

# Markov Chain Monte Carlo

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<https://github.com/roboticcam/machine-learning-notes>

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# Metropolis Hasting Algorithm

1. initialise  $x^{(0)}$
  2. **for**  $i = 0$  to  $N - 1$ 
    - $u \sim U(0, 1)$
    - $x^* \sim q(x^* | x^{(i)})$
    - if**  $u < \min \left( 1, \frac{\pi(x^*)q(x | x^*)}{\pi(x)q(x^* | x)} \right)$ 
      - $x^{(i+1)} = x^*$
    - else**
      - $x^{(i+1)} = x^{(i)}$
- ▶ The take-home message here, is that it does not “disgard” samples like rejection sampling. It simply “repeats” samples.
  - ▶ If the same sample repeats too many times, it has **bad mixing**
  - ▶ see demo for an example.

# Metropolis Hasting - Why it work?

- ▶  $K(x \rightarrow x^*)$  includes the joint density of the following:
  1. Propose  $x^*$  from  $q(x^*|x)$ ,
  2. then accept  $x^*$  with ratio  $\alpha(x^*, x) = \min\left(1, \frac{\pi(x^*)q(x|x^*)}{\pi(x)q(x^*|x)}\right)$
- ▶ very easily verify it satisfy **detailed balance**:

$$\begin{aligned}\pi(x)q(x^*|x)\alpha(x^*, x) &= \pi(x)q(x^*|x) \min\left(1, \frac{\pi(x^*)q(x|x^*)}{\pi(x)q(x^*|x)}\right) \\ &= \min(\pi(x)q(x^*|x), \pi(x^*)q(x|x^*)) \\ &= \pi(x^*)q(x|x^*) \min\left(1, \frac{\pi(x)q(x^*|x)}{\pi(x^*)q(x|x^*)}\right) \\ &= \pi(x^*)q(x|x^*)\alpha(x, x^*)\end{aligned}$$

- ▶ note that  $\alpha(x^*, x) \neq \alpha(x, x^*)$
- ▶ **Exercise** wait a second, are we missing anything here?

# Metropolis Hasting - Missing the self transition part

- ▶ when  $x^*$  is accepted, it's accepted on a specific value  $\sim q(\cdot)$
- ▶ when  $x^*$  is discarded for a  $x$  repeat,  $x^*$  can be a **range of values**  $\sim q(\cdot)$ :

$$\begin{cases} p(x^* \neq x) &= \alpha(x) \\ p(x^* = x) &= 1 - \alpha(x) \end{cases}$$

$$\begin{aligned} p(x^* \neq x) &= \alpha(x) = \int_{x^*} p(x^* \neq x | x^*, x) q(x^* | x) dx^* \\ &= \int_{x^*} \alpha(x^*, x) q(x^* | x) dx^* \end{aligned}$$

$$p(x^* = x) = 1 - \alpha(x) = 1 - \int_{x^*} \alpha(x^*, x) q(x^* | x) dx^*$$

$$K(x \rightarrow x^*) = q(x^* | x) \alpha(x^*, x) + \underbrace{\delta_x(x^*)}_{=0: \text{when } x \neq x^*} (1 - \alpha(x))$$
$$\qquad \qquad \qquad \underbrace{\hspace{10em}}_{=\delta_{x^*}(x)(1-\alpha(x^*))}$$

# Two stage acceptance rule

let  $\pi(x) \propto L(x)\pi^P(x)$ :

$$\begin{aligned}\alpha(x^*, x) &= \min \left( 1, \frac{\pi(x^*)q(x|x^*)}{\pi(x)q(x^*|x)} \right) \\ \Rightarrow \alpha(x^*, x) &= \min \left( 1, \underbrace{\frac{\pi^P(x^*)q(x|x^*)}{\pi^P(x)q(x^*|x)}}_{\text{cheaper to compute}} \right) \min \left( 1, \frac{L(x^*)}{L(x)} \right)\end{aligned}$$

# Hamiltonian Metropolis Hasting (HMC)

- ▶ Let Hamiltonian to be  $H(q, p)$
- ▶ where  $q$  is the position and  $p$  is the momentum, for each dimension  $i$ :

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

- ▶ For HMC, we usually use Hamiltonian function:

$$H(q, p) = U(q) + K(p)$$

- ▶ As an example:

$$H(q, p) = U(q) + K(p) = \frac{q^2}{2} + \frac{p^2}{2}$$

- ▶ the solution is:

$$q(t) = r \cos(a + t) \quad p(t) = -r \sin(a + t)$$

# Reversibility of Hamiltonian dynamics

- ▶ Let a mapping function  $T_s$  and its inverse  $T_{-s}$ :

$$\begin{aligned}T_s(q(t), p(t)) &= (q(t+s), p(t+s)) \\ T_{-s}(q(t+s), p(t+s)) &= (q(t), p(t))\end{aligned}$$

- ▶ are invariant under a reversal of the direction of time  $t \rightarrow -t$ , when  $q_i$  and  $p_i$  are changed to:

$$q_i \rightarrow q_i \quad p_i = \frac{dq_i}{dt} \rightarrow \frac{dq_i}{d(-t)} = -p_i$$

- ▶ this implies:

$$\frac{dq_i}{d(-t)} = -\frac{\partial H}{\partial p_i} \quad \frac{d(-p_i)}{d(-t)} = -\frac{\partial H}{\partial q_i}$$

- ▶ or:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

- ▶ form of equations does not change: rate of change is the reversed.
- ▶ at  $t$ , evolution is stopped, sign of velocity is reversed
- ▶ system is allowed to evolve once again for another time interval  $t$ ; return to its original starting point

# Gibbs sampling

Gibbs sampling algorithm:

- ▶ given a starting sample  $(x_1, y_1, z_1)^\top$
- ▶ you want to sample

$$\{(x_2, y_2, z_2)^\top, (x_3, y_3, z_3)^\top, \dots, (x_N, y_N, z_N)^\top\} \sim P(x, y, z)$$

- ▶ Then the algorithm goes:

$$x_2 \sim P(x|y_1, z_1)$$

$$y_2 \sim P(y|x_2, z_1)$$

$$z_2 \sim P(z|x_2, y_2)$$

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$$x_3 \sim P(x|y_2, z_2)$$

$$y_3 \sim P(y|x_3, z_2)$$

$$z_3 \sim P(z|x_3, y_3)$$

...



# Gibbs sampling Toy Example

In this toy example, let's sample:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right)$$

$$x_1 | x_2 \sim \mathcal{N} \left( \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (x_2 - \mu_2), \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \right)$$

$$x_2 | x_1 \sim \mathcal{N} \left( \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (x_1 - \mu_1), \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \right)$$

# A special case of M-H

Looking at the M-H acceptance ratio

- ▶ Let  $\mathbf{x} = x_1, \dots, x_D$ .
- ▶ When sampling  $k^{\text{th}}$  component,  $q_k(\mathbf{x}^*|\mathbf{x}) = \pi(x_k^*|\mathbf{x}_{-k})$
- ▶ When sampling  $k^{\text{th}}$  component,  $\mathbf{x}_{-k}^* = \mathbf{x}_{-k}$

$$\frac{\pi(\mathbf{x}^*)q(\mathbf{x}|\mathbf{x}^*)}{\pi(\mathbf{x})q(\mathbf{x}^*|\mathbf{x})} = \frac{\pi(\mathbf{x}^*)\pi(x_k|\mathbf{x}_{-k}^*)}{\pi(\mathbf{x})\pi(x_k^*|\mathbf{x}_{-k})} = \frac{\pi(x_k^*|\mathbf{x}_{-k}^*)\pi(x_k|\mathbf{x}_{-k}^*)}{\pi(x_k|\mathbf{x}_{-k})\pi(x_k^*|\mathbf{x}_{-k})} = 1$$

# Collapsed Gibbs sampling

- ▶ Treats  $(x, y)$  as a single variable

$$\begin{aligned}(x_2, y_2) &\sim P(x, y|z_1) &\implies x_2 &\sim p(x|z_1) &y_2 &\sim p(y|x_2, z_1) \\ z_2 &\sim P(z|x_2, y_2)\end{aligned}$$

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$$\begin{aligned}(x_3, y_3) &\sim P(x, y|z_2) &\implies x_3 &\sim p(x|z_2) &y_3 &\sim p(y|x_3, z_2) \\ z_3 &\sim P(z|x_3, y_3)\end{aligned}$$

...

- ▶ However, we need to know how to compute:

$$P(x|z) = \int_y P(x, y|z) dy$$

- ▶ The algorithm reduces **auto-correction**.

# What is auto-correction

- ▶ lag-k **autocovariance** of the functional  $g(X_1), g(X_2)$

$$\gamma(k) = \text{cov}(g(X_i), g(X_{i+k}))$$

- ▶ lag-k **autocorrelation** of the functional  $g(X_1), g(X_2)$

$$\frac{\gamma(k)}{\gamma(0)}$$

- ▶ need to perform **thinning** to make samples more like drawn using i.i.d
- ▶ Let's look at an autocorrelation **demo** for computing multivariate Gaussian distribution of having 2-D, ... 5-D.
- ▶ **Exercise** what would be an appropriate  $g(\cdot)$  used here?
- ▶ **Homework** you need to write a similar code

# Parallel Gibbs sampling

- ▶ You can see the algorithm won't "parallelise".
- ▶ However, under some models (and clever work-around) machine learning researcher able to parallelise some Gibbs sampling scheme for various models, typically, using

$$p(x_1, x_2, \dots, x_n) = \int_u p(x_1, x_2, \dots, x_n | u) p(u) du$$

and also have the property that:

$$p(x_1, x_2, \dots, x_n | u) = \prod_{i=1}^n p(x_i | u)$$

- ▶ Well, make sense to perform inference to **Big data** with CUDA, multiple processors.

# Convergence Diagnostics

- ▶ The question is when to stop sampling.
- ▶ **word of caution:** individual sample do not converge. It's the entire distribution.
- ▶ sample will generally be correlated with each other, slowing the algorithm in its attempt to sample from the entire stationary distribution
- ▶ run **convergence diagnostics**: *Cowles, M.K.; Carlin, B.P. (1996). "Markov chain Monte Carlo convergence diagnostics: a comparative review". Journal of the American Statistical Association. 91: 883 - 904.*
- ▶ or using R Package 'coda'

- Potts Model:

$$M(\Pi) \propto \exp \left( \sum_{i < j} \beta_{ij} \mathbf{1}_{z_i = z_j} \right)$$

- Swendsen-Wang algorithm: The joint density between **nodes**  $\Pi$  and edges  $r_{ij} \in \{0, 1\}$ :

$$P(\Pi, \mathbf{r}) = P(\Pi) p(\mathbf{r} | \Pi)$$

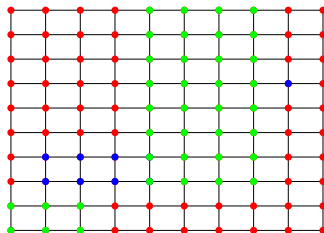
- each edges can be sampled independently:

$$P(r_{ij} = 0 | \Pi) = \exp(-\beta_{ij} \mathbf{1}_{z_i = z_j}) = q_{ij}$$

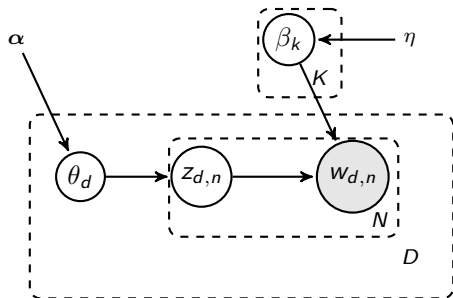
$$P(\mathbf{r} | \Pi) = \prod_{1 \leq i < j \leq n} P(r_{ij} | \Pi)$$

- the **trick** is to sample the nodes condition on the edges:

$$P(\Pi | \mathbf{r}) = \prod_{1 \leq i < j \leq n} [\exp(\beta_{ij} \mathbf{1}_{z_i = z_j}) - 1]^{r_{ij}}$$



# A real sampling example: Latent Dirichlet Allocation



- ▶  $\beta_k \sim \text{Dir}(\eta, \dots, \eta)$  for  $k \in \{1, \dots, K\}$ .
- ▶ For each document  $d$ :
  - $\theta \sim \text{Dir}(\alpha, \dots, \alpha)$
  - For each word  $w \in \{1, \dots, N\}$ :
    - $z_{dn} \sim \text{Mult}(\theta_d)$
    - $w_{dn} \sim \text{Mult}(\beta_{z_{dn}})$



# Basic tools: Multinomial-Dirichlet

## Posterior

$$\begin{aligned} & P(p_1, \dots, p_k | n_1, \dots, n_k) \\ & \propto \underbrace{\frac{\Gamma(\sum_{i=1}^k \alpha_i)}{\prod_{i=1}^k \Gamma(\alpha_i)} \prod_{i=1}^k p_i^{\alpha_i-1}}_{\text{Dir}(p_1, \dots, p_k | \alpha_1, \dots, \alpha_k)} \underbrace{\frac{n!}{n_1! \dots n_k!} \prod_{i=1}^k p_i^{n_i}}_{\text{Mult}(n_1, \dots, n_k | p_1, \dots, p_k)} \\ & \propto \prod_{i=1}^k p_i^{\alpha_i-1} \prod_{i=1}^k p_i^{n_i} = \prod_{i=1}^k p_i^{\alpha_i-1+n_i} \\ & = \text{Dir}(p_1, \dots, p_k | \alpha_i + n_i, \dots, \alpha_k + n_k) \end{aligned}$$

## Marginal

$$\begin{aligned} p(n_1, \dots, n_k) &= \int_{p_1, \dots, p_k} P(p_1, \dots, p_k, n_1, \dots, n_k) \\ &= \frac{\Gamma(\sum_{i=1}^k \alpha_i)}{\prod_{i=1}^k \Gamma(\alpha_i)} \frac{n!}{n_1! \dots n_k!} \int_{p_1, \dots, p_k} \prod_{i=1}^k p_i^{\alpha_i-1+n_i} \\ &= \frac{N!}{n_1! \dots n_k!} \times \frac{\Gamma(\sum_{i=1}^k \alpha_i)}{\prod_{i=1}^k \Gamma(\alpha_i)} \times \frac{\prod_{i=1}^k \Gamma(\alpha_i + n_i)}{\Gamma(N + \sum_{i=1}^k \alpha_i)} \end{aligned}$$

# Gibbs sampling for Latent Dirichlet Allocation

The parameters of the model include:

- ▶  $\{\beta_k\}_{k=1}^K$  each  $\beta_k$  has dimension  $V$  (vocab)
- ▶  $\{\theta_d\}_{d=1}^D$
- ▶  $\{z_{dn} \in \{1 \dots D\}, n \in \{1 \dots N\}\}$

since everything **conjugate**, posterior inference is easy:

- ▶ start with random initial values to all the variables
- ▶  $\beta_k \sim \text{Dir}(\eta + N_1^{(v)}, \dots, \eta + N_K^{(v)})$  for  $k \in \{1, \dots, K\}$   
where  $N_v^{(v)} = \#(\{w_{dn} = v \text{ AND } z_{dn} = k\})$
- ▶ For each document  $d$ :  
 $\theta_d \sim \text{Dir}(\alpha + N_1^{(d)}, \dots, \alpha + N_K^{(d)})$   
where  $N_k^{(d)} = \#(\{z_{dn} = k\})$   
For each word  $w \in \{1, \dots, N\}$ :

- ▶  $\beta_k \sim \text{Dir}(\eta, \dots, \eta)$  for  $k \in \{1, \dots, K\}$ .
- ▶ For each document  $d$ :  
 $\theta \sim \text{Dir}(\alpha, \dots, \alpha)$   
For each word  
 $w \in \{1, \dots, N\}$ :  
 $z_{dn} \sim \text{Mult}(\theta_d)$   
 $w_{dn} \sim \text{Mult}(\beta_{z_{dn}})$

$$\begin{aligned}\Pr(z_{dn} = k) &= \Pr(w_{dn} | z_{dn}, \beta_k) p(z_{dn} | \theta_d) \\ &\propto \beta_{k, w_{dn}} \theta_d\end{aligned}$$

# Exercise and Homework for LDA

- ▶ **Exercise** For the Gibbs sampling of each of the set of variables, verify they are true, i.e.,

$$\begin{aligned} p\left(\beta_k | \{\beta_j\}_{j=1, j \neq k}^K, \{\theta_d\}_{d=1}^D, \{z_{d \in \{1 \dots D\}, n \in \{1 \dots N\}}\}\right) \\ &= \text{Dir}(\eta + N_1^{(v)}, \dots, \eta + N_V^{(v)}) \\ p\left(\theta_d | \{\beta_j\}_{j=1, j \neq k}^K, \{\theta_j\}_{j=1, j \neq d}^D, \{z_{d \in \{1 \dots D\}, n \in \{1 \dots N\}}\}\right) \\ &= \text{Dir}(\alpha + N_1^{(d)}, \dots, \alpha + N_K^{(d)}) \\ p\left(z_{dn} = k | \{\beta_j\}_{j=1, j \neq k}^K, \{\theta_d\}_{d=1}^D, \{z_{d \in \{1 \dots D\}, j \in \{1 \dots N\}, j \neq n}\}\right) \\ &\propto \beta_{k, w_{dn}} \theta_d \end{aligned}$$

- ▶ **Homework** generate a set of synthetic values for all variables and  $\{w_{dn}\}$ 
  - ▶ think about the structure for each of the variables
  - ▶ caution: MATLAB has no dirichlet generator, what is the alternative?

# Collapsed sampling for LDA

- ▶ we may only interested in sampling  $\{z_d \in \{1 \dots D\}, n \in \{1 \dots N\}\}$
- ▶ we could collapse both  $\{\beta_j\}_{j=1, j \neq k}^K$  and  $\{\theta_d\}_{d=1}^D$ ,

$$p(z_{dn} | \mathbf{z}_{-dn}, \mathbf{w})$$

where  $\mathbf{z}_{-dn}$  are all the  $\mathbf{z}$  except  $z_{dn}$

$$\begin{aligned} \Pr(z_{dn} | \mathbf{z}_{-dn}, \mathbf{w}) &\propto \Pr(z_{dn}, \mathbf{z}_{-dn}, w_{dn}, \mathbf{w}_{-dn}) \\ &= \Pr(w_{dn} | z_{dn}, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \Pr(z_{dn}, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \\ &= \Pr(w_{dn} | z_{dn}, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \Pr(z_{dn} | \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \Pr(\mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \\ &\propto \Pr(w_{dn} | z_{dn}, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \underbrace{\Pr(z_{dn} | \mathbf{z}_{-dn})}_{\text{there is no } \mathbf{w}, \text{prior}} \end{aligned}$$

- ▶ note that, previously,  
 $\Pr(w_{dn} | z_{dn}, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}, \beta) = \Pr(w_{dn} | z_{dn}, \beta_k) = \beta_{z_{dn}, w_{dn}}$

look at:  $p(z_{dn} = i | \mathbf{z}_{-dn})$

$$\Pr(z_{dn} | \mathbf{z}_{-dn}, \mathbf{w}) \propto p(w_{dn} | z_{dn}, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \underbrace{\Pr(z_{dn} | \mathbf{z}_{-dn})}$$

- ▶ Looking at  $\Pr(z_{dn} = i | \mathbf{z}_{-dn})$  using  $i$  instead of loop index  $k$ :

$$\begin{aligned} \Pr(z_{dn} = i | \mathbf{z}_{-dn}) &= \int_{\theta_d} p(z_{dn} = i, \theta_d | \mathbf{z}_{-dn}) d\theta_d \\ &= \int_{\theta_d} \Pr(z_{dn} = i | \theta_d) p(\theta_d | \mathbf{z}_{-dn}) d\theta_d \\ &\propto \int_{\theta_d} \Pr(z_{dn} = i | \theta_d) \underbrace{\Pr(\mathbf{z}_{-dn} | \theta_d) p(\theta_d)} d\theta_d \\ &= \int_{\theta_d} \text{Mult}(z_{dn} = i | \theta_d) \underbrace{\text{Dir}(\alpha + N_1^{(d)}, \dots, \alpha + N_K^{(d)})} d\theta_d \\ &= \frac{\Gamma(\sum_{k=1}^K (\alpha + N_k^{(d)}))}{\prod_{k=1}^K \Gamma(\alpha + N_k^{(d)})} \times \frac{\Gamma((\alpha + N_i^{(d)}) + 1) \left( \prod_{k=1, k \neq i}^K \Gamma((\alpha + N_k^{(d)})) \right)}{\Gamma(1 + \sum_{k=1}^K (\alpha + N_k^{(d)}))} \\ &= \frac{\alpha + N_i^{(d)}}{\sum_{k=1}^K (\alpha + N_k^{(d)})} = \frac{\alpha + N_i^{(d)}}{K\alpha + N^{(d)}} \end{aligned}$$

- ▶  $N_i^{(d)}, N^{(d)}$  are counted without  $z_{dn}$ , i.e.  $N_k^{(d)} = \#(\{z_{dn \neq dn} = i\})$

look at:  $p(w_{dn}|z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn})$

$$\Pr(z_{dn}|\mathbf{z}_{-dn}, \mathbf{w}) \propto \underbrace{p(w_{dn}|z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn})}_{\text{using } i \text{ instead of loop index } k} \Pr(z_{dn}|\mathbf{z}_{-dn})$$

- ▶ Looking at  $\Pr(w_{dn}|z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn})$  using  $i$  instead of loop index  $k$ :

$$\begin{aligned} \Pr(w_{dn}|z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) &= \int_{\beta} \Pr(w_{dn}, \beta|z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) d\beta \\ &= \int_{\beta} \Pr(w_{dn}|\beta, z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \underbrace{p(\beta, z_{dn} = i|\mathbf{z}_{-dn}, \mathbf{w}_{-dn})}_{\text{using } i \text{ instead of loop index } k} p(\mathbf{z}_{-dn}, \mathbf{w}_{-dn}) d\beta \\ &\propto \int_{\beta_i} \Pr(w_{dn}|\beta, z_{dn} = i) \underbrace{p(\beta_i|\mathbf{z}_{-dn}, \mathbf{w}_{-dn})}_{\text{using } i \text{ instead of loop index } k} d\beta_i \\ &= \int_{\beta_i} \beta_{i, w_{dn}} \underbrace{\text{Dir}(\eta + N_1^{(v)}, \dots, \eta + N_V^{(v)})}_{\text{using } i \text{ instead of loop index } k} d\beta_i \end{aligned}$$

this is just the expectation of  $\beta_{i, w_{dn}}$ , i.e., the  $w_{dn}^{\text{th}}$  component of vector  $\beta_i$

- ▶ using expectation of Dirichlet distribution:

$$\Pr(w_{dn}|z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) = \frac{\eta + N_{w_{dn}}^{(v)}}{\sum_{v \in \{1, \dots, V\}} \eta + N_{w_{dn}}^{(v)}} = \frac{\eta + N_{w_{dn}}^{(v)}}{V\eta + N^{(v)}}$$

where  $N_v^{(v)} = \#(\{w_{\tilde{dn} \neq dn} = v \text{ AND } z_{\tilde{dn} \neq dn} = i\})$

# Putting things together

$$\begin{aligned}\Pr(z_{dn} = i | \mathbf{z}_{-dn}, \mathbf{w}) &\propto \Pr(w_{dn} | z_{dn} = i, \mathbf{z}_{-dn}, \mathbf{w}_{-dn}) \Pr(z_{dn} = i | \mathbf{z}_{-dn}) \\ &= \frac{\eta + N_{w_{dn}}^{(v)}}{V\eta + N^{(v)}} \frac{\alpha + N_i^{(d)}}{K\alpha + N^{(d)}}\end{aligned}$$

where:

- ▶  $N_k^{(d)} = \#(\{z_{\tilde{dn} \neq dn} = i\})$
- ▶  $N_v^{(v)} = \#(\{w_{\tilde{dn} \neq dn} = v \text{ AND } z_{\tilde{dn} \neq dn} = i\})$

# What about $\beta$ and $\theta_d$

- **Exercise** think about what you are going to do for  $\beta$  and  $\theta_d$  when  $\mathbf{z}$  are available



# Slice Sampling - joint density with auxiliary variable and marginal

- ▶ given some un-normalised function  $f(x)$ , where

$$Z = \int f(x) dx \quad \pi(x) = \frac{f(x)}{Z}$$

- ▶ Introduce auxiliary variable  $u$  a joint distribution over  $(x, u)$  is defined as:

$$\pi(x, u) = \begin{cases} 1/Z & \text{if } 0 < u < f(x) \\ 0 & \text{otherwise} \end{cases}$$

- ▶ The joint density of  $(x, u)$  is uniform over the region

$$\{(x, u) : 0 < u < f(x)\}$$

- ▶ Marginal distribution over  $x$  is:

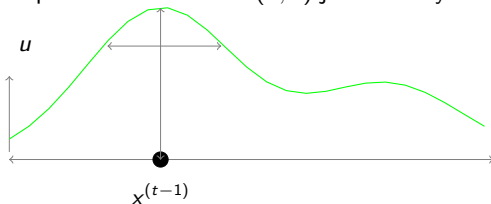
$$\pi(x) = \int_0^{f(x)} \frac{1}{Z} du = \frac{f(x)}{Z} = \pi(x)$$

- ▶ if  $\pi(x) \propto L(x)\pi^p(x)$ :

$$\begin{aligned} u &\sim U(0, L(x^{(t-1)})) & x^{(t)} &\sim U(1[\pi(x) > u\pi^p(x)]) \\ \implies x^{(t)} &\sim U(1[L(x) > u]) \end{aligned}$$

# Slice Sampling - conditional

- ▶ Top-down view of the  $\pi(u, x)$  joint density:



- ▶ using gibbs sampling:

$$u \sim U(0, \pi(x^{(t-1)}))$$

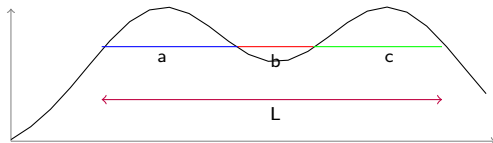
$$x^{(t)} \sim U(\mathbf{1}[\pi(\cdot) > u])$$

- ▶ Very powerful technique, been working with it in a number of non-parametric Bayes settings.

# Slice Sampling - Shrink algorithm

- ▶ Usually, its **not** simple to sample  $x^{(t)} \sim \mathbf{1}[p(x) > u]$ , given  $p(x)$  is usually not a concave function.
- ▶ We need to use “shrinkage algorithm” or “expansion algorithm”
- ▶ to see why “shrinkage” targets the right distribution:

# Shrinkage algorithm



$$\Pr(X^{(t)} \in a \rightarrow X^{(t+1)} \in a) = \frac{a+b}{L}$$

$$\Pr(X^{(t)} \in a \rightarrow X^{(t+1)} \in c) = \frac{c}{L}$$

$$\Pr(X^{(t)} \in c \rightarrow X^{(t+1)} \in a) = \frac{a}{L}$$

$$\Pr(X^{(t)} \in c \rightarrow X^{(t+1)} \in c) = \frac{b+c}{L}$$

Therefore,

$$\begin{aligned}\Pr(X^{(t+1)} \in a) &= \Pr(X^{(t)} \in a \rightarrow X^{(t+1)} \in a) \Pr(X^{(t)} \in a) + \Pr(X^{(t)} \in c \rightarrow X^{(t+1)} \in a) \Pr(X^{(t)} \in c) \\ &= \frac{a+b}{L} \frac{a}{L} + \frac{a}{L} \frac{c}{L} = \frac{a^2 + ab + ac}{L^2} = \frac{a}{L} = \Pr(X^{(t)} \in a)\end{aligned}$$

$$\begin{aligned}\Pr(X^{(t+1)} \in c) &= \Pr(X^{(t)} \in a \rightarrow X^{(t+1)} \in c) \Pr(X^{(t)} \in a) + \Pr(X^{(t)} \in c \rightarrow X^{(t+1)} \in c) \Pr(X^{(t)} \in c) \\ &= \frac{c}{L} \frac{a}{L} + \frac{b+c}{L} \frac{c}{L} = \frac{ac + bc + c^2}{L^2} = \frac{c}{L} = \Pr(X^{(t)} \in c)\end{aligned}$$

$$\Pr(X^{(t+1)}) = \Pr(X^{(t)})$$

# Elliptical Slice Sampling

Murray, Iain, and Ryan P. Adams. "Slice sampling covariance hyperparameters of latent Gaussian models.", *NIPS 2010*

1. choose ellipse:  $v \sim \mathcal{N}(0, \Sigma)$
2. log-likelihood threshold:

$$u \sim U(0, 1)$$
$$\log(y) = \log(L(x)) + \log(u) \implies y = uL(x)$$

3. draw an initial proposal, and defining a bracket:

$$\theta \sim U(0, 2\pi)$$
$$[\theta_{\min}, \theta_{\max}] = [\theta - 2\pi, \theta]$$

4.  $x^* = x \cos(\theta) + v \sin(\theta)$
5. if  $\log(L(x^*)) > \log(y)$ , i.e.,  $L(x^*) > uL(x)$  (this is similar to slice sampling)
6.     **accept:** return  $x^*$
7. **else**  
    shrink the bracket - the following procedure only "shrink" one-side:
8.     **if**  $\theta < 0$  **then:**  $\theta_{\min} = \theta$  **else:**  $\theta_{\max} = \theta$   
        think about what happens when:  $(\theta_{\max} > 0, \theta_{\min} > 0)$ ,  $(\theta_{\max} < 0, \theta_{\min} < 0)$  and  $(\theta_{\max} > 0, \theta_{\min} < 0)$   
        try a new point:
9.      $\theta \sim U(\theta_{\min}, \theta_{\max})$
10.    **Goto** step 4

# detailed balance

- let's look at again  $K(x \rightarrow x^*)$  extended to variables  $u$  and  $v$ :

$$\begin{aligned}
 & \pi(x)K(x \rightarrow x^*) \\
 &= \underbrace{\pi(x)}_{L(x)\mathcal{N}(0,\Sigma)} \underbrace{p(\text{height}|x)}_{\pi(u|x)} \underbrace{p(\text{shape})}_{\pi(v)} \pi(x^*|\text{height, shape}) \mathbf{1}(\mathcal{E}(x, u, v), \mathcal{E}(x^*, u^*, v^*)) \\
 &= L(x)\mathcal{N}(x|0, \Sigma) \underbrace{\frac{1}{L(x)}}_{\text{height - not } \pi(x)} \underbrace{\mathcal{N}(v|0, \Sigma)}_{\text{shape}} \underbrace{p(\{\theta_k\}, x^*|\mathcal{E}(x, u, v), x)}_{\text{shrink ellipse to accept } x^*} \mathbf{1}(\mathcal{E}(x, u, v), \mathcal{E}(x^*, u^*, v^*)) \\
 &= \mathcal{N}(x|0, \Sigma)\mathcal{N}(v|0, \Sigma)p(\{\theta_k\}, x^*|\mathcal{E}(x, u, v), x) \mathbf{1}(\mathcal{E}(x, u, v), \mathcal{E}(x^*, u^*, v^*))
 \end{aligned}$$

- In order to prove **reversibility**:

$$\begin{aligned}
 \pi(x)K(x \rightarrow x^*) &= \pi(x^*)K(x^* \rightarrow x) \implies \\
 & \mathcal{N}(x|0, \Sigma)\mathcal{N}(v|0, \Sigma)p(\{\theta_k\}, x^*|\underbrace{\mathcal{E}(x, u, v), x}_{\text{same ellipse}}) \\
 &= \mathcal{N}(x^*|0, \Sigma)\mathcal{N}(v^*|0, \Sigma)p(\{\theta'_k\}, x|\underbrace{\mathcal{E}(x^*, u^*, v^*), x^*}_{\text{same ellipse}})
 \end{aligned}$$

- here comes a central thing **clever idea**, can we always find a  $v'$  such that:  
**firstly**  $\text{ellipse}(x, u, v) = \text{ellipse}(x^*, u^*, v^*)$   
**secondly**  $\mathcal{N}(x|0, \Sigma)\mathcal{N}(v|0, \Sigma) = \mathcal{N}(x^*|0, \Sigma)\mathcal{N}(v^*|0, \Sigma)$

# “Same-dimension” rotation factor of Gaussian

$$\text{Let } \begin{bmatrix} x'_1 \\ v'_1 \end{bmatrix} = \mathcal{R}(\theta) \begin{bmatrix} x_1 \\ v_1 \end{bmatrix} \text{ and } \begin{bmatrix} x'_2 \\ v'_2 \end{bmatrix} = \mathcal{R}(\theta) \begin{bmatrix} x_2 \\ v_2 \end{bmatrix}$$

$$\text{Collectively, we write the above as: } \begin{bmatrix} \mathbf{x}' \\ \mathbf{v}' \end{bmatrix} = \mathcal{R}(\theta) \begin{bmatrix} \mathbf{x} \\ \mathbf{v} \end{bmatrix} \implies \begin{bmatrix} \mathbf{x} \\ \mathbf{v} \end{bmatrix} = \mathcal{R}(-\theta) \begin{bmatrix} \mathbf{x}' \\ \mathbf{v}' \end{bmatrix}$$

$$\begin{aligned} & \mathcal{N}(\mathbf{x}'|0, \Sigma)\mathcal{N}(\mathbf{v}'|0, \Sigma) \\ &= \exp \left[ \frac{-1}{2} \left( \Sigma_{1,1}(x'^2_1 + v'^2_1) + 2\Sigma_{1,2}(x'_1x'_2 + v'_1v'_2) + \Sigma_{2,2}(x'^2_2 + v'^2_2) \right) \right] \end{aligned}$$

We know that,

$$\begin{aligned} x'_1x'_2 + v'_1v'_2 &= [\cos(\theta)x_1 - \sin(\theta)v_1][\cos(\theta)x_2 - \sin(\theta)v_2] + [\sin(\theta)x_1 + \cos(\theta)v_1][\sin(\theta)x_2 + \cos(\theta)v_2] \\ &= \cos^2(\theta)x_1x_2 - \cos(\theta)\sin(\theta)x_1v_2 - \sin(\theta)\cos(\theta)v_1x_2 + \sin^2(\theta)v_1v_2 \\ &\quad + \sin^2(\theta)x_1x_2 + \cos(\theta)\sin(\theta)v_1x_2 + \sin(\theta)\cos(\theta)x_1v_2 + \cos^2(\theta)v_1v_2 \\ &= x_1x_2 + v_1v_2 \end{aligned}$$

It is then obvious that,

$$\mathcal{N}(\mathbf{x}'|0, \Sigma)\mathcal{N}(\mathbf{v}'|0, \Sigma) = \mathcal{N}(\mathbf{x}|0, \Sigma)\mathcal{N}(\mathbf{v}|0, \Sigma)$$