Lecture January 28

GM - PDF

$$P_T(\vec{R};\vec{\alpha}) = \frac{|\psi_T(\vec{R};\vec{\alpha})|^2}{\int d\vec{R}\, |\psi_T(\vec{R};\vec{\alpha})|^2}$$

$$\vec{R} = \{\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots \vec{r}_N\}$$

$$\vec{\alpha} = \{\alpha_1, \alpha_2, \alpha_3, \dots \alpha_M\}$$

$P_T(\vec{R};\vec{\alpha}) \rightarrow P_i^{(n)}$ (we have model for this)

Markov chain:

$$\boxed{P_i^{(n+1)} = \sum_j W(j \rightarrow i) P_j^{(n)}}$$

stochastic matrix (unknown)

W with matrix elements w_{ij} $\quad W \in \mathbb{R}^{n \times n}$

$$\sum^{n} w_{ij} = 1$$

$j=1$

Example : $\mathbb{R}^{3\times 3}$

$$W = \begin{bmatrix} \frac{1}{2} & 0 & 1 \\ 0 & 1/3 & 0 \\ 1/2 & 2/3 & 0 \end{bmatrix}$$

$\lambda_{max} = \underline{1}$, If a Markov chain converges, it converges to the most likely state, this is the state with $\lambda_{max} = 1$

$$\lim_{n\to\infty} p_i^{(n)} \to p_i^{(\infty)}$$

$$p_i^{(n)} = p_i^{(n-1)}$$

$$p^{T(n)} = [p_1^{(n)}, p_2^{(n)} \ldots]$$

Markov chain

$$p^{(n)} = W p^{(n-1)}$$

$$\lim_{n\to\infty} p^{(n)} = p^{(ss)}$$

$$p^{(ss)} = W p^{(ss)}$$

$p^{(0)}$ expand in the eigen vectors of W, v

$$p^{(0)} = \sum_{i=0}^{n-1} a_i v_i$$

$$p^{(1)} = W p^{(0)} \qquad W v_i = \lambda_i v_i$$

$$= \sum_{i=0}^{n-1} a_i \lambda_i v_i$$

$$p^{(2)} = W p^{(1)} = \sum_{i=0} a_i \lambda_i \underbrace{W v_i}_{\lambda_i v_i}$$

$$= \sum_{i=0}^{n-1} a_i \lambda_i^2 v_i$$

$$\lambda = \{ \lambda_0, \lambda_1, \dots \lambda_n \}$$

$$\lambda_0 \geq \lambda_1 \geq \lambda_2 \dots \geq \lambda_n$$

$$p^{(n)} = \sum_{i=0}^{n-1} a_i \lambda_i^n v_i$$

$n \quad n-1 \quad n$

$$\lim_{n\to\infty} = a_0\lambda_0^{n} v_0 + \sum_{i=1} a_i \lambda_i^{n} v_i$$

$$= a_0 \lambda_0^{n} v_0$$

most likely state

$P_i^{(n)}$ is a multidimensional

Difficult to sample (and calculate the norm)

W = is unknown, we will make a model

$$W(j\to i) = A(j\to i)\; T(j\to i)$$

acceptance for making a move

Transition likelihood

$$A \in \mathbb{R}^{n\times n}$$

$n \times n$

$T \in \mathbb{R}$

$$\sum_j a_{ij} = 1 = \sum_j t_{ij}$$

Detailed Balance

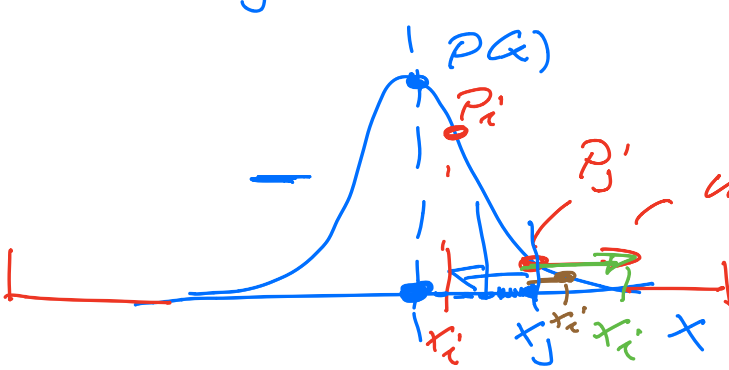
$$\frac{P_i}{P_j} = \frac{W(j \to i)}{W(i \to j)} = \frac{A(j\to i)\,T(j \to i)}{A(i \to j)\,T(i \to j)}$$

cancel out the norm of P_i

Brute force MC : $\boxed{T(j \to i) = \frac{1}{N} = T(i \to j) = \frac{1}{N}}$

$$\frac{P_i}{P_j} = \frac{A(j \to i)}{A(i \to j)}$$

Metropolis algorithm ratio



uniform Distribution for the jumping of a random walker.

$$\boxed{\frac{P_i}{P_j} > 1} \quad \Big(\underbrace{x_i = x_j}_{\text{allowed state.}} \Rightarrow \frac{P_i}{P_j} = 1\Big)$$

$$\frac{P_i}{P_j} = 0$$

$$\frac{P_i}{P_j} \geq 0$$

$$\frac{P_i}{P_j} < 1$$

$$0 \leq P_i, P_j \leq 1$$

max value $P_i, P_j = 1$

$$0 \leq A(j \to i) \leq 1$$

Metropolis

$A(j \to i)$ is unknown.

if $\dfrac{P_i}{P_j} \geq 1$ $A(j \to i)$ takes max value $= 1$

$$\frac{P_i}{P_j} = \frac{1}{A(i \to j)} \quad 0 \leq A(i \to j) < 1$$

$$0 \leq \frac{P_i}{P_j} < 1 \quad 0 \leq A(j \to i) < 1$$

$$A(i \to j) = 1$$

Metropolis algo

$$A(j \to i) = \min\left(1, \frac{P_i}{P_j}\right)$$

$$\boxed{\frac{P_i}{P_j} = \frac{A(j \to i)}{A(i \to j)}} < 1$$

$$A(j \to i) < A(i \to j) = 1$$

$r \in [0,1]$

$$\boxed{\text{accept if } \quad r \le P_i / P_j}$$

$$\frac{P_i}{P_j} = \frac{|\Psi(\vec{R}_i ; \vec{\alpha})|^2}{|\Psi(\vec{R}_j ; \vec{\alpha})|^2}$$

$$\vec{R}_i = \left\{ \vec{r}_1^{(i)}, \vec{r}_2^{(i)}, \vec{r}_3^{(i)}, \ldots \vec{r}_N^{(i)} \right\}$$

Move of all particles,

Possible model:

$$\Psi_T(\vec{R}_i) = \varphi_1(r_1^{(i)})\varphi_2(r_2^{(i)}) \ldots$$

$$\varphi_N(r_N^{(i)}) \prod_{k>l} f(r_{kl}^{(i)})$$

$$r_{kl}^{(i)} = |\vec{r}_k^{(i)} - \vec{r}_l^{(i)}|$$

Move one particle at the time

$$\frac{|\varphi_1(r_1^{(i)})\,\varphi_2(r_2^{(j)})\,\varphi_3(r_3^{(j)})\cdots|^2}{|\varphi_1(r_1^{(j)})\,\varphi_2(r_2^{(j)})\cdots}$$

Metropolis algo, general case

$$T(i\to j) \neq T(j\to i)$$

$$\frac{P_i}{P_j} = \frac{T(j\to i)\,A(j\to i)}{T(i\to j)\,A(i\to j)}$$

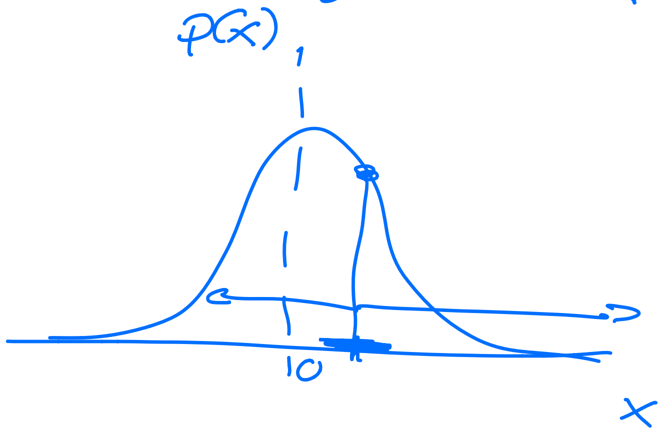
we will develop a model for this

No need for stepsize

Importance sampling

Fokker-Planck eq.

Langevin - eq



$$\frac{P_i \, T(i \to j)}{P_j \, \underbrace{T(j \to i)}_{\text{we have a model}}} = \frac{A(j \to i)}{A(i \to j)}$$

Metropolis-Hastings algo

$$A(j \to i) = \mathrm{MIN}\left(1, \frac{P_i \, T(i \to j)}{P_j \, T(j \to i)}\right)$$