{L})$
  if $y < f(x_1)$ and $\text{Accept}(x_1)$ then
    exit loop
  if $x_1 < x_0$ then $\bar{L} \leftarrow x_1$
    else $\bar{R} \leftarrow x_1$

Figure: The shrinkage procedure to create a new sample x_1.

Convergence diagnosis

- Gelman-Rubin-Brooks (1992, 1998) monitor convergence by the estimated *scale reduction factor*

$$\sqrt{\hat{R}} = \sqrt{\left(\frac{N-1}{N} + \frac{m+1}{mN}\frac{B}{W}\right)\frac{df}{df-2}} \tag{18}$$

- Here, we run a small number (m) of parallel chains for $2N$ iterations each. B/N is the variance between the means from the m parallel chains. W is the average of the m within-chain variances, and df is the degrees of freedom of an approximating t density to the posterior distribution.
- The authors show it must approach 1 as $N \to \infty$.
- Geweke's test (1992): test equality of the means for the first segment (usually the first 10% of samples) and the last segment (usually the last 50% of samples) of a Markov chain.
- `R` packages `MCMC` and `coda`.