18-5-2023

Simulated Annealing with MCMC

$|A| < \infty$

$\forall x \in A \quad : \quad N(x) = \{\text{γειτονικά στοιχεία του } x\}$

$N(x) \subseteq A$

$\{X_1, X_2, \ldots\}$ M Chain

$X_n = x \implies X_{n+1}$ διακρ. ομ. $N(x)$

$$q(x,y) = P(X_{n+1} = y \mid X_n = x) = \frac{1}{|N(x)|}, \quad y \in N(x)$$

Θέλουμε $\pi(x) = c\, e^{\lambda V(x)}$, $\quad b(x) = e^{\lambda V(x)}$

$$a(x,y) = \min\left\{ \frac{b(y)\, q(y,x)}{b(x)\, q(x,y)}, 1 \right\} =$$

$$= \min\left\{ \frac{e^{\lambda V(y)} / |N(y)|}{e^{\lambda V(x)} / |N(x)|}, 1 \right\}$$

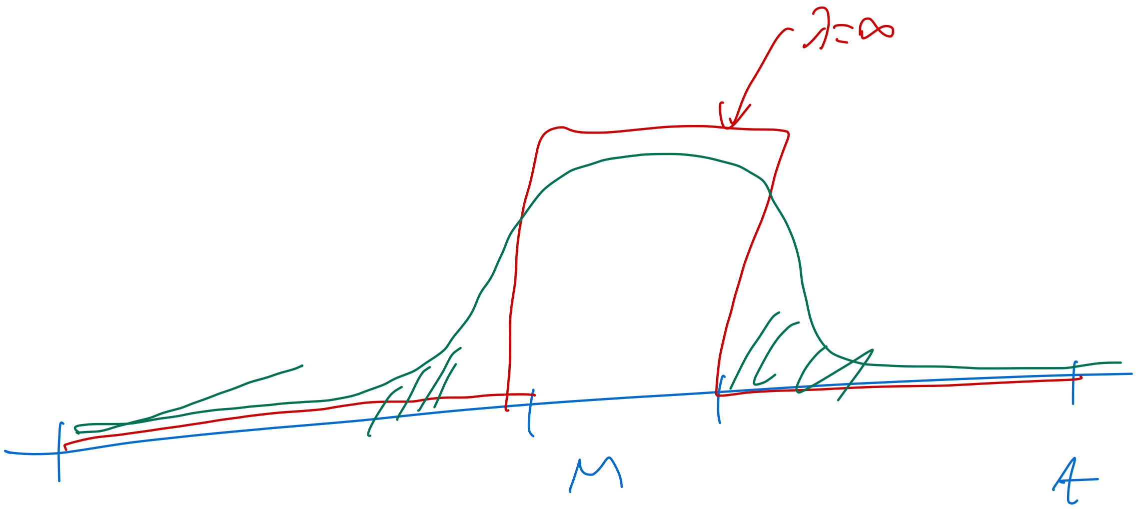
Αν $|N(x)| = K =$ σταθ

$$\Longrightarrow \quad a(x,y) = \min\left\{ e^{\lambda(V(y)-V(x))}, 1 \right\}$$

Αν $V(y) \geq V(x) \Rightarrow a(x,y) = 1$

$V(y) < V(x) \Rightarrow a(x,y) = \underbrace{e^{\lambda(V(y)-V(x))}}_{<1}$

$\forall \lambda > 0 \quad \underline{\{\tilde{X}_1, \tilde{X}_2, \ldots\}}$ στάσιμη $P_\lambda(\cdot)$



Παρατήρηση: Αν $X_n = x$, $X_{n+1} = y$

$$a_n(x,y) = \min\left\{ e^{\lambda_n(V(y)-V(x))}, 1 \right\}$$

$\lambda_n \longrightarrow \infty$ ("αργά")

$$\lambda_n \approx C \log(n+1)$$

Traveling Salesman Problem (NP-Complete)

Knapsack

$$\max \sum c_i x_i$$
$$\sum a_i x_i \le b$$
$$x_i \ge 0$$

LP

$x_1 \ge 0$

$$\frac{c_1}{a_1} \ge \frac{c_2}{a_2} \quad \cdots \qquad x_j : 0$$

$x_i \in \mathbb{Z}$?

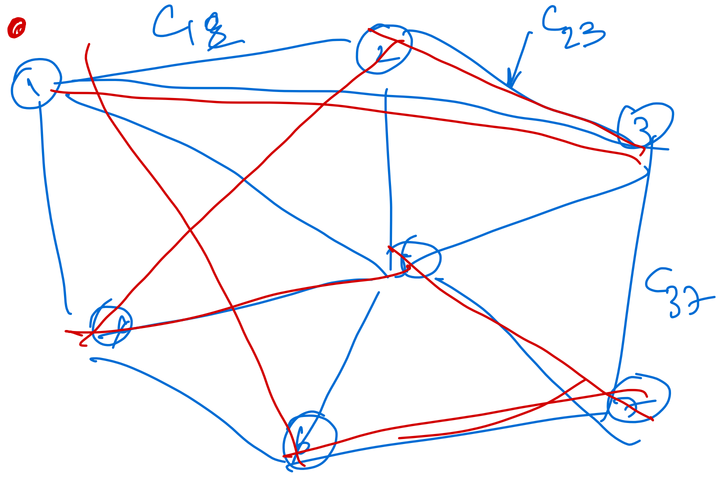
IP

NP-complete

integer knapsack

$$\max \sum c_i x_i$$
$$\sum a_i x_i \le b$$
$$x_i \ge 0, \quad x \in \mathbb{Z}$$

Traveling Salesman Problem (TSP)



tour → 1 − 3 − 2 − 4 − 5 − 7 − 6 − 1

tour μέγιστης αξίας

Παράδειγμα

$\exists$ ακμή (i,j) $\forall i,j$, $i=1,\dots,r$, $j=1,\dots,r$

$\exists$ συνάρτηση $v(i,j)$ αξία ακμής

Έστω $x=(x_1,\dots,x_r)$: μετάθεση $(1,2,\dots,r)$

$$\boxed{V(x)=\sum_{i=1}^{r-1} v(x_i,x_{i+1})}$$

$$A=\{x : \text{μετάθεση του } (1,2,\dots,r)\}$$

$$|A| = r!$$

$N(x)$

$(r=5)$

π.χ. $x = (1, 3, 2, 5, 4)$

τυχαία

$y = (1, 5, 2, 3, 4)$

$N(x) = \binom{5}{2}$

Sampling - Importance Resampling

$\boxed{\theta = E_f(h(x))}$

$f \leftarrow$ θέλουμε γεννήτρια

$g \leftarrow \exists$ γεννήτρια

Accept reject

$Y \sim g$

accept με πιθ. $\propto \boxed{\frac{f(x)}{g(x)} = w(x)}$

διορθώνω την καταλληλη αλλαγή της πιθ. αποδ.

Importance Sampling

$$E_f(h(x)) = E_g(w(x) \cdot h(x))$$

$$Y \sim g \longrightarrow \tilde{h}(Y) = w(Y)\,h(Y)$$

Έστω ότι δημιουργούμε $Y_1, \dots, Y_m \sim g$

$y_1 \quad y_2 \quad y_3 \; \dots \quad y_m \sim g$

$w(y_1) \quad w(y_2) \quad \dots \quad w(y_m)$

Ac/Rej: δέχομαι από ρ δέχομαι από ρ δέχομαι από ρ $\longrightarrow$ υποσ. $\{y_1, \dots, y_m\} \sim f$

IS: $\tilde{h}_1 = h(y_1)w(y_1) \; \dots \dots \; \tilde{h}(y_m) w(y_m)$

SIR
Sampling / Importance Resampling

$$\underset{w_1}{\overset{y_1}{|}} \quad \underset{w_2}{\overset{y_2}{|}} \quad \cdots \quad \underset{w_m}{\overset{y_m}{|}}$$

Sampling from $\{y_1, \ldots, y_m\}$ με πιθ. επιλογής $P(X=y_j) = \dfrac{w_j}{\sum_{j=1}^{m} w_j} = c\, w_j$

$$X \xrightarrow[m\to\infty]{\mathcal{D}} f$$

$$\boxed{\lim_{m\to\infty} P(X\in A) = \int_A f(y)\,dy \qquad \forall A}$$

Εστω $g(x) = c\, g_0(x)$ c: άγνωστη

Acc/Rej , IS δεν εφαρμόζονται.

Όμως μέσω MCMC $\sim g$
κ' SIR
} εφικτή

Αλγόριθμος

① Δημιουργούμε $Y_1, \dots, Y_m \sim g$ iid

② $$W_i = \frac{f(Y_i)}{g(Y_i)}, \quad i = 1, \dots, m$$

③ $$X \in \{Y_1, \dots, Y_m\} : P(X = y_i) = \frac{w_i}{\sum_{i=1}^{m} w_i}$$

Θ : $$\lim_{m \to \infty} P(X \in A) = \int_A f(y)\,dy = P_f(X \in A)$$

Απόδειξη

$$P(X \in A) = E\left(1(X \in A)\right) =$$

$$= E_g\left[\underbrace{E\left(1(X \in A) \mid Y_1, \dots, Y_m\right)}_{m(Y_1, \dots, Y_m)}\right]$$

Αρκεί ν.δ.ο. $$\lim_{m \to \infty} m(Y_1, \dots, Y_m) \to \int_A f(y)\,dy = \theta$$

μ-π.σ.σ.
(g)

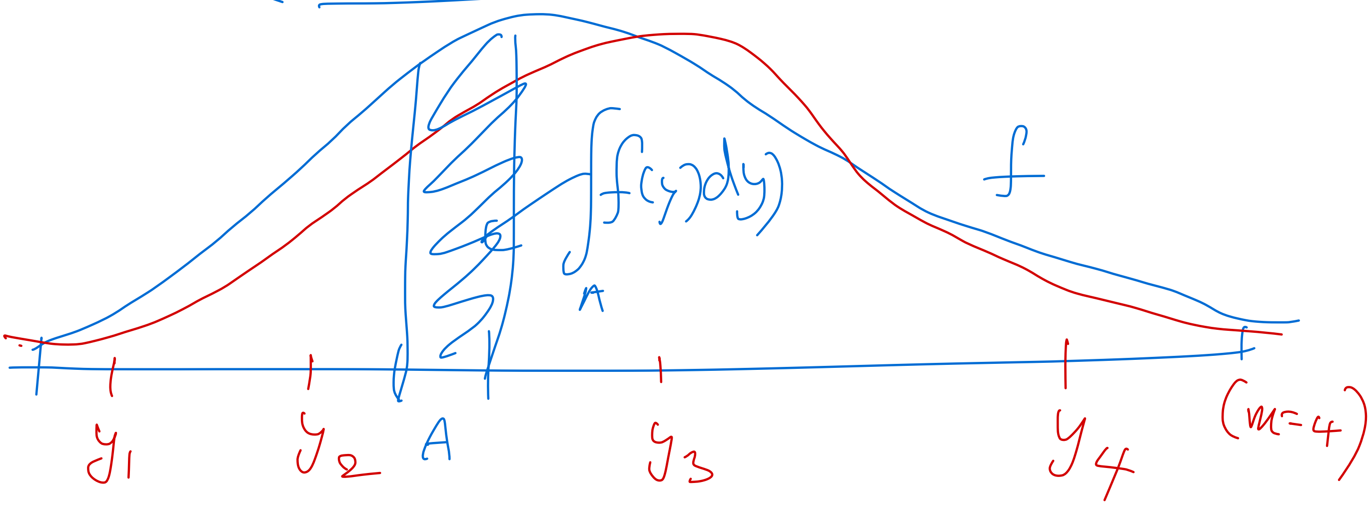
Τότε $$E\left(m(Y_1, \dots, Y_m)\right) \xrightarrow{m \to \infty} \theta$$

Επειδή $m \le 1 \quad \forall\, Y_1, \dots, Y_m$

Θ. φραγμένης σύγκλισης

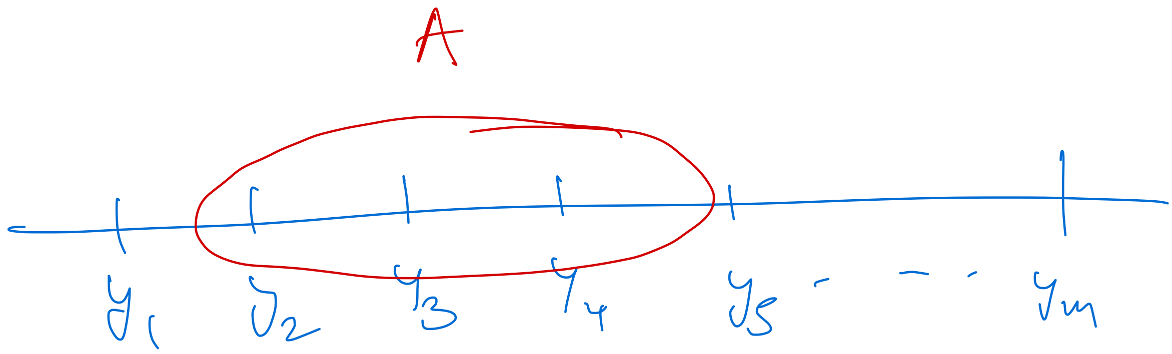
(bounded convergence)

$$\Rightarrow \; E\big(m(Y_1, \dots, Y_m)\big) \to \theta \, .$$



$$x \in \{y_1, y_2, y_3, y_4\}$$

$$m(y_1,\dots,y_m) = P(X\in A \mid Y_1=y_1,\dots,Y_m=y_m)$$



$$P(X\in A\mid y_1,\dots,y_m) = \sum_{i=1}^{m} 1(y_i\in A)\,\frac{w_i}{\sum w_i} = \frac{\sum_{i=1}^{m} 1(y_i\in A)\, w_i}{\sum_{i=1}^{m} w_i}$$

$m(y_1,\dots,y_m)$

$$\Rightarrow \boxed{m(Y_1,\dots,Y_m) = \frac{\sum_{i=1}^{m} 1(Y_i\in A)\cdot W_i}{\sum_{i=1}^{m} W_i}}$$

$$W_i = \frac{f(Y_i)}{g(Y_i)}, \quad i=1,\dots,m$$

Θ.δ.ο. $\displaystyle \frac{1}{m}\sum_{i=1}^{m} 1(Y_i\in A)\, W_i \longrightarrow \theta_1$

$$\frac{1}{m}\sum_{i=1}^{m} W_i \longrightarrow \theta_2$$

$$\frac{1}{m}\sum_{i=1}^{m} w_i \to E_g\left(\frac{f(X)}{g(X)}\right) = 1.$$

$$\frac{1}{m}\sum_{i=1}^{m} w_i \to E_g\left[1(Y\in A)\frac{f(Y)}{g(Y)}\right]$$

$$= \int_A \frac{f(y)}{g(y)}\cdot g(y)\,dy = \int_A f(y)\,dy.$$