

BIOS 731

Advanced Statistical Computing

Fall 2020

Lecture 12

Introduction to SMC

Steve Qin

Metropolis-Hastings Algorithm

- Start with any $X^{(0)}=x_0$, and a “*proposal chain*” $T(x,y)$
- Suppose $X^{(t)}=x_t$. At time $t+1$,
 - **Draw** $y \sim T(x_t, y)$ (i.e., propose a move for the next step)
 - Compute “*goodness ratio*”

$$r = \frac{\pi(y)T(y, x_t)}{\pi(x_t)T(x_t, y)}$$
 - **Acceptance/Rejection decision:** Let

$$X^{(t+1)} = \begin{cases} y, & \text{with } p = \min\{1, r\} \\ x_t, & \text{with } 1 - p \end{cases}$$

Remarks

- How to choose a good proposal function is crucial.
- Sometimes tuning is needed.
 - Rule of thumb: 30% acceptance rate
- Convergence is slow for high dimensional cases.

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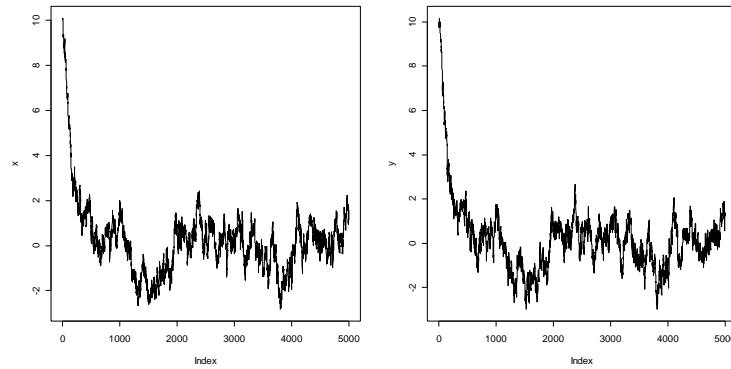
Summary on M-H algorithm

- Needs to know the density function of the target distribution (not necessarily to be complete)
- Up to a normalizing constant
- Easy to implement, ideal for homogeneous set of parameters (not too many).
- Require burn-in
- Monitor convergence

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Convergence

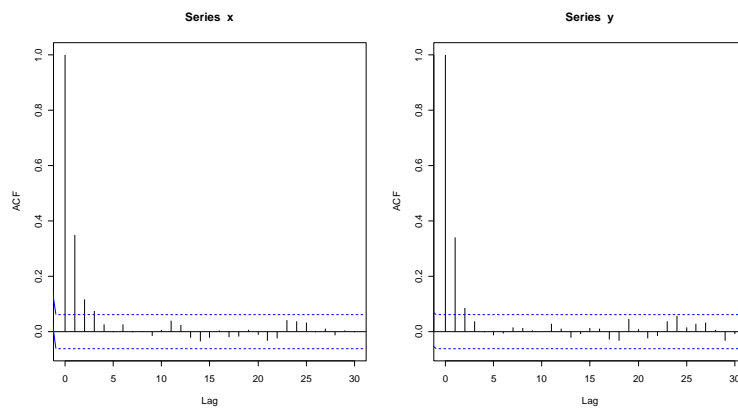
- Trace plot



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Convergence

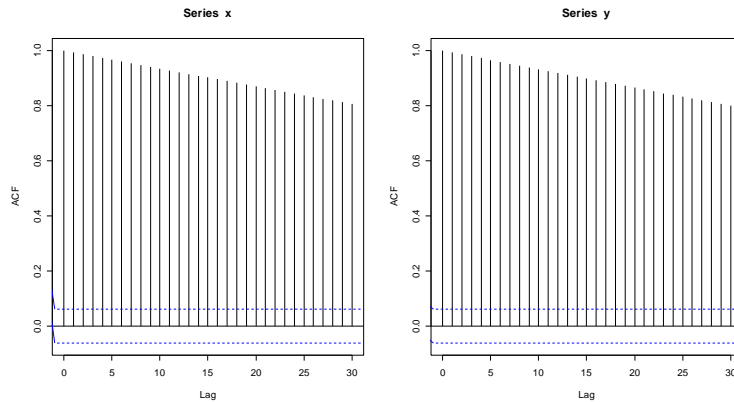
- Autocorrelation plot Good



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Convergence

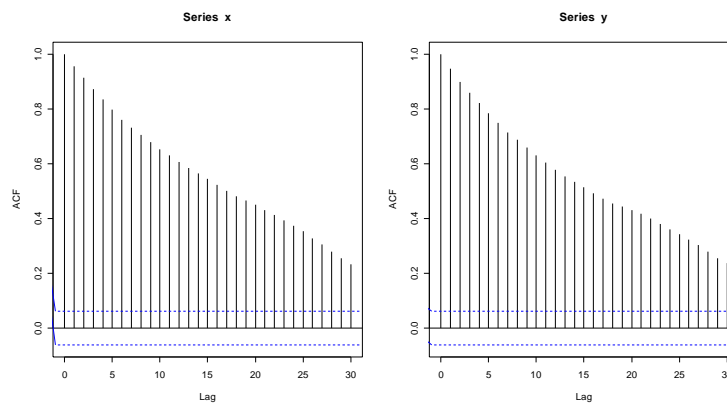
- Autocorrelation plot Bad $s = 0.5$



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Convergence

- Autocorrelation plot Okay $s = 3.0$



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References

- Metropolis et al. 1953,
- Hastings 1973,
- Tutorial paper:
Chib and Greenberg (1995). Understanding the Metropolis--Hastings Algorithm. *The American Statistician* **49**, 327-335.

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Gibbs Sampler

- **Purpose:** Draw random samples from a joint distribution (high dimensional)

$$x = (x_1, x_2, \dots, x_n) \text{ Target } \pi(x)$$

- **Method:** Iterative conditional sampling

$$\forall i, \text{ draw } x_i \sim \pi(x_i | x_{[-i]})$$

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Illustration of Gibbs Sampler

- Suppose the **target distribution is:**

$$(X, Y) \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$$

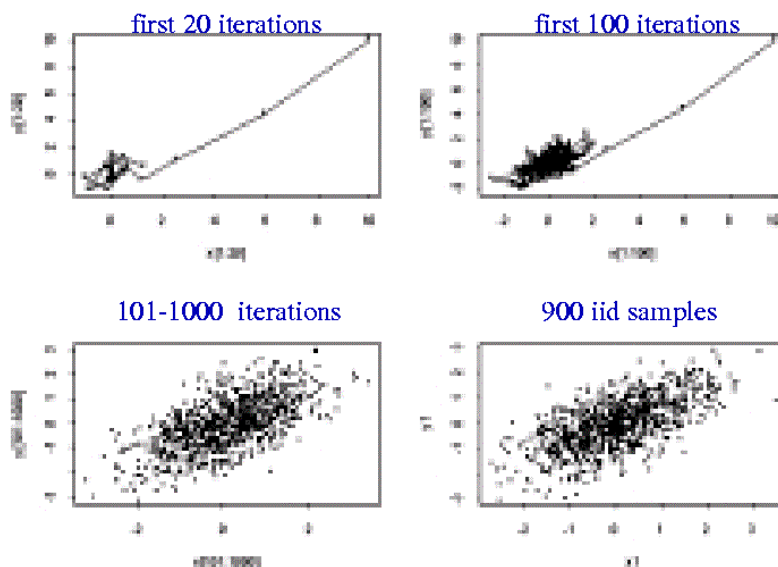
- Gibbs sampler:**

$$[X|Y = y] \sim N(\rho y, 1 - \rho^2)$$

$$[Y|X = x] \sim N(\rho x, 1 - \rho^2)$$

Start from, say, $(X, Y) = (10, 10)$, we can take a look at the trajectories. We took $\rho = 0.6$.

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References

- Geman and Geman 1984,
- Gelfand and Smith 1990,
- Tutorial paper:
Casella and George (1992). Explaining the Gibbs sampler. *The American Statistician*, **46**, 167-174.

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Summary of Gibbs sampler

- Special case of MH algorithm
- The most popular MCMC method, generally more efficient than MH.
- Require some mathematical derivation.
- Verify convergence of the sequence
- Require burn in.
- Use multiple chains
- Be careful of *pseudo* Gibbs sampler!

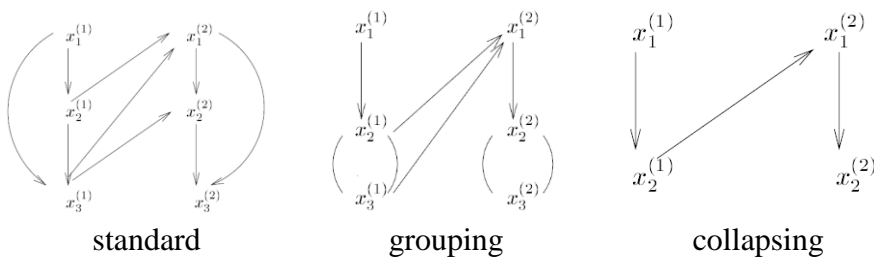
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Collapsing and grouping

- Want to sample from $\mathbf{X} = (x_1, x_2, \dots, x_d)$
- Regular Gibbs sampler:
 - Sample $x_1^{(t+1)}$ from $\pi(x_1^{(t+1)} \mid x_2^{(t)}, x_3^{(t)}, \dots, x_d^{(t)})$,
 - Sample $x_2^{(t+1)}$ from $\pi(x_2^{(t+1)} \mid x_1^{(t)}, x_3^{(t)}, \dots, x_d^{(t)})$,
 - ...
 - Sample $x_d^{(t+1)}$ from $\pi(x_d^{(t+1)} \mid x_2^{(t)}, x_3^{(t)}, \dots, x_{d-1}^{(t)})$,
- Alternatively:
 - Grouping: $\mathbf{x}_{d-1}' = (x_{d-1}, x_d)$.
 - Collapsing, i.e., integrate out x_d : $\mathbf{X}^- = (x_1, x_2, \dots, x_{d-1})$

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The three-schemes



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Examples

- Murray's data
- Bivariate Gaussian with mean 0 and unknown covariance matrix Σ

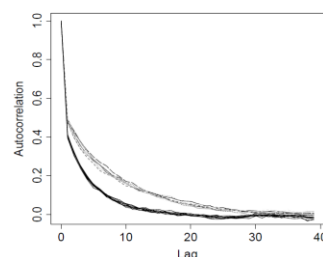
1	1	-1	-1	2	2	-2	-2	*	*	*	*
1	-1	1	-1	*	*	*	*	2	2	-2	-2

standard

$$\Sigma \mid y_{obs}, y_{mis}, \\ y_{mis} \mid y_{obs}, \Sigma.$$

collapsing

$$y_{mis,i} \mid y_{obs}, y_{mis,[-i]}.$$



Remarks

- Avoid introducing unnecessary parameters into a Gibbs sampler,
- Do as much analytical work as possible,
- However, introducing some clever auxiliary variables can greatly improve computation efficiency.

An example

Design a Gibbs Sampler:

$$- x|y \sim N(y, 1) ,$$

$$- y|x \sim N(x, 1) .$$

```
n <- 1000
x <- rep(NA,n)
y <- rep(NA,n)
x[1] <- 0
y[1] <- 0
for(i in 1:(n-1)) {
  x[i+1] <- rnorm(1,y[i],1)
  y[i+1] <- rnorm(1,x[i+1],1)
}
plot(x,y)
```

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- Doesn't seem to converge.
- Unable to find a joint distribution $F(X,Y)$ satisfies
 - $x|y \sim N(y, 1) ,$
 - $y|x \sim N(x, 1) .$

Pseudo Gibbs Sampler

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Convergence Diagnostics

Patrick Lam

Within Chain Variance

$$W = \frac{1}{m} \sum_{j=1}^m s_j^2$$

where

$$s_j^2 = \frac{1}{n-1} \sum_{i=1}^n (\theta_{ij} - \bar{\theta}_j)^2$$

s_j^2 is just the formula for the variance of the j th chain. W is then just the mean of the variances of each chain.

W likely underestimates the true variance of the stationary distribution since our chains have probably not reached all the points of the stationary distribution.

Between Chain Variance

$$B = \frac{n}{m-1} \sum_{j=1}^m (\bar{\theta}_j - \bar{\bar{\theta}})^2$$

where

$$\bar{\bar{\theta}} = \frac{1}{m} \sum_{j=1}^m \bar{\theta}_j$$

This is the variance of the chain means multiplied by n because each chain is based on n draws.

Estimated Variance

We can then estimate the variance of the stationary distribution as a weighted average of W and B .

$$\hat{\text{Var}}(\theta) = \left(1 - \frac{1}{n}\right)W + \frac{1}{n}B$$

Because of overdispersion of the starting values, this overestimates the true variance, but is unbiased if the starting distribution equals the stationary distribution (if starting values were not overdispersed).

Gelman and Rubin Multiple Sequence Diagnostic

Steps (for each parameter):

1. Run $m \geq 2$ chains of length $2n$ from overdispersed starting values.
2. Discard the first n draws in each chain.
3. Calculate the within-chain and between-chain variance.
4. Calculate the estimated variance of the parameter as a weighted sum of the within-chain and between-chain variance.
5. Calculate the potential scale reduction factor.

Potential Scale Reduction Factor

The potential scale reduction factor is

$$\hat{R} = \sqrt{\frac{\hat{\text{Var}}(\theta)}{W}}$$

When \hat{R} is high (perhaps greater than 1.1 or 1.2), then we should run our chains out longer to improve convergence to the stationary distribution.

If we have more than one parameter, then we need to calculate the potential scale reduction factor for each parameter.

We should run our chains out long enough so that all the potential scale reduction factors are small enough.

We can then combine the mn total draws from our chains to produce one chain from the stationary distribution.

Sequential Monte Carlo

Accept-reject method

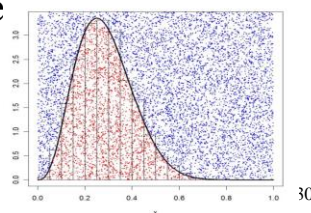
- The accept-reject method
 1. Generate $X \sim g$, $U \sim \text{Uniform}(0,1)$,
 2. Accept $Y = X$ if $U \leq f(X)/Mg(X)$,
 3. Repeat.

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Accept-reject method example

- *Beta* (α, β) , $\alpha \geq 1$, $\beta \geq 1$,
 simulate $Y \sim \text{Uniform}(0,1)$ and
 $U \sim \text{Uniform}(0,m)$,
 m is the max of the Beta density.
 select $X = Y$ if under curve

what is the acceptance rate?



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Importance sampling

- A variance reduction technique.
- Certain values of the input random variables have more impact on the parameter being estimated than others.
- If these "important" values are emphasized by sampling more frequently, then the estimator variance can be reduced.
- Marshall (1956) suggested that one should focus on the region(s) of "importance" so as to save computational resource.
- Essential in high-dimensional models.

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Importance sampling

- *Importance sampling:*

to evaluate $E_f[h(X)] = \int h(x)f(x)dx$

based on generating a sample X_1, \dots, X_n from a given distribution g and approximating

$$E_f[h(X)] \approx \frac{1}{m} \sum_{j=1}^m \frac{f(X_j)}{g(X_j)} h(X_j)$$

which is based on

$$E_f[h(X)] = \int_{\mathbb{R}^n} h(x) \frac{f(x)}{g(x)} g(x) dx$$

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The algorithm

- To evaluate $\mu = E_{\pi}[h(X)] = \int h(x)\pi(x)dx$.
 - Draw $x^{(1)}, \dots, x^{(m)}$ from a trial distribution $g()$.
 - Calculate the *importance weight*

$$w^{(j)} = \pi(x^{(j)} / g(x^{(j)})), \quad \text{for } j=1, \dots, m.$$
 - Approximate μ by $\hat{\mu} = \frac{w^{(1)}h(x^{(1)}) + \dots + w^{(m)}h(x^{(m)})}{w^{(1)} + \dots + w^{(m)}}.$
- Remark: $\hat{\mu}$ is better than the unbiased estimator $\tilde{\mu} = \frac{1}{m} \{w^{(1)}h(x^{(1)}) + \dots + w^{(m)}h(x^{(m)})\}.$
why?

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The basic methodology of importance sampling

- To choose a distribution which "encourages" the important values.
- This use of "biased" distributions will result in a biased estimator if it is applied directly.
- Weight to correct for the use of the biased distribution to ensure unbiasedness.
- The weight is given by the likelihood ratio,

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Importance sampling example

- Small tail probabilities:

$$Z \sim N(0,1), P(Z > 4.5)$$

naïve: simulate $Z_i \sim N(0,1), i=1, \dots, M$.

calculate

$$P(Z > 4.5) \approx \frac{1}{M} \sum_{i=1}^M I(Z_i > 4.5)$$

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Importance sampling example

Let $Y \sim TExp(4.5, 1)$ with density

$$f_Y(y) = e^{-(y-4.5)} / \int_{4.5}^{\infty} e^{-x} dx.$$

Now simulated from f_Y and use importance sampling, we obtain

$$P(Z > 4.5) \approx \frac{1}{M} \sum_{i=1}^M \frac{\varphi(Y_i)}{f_Y(Y_i)} I(Y_i > 4.5) = .000003377.$$

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Importance sampling example

```
## theoretical value
p0=1-pnorm(4.5)
## sample directly from normal distribution
## this needs large number of samples
z=rnorm(10000000)
p1=mean(z>4.5)

## importance sampling
n0=10000
Y=rexp(n0, 1)+4.5
a=dnorm(Y)/dexp(Y-4.5)
p2=mean(a[Y>4.5])

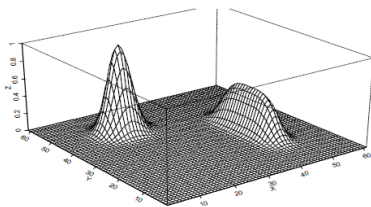
c(p0, p1, p2) ##
[1] 3.397673e-06 2.600000e-06 3.418534e-06
```

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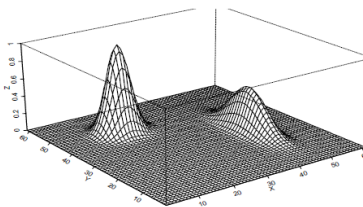
Another example

$$f(x, y) = 0.5e^{-90(x-0.5)^2-45(y+0.1)^4} + e^{-45(x+0.4)^2-60(y-0.5)^2}$$

(a)



(b)



- Both grid-point method and vanilla Monte Carlo methods wasted resources on “boring” desert area.

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Another example

- Use proposal function

$$g(x, y) \propto 0.5e^{-90(x-0.5)^2-10(y+0.1)^2} + e^{-45(x+0.4)^2-60(y-0.5)^2},$$

with $(x, y) \in [-1, 1] \times [-1, 1]$, a truncated mixture of bivariate Gaussian

$$0.46\mathcal{N}\left[\begin{pmatrix} 0.5 \\ -0.1 \end{pmatrix}, \begin{pmatrix} \frac{1}{180} & 0 \\ 0 & \frac{1}{20} \end{pmatrix}\right] + 0.54\mathcal{N}\left[\begin{pmatrix} -0.4 \\ 0.5 \end{pmatrix}, \begin{pmatrix} \frac{1}{90} & 0 \\ 0 & \frac{1}{120} \end{pmatrix}\right]$$

Vanilla Monte Carlo

$$\hat{\mu} = 0.1307$$

$$\text{std}(\hat{\mu}) = 0.009$$

Importance Sampling

$$\hat{\mu} = 0.1259$$

$$\text{std}(\hat{\mu}) = 0.0005$$

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Sequential importance sampling

- For high dimensional problem, how to design trial distribution is challenging.
- Suppose the target density of $\mathbf{x} = (x_1, x_2, \dots, x_d)$ can be decomposed as

$$\pi(\mathbf{x}) = \pi(x_1)\pi(x_2 | x_1) \cdots \pi(x_d | x_1, \dots, x_{d-1})$$

then constructed trial density as

$$g(\mathbf{x}) = g_1(x_1)g_2(x_2 | x_1) \cdots g_d(x_d | x_1, \dots, x_{d-1})$$

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Sequential importance sampling

$$w(\mathbf{x}) = \frac{\pi(x_1)\pi(x_2 | x_1) \cdots \pi(x_d | x_1, \dots, x_{d-1})}{g_1(x_1)g_2(x_2 | x_1) \cdots g_d(x_d | x_1, \dots, x_{d-1})}$$

Suggest a recursive way of computing and monitoring importance weight. Denote

$$\mathbf{x}_t = (x_1, x_2, \dots, x_t)$$

then we have

$$w_t(\mathbf{x}_t) = w_{t-1}(\mathbf{x}_{t-1}) \frac{\pi(x_t | \mathbf{x}_{t-1})}{g_t(x_t | \mathbf{x}_{t-1})}$$

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Sequential importance sampling

- Advantages of the recursion scheme
 - Can stop generating further components of \mathbf{x} if the partial weight is too small.
 - Can take advantage of $\pi(x_t | \mathbf{x}_{t-1})$ in designing $g_t(x_t | \mathbf{x}_{t-1})$
- However, the scheme is impractical since requires the knowledge of marginal distribution $\pi(\mathbf{x}_t)$.

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Sequential importance sampling

- Add another layer of complexity:
- Introduce a sequence of “auxiliary distributions” $\pi_1(x_1)\pi_2(\mathbf{x}_2)\pi_d(\mathbf{x})$ such that $\pi_t(\mathbf{x}_t)$ is a reasonable approximation of the marginal distribution $\pi(\mathbf{x}_t)$, for $t = 1, \dots, d-1$ and $\pi_d = \pi$.
- Note the π_d are only required to be known up to a normalizing constant.

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The SIS procedure

For $t = 2, \dots, d$,

- Draw $X_t = x_t$ from $g_t(x_t | x_{t-1})$, and let $\mathbf{x}_t = (\mathbf{x}_{t-1}, x_t)$
- Compute $u_t = \frac{\pi_t(\mathbf{x}_t)}{\pi_{t-1}(\mathbf{x}_{t-1}) g_t(x_t | \mathbf{x}_{t-1})}$ and let $w_t = w_{t-1} u_t$
- u_t : incremental weight.
- The key idea is to break a difficult task into manageable pieces.
- If w_t is getting too small, reject.

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An application example of SIS

- Assume
 - Constant population size N ,
 - Evolve in non-overlapping generation,
 - The chromosomal region is sufficiently small,
 - No recombination,
 - “haplotype”: each chromosome only has one parent.

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Population genetics example

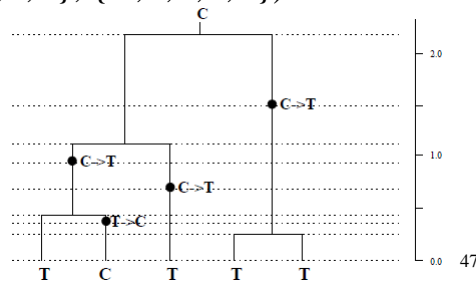
- Notation:
 - E : set of all possible genetic types,
 - μ : mutation rate per chromosome per generation,
 - $P = (P_{\alpha\beta})$: the mutation transition matrix,
 - If a parental segment of type $\alpha \in E$,

its progeny is $\begin{cases} \alpha & \text{with prob. } 1 - \mu, \\ \beta & \text{with prob. } \mu P_{\alpha\beta}. \end{cases}$

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Example data

- From Stephens and Donnelly (2000)
- $E = \{C, T\}$
- The history $H = (H_{-k}, H_{-(k-1)}, \dots, H_{-1}, H_0)$
 $= (\{C\}, \{C, C\}, \{C, T\}, \{C, C, T\}, \{C, T, T\}, \{T, T, T\},$
 $\{T, T, T, T\}, \{C, T, T, T, T\}, \{C, T, T, T, T\})$



Coalescence example

- Use $H = (H_{-m}, \dots, H_{-1}, H_0)$ to denote the whole ancestral history (unobserved) of the 5 individuals.
- Compute the likelihood function

$$p_{\theta}(H) = p_{\theta}(H_{-k}) p_{\theta}(H_{-k+1} | H_{-k}) \cdots p_{\theta}(H_0 | H_{-1}) p_{\theta}(\text{stop} | H_0)$$

$p_{\theta}(H_{-k}) = \pi_0(H_{-k})$ π_0 is the stationary distribution of P .

$$p_{\theta}(H_i | H_{i-1}) = \begin{cases} \frac{n_{\alpha}}{n} \frac{\theta}{n-1+\theta} P_{\alpha\beta} & \text{if } H_i = H_{i-1} - \alpha + \beta \\ \frac{n_{\alpha}}{n} \frac{n-1}{n-1+\theta} & \text{if } H_i = H_{i-1} + \alpha \\ 0 & \text{otherwise,} \end{cases}$$

Coalescence calculation

- For $i = -(k-1), \dots, 0$

$$p_{\theta}(H_i | H_{i-1}) = \begin{cases} \frac{n_{\alpha}}{n} \frac{\theta}{n-1+\theta} P_{\alpha\beta} & \text{if } H_i = H_{i-1} - \alpha + \beta \\ \frac{n_{\alpha}}{n} \frac{n-1}{n-1+\theta} & \text{if } H_i = H_{i-1} + \alpha \\ 0 & \text{otherwise,} \end{cases}$$

$$p_{\theta}(\text{stop} | H_0) = \sum_{\alpha} \frac{n_{\alpha}}{n} \frac{n-1}{n-1+\theta}.$$

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Notations

- n is the sample size at generation H_{i-1}
- n_{α} is the number of chromosome of type α in the sample.
- $\theta = 2N\mu/\nu$.
- N population size.
- ν^2 is the variance of the number of progeny of a random chromosome.

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Strategies to estimate θ

- To get MLE, we need to compute likelihood

$$p_{\theta}(H_0) = \sum_{\mathcal{H}: \text{compatible with } H_0} p_{\theta}(\mathcal{H}).$$

- Naïve Monte Carlo won't work because of compatibility issue.
- An alternative is to simulate \mathbf{H} backward starting from H_0 and use weight to correct bias.

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An SIS approach

- Simulate H_{-1}, H_{-1}, \dots , from a trial distribution built up sequentially by revering the forward sampling probability at a fixed θ_0 . That is, for $i=1, \dots, k$, we have

$$g_i(H_{-i} | H_{-i+1}) = \frac{p_{\theta_0}(H_{-i} | H_{-i+1})}{\sum_{\text{all } H'_{-i}} p_{\theta_0}(H_{-i} | H'_{-i+1})},$$

the final trial distribution

$$g(\mathbf{H}) = g_1(H_{-1} | H_0) \cdots g_k(H_{-k} | H_{-k+1})$$

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An SIS approach

- By simulating from $g()$ multiple copies of the history, $H^{(j)}$, $j=1, \dots, m$, we can approximate the likelihood function as

$$\hat{p}_{\theta}(H_0) = \frac{1}{m} \sum_{j=1}^m \frac{p_{\theta}(H^{(j)})}{g(H^{(j)})}.$$

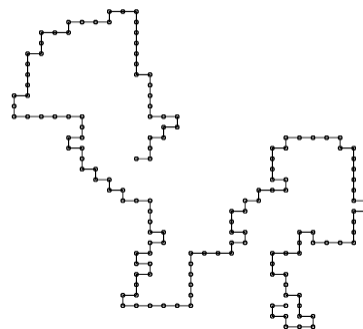
- Note the choice of θ_0 can influence the final result.

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Other examples of SIS

- Growing a polymer
 - Self avoid walk
- Sequential imputation for statistical missing data problem.
- More and details of these examples, see Liu 2001.

A Self-Avoiding Walk of Length N=150



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