

Approximate marginalization / Bayesian updates / inference

- Variational method
- Sampling methods

ORIE 4742 - Info Theory and Bayesian ML

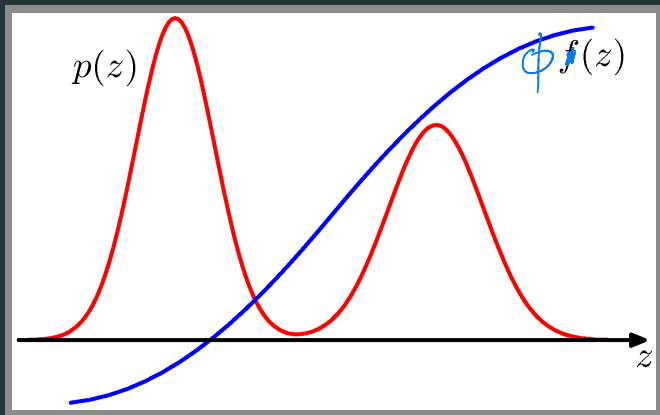
Monte Carlo Techniques

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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 \equiv regular algorithm +
fn to generate $U[0,1]$

- pseudorandomness and seed

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

- advantage: calculations are repeatable

- estimate variance

deterministic fn
whose outputs 'look random'
(ie, any calculation is approx the same)

if $X_i \sim F$

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

$$\underbrace{\text{assume } X_i \text{ are i.i.d.}}_{\rightarrow} \cdot \text{Var}(Z_L) = \frac{1}{L} E[(\mu - \phi(x_i))^2]$$

(ie, $Z_L \in \mu \pm 2\sqrt{\text{Var}(Z_L)}$ w.p. 95%)

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

- use CIs to indicate
how good your estimate is

- MCMC - $X_i \sim F$, dependent

- ϕ may be very large for low probability X

monte carlo sampling techniques

basic methods (iid samples)

- inversion
- distribution-specific techniques (Box-Muller for Gaussians)
- rejection sampling
- importance sampling
- advanced techniques (adaptive rejection sampling, SIR)

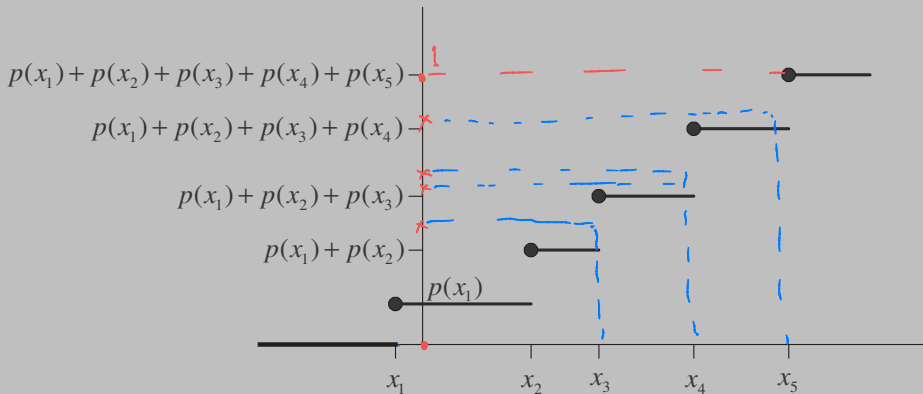
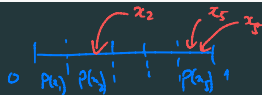
markov-chain monte carlo (MCMC)

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

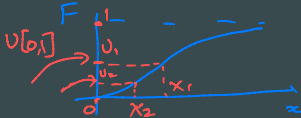
X continuous r.v. with pdf f and c.d.f. $F(\cdot)$

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

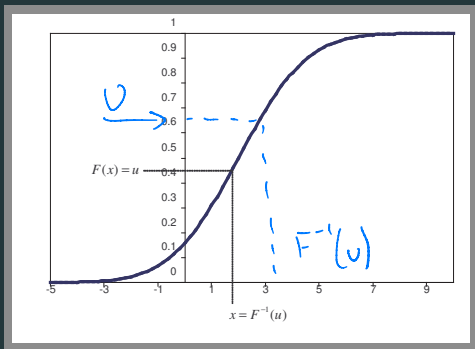
inversion method

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

1. generate $U \sim U[0, 1]$.
2. return $X_0 = F^{-1}(U)$.



intuition/proof for inversion method



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

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

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

$$= F(x)$$

\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 λ , with cdf

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

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

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

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

Box-Muller method for Gaussian r.v.

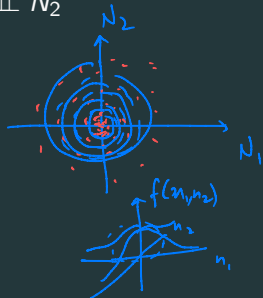
- generate $N_1 \sim \mathcal{N}(0, 1)$, $N_2 \sim \mathcal{N}(0, 1)$, $N_1 \perp N_2$
- in polar coordinates $(N_1, N_2) = (R \cos \theta, R \sin \theta)$

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

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

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

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



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

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

the Box-Muller Method

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

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

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

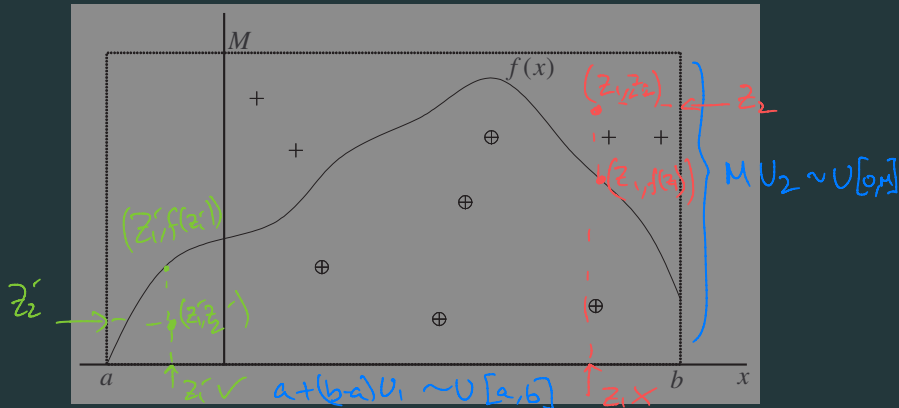
- Generate $\frac{R^2}{2} = -\ln(1-U_1)$, $\theta = 2\pi U_2$
- Set $N_1 = R \cos \theta$, $N_2 = R \sin \theta$

rejection sampling

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

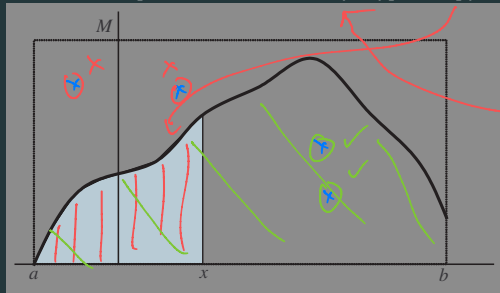
rejection sampling

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



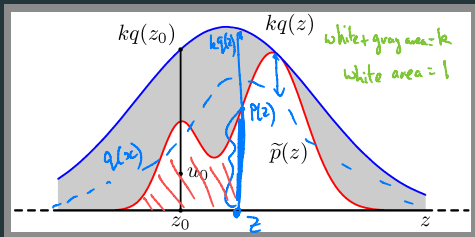
$$\begin{aligned} & \mathbb{P}[Z_1 \leq x | Z_1 \text{ accepted}] \\ &= \frac{\mathbb{P}[Z_1 \leq x \text{ AND } Z_1 \text{ accepted}]}{\mathbb{P}[Z_1 \text{ accepted}]} \end{aligned}$$

$\mathbb{P}[Z_1 \text{ accepted}] \propto$ green shaded area

$\mathbb{P}[Z_1 \text{ accepted}, Z_1 \leq x] \propto$ red shaded area

$$\begin{aligned} &= \frac{\text{Shaded area in red}}{\text{Shaded area in green}} \\ &= F(x) \end{aligned}$$

generalized rejection sampling

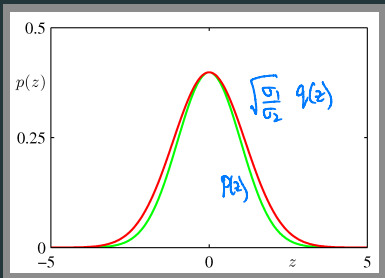


- Suppose we have a sampler for $Z \sim Q$
- Want - $X \sim P$
- Suppose $\max_z \frac{p(z)}{q(z)} \leq k(z)$

$$\Rightarrow p(x) \leq kq(x) \quad \forall x \in \mathbb{R}$$

- Algo - generate $Z_1 \sim Q$.
- accept Z_1 with probability $\frac{p(Z_1)}{kq(Z_1)}$, else reject
- (equiv, generate $Z_2 = kq(Z_1) U_2$, accept if $Z_2 < p(Z_1)$)

rejection sampling: running time in high dimensions



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

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

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

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

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

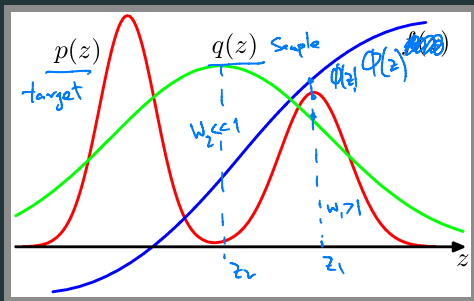
• Q: What if $Z \sim N(0, \sigma_1 I_d)$, $X \sim N(0, \sigma_2 I_d)$
 $\Rightarrow IP[\text{Acceptance}] = 1/k^d = \left(\frac{\sigma_2}{\sigma_1}\right)^{d/2} \ll 1 \Rightarrow$ Need many samples

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 $w_i = p(Z_i)/q(Z_i)$ importance sampling weights



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

importance sampling: unknown normalization

- Suppose $p(x) = \frac{1}{z_p} \tilde{p}(x)$, $q(x) = \frac{1}{z_q} \tilde{q}(x)$, $y_i \sim q$

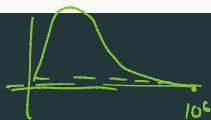
- $$\begin{aligned} \mathbb{E}[\phi(x)] &= \int \phi(x) \frac{\tilde{p}(x)}{z_p} dx \\ &= \left(\frac{z_q}{z_p}\right) \int \phi(x) \underbrace{\left(\frac{\tilde{p}(x)}{\tilde{q}(x)}\right)}_{w(x) = \tilde{p}(x)/\tilde{q}(x)} \cdot \frac{\tilde{q}(x)}{z_q} dx \\ &= (z_q/z_p) \mathbb{E}_q[\phi(y) w(y)] \end{aligned}$$

- $$1 = \int p(x) dx = \frac{z_q}{z_p} \int \frac{\tilde{p}(x)}{\tilde{q}(x)} q(x) dx = \frac{z_q}{z_p} \mathbb{E}[w(y)]$$

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

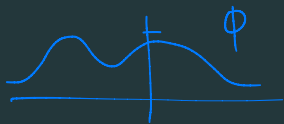
importance sampling: comments

$$E[\phi(x)] \approx \frac{1}{L} \sum \frac{P(z_i)}{q(z_i)} \phi(z_i)$$



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

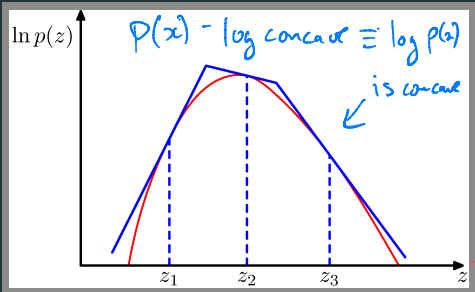
depends on $\max \phi(z_i) w(z_i)$



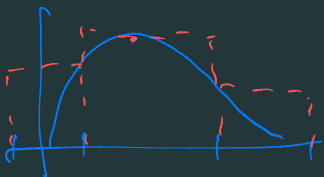
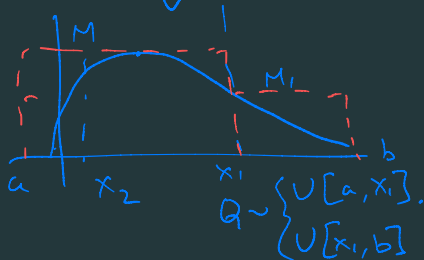
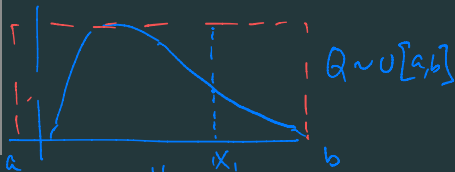
- Problem - If $P(z)/q(z)$ is large for some z , then high variance

- Practice - choose q s.t. $\frac{P(z)}{q(z)} \phi(z)$ is not too large
want this to be small $\leftarrow 1/10^6$

(advanced) adaptive rejection sampling

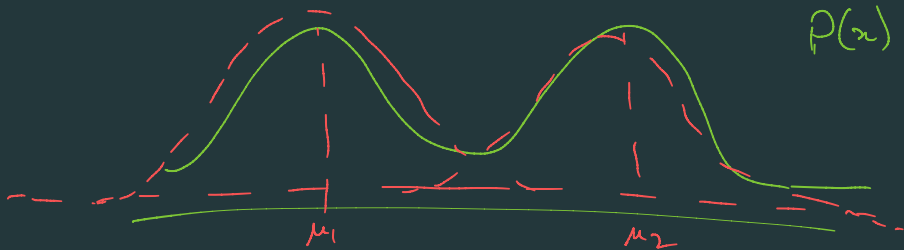


Idea - Keep improving the 'proposal dist' Q

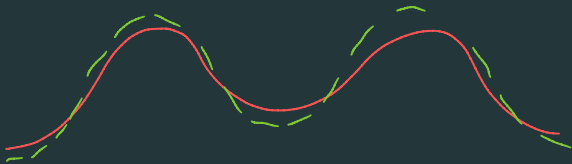


$k = \frac{\text{Area under red}}{\text{Area under blue}}$

Eg



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



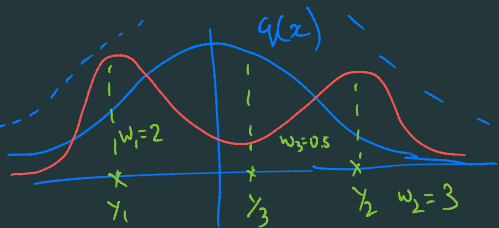
(advanced) sampling-importance-resampling (SIR/bootstrap)

• SIR heuristic

- Generate $y_1, y_2, \dots, y_L \sim \theta$

- Compute $w_i = \frac{p(y_i)}{q(y_i)}$

- Resample $\tilde{y}_1, \tilde{y}_2, \dots, \tilde{y}_L$ from dist $\tilde{p} \sim \left\{ y_i \text{ w.p. } w_i / \sum w_i \right\}$



• Eg - $\tilde{p} = \begin{cases} y_1 \text{ w.p. } 2/5.5 \\ y_2 \text{ w.p. } 3/5.5 \\ y_3 \text{ w.p. } 0.5/5.5 \end{cases}$

- Claim - $AsL \rightarrow \infty, \tilde{p} \rightarrow P$

disadvantage

$\tilde{p} \approx P$
(not exact samples)

advantage

(no sample rejected)

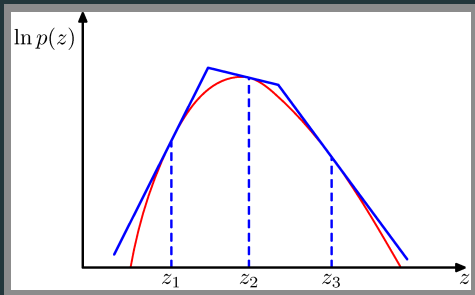
the Box-Muller Method

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

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

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

(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

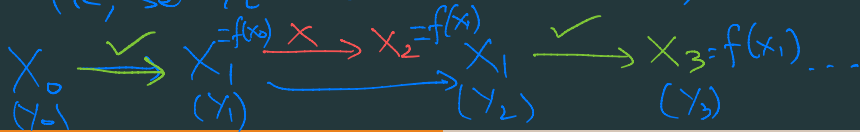
$$X_1, X_2, X_3, \dots, X_L \rightarrow Y_1, Y_2, Y_3, \dots, Y_L$$

✓ ✓ ✗ ✓

- Method 3 - Generate $X_1, X_2 = f(X_1), X_3 = f(X_2), \dots$

- Accept/Reject X_t w.p. $A(X_{t-1}, X_t)$

(ie, 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

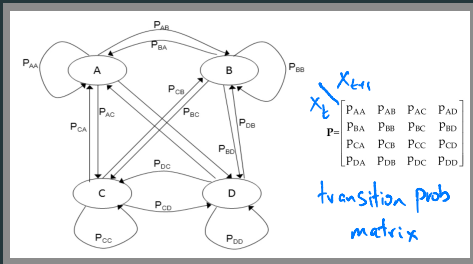
iff
$$P(X_i | X_1, X_2, \dots, X_{i-1}) = P(X_i | X_{i-1})$$

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 Bayes Net!

- State-space = $\{A, B, C, D\}$

- $P(X_{t+1}=A | X_t=B) = \underline{\underline{P_{BA}}}$

does not depend on X_{t-1}

• $\sum P_{Ax} = 1 \forall A \equiv$ Each row-sum of $P = 1, P_{ij} \geq 0 \forall ij$
x: outgoing edges
 (stochastic matrix)

• Directed (not necessarily, acyclic) graph

• Let $\pi_t \leftarrow$ row vector \equiv Distribution of $X_t = P[X_t=x | X_0]$

Then $\pi_{t+1} = \pi_t \cdot P = \begin{bmatrix} \pi_t \end{bmatrix} \begin{bmatrix} \cdot & P & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$

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)

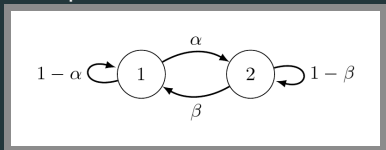
1) X_t can get 'absorbed'
 (not interesting for us --)



2) π_t can 'converge' to a fixed distrib π 'steady-state dist'

(recall $\pi_t = \pi_{t-1} P \Rightarrow \pi = \pi P$)

example:

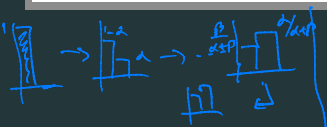


$\pi_0 = (1, 0)$ (i.e., start at '1')

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

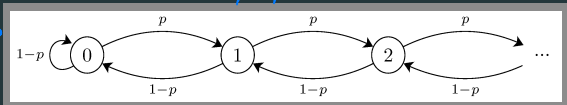
\vdots

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



markov chains: example (infinite Markov Chain)

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



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

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

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

all else is 0

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

• Steady-state $\pi(i)$

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

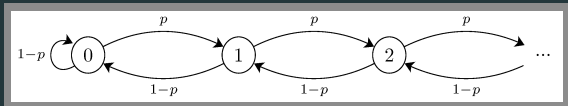
• Claim - $\pi(i) = \frac{1}{2} \left(\frac{p}{1-p}\right)^i$ (assuming $p < \frac{1}{2}$)
 $\Rightarrow Z = \sum \left(\frac{p}{1-p}\right)^i$

'Proof': $\forall i > 0, \sum_j \pi(j) P_{ji} = \frac{1}{2} \left(\frac{p}{1-p}\right)^i \cdot (p + 1-p)$

$$\sum_j \pi(j) P_{ji} = \frac{1}{2} \left(\left(\frac{p}{1-p}\right)^{i-1} \cdot p + \left(\frac{p}{1-p}\right)^{i+1} (1-p) \right)$$

markov chains: reversibility

(idea 'borrowed' from physics)



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

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

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

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

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

Pf - check $(*) \Rightarrow (**)$

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

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

- if $i = j+1$

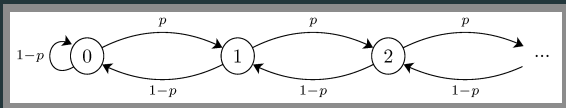
$$\frac{1}{2} \left(\frac{p}{1-p} \right)^i \cdot (1-p)$$

$$\pi(i) P_{ij}$$

$$\frac{1}{2} \left(\frac{p}{1-p} \right)^{i-1} \cdot p$$

$$\pi(i-1) P_{ji}$$

Markov chains: the ergodic theorem



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

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

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

$X \sim \pi$ 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 $\mathbb{E}_{x \sim P}[\phi(x)]$)

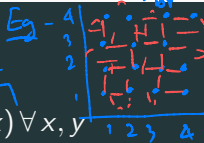
- This requires the MC R to have steady-state dist as P (i.e., want $P = PR$)

the Metropolis algorithm

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

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

$\Theta \equiv$ move to random place

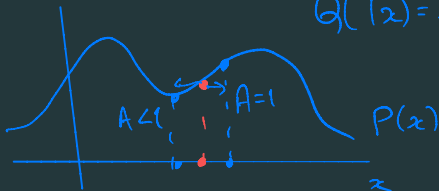


Metropolis sampling

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 $A(Y_t, Z_{t-1}) = \min\left\{1, \frac{\tilde{P}(Y_t)}{\tilde{P}(Z_{t-1})}\right\}$
else **reject** and set $Z_t = Z_{t-1}$

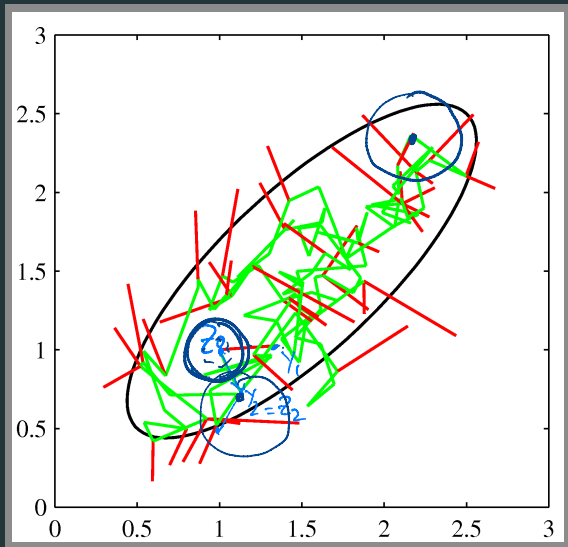


$$Q(x|z) = \frac{1}{2} \exp\left(-\frac{|x-z|}{2}\right)$$

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

$$Q(x|y) = N(0, \sigma I)$$



Metropolis algorithm: proof of correctness

• Want to show P is a steady state distⁿ

$$\begin{aligned} - \forall x, y, R_{xy} &= P[x \rightarrow y] = Q(y|x) \cdot A(x, y) \\ R_{xx} &= \sum_y Q(y|x) (1 - A(x, y)) \end{aligned}$$

- Now we check local balance, i.e., $\forall x, y$

$$P(x) R_{xy} = P(x) \cdot Q(y|x) \cdot \max\left(1, \frac{\tilde{P}(y)}{P(x)}\right)$$

|| Symmetric

$$P(y) R_{yx} = P(y) \cdot Q(x|y) \cdot \max\left(1, \frac{\tilde{P}(x)}{P(y)}\right)$$

Also $\forall x, y$, 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 $A(Y_t, Z_{t-1}) = \min \left\{ 1, \frac{\tilde{P}(Y_t)Q(Z_{t-1}|Z_t)}{\tilde{P}(Z_{t-1})Q(Z_t|Z_{t-1})} \right\}$
else **reject** and set $Z_t = Z_{t-1}$

Gibbs sampling

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

Gibbs sampling

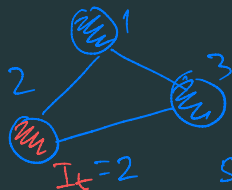
1. choose initial $X_0 = (X_0(1), X_0(2), \dots, X_0(n))$
2. to obtain sample t :

pick I_t uniformly at random (alternate - pick in round robin order)

set $\underline{X_t(i)} = X_{t-1}(i)$ for $i \neq I_t$ ie, $I_1=1, I_2=2, \dots, I_n=n, I_{n+1}=1, I_{n+2}=2, \dots$

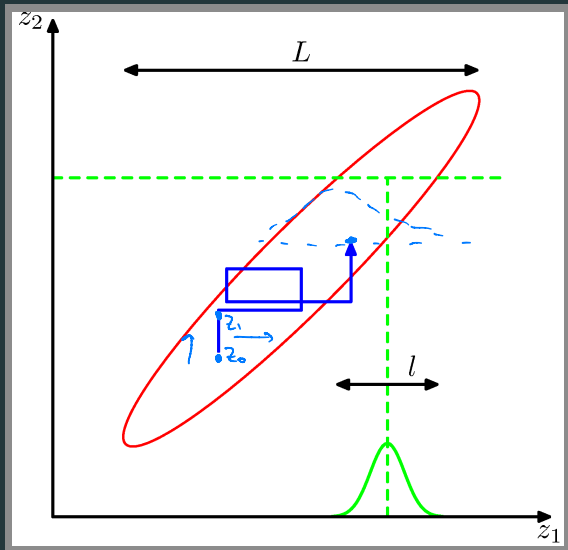
set $\underline{X_t(I_t)} \sim P(\cdot | X_{t-1} \setminus X_{t-1}(I_t))$

ie, fix all $X(i)$ 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

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

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

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

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