

Approximate marginalization / Bayesian updates / inference

- Variational method
- Sampling methods

## ORIE 4742 - Info Theory and Bayesian ML

### Monte Carlo Techniques

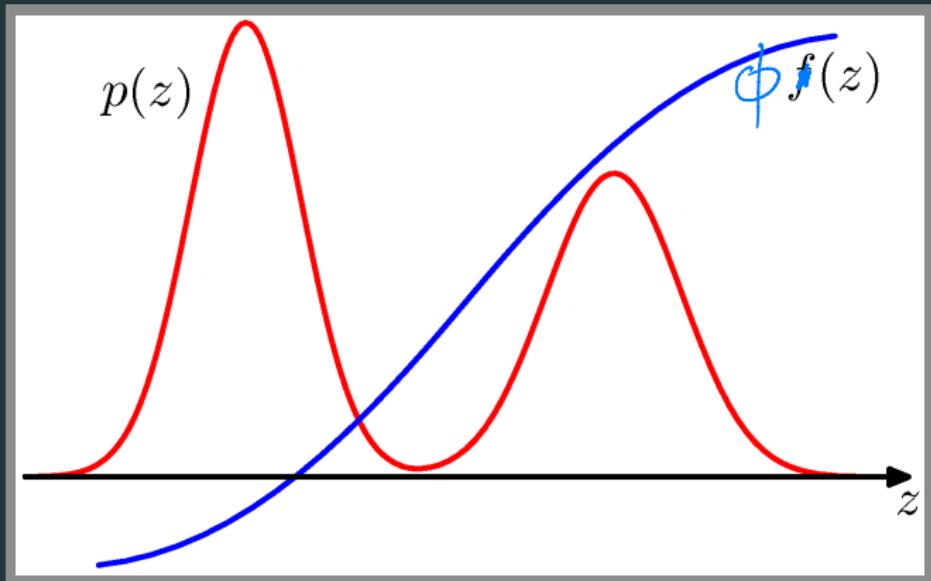
---

April 16, 2020

Sid Banerjee, ORIE, Cornell

Today's lecture - Bishop Ch 11  
( $\approx$  Mackay Ch 29)

## why Monte Carlo?



- Task - compute  $E[\phi(x)]$ ,  $x \sim F$
- Approximation -  $X_1, X_2, \dots, X_L \sim F$ ,  $E[\phi(x)] \approx \frac{1}{L} \sum_{i=1}^L \phi(x_i)$

## monte carlo basics

- primitive: `rand()`

Any simulation / randomized algo = regular algorithm + fn to generate  $\mathbb{U}[0,1]$

- pseudorandomness and seed

- $X_1, X_2, \dots, X_L = g(\underline{\text{seed}})$

- advantage: calculations are repeatable

- estimate variance

$$\overline{x} \sim F \cdot \frac{\mathbb{E}[\phi(x)]}{\mu} = \mathbb{E}\left[\underbrace{\frac{1}{L} \sum_{i=1}^L \phi(x_i)}_{z_L}\right] = \frac{1}{L} \sum_{i=1}^L \mathbb{E}[\phi(x)]$$

deterministic fn  
whose outputs 'look random'  
(ie, any calculation is approx the same)  
if  $x_i \sim F$

assume  $x_i$  are  $\perp \!\!\! \perp$   $\rightarrow \text{Var}(z_L) = \frac{1}{L} \mathbb{E}[(\mu - \phi(x_i))^2]$   $\left( \text{ie, } z_L \in \mu \pm 2\sqrt{\text{Var}(z_L)} \text{ w.p. } 95\% \right)$

- issues: non-independence, 'rare-events'

- MCMC -  $x_i \sim F$ , dependent

- $\phi$  may be very large for low probability  $X$

- use CIs to indicate how good your estimate is

# monte carlo sampling techniques

basic methods (iid samples)

- <sup>last class</sup>
- inversion
  - distribution-specific techniques (Box-Muller for Gaussians)
  - rejection sampling
  - importance sampling
  - advanced techniques (adaptive rejection sampling, SIR)

markov-chain monte carlo (MCMC)

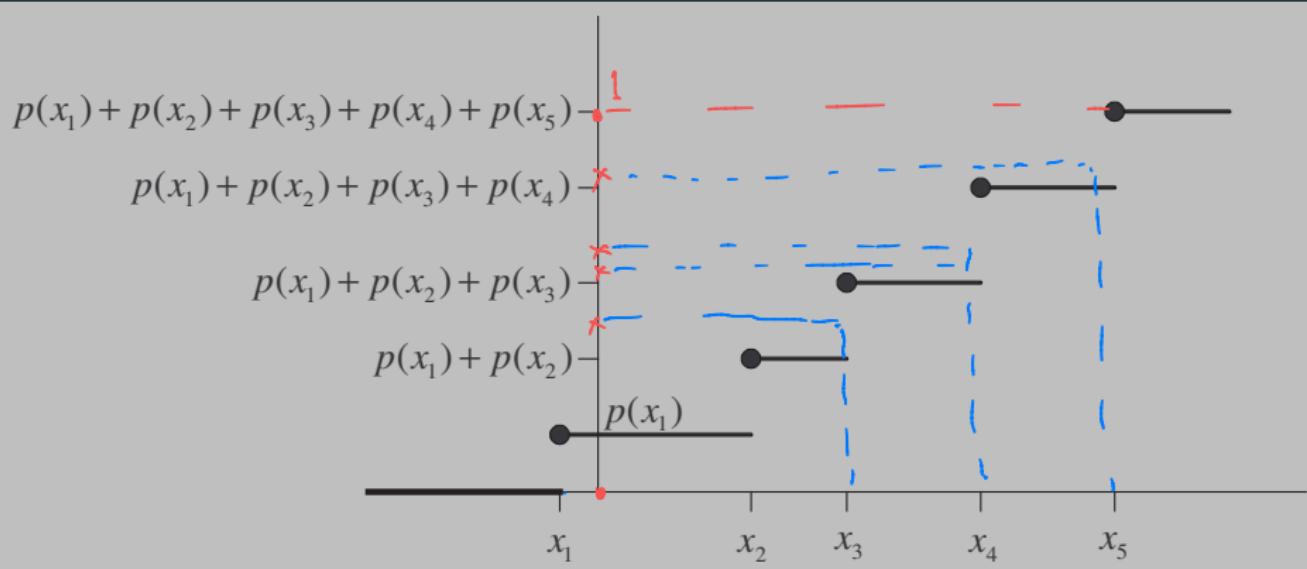
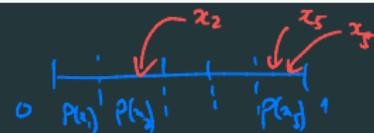
To day

- Metropolis-Hastings
- Gibbs sampling
- advanced techniques (slice sampling, Hamiltonian MC)



## warmup: simulating discrete rv

$X$  takes values  $x_1 \leq x_2 \leq \dots \leq x_5$ ,  $\mathbb{P}[X = x_i] = p(x_i)$



## the inversion method

$X$  continuous r.v. with pdf  $f$  and c.d.f.  $F(\cdot)$

- want to generate samples of  $X$ .
- $F(\cdot)$  non-decreasing  $\implies$  can define inverse  $F^{-1}(\cdot)$
- $F(x) = u \iff F^{-1}(u) = x$

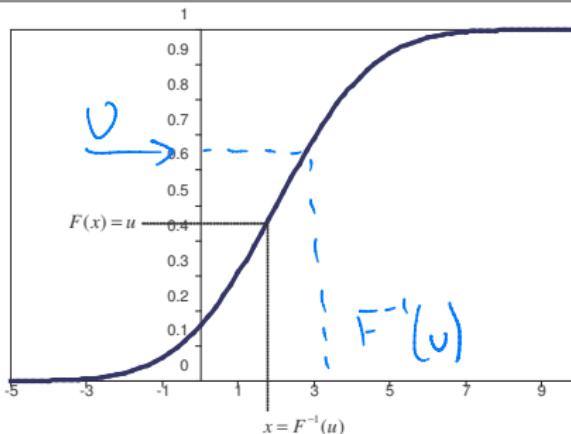
### inversion method

given desired cdf  $F$  (continuous, increasing), generate sample  $X_0 \sim F$  as:

1. generate  $U \sim U[0, 1]$ .
2. return  $X_o = F^{-1}(U)$ .



## intuition/proof for inversion method



$$X \sim F^{-1}(U)$$

$$\mathbb{P}[X \leq x] = \mathbb{P}[F^{-1}(U) \leq x]$$

$$= \mathbb{P}[U \leq F(x)]$$

$$= F(x)$$

$\Rightarrow$  CDF of  $X$  is  $F$

• Problem -  $F^{-1}(\cdot)$  may not be simple

## inversion method example

generate samples of an exponential r.v. with parameter  $\lambda$ , with cdf

$$F(x) = \begin{cases} 1 - e^{-\lambda x} & \text{if } x \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

$$\Rightarrow F^{-1}: y = 1 - e^{-\lambda x} \Rightarrow x = \underbrace{-\frac{1}{\lambda} \ln(1-y)}$$

$$\Rightarrow X = -\frac{1}{\lambda} \ln(1-U) \sim \text{Exp}(\lambda)$$

$\nwarrow \sim U[0,1]$

# Box-Muller method for Gaussian r.v.

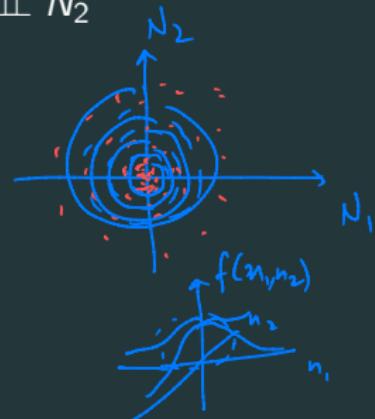
- generate  $N_1 \sim \mathcal{N}(0, 1)$ ,  $N_2 \sim \mathcal{N}(0, 1)$ ,  $N_1 \perp\!\!\!\perp N_2$
- in polar coordinates  $(N_1, N_2) = (R \cos \theta, R \sin \theta)$

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2\pi} e^{-x^2/2} e^{-y^2/2} dx dy = 1$$

$$x = r \cos \theta, y = r \sin \theta$$

$$\Rightarrow \int_0^{\infty} \int_0^{2\pi} \underbrace{\frac{1}{2\pi}}_{f(\theta)} \cdot \underbrace{r e^{-r^2/2}}_{f(r)} dr d\theta = 1$$

$$= \left( \int_0^{2\pi} \frac{d\theta}{2\pi} \right) \left( \int_0^{\infty} r e^{-r^2/2} dr \right)$$



$$\theta \sim \text{Unif}[0, 2\pi]$$

$$\frac{R^2}{2} \sim \text{Exp}(1)$$

## the Box-Muller Method

$$(N_1, N_2) = (R \cos \theta, R \sin \theta) \quad , \quad N_1 \perp\!\!\!\perp N_2$$

$\theta \sim U[0, 2\pi]$ , and independent of  $R$ .

$$R = \sqrt{N_1^2 + N_2^2} = \sqrt{2X}, \quad \text{where } X \sim Exp(1)$$

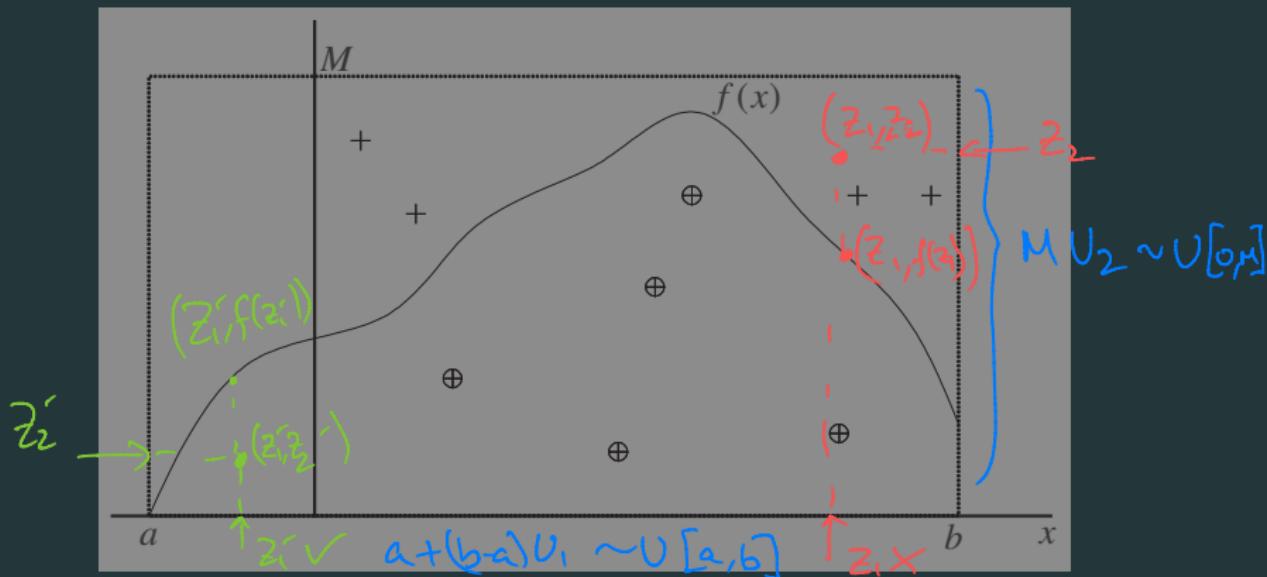
- Generate  $\frac{R^2}{2} = -\ln(1-U_1)$ ,  $\theta = 2\pi U_2$
- Set  $N_1 = R \cos \theta$ ,  $N_2 = R \sin \theta$

# rejection sampling

want samples of a rv  $X \in [a, b]$ , with pdf  $f(x) \leq M$

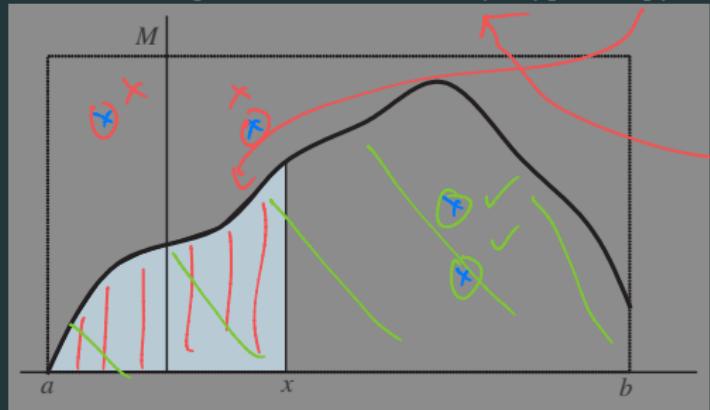
## rejection sampling

1. Generate  $U_1, U_2 \sim U[0, 1]$ , and set  $Z_1 = a + (b - a)U_1$ ,  $Z_2 = MU_2$
2. if  $Z_2 \leq f(Z_1)$ , return  $X_o = Z_1$ ; else, reject and repeat



## rejection sampling: proof of correctness

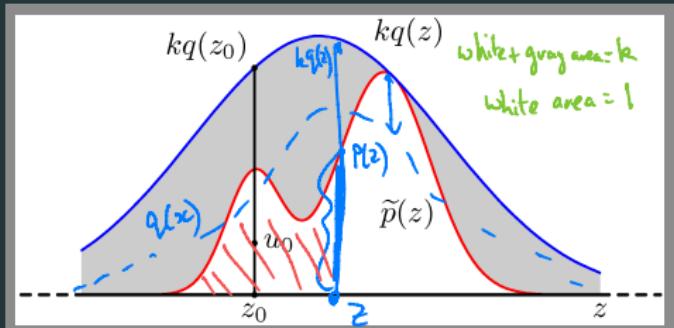
observe:  $\mathbb{P}[Z_1 \leq x, Z_2 \leq f(Z_1)] = \mathbb{P}[(Z_1, Z_2) \in \text{shaded region in figure}]$



$$\begin{aligned}\mathbb{P}[Z_1 \leq x | Z_1 \text{ accepted}] \\ = \frac{\mathbb{P}[Z_1 \leq x \text{ AND } Z_1 \text{ accepted}]}{\mathbb{P}[Z_1 \text{ accepted}]}\end{aligned}$$

$$\begin{aligned}\mathbb{P}[Z_1 \text{ accepted}] &\propto \text{green shaded area} \\ \mathbb{P}[Z_1 \text{ accepted}, Z_1 \leq x] &\propto \text{red shaded area} \\ &= \frac{\text{Shaded area in red}}{\text{Shaded area in green}} \\ &= F(x)\end{aligned}$$

## generalized rejection sampling



• Suppose we have a Sampler for  $Z \sim Q$

• Want -  $X \sim P$

• Suppose  $\max_z \frac{P(z)}{q(z)} \leq K$

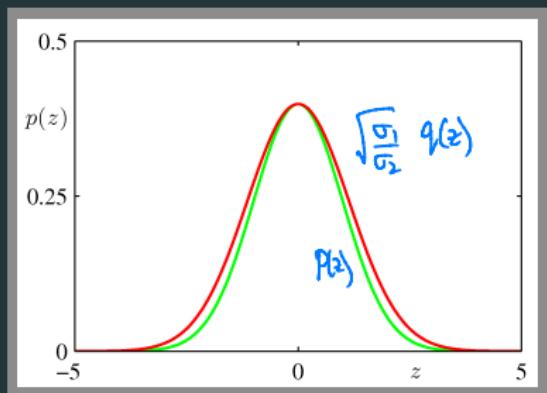
$$\Rightarrow P(z) \leq Kq(z) \quad \forall z \in \mathbb{R}$$

• Algo - generate  $Z \sim Q$ .

- accept  $Z_1$  with probability  $\frac{P(z_1)}{Kq(z_1)}$ , else reject

(equiv, generate  $Z_2 = Kq_1(z_1) + U_2$ , accept if  $Z_2 < P(z_1)$ )

## rejection sampling: running time in high dimensions



Eg -  $Z \sim N(0, \sigma_1)$ , want  $X \sim N(0, \sigma_2)$

$$\cdot q(z) = \frac{1}{\sqrt{2\pi}\sigma_1} e^{-z^2/2\sigma_1^2}, \quad p(z) = \frac{1}{\sqrt{2\pi}\sigma_2} e^{-z^2/2\sigma_2^2}$$

$$\cdot \frac{p(z)}{q(z)} \leq \sqrt{\frac{\sigma_1}{\sigma_2}}$$

$$\Rightarrow Z \sim N(0, \sigma_1), \text{ accept w.p. } \frac{e^{-z^2/2\sigma_2^2}}{e^{-z^2/2\sigma_1^2}} \cdot \sqrt{\frac{\sigma_1}{\sigma_2}}$$

$$- \boxed{P[\text{Acceptance}] = \frac{1}{k}} = \sqrt{\frac{\sigma_2}{\sigma_1}} \Rightarrow E[\# \text{ of samples for 1 acceptance}] = k = \sqrt{\frac{\sigma_1}{\sigma_2}}$$

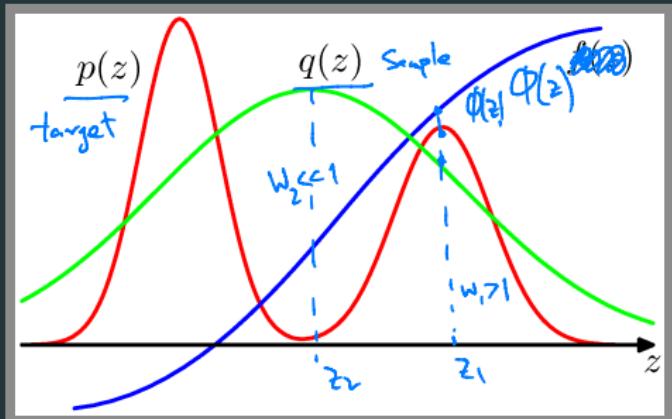
- Q: What if  $Z \sim N(0, \sigma_1 I_d)$ ,  $X \sim N(0, \sigma_2 I_d)$   
 $\Rightarrow P[\text{Acceptance}] = \frac{1}{k^d} = \left(\frac{\sigma_2}{\sigma_1}\right)^{d/2} \ll 1 \Rightarrow$  Need many samples

# importance sampling

- given function  $\phi(\cdot)$ , want  $\mathbb{E}[\phi(X)]$  where  $X \sim P$
- can generate samples  $Z \sim Q$

## importance sampling

1. generate  $Z_1, Z_2, \dots, Z_L \sim Q$
2. compute  $\mathbb{E}[\phi(X)] = \frac{1}{L} \sum_{i=1}^L w_i \phi(Z_i)$ , where  $w_i = p(Z_i)/q(Z_i)$



$$\begin{aligned}\mathbb{E}_P[\phi(x)] &= \int_{\mathbb{R}^d} \phi(x) p(x) dx \\ &= \int_{\mathbb{R}^d} \phi(x) \underbrace{\left( \frac{p(x)}{q(x)} \right)}_{w(x)} q(x) dx \\ &= \mathbb{E}_Q \left[ \underbrace{w(z)}_{\tilde{w}(z)} \phi(z) \right] \\ &\approx \frac{1}{L} \sum_{i=1}^L \left( \frac{p(z_i)}{q(z_i)} \right) \phi(z_i)\end{aligned}$$

## importance sampling: unknown normalization

- Suppose  $P(x) = \frac{1}{Z_p} \tilde{P}(x)$ ,  $q_v(x) = \frac{1}{Z_q} \tilde{q}_v(x), Y_i \sim Q$

- $$\begin{aligned}\mathbb{E}[\phi(x)] &= \int \phi(x) \frac{\tilde{P}(x)}{Z_p} dx \\ &= \left( \frac{Z_q}{Z_p} \right) \int \phi(x) \underbrace{\left( \frac{\tilde{P}(x)}{\tilde{q}_v(x)} \right)}_{w(x) = \tilde{P}(x)/\tilde{q}_v(x)} \cdot \frac{\tilde{q}_v(x)}{Z_q} dx \\ &= \left( Z_q / Z_p \right) \mathbb{E}_Q[\phi(Y) w(Y)]\end{aligned}$$

- $$1 = \int P(x) dx = \frac{Z_q}{Z_p} \int \frac{\tilde{P}(x)}{\tilde{q}_v(x)} q_v(x) dx = \frac{Z_q}{Z_p} \mathbb{E}[w(Y)]$$

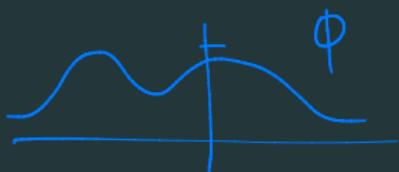
$$\Rightarrow \mathbb{E}[\phi(x)] = \frac{\mathbb{E}_Q[\phi(Y) w(Y)]}{\mathbb{E}[w(Y)]} \approx \sum_{i=1}^L \frac{w_i}{\sum_j w_j} \cdot \phi(Y_i)$$

## importance sampling: comments

$$\mathbb{E}[\phi(x)] \approx \frac{1}{L} \sum \underbrace{\frac{p(z_i)}{q(z_i)}}_{\gg 1} \underbrace{\phi(z_i)}_{\phi(x) \leq 1}$$

$$\frac{1}{L} \text{Var} \left( \phi(z_i) w(z_i) \right)$$

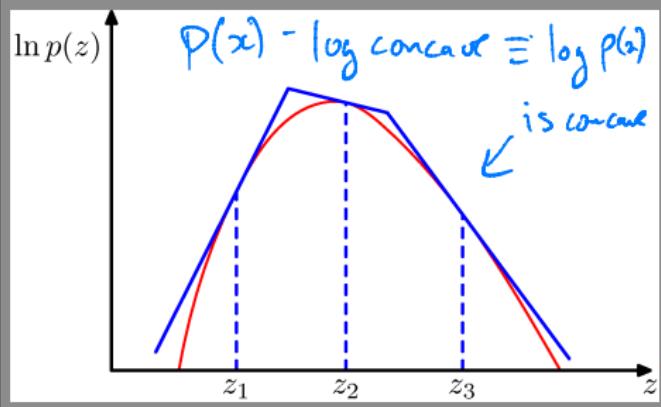
depends on  $\max \phi(z_i) w(z_i)$



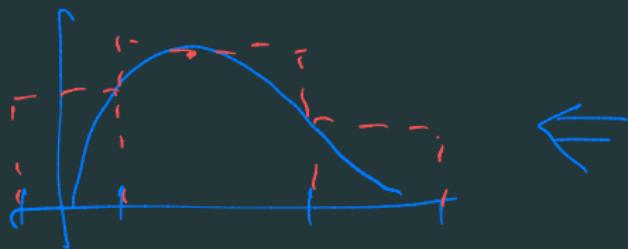
- Problem - If  $p(z)/q(z)$  is large for some  $z$ , then  
high variance

- Practice - Choose  $q$  s.t.  $\left[ \frac{p(z)}{q(z)} \right] \left[ \phi(z) \right]$  is not too large  
want this to be small  $\rightarrow t \approx 10^6$

## (advanced) adaptive rejection sampling



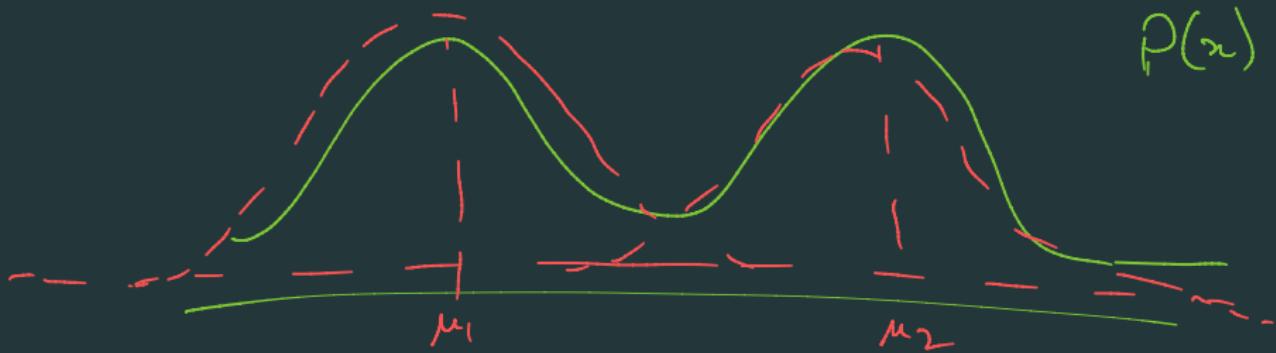
Idea - Keep improving the  
'proposal dist'  $Q$



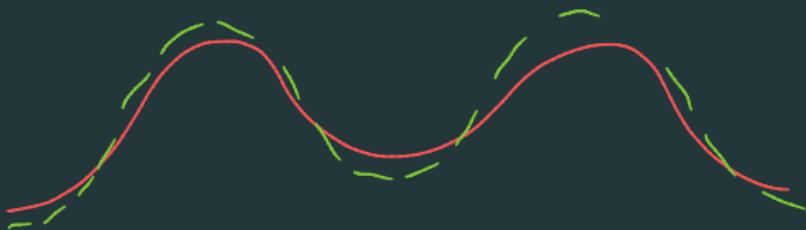
$$k = \frac{\text{Area under red}}{\text{Area under blue}}$$



Eg



$$q_V = \underbrace{\frac{0.9}{2} N(\mu_1, 1)}_{\text{---}} + \underbrace{\frac{0.9}{2} N(\mu_2, 1)}_{\text{---}} + 0.1 V [-10^6, 10^6]$$



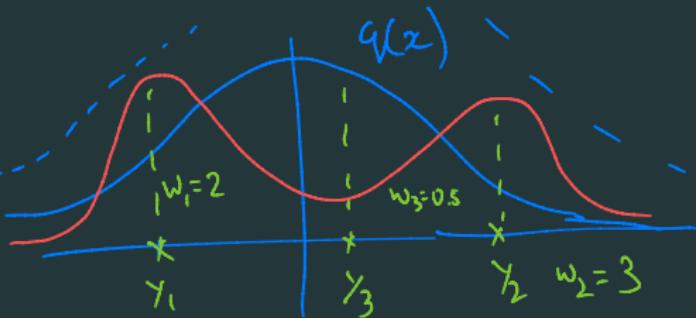
## (advanced) sampling-importance-resampling (SIR/bootstrap)

- SIR heuristic

- Generate  $\gamma_1, \gamma_2, \dots, \gamma_L \sim Q$

- Compute  $w_i = \frac{P(\gamma_i)}{q(\gamma_i)}$

- Resample  $\tilde{\gamma}_1, \tilde{\gamma}_2, \dots, \tilde{\gamma}_L$  from dist  $\tilde{P} \sim \left\{ \gamma_i \text{ wp } w_i / \sum w_i \right\}$



- Eg -  $\tilde{P} = \left\{ \begin{array}{l} \gamma_1 \text{ wp } 2/5.5 \\ \gamma_2 \text{ wp } 3/5.5 \\ \gamma_3 \text{ wp } 0.5/5.5 \end{array} \right.$

- Claim - As  $L \nearrow \infty$ ,  $\tilde{P} \rightarrow P$

disadvantage  
 $\tilde{P} \approx P$   
(not exact samples)  
advantage  
(no sample rejected)





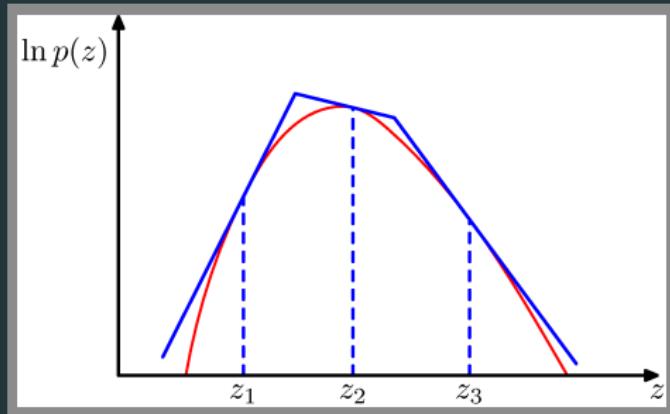
## the Box-Muller Method

$$(N_1, N_2) = (R \cos \theta, R \sin \theta)$$

$\theta \sim U[0, 2\pi]$ , and independent of  $R$ .

$$R = \sqrt{N_1^2 + N_2^2} = \sqrt{2X}, \quad \text{where } X \sim Exp(1)$$

## (advanced) adaptive rejection sampling





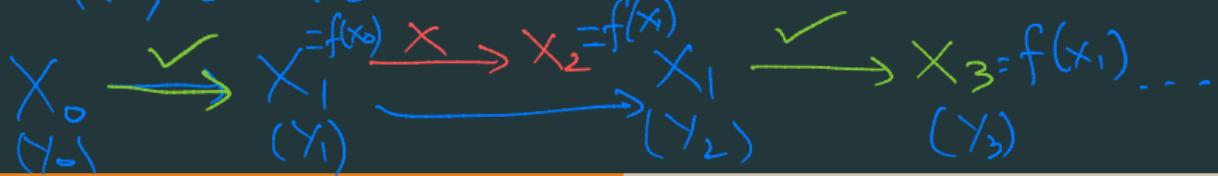
## MCMC: the basic idea

- Method 1 - Generate  $X_1, X_2, \dots, X_L$  iid from  $P$   
(Inversion Sampling, Importance Sampling)
- Method 2 - Generate  $X_1, \dots, X_L$  iid, accept/reject samples

$$\checkmark X_1 \checkmark X_2 \checkmark X_3, \dots, \checkmark X_L \rightarrow Y_1, Y_2, Y_3, \dots, Y_L$$

- Method 3 - Generate  $X_1, X_2 = f(X_1), X_3 = f(X_2), \dots$   
- Accept/Reject  $X_t$  w.p.  $A(X_{t-1}, X_t)$

(i.e., set  $Y_t = X_t$  or set  $Y_t = X_{t-1}$ )



## markov chains: basic definition

Seq of r.v.  $X_1, X_2, \dots, X_n$  is a MC  
iff  $P(X_i | X_1, X_2, \dots, X_{i-1}) = P(X_i | X_{i-1})$

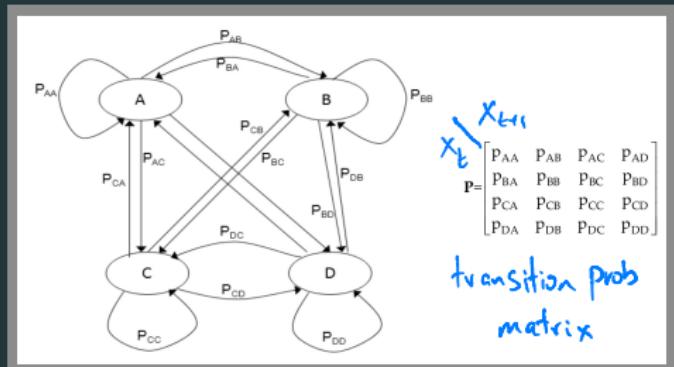
BayesNet for MC



- Check -  $P(X_i, X_{i+2} | X_{i+1}) = P(X_i | X_{i+1}) \cdot P(X_{i+2} | X_{i+1})$   
(d-separation)

# markov chains: state-space and transition matrix

(time-invariant)



Note - This is not a BayesNet!

- State-Space  $\equiv \{A, B, C, D\}$
- $P(X_{t+1} = A | X_t = B) = \underline{P_{BA}}$

*transition prob  
matrix*

$$P = \begin{bmatrix} & X_{t+1} \\ X_t & \begin{bmatrix} P_{AA} & P_{AB} & P_{AC} & P_{AD} \\ P_{BA} & P_{BB} & P_{BC} & P_{BD} \\ P_{CA} & P_{CB} & P_{CC} & P_{CD} \\ P_{DA} & P_{DB} & P_{DC} & P_{DD} \end{bmatrix} \end{bmatrix}$$

- $\sum_{x: \text{outgoing edges}} P_{Ax} = 1 \quad \forall A \equiv$  Each row-sum of  $P = 1, P_{ij} \geq 0 \quad \forall i, j$  (stochastic matrix)
- Directed (not necessarily, acyclic) graph
- Let  $\Pi_t \stackrel{\text{row vector}}{\equiv} \text{Distribution of } X_t = P[X_t = z | X_0]$
- Then  $\Pi_{t+1} = \Pi_t \cdot P = \begin{bmatrix} \Pi_t \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} \cdot & P & \cdot \end{bmatrix}$

## markov chains: steady-state

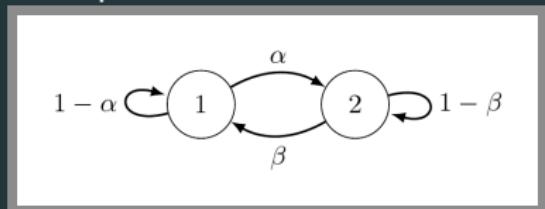
Q. - Given  $X_1, X_2, X_3, \dots$  from a time invariant MC,  
 what can we say about  $\lim_{t \rightarrow \infty} X_t$  (or  $X_t$  for large  $t$ )

1)  $X_t$  can get 'absorbed'  
 (not interesting for us ...)



2)  $\pi_t$  can 'converge' to a fixed distrib  $\pi$  'steady state dist'  
 (recall  $\pi_t = \pi_{t-1}P$   $\Rightarrow \pi = \pi P$ )

example:

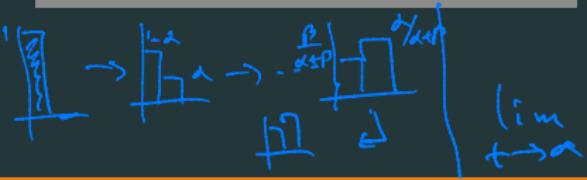


$$\pi_0 = (1, 0) \quad (\text{i.e., start at '1'})$$

$$\pi_1 = (1, 0) \begin{pmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{pmatrix} = (1-\alpha, \alpha)$$

$$\vdots$$

$$\lim_{t \rightarrow \infty} \pi_t = \pi = \left( \frac{\beta}{\alpha+\beta}, \frac{\alpha}{\alpha+\beta} \right)$$



# markov chains: example (infinite Markov Chain)

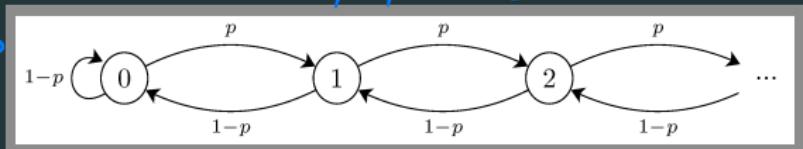
the 1-d random walk on  $\{0, 1, 2, \dots\}$

$$P[X_t=i+1|X_{t-1}=i] = p$$

$$P[X_t=i-1|X_{t-1}=i] = 1-p$$

all else is 0

$$(P[X_t=0|X_{t-1}=0]=1-p)$$



$$P = \begin{pmatrix} 1-p & p & 0 & \dots \\ 0 & 1-p & p & \dots \\ 0 & 0 & 1-p & \dots \\ \vdots & & & \ddots \end{pmatrix}$$

- Steady-state  $\pi(i)$

$$\sum_j \pi(j) P_{ij} = \sum_j \pi(j) P_{ji} \quad \forall i$$

- Claim -  $\pi(i) = \frac{1}{Z} \left(\frac{p}{1-p}\right)^i$  (assuming  $p < \frac{1}{2}$ )  

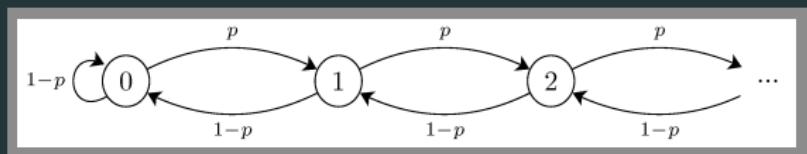
$$\Rightarrow Z = \sum_i \left(\frac{p}{1-p}\right)^i < \infty$$

'Proof':  $\forall i > 0, \sum_j \pi(j) P_{ij} = \frac{1}{Z} \left(\frac{p}{1-p}\right)^i \cdot (p + 1-p)$

$$\sum_j \pi(j) P_{ji} = \frac{1}{Z} \left(\left(\frac{p}{1-p}\right)^{i-1} \cdot p + \left(\frac{p}{1-p}\right)^{i+1} (1-p)\right)$$

## markov chains: reversibility

(idea 'borrowed' from physics)



- Steady-state  $\pi(i)$  (Global balance)

$$\sum_j \pi(j) P_{ij} = \sum_j \pi(j) P_{ji} \quad \forall i$$

- (Easier) Local balance -  $\forall i, j$

$$\pi(i) P_{ij} = \pi(j) P_{ji} \quad (\star)$$

- 'Magic Thm' - If local balance holds  $\forall i, j \Rightarrow \pi$  is steady-state dist

Pf - Check  $(\star) \Rightarrow \text{(*)}$

$$\pi(i) = \frac{1}{Z} \left( \frac{p}{1-p} \right)^i$$

- Check local balance  $\oplus$

$$\forall i, j - \text{if } i \neq j-1 \text{ or } j+1, \\ \text{then } P_{ij} = P_{ji} = 0 \Rightarrow \text{True}$$

$$- \text{ if } i = j+1$$

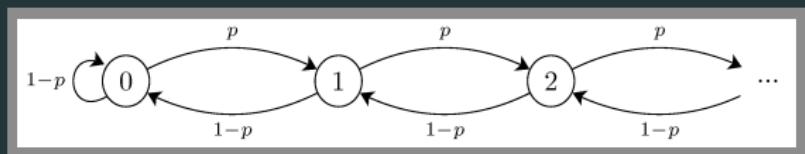
$$\frac{1}{Z} \left( \frac{p}{1-p} \right)^i \cdot (i-p)$$

$$\pi(i) \quad P_{ii}$$

$$\frac{1}{Z} \left( \frac{p}{1-p} \right)^{i-1} \cdot p$$

$$\pi(i-1) = \pi(i) \quad P_{ii}$$

## Markov chains: the ergodic theorem



Ergodic  $\Rightarrow$   
averages over time  
= averages over 'space'

- Let  $\pi$  be steady-state dist of MC with trans mat  $P$   
(ie,  $\pi = \pi P$ )  
state-space of MC
- Then for any fn  $\phi(x), x \in S$ ,

$$\mathbb{E}_{X \sim \pi} [\phi(x)] = \lim_{T \rightarrow \infty} \frac{1}{T} \mathbb{E} \left[ \sum_{t=0}^{T-1} \phi(X_t) \right]$$

space-average      time average

where  $X_0 \rightarrow X_1 \rightarrow X_2 \rightarrow \dots \rightarrow X_T$  are from the MC

## Markov-chain monte carlo

Recall - Basic MCMC recipe

- Start at  $X_0$
- At time  $t$ , compute  $Y_t = f(X_{t-1})$
- Set  $X_{t+1} = \begin{cases} Y_t & \text{w.p. } A(X_{t-1}, Y_t) \\ X_{t-1} & \text{otherwise} \end{cases}$ 

Some  
MC  
with  
trans  
mat  
 $R$
- Compute  $\frac{1}{L} \sum_{t=1}^L \phi(X_t)$ 

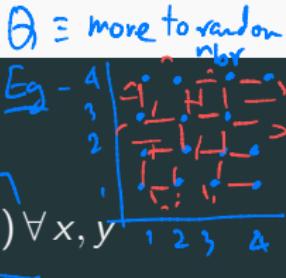
want this to  
be  $E_{X \sim P}[\phi(X)]$
- This requires the MC  $R$  to have steady-state dist as  $P$  (ie., want  $P = PR$ )

# the Metropolis algorithm

- target distribution  $P(x) = \tilde{P}(x)/Z$

- proposal distribution(s)  $Q(x|y)$ , with  $Q(x|y) = Q(y|x) \forall x, y$

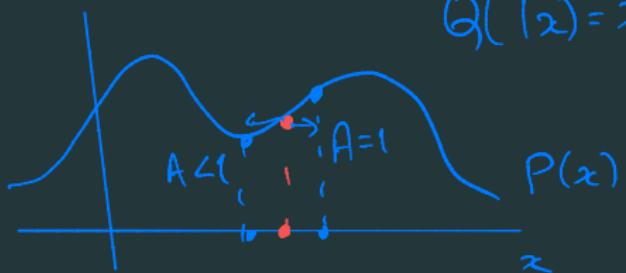
Symmetric



## Metropolis sampling

1. choose initial  $Z_0$
2. to obtain sample  $t$ , generate  $Y_t \sim Q(\cdot|Z_{t-1})$

3. accept  $Z_t = Y_t$  with probability  $A(Y_t, Z_{t-1}) = \max \left\{ 1, \frac{\tilde{P}(Y_t)}{\tilde{P}(Z_{t-1})} \right\}$   
else reject and set  $Z_t = Z_{t-1}$

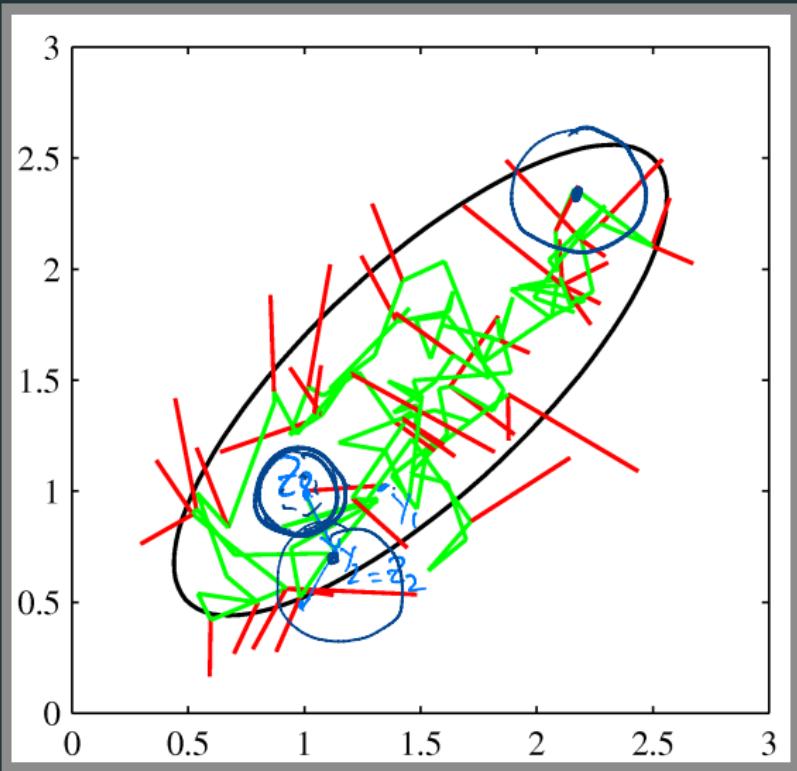


$$Q(z|x) = x + 1 \text{ w.p. } \frac{1}{2}$$

i.e., if  $\tilde{P}(Y_t) \geq \tilde{P}(Z_{t-1})$ ,  
then move, else move  
with prob  $\frac{\tilde{P}(Y_t)}{\tilde{P}(Z_{t-1})}$

# Metropolis for 2-d Gaussian

$$\begin{aligned} Q(x|y) \\ = N(0, \sigma^2 I) \end{aligned}$$



## Metropolis algorithm: proof of correctness

- Want to show  $P$  is a steady state dist<sup>n</sup>
- $\forall x, y, R_{xy} = P[x \rightarrow y] = Q(y|x) \cdot A(x,y)$ 
$$R_{xx} = \sum_y Q(y|x) (1 - A(x,y))$$
- Now we check local balance, ie,  $\forall x, y$ 
$$P(x) R_{xy} = P(x) \cdot Q(y|x) \cdot \max\left(1, \frac{\tilde{P}(y)}{\tilde{P}(x)}\right)$$
$$\text{if Symmetric}$$
$$P(y) R_{yx} = P(y) \cdot Q(x|y) \cdot \max\left(1, \frac{\tilde{P}(x)}{\tilde{P}(y)}\right)$$
$$\text{if } \forall x, y, \text{ if } P(x) \geq P(y) \Rightarrow A(x,y) = 1, A(y,x) = P(x)/P(y)$$

# Metropolis-Hastings

- target distribution  $P(x) = \tilde{P}(x)/Z$
- proposal distribution(s)  $Q(x|y)$

## Metropolis-Hastings sampling

1. choose initial  $Z_0$
2. to obtain sample  $t$ , generate  $Y_t \sim Q(\cdot|Z_{t-1})$
3. accept  $Z_t = Y_t$  with prob  $A(Y_t, Z_{t-1}) = \max \left\{ 1, \frac{\tilde{P}(Y_t)Q(Z_{t-1}|Z_t)}{\tilde{P}(Z_{t-1})Q(Z_t|Z_{t-1})} \right\}$   
else **reject** and set  $Z_t = Z_{t-1}$

# Gibbs sampling

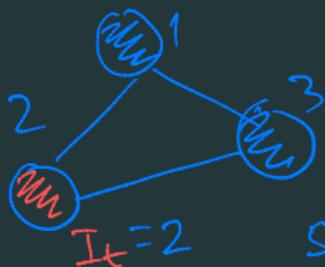
- target distribution  $P(x(1), x(2), \dots, x(n))$

## Gibbs sampling

1. choose initial  $X_0 = (X_0(1), X_0(2), \dots, X_0(n))$
2. to obtain sample  $t$ :

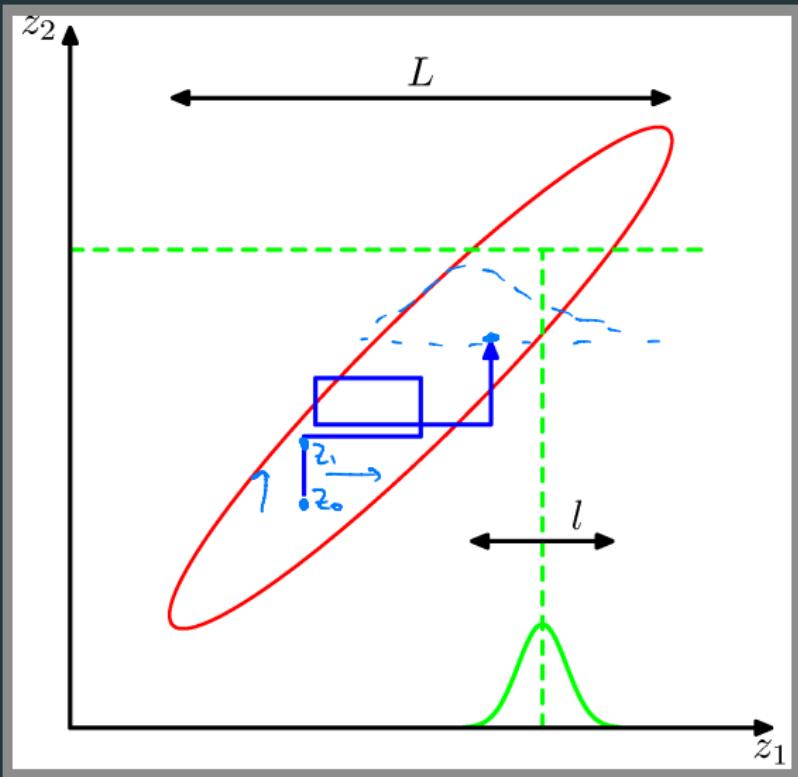
pick  $I_t$  uniformly at random (alternate- pick in round robin order)  
set  $\underline{X_t(i)} = X_{t-1}(i)$  for  $i \neq I_t$  i.e.,  $I_1=1, I_2=2, \dots, I_n=n, I_{n+1}=1, I_{n+2}=2, \dots$   
set  $\underline{X_t(I_t)} \sim P(\cdot | \underline{X_{t-1}} \setminus X_{t-1}(I_t))$

$\xrightarrow{\text{i.e., fix all } X(i) \text{ except } I_t}$



Sample  $X_t(2) \sim P(x_2 | x_1, x_3)$

## Gibbs sampling for 2-d Gaussian



$$Z_0 = \{Z_0(1), Z_0(2)\}$$

$$I_1 = 2$$

$$I_2 = 1$$

$$I_3 = 2$$

$$I_4 = 1$$

⋮

## Gibbs sampling: proof of correctness

$$\cdot R_{(x_1, x_2) \rightarrow (x'_1, x_2)} = \underbrace{P[I_t=1]}_{1/2} \cdot P[x'_1 | x_2]$$

$$R_{(x'_1, x_2) \rightarrow (x_1, x_2)} = \frac{1}{2} \cdot P(x_1 | x_2)$$

Claim.  $\pi(x_1, x_2) = P(x_1, x_2)$  is a steady state dist

$$\text{i.e. } \underbrace{P(x_1, x_2)}_{P(x_2)P(x_1 | x_2)} \cdot \frac{1}{2} \cdot P[x'_1 | x_2] = \underbrace{P(x'_1, x_2)}_{P(x_2)P(x'_1 | x_2)} \cdot \frac{1}{2} \cdot P(x_1 | x_2)$$