CSC696H: Advanced Topics in Probabilistic Graphical Models

Monte Carlo Methods

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Some material from:
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Outline

- Monte Carlo Estimation
- Sequential Monte Carlo
- Markov Chain Monte Carlo

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- Monte Carlo Estimation
- Sequential Monte Carlo
- Markov Chain Monte Carlo

Motivation for Monte Carlo Methods

- Now consider computing the expectation of a function $f(z)$ over $p(z)$.
- Recall that this looks like $E_{p(z)}[f] = \int_z f(z)p(z)dz$
- How can we approximate or estimate E[f]?

A bad plan…

Discretize the space where z lives into L blocks

Then compute $E_{p(z)}[f] \cong \frac{1}{L}\sum_{l=1}^{L} p(z)f(z)$

Scales poorly with dimension of Z

A better plan…

Given independant samples $z^{(l)}$ from $p(z)$

Estimate $E_{p(z)}[f] \cong \frac{1}{L}\sum_{l=1}^{L} f(z)$

Motivation for Monte Carlo Methods

- Generally, Z lives in a very high dimensional space.
- Generally, regions of high $p(z)$ is very little of that space.
- IE, the probability mass is very localized.
- Watching samples from $p(z)$ should provide a good maximum (one of our inference problems)

Motivation for Monte Carlo Methods

- Real problems are typically complex and high dimensional.

- Suppose that we *could* generate samples from a distribution that is proportional to one we are interested in.

- Typically we want posterior samples,

$$p(z \mid \mathcal{D}) = \frac{p(z)p(\mathcal{D} \mid z)}{p(\mathcal{D})} \propto \widetilde{p}(z)$$

Unnormalized posterior

Don't know marginal likelihood / normalizer

- Typically, $\widetilde{p}(z)$ is easier to evaluate (though not always)

Inference (and related) Tasks

- Simulation: $x \sim p(x) = \frac{1}{Z} f(x)$
- Compute expectations: $\mathbb{E}[\phi(x)] = \int p(x)\phi(x)\, dx$
- Optimization: $x^* = \arg\max_x f(x)$
- Compute normalizer / marginal likelihood: $Z = \int f(x)\, dx$

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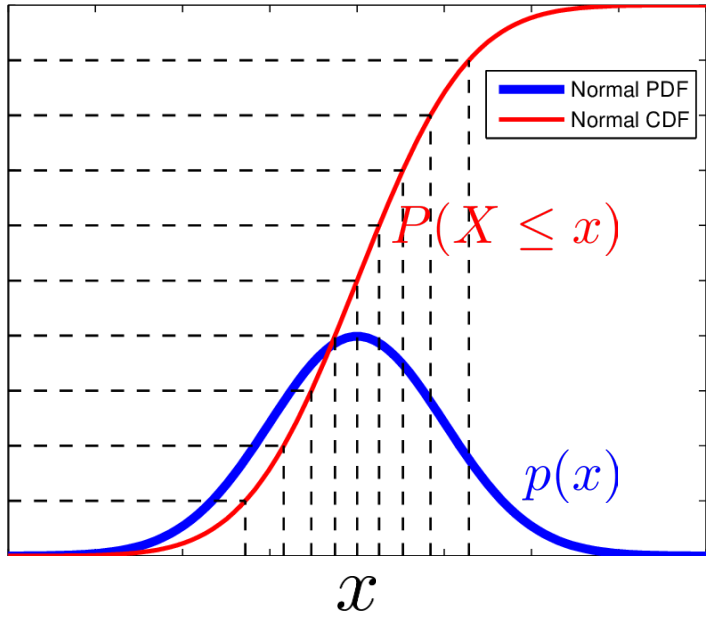
Sampling Continuous RVs

Recall that the CDF is the integral of the PDF and (left) tail probability,

$$P(X \leq x) = \int_{-\infty}^{x} p(X = t)\, dt$$

Observation 1 Equally spaced intervals of CDF correspond to regions of equal event probability

Observation 2 The same events have unequal regions under PDF



Question Given samples $\{x_i\}_{i=1}^{N} \sim p(x)$ what is the probability distribution of the CDF values,

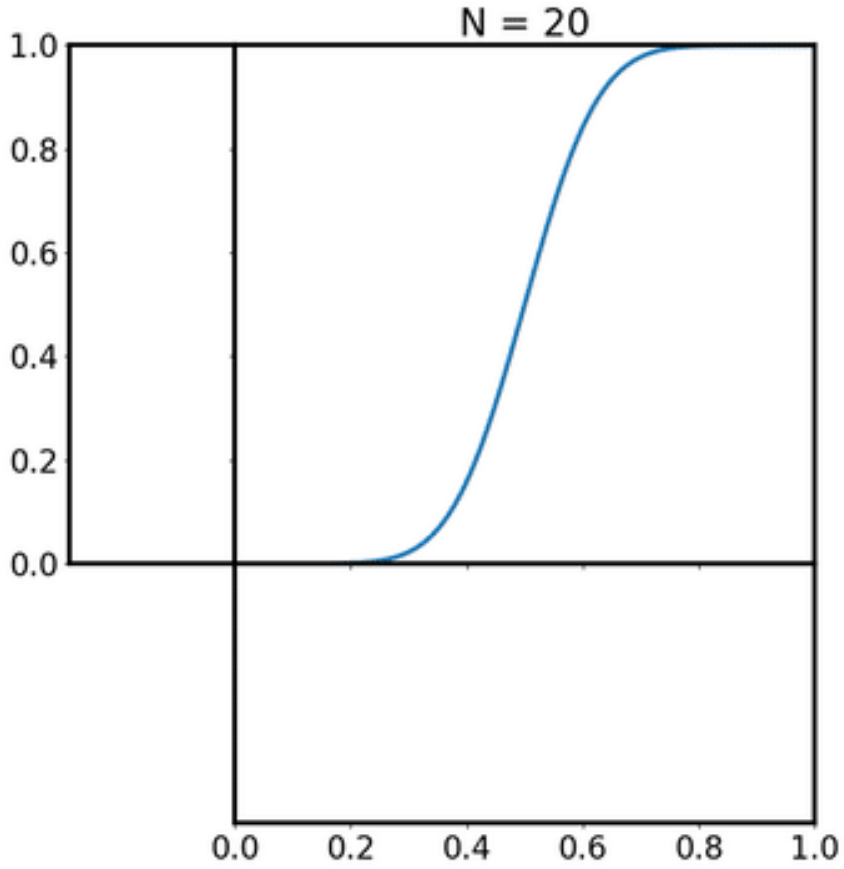
$$\{P(X \leq x_i)\}_{i=1}^{N} \sim ???$$

Sampling Continuous RVs

Answer The CDF of iid samples has a **standard uniform** distribution!

$$\{P(X \leq x_i)\}_{i=1}^{N} \sim \text{Uniform}(0, 1)$$

This property is called the **probability integral transform**



Question How can we use this fact to sample *any* RV?

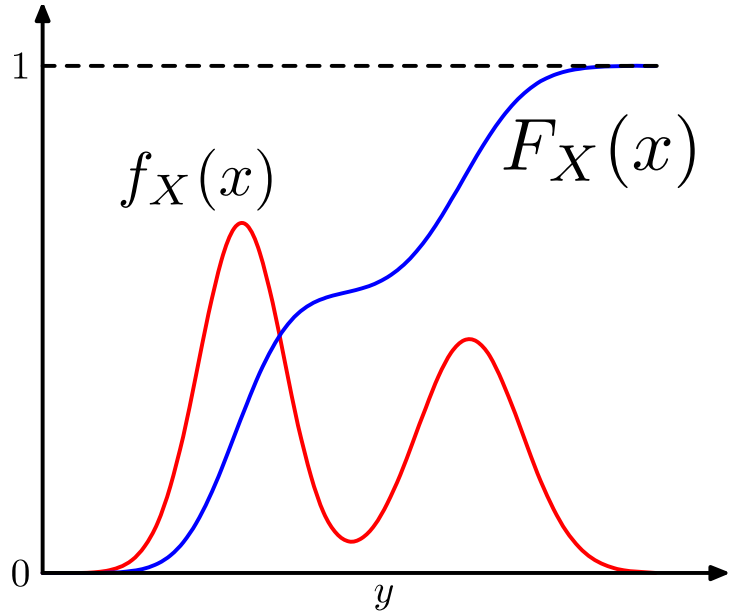
Answer Apply this relationship in reverse:

1. Sample iid standard uniform RVs
2. Compute *inverse* CDF
3. Result are samples from the target

Inverse Transform Sampling

- Input: Independent standard uniform variables $U_1, U_2, U_3, \ldots$
- We can use these to exactly sample from any continuous distribution using the cumulative distribution function:

$$F_X(x) = P(X \leq x) = \int_{-\infty}^{x} f_X(z)\, dz$$



- Assuming continuous CDF is invertible:

$$h(u) = F_X^{-1}(u)$$
$$X_i = h(U_i)$$

Requires us to have access to inverse CDF

$$P(X_i \leq x) = P(h(U_i) \leq x) = P(U_i \leq F_X(x)) = F_X(x)$$

This function transforms uniform variables to our target distribution!

Inverse Transform Sampling

- Very nice trick that applies to *all* continuous RVs (in theory)
- Yay, we know how to sample any RV right? Wrong…
- Don't always have the *inverse* CDF (or cannot calculated it)
- Doesn't extend easily to multivariate RVs (that's why I only showed 1-dimensional)

Rejection Sampling

Assume

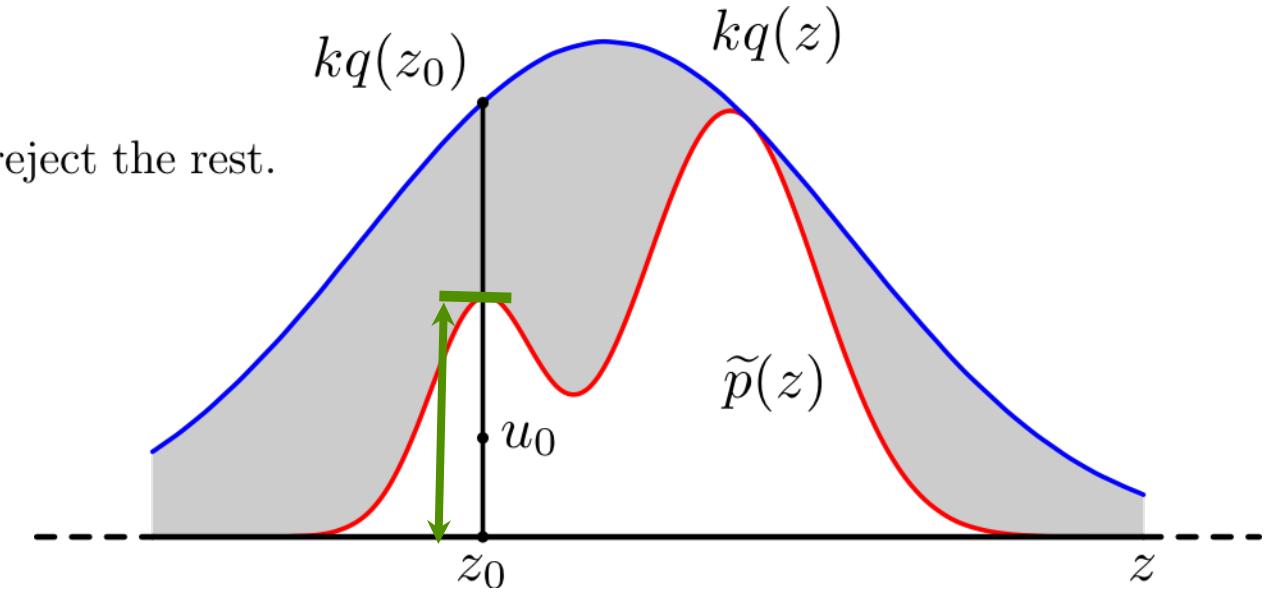
- Access to easy-to-sample distribution $q(z)$
- Constant *k* such that $\tilde{p}(z) \leq k \cdot q(z)$

Proposal Distribution
Where we can use one of methods on previous slides to sample efficiently

Algorithm

1) Sample $q(z)$

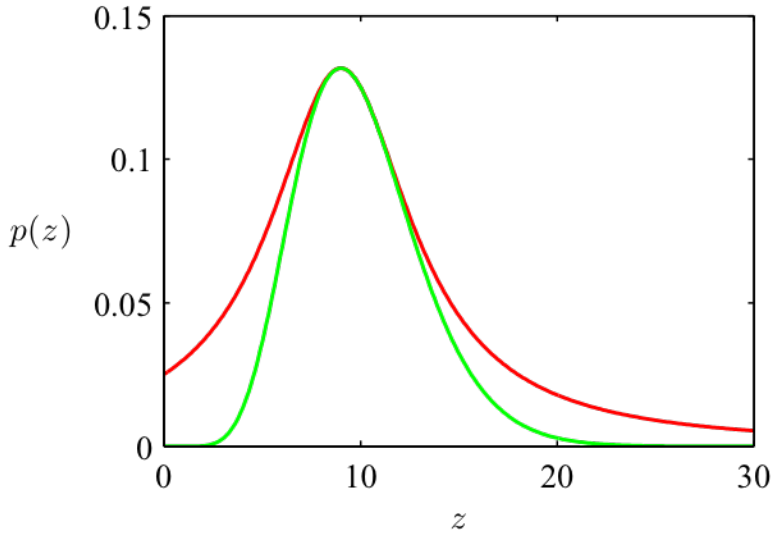
2) Keep samples in proportion to $\frac{\tilde{p}(z)}{k \bullet q(z)}$ and reject the rest.



Example Uses Gaussian proposal q to draw samples from multimodal distribution p

Rejection Sampling

- Rejection sampling is hopeless in high dimensions, but is useful for sampling low dimensional “building block” functions.
- For example, the Box-Muller method for generating samples from a Gaussian uses rejection sampling.



A second example where a gamma distribution is approximated by a Cauchy proposal distribution.

Inference (and related) Tasks

- Simulation: $x \sim p(x) = \frac{1}{Z} f(x)$
- Compute expectations: $\mathbb{E}[\phi(x)] = \int p(x)\phi(x)\, dx$
- Optimization: $x^* = \arg\max_x f(x)$
- Compute normalizer / marginal likelihood: $Z = \int f(x)\, dx$

Monte Carlo Integration

One reason to sample a distribution is to approximate expected values under that distribution…

Expected value of function $f(x)$ w.r.t. distribution $p(x)$ given by,

$$\mathbb{E}_p[f(x)] = \int p(x) f(x)\, dx \equiv \mu$$

- Doesn't always have a closed-form for arbitrary functions
- Suppose we have iid samples: $\{x_i\}_{i=1}^N \sim p(x)$
- *Monte Carlo* estimate of expected value,

$$\hat{\mu}_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \approx \mathbb{E}_p[f(x)]$$

Monte Carlo Integration

$$\hat{\mu}_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \approx \mathbb{E}_p[f(x)]$$

- Expectation estimated from *empirical distribution* of L samples:

$$\hat{p}_N(x) = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}(x) \qquad \{x_i\}_{i=1}^{N} \sim p(x)$$

- The *Dirac delta* is *loosely* defined as a piecewise function:

$$\delta_{x_i}(x) = \begin{cases} +\infty & x = x_i \\ 0 & x \neq x_i \end{cases}$$

Caveat This is technically incorrect. Dirac is only well-defined within integrals, $\int \delta_{\bar{x}}(x) f(x)\, dx = f(\bar{x})$ but it gets the intuition across.

- For any *N* this estimator, a random variable, is *unbiased*:

$$\mathbb{E}[\hat{\mu}_N] = \frac{1}{N}\sum_{i=1}^{N} f(x_i) = \mathbb{E}_p[f(x)]$$

Monte Carlo Asymptotics

$$\hat{\mu}_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \approx \mathbb{E}_p[f(x)]$$

- Estimator variance reduces at rate 1/N:

$$\mathrm{Var}[\hat{\mu}_N] = \frac{1}{N}\mathrm{Var}[f] = \frac{1}{N}\mathbf{E}\left[(f(x)-\mu)^2\right]$$

Independent of dimensionality of random variable X

- If the true variance is **finite** have *central limit theorem*:

$$\sqrt{N}(\hat{\mu}_N - \mu) \underset{N\to\infty}{\Longrightarrow} \mathcal{N}(0, \mathrm{Var}[f])$$

- Even if true variance is **infinite** have *laws of large numbers*:

Weak Law

$$\lim_{N\to\infty} \Pr\left(|\hat{\mu}_N - \mu| < \epsilon\right) = 1, \qquad \text{for any} \epsilon > 0$$

Strong Law

$$\Pr\left(\lim_{N\to\infty} \hat{\mu}_N = \mu\right) = 1$$

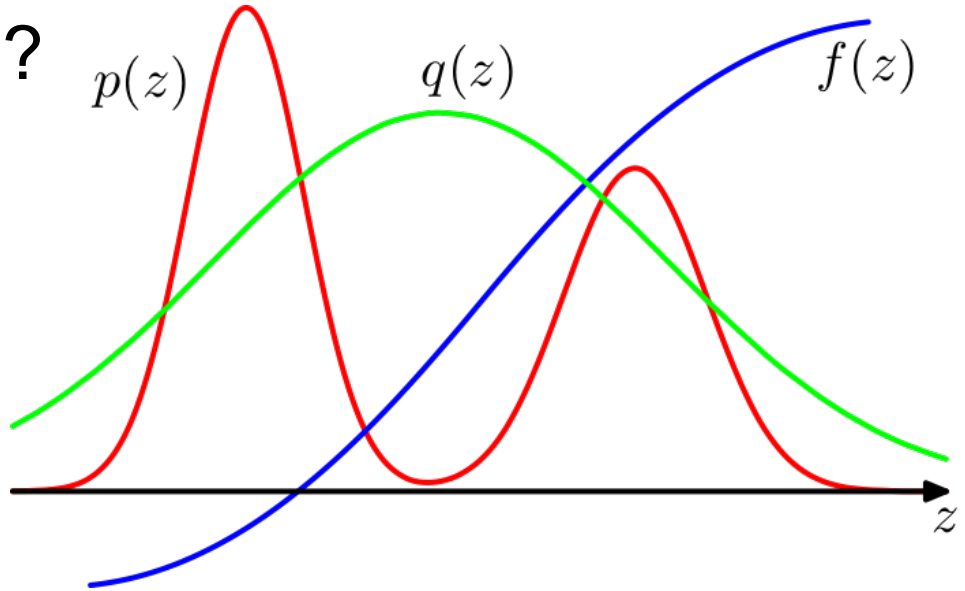
Importance Sampling

Can we estimate $\mathbb{E}_p[f]$ without sampling p(z)?

$$\mathbb{E}_p[f] = \int f(z)p(z)\,dz$$

q(z) is an easy-to-sample proposal distribution

$$= \int f(z)\frac{p(z)}{q(z)}q(z)\,dz$$



Monte Carlo estimate over samples $\{z_i\}_{i=1}^N \sim q$ from proposal q(z):

$$\mathbb{E}_p[f] \approx \frac{1}{N}\sum_{i=1}^{N}\frac{p(z_i)}{q(z_i)}f(z_i)$$

Key: We can sample from an "easy" distribution q(z) instead!

Importance Sampling

IS weights are the ratio of target / proposal distributions:

$$\mathbb{E}_p[f] \approx \frac{1}{N}\sum_{i=1}^{N} w_i f(z_i) \qquad \text{where} \qquad w_i = \frac{p(z_i)}{q(z_i)}$$

But we often do not know the normalizer of the target distribution,

$$p(z) = \frac{1}{Z_p}\widetilde{p}(z) \qquad \text{where} \qquad Z_p = \int \widetilde{p}(z)\, dz$$

Can only evaluate unnormalized target

Can we evaluate IS estimate in terms of unnormalized weights?

$$\widetilde{w}_i = \frac{\widetilde{p}(z_i)}{q(z_i)}$$

Yes! Let's see how…

Importance Sampling (Normalized)

Recall, the importance sampling estimate is given by,

$$\mathbb{E}_p[f] \approx \frac{1}{N} \sum_{i=1}^{N} \frac{p(z_i)}{q(z_i)} f(z_i)$$

With normalized target and proposal distributions, respectively:

$$p(z) = \frac{1}{Z_p} \widetilde{p}(z) \qquad\qquad q(z) = \frac{1}{Z_p} \widetilde{q}(z)$$

Substitute and pull out ratio of normalizers,

$$\mathbb{E}_p[f] \approx \left(\frac{Z_q}{Z_p} \right) \frac{1}{N} \sum_{i=1}^{N} \frac{\widetilde{p}(z_i)}{\widetilde{q}(z_i)} f(z_i)$$

Need to compute this… ←

→ **Easy to compute**

Importance Sampling (Normalized)

Idea Compute importance sampling estimate of target normalizer:

$$Z_p = \int \widetilde{p}(z)\, dz = \int \frac{\widetilde{p}(z)}{q(z)} q(z)\, dz \approx \frac{1}{N} \sum_{i=1}^{N} \frac{\widetilde{p}(z_i)}{q(z_i)}$$

Typically we have normalized proposal $q(z)$ so $Z_q = 1$ and,

$$\frac{Z_p}{Z_q} \approx \frac{1}{N} \sum_{i=1}^{N} \frac{\widetilde{p}(z_i)}{q(z_i)} = \frac{1}{N} \sum_{i=1}^{N} \widetilde{w}_i$$

Where $\widetilde{w}_i$ are our *unnormalized importance weights,*

$$\widetilde{w}_i = \frac{\widetilde{p}(z_i)}{q(z_i)}$$

We can compute this!

Importance Sampling (normalized)

Given samples $\{z_i\}_{i=1}^N \sim q$ we can write the IS estimate as,

$$\mathbb{E}_p[f] \approx \left(\frac{Z_q}{Z_p}\right) \frac{1}{N} \sum_{i=1}^{N} \widetilde{w}_i f(z_i)$$

The ratio of normalizers is approximated by normalized weights,

$$\frac{Z_p}{Z_q} \approx \frac{1}{N} \sum_{i=1} \widetilde{w}_i$$

Substituting the normalized weights yields,

$$\mathbb{E}_p[f] \approx \frac{\sum_{i=1}^{N} \widetilde{w}_i f(z_i)}{\sum_{j=1}^{N} \widetilde{w}_j} \qquad \text{where} \qquad \widetilde{w}_j = \frac{\widetilde{p}(z_j)}{\widetilde{q}(z_j)}$$

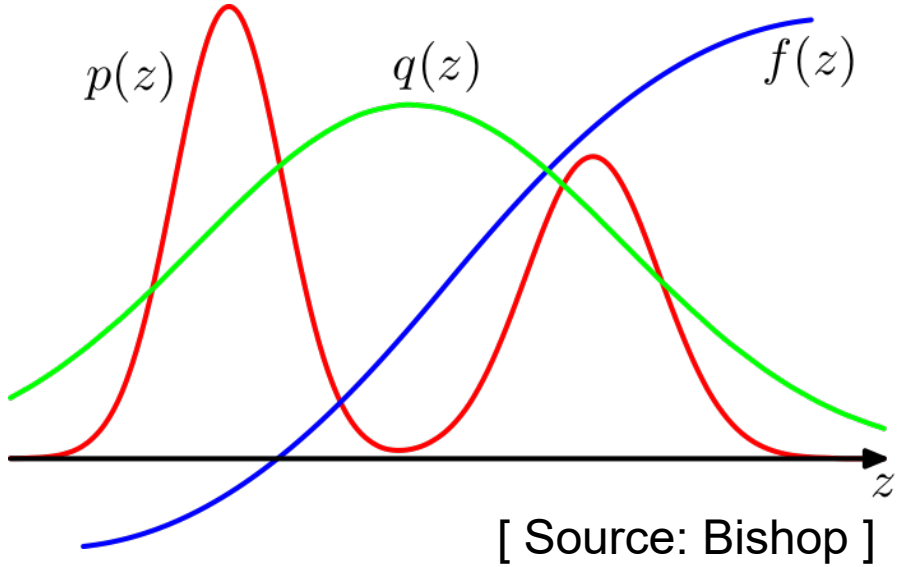
Importance Sampling On-A-Slide

1. Simulate from tractable distribution

$$\{z_i\}_{i=1}^{N} \sim q(z)$$

2. Compute importance weights & normalize

$$\widetilde{w}_i = \frac{\widetilde{p}(z_i)}{q(z_i)} \qquad w_i = \frac{\widetilde{w}_i}{\sum_{i=1}^{N} \widetilde{w}_i}$$



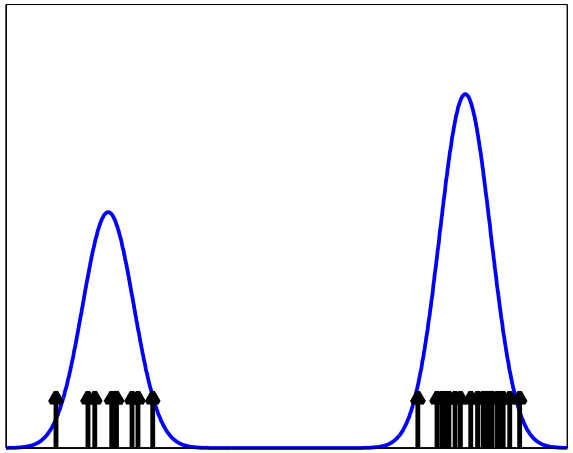
[Source: Bishop]

3. Compute importance-weighted expectation

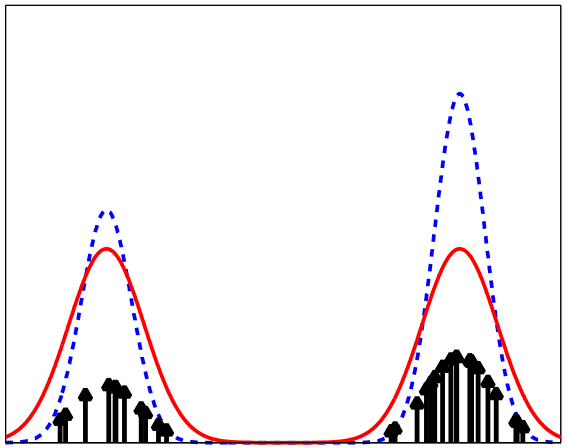
$$\mathbf{E}_p[f(z)] \approx \sum_{i=1}^{N} w_i f(z_i) \equiv \hat{f}$$

Note There is no 1/N term since it is part of the normalized IS weights

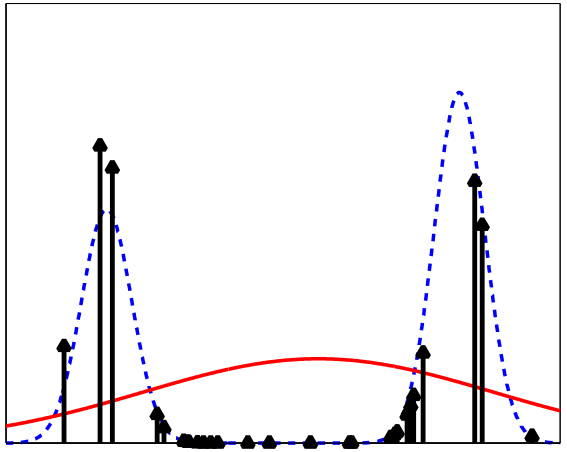
Selecting Proposal Distributions



Target Distribution



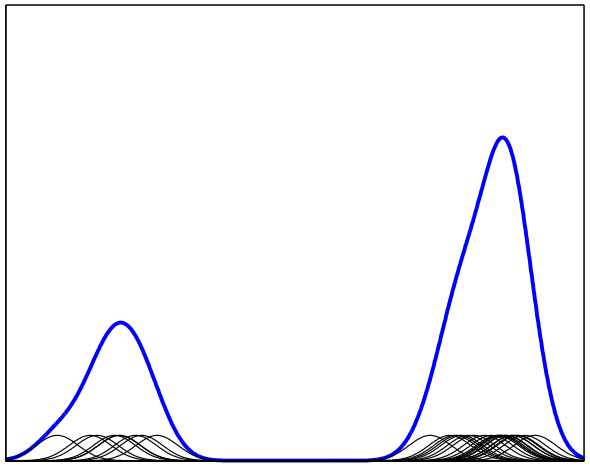
Good Proposal

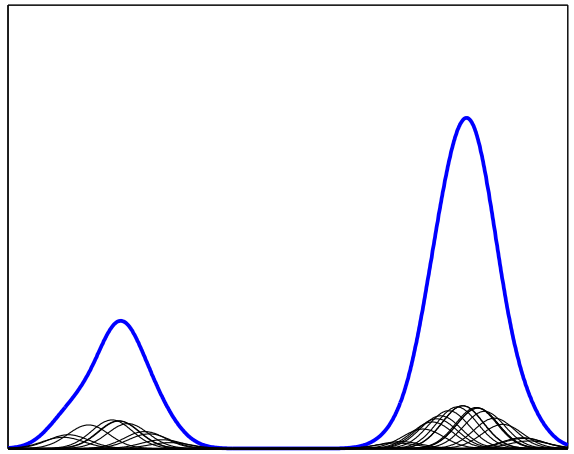


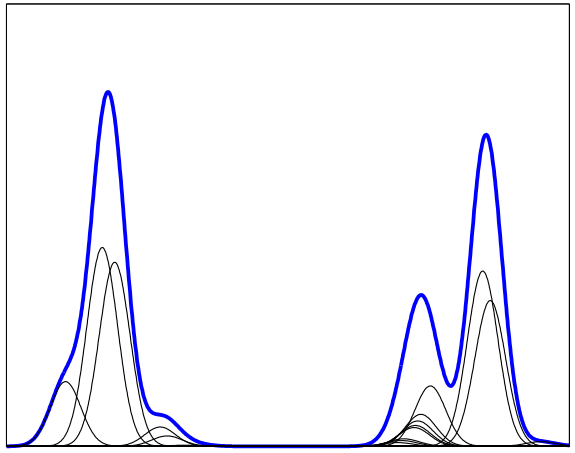
Poor Proposal

Kernel or Parzen window estimators interpolate to predict density:

$$\hat{p}(x) = \sum_{\ell=1}^{L} w^{(\ell)} \mathcal{N}(x; x^{(\ell)}, \Lambda) \qquad w^{(\ell)} \propto \frac{p(x^{(\ell)})}{q(x^{(\ell)})}$$







Importance Sampling

Q: What is a good proposal distribution?

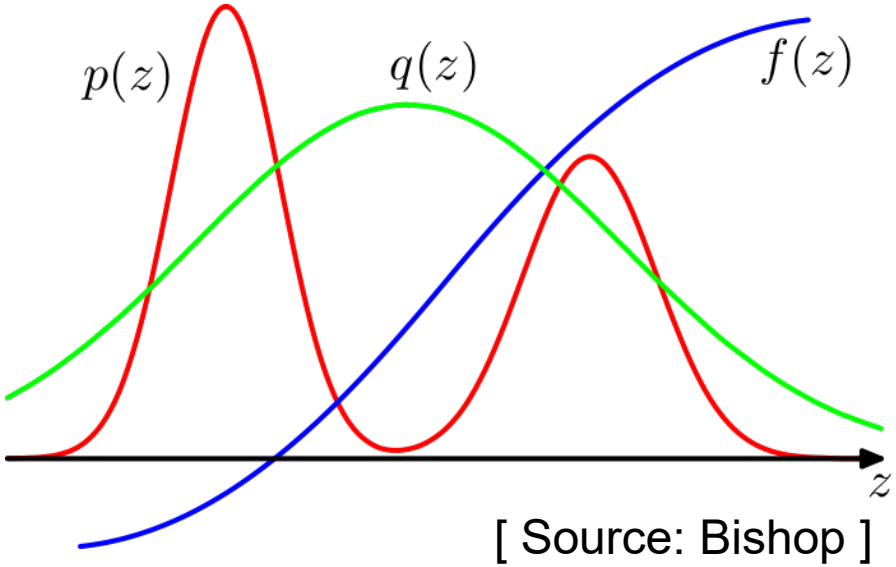
A: Minimize estimator variance

$$q^* = \arg\min_q \mathrm{Var}_q(\hat{f})$$

Minimum variance obtained when,

$$q^* \propto |f(z)|p(z)$$

E.g. can do better than q=p



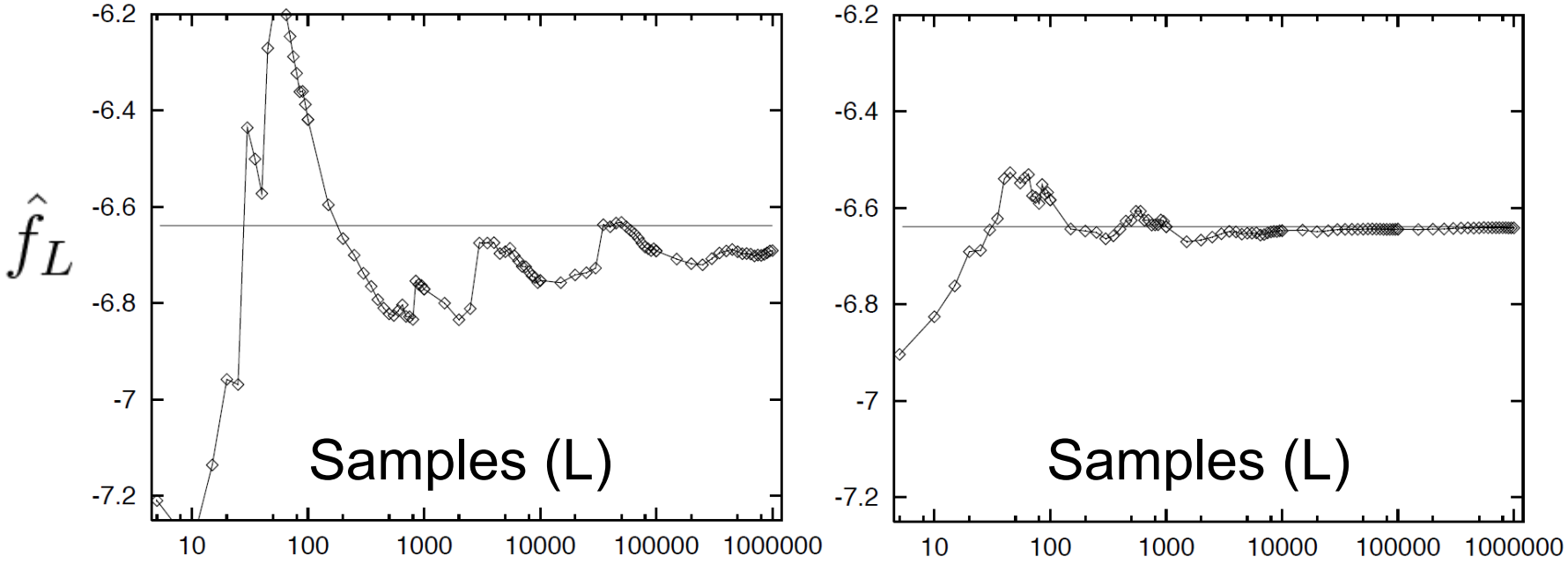
[Source: Bishop]

Estimator variance scales catastrophically with dimension:

e.g. for N-dim. X and Gaussian q(x): $\mathrm{Var}_{q^*}(\hat{f}) = \exp(\sqrt{2N})$

Selecting Proposal Distributions

- For a toy one-dimensional, heavy-tailed target distribution:



Gaussian Proposal *Cauchy (Student's-t) Proposal*

Empirical variance of weights may not predict estimator variance!

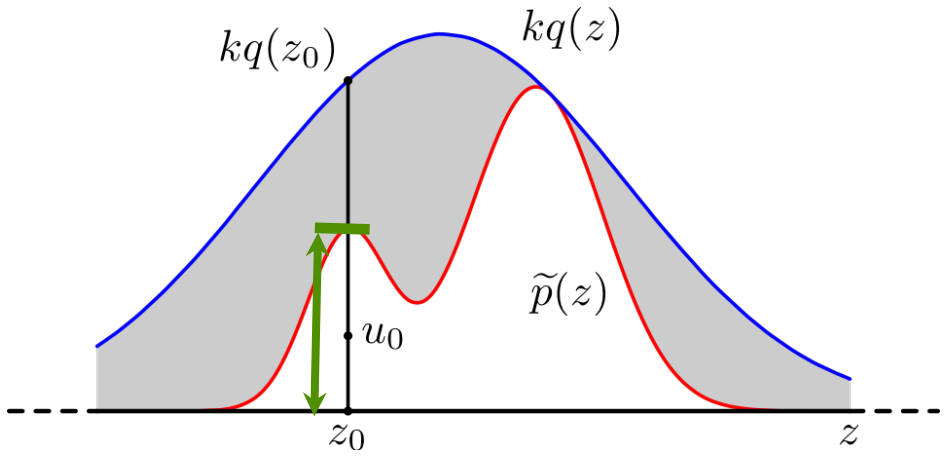
- Always (asymptotically) unbiased, but variance of estimator can be enormous unless weight function bounded above:

$$\mathbb{E}_q[\hat{f}_L] = \mathbb{E}_p[f] \qquad \mathrm{Var}_q[\hat{f}_L] = \frac{1}{L}\mathrm{Var}_q[f(x)w(x)] \qquad w(x) = \frac{p(x)}{q(x)}$$

Monte Carlo Methods Summary

Rejection sampling

- Choose q such that: $\widetilde{p}(z) \leq k \cdot q(z)$
- Sample q(z) and keep with probability: $\frac{\widetilde{p}(z)}{k \cdot q(z)}$

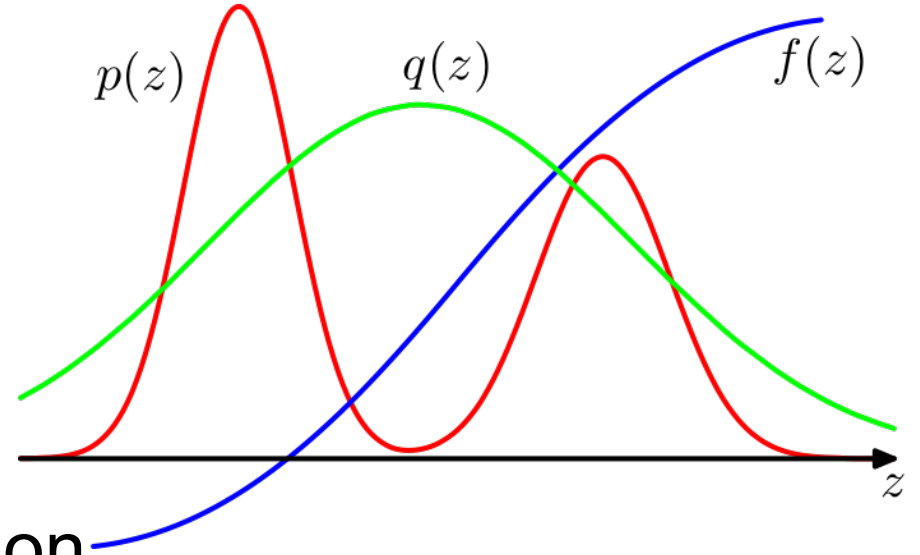


Pro: Efficient, easy to implement

Con: Acceptance rate evaporates as dimension increases

Importance Sampling

$$\mathbf{E}_p[f(z)] \approx \sum_{l=1}^{L} \frac{\widetilde{r}^{(l)}}{\sum_{i=1}^{L} \widetilde{r}^{(i)}} f(z^{(l)}) \qquad \widetilde{r}^{(l)} = \frac{\widetilde{p}(z^{(l)})}{q(z^{(l)})}$$



Pro: Efficient, easy to implement

Con: Variance grows exponentially in dimension

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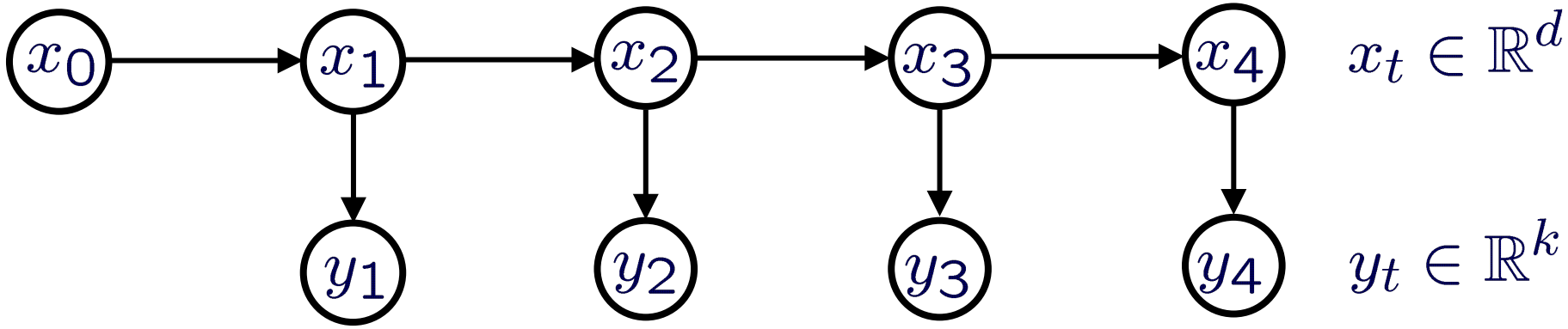
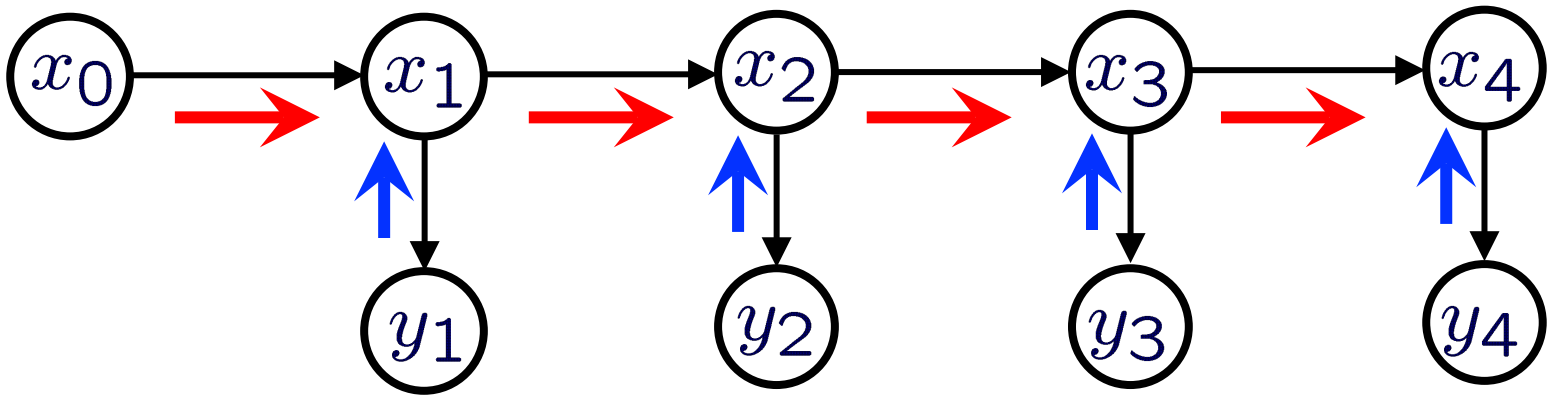
Non-linear State Space Models



$$x_{t+1} = f(x_t, w_t) \qquad w_t \sim \mathcal{F}$$
$$y_t = g(x_t, v_t) \qquad v_t \sim \mathcal{G}$$

- State dynamics and measurements given by potentially complex *nonlinear functions*
- Noise sampled from *non-Gaussian* distributions
- Usually no closed form for messages or marginals

Sequential Importance Sampling (SIS)



- Suppose interested in some complex, global function of state:

$$\mathbb{E}[f] = \int f(x)p(x \mid y)\, dx \approx \sum_{\ell=1}^{L} w_\ell f(x^{(\ell)}) \qquad w_\ell \propto \frac{p(x^{(\ell)} \mid y)}{q(x^{(\ell)} \mid y)} \qquad x^{(\ell)} \sim q(x \mid y)$$

- Construct efficient proposal using Markov structure

$$q(x \mid y) = q(x_0) \prod_{t=1}^{T} q(x_t \mid x_{t-1}, y_t) \qquad q(x_t \mid x_{t-1}, y_t) \approx p(x_t \mid x_{t-1}, y)$$

Computing the weights is easy with this type of proposal!

Recursive Weight Updating

Recall the importance weights are given by,

$$w^{(\ell)} \propto \frac{p(x^{(\ell)} \mid y)}{q(x^{(\ell)} \mid y)} \propto \frac{p(x^{(\ell)}, y)}{q(x^{(\ell)} \mid y)}$$

Plugging in the factorization of p and q weights at time t are:

$$w_t^{(\ell)} \propto \frac{p(x_0^{(\ell)})}{q(x_0^{(\ell)})} \frac{p(x_1^{(\ell)} \mid x_0^{(\ell)}) p(y_1 \mid x_1^{(\ell)})}{q(x_1^{(\ell)} \mid x_0^{(\ell)}, y_1)} \cdots \frac{p(x_t^{(\ell)} \mid x_{t-1}^{(\ell)}) p(y_t \mid x_t^{(\ell)})}{q(x_t^{(\ell)} \mid x_{t-1}^{(\ell)}, y_t)}$$

Therefore, by recursion we have that weights at time $t+1$ are:

$$w_{t+1}^{(\ell)} \propto w_t^{(\ell)} \frac{p(x_{t+1}^{(\ell)} \mid x_t^{(\ell)}) p(y_{t+1} \mid x_{t+1}^{(\ell)})}{q(x_{t+1}^{(\ell)} \mid x_t^{(\ell)}, y_t)}$$

Sequential Importance Sampling (SIS)

For ℓ = 1,…,N

Sample initial N particles from proposal prior: $x_0^{(\ell)} \sim q_0$

Compute initial importance weights: $w_0^{(\ell)} \propto p(x_0^{(\ell)}) \div q(x_0^{(\ell)})$

For t=1,…T

For ℓ =1,…N

Propagate particles: $x_t^{(\ell)} \sim q(x_t \mid x_{t-1}^{(\ell)}, y_t)$

Compute *unnormalized* weights,

$$\widetilde{w}_t^{(\ell)} = w_{t-1}^{(\ell)} \frac{p(x_t^{(\ell)}|x_{t-1}^{(\ell)})p(y_t|x_t^{(\ell)})}{q(x_t^{(\ell)}|x_{t-1}^{(\ell)},y_t)}$$

Normalize weights: $w_t^{(\ell)} = \widetilde{w}_t^{(\ell)} \div \sum_i \widetilde{w}_t^{(i)}$

Filter mean estimate: $\hat{x}_t = \sum_\ell w_t^{(\ell)} x_t^{(\ell)}$

Particle Filters: The Movie

(M. Isard, 1996)

Weight Degeneration

Sequential importance sampling does not work!

- Sample trajectories $x^{(\ell)}$ are high-dimensional and become unlikely
- In time, unnormalized weights approach zero with high probability,

$$\lim_{t\to\infty} \widetilde{w}_t^{(\ell)} = 0$$

- Normalized weights approach *one-hot vector,*

$$w_t^{(\ell)} = \widetilde{w}_t^{(\ell)} \div \sum_i \widetilde{w}_t^{(i)} = \begin{cases} 1 & \text{if } \widetilde{w}_t^{(\ell)} = \max \widetilde{w}_t \\ 0 & \text{otherwise} \end{cases}$$

Particle Resampling

$$p(x_t \mid y_{\bar{t}}) \approx \sum_{\ell=1}^{L} \omega_t^{(\ell)} \delta_{x_t^{(\ell)}}(x_t)$$

where $y_{\bar{t}} = \{y_1, \ldots, y_t\}$

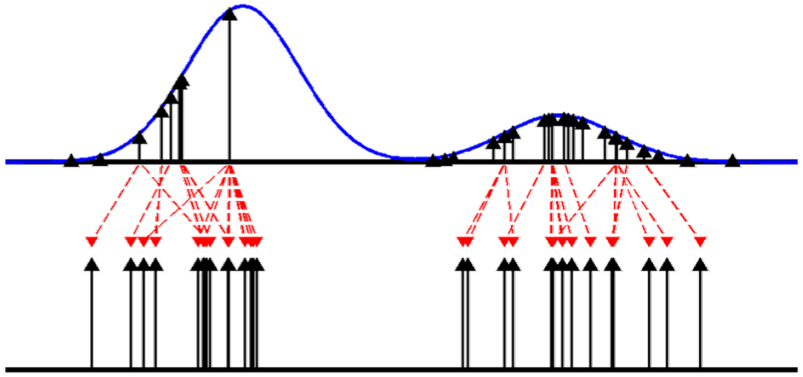
$$p(x_t \mid y_{\bar{t}}) \approx \sum_{\ell=1}^{L} \frac{1}{L} \delta_{\bar{x}_t^{(\ell)}}(x_t)$$

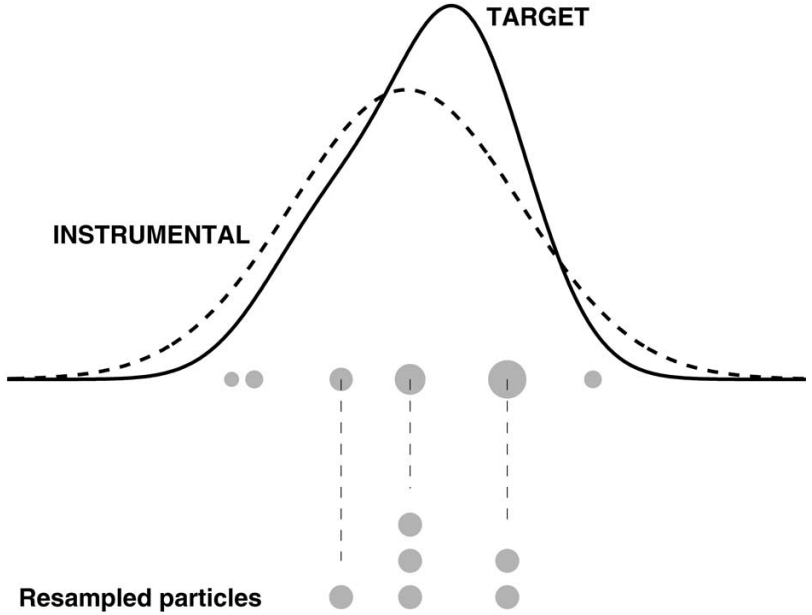
$$\bar{x}_t^{(\ell)} = x_t^{(j_\ell)}$$

$$j_\ell \sim \mathrm{Cat}(\omega_t)$$

Resample with replacement produces random discrete distribution with same mean as original distribution

While remaining unbiased, resampling avoids degeneracies in which most weights go to zero





Sequential IS with Resampling : Particle Filter

Initialize: N samples $\widetilde{x}_0^{(\ell)} \sim q_0$ and weights $w_0^{(\ell)} \propto p(x_0^{(\ell)}) \div q(x_0^{(\ell)})$

For t=1,…T

If Resampling:

Resample $x_{t-1}^{(\ell)}$ from $\widetilde{x}_{t-1}$ according to normalized weights w_{t-1} (with replacement)

Set uniform weights $w_{t-1} = 1/N$

Else: Set $x_{t-1} = \widetilde{x}_{t-1}$

For ℓ=1,…N

Propagate particles: $x_t^{(\ell)} \sim q(x_t \mid x_{t-1}^{(\ell)}, y_t)$

Compute *unnormalized* weights, $\widetilde{w}_t^{(\ell)} = w_{t-1}^{(\ell)} \frac{p(x_t^{(\ell)}|x_{t-1}^{(\ell)})p(y_t|x_t^{(\ell)})}{q(x_t^{(\ell)}|x_{t-1}^{(\ell)},y_t)}$

Normalize weights: $w_t^{(\ell)} = \widetilde{w}_t^{(\ell)} \div \sum_i \widetilde{w}_t^{(i)}$

Filter mean estimate: $\hat{x}_t = \sum_\ell w_t^{(\ell)} x_t^{(\ell)}$

“Bootstrap” Proposal

Recall that the full proposal distribution factorizes as,

$$q(x \mid y) = q(x_0) \prod_{t=1}^{T} q(x_t \mid x_{t-1}, y_t)$$

A convenient choice is to sample from the prior distribution,

$$q(x) = p(x_0) \prod_{t=1}^{T} p(x_t \mid x_{t-1})$$

This is easy to sample, and weight updates simplify,

$$w_{t+1}^{(\ell)} \propto w_t^{(\ell)} \frac{p(x_{t+1}^{(\ell)} \mid x_t^{(\ell)}) p(y_{t+1} \mid x_{t+1}^{(\ell)})}{p(x_{t+1}^{(\ell)} \mid x_t^{(\ell)})} = w_t^{(\ell)} p(y_{t+1} \mid x_{t+1}^{(\ell)})$$

“Correct” weights with data likelihood

Bootstrap Particle Filter

Initialize: N samples $\widetilde{x}_0^{(\ell)} \sim q_0$ and weights $w_0^{(\ell)} \propto p(x_0^{(\ell)}) \div q(x_0^{(\ell)})$

For t=1,…T

If Resampling:

Resample $x_{t-1}^{(\ell)}$ from $\widetilde{x}_{t-1}$ according to normalized weights w_{t-1} (with replacement)

Set uniform weights $w_{t-1} = 1/N$

Else: Set $x_{t-1} = \widetilde{x}_{t-1}$

For ℓ=1,…N

Propagate particles: $\widetilde{x}_t^{(\ell)} \sim p(x_t \mid x_{t-1}^{(\ell)})$ ←

Compute *unnormalized* weights, $\widetilde{w}_t^{(\ell)} = w_{t-1}^{(\ell)} p(y_t \mid \widetilde{x}_t^{(\ell)})$ ←

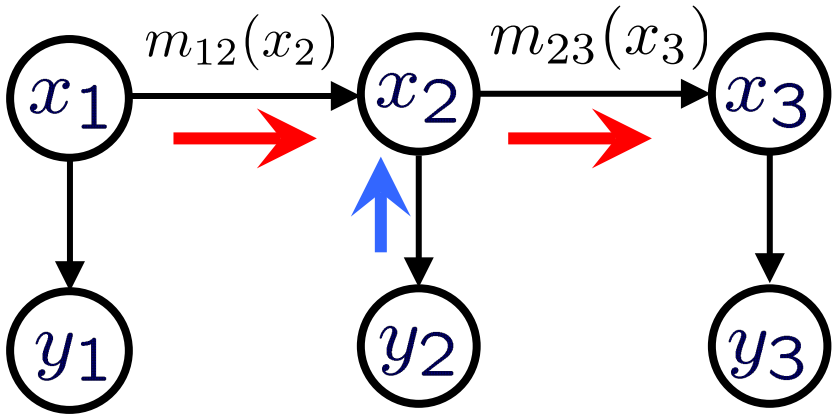
Changes for Bootstrap

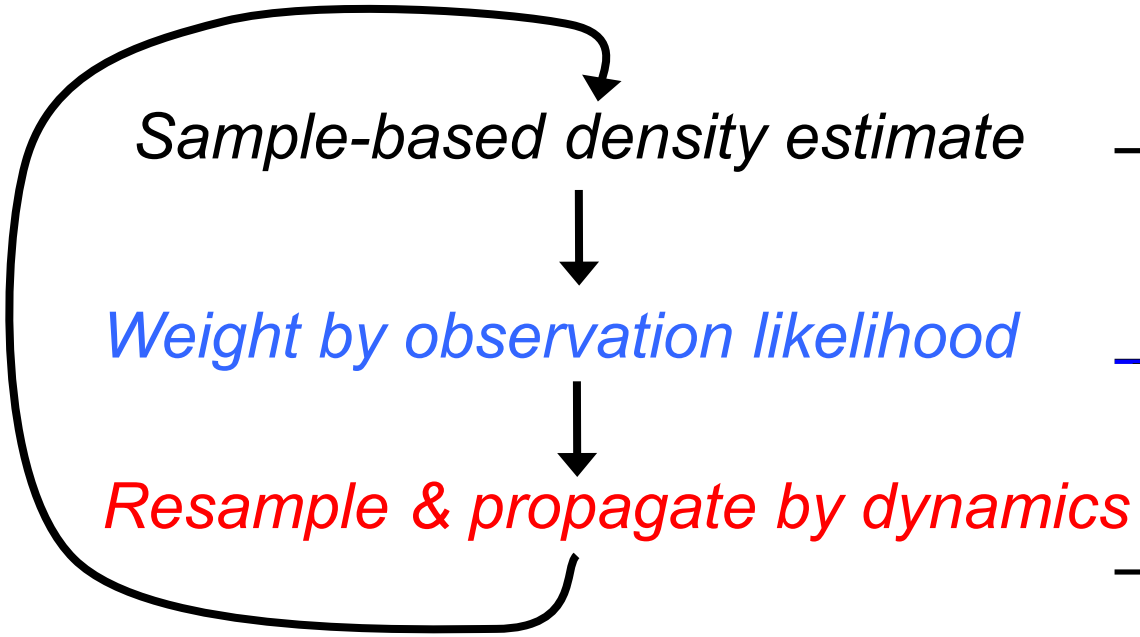
Normalize weights: $w_t^{(\ell)} = \widetilde{w}_t^{(\ell)} \div \sum_i \widetilde{w}_t^{(i)}$

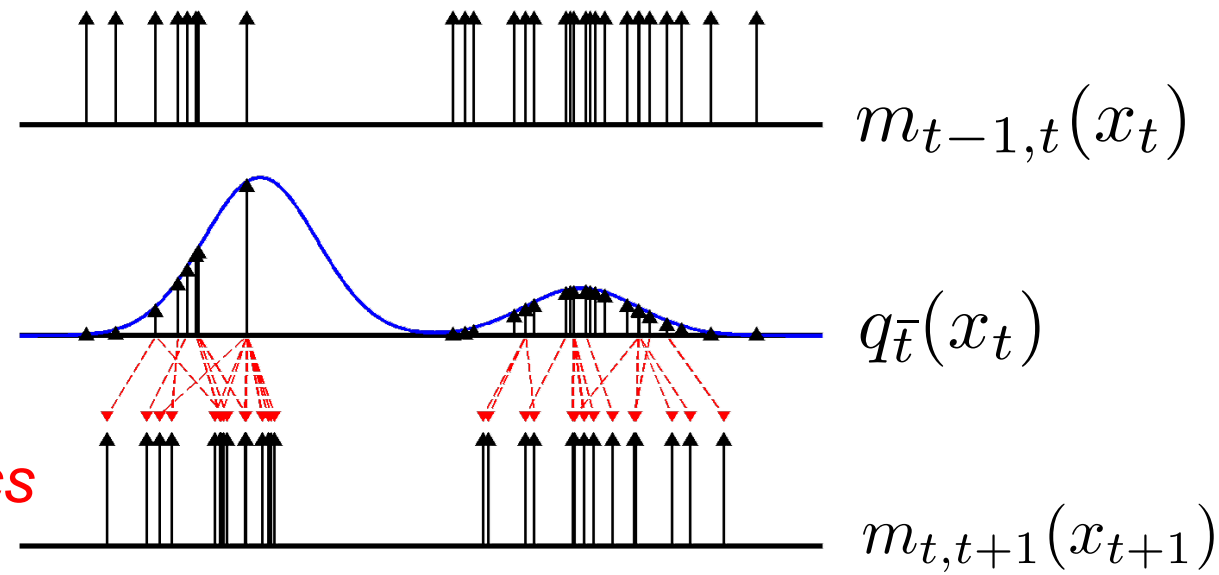
Filter mean estimate: $\hat{x}_t = \sum_\ell w_t^{(\ell)} x_t^{(\ell)}$

Particle Filtering Algorithms

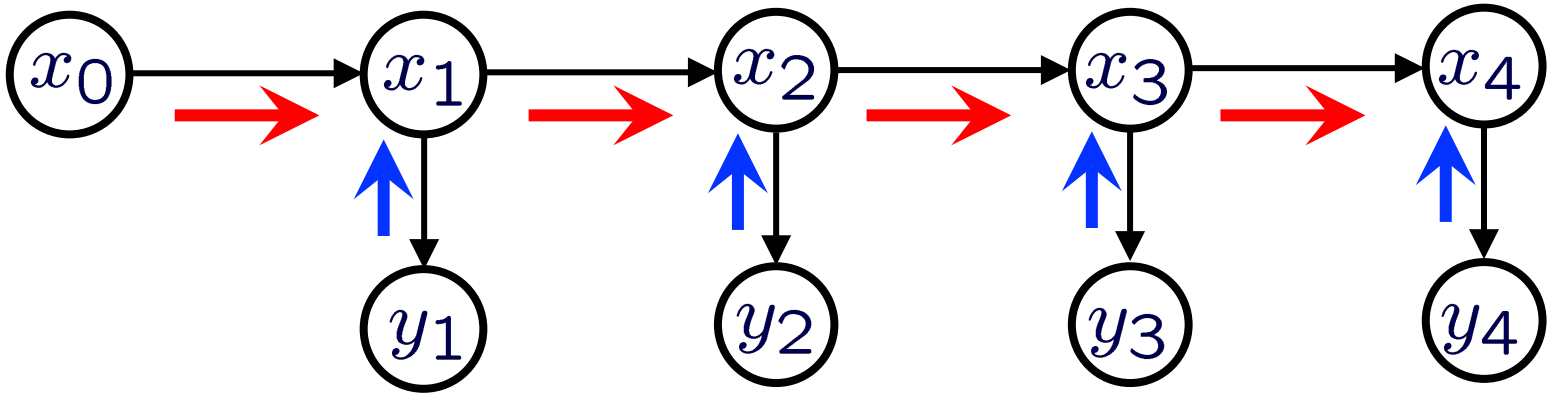
- Represent state estimates using a set of samples
- Propagate over time using *sequential importance sampling with resampling*







BP for State-Space Models



$$m_{t-1,t}(x_t) \propto p(x_t \mid y_{\overline{t-1}}) \qquad \text{where} \quad y_{\bar{t}} = \{y_1, \ldots, y_t\}$$

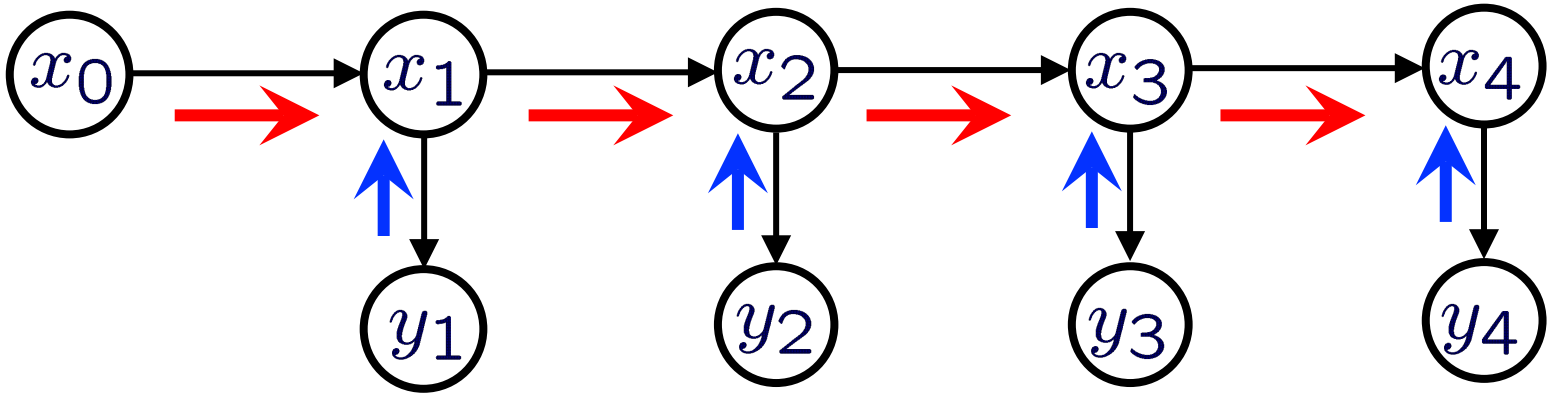
$$m_{t-1,t}(x_t)\, p(y_t \mid x_t) \propto p(x_t \mid y_{\bar{t}}) = q_{\bar{t}}(x_t)$$

Prediction (Integral/Sum step of BP):

$$m_{t-1,t}(x_t) \propto \int p(x_t \mid x_{t-1}) q_{\overline{t-1}}(x_{t-1})\, dx_{t-1}$$

Inference (Product step of BP): $q_{\bar{t}}(x_t) = \dfrac{1}{Z_t} m_{t-1,t}(x_t) p(y_t \mid x_t)$

Particle Filter: Measurement Update



Incoming message: A set of *L* weighted particles

$$m_{t-1,t}(x_t) \approx \sum_{\ell=1}^{L} w_{t-1,t}^{(\ell)} \delta(x_t, x_t^{(\ell)}) \qquad \sum_{\ell=1}^{L} w_{t-1,t}^{(\ell)} = 1$$

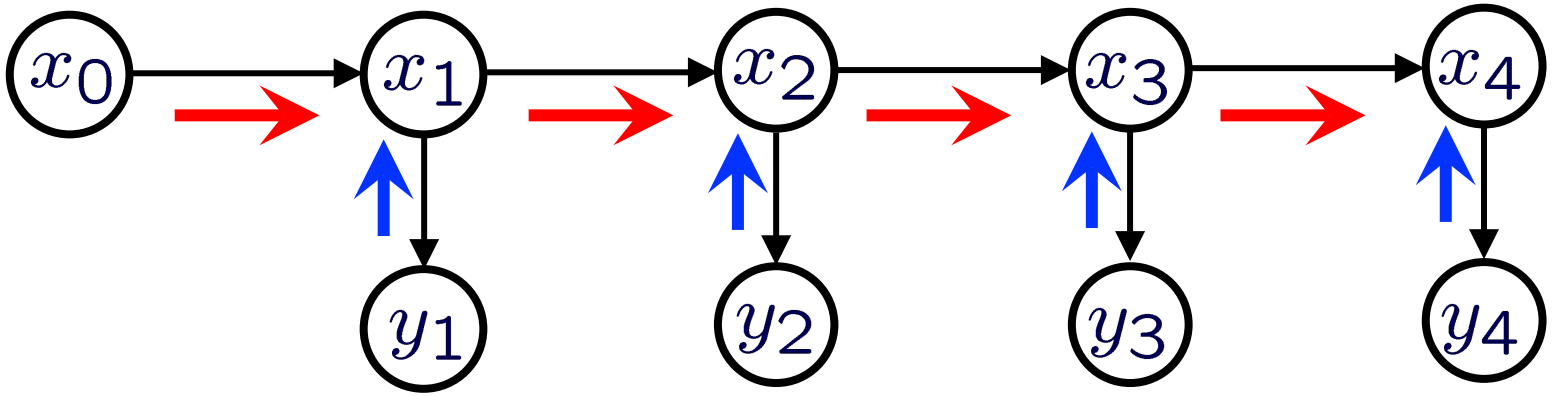
Bayes' Rule: Posterior at particles proportional to prior times likelihood

$$q_{\overline{t}}(x_t) \propto m_{t-1,t}(x_t)\, p(y_t \mid x_t) \propto \sum_{\ell=1}^{L} w_{t-1,t}^{(\ell)}\, p(y_t \mid x_t^{(\ell)})\, \delta(x_t, x_t^{(\ell)})$$

$$q_{\overline{t}}(x_t) = \sum_{\ell=1}^{L} w_t^{(\ell)} \delta(x_t, x_t^{(\ell)}) \qquad w_t^{(\ell)} \triangleq \frac{w_{t-1,t}^{(\ell)}\, p(y_t \mid x_t^{(\ell)})}{\sum_{m=1}^{L} w_{t-1,t}^{(m)}\, p(y_t \mid x_t^{(m)})}$$

*Variance of importance weights **increases** with each update*

Particle Filter: Sample Propagation



State Posterior Estimate: A set of *L* weighted particles

$$q_t(x_t) = \sum_{\ell=1}^{L} w_t^{(\ell)} \delta(x_t, x_t^{(\ell)}) \qquad \sum_{\ell=1}^{L} w_t^{(\ell)} = 1$$

Prediction: Sample next state conditioned on current particles

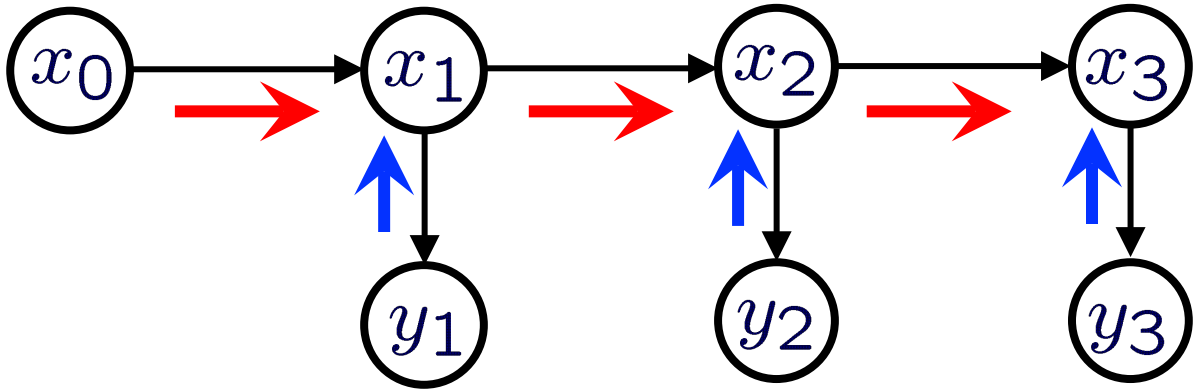
$$m_{t,t+1}(x_{t+1}) = \sum_{\ell=1}^{L} w_{t,t+1}^{(\ell)} \delta(x_{t+1}, x_{t+1}^{(\ell)})$$

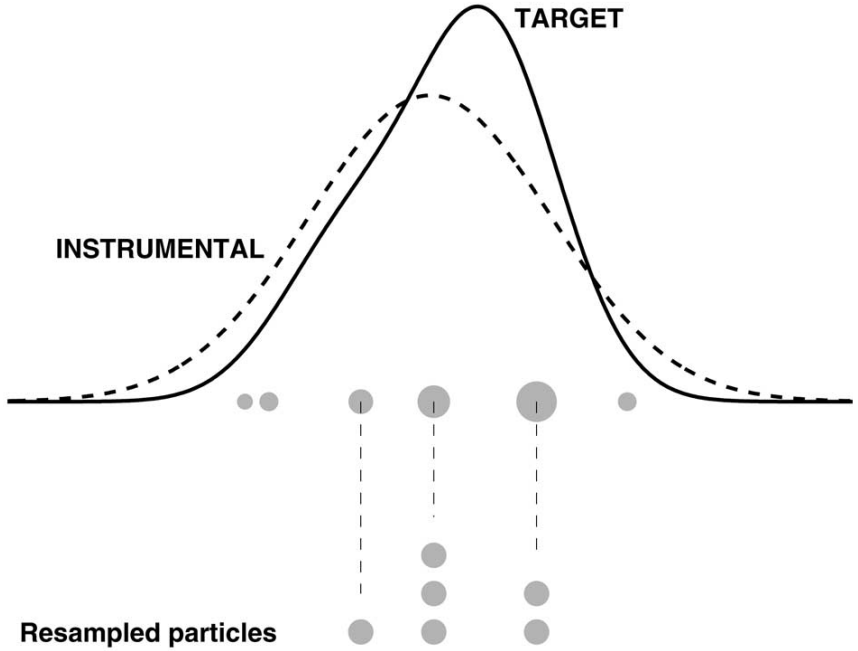
$$x_{t+1}^{(\ell)} \sim p(x_{t+1} \mid x_t^{(\ell)})$$

$$w_{t,t+1}^{(\ell)} = w_t^{(\ell)}$$

Assumption for now: Can exactly simulate temporal dynamics

Particle Filter: Resampling





State Posterior Estimate:

$$q_{\bar{t}}(x_t) = \sum_{\ell=1}^{L} w_t^{(\ell)} \delta(x_t, x_t^{(\ell)})$$

Prediction: Sample next state conditioned on randomly chosen particles

$$m_{t,t+1}(x_{t+1}) = \sum_{\ell=1}^{L} w_{t,t+1}^{(\ell)} \delta(x_{t+1}, x_{t+1}^{(\ell)})$$

$$\tilde{x}_t^{(\ell)} \sim q_{\bar{t}}(x_t)$$

$$x_{t+1}^{(\ell)} \sim p(x_{t+1} \mid \tilde{x}_t^{(\ell)})$$

$$w_{t,t+1}^{(\ell)} = 1/L$$

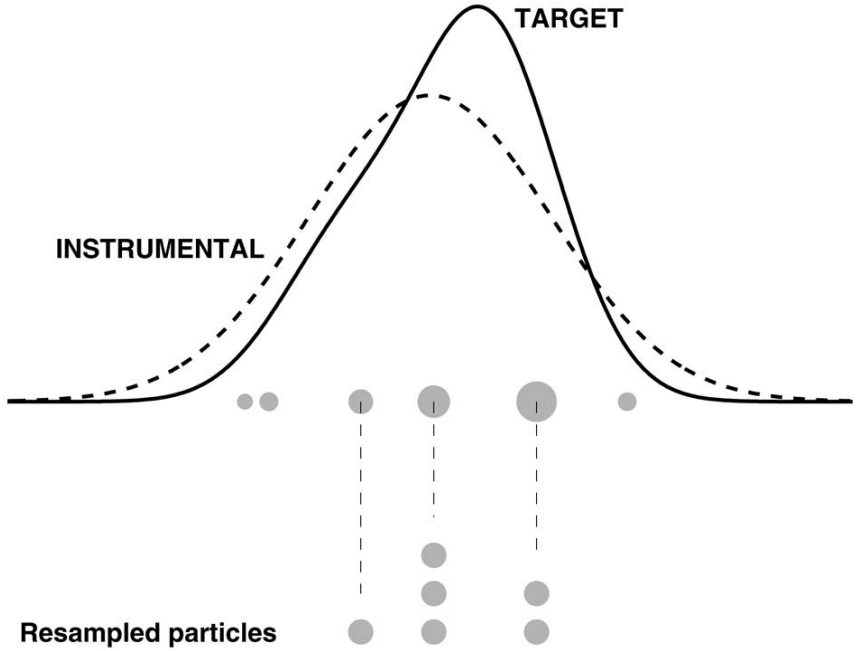
Resampling with replacement preserves expectations, but increases the variance of subsequent estimators

Particle Filter: Resampling

Effective Sample Size:

$$L_{\text{eff}} = \left(\sum_{\ell=1}^{L} \left(w^{(\ell)} \right)^2 \right)^{-1}$$

$$1 \leq L_{\text{eff}} \leq L$$



State Posterior Estimate:

$$q_{\bar{t}}(x_t) = \sum_{\ell=1}^{L} w_t^{(\ell)} \delta(x_t, x_t^{(\ell)})$$

Prediction: Sample next state conditioned on randomly chosen particles

$$m_{t,t+1}(x_{t+1}) = \sum_{\ell=1}^{L} w_{t,t+1}^{(\ell)} \delta(x_{t+1}, x_{t+1}^{(\ell)})$$

$$\tilde{x}_t^{(\ell)} \sim q_{\bar{t}}(x_t)$$

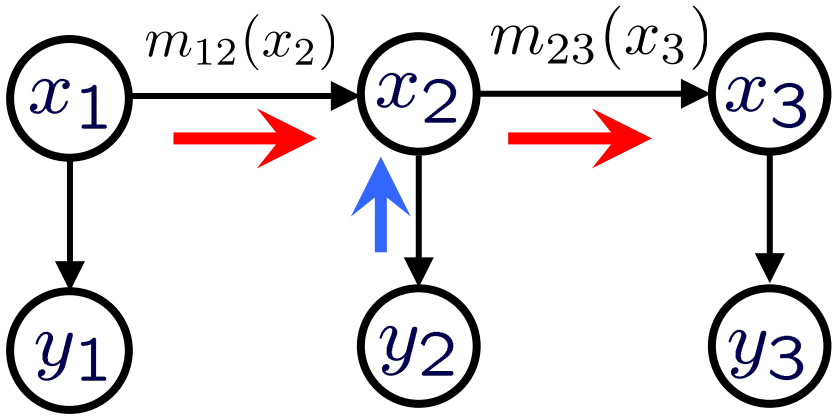
$$x_{t+1}^{(\ell)} \sim p(x_{t+1} \mid \tilde{x}_t^{(\ell)})$$

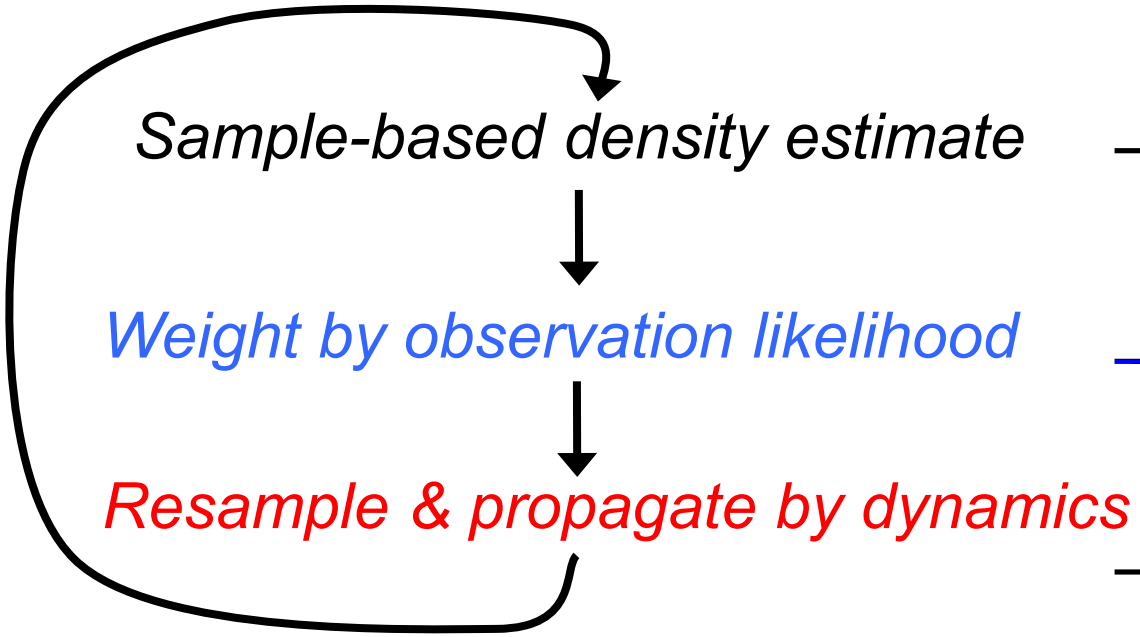
$$w_{t,t+1}^{(\ell)} = 1/L$$

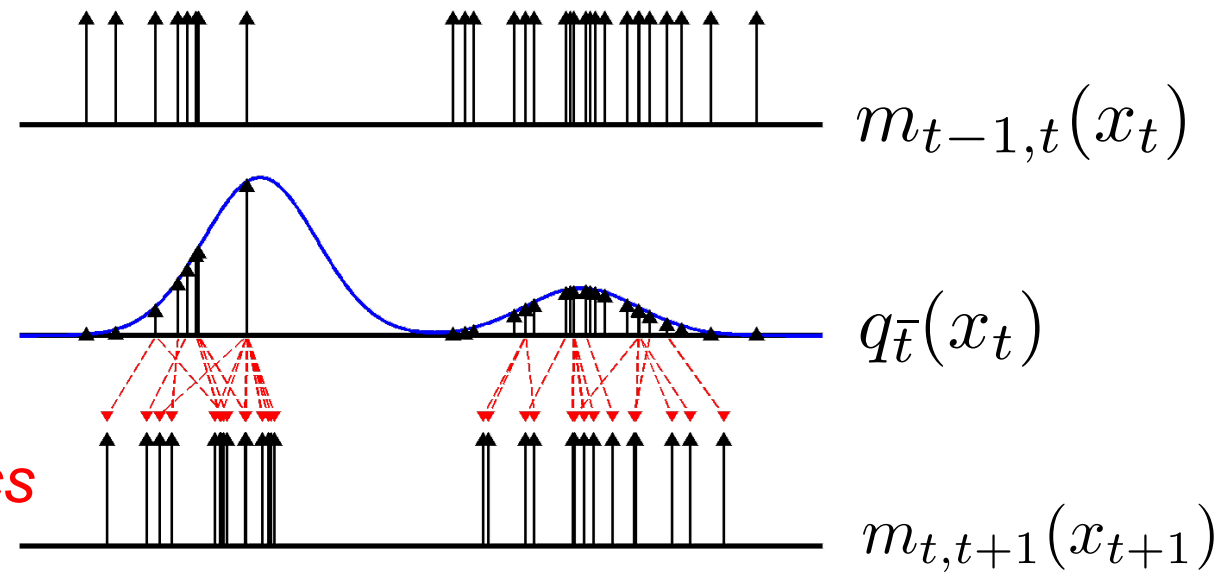
Resampling with replacement preserves expectations, but increases the variance of subsequent estimators

Particle Filtering Algorithms

- Represent state estimates using a set of samples
- Propagate over time using *sequential importance sampling with resampling*

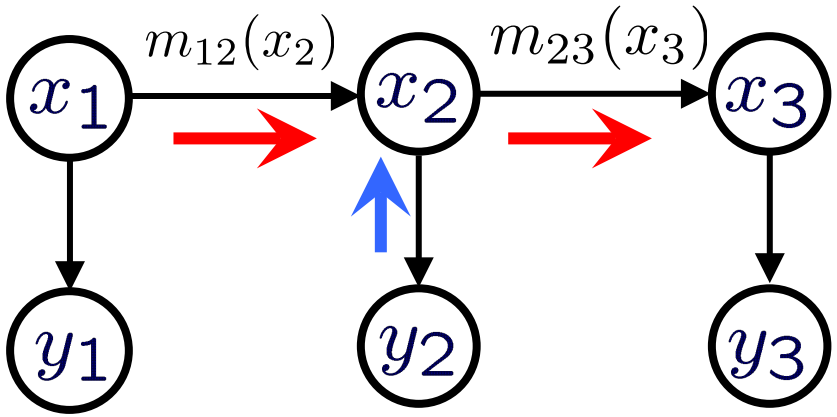






Bootstrap Particle Filter Summary

- Represent state estimates using a set of samples
- Propagate over time using *sequential importance sampling with resampling*



Assume sample-based approximation of incoming message:

$$m_{t-1,t}(x_t) = p(x_t \mid y_{t-1}, \ldots, y_1) \approx \sum_{\ell=1}^{L} \frac{1}{L} \delta_{x_t^{(\ell)}}(x_t)$$

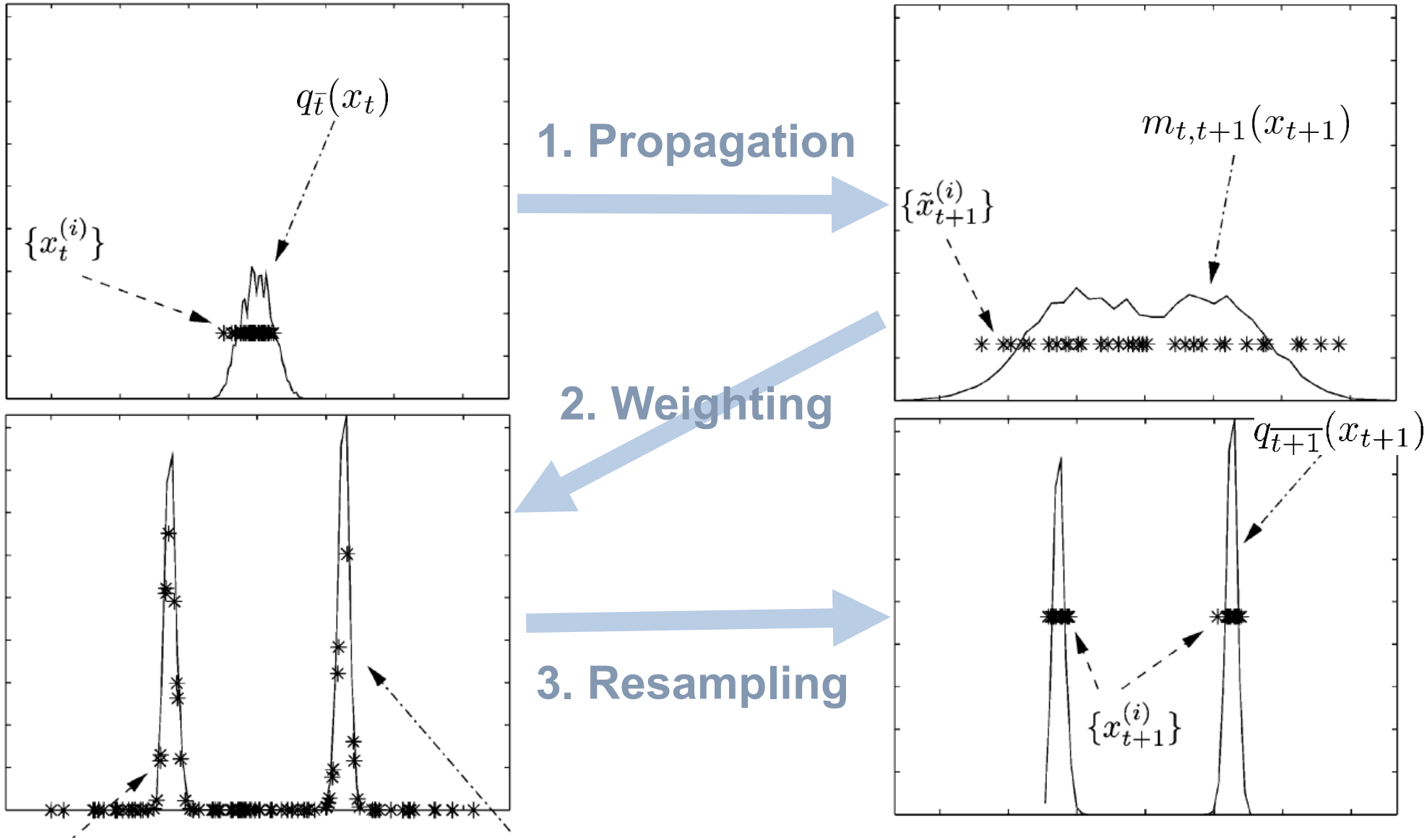
Account for observation via importance weights:

$$p(x_t \mid y_t, y_{t-1}, \ldots, y_1) \approx \sum_{\ell=1}^{L} w_t^{(\ell)} \delta_{x_t^{(\ell)}}(x_t) \qquad w_t^{(\ell)} \propto p(y_t \mid x_t^{(\ell)})$$

Sample from forward dynamics distribution of next state:

$$m_{t,t+1}(x_{t+1}) \approx \sum_{m=1}^{L} \frac{1}{L} \delta_{x_{t+1}^{(m)}}(x_{t+1}) \qquad x_{t+1}^{(m)} \sim \sum_{\ell=1}^{L} w_t^{(\ell)} p(x_{t+1} \mid x_t^{(\ell)})$$

Bootstrap Particle Filter Summary

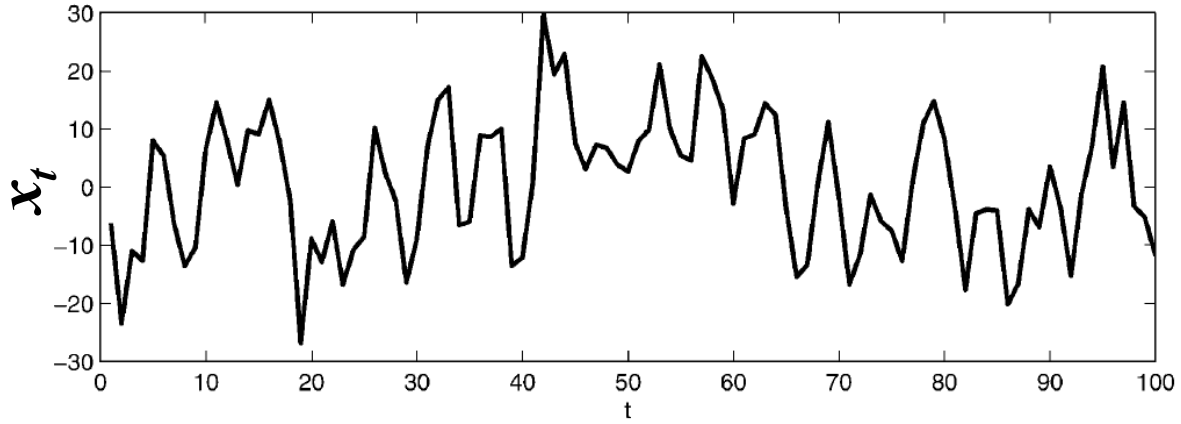


[Source: Cappe]

Toy Nonlinear Model

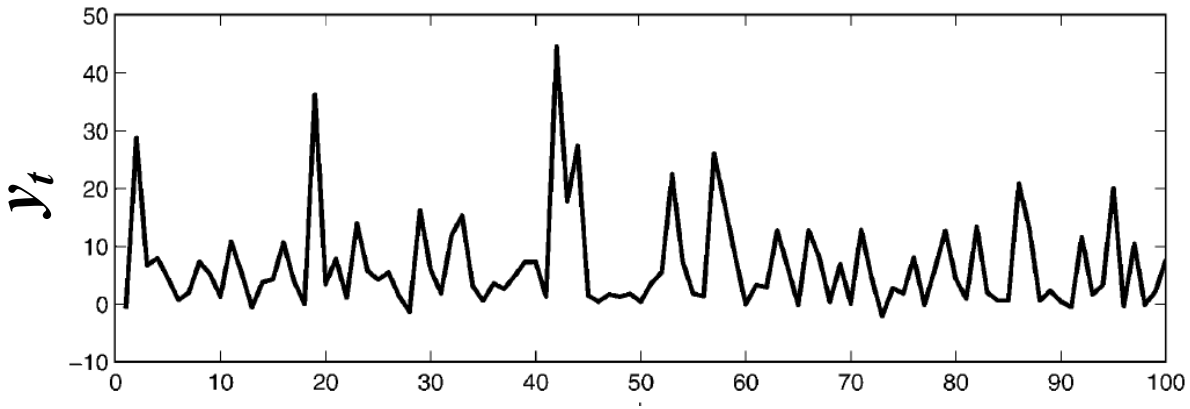
Nonlinear dynamics and observation model…

Dynamics



$$x_t = \frac{x_{t-1}}{2} + 25\frac{x_{t-1}}{1+x_{t-1}^2} + 8\cos(1.2t) + u_t$$

Measurement

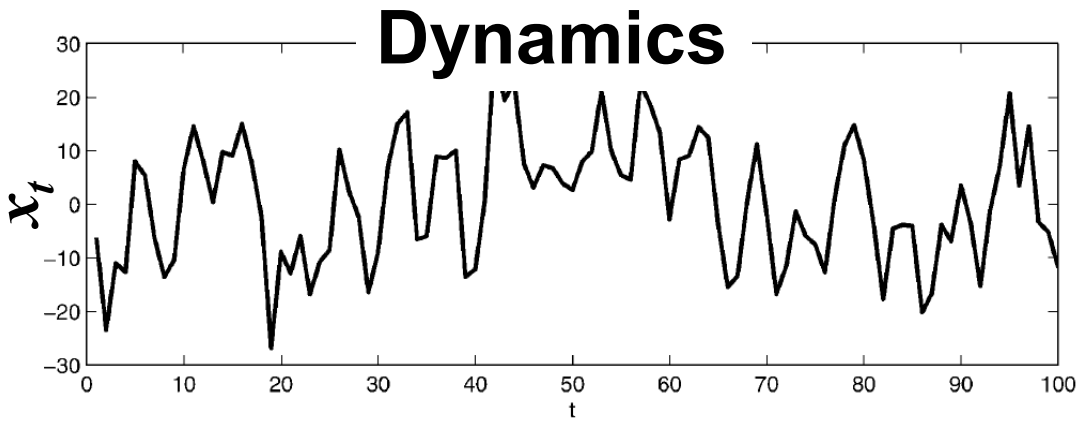


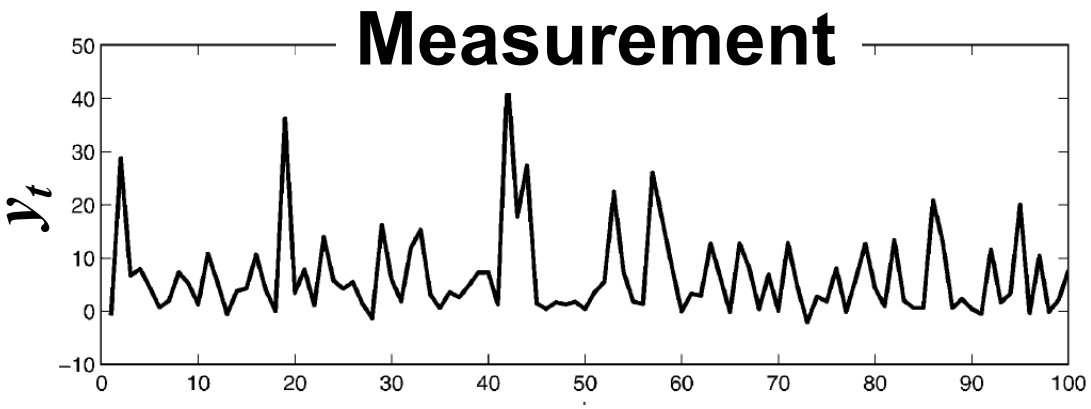
$$y_t = \frac{x_t^2}{20} + v_t$$

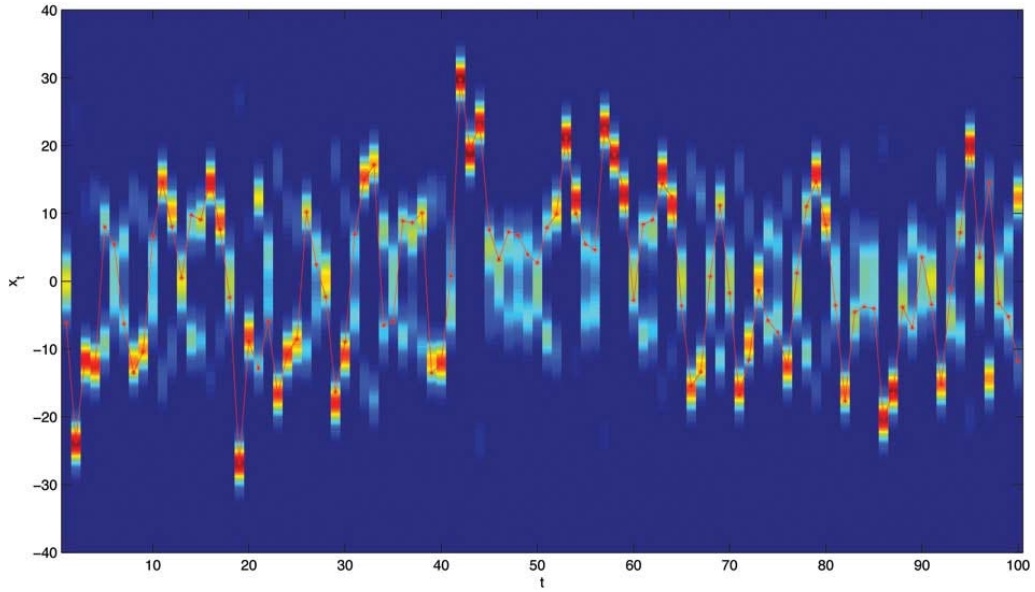
Gaussian noise model, $u_t \sim \mathcal{N}(0, \sigma_x^2)$ and $v_t \sim \mathcal{N}(0, \sigma_y^2)$

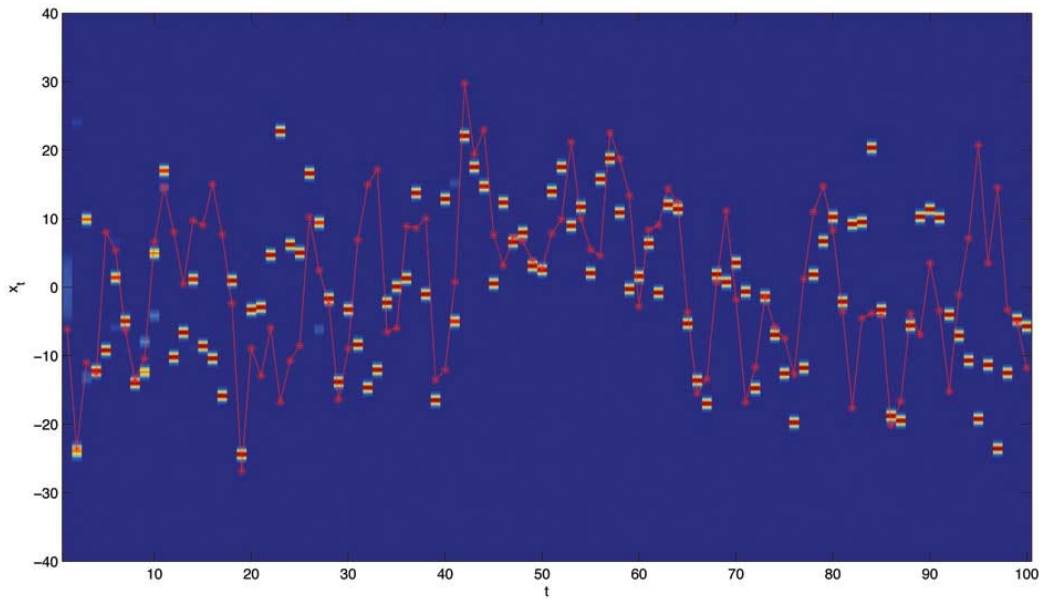
…filter equations lack closed form.

Toy Nonlinear Model









Particle Filter Marginal KDEs

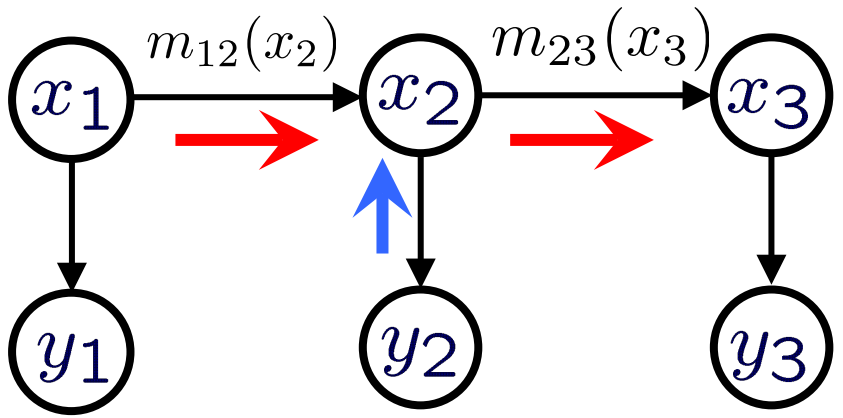
Full Sequence Importance Sampling

What is the probability that a state sequence, sampled from the prior model, is consistent with all observations?

A More General Particle Filter

- Assume sample-based approximation of previous state's marginal:

$$p(x_{t-1} \mid y_{t-1}, \ldots, y_1) \approx \sum_{\ell=1}^{L} \frac{1}{L} \delta_{x_{t-1}^{(\ell)}}(x_{t-1})$$



- Sample from a *proposal distribution q*:

$$x_t^{(\ell)} \sim q(x_t \mid x_{t-1}^{(\ell)}, y_t) \approx p(x_t \mid x_{t-1}^{(\ell)}, y_t)$$

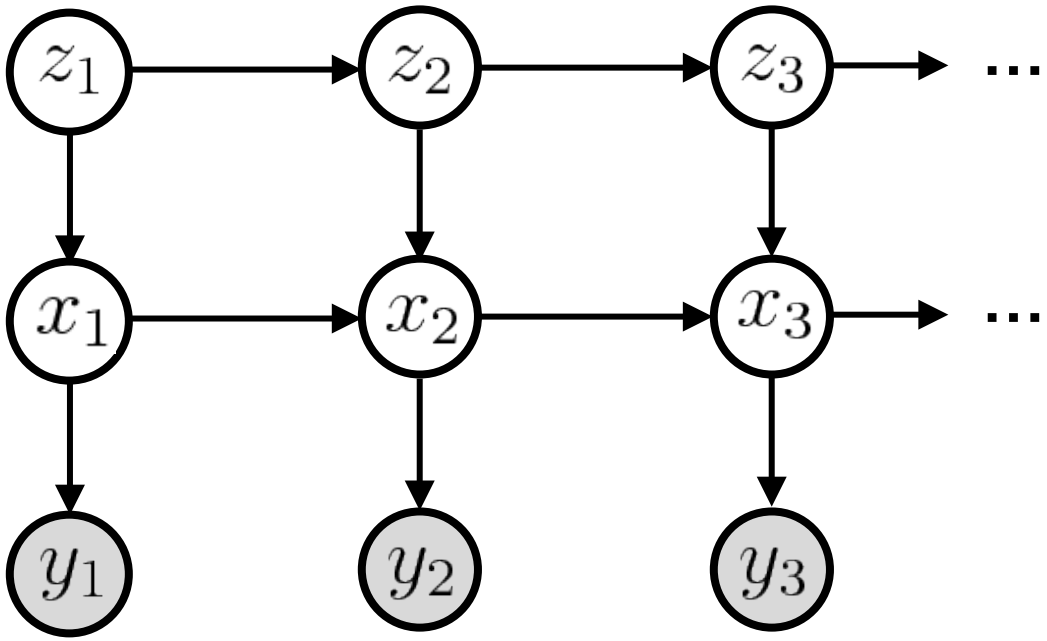
- Account for *observation and proposal* via importance weights:

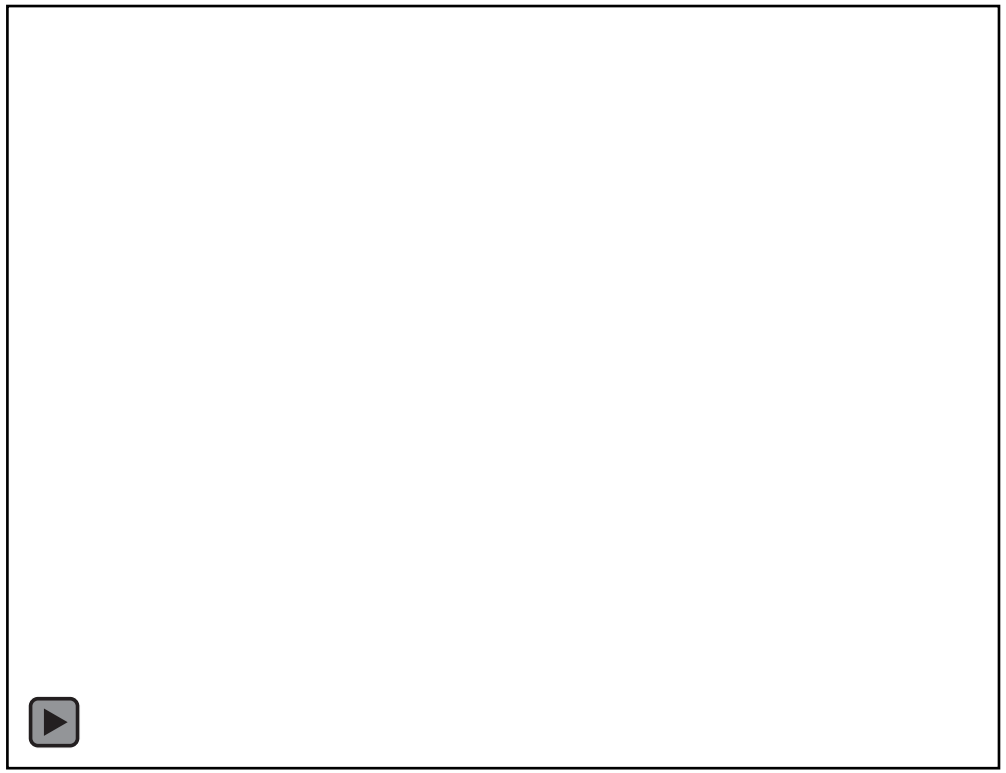
$$w_t^{(\ell)} \propto \frac{p(x_t^{(\ell)} \mid x_{t-1}^{(\ell)}) p(y_t \mid x_t^{(\ell)})}{q(x_t^{(\ell)} \mid x_{t-1}^{(\ell)}, y_t)}$$

- Resample to avoid particle degeneracy:

$$p(x_t \mid y_t, \ldots, y_1) \approx \sum_{\ell=1}^{L} \frac{1}{L} \delta_{x_t^{(\ell)}}(x_t) \qquad x_t^{(\ell)} \sim \sum_{m=1}^{L} w_t^{(m)} \delta_{x_t^{(m)}}(x_t)$$

Switching State-Space Model





Colors indicate 3 writing modes

[Video: Isard & Blake, ICCV 1998.]

Discrete switching state:

$$z_t \mid z_{t-1} \sim \mathrm{Cat}(\pi(z_{t-1}))$$

With stochastic transition matrix π

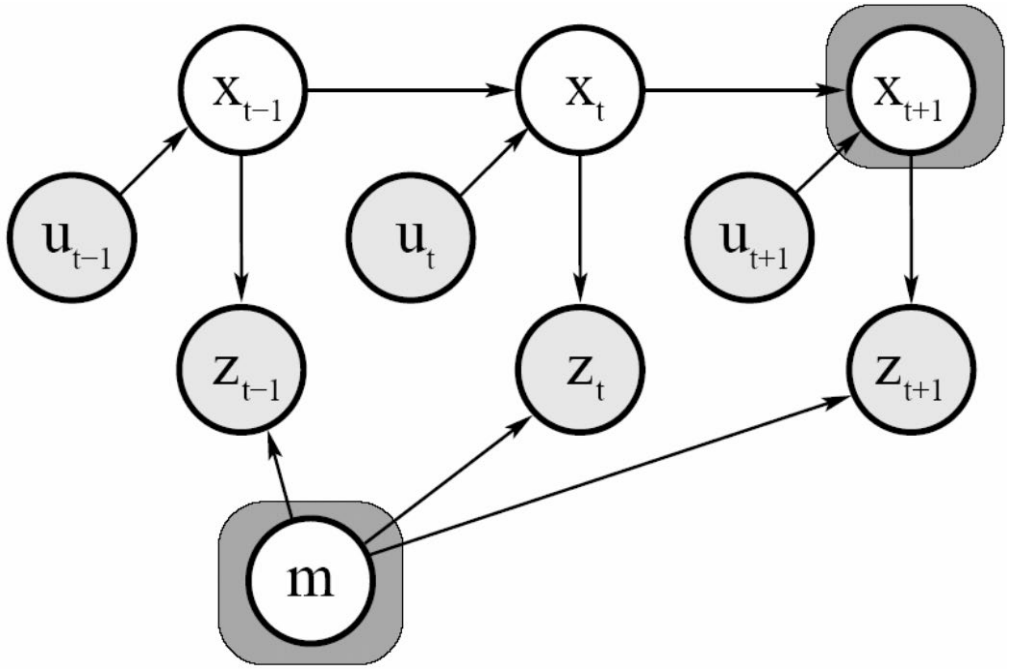
Switching state selects dynamics:

$$x_t \mid x_{t-1} \sim \mathcal{N}(A_{z_t} x_{t-1}, \Sigma_{z_t})$$

(e.g. Nonlinear Gaussian)

Example: Particle Filters for SLAM

Simultaneous Localization & Mapping (FastSLAM, Montemerlo 2003)



$$p(x_t, m \mid z_{1:t}, u_{1:t})$$

x_t = State of the robot at time t

m = Map of the environment

$z_{1:t}$ = Sensor inputs from time 1 to t

$u_{1:t}$ = Control inputs from time 1 to t

Raw odometry (controls)

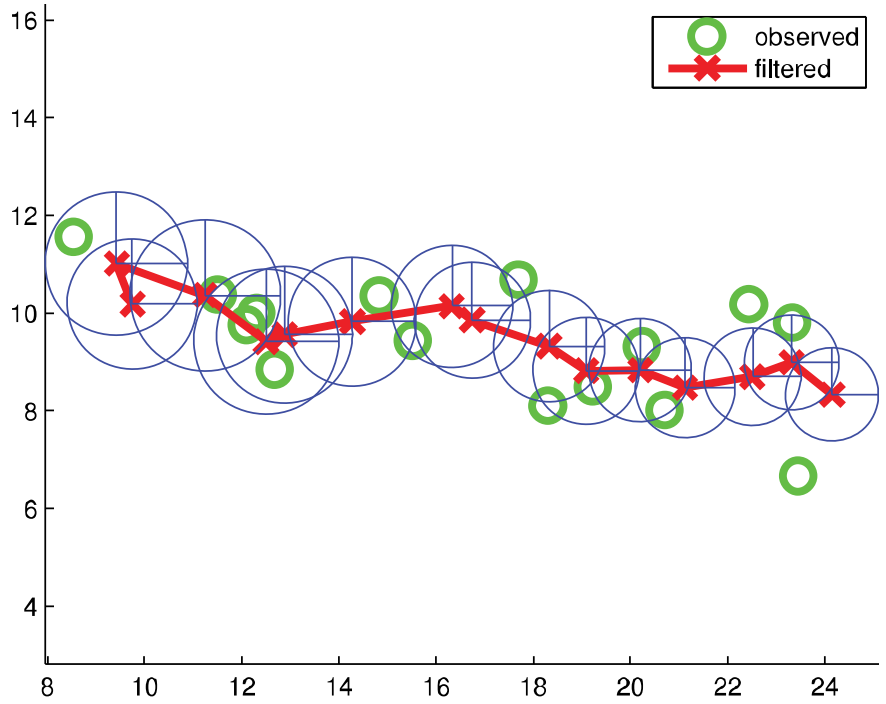
True trajectory (GPS)

Inferred trajectory & landmarks

Dynamical System Inference

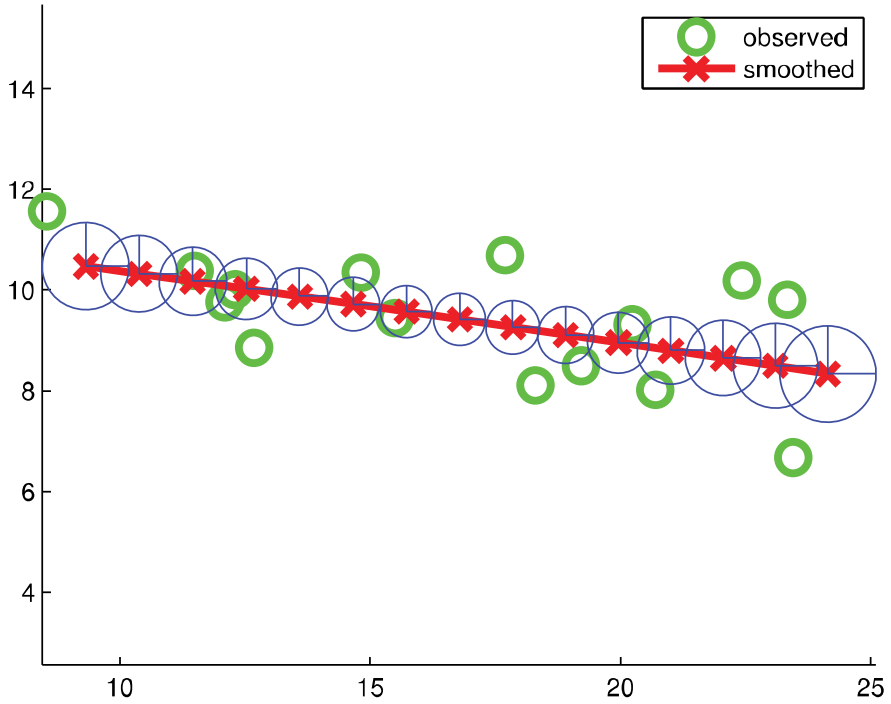
Define shorthand notation: $y_1^{t-1} \triangleq \{y_1, \ldots, y_{t-1}\}$

Filtering



Compute $p(x_t \mid y_1^t)$ at each time t

Smoothing

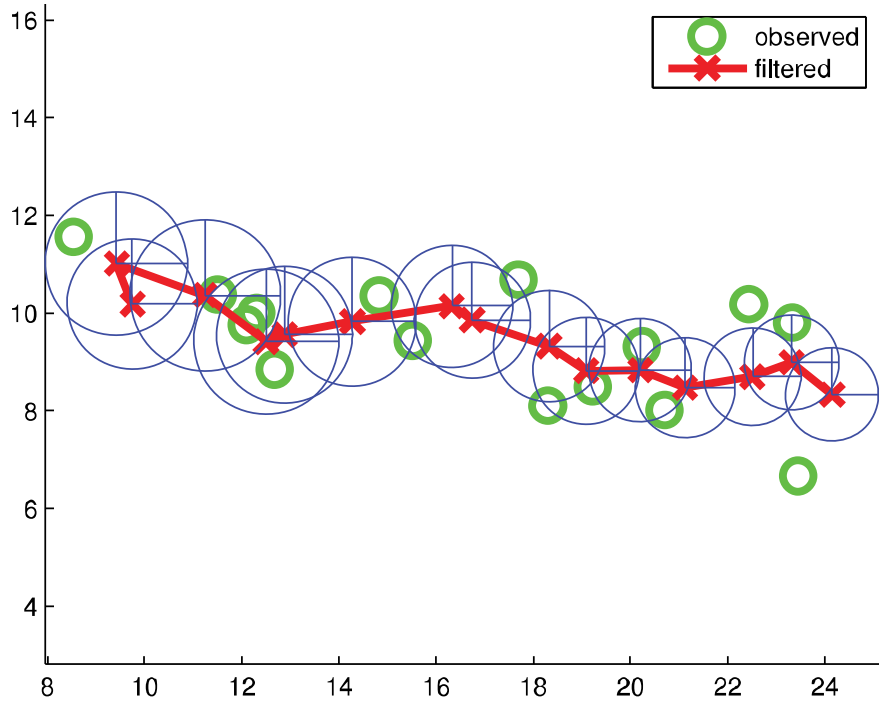


Compute full posterior marginal $p(x_t \mid y_1^T)$ at each time t

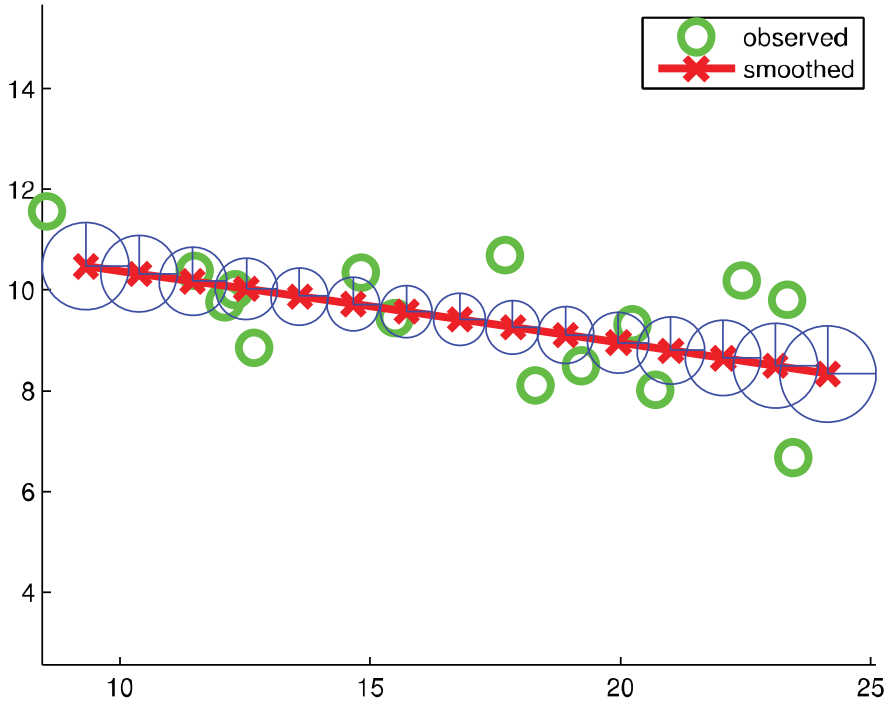
Dynamical System Inference

Define shorthand notation: $y_1^{t-1} \triangleq \{y_1, \ldots, y_{t-1}\}$

Filtering

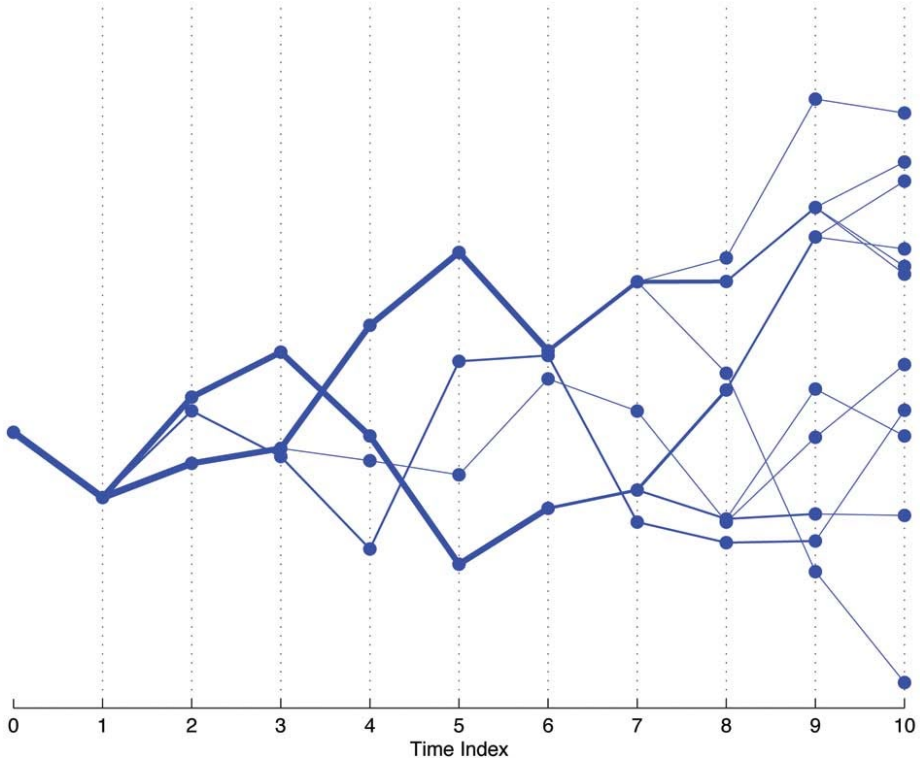


Smoothing



If estimates at time t are not needed *immediately*, then better *smoothed* estimates are possible by incorporating future observations

A Note On Smoothing



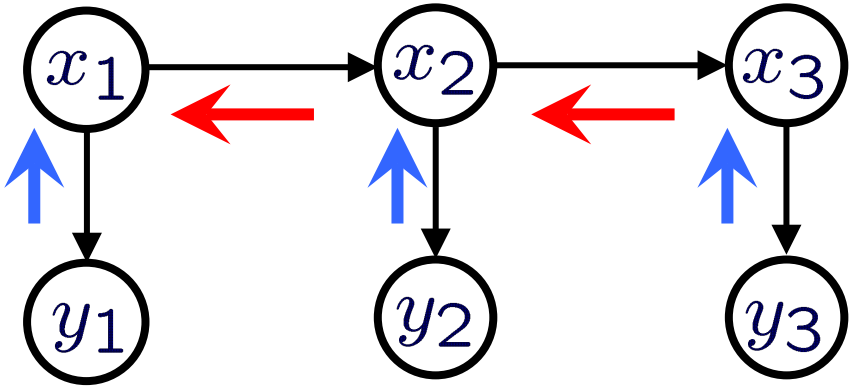
- Each resampling step discards states and they cannot subsequently restored
- Resampling introduces dependence across trajectories (common ancestors)
- Smoothed marginal estimates are generally poor
- Backwards simulation improves estimates of smoothed trajectories

Particle Filter Smoothing

Smoothing distribution factorizes as,

$$p(x_1^T \mid y_1^T) = p(x_T \mid y_1^T) \prod_{t=1}^{T-1} p(x_t \mid x_{t+1}, y_1^T)$$

$$= p(x_T \mid y_1^T) \prod_{t=1}^{T-1} p(x_t \mid x_{t+1}, y_1^t)$$



Markov property removes dependence on $y_{t+1} \ldots y_T$

Filter distribution at time T

Suggests an algorithm to sample from $p(x_1^T \mid y_1^T)$:

1. Compute and store filter marginals, $p(x_t \mid y_1^t)$ for t=1,…,T
2. Sample final state from full posterior marginal, $x_T \sim p(x_T \mid y_1^T)$
3. Sample in reverse for t=(T-1),(T-2),…,2,1 from, $x_t \sim p(x_t \mid x_{t+1}, y_1^t)$

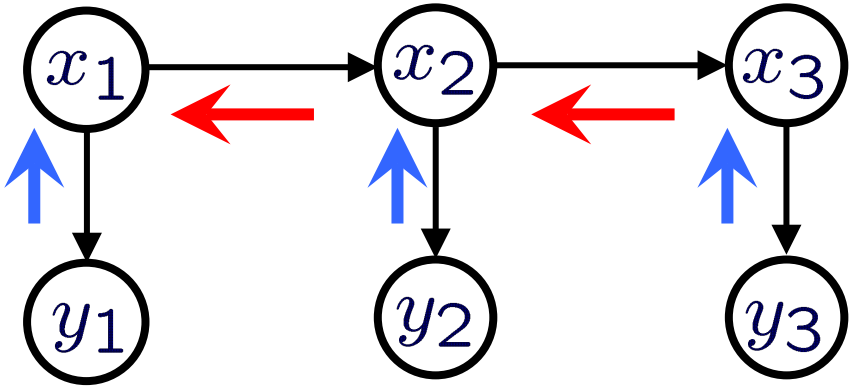
Use resampling idea to sample from current particle trajectories in reverse

Particle Filter Smoothing

Reverse conditional given by def'n of conditional prob.:

$$p(x_t \mid x_{t+1}, y_1^t) = \frac{p(x_{t+1} \mid x_t) p(x_t \mid y_1^t)}{p(x_{t+1} \mid y_1^t)}$$

$$\propto p(x_{t+1} \mid x_t) p(x_t \mid y_1^t)$$



Forward pass sample-based filter marginal estimates:

$$p(x_t \mid y_1^t) \approx \sum_{\ell=1}^{L} w_t^{(\ell)} \delta(x_t - x_t^{(\ell)})$$

Thus particle estimate of reverse prediction is:

$$p(x_t \mid x_{t+1}, y_1^T) \approx \sum_{\ell=1}^{L} \rho_t^{(\ell)}(x_{t+1}) \delta(x_t - x_t^{(i)}) \quad \text{where} \quad \rho_t^{(i)}(x_{t+1}) = \frac{w_t^{(i)} p(x_{t+1} \mid x_t^{(i)})}{\sum_{l=1}^{L} w_t^{(l)} p(x_{t+1} \mid x_t^{(l)})}$$

Particle Filter Smoothing

Algorithm 5 Particle Smoother

for $t = 0$ to T **do** ▷ Forward Pass Filter

Run Particle filter, storing at each time step the particles and weights $\{x_t^{(i)}, \omega_t^{(i)}\}_{1 \leq i \leq L}$

end for

Choose $\widetilde{x}_T = x_T^{(i)}$ with probability $\omega_t^{(i)}$.

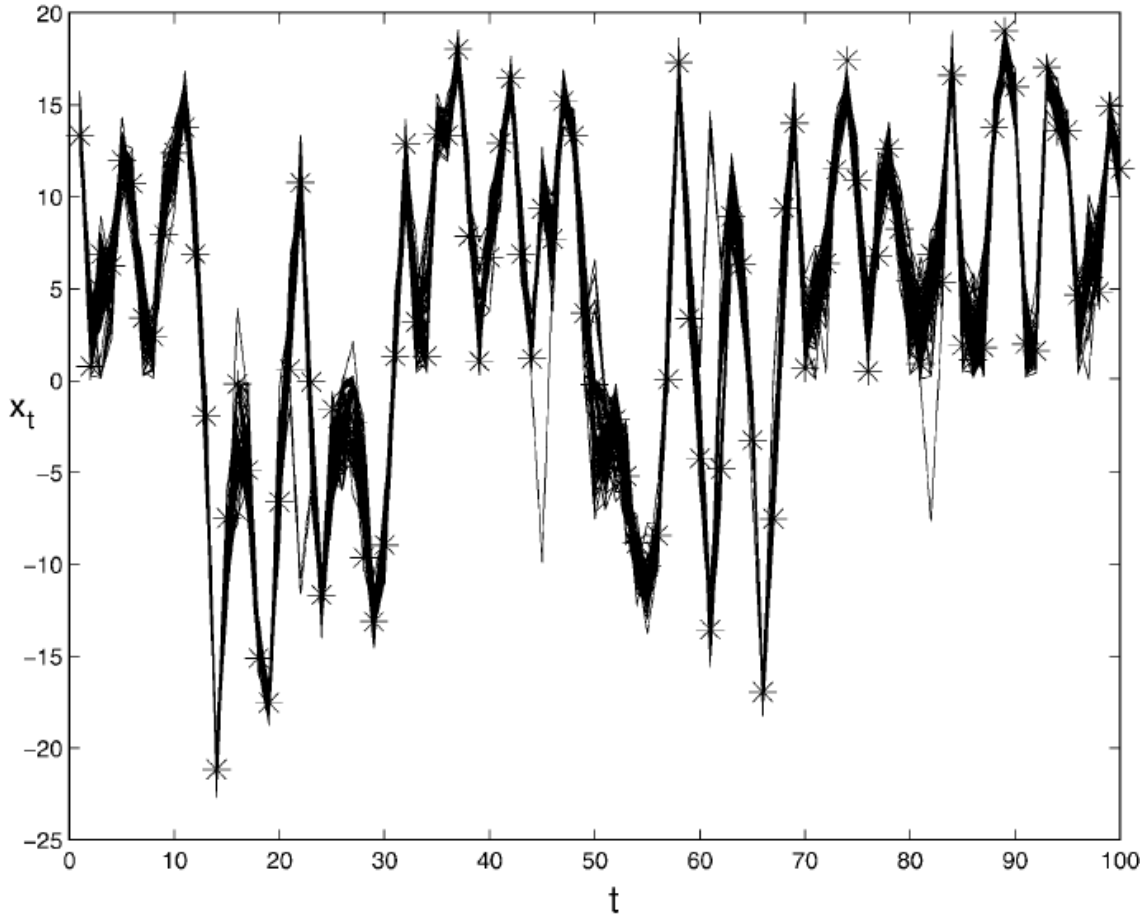
for $t = T - 1$ to 1 **do** ▷ Backward Pass Smoother

Calculate $\rho_t^{(i)} \propto \omega_t^{(i)} p(\tilde{x}_{t+1} \mid x_t^{(i)})$ for $i = 1, \ldots, L$ and normalize the modified weights.

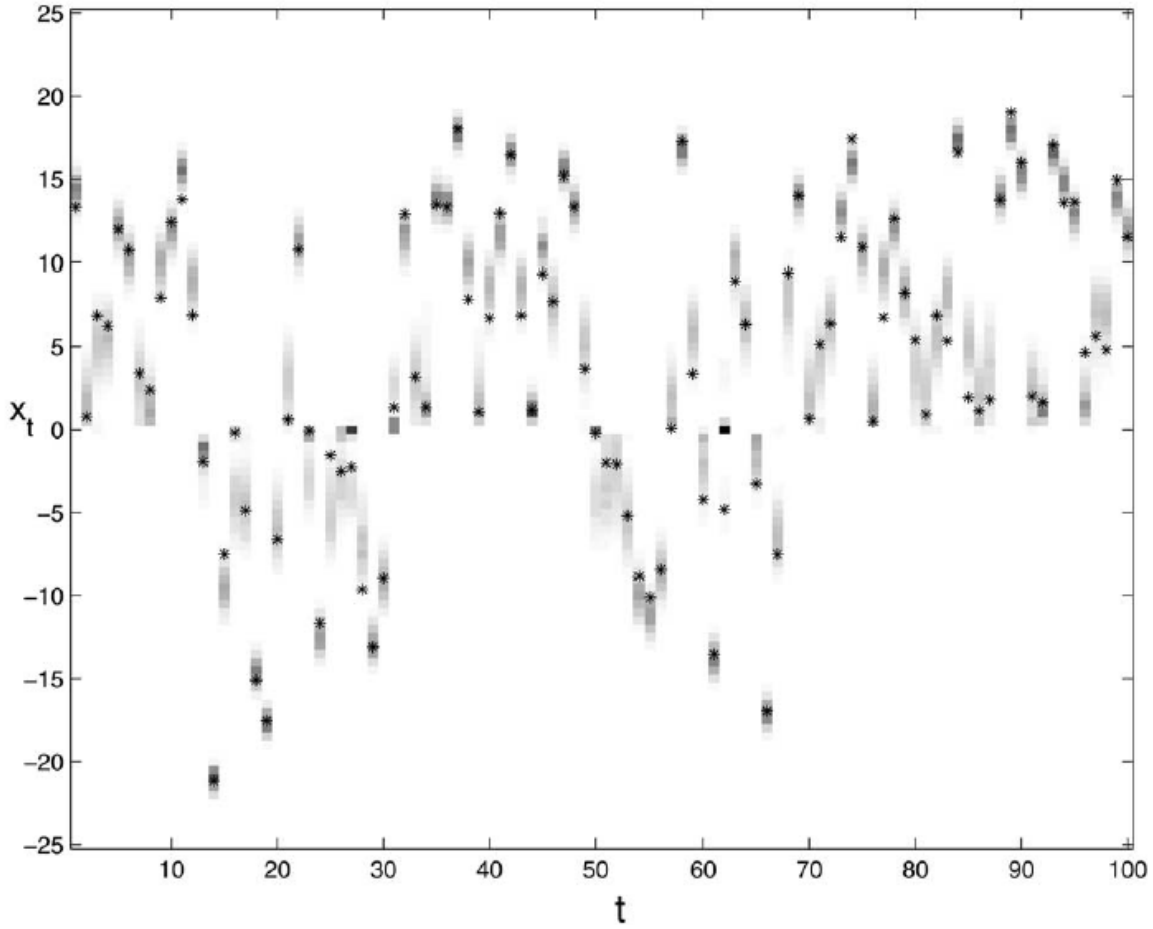
Choose $\widetilde{x}_t = x_t^{(i)}$ with probability $\rho_t^{(i)}$.

end for

Particle Smoothing Example



Smoothing trajectories for T=100.
True states (*).



Kernel density estimates based on smoothed trajectories.True states (*).

Additional Particle Filter Topics

- Auxiliary particle filter – bias samples towards those more likely to “survive”
- Rao-Blackwell PF – analytically marginalize tractable sub-components of the state (e.g. linear Gaussian terms)
- MCMC PF – apply MC kernel with correct target $p(x_1^t \mid y_1^t)$ to sample trajectory prior to the resampling step
- Other smoothing topics:
  - Generalized two-filter smoothing
  - MC approximation of posterior marginals $p(x_t \mid y_1^T)$
- *Maximum a posteriori* (MAP) particle filter
- Maximum likelihood parameter estimation using PF

Sequential Monte Carlo Summary

- Importance sampling for inference in nonlinear dynamical systems
- Using model dynamics as proposal allows recursive weight updates

$$q(x \mid y) = q(x_0) \prod_{t=1}^{T} p(x_t \mid x_{t-1}) \qquad w_t^{(\ell)} \propto w_{t-1}^{(\ell)} p(y_t \mid x_t^{(\ell)})$$

- All but one weight go to zero as prior/posterior diverge (degeneracy)
- Periodic resampling (with replacement) avoids weight degeneracy
- Each resampling step increases estimator variance (use sparingly)
- In practice, resample when effective sample size (ESS) below thresh

Outline

- Monte Carlo Estimation
- Sequential Monte Carlo
- Markov Chain Monte Carlo

Monte Carlo Estimation

One reason to sample a distribution is to approximate expected values under that distribution…

Expected value of function $f(x)$ w.r.t. distribution $p(x)$ given by,

$$\mathbb{E}_p[f(x)] = \int p(x)f(x)\,dx \equiv \mu$$

- Doesn't always have a closed-form for arbitrary functions
- Suppose we have iid samples: $\{x_i\}_{i=1}^N \sim p(x)$
- *Monte Carlo* estimate of expected value,

$$\hat{\mu}_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \approx \mathbb{E}_p[f(x)]$$

Samples must be independent!

Markov chain Monte Carlo methods

- The approximations of expectation that we have looked at so far have assumed that the samples are independent draws.
- This sounds good, but in high dimensions, we do not know how to get good independent samples from the distribution.
- MCMC methods drop this requirement.
- Basic intuition
  - If you have finally found a region of high probability, stick around for a bit, enjoy yourself, grab some more samples.

Markov chain Monte Carlo methods

- Samples are conditioned on the previous one (this is the Markov chain).
- MCMC is often a good hammer for complex, high dimensional, problems.
- Main downside is that it is not “plug-and-play”
  - Doing well requires taking advantage to the structure of your problem
  - MCMC tends to be expensive (but take heart---there may not be any other solution, and at least your problem is being solved).
  - If there are faster solutions, you can incorporate that (and MCMC becomes a way to improve/select these good guesses).

Metropolis Algorithm

We want samples $z^{(1)}, z^{(2)}, \ldots$.

Again, write $p(z) = \tilde{p}(z)/Z$

Assume that $q\left(z \middle| z^{(prev)}\right)$ can be sampled easily

Also assume that $q(\ \ )$ is symmetric, i.e., $q\left(z_A \middle| z_B\right) = q\left(z_B \middle| z_A\right)$

For example, $q\left(z \middle| z^{(prev)}\right) \sim \mathbb{N}\left(z; z^{(prev)}, \sigma^2\right)$

Metropolis Algorithm

While not_bored

{

Sample $q\left(z \middle| z^{(prev)}\right)$

Accept with probability $A\left(z, z^{(prev)}\right) = \min\left(1, \frac{\tilde{p}(z)}{\tilde{p}\left(z^{(prev)}\right)}\right)$

If accept, emit z, otherwise, emit $z^{(prev)}$.

}

Always emit one or the other

If things get better, always accept. If they get worse, sometimes accept.

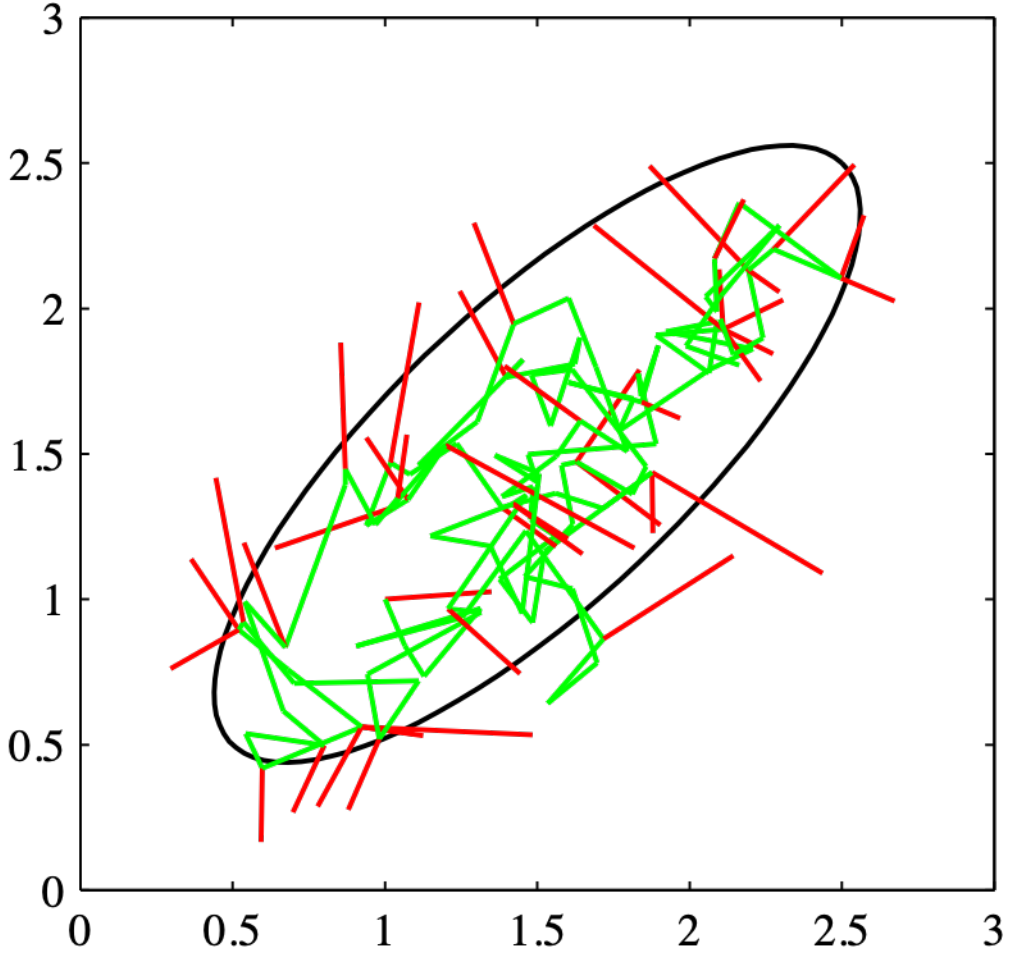
Metropolis Algorithm

Note that

$$A\left(z, z^{(prev)}\right) = \min\left(1, \frac{\tilde{p}(z)}{\tilde{p}\left(z^{(prev)}\right)}\right) = \min\left(1, \frac{p(z)}{p\left(z^{(prev)}\right)}\right)$$

So we do not need to normalize $p(z)$

Metropolis Example



Green follows accepted proposals
Red are rejected moves.

Markov chain view

Denote an initial probability distribution by $p\left(z^{(1)}\right)$

Define transition probabilities by:

$$T\left(z^{(prev)}, z\right) = p\left(z \middle| z^{(prev)}\right) \qquad \text{(a probability distribution)}$$

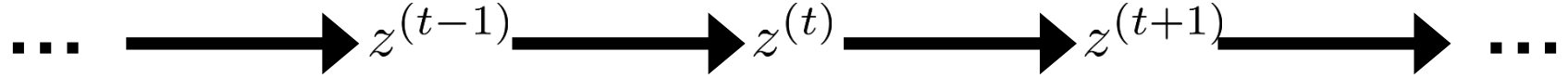
T can change over time, but for now, assume that it
it is always the same (homogeneous chain)

A given chain evolves from a sample of $p\left(z^{(1)}\right)$, and is
an instance from an essemble of chains.

Markov Chain Monte Carlo (MCMC)

- Stochastic 1st order Markov process with transition kernel:

$$T(z^{(t)} \mid z^{(t-1)})$$



- Each $x^{(t)}$ full N-dimensional state vector
- MCMC samples $\ldots, z^{(t-1)}, z^{(t)}, z^{(t+1)}, \ldots$ **not independent**
- New superscript notation indicates dependence:

$\{z^{(\ell)}\}_{\ell=1}^{L}$ **Independent**

$\{z^{(t)}\}_{t=1}^{T}$ **Dependent**

Key Question: How many MCMC samples T are needed to draw L independent samples from p(x)?

Stationary Markov chains

- Recall that our goal is to have our Markov chain emit samples from our **target distribution** $p(z)$.
- This implies that the distribution being sampled at time $t+1$ would be the same as that of time t (**stationary**).
- If our stationary (target) distribution is $p()$, then if we imagine an ensemble of chains, they are in each state with (long-run) probability $p()$.
  - On average, a switch from s1 to s2 happens as often as going from s2 to s1, otherwise, the percentage of states would not be stable.

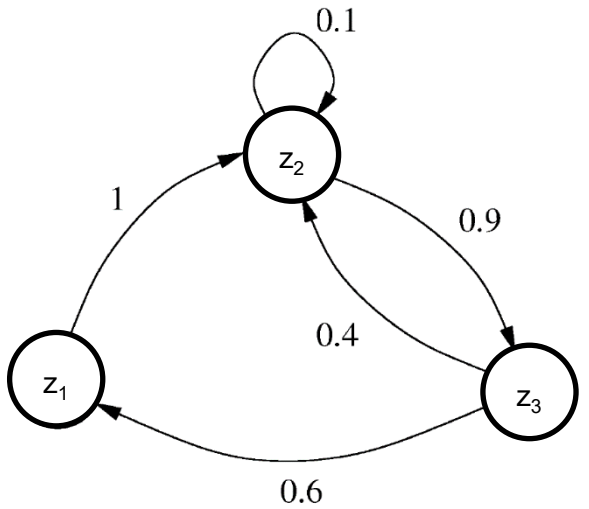
Markov Chain Monte Carlo (MCMC)

- Stochastic 1st order Markov process with transition kernel:

$$T(z^{(t)} \mid z^{(t-1)})$$

$$\ldots \longrightarrow z^{(t-1)} \longrightarrow z^{(t)} \longrightarrow z^{(t+1)} \longrightarrow \ldots$$

E.g. Let, $T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.1 & 0.9 \\ 0.6 & 0.4 & 0 \end{bmatrix}$



[Source: Andrieu et al.]

- Initial state dist'n: $\mu(z^{(1)}) = (0.5, 0.2, 0.3)$
- Repeated transitions converge to target

$$\mu(z^{(1)}) \cdot T \cdot T \cdot \ldots T = (0.2, 0.4, 0.4) = p(z)$$

True for <u>any</u> initial state distribution

How can we formalize this?

Detailed balance

- Detailed balance is defined by:

$$p(z)T(z,z') = p(z')T(z',z)$$

(We assume that $T(\bullet) > 0$)

- Detailed balance is a sufficient condition for *p()* to be a stationary distribution with respect to the positive T.

Sufficient but *not* necessary

Detailed balance implies stationary

$$p(z) = \sum_{z'} p^{(prev)}(z') T(z', z)$$

(because?)

Detailed balance implies stationary

$$p(z) = \sum_{z'} p^{(prev)}(z') T(z', z) \qquad \text{(marginalization)}$$

$$= \sum_{z'} p^{(prev)}(z) T(z, z') \qquad \textbf{(because?)}$$

Detailed balance implies stationary

$$
\begin{aligned}
p(z) &= \sum_{z'} p^{(prev)}(z')T(z',z) && \text{(marginalization)} \\
&= \sum_{z'} p^{(prev)}(z)T(z,z') && \text{(detailed balance)} \\
&= p^{(prev)}(z)\sum_{z'} T(z,z') && \textbf{(because?)}
\end{aligned}
$$

Detailed balance implies stationary

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p(z) &= \sum_{z'} p^{(prev)}(z')T(z',z) && \text{(marginalization)} \\
&= \sum_{z'} p^{(prev)}(z)T(z,z') && \text{(detailed balance)} \\
&= p^{(prev)}(z)\sum_{z'} T(z,z') && \text{(moving constant out of sum)} \\
&= p^{(prev)}(z)\sum_{z'} p(z'|z) && \textbf{(because?)}
\end{aligned}
$$

Detailed balance implies stationary

$$
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&= p^{(prev)}(z)\sum_{z'} T(z,z') && \text{(moving constant out of sum)} \\
&= p^{(prev)}(z)\sum_{z'} p(z'|z) && \text{(definition of T)} \\
&= p^{(prev)}(z)\sum_{z'} \frac{p(z',z)}{p(z)} && \textbf{(because?)}
\end{aligned}
$$

Detailed balance implies stationary

$$
\begin{aligned}
p(z) &= \sum_{z'} p^{(prev)}(z')T(z',z) && \text{(marginalization)} \\
&= \sum_{z'} p^{(prev)}(z)T(z,z') && \text{(detailed balance)} \\
&= p^{(prev)}(z)\sum_{z'} T(z,z') && \text{(moving constant out of sum)} \\
&= p^{(prev)}(z)\sum_{z'} p(z'|z) && \text{(definition of T)} \\
&= p^{(prev)}(z)\sum_{z'} \frac{p(z',z)}{p(z)} && \text{(definition of "|")} \\
&= p^{(prev)}(z)\frac{p(z)}{p(z)} && \textbf{(because?)}
\end{aligned}
$$

Detailed balance implies stationary

$$
\begin{aligned}
p(z) &= \sum_{z'} p^{(prev)}(z')T(z',z) && \text{(marginalization)} \\
&= \sum_{z'} p^{(prev)}(z)T(z,z') && \text{(detailed balance)} \\
&= p^{(prev)}(z)\sum_{z'} T(z,z') && \text{(moving constant out of sum)} \\
&= p^{(prev)}(z)\sum_{z'} p(z'|z) && \text{(definition of T)} \\
&= p^{(prev)}(z)\sum_{z'} \frac{p(z',z)}{p(z)} && \text{(definition of "|")} \\
&= p^{(prev)}(z)\frac{p(z)}{p(z)} && \text{(marginalization)} \\
&= p^{(prev)}(z) && \textbf{(because?)}
\end{aligned}
$$

Detailed balance implies stationary

$$
\begin{aligned}
p(z) &= \sum_{z'} p^{(prev)}(z') T(z', z) && \text{(marginalization)} \\
&= \sum_{z'} p^{(prev)}(z) T(z, z') && \text{(detailed balance)} \\
&= p^{(prev)}(z) \sum_{z'} T(z, z') && \text{(moving constant out of sum)} \\
&= p^{(prev)}(z) \sum_{z'} p(z' | z) && \text{(definition of T)} \\
&= p^{(prev)}(z) \sum_{z'} \frac{p(z', z)}{p(z)} && \text{(definition of "|")} \\
&= p^{(prev)}(z) \frac{p(z)}{p(z)} && \text{(marginalization)} \\
&= p^{(prev)}(z) && \text{(canceling)}
\end{aligned}
$$

Detailed balance (continued)

- Detailed balance (**for *p()***) means that *if* our chain was generating samples from *p()*, it would continue to due so.
  - We will address how it gets there soon.
  - For MCMC algorithms like Metropolis, it is important that the stationary state is the distribution **we want** (most Markov chains converge to *something*),

- Does the Metropolis algorithm have detailed balance?

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

For detailed balance, we need to show (in general)

$p(z')T(z',z) = p(z)T(z,z')$

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

For detailed balance, we need to show (in general)

$$p(z')T(z',z) = p(z)T(z,z')$$

In Metropolis this is

$$p(z')q(z|z')A(z,z') = p(z)q(z'|z)A(z',z)$$

Probability of transition from z to z' is the probability that z' is proposed, **and** it is accepted.

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

$$p(z')q(z|z')A(z,z') = q(z|z')\min(p(z'),p(z))$$ **(because?)**

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

$$p(z')q(z|z')A(z,z') = q(z|z')\min(p(z'),p(z)) \qquad \text{(bring } p(z') \text{ into } A\text{)}$$

$$= q(z'|z)\min(p(z'),p(z)) \qquad \textbf{(because?)}$$

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

$$
\begin{aligned}
p(z')q(z|z')A(z,z') &= q(z|z')\min(p(z'),p(z)) && \text{(bring } p(z') \text{ into } A\text{)} \\
&= q(z'|z)\min(p(z'),p(z)) && \text{q() is symmetric} \\
&= p(z)q(z'|z)\min\left(\frac{p(z')}{p(z)},1\right) && \textbf{(because?)}
\end{aligned}
$$

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

$$
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&= q(z'|z)\min(p(z'),p(z)) && \text{q() is symmetric} \\
&= p(z)q(z'|z)\min\left(\frac{p(z')}{p(z)},1\right) && \text{(divide the min() by } p(z)\text{)} \\
&= p(z)q(z'|z)\min\left(1,\frac{p(z')}{p(z)}\right) && \text{(switch order in min())} \\
&= p(z)q(z'|z)A(z',z) && \textbf{(because?)}
\end{aligned}
$$

Metropolis has detailed balance

Recall that in Metropolis, $A(z,z') = \min\left(1, \frac{p(z)}{p(z')}\right)$

$$
\begin{aligned}
p(z')q(z|z')A(z,z') &= q(z|z')\min(p(z'),p(z)) && \text{(bring } p(z') \text{ into } A) \\
&= q(z'|z)\min(p(z'),p(z)) && \text{q() is symmetric} \\
&= p(z)q(z'|z)\min\left(\frac{p(z')}{p(z)},1\right) && \text{(divide the min() by } p(z)) \\
&= p(z)q(z'|z)\min\left(1,\frac{p(z')}{p(z)}\right) && \text{(switch order in min())} \\
&= p(z)q(z'|z)A(z',z) && \text{(definition of } A(z',z))
\end{aligned}
$$

Ergodic chains

- Different starting probabilities will give different chains
- We want our chains to converge (in the limit) to the same stationary state, regardless of starting distribution.
- Such chains are called ergodic, and the common stationary state is called the equilibrium state.
- Ergodic chains have a unique equilibrium.

When do our chains converge?

- Important theorem tells us that for finite state spaces* our chains converge to equilibrium under two relatively weak conditions.
  - (1) Irreducible
    - We can get from any state to any other state
  - (2) Aperiodic
    - The chain does not get trapped in cycles
- These are true for detailed balance (there exists a stationary state) with T>0 (you can get there).
  - Detailed balance is sufficient, but not necessary for convergence—it is a stronger property than (1) & (2)

*Infinite or uncountable state spaces introduces additional complexities, but the main thrust is similar.

Evolution of ergodic chains

Let $p^{(t)}(z)$ be the distribution at some time (e.g., initial distribution)

Let $\pi(z)$ be the stationary distribution

Let $p^{(t)}(z) = \pi(z) - \Delta^{(t)}(z)$

What is $p^{(t+1)}(z)$ in terms of $\pi(z)$?

Evolution of ergodic chains

Let $p^{(t)}(z)$ be the distribution at some time (e.g., initial distribution)

Let $\pi(z)$ be the stationary distribution

Let $p^{(t)}(z) = \pi(z) - \Delta^{(t)}(z)$

$$
\begin{aligned}
p^{(t+1)}(z) &= \sum_{z'} p^{(t)}(z')\, T(z,z') \\
&= \sum_{z'} \pi(z')\, T(z,z') - \sum_{z'} \Delta^{(t)}(z')\, T(z,z') \\
&= \pi(z) - \Delta^{(t+1)}(z)
\end{aligned}
$$

Evolution of ergodic chains

Let $p^{(t)}(z) = \pi(z) - \Delta^{(t)}(z)$

$$p^{(t+1)}(z) = \sum_{z'} p^{(t)}(z')\, T(z,z')$$

$$= \sum_{z'} \pi(z')\, T(z,z') - \sum_{z'} \Delta^{(t)}(z')\, T(z,z')$$

$$= \pi(z) - \Delta^{(t+1)}(z)$$

Cannot die!

Dies out

Evolution of ergodic chains

$$
\begin{aligned}
p^{(t+1)}(z) &= \sum_{z'} p^{(t)}(z')\, T(z,z') \\
&= \sum_{z'} \pi(z')\, T(z,z') - \sum_{z'} \Delta^{(t)}(z')\, T(z,z') \\
&= \pi(z) - \Delta^{(t+1)}(z)
\end{aligned}
$$

Claim that $\left|\Delta^{(t)}(z)\right| < (1-v)^t$

where $v = \min_{z} \min_{z':\pi(z')>0} \dfrac{T(z,z')}{\pi(z)}$

and we have $0 < v \leq 1$

Matrix-vector representation

Chains (think ensemble) evolve according to:

$$p(z) = \sum_{z'} p(z')\, T(z', z)$$

Matrix vector representation:

$$\mathbf{p} = \mathbf{T}\mathbf{p}'$$

And, after n iterations after a starting point:

$$\mathbf{p}^{(n)} = \mathbf{T}^N \mathbf{p}^{(0)}$$

Matrix representation

A single transition is given by

$$\mathbf{p} = \mathbf{T}\mathbf{p}'$$

Note what happens for stationary state:

$$\mathbf{p}^* = \mathbf{T}\mathbf{p}^*$$

What does this equation look like?

So, $\mathbf{p}^*$ is an eigenvector with eigenvalue one.

Matrix representation

A single transition is given by

$$\mathbf{p} = \mathbf{T}\mathbf{p}'$$

Note what happens for stationary state:

$$\mathbf{p}^* = \mathbf{T}\mathbf{p}^*$$

So, $\mathbf{p}^*$ is an eigenvector with eigenvalue one.

And, intutively, if things converge, $\mathbf{p}^* = \mathbf{T}^\infty \mathbf{p}^{(0)}$ For any $\mathbf{p}^{(0)}$!

Aside on stochastic matrices

- A right (row) stochastic matrix has non-negative entries, and its rows sum to one.
- A left (column) stochastic matrix has non-negative entries, and its columns sum to one.
- A doubly stochastic matrix has both properties.

Aside on stochastic matrices

- In our problem, T is a left (column) stochastic matrix.
  - If you want to be right handed, take the transpose

- The column vector, **p**, also has non-negative elements, that sum to one (stochastic vector).

Aside on stochastic matrices

- In our problem, T is a left (column) stochastic matrix.
  - If you want to be right handed, take the transpose
- The column vector, **p**, also has non-negative elements, that sum to one (stochastic vector).
- Fun facts
  - The product of a stochastic matrix and vector is a stochastic vector.
  - The product of two stochastic matrices is a stochastic matrix.

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = ?$$

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = E\Lambda^N E^{-1}$$

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = E\Lambda^N E^{-1}$$

T^N cannot grow without bound, Why not?

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = E\Lambda^N E^{-1}$$

T^N cannot grow without bound,

because it is a stochastic matrix.

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = E\Lambda^N E^{-1}$$

T^N cannot grow without bound,

because it is a stochastic matrix.

Logic:

- Product of stochastic matrix is a stochastic matrix
- Columns of (left) stochastic matrix sum to 1
- Power is a bunch of products

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = E\Lambda^N E^{-1}$$

Since T^N cannot grow without bound, the eigenvalue magnitudes (remember they can be complex) are inside [0,1].

Aside on (stochastic) matrix powers

Consider the eigenvalue decomposition of T, $T = E\Lambda E^{-1}$

$$\mathrm{T}^N = E\Lambda^N E^{-1}$$

Since T^N cannot grow without bound, the eigenvalue magnitudes (remember they can be complex) are inside [0,1].

In fact, for our situation, the second biggest absolute value of the eigenvalues is less than one (not so easy to prove), which also means the biggest one is 1 (otherwise T will go to zero).

Aside on (stochastic) matrix powers

We have $\mathrm{T}^N = E\Lambda^N E^{-1}$

$$\Lambda = \begin{pmatrix} 1 & & & \\ & \lambda_2 & & \\ & & \cdots & \\ & & & \lambda_K \end{pmatrix} \quad \text{and} \quad \Lambda^\infty = \begin{pmatrix} & & ? & \end{pmatrix}$$

Aside on (stochastic) matrix powers

We have $\mathrm{T}^N = E\Lambda^N E^{-1}$

$$\Lambda = \begin{pmatrix} 1 & & & \\ & \lambda_2 & & \\ & & \bullet\bullet\bullet & \\ & & & \lambda_K \end{pmatrix} \quad \text{and} \quad \Lambda^\infty = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & \bullet\bullet\bullet & \\ & & & 0 \end{pmatrix}$$

Aside on (stochastic) matrix powers

We have $\mathrm{T}^N = E\Lambda^N E^{-1}$

$$\Lambda = \begin{pmatrix} 1 & & & \\ & \lambda_2 & & \\ & & \cdots & \\ & & & \lambda_K \end{pmatrix} \quad \text{and} \quad \Lambda^\infty = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & \cdots & \\ & & & 0 \end{pmatrix}$$

$$\Lambda^\infty E^{-1} = \begin{pmatrix} & ? & \\ & & \end{pmatrix}$$

Aside on (stochastic) matrix powers

We have $\mathrm{T}^N = E\Lambda^N E^{-1}$

$$\Lambda = \begin{pmatrix} 1 & & & \\ & \lambda_2 & & \\ & & \bullet\bullet\bullet & \\ & & & \lambda_K \end{pmatrix} \quad \text{and} \quad \Lambda^\infty = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & \bullet\bullet\bullet & \\ & & & 0 \end{pmatrix}$$

$$\Lambda^\infty E^{-1} = \begin{pmatrix} E^{-1}(1,:) \\ \mathbf{0}^T \\ \cdots \\ \mathbf{0}^T \end{pmatrix}$$

Aside on (stochastic) matrix powers

Write $\mathbf{p}$ in terms of the eigen basis

$$\mathbf{p} = \sum_i a_i \mathbf{e}_i$$

$$E^{-1}(1,:) \bullet \mathbf{p} = \sum_i a_i E^{-1}(1,:) \bullet \mathbf{e}_i = a_1$$

Aside on (stochastic) matrix powers

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$E^{-1} \bullet E = I$

And the columns of E are $\mathbf{e}_i$

So, $E^{-1}(1,:) \bullet E = (1,0,0,\cdots.0)$

(first row of the inverse), and

so $E^{-1}(1,:) \bullet \mathbf{e}_1 = 1$

and $E^{-1}(1,:) \bullet \mathbf{e}_{i \neq 1} = 0$

Aside on (stochastic) matrix powers

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(first row of the inverse), and
so $E^{-1}(1,:) \bullet \mathbf{e}_1 = 1$
and $E^{-1}(1,:) \bullet \mathbf{e}_{i \neq 1} = 0$

and, $$\Lambda^{\infty} E^{-1} \mathbf{p} = \begin{pmatrix} E^{-1}(1,:) \bullet \mathbf{p} \\ 0 \\ \cdots \\ 0 \end{pmatrix} = \begin{pmatrix} a_1 \\ 0 \\ \cdots \\ 0 \end{pmatrix}$$

Aside on (stochastic) matrix powers

Recall that we are studying $\mathrm{E}\Lambda^{\infty}E^{-1}\mathbf{p}$

$$\Lambda^{\infty}E^{-1}\mathbf{p} = \begin{pmatrix} a_1 \\ 0 \\ \dots \\ 0 \end{pmatrix}$$

So, $\mathrm{E}\,\Lambda^{\infty}E^{-1}\mathbf{p} = \ ?$

Aside on (stochastic) matrix powers

Recall that we are studying $\mathrm{E}\Lambda^{\infty}E^{-1}\mathbf{p}$

$$\Lambda^{\infty}E^{-1}\mathbf{p} = \begin{pmatrix} a_1 \\ 0 \\ \dots \\ 0 \end{pmatrix}$$

So, $\mathrm{E}\ \Lambda^{\infty}E^{-1}\mathbf{p} = a_1\mathbf{e_1}$

Aside on (stochastic) matrix powers

So, $\mathbf{p}^* = \mathrm{E}\Lambda^{\infty}E^{-1}\mathbf{p}$

u_1

$\mathrm{E}\Lambda^{\infty}E^{-1}\mathbf{p} = \mathbf{p}^*$ no mater what the initial point $\mathbf{p}$ is.

So, glossing over details, we have convergence to equilibrium.

Optional

Justification relies on Perron Frobenius theorem

Let $A = (a_{ij})$ be an $n \times n$ positive matrix: $a_{ij} > 0$ for $1 \le i, j \le n$. Then the following statements hold.

1. There is a positive real number r, called the **Perron root** or the **Perron–Frobenius eigenvalue**, such that r is an eigenvalue of A and any other eigenvalue λ (possibly, complex) is strictly smaller than r in absolute value, $|\lambda| < r$. Thus, the spectral radius $\rho(A)$ is equal to r.
2. The Perron–Frobenius eigenvalue is simple: r is a simple root of the characteristic polynomial of A. Consequently, the eigenspace associated to r is one-dimensional. (The same is true for the left eigenspace, i.e., the eigenspace for A^T.)
3. There exists an eigenvector $v = (v_1,\ldots,v_n)$ of A with eigenvalue r such that all components of v are positive: $A\,v = r\,v$, $v_i > 0$ for $1 \le i \le n$. (Respectively, there exists a positive left eigenvector w: $w^T A = r\,w^T$, $w_i > 0$.)
4. There are no other positive (moreover non-negative) eigenvectors except v (respectively, left eigenvectors except w), i.e. all other eigenvectors must have at least one negative or non-real component.
5. $\lim_{k\to\infty} A^k/r^k = vw^T$, where the left and right eigenvectors for A are normalized so that $w^T v = 1$. Moreover, the matrix vw^T is the projection onto the eigenspace corresponding to r. This projection is called the **Perron projection**.
6. **Collatz–Wielandt formula**: for all non-negative non-zero vectors x, let $f(x)$ be the minimum value of $[Ax]_i / x_i$ taken over all those i such that $x_i \neq 0$. Then f is a real valued function whose maximum is the Perron–Frobenius eigenvalue.
7. A "Min-max" Collatz–Wielandt formula takes a form similar to the one above: for all strictly positive vectors x, let $g(x)$ be the maximum value of $[Ax]_i / x_i$ taken over i. Then g is a real valued function whose minimum is the Perron–Frobenius eigenvalue.
8. The Perron–Frobenius eigenvalue satisfies the inequalities

$$\min_i \sum_j a_{ij} \le r \le \max_i \sum_j a_{ij}.$$

From Wikipedia

Main points about P-F for positive square matrices

- The maximal eigenvalue is strictly maximal and real valued (item 1).
- Its eigenvector (as computed by software*) has all positive (or negative) real components (item 3).
- The maximal eigenvalue of a stochastic matrix has absolute value 1 (item 8 applied to stochastic matrix).

*P-F says that the positive version exists, but software might hand you the negative of that, but you can negate it to be consistent with P-F.

Summary on matrix version of stationarity

$\mathbf{p}^* = \mathbf{T}\mathbf{p}^*$ is an eigenvector with eigenvalue one.

We have written it as $\mathbf{p}^* \parallel \mathbf{e}^1$ because $\mathbf{e}^1$ is the eigenvector normalized to norm 1 (not stochastic).

Intuitively (perhaps), T will reduce any component of p orthogonal to p^*, and T^N will kill off such components as $\mathrm{N} \to \infty$.

Neal ’93 provides an algebraic proof which does not rely on spectral theory.

MCMC so far

- Under reasonable conditions (ergodicity) ensembles of chains over discretized states converge to an equilibrium state (stationary distribution)

- Easiest way to prove (or check) that this is the case is to show **detailed balance** and use T>0 (sufficient but not necessary)

- There is a nice analogy with powers of stochastic matrices, which converge to an operator based on the largest magnitude eigenvector (with |eigenvalue|=1)

- In theory, to use MCMC for sampling a distribution, we simply need to ensure that our target distribution is the equilibrium state.

- In practice we do not know even know if we have visited the best place yet. (The ensemble metaphor runs into trouble if you have a small number of chains compared to the number of states).

MCMC Theory vs. Practice

- The time it takes to get reasonably close to equilibrium (where samples come from the target distribution) is called “burn in” time.
  - I.E., how long does it take to forget the starting state.
  - There is no general way to know when this has occurred.
- The average time it takes to visit a state is called “hit time”.
- What if we really want independent samples?
  - In theory we can take every N^{th} sample (some theories about how long to wait exist, but it depends on the algorithm and distribution).

MCMC for ML in practice

- We use MCMC for machine learning problems with very complex distributions over high dimensional spaces.

- Variables can be either discrete or continuous (often both)

- Despite the gloomy worst case scenario, MCMC is often a good way to find good solutions (either by MAP or integration).
  - Key reason is that there is generally structure in our distributions.
  - We need to exploit this knowledge in our proposal distributions.
  - Instead of getting hung up about whether you actually have convergence
    - Enjoy that fact that what you are doing is principled and can improve any answer (with respect to your model) that you can get by other means
      - Your model should be able to tell you which proposed solution are good.

A View of Metropolis

[Source: D. MacKay]

Transition kernel with target distribution:

$$p(x) = \frac{1}{Z}\tilde{p}(x)$$

1. Sample proposal: $x' \mid x^{(t-1)} \sim q(\cdot)$
2. Accept with probability:

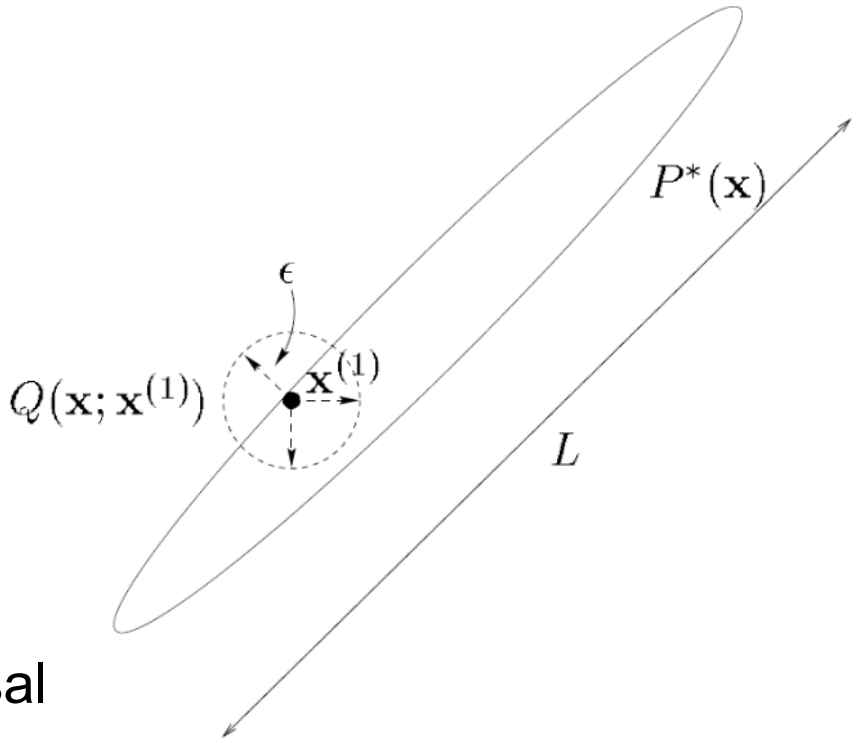
$$\min\{1, a\} \quad \text{where} \quad a = \frac{\tilde{p}(x')}{p(x^{(t-1)})}$$

Proposal must be symmetric

$$q(x^{(t)} \mid x^{(t-1)}) = q(x^{(t-1)} \mid x^{(t)})$$

Example: Symmetric Gaussian proposal

$$q(x^{(t)} \mid x^{(t-1)}) = \mathcal{N}(x^{(t-1)}, \epsilon^2)$$

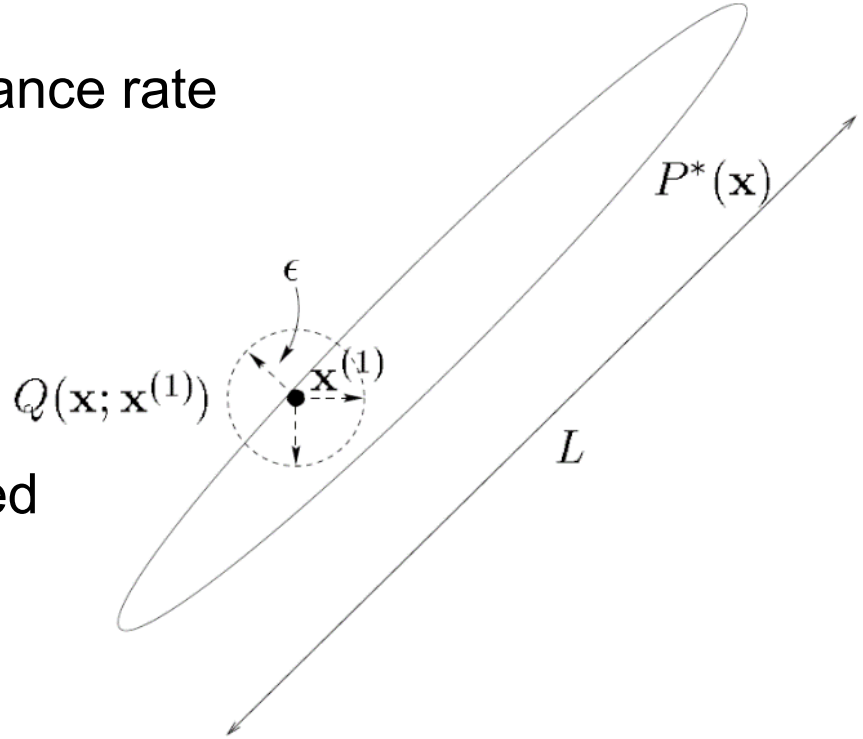


Metropolis Efficiency

How many samples needed for an independent sample?

Consider Gaussian proposal: $q(x^{(t)} \mid x^{(t-1)}) = \mathcal{N}(x^{(t-1)}, \epsilon^2)$ [Source: D. MacKay]

- Typically $\epsilon \ll L$ for adequate acceptance rate
- Leads to random walk dynamics that are slow to converge
- Rule of Thumb:
  If average acceptance is $f \in (0, 1)$ need to run for roughly $T \approx (L/\epsilon)^2 / f$ iterations for an independent sample

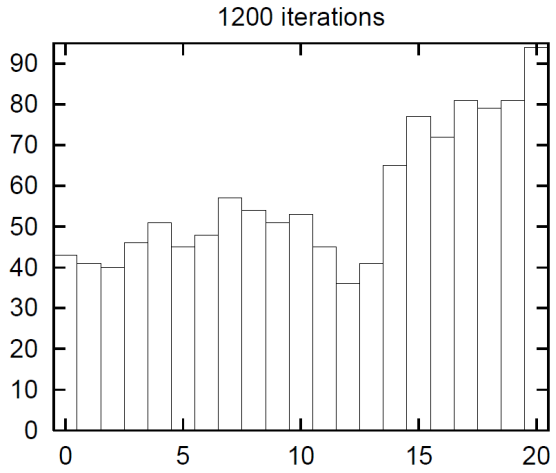


This is only a lower bound (and potentially very loose)

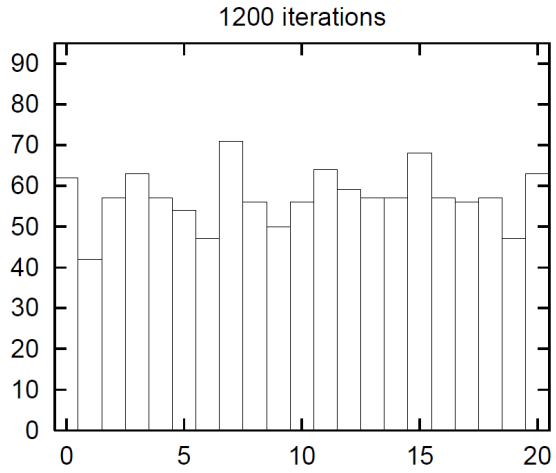
Example: Random Walk Dynamics

State evolution for t=1…600, horizontal bars denote intervals of 50

Metropolis



Independent



[Source: D. MacKay]

Target: $p(x) = \begin{cases} \frac{1}{21} & x \in \{0, \ldots, 20\} \\ 0 & \text{otherwise} \end{cases}$

Proposal: $q(x' \mid x) = \begin{cases} \frac{1}{2} & x' = x \pm 1 \\ 0 & \text{otherwise} \end{cases}$

From $x_0 = 10$ need ~400 steps to reach both end states (0 and 20). So, ~400 steps to generate 1 independent sample!

Very important to avoid random walk dynamics

Beyond the Metropolis Method

Metropolis requires the proposal to be symmetric,

$$q(z' \mid z) = q(z \mid z')$$

This often results in a chain that takes a long time to converge to a stationary distribution (long burn in time)

Example The most common proposal (Gaussian),

$$q(z' \mid z) = \mathcal{N}(z' \mid z, \sigma^2 I)$$

exhibits random walk dynamics that are inefficient

Metropolis-Hastings relaxes this symmetry requirement…

Metropolis-Hastings MCMC method

While not_bored

{

Sample $q\left(z \middle| z^{(prev)}\right)$

Accept with probability $A\left(z, z^{(prev)}\right) = \min\left(1, \frac{\tilde{p}(z) q\left(z^{(prev)} \middle| z\right)}{\tilde{p}\left(z^{(prev)}\right) q\left(z \middle| z^{(prev)}\right)}\right)$

If accept, emit z, otherwise, emit $z^{(prev)}$.

}

Does Metropolis-Hastings converge to the target distribution?

- Like Metropolis, but now q() is not necessarily symmetric.
- If Metropolis-Hastings has detailed balance, then it converges to the target distribution under weak conditions.
  - The converse is not true, but generally samplers of interest will have detailed balance

Does Metropolis-Hastings have detailed balance?

To show detailed balance we need to show

$$p(z')q(z|z')A(z,z') = p(z)q(z'|z)A(z',z)$$

$$p(z')q(z|z')A(z,z') = \min\left(p(z')q(z|z'), p(z)q(z'|z)\right)$$

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$$p(z')q(z|z')A(z,z') = \min\left(p(z')q(z|z'), p(z)q(z'|z)\right)$$

$$\left\{ \text{Recall that} \quad A(z,z') = \min\left(1, \frac{p(z)q(z'|z)}{p(z')q(z|z')}\right) \right\}$$

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$$p(z')q(z|z')A(z,z') = \min\left(p(z')q(z|z'), p(z)q(z'|z)\right)$$

$$= p(z)q(z'|z)\min\left(\frac{p(z')}{p(z)}\frac{q(z|z')}{q(z'|z)}, 1\right)$$

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Does Metropolis-Hastings have detailed balance?

To show detailed balance we need to show

$$p(z')q(z|z')A(z,z') = p(z)q(z'|z)A(z',z)$$

$$\begin{aligned}
p(z')q(z|z')A(z,z') &= \min\left(p(z')q(z|z'), p(z)q(z'|z)\right) \\
&= p(z)q(z'|z)\min\left(\frac{p(z')}{p(z)}\frac{q(z|z')}{q(z'|z)}, 1\right) \\
&= p(z)q(z'|z)\min\left(1, \frac{p(z')}{p(z)}\frac{q(z|z')}{q(z'|z)}\right) \\
&= p(z)q(z'|z)A(z',z)
\end{aligned}$$

Metropolis-Hastings comments

- Again it does not matter if we use unnormalized probabilities in the M-H acceptance ratio A(z,z')
- It should be clear that the Metropolis method (where q() is symmetric) is a special case of M-H
- q(z'|z) can be anything, but you need to specify the reverse move q(z|z'), which can be tricky

MCMC So Far…

Metropolis Algorithm

- Sample RV from proposal $z \sim q(z \mid z^{(\text{prev})})$
- Proposal must be *symmetric* $q(z \mid z^{(\text{prev})}) = q(z^{(\text{prev})} \mid z)$
- Accept with probability $\min\left\{1, \widetilde{p}(z) \div \widetilde{p}(z^{(\text{prev})})\right\}$

Metropolis-Hastings Algorithm

- Proposal does not have to be symmetric
- Accept with probability

$$\min\left\{1, \frac{\widetilde{p}(z)q(z^{(\text{prev})} \mid z)}{\widetilde{p}(z^{(\text{prev})})q(z \mid z^{(\text{prev})})}\right\}$$

Both methods require choosing proposal, which can be hard

Gibbs Sampling

Let $p(x)$ be the target distribution on random variables,

$$x_1, x_2, \ldots, x_N$$

Consider the *complete conditional distribution* x_i

$$p(x_i \mid x_{\neg i})$$

where $x_{\neg i} = \{x_1, x_2, \ldots, x_N\} \backslash x_i$ all RVs *except* x_i

Idea Don't sample all RVs from one proposal. Sample each from its corresponding complete conditional,

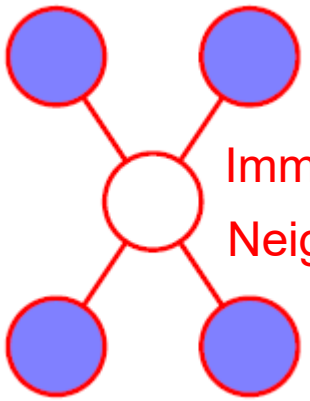
$$q_i(x_i \mid x_{\neg i}) = p(x_i \mid x_{\neg i})$$

We call this method Gibbs Sampling

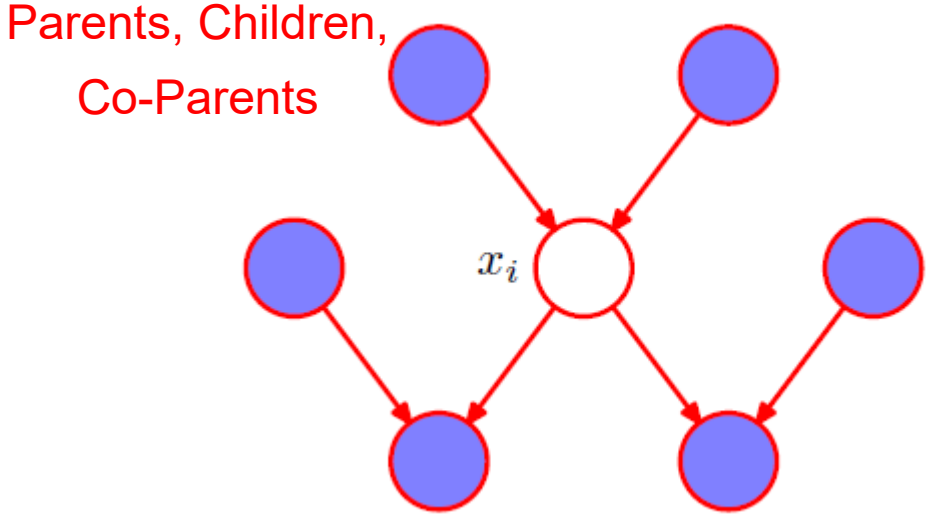
Gibbs Sampling

Recall that an RV is conditionally independent of all RVs given its *Markov Blanket*

MRF



Bayes Net



So complete conditionals only depend on Markov Blanket,

$$p(x_i \mid x_{\neg i}) = p(x_i \mid x_{\mathrm{Mb}(i)})$$

[Source: Bishop, C. PRML]

Consider a set of N variables, z_1, z_1, ...,z_N. Then Gibbs says

Initialize $\left\{ z_i^{(0)} : i = 1,...,N \right\}$

While not_bored

{

For i=1 to N

{

Sample $z_i^{(\tau+1)} \sim p\left(z_i \middle| z_1^{(\tau+1)},...,z_{i-1}^{(\tau+1)},z_{i+1}^{(\tau)},...,z_M^{(\tau)} \right)$

Always accept (i.e., emit $z = z_1^{(\tau+1)},...,z_{i-1}^{(\tau+1)},z_i^{(\tau+1)},z_{i+1}^{(\tau)},...,z_M^{(\tau)}$)

}

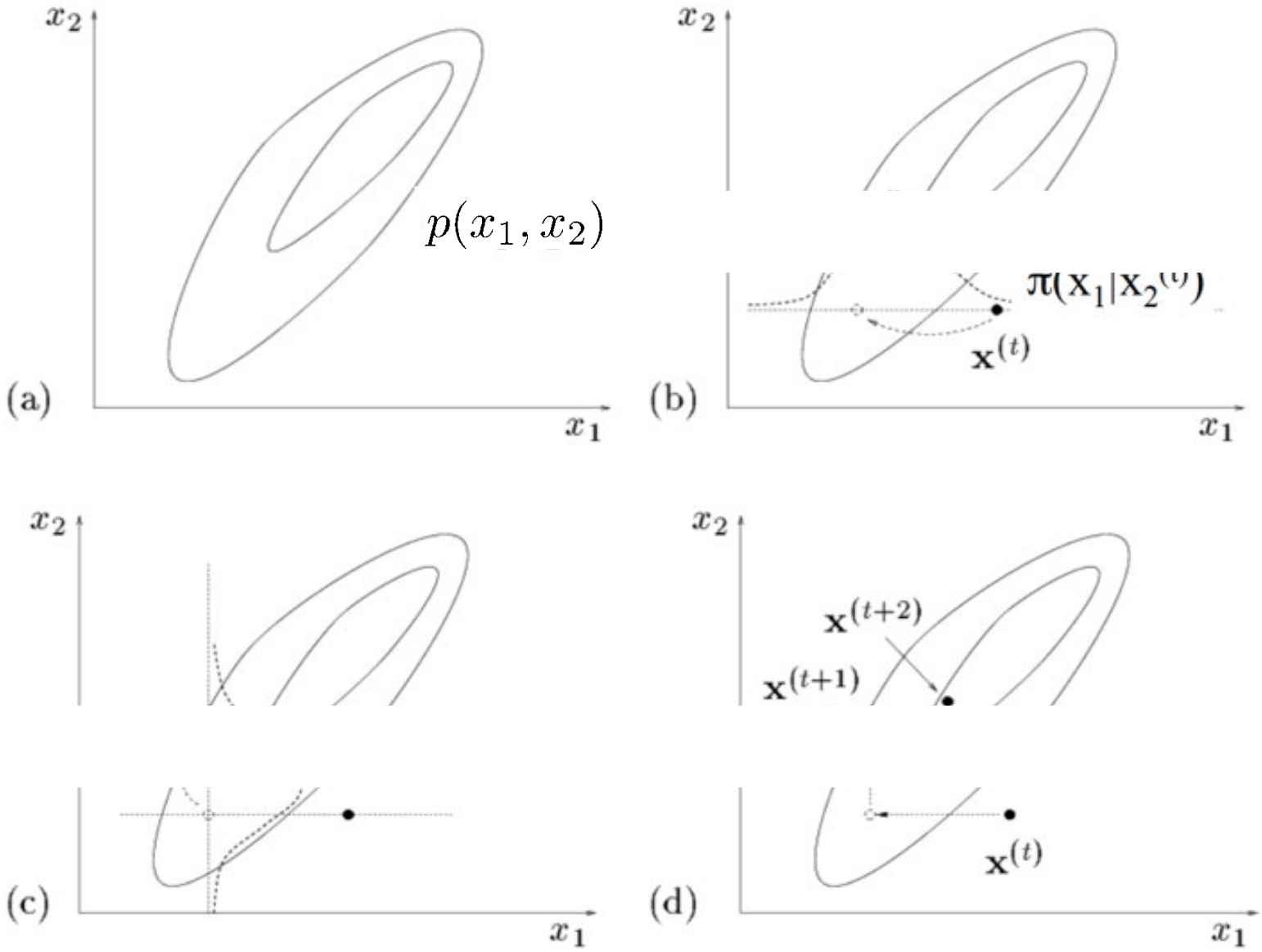
}

Can choose any order (or randomize)

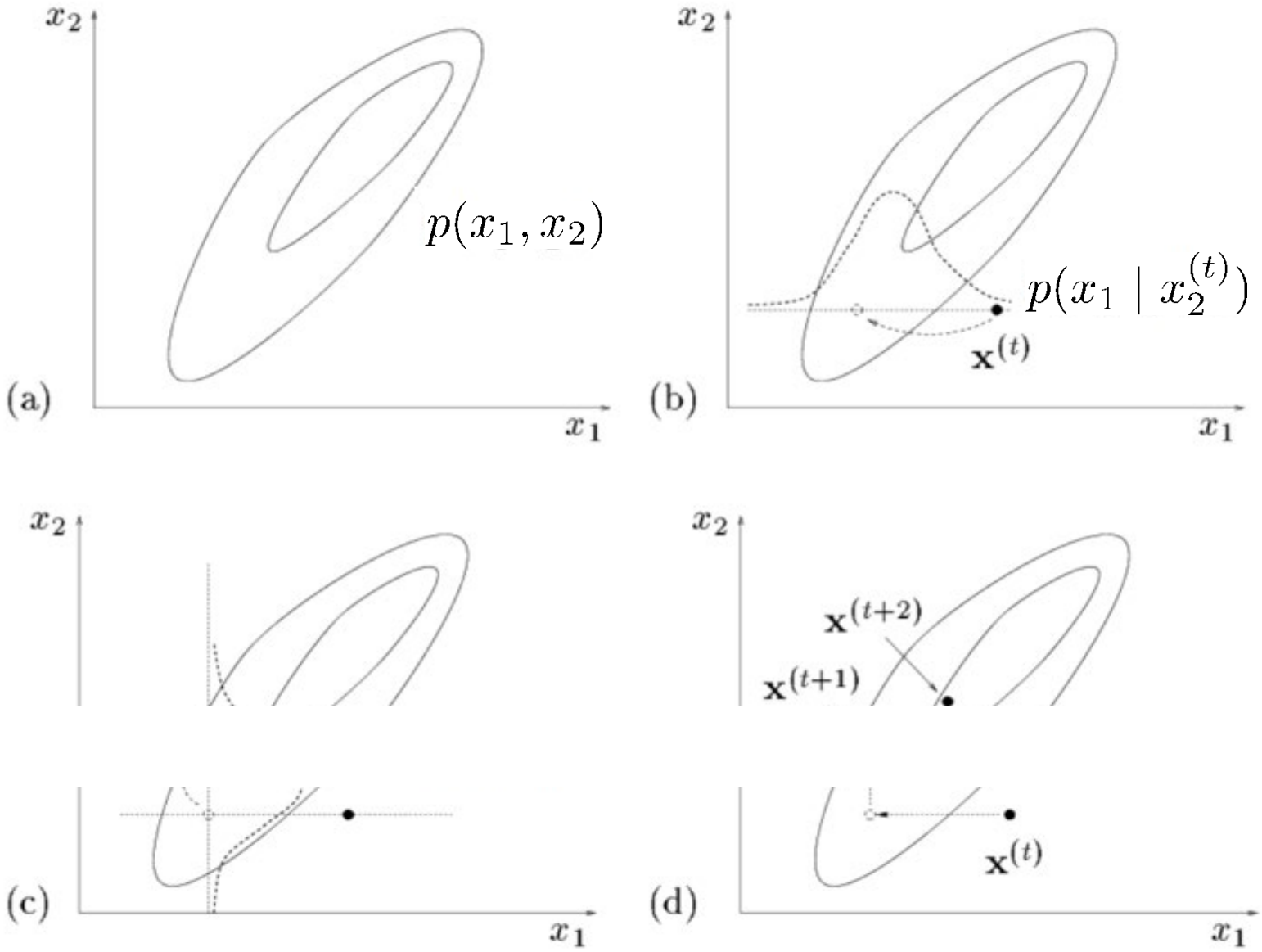
Condition on most recent samples

Gibbs sampling

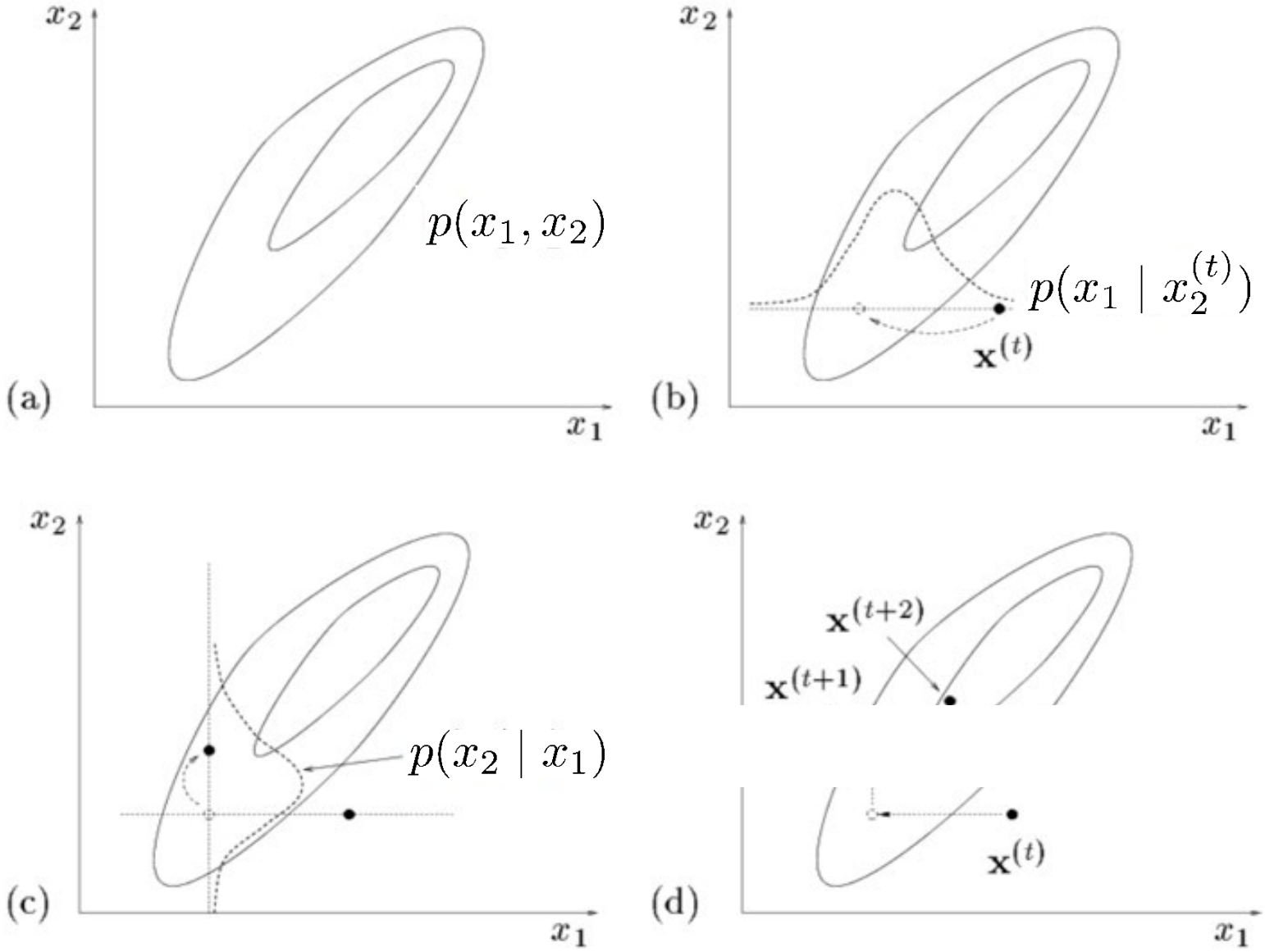
- Gibbs sampling is special case of M-H (but we always accept)
- Unlike M-H we *do not have to choose proposal*
- The proposal distribution will be cycle over $p(z_i \mid z_{\neg i})$
- Transition function T() varies (cycles) over time
  - Relaxation of our assumption used to provide intuition about convergence
  - It still OK because the concatenation of the T() for a cycle converge
- We must be able to compute and sample from $p(z_i \mid z_{\neg i})$
  - This is not always possible in general!
- This is **not** the sample as sampling from the generative model, e.g. Ancestral Sampling in a Bayes Net samples from $p(z_i \mid z_{\mathrm{Pa}(i)})$



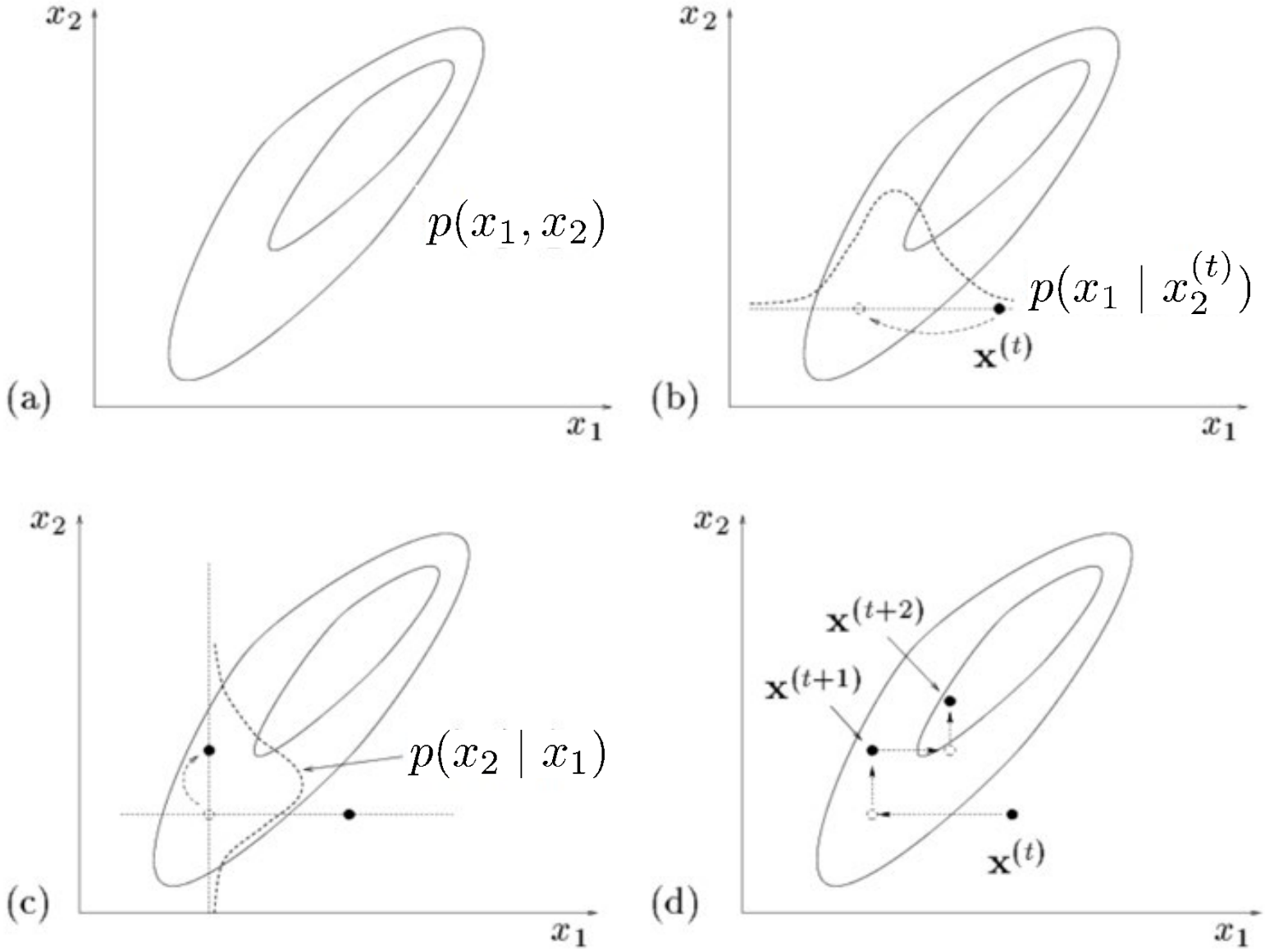
(Source: D. MacKay)



(Source: D. MacKay)



(Source: D. MacKay)



(Source: D. MacKay)

Examples of Gibbs

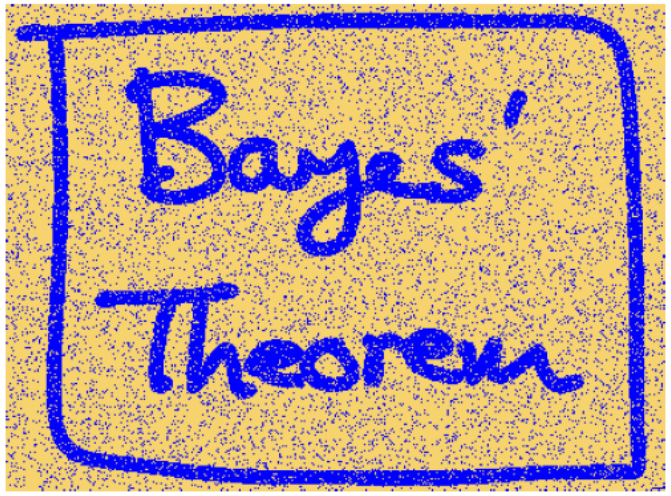
- Gibbs can be very good if one can compute and sample from the complete conditional distributions

- This is often feasible for MRFs of discrete RVs
  - Typical examples include symmetric systems like the Markov random field grids we had for images
  - Complete conditionals only depend on immediate neighboring pixels

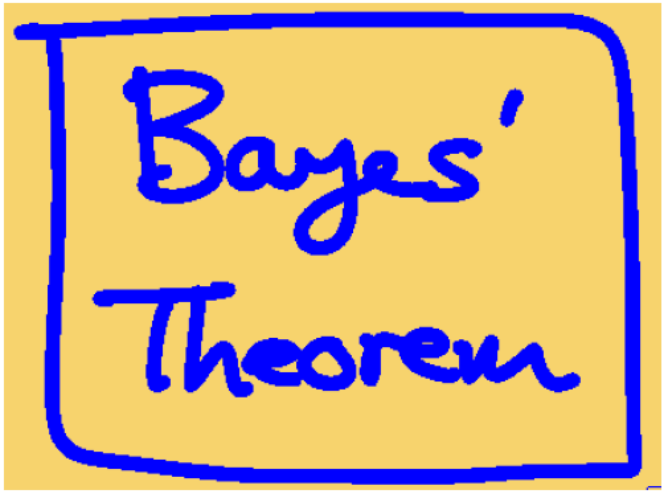
- Continuous models are more complicated, and typically restricted to *exponential family distributions* (we will discuss in the next lecture)

Example: Image Denoising

Noisy Image



Latent Image

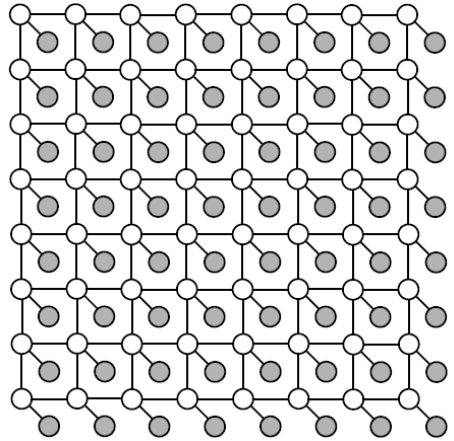


Problem Given observed image corrupted by i.i.d. noise, infer "clean" denoised image.

[Source: Bishop, C. PRML]

Example: Image Denoising

Use a “grid graph” where each pixel is connected to its up/down/left/right neighbors,



$$p(x \mid y) \propto \prod_i \phi_i(x_i, y_i) \prod_{j \in \Gamma(i)} \phi_{ij}(x_i, x_j)$$

Where $x_i, y_i \in \{-1, +1\}$ for convenience

Observation noise

Observation Likelihood: $\log \phi_i(x_i) = \eta x_i y_i$

Pairwise Similarity: $\log \phi_{ij}(x_i, x_j) = \beta x_i x_j$

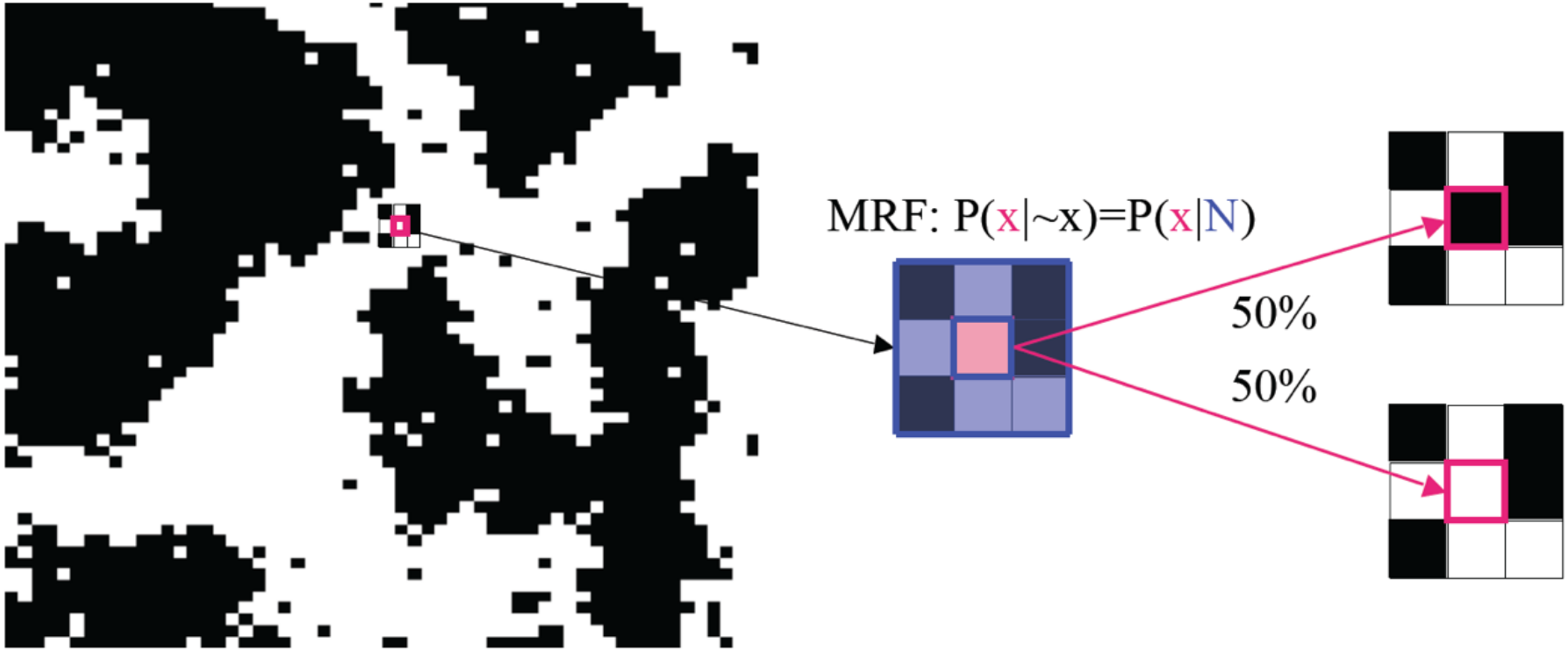
Smoothness prior

Complete conditional only depends on immediate neighbors,

$$p(x_i \mid x_{\neg i}) \propto \phi_i(x_i, y_i) \prod_{j \in \in \Gamma(i)} \phi_{ij}(x_i, x_j)$$

Normalizer only requires summing over 4 neighbors $\mathcal{O}(2^4)$

Examples of Gibbs



(From Dellaert and Zhu tutorial)

Examples of Gibbs

Weak Affinity to Neighbors

Strong Affinity to Neighbors

(From Dellaert and Zhu tutorial)

Gibbs as Metropolis Hastings (M-H)

To see Gibbs as MH, and to understand why we always accept, consider that if it were MH, then our proposal distribution, $q_i()$, for a given variable, i, would be

$$q_i\left(\mathbf{z}^*\middle|\mathbf{z}\right) = p\left(z_i^*\middle|\mathbf{z}_{\backslash \mathrm{i}}\right) \quad \text{and} \quad q_i\left(\mathbf{z}\middle|\mathbf{z}^*\right) = p\left(z_i\middle|\mathbf{z}_{\backslash \mathrm{i}}^*\right)$$

And we have $\mathbf{z}_{\backslash \mathrm{i}}^* = \mathbf{z}_{\backslash \mathrm{i}}$ because only i changes.

The "*" here means next state, NOT stationary state.

Gibbs as M-H

$$\mathrm{A}\left(\mathbf{z}^{*},\mathbf{z}\right)=\min\left[1,\frac{p\left(\mathbf{z}^{*}\right)q_i\left(\mathbf{z}\middle|\mathbf{z}^{*}\right)}{p\left(\mathbf{z}\right)q_i\left(\mathbf{z}^{*}\middle|\mathbf{z}\right)}\right]$$

(def'n of A())

Gibbs as M-H

$$\mathrm{A}\left(\mathbf{z}^*, \mathbf{z}\right) = \min\left(1, \frac{p\left(\mathbf{z}^*\right) q_i\left(\mathbf{z} \middle| \mathbf{z}^*\right)}{p\left(\mathbf{z}\right) q_i\left(\mathbf{z}^* \middle| \mathbf{z}\right)}\right) \qquad \text{(def'n of A())}$$

$$= \min\left(1, \frac{p\left(\mathbf{z}^*_{\setminus i}\right) p\left(z_i^* \middle| \mathbf{z}^*_{\setminus i}\right) q_i\left(\mathbf{z} \middle| \mathbf{z}^*\right)}{p\left(\mathbf{z}_{\setminus i}\right) p\left(z_i \middle| \mathbf{z}_{\setminus i}\right) q_i\left(\mathbf{z}^* \middle| \mathbf{z}\right)}\right) \qquad \textbf{(because?)}$$

Gibbs as M-H

$$\mathrm{A}\left(\mathbf{z}^*, \mathbf{z}\right) = \min\left(1, \frac{p\left(\mathbf{z}^*\right) q_i\left(\mathbf{z} \middle| \mathbf{z}^*\right)}{p\left(\mathbf{z}\right) q_i\left(\mathbf{z}^* \middle| \mathbf{z}\right)}\right)$$

(def'n of A())

$$= \min\left(1, \frac{p\left(\mathbf{z}^*_{\setminus i}\right) p\left(z^*_i \middle| \mathbf{z}^*_{\setminus i}\right) q_i\left(\mathbf{z} \middle| \mathbf{z}^*\right)}{p\left(\mathbf{z}_{\setminus i}\right) p\left(z_i \middle| \mathbf{z}_{\setminus i}\right) q_i\left(\mathbf{z}^* \middle| \mathbf{z}\right)}\right)$$

(def'n of "bar")

$$= \min\left(1, \frac{p\left(\mathbf{z}^*_{\setminus i}\right) p\left(z^*_i \middle| \mathbf{z}^*_{\setminus i}\right) p\left(z_i \middle| \mathbf{z}^*_{\setminus \mathrm{i}}\right)}{p\left(\mathbf{z}_{\setminus i}\right) p\left(z_i \middle| \mathbf{z}_{\setminus i}\right) p\left(z^*_i \middle| \mathbf{z}_{\setminus \mathrm{i}}\right)}\right)$$

(because?)

Gibbs as M-H

$$\mathrm{A}\left(\mathbf{z}^*,\mathbf{z}\right) = \min\left(1, \frac{p\left(\mathbf{z}^*\right) q_i\left(\mathbf{z}\middle|\mathbf{z}^*\right)}{p\left(\mathbf{z}\right) q_i\left(\mathbf{z}^*\middle|\mathbf{z}\right)}\right) \qquad \text{(def'n of A())}$$

$$= \min\left(1, \frac{p\left(\mathbf{z}^*_{\setminus i}\right) p\left(z^*_i\middle|\mathbf{z}^*_{\setminus i}\right) q_i\left(\mathbf{z}\middle|\mathbf{z}^*\right)}{p\left(\mathbf{z}_{\setminus i}\right) p\left(z_i\middle|\mathbf{z}_{\setminus i}\right) q_i\left(\mathbf{z}^*\middle|\mathbf{z}\right)}\right) \qquad \text{(def'n of "bar")}$$

$$= \min\left(1, \frac{p\left(\mathbf{z}^*_{\setminus i}\right) p\left(z^*_i\middle|\mathbf{z}^*_{\setminus i}\right) p\left(z_i\middle|\mathbf{z}^*_{\setminus \mathrm{i}}\right)}{p\left(\mathbf{z}_{\setminus i}\right) p\left(z_i\middle|\mathbf{z}_{\setminus i}\right) p\left(z^*_i\middle|\mathbf{z}_{\setminus \mathrm{i}}\right)}\right) \qquad \text{(Gibbs, coloring)}$$

$$= \min(1,1) \qquad \text{(cancel colors using } \mathbf{z}^*_{\setminus i} = \mathbf{z}_{\setminus i} \text{ , as only } z_i \text{ changes)}$$

$$= 1$$

Gibbs Sampling Extensions

Standard Gibbs suffers same random walk behavior as M-H
(but no adjustable parameters, so that's a plus…)

Block Gibbs Jointly sample subset $S \subset \mathcal{V}$ from $p(x_S \mid x_{\neg S})$

- Reduces random walk caused by highly correlated variables
- Requires that conditional $p(x_S \mid x_{\neg S})$ can be sampled efficiently

Collapsed Gibbs Marginalize some variables out of joint:

$$p(x_{\mathcal{V} \setminus S}) = \int p(x) dx_S$$

- Reduces dimensionality of space to be sampled
- Requires that marginals are computable in closed-form

Combined samplers

Different samplers fail in different ways, so combine them…

1. Initialise $x^{(0)}$.
2. For $i = 0$ to $N - 1$
   - Sample $u \sim \mathcal{U}_{[0,1]}$.
   - If $u < \nu$

     Apply the MH algorithm with a global proposal.
   - else

     Apply the MH algorithm with a random walk proposal.

…can also combine with Gibbs proposals

Mixing MCMC Kernels

Can do this more generally….

Consider a set of MCMC kernels $T_1, T_2, \ldots, T_K$ all having target distribution p(x) then the mixture:

$$T = \sum_{k=1}^{K} \pi_k T_k$$

Mixing weights

Is a valid MCMC kernel with target distribution p(x)

Mixture MCMC Transition kernel given by:

1. Sample $k \sim \pi$
2. Sample $x^{(t+1)} \sim T_k(x \mid x^{(t)})$

Inference (and related) Tasks

- Simulation: $x \sim p(x) = \frac{1}{Z} f(x)$
- Compute expectations: $\mathbb{E}[\phi(x)] = \int p(x)\phi(x)\, dx$
- Optimization: $x^* = \arg\max_x f(x)$
- Compute normalizer: $Z = \int f(x)\, dx$

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Simulated Annealing

- Analogy with physical systems
- Relevant for optimization (not integration)
- Powers of probability distributions emphasize the peaks
- If we are looking for a maximum within a lot of distracting peaks, this can help.

Simulated Annealing

- Define a temperature T, and a cooling schedule (black magic part)
- Lower temperatures correspond to emphasized maximal peaks.
  - Hence we exponentiate by (1/T).
- The terminology makes sense because the number of states accessible to a physical system decreases with temperature.

Simulated Annealing

1. Initialise $x^{(0)}$ and set $T_0 = 1$.
2. For $i = 0$ to $N - 1$
   - Sample $u \sim \mathcal{U}_{[0,1]}$.
   - Sample $x^\star \sim q(x^\star | x^{(i)})$.
   - If $u < \mathcal{A}(x^{(i)}, x^\star) = \min\left\{1, \frac{p^{\frac{1}{T_i}}(x^\star) q(x^{(i)}|x^\star)}{p^{\frac{1}{T_i}}(x^{(i)}) q(x^\star|x^{(i)})}\right\}$

     $$x^{(i+1)} = x^\star$$

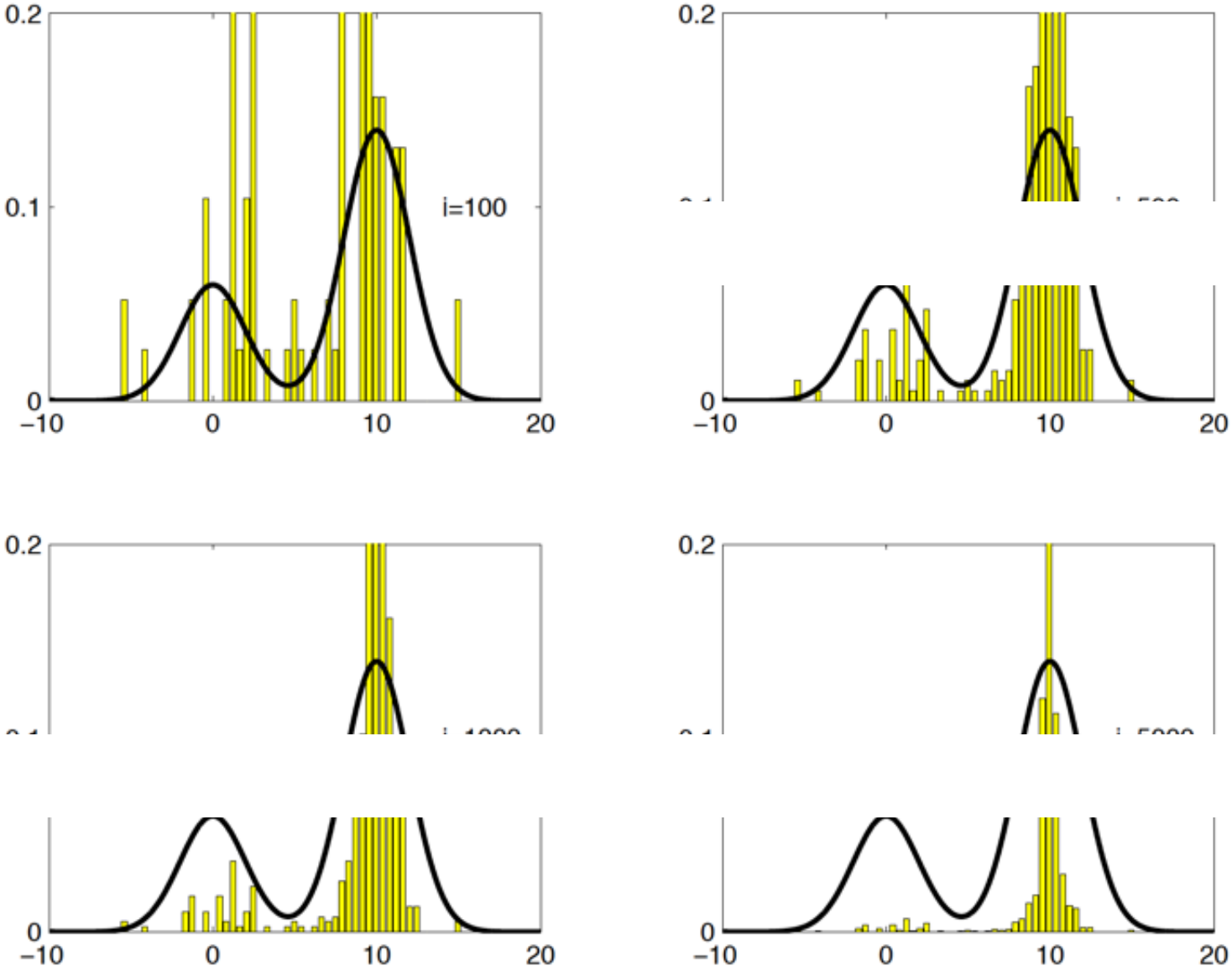
     else

     $$x^{(i+1)} = x^{(i)}$$

   - Set T_{i+1} according to a chosen cooling schedule.

Basically M-H but we are *annealing* target distribution with temperature T

(From Andrieu et al)



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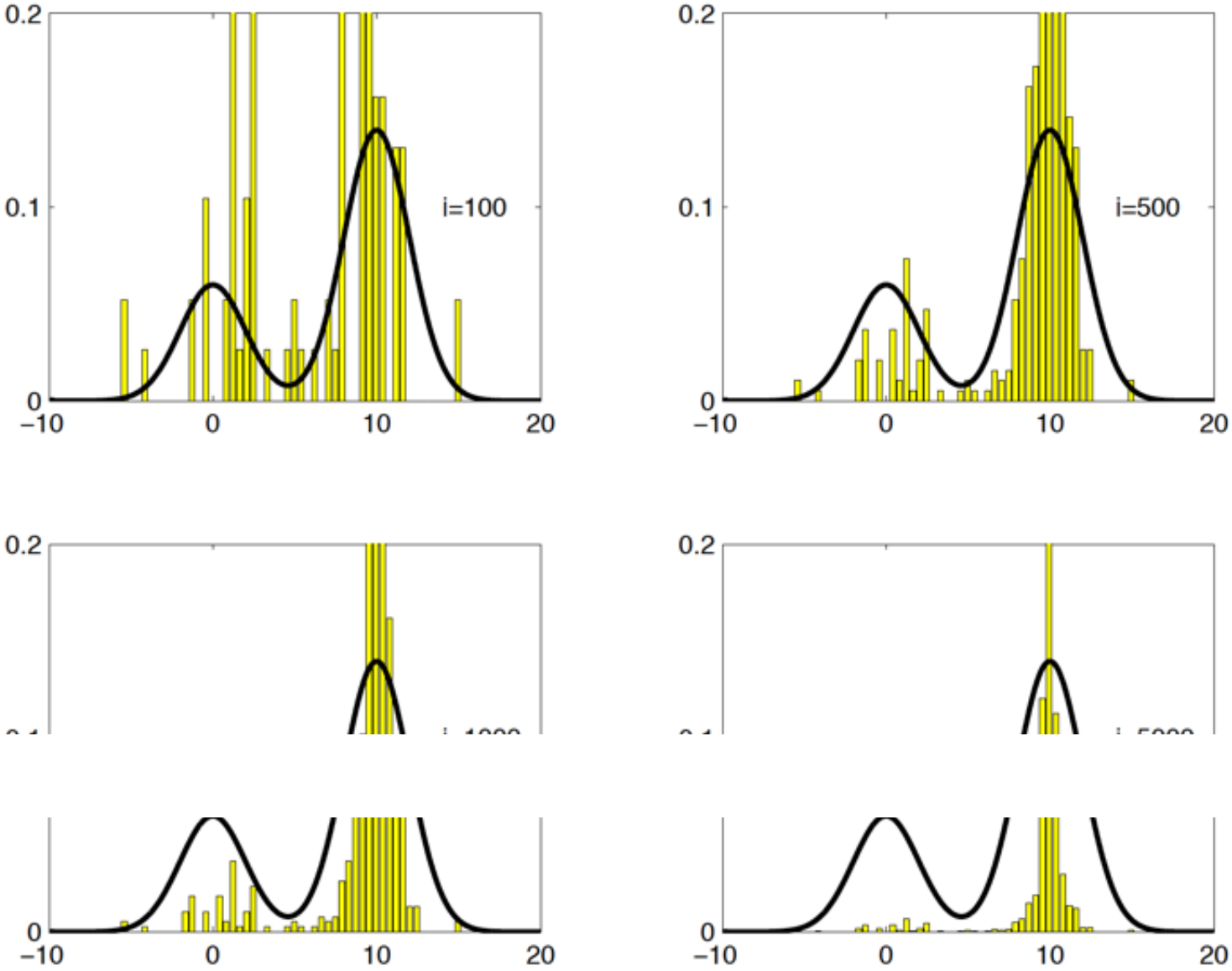

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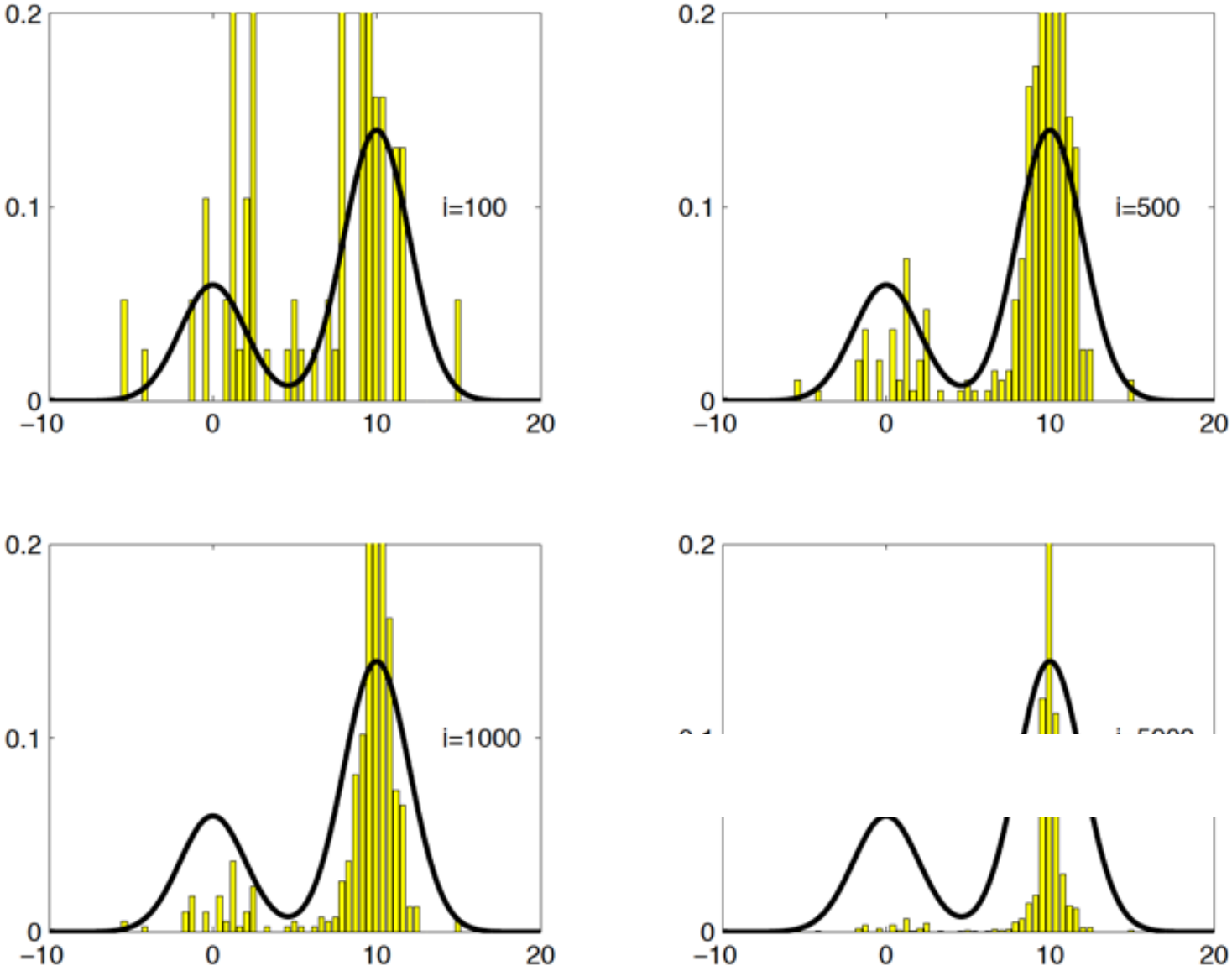

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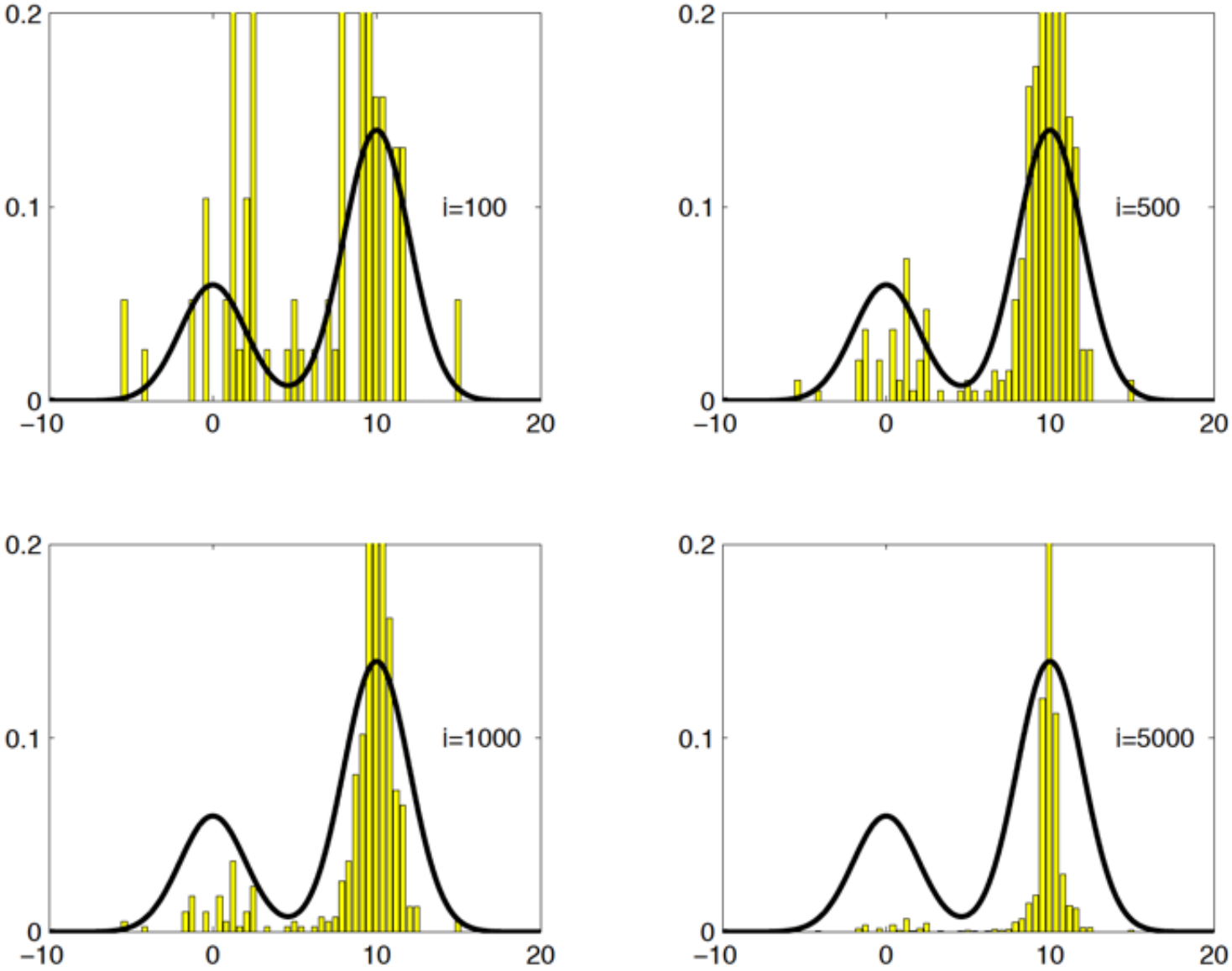


(From Andrieu et al)

Simulated Annealing

Let *annealing distribution* at temp τ be given by:

$$p_\tau(x) \propto (f(x))^{1/\tau}$$

As $\tau \to 0$ we have:

$$\lim_{\tau \to 0} p_\tau(x) = \delta(x^*) \qquad \text{where} \qquad x^* = \arg\max_x f(x)$$

Simulated Annealing (SA) for Global Optimization:
Annealing schedule $\tau_0 \geq \ldots \geq \tau_t \geq \ldots \geq 0$

1. Sample $x^{(t)}$ from MCMC kernel T_t with target $p_{\tau_t}(x)$
2. Set τ_{t+1} according to annealing schedule

SA for Convergence: $\tau_0 \geq \ldots \geq 1$ Final temperature = 1

MCMC Summary

- Markov chain induced by MCMC transition kernel T(z,z')
- Converges to stationary distribution iff chain is **ergodic**
  - Chain is ergodic if it is **irreducible** (can get from any z to any z') and **aperiodic** (doesn't get trapped in cycles)
- Easier to prove **detailed balance,** which implies ergodicity

$$p(z)T(z,z') = p(z')T(z',z)$$

- Metropolis algorithm samples from symmetric proposal q(z'|z) and accepts sample z' with probability,

$$A = \min\left(1, \frac{\widetilde{p}(z')}{\widetilde{p}(z)}\right)$$

MCMC Summary

- Metropolis-Hastings allows non-symmetric proposal q(z'|z) and accepts sample z' with probability,

$$A = \min\left(1, \frac{\widetilde{p}(z')}{\widetilde{p}(z)} \frac{q(z \mid z')}{q(z' \mid z)}\right)$$

- Gibbs sampler on random vector $z = (z_1, \ldots, z_d)^T$ successively samples from *complete conditionals*,

$$\begin{aligned}
z_1^{\text{new}} &\sim p(z_1 \mid z_2^{\text{old}}, \ldots, z_d^{\text{old}}) \\
z_2^{\text{new}} &\sim p(z_2 \mid z_1^{\text{new}}, z_3^{\text{old}}, \ldots, z_d^{\text{old}}) \\
&\cdots \\
z_d^{\text{new}} &\sim p(z_d \mid z_1^{\text{new}}, \ldots, z_{d-1}^{\text{new}})
\end{aligned}$$

- Gibbs is instance of M-H which *always accepts*

MCMC Summary

- Simulated annealing adjusts target distribution at each stage with temperature T

$$(p(z))^{\frac{1}{T_i}}$$

- For decreasing temperatures $\lim T_i \to 0$ support of target approaches set of global maximizers
  - Convenient to use for global maximization
  - Can prove that this will find the global maximum in the limit (need to wait for the heat death of the universe, however…)
- For increasing temp ending at $\lim T_i \to 1$ approaches $p(x)$
  - Helps avoid getting stuck in local optima

Monte Carlo Methods Summary

- Simulation: $x \sim p(x) = \frac{1}{Z} f(x)$ **Rejection sampling, MCMC**
- Compute expectations: $\mathbb{E}[\phi(x)] = \int p(x)\phi(x)\, dx$ **Importance sampling or any simulation method**
- Optimization: $x^* = \arg\max_x f(x)$ **Simulated annealing**
- Compute normalizer / marginal likelihood: $Z = \int f(x)\, dx$ **Reverse importance sampling (Did not cover)**

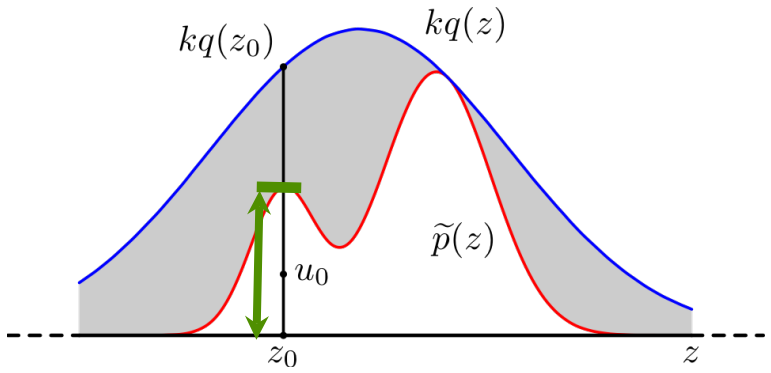
Monte Carlo Methods Summary

- In complex models we often have no other choice than to simulate realizations

- Rejection sampler choose proposal/constant s.t. $\widetilde{p}(z) \leq kq(z)$

1) Sample $q(z)$

2) Keep samples in proportion to $\dfrac{\tilde{p}(z)}{k \bullet q(z)}$ and reject the rest.



- Monte carlo estimate via independent samples $\{z^{(i)}\}_{i=1}^{L} \sim p$,

$$\mathbf{E}_p[f] \approx \frac{1}{L} \sum_{i=1}^{L} f(z^{(i)})$$

- Unbiased
- Consistent
- Law of large numbers
- Central limit theorem (if f is finite variance)

Monte Carlo Methods Summary

- Importance sampling estimate over samples $\{z^{(i)}\}_{i=1}^{L} \sim q$,

$$\mathbf{E}_p[f] \approx \sum_{i=1}^{L} w^{(i)} f(z^{(i)})$$

$$w^{(i)} \propto \frac{\widetilde{p}(z^{(i)})}{q(z^{(i)})}$$

Proposal

Importance Weights

- Avoids simulation of *p(z)* but variance scales exponentially with dim.
- Sequential importance sampling extends IS for sequence models, with proposal given by dynamics,

$$q(z) = q(z_0) \prod_{t=1}^{T} p(z_t \mid z_{t-1})$$

"Bootstrap" Particle Filter

$$w_t(z^{(i)}) \propto w_{t-1}(z^{(i-1)}) p(y_t \mid z_t^{(i)})$$

Recursively update weights

- **Resampling** step necessary to avoid weight degeneracy

Monte Carlo Methods Summary

- Lots of other methods to explore…
  - Hamiltonian Monte Carlo
  - Slice Sampling
  - Reversible Jump MCMC (and other *transdimensional samplers*)
  - Parallel Tempering

- Some good resources if you are interested…

Neal, R. “Probabilistic Inference Using Markov Chain Monte Carlo Methods”, U. Toronto, 1993
MacKay, D. J. “Introduction to Monte Carlo Methods”, Cambridge U., 1998
Andrieu, C., et al., “Introduction to MCMC for Machine Learning”, 2001