School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Approximate Inference: Advanced Topics in MCMC

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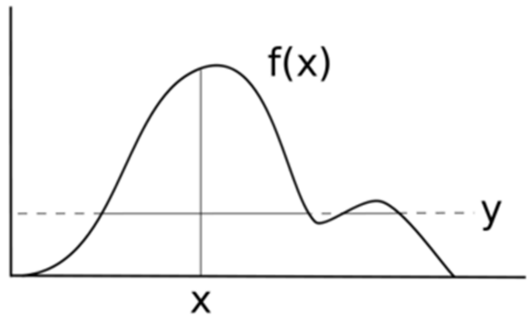
Lecture 18, March 24, 2014



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Recap of MCMC

- Markov Chain Monte Carlo methods use adaptive proposals Q(x'|x) to sample from the true distribution P(x)

- Metropolis-Hastings allows you to specify any proposal Q(x'|x)
  - But choosing a good Q(x'|x) requires care

- Gibbs sampling sets the proposal Q(x'|x) to the conditional distribution P(x'|x)
  - Acceptance rate always 1!
  - But remember that high acceptance usually entails slow exploration
  - In fact, there are better MCMC algorithms for certain models

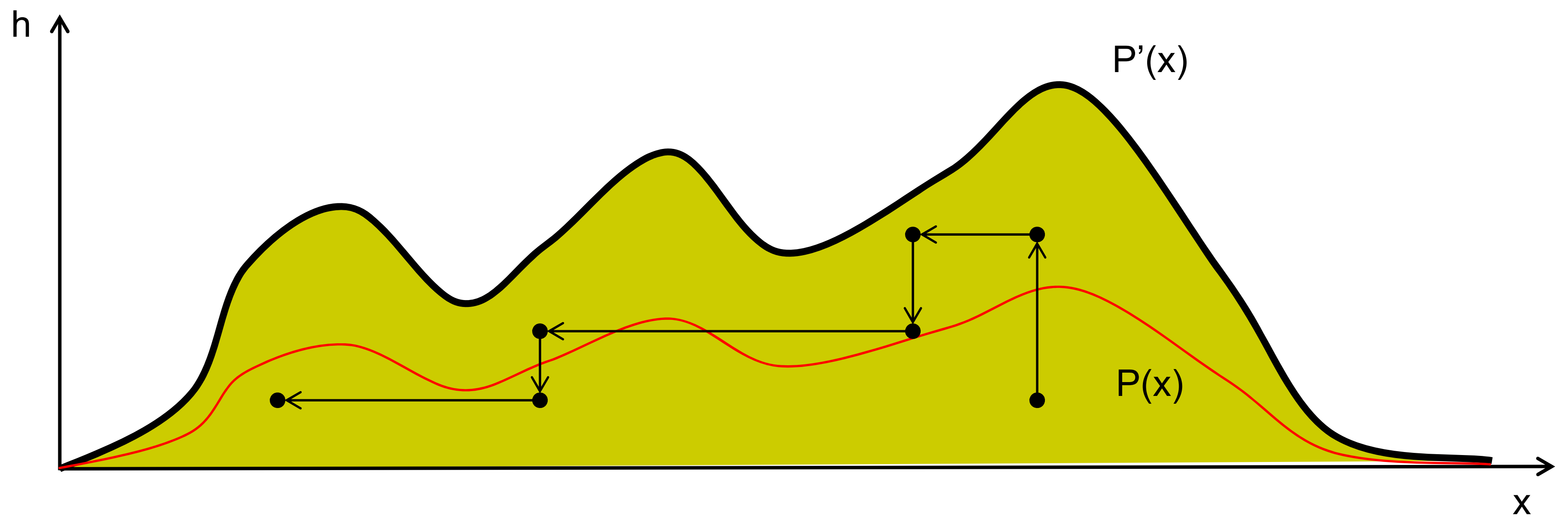
- Knowing when to halt burn-in is an art

Auxiliary Variables

- Advanced MCMC algorithms rely on auxiliary variables
  - Auxiliary variables are extra r.v.s not from the original model
  - They are random-valued intermediate quantities that allow us to sample model r.v.s in creative ways
- Suppose x is an r.v. and v is an a.v.. Generally, we use a.v.s when:
  - P(x|v) and P(v|x) have simple forms
  - P(x,v) is easy to navigate

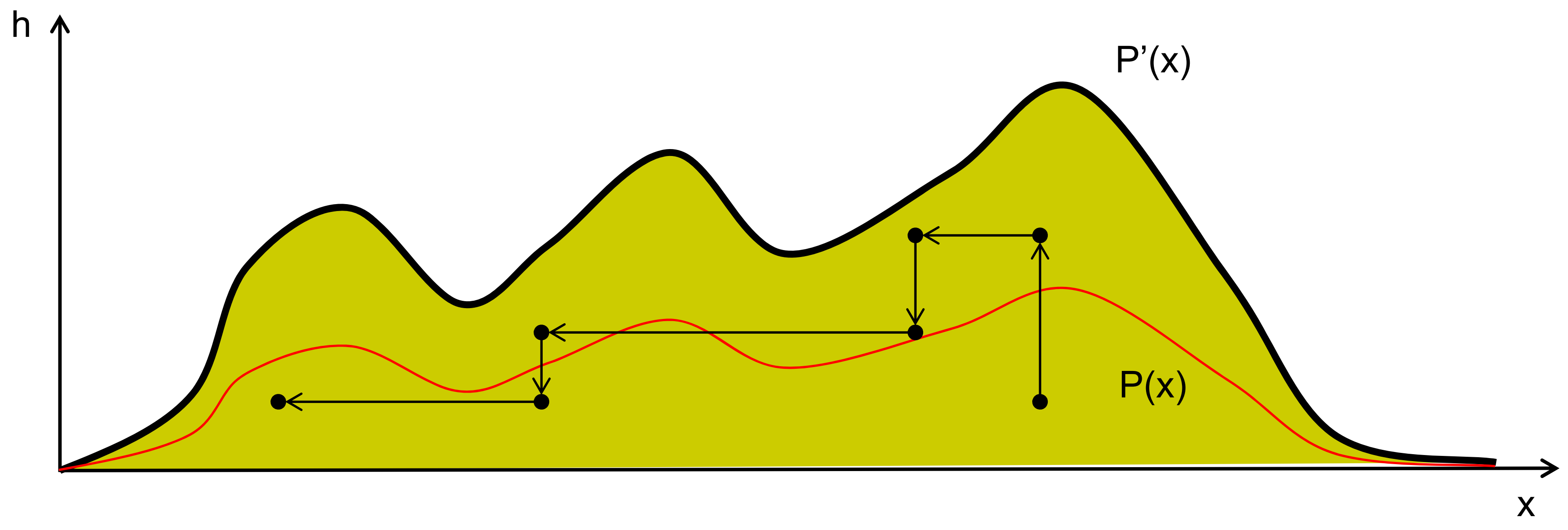
Slice Sampling

- Slice sampling is an auxiliary variable MCMC algorithm
  - Key idea: uniformly sample the area under P'(x) = aP(X), instead of P(x)
  - Never evaluate expensive P(x), only evaluate cheap P'(x)



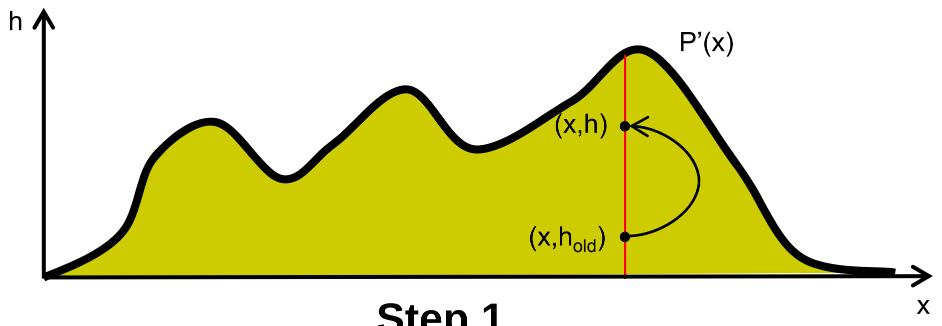
Slice Sampling

- When is Slice sampling useful?
  - Ex: Markov Random Fields where P(x) = (1/a) * exp(bx)
  - Normalizer (1/a) usually intractable to evaluate!
  - Slice sampling only requires (easy) evaluation of P'(x) = exp(bx)

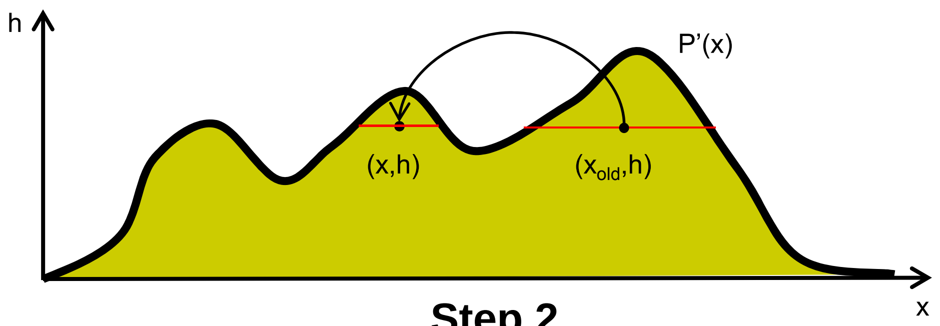


Slice Sampling

- Slice sampling uses an a.v. h (in addition to the r.v. x)
  - The pair (x,h) is the position of the sampler in the area under P'(x)
- We only need to know P'(x) = aP(x) for some unknown a
- The algorithm iterates between two steps:
  - Step 1: sample h from $Q(h \mid x) = Uniform[0, P'(x)]$
  - Step 2: sample x from $Q(x \mid h) \propto \begin{cases} 1 & \text{if } P'(x) \geq h \\ 0 & \text{otherwise} \end{cases}$ (uniform dist. on all x s.t. P'(x)≥h)



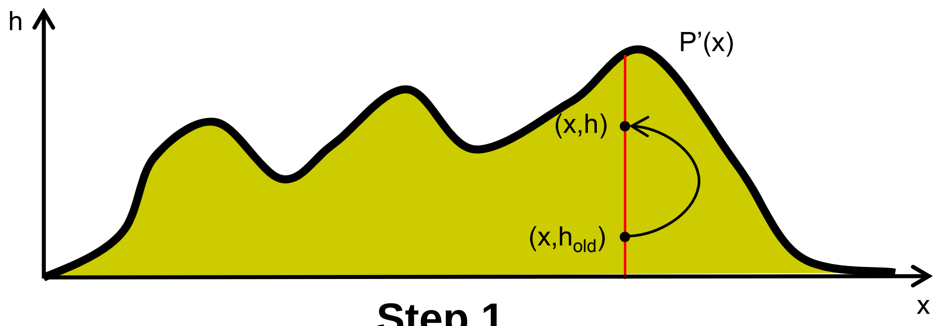
Step 1



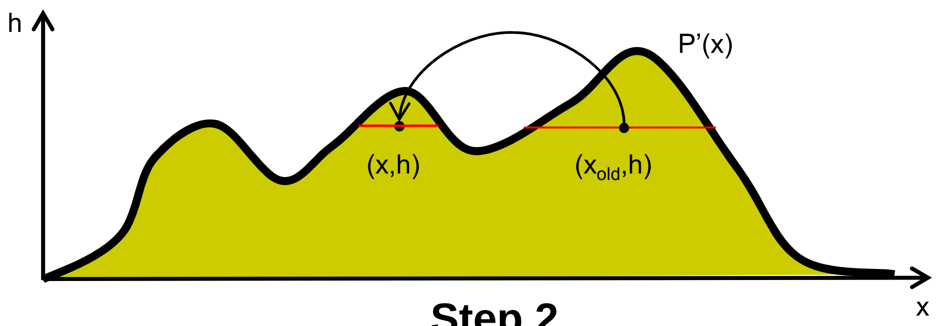
Step 2

Slice Sampling

- The algorithm iterates between two steps:
  - Step 1: sample h from $Q(h\,|\,x) = Uniform[0, P'(x)]$
  - Step 2: sample x from $Q(x\,|\,h) \propto \begin{cases} 1 & \text{if } P'(x) \geq h \\ 0 & \text{otherwise} \end{cases}$ (uniform dist. on all x s.t. P'(x)≥h)
- Step 2 requires finding the set {x s.t. P'(x)≥h}
  - Alternative 1: rejection sampling (reject whenever we get x s.t. P'(x)<h)
  - Alternative 2: "Bracketing" technique (to be presented shortly)



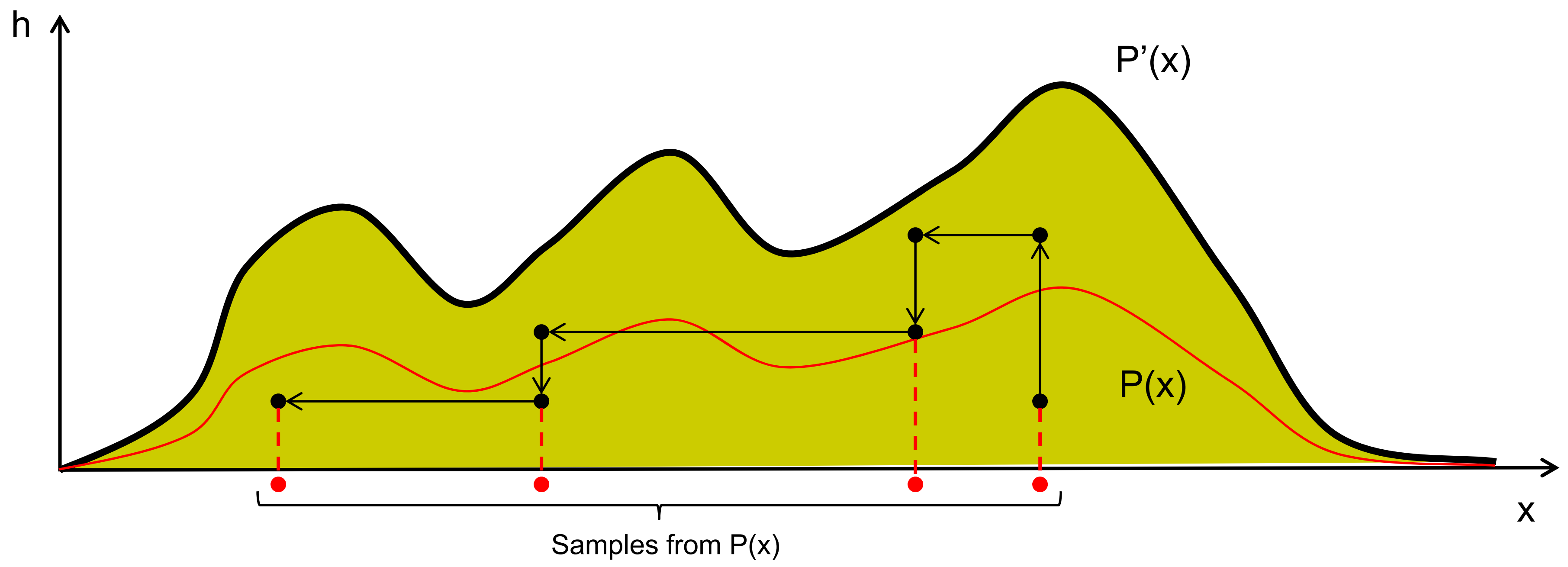
Step 1



Step 2

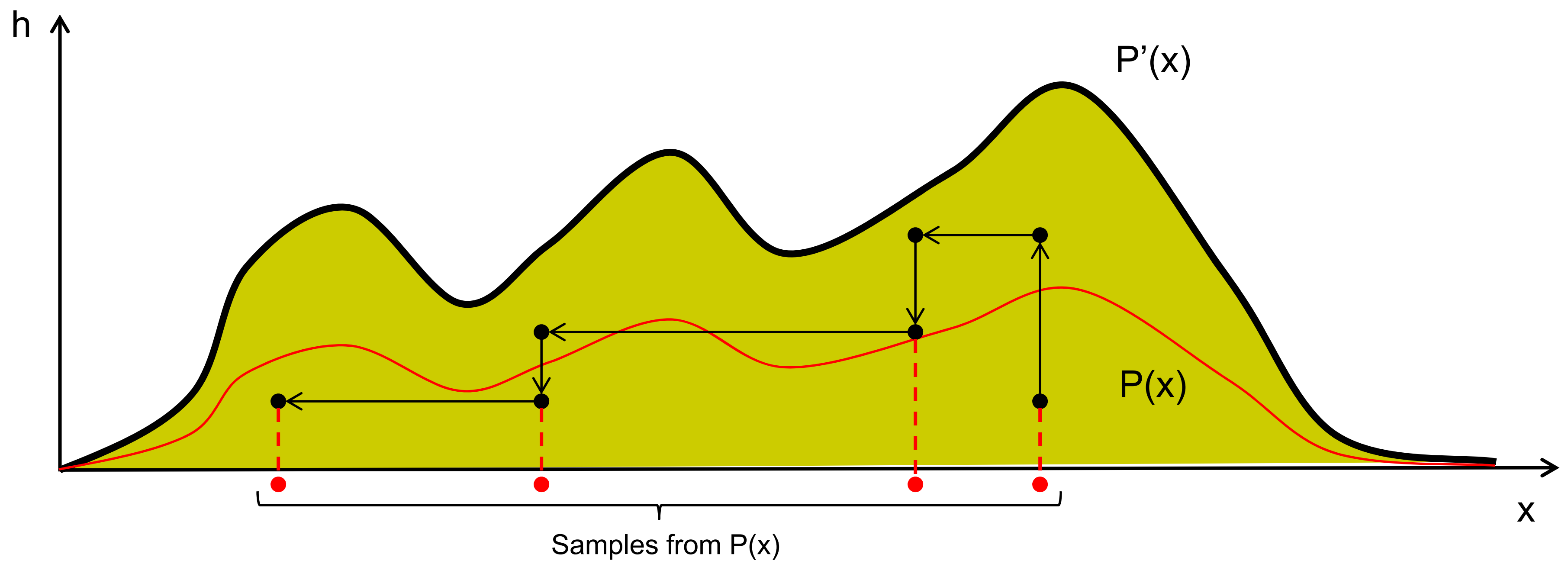
Why does this work?

- At convergence, the samples (x,h) will be uniformly distributed under the area of P'(x)
- If we marginalize out h, we get samples from P(x) = (1/a)P'(x)
  - Never needed to evaluate normalizer (1/a)!



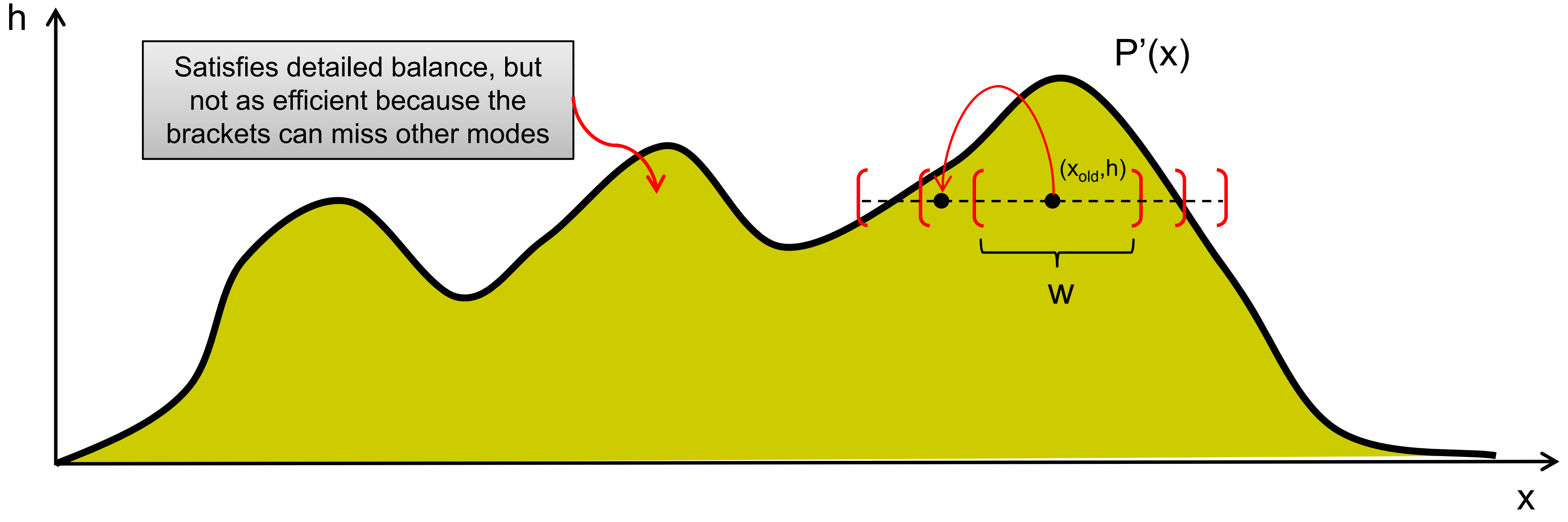
Why does this work?

- How to marginalize out h?
  - We have samples (x_1,h_1), (x_1,h_2), (x_2,h_2), (x_2,h_3), …
  - Marginalization is just dropping h from the samples
  - After dropping h, left with x_1, x_2, x_3, … which are samples from P(x)!



Handling difficult Q(x|h)

- Step 2 (sampling Q(x|h)) may not be easy
  - For complex distributions, cannot analytically find {x s.t. P'(x) ≥ h}
  - However, we can still easily evaluate P'(x) at any x…
- Solution: "bracketing" strategy
  1. Draw a random bracket width w, and place the bracket on (x_{old},h)
  2. Expand the bracket until the endpoints a, b are "above P'(x)": i.e. P'(a) < h and P'(b) < h
  3. Uniformly sample from within the bracket (reject samples x s.t. P'(x) < h)

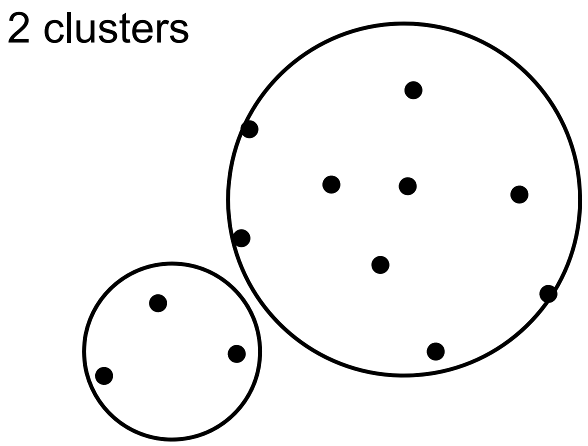

h
Satisfies detailed balance, but not as efficient because the brackets can miss other modes
P'(x)
(x_{old},h)
w
x

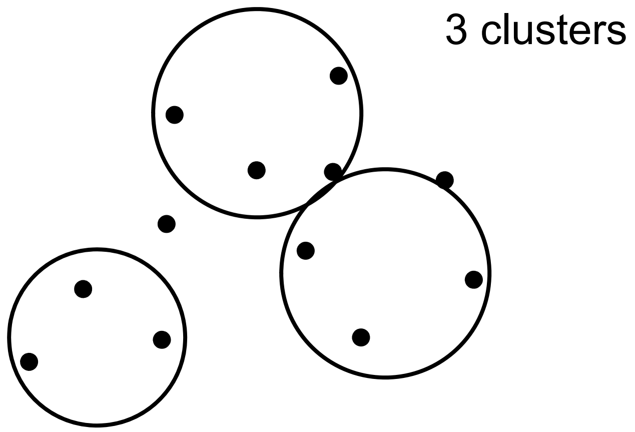
How to Sample from Different Model Spaces?

- Detailed Balance

$$\pi(x')T(x \mid x') = \pi(x)T(x' \mid x)$$

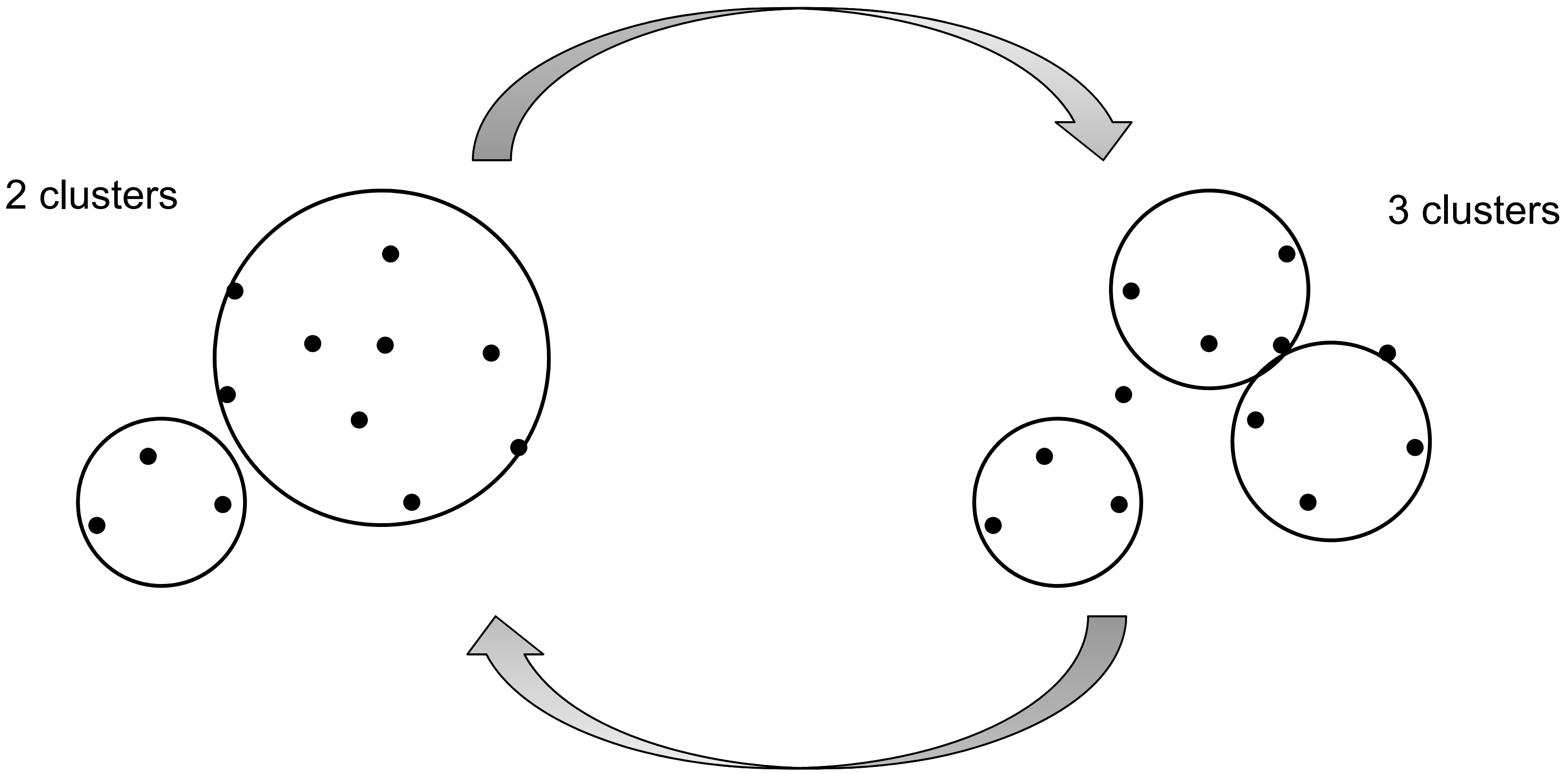
- Why we need detailed balance?
  - Stationary distribution $\pi(x)$!
  - Then how can such a $\pi(x)$ handle the following case?





Reversible Jump MCMC

- An MCMC algorithm that allows for model selection
  - Examples: choosing # clusters K, or even switching between two completely different models $P_1(x)$ and $P_2(x)$



RJMCMC

- Definitions:
  - x – model r.v.s (the number of x's can change depending on the model)
  - u – auxiliary variables used to perform "dimension matching"
  - m – an indicator representing which model we are currently using
  - P(x|m) – probability distribution for r.v.s x assuming model m
- RJMCMC uses two types of proposal distribution:
  - j(m'|m) – model proposal; switches from model m to m'. Must be reversible!
  - q(x',u'|m→m',x,u) – data proposal; proposes (x',u') under the new model m', starting from (x,u) under the previous model m
- RJMCMC also requires a mapping function:
  - $h_{m,m'}(x,u)$ – explains how (x,u) under model m maps to (x',u') under m'

The mapping function h()

- Properties of $h_{m,m'}(x,u)$:
  - Is deterministic (non-random)
  - Takes a vector (x,u) as input, and outputs a vector (x',u')
    - Dimension of x is usually different from x' (and likewise for u,u')
  - Must be bijective (one-to-one) so that its inverse is well-defined

- Simple example: switching from 2 clusters to 3 clusters
  - Let x_1, x_2 be the first 2 cluster centers
  - Randomly draw an a.v. u to be the 3rd cluster center
  - Then

$$h_{2,3}(x_1, x_2, u) = \begin{bmatrix} x_1' = x_1 \\ x_2' = x_2 \\ x_3' = u \end{bmatrix}$$

    - i.e. $h_{2,3}()$ maps a 2-cluster model to a 3-cluster model by setting the 3rd cluster center x_3' to u (dimension matching)

RJMCMC Algorithm

1. Initialize x,u,m
2. Repeat until convergence:
   1. Propose a new model m' using j(m'|m)
   2. Propose a new model state (x',u') using q(x',u'|m→m',x,u)
   3. Compute the acceptance probability:

$$A(m',x',u' \mid m,x,u) = \min\left(1, \frac{P(x' \mid m')}{P(x \mid m)} \times \overbrace{\frac{j(m \mid m')}{j(m' \mid m)} \times \frac{q(x,u \mid m' \to m, x', u')}{q(x',u' \mid m \to m', x, u)} \times \left|\det \frac{\partial h_{m,m'}(x,u)}{\partial (x,u)}\right|}^{\boxed{\text{Equivalent to MH algorithm's inv. ratio of proposals } Q(x|x')/Q(x'|x)}}\right)$$

Ratio of model probs.

Inv. ratio of model proposals

Inv. ratio of data proposals

Absolute value of the determinant
of the Jacobian of h()

The abs-det-Jacobian term

$$\boxed{\left|\det \frac{\partial h_{m,m'}(x,u)}{\partial(x,u)}\right|}$$

- A "Jacobian" is a matrix of all 1st derivatives
  - Example: 2-clusters to 3-clusters; recall $h_{2,3}(x_1,x_2,u) = \begin{bmatrix} x_1' = x_1 \\ x_2' = x_2 \\ x_3' = u \end{bmatrix}$

The Jacobian is $\dfrac{\partial h_{2,3}(x_1,x_2,u)}{\partial(x_1,x_2,u)} = \begin{bmatrix} \partial x_1'/\partial x_1 & \partial x_1'/\partial x_2 & \partial x_1'/\partial u \\ \partial x_2'/\partial x_1 & \partial x_2'/\partial x_2 & \partial x_2'/\partial u \\ \partial x_3'/\partial x_1 & \partial x_3'/\partial x_2 & \partial x_3'/\partial u \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

thus $\left|\det \dfrac{\partial h_{2,3}(x_1,x_2,u)}{\partial(x_1,x_2,u)}\right| = 1$

In general, we construct h() so that the abs-det-Jacobian term is trivial (e.g. 1)

The Jacobian term

$$\boxed{\left|\det \frac{\partial h_{m,m'}(x,u)}{\partial(x,u)}\right|}$$

- Why do we need the Jacobian?
  - It arises from a change of variables during integration!
  - Consider the detailed balance equation; take integrals on both sides:

$$\int P(x)g(x',u' \mid x,u)A(x',u' \mid x,u)dxdu = \int P(x')g(x,u \mid x',u')A(x,u \mid x',u')dx'du'$$

    - g() combines the model proposal j() and the data proposal q()
    - For simplicity, we omit the model indicator m, because the dimensionality of (x,u) completely identifies which model m the system is in
  - Now perform a change of variables from (x',u') to (x,u) on the RHS:

$$\int P(x)g(x',u' \mid x,u)A(x',u' \mid x,u)dxdu = \int P(x')g(x,u \mid x',u')A(x,u \mid x',u')\left|\det \frac{\partial h_{(x,u),(x',u')}(x,u)}{\partial(x,u)}\right|dxdu$$

  - The equation above holds if, for all x,x',u,u',

$$P(x)g(x',u' \mid x,u)A(x',u' \mid x,u) = P(x')g(x,u \mid x',u')A(x,u \mid x',u')\left|\det \frac{\partial h_{(x,u),(x',u')}(x,u)}{\partial(x,u)}\right|$$

The Jacobian term

$$\boxed{\left|\det \frac{\partial h_{m,m'}(x,u)}{\partial(x,u)}\right|}$$

- Why do we need the Jacobian?
  - The detailed balance condition holds if, for all x,x',u,u',

$$P(x)g(x',u'\mid x,u)A(x',u'\mid x,u) = P(x')g(x,u\mid x',u')A(x,u\mid x',u')\left|\det \frac{\partial h_{(x,u),(x',u')}(x,u)}{\partial(x,u)}\right|$$

  - We can now construct an acceptance probability that satisfies detailed balance (see previous lecture, MH algorithm):

$$A(x',u'\mid x,u) = \min\left(1, \frac{P(x')}{P(x)} \times \frac{g(x,u\mid x',u')}{g(x',u'\mid x,u)} \times \left|\det \frac{\partial h_{(x,u),(x',u')}(x,u)}{\partial(x,u)}\right|\right)$$

  - Restoring the model indicator m, we get

$$A(m',x',u'\mid m,x,u) = \min\left(1, \frac{P(x'\mid m')}{P(x\mid m)} \times \frac{j(m\mid m')}{j(m'\mid m)} \times \frac{q(x,u\mid m'\to m,x',u')}{q(x',u'\mid m\to m',x,u)} \times \left|\det \frac{\partial h_{m,m'}(x,u)}{\partial(x,u)}\right|\right)$$

Question:

- What is our stationary distribution in our RJMCMC?

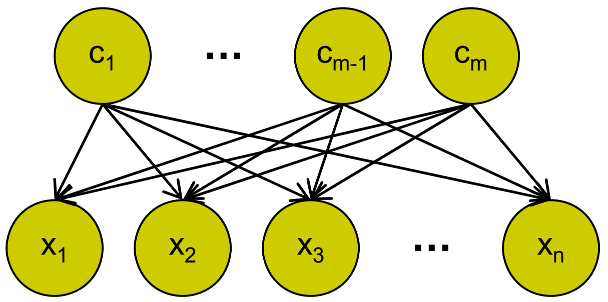
RJMCMC Example: Clustering

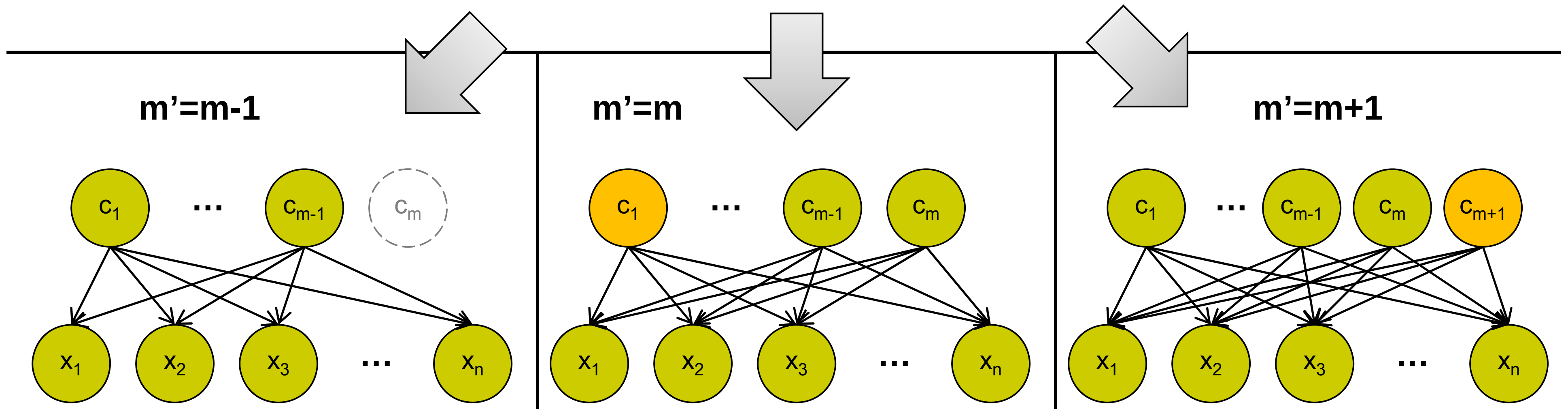
- Models: Let m = 1,2,3,… denote the number of clusters
  - P(x,c|m) - probability of (observed) data x and (unknown) cluster centers c, assuming m clusters
    - Can be a Gaussian mixture model or any other clustering model. For this example, we don't need to know its exact form.

- Proposal distributions:
  - j(m'|m) – switches from m to m' clusters, where m' = {m-1,m,m+1}
    - m' = m-1 is used to decrease the number of clusters
    - m' = m+1 is used to increase the number of clusters
    - m' = m is used to change cluster centers c
  - q(x',c',u'|m→m',x,c,u) – form differs depending on m' and m
  - $h_{m,m'}(c,u)$ – again, form differs depending on m' and m
  - abs-det-Jacobian – turns out that this is always 1!

RJMCMC Example: Clustering

Starting state: m cluster centers





Remove cluster (e.g. c_m)

Change cluster center(e.g. c_1)

Add cluster

RJMCMC Example: Clustering

- We set j() as follows:

$$j(m' \mid m) = \begin{cases} 0.5 - p & \text{if } m' = m - 1 \\ 2p & \text{if } m' = m \\ 0.5 - p & \text{if } m' = m + 1 \end{cases}$$

"Explore cluster centers c 2p of the time, change the number of clusters 1-2p of the time"

Notice that reverse moves have the same probability as forward moves

- For q(), h() and the Jacobian, consider the 3 cases separately:
  - m' = m (change cluster center):
    - u, u' are used to change the value of some c_i
    - First, pick a cluster center i in {1,…,m} to change assignment (at uniform)
    - Next, draw a new cluster center u according to some proposal $q_{center}(u)$
    - Finally, set $c'_i = u$

$$q(x', c', u' \mid m \to m', x, c, u) = \frac{1}{m} \times q_{center}(u) \quad \text{and} \quad h_{i,m,m'=m}(c,u) = \begin{bmatrix} c'_1 \\ c'_2 \\ \vdots \\ c'_m \\ u' \end{bmatrix}$$

where $c'_j = c_j$ if $j \neq i$, and $c'_i = u$, and $u' = c_i$

RJMCMC Example: Clustering

- For q(), h() and the Jacobian, consider the 3 cases separately:
  - m' = m (change cluster center):
    - What does the abs-det-Jacobian look like?
    - Recall that $h_{i,m,m'=m}(c,u)$ sets $c'_j = c_j$ for all $j \neq i$, and $c'_i = u$, and $u' = c_i$
    - Let's say we're changing c_i, where $i = m$

$$\frac{\partial h_{i=m,m,m'=m}(c,u)}{\partial(c,u)} = \begin{bmatrix} \partial c'_1/\partial c_1 & \partial c'_1/\partial c_2 & \cdots & \partial c'_1/\partial c_m & \partial c'_1/\partial u \\ \partial c'_2/\partial c_1 & \partial c'_2/\partial c_2 & & \partial c'_2/\partial c_m & \partial c'_2/\partial u \\ \vdots & & \ddots & & \vdots \\ \partial c'_m/\partial c_1 & \partial c'_m/\partial c_2 & & \partial c'_m/\partial c_m & \partial c'_m/\partial u \\ \partial u'/\partial c_1 & \partial u'/\partial c_2 & \cdots & \partial u'/\partial c_m & \partial u'/\partial u \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

Therefore $\left|\det \frac{\partial h_{i=m,m,m'=m}(c,u)}{\partial(c,u)}\right| = |-1| = 1$

In fact, the abs-det-Jacobian is 1 for any choice of i!

RJMCMC Example: Clustering

- For q(), h() and the Jacobian, consider the 3 cases separately:
  - m' = m-1 (remove a cluster):
    - u is empty, and u' matches the cluster to be removed
    - Pick a cluster center i in {1,…,m} to remove (at uniform)

$$q(x',c',u' \mid m \to m', x, c, u) = \frac{1}{m}$$ and $$h_{i,m,m'=m-1}(c,u) = \begin{bmatrix} c'_1 \\ c'_2 \\ \vdots \\ c'_{m-1} \\ u' \end{bmatrix}$$ where $c'_j = c_j$ if $j < i$, and $c'_j = c_{j+1}$ if $j > i$, and $u' = c_i$

RJMCMC Example: Clustering

- For q(), h() and the Jacobian, consider the 3 cases separately:
  - m' = m-1 (remove a cluster):
    - For the Jacobian, let's assume we're removing cluster c_i where i = m
    - Thus we set $c'_j = c_j$ for all j < m, and $u' = c_m$

$$\frac{\partial h_{i=m,m,m'=m-1}(c,u)}{\partial(c,u)} = \begin{bmatrix} \partial c'_1/\partial c_1 & \partial c'_1/\partial c_2 & \cdots & \partial c'_1/\partial c_{m-1} & \partial c'_1/\partial c_m \\ \partial c'_2/\partial c_1 & \partial c'_2/\partial c_2 & & \partial c'_2/\partial c_{m-1} & \partial c'_2/\partial c_m \\ \vdots & & \ddots & & \vdots \\ \partial c'_{m-1}/\partial c_1 & \partial c'_{m-1}/\partial c_2 & & \partial c'_{m-1}/\partial c_{m-1} & \partial c'_m/\partial c_m \\ \partial u'/\partial c_1 & \partial u'/\partial c_2 & \cdots & \partial u'/\partial c_{m-1} & \partial u'/\partial c_m \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}$$

Therefore $$\left|\det \frac{\partial h_{i=m,m,m'=m-1}(c,u)}{\partial(c,u)}\right| = |1| = 1$$

Again, the abs-det-Jacobian is 1 for any choice of i!

RJMCMC Example: Clustering

- For q(), h() and the Jacobian, consider the 3 cases separately:
  - m' = m+1 (add a cluster):
    - u is the center of the cluster to be added, and u' is empty
    - We draw a cluster center u according to some proposal $q_{center}(u)$

$q(x',c',u' \mid m \to m', x, c, u) = q_{center}(u)$ and $h_{i,m,m'=m+1}(c,u) = \begin{bmatrix} c'_1 \\ c'_2 \\ \vdots \\ c'_m \\ c'_{m+1} \end{bmatrix}$ where $c'_j = c_j$ for all $j \le m$, and $c'_{m+1} = u$

RJMCMC Example: Clustering

- For q(), h() and the Jacobian, consider the 3 cases separately:
  - m' = m+1 (add a cluster):
    - For the Jacobian, recall we set $c'_j = c_j$ for all $j \le m$, and $c'_{m+1} = u$

$$\frac{\partial h_{m,m'=m+1}(c,u)}{\partial(c,u)} = \begin{bmatrix} \partial c'_1/\partial c_1 & \partial c'_1/\partial c_2 & \cdots & \partial c'_1/\partial c_m & \partial c'_1/\partial u \\ \partial c'_2/\partial c_1 & \partial c'_2/\partial c_2 & & \partial c'_2/\partial c_m & \partial c'_2/\partial u \\ \vdots & & \ddots & & \vdots \\ \partial c'_m/\partial c_1 & \partial c'_m/\partial c_2 & & \partial c'_m/\partial c_m & \partial c'_m/\partial u \\ \partial c'_{m+1}/\partial c_1 & \partial c'_{m+1}/\partial c_2 & \cdots & \partial c'_{m+1}/\partial c_m & \partial c'_{m+1}/\partial u \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}$$

Therefore $\left| \det \frac{\partial h_{m,m'=m+1}(c,u)}{\partial(c,u)} \right| = |1| = 1$

RJMCMC Example: Clustering

- Notice the following important properties:
  - All model changes j(m'|m) are all reversible
    - We can get to any number of clusters m
    - We can change the location of any cluster i
    - This ensures we converge to the stationary distribution
  - abs-det-Jacobian is always 1
    - We designed our r.v. mappings h() to make this true!

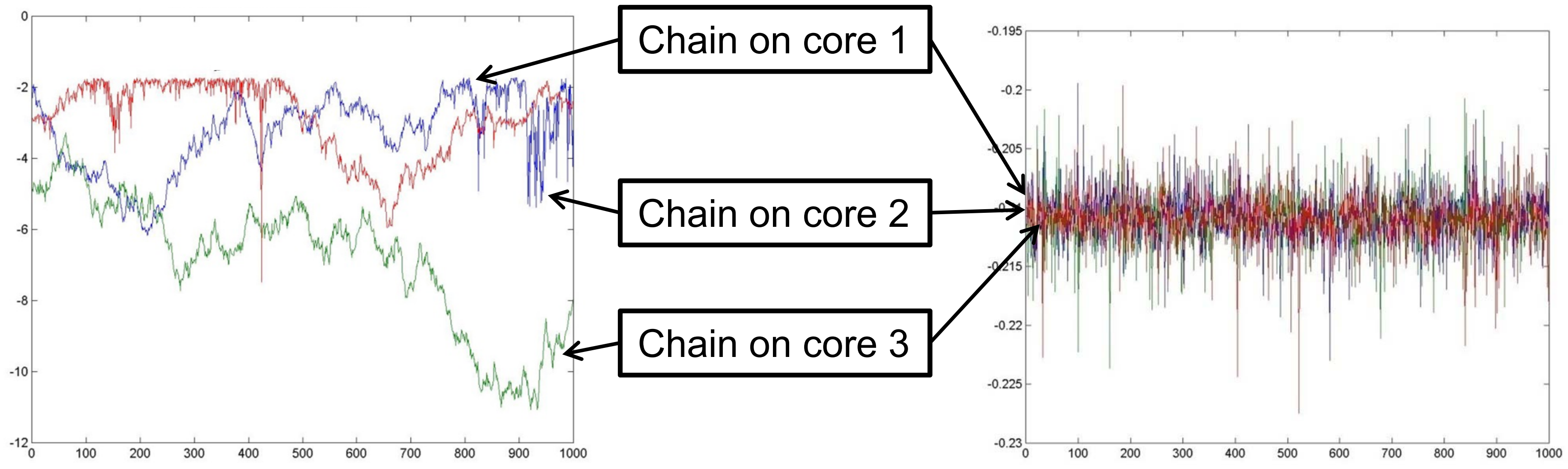
- Take note:
  - For most mixture models, we can't simply use P(x,c|m). We need to introduce hidden cluster assignment variables z for each data point x, and incorporate them into the proposals.
    - The basic principle of RJMCMC remains the same, though

Large-scale MCMC

- Modern datasets can be very large
  - Millions of data points
  - Require Gigabytes of memory
  - E.x. Yahoo web graph has ~1.4 billion nodes and 6.6 billion edges
- So far, we have not explained how to take advantage of parallelism in MCMC
  - Without parallelism, we cannot use large datasets!
- In the rest of this lecture, we will cover techniques that permit multiple CPUs/cores to be used with MCMC

Taking Multiple Chains

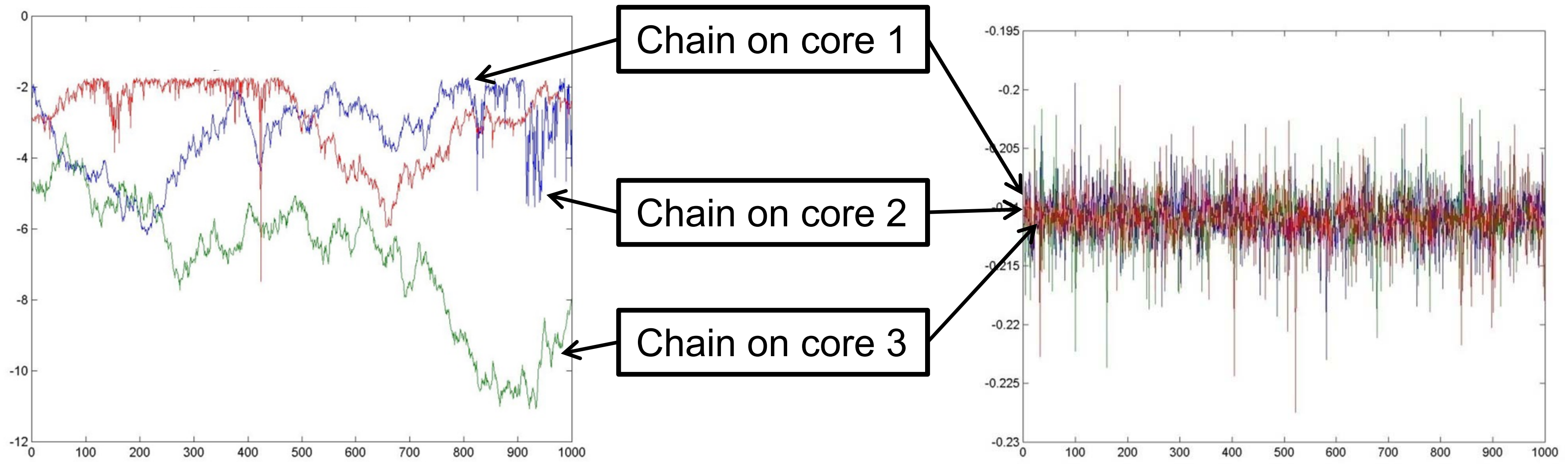
- Proper use of MCMC actually requires parallelism
  - To determine convergence, you need to take multiple MCMC chains
  - Chains are independent, so you can run one chain per CPU
  - Once converged, you can combine samples from all chains



Not converged **Converged**

Taking Multiple Chains

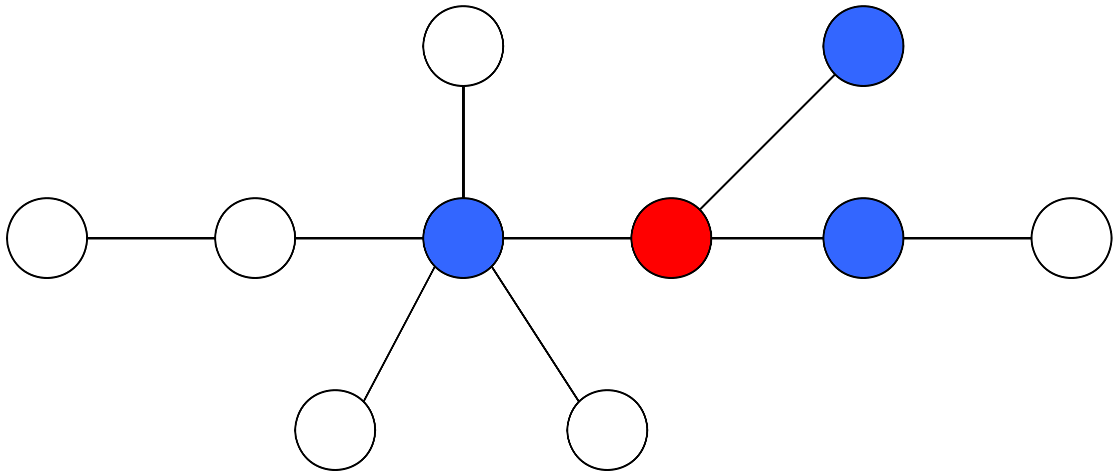
- Taking multiple chains doesn't solve all issues, though
  - If burn-in is long, then all chains will take a long time to converge!
  - We need a way to take each sample faster…



Not converged **Converged**

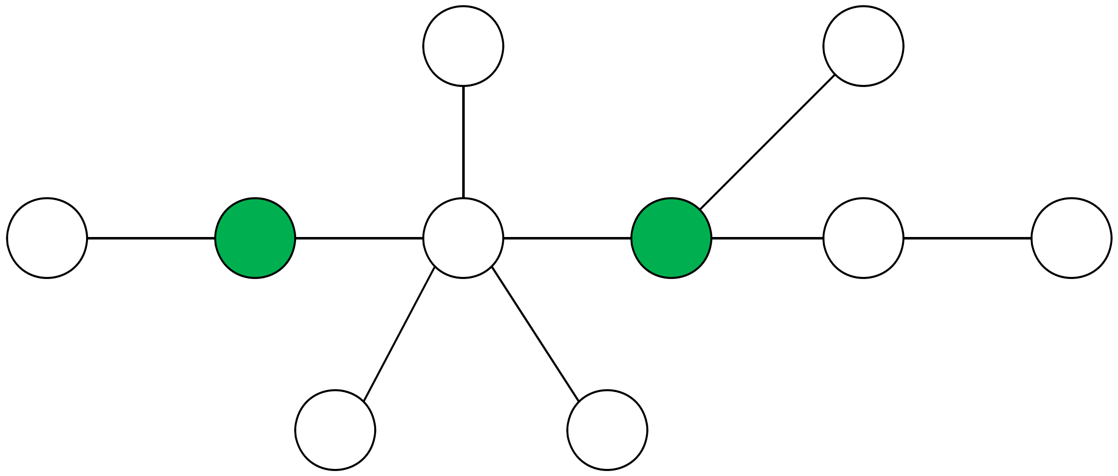
Parallel Gibbs Sampling

- Recall that in MRFs, we Gibbs sample by sampling from P(x|MB(x)), the conditional distribution of x given its Markov Blanket MB(x)
  - For MRFs, the Markov Blanket of x is just its neighbors
  - In the MRF below, the red node's Markov Blanket consists of the blue nodes



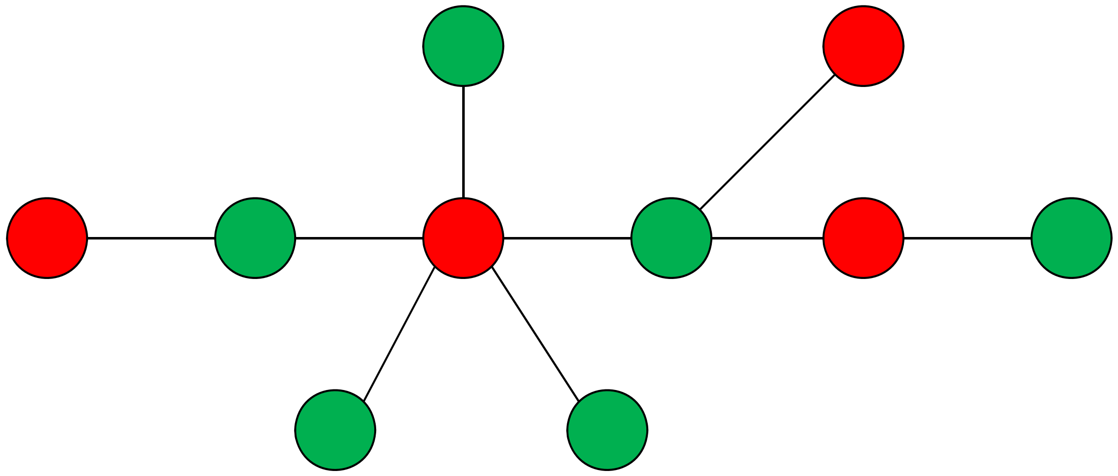
Parallel Gibbs Sampling

- Observe that we can Gibbs sample the two green nodes simultaneously
  - Neither node is part of the other's Markov Blanket, so their conditional distributions do not depend on each other
  - Sampling one of the green nodes doesn't change the conditional distribution of the other node!



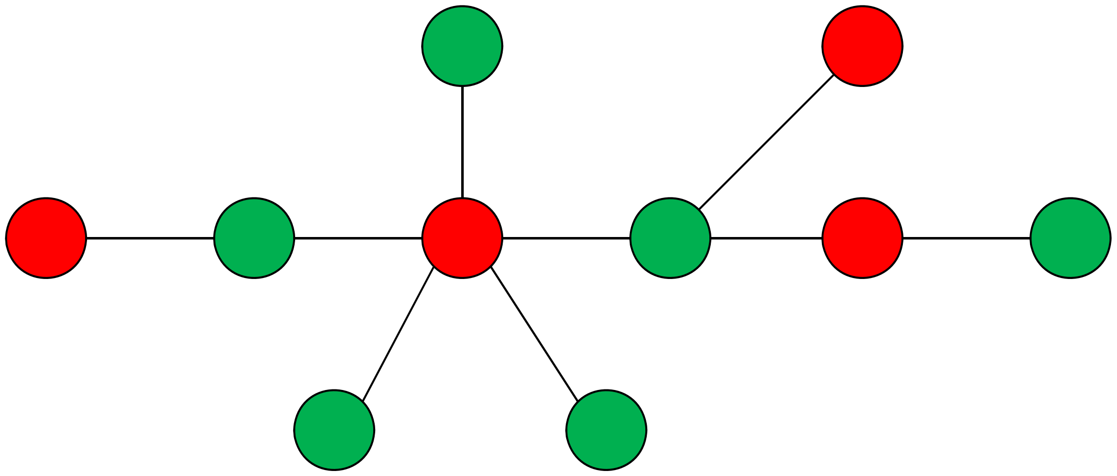
Parallel Gibbs Sampling

- How do we generalize this idea to the whole graph?
  - Find subsets of nodes, such that all nodes in a given subset are not in each other's Markov Blankets, and the subsets cover the whole graph
    - The subsets should be as large as possible
      - Because we can Gibbs sample all nodes in a subset at the same time
    - At the same time, we want as few subsets as possible
      - The Markov Blankets of different subsets overlap, so they cannot be sampled at the same time. We must process the subsets sequentially.



Parallel Gibbs Sampling

- We can find these covering subsets with k-coloring algorithms (Gonzales et al., 2011)
  - A k-coloring algorithm colors a graph using k colors, such that:
    - Every node gets one color
    - No edge has two nodes of the same color
- Trees always admit a 2-coloring (e.g. below)
  - Assign one color to some node, and alternate colors as you move away



Parallel Gibbs Sampling

- Bipartite graphs are always 2-colorable
  - Color each side of the bipartite graph with opposite colors
  - e.x. Latent Dirichlet Allocation model is bipartite

- However, not all graphs have k-colorings for all $k \geq 2$
  - In the worst case, a graph with n nodes can require n colors
    - The full clique is one such graph
  - Determining if a graph is k-colorable for $k > 2$ is NP-complete
  - In practice, we employ heuristics to find k-colorings

- Instead of using k-colorings, why not just Gibbs sample all variables at the same time?
  - The Markov Chain may become non-ergodic, and is no longer guaranteed to converge to the stationary distribution!

Online MCMC

- In "online" algorithms, we need to process new data points one-at-a-time
  - Moreover, we have to "forget" older data points because memory is finite
- For such applications to be viable, we can only afford constant time work per new data point
  - Otherwise we will reach a point where new data can no longer be processed in a reasonable amount of time
- What MCMC techniques can we use to make an online algorithm?

Sequential Monte Carlo

- SMC is a generalization of Particle Filters
  - Recall that PFs incrementally sample $P(X_t|Y_{1:t})$, where the Xs are latent r.v.s and the Ys are observations under a state-space model
  - SMC does not assume the GM is a state-space model, or has any particular structure at all

- Suppose we have n r.v.s $x_1,\ldots,x_n$
  - SMC first draws samples from the marginal distribution $P(x_1)$, then $P(x_{1:2})$, and so on until $P(x_{1:n})$
  - Key idea: Construct proposals such that we sample from $P(x_{1:k+1})$ in constant time, given samples from $P(x_{1:k})$
  - Like other MCMC algorithms, we only require that we can evaluate $P'(x_{1:n}) = aP(x_{1:n})$ for some unknown a

Sequential Importance Sampling

- SIS is the foundation of Sequential Monte Carlo
  - It allows new variables to be sampled in constant time, without resampling older variables

- SIS uses proposal distributions with the following structure:

$$q_n(x_{1:n}) = q_{n-1}(x_{1:n-1})q_n(x_n \mid x_{1:n-1})$$
$$= q_1(x_1)\prod_{k=2}^{n} q_k(x_k \mid x_{1:k-1})$$

  - Notice we can propose x_{k+1} if we've already drawn $x_{1:k}$, without having to redraw $x_{1:k}$

Sequential Importance Sampling

- In normalized importance sampling, recall how the sample weights w^i are defined:

$$\langle f(X) \rangle_P = \sum_i f(x^i) w^i$$

where $w^i = \frac{r^i}{\sum_j r^j}$ and $r^i = \frac{P'(x^i)}{Q(x^i)}$

- In SIS, the unnormalized weights r can be rewritten as a telescoping product:

$$\begin{aligned} r(x_{1:n}) &= \frac{P'_n(x_{1:n})}{q_n(x_{1:n})} \\ &= \frac{P'_{n-1}(x_{1:n-1})}{q_{n-1}(x_{1:n-1})} \frac{P'_n(x_{1:n})}{P'_{n-1}(x_{1:n-1}) q_n(x_n \mid x_{1:n-1})} \\ &= r_{n-1}(x_{1:n-1}) \alpha_n(x_{1:n}) \\ &= r_1(x_1) \prod_{k=2}^{n} \alpha_k(x_{1:k}) \end{aligned}$$

where $\alpha_n(x_{1:n}) = \frac{P'_n(x_{1:n})}{P'_{n-1}(x_{1:n-1}) q_n(x_n \mid x_{1:n-1})}$

Sequential Importance Sampling

$$r(x_{1:n}) = r_1(x_1)\prod_{k=2}^{n}\alpha_k(x_{1:k}) \qquad \text{where} \qquad \alpha_n(x_{1:n}) = \frac{P'_n(x_{1:n})}{P'_{n-1}(x_{1:n-1})q_n(x_n \mid x_{1:n-1})}$$

- This means the unnormalized weights r can be computed incrementally
  - Compute α_n and use it to update $r(x_{1:n-1})$ to $r(x_{1:n})$
    - NB: For this update to be constant time, we also require $P'_n(x_{1:n})$ to be computable from $P'_{n-1}(x_{1:n-1})$ in constant time
  - We remember the unnormalized weights r at each iteration, and compute the normalized weights w as needed from r

- Thus, we can sample x AND compute the normalized weights w using constant time per new variable x_n
  - So SIS meets the requirements for an online inference algorithm!

- Even better, the samples don't depend on each other
  - Assign one CPU core per sample to make the SIS algorithm parallel!

Sequential Importance Sampling

- SIS algorithm:
  - At time n = 1
    - Draw samples $x^i_1 \sim q_1(x_1)$
    - Compute unnormalized weights $r_1^i = P_1'(x_1^i)/q_1(x_1^i)$
    - Compute normalized weights w^i_1 by normalizing r^i_1
  - At time n ≥ 2
    - Draw samples $x^i_n \sim q_n(x_n|x^i_{1:n-1})$
    - Compute unnormalized weights $r_n^i = r_{n-1}^i \alpha_n(x_{1:n}^i) = r_{n-1}^i \dfrac{P_n'(x_{1:n}^i)}{P_{n-1}'(x_{1:n-1}^i) q_n(x_n^i \mid x_{1:n-1}^i)}$
    - Compute normalized weights w^i_n by normalizing r^i_n

Sequential Importance Sampling

- But we are not done yet!
- Unfortunately, SIS suffers from a severe drawback: the variance of the samples increases exponentially with n!
  - See eq (31) of Doucet's SMC tutorial for an example
- Resampling at each iteration will decrease the sample variance!
  - Similar to weighted resampling from the first MC lecture!

Multinomial Resampling

- Suppose we have m samples $x^1,\ldots,x^m$ with corresponding importance weights $w^1,\ldots,w^m$

- Construct a categorical distribution from these samples:
  - This distribution has m categories (choices)
  - The probability of drawing category k is w^k
  - Drawing category k gets us x^k

- To resample, just draw N times from this distribution
  - Note that N can be greater/less than m!

- For more advanced strategies such as systematic and residual resampling, refer to page 13 of Doucet's SMC tutorial

Why Resample?

- Apart from decreasing variance, there are other reasons…

- Resampling removes samples x^k with low weights w^k
  - Low-weight samples come from low-probability regions of P(x)
    - We want to focus computation on high-probability regions of P(x)
  - Notice that each sample gets an equal amount of computation, regardless of its weight w_k
    - Resampling ensures that more computation is spent on samples x_k that come from high-probability regions of P(x)

- Resampling prevents a small number of samples x_k from dominating the empirical distribution
  - Resampling resets all weights w_k to 1/N
    - This prevents sample weights w_k from growing until they reach 1

Sequential Monte Carlo

- The SMC algorithm is just SIS with resampling:
  - At time n = 1
    - Draw samples $x^i_1 \sim q_1(x_1)$
    - Compute unnormalized weights $r_1^i = P_1'(x_1^i) / q_1(x_1^i)$
    - Compute normalized weights w^i_1 by normalizing r^i_1
    - Resample w^i_1, x^i_1 into N equally-weighted particles x^i_1
  - At time n ≥ 2
    - Draw samples $x^i_n \sim q_n(x_n|x^i_{1:n-1})$
    - Compute unnormalized weights $r_n^i = r_{n-1}^i \alpha_n(x_{1:n}^i) = r_{n-1}^i \dfrac{P_n'(x_{1:n}^i)}{P_{n-1}'(x_{1:n-1}^i) q_n(x_n^i \mid x_{1:n-1}^i)}$
    - Compute normalized weights w^i_n by normalizing r^i_n
    - Resample w^i_n,$x^i_{1:n}$ into N equally-weighted particles $x^i_{1:n}$

Summary

- Slice sampling
    - Samples from area under P(x)
- Reverse Jump MCMC
    - Allows us to switch between different models P(x)
- Parallel Gibbs sampling
    - Exploit graph colorings to sample same-colored nodes in parallel
- Sequential Monte Carlo
    - Uses incremental proposal distributions
    - Provides a framework for designing online, parallel MCMC algorithms