

Evolutionary Monte Carlo methods

P. Del Moral

UNSW, Sydney, School of Mathematics & Statistics

Mini Course, Iasi University, June 2015

Part IV - Illustrations - Exercises - Solutions

A dozen of examples

- Filtering, HMM, IKF,...
- Importance sampling, rare events,...
- Interacting SA, subset simulation,...
- Confinement, Polymers,...

Laboratory examples

Particle-MCMC methodologies

- Independent Metropolis-Hastings scheme
- Frozen particle path & Particle Gibbs sampler

7 Exercises with solutions

A dozen of examples

Filtering, HMM, IKF,...

Importance sampling, rare events,...

Interacting SA, subset simulation,...

Confinement, Polymers,...

Laboratory examples

Particle-MCMC methodologies

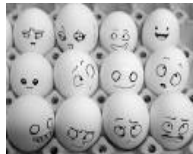
7 Exercises with solutions



A Dozen of Examples



www.flickr.com/photos/13041170



1) Filtering problems $(X_n, Y_n) = (\text{Signal}, \text{Observation})$

FK model for the posterior distributions

$$G_n(x_n) = p(y_n|x_n) \Rightarrow Q_n(f) = \mathbb{E}(f(X_0, \dots, X_n) \mid Y_p = y_p, p < n)$$

$$\eta_n(f) = \mathbb{E}(f(X_n) \mid Y_p = y_p, p < n)$$

and

$$Z_{n+1} = p_n(y_0, \dots, y_n)$$

2) Filtering the noise ($\mathcal{X}_0 := W_0$)

$$\begin{cases} \mathcal{X}_n := F_n(\mathcal{X}_{n-1}, W_n) & \rightsquigarrow \mathcal{X}_n = \varphi_n(W_0, \dots, W_n) \\ \mathcal{Y}_n = H_n(\mathcal{X}_n, V_n) \stackrel{\text{ex.}}{=} h_n(\mathcal{X}_n) + V_n & \text{with } V_n \sim \mathcal{N}(0, 1) \end{cases}$$

Bayes' rule

$$p(w_0, \dots, w_n \mid y_0, \dots, y_{n-1}) \propto \left\{ \prod_{0 \leq k < n} \underbrace{p(y_k \mid (w_0, \dots, w_k))}_{:= G_k(w_0, \dots, w_k)} \right\} p(w_0, \dots, w_n)$$

\Downarrow

FK model with the Markov chain $X_n = (W_0, \dots, W_n)$ and the functions

$$G_n(X_n) = p(y_n \mid (w_0, \dots, w_n)) \stackrel{\text{ex.}}{\propto} e^{-\frac{1}{2}(y_n - h_n(\varphi_n(w_0, \dots, w_n)))^2}$$

\Downarrow

$$\eta_n(f) = \mathbb{E}(f(W_0, \dots, W_n) \mid Y_p = y_p, p < n)$$

3) Markov restriction/Confinements

$$G_n(x_n) = 1_{A_n}(x_n) \Rightarrow Q_n(f) = \mathbb{E}(f(X_0, \dots, X_n) \mid X_p \in A_p, p < n)$$

$$\eta_n(f) = \mathbb{E}(f(X_n) \mid X_p \in A_p, p < n)$$

and

$$Z_{n+1} = \mathbb{P}(X_p \in A_p, p \leq n)$$

4) Self-avoiding walks X'_n SRW on \mathbb{Z}^2 (starts at the origin)

$$X_n = (X'_0, \dots, X'_n) \quad \text{and} \quad G_n(X_n) = 1_{\notin \{X'_0, \dots, X'_{n-1}\}}(X'_n)$$

\Downarrow

$$\eta_n(f) = \mathbb{E}(f(X'_0, \dots, X'_n) \mid X'_p \neq X'_q, 0 \leq p < q < n)$$

and

$$\mathcal{Z}_n = \mathbb{P}(X'_p \neq X'_q, 0 \leq p < q < n) = \frac{1}{4^n} \times \#\{\text{non intersecting } n\text{-paths}\}$$

5) Top-spectrum approximations $E = \{1, \dots, d\}$

$$Q(i, j) = \sum_j Q(i, j) \times \frac{Q(i, j)}{\sum_j Q(i, j)} := G(i) \times M(i, j)$$

When Q is symmetric

$$Q(i, j) = Q(j, i) \Leftrightarrow \underbrace{\frac{G(i)}{\sum_k G(k)}}_{:=\mu(i)} M(i, j) = \underbrace{\frac{G(j)}{\sum_k G(k)}}_{:=\mu(j)} M(j, i)$$

\Downarrow

\rightsquigarrow **Spectral theorem:**

$$Q^n(i, j) = \sum_{0 \leq k < d} \lambda_k^n \varphi_k(i) \varphi_k(j)$$

with $\lambda_k \downarrow$, eigen-vectors $Q(\varphi_k) = \lambda_k \varphi_k$ orthonormal basis of $\mathbb{L}_2(\mu)$.

FK interpretation (X_k Markov with transitions M_k)

$$\begin{aligned} Q^n(\mathbf{i}_0, \mathbf{i}_n) &= \sum_{1 \leq j_0, \dots, j_n \leq d} \underbrace{\mathbf{1}_{\mathbf{i}_0}(j_0)}_{=\eta_0(j_0)} G(j_0) M(j_0, j_1) \dots G(j_{n-1}) M(j_{n-1}, j_n) \underbrace{\mathbf{1}_{\mathbf{i}_n}(j_n)}_{=f(j_n)} \\ &= \mathbb{E} \left(f(X_n) \prod_{0 \leq k < n} G_k(X_k) \right) \end{aligned}$$

Long time behavior (power method)

$$Q^n(i_0, i_n) \simeq_{n \uparrow} \lambda_0^n \varphi_0(i_0) \varphi_0(i_n) \Rightarrow \mathcal{Z}_n = \lambda_0^n \times \text{cte} \Rightarrow \frac{1}{n} \log \mathcal{Z}_n \simeq \log \lambda_0$$

and

$$\eta_n(f) = \frac{Q^n(i_0, i_n)}{\sum_{1 \leq j_n \leq d} Q_n(i_0, j_n)} \simeq_{n \uparrow} \frac{\varphi_0(i_n)}{\sum_{j_n} \varphi_0(j_n)}$$

Particle approximations:

Replace η_n and \mathcal{Z}_n by their approximations η_n^N and \mathcal{Z}_n^N ...

6) Twisted/Importance sampling

$$X_n = (X'_n, X'_{n+1}) \quad \text{and} \quad G_n(X_n) = e^{V_n(X'_n) - V_{n-1}(X'_{n-1})}$$

$$\Downarrow (V_0 = 0)$$

$$Q_{n+1}(f) \propto \mathbb{E} \left(f((X'_0, X'_1), \dots, (X'_{n+1}, X'_{n+2})) \underbrace{e^{V_n(X'_n)}}_{\text{favor path with high } V_n(X'_n)} \right)$$

and

$$Z_{n+1} = \mathbb{E} \left(e^{V_n(X'_n)} \right)$$

Applications

$$f((X'_0, X'_1), \dots, (X'_{n+1}, X'_{n+2})) = \underbrace{1_{V_n(X'_n) \geq a}}_{= 0 \text{ for paths with small } V_n(X'_n)} e^{-V_n(X'_n)}$$

\rightsquigarrow Particle algorithm drives paths to V_n -high terminal values!

7) \oplus 8) = Boltzmann-Gibbs measures

- ▶ **7) BG meas.** $\pi_n(dx) = \frac{1}{Z_{\beta_n}} e^{-\beta_n V(x)} \lambda(dx)$, with $\beta_n \uparrow$.

$$G_n(x) = e^{-(\beta_{n+1}-\beta_n)V(x)} \quad \text{and} \quad M_n \quad \text{s.t.} \quad \pi_n = \pi_n M_n \quad (\pi_n\text{-Shaker})$$

\Downarrow

$$\eta_n = \pi_n \quad \text{and} \quad Z_{\beta_n}/Z_{\beta_0} = \mathcal{Z}_n$$

- ▶ **8) Tails/Restricted meas.** $\pi_n(dx) = \frac{1}{Z_{A_n}} 1_{A_n}(x) \lambda(dx)$, with $A_n \downarrow$

$$G_n(x) = 1_{A_{n+1}}(x) \quad \text{and} \quad M_n \quad \text{s.t.} \quad \pi_n = \pi_n M_n \quad (A_n\text{-Shaker})$$

\Downarrow

$$\eta_n = \pi_n \quad \text{and} \quad Z_{A_n}/Z_{A_0} = \mathcal{Z}_n$$

Applications: Ising, Glauber, Potts models, Black-box problems, rare events, tail probabilities,...

9) "Product" measures (with any $h_k \geq 0$)

Target product type measures

$$\pi_n(dx) = \frac{1}{Z_n} \left\{ \prod_{0 \leq k \leq n} h_k(x) \right\} \lambda(dx)$$

FK model

$$G_n = h_{n+1} \quad \text{and} \quad M_n \quad \text{s.t.} \quad \pi_n = \pi_n M_n \quad (\pi_n\text{-Shaker})$$

\Downarrow

$$\eta_n = \pi_n \quad \text{and} \quad Z_n/Z_0 = \mathcal{Z}_n$$

Important observation: "Product" \supset BG \cup Restrictions

$$\prod_{0 \leq k \leq n} 1_{A_k} = 1_{A_n} \quad \text{and} \quad \prod_{0 \leq k \leq n} e^{-(\beta_k - \beta_{k-1})V} = e^{-(\beta_n - \beta_0)V}$$

10) HMM $\Theta \sim p(\theta)d\theta \rightsquigarrow (X_n, Y_n)$ linear-Gauss filtering

$$\underbrace{p(\theta | (y_0, \dots, y_n))d\theta}_{:=\pi_n(d\theta)} = \frac{1}{Z_n} \left\{ \prod_{0 \leq k \leq n} \underbrace{p(y_k | \theta, (y_0, \dots, y_{k-1}))}_{:=h_k(\theta) \text{ (using Kalman)}} \right\} \underbrace{p(\theta)d\theta}_{:=\lambda(d\theta)}$$

FK model

$$G_n = h_{n+1} \quad \text{and} \quad M_n \quad \text{s.t.} \quad \pi_n = \pi_n M_n \quad (\pi_n\text{-Shaker})$$

\Downarrow

$$\eta_n = \pi_n \quad \text{and} \quad Z_n/Z_0 = \mathcal{Z}_n$$

Important observation to compute $h_k(\theta)$:

$$\begin{aligned} & p(y_k | \theta, (y_0, \dots, y_{k-1})) \\ &= \int \underbrace{p(y_k | \theta, x_k, (y_0, \dots, y_{k-1}))}_{= \text{(ex.) Law of } Y_k = C_k(\theta)x_k + V_k} \underbrace{p(x_k | \theta, (y_0, \dots, y_{k-1})) dx_k}_{= \text{Kalman-predictor}} \end{aligned}$$

11) HMM $\Theta \sim p(\theta)d\theta \rightsquigarrow (X_n, Y_n)$ nonlinear filtering

$$p(\theta | (y_0, \dots, y_n)) \propto \left\{ \prod_{0 \leq k \leq n} \underbrace{p(y_k | \theta, (y_0, \dots, y_{k-1}))}_{h_k(\theta) \simeq \bar{h}_k(\theta, \xi^\theta)} \right\} p(\theta)$$

(using particle filters)

Particle filter estimation

$$p(y_k | \theta, (y_0, \dots, y_{k-1})) = \int p(y_k | \theta, x_k (y_0, \dots, y_{k-1})) \overbrace{p(x_k | \theta, (y_0, \dots, y_{k-1}))}^{= \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_k^{\theta, i}}} dx_k = \bar{h}_k(\theta, \xi^\theta)$$

Unbiased estimation

$$\mathbb{E} \left(\prod_{0 \leq k \leq n} \bar{h}_k(\Theta, \xi^\Theta) \mid \Theta = \theta \right) = p((y_0, \dots, y_n) | \theta) = \prod_{0 \leq k \leq n} h_k(\theta)$$

\rightsquigarrow **Extended target with θ -marginal** $= \pi_n$

$$\bar{\pi}_n(d(\theta, \xi^\theta)) = \left\{ \prod_{0 \leq k \leq n} \bar{h}_k(\theta, \xi^\theta) \right\} \times p(d\theta) p(d\xi^\theta | \theta)$$

Conclusion

$$\bar{\pi}_n(d(\theta, \xi^\theta)) = \left\{ \prod_{0 \leq k \leq n} \bar{h}_k(\theta, \xi^\theta) \right\} \times p(d\theta) p(d\xi^\theta | \theta)$$

Extended "product" measure $\bar{\theta} = (\theta, \xi^\theta)$

$$\bar{\pi}_n(d\bar{\theta}) \propto \overbrace{\left\{ \prod_{0 \leq k \leq n} \bar{h}_k(\bar{\theta}) \right\}}^{:= H_n(\bar{\theta})} \times p(d\bar{\theta})$$

\Leftrightarrow FK model

$$G_n = \bar{h}_{n+1} \quad \text{and} \quad M_n \quad \text{s.t.} \quad \bar{\pi}_n = \bar{\pi}_n M_n \quad (\bar{\pi}_n\text{-Shaker}) \Rightarrow \eta_n = \bar{\pi}_n$$

Example of $\bar{\pi}_n$ -Shaker = MH

$$\bar{\theta} = (\theta, \xi^\theta) \longrightarrow \bar{\theta}' = (\theta', \xi^{\theta'}) \sim \bar{q}(d\bar{\theta}'|\bar{\theta}) := q(d\theta'|\theta) p(d\xi^{\theta'}|\theta')$$

\Downarrow

$$\begin{aligned} \frac{\bar{\pi}_n(d\bar{\theta}')\bar{q}(d\bar{\theta}|\bar{\theta}')}{\bar{\pi}_n(d\bar{\theta})\bar{q}(d\bar{\theta}|\bar{\theta}')} &= \frac{H_n(\bar{\theta}')}{H_n(\bar{\theta})} \times \frac{p(d\theta') p(d\xi^{\theta'}|\theta') q(d\theta|\theta') p(d\xi^\theta|\theta)}{p(d\theta) p(d\xi^\theta|\theta) q(d\theta'|\theta) p(d\xi^{\theta'}|\theta')} \\ &= \frac{H_n(\bar{\theta}')}{H_n(\bar{\theta})} \times \underbrace{\frac{p(d\theta') q(d\theta|\theta')}{p(d\theta) q(d\theta'|\theta)}}_{=1 \text{ if reversible}} \end{aligned}$$

12) Θ_n Markov $\rightsquigarrow (X_n, Y_n)$ Partial linear-Gauss filtering

$$p((\theta_0, \dots, \theta_n) \mid (y_0, \dots, y_n))$$

$$\propto \left\{ \prod_{0 \leq k \leq n} \underbrace{p(y_k \mid (\theta_0, \dots, \theta_{k-1}), \theta_k, (y_0, \dots, y_{k-1}))}_{=G_k(\theta_0, \dots, \theta_k)} \right\} \times p(\theta_0, \dots, \theta_n)$$

Important observation to compute G_k :

$$G_k(\theta_0, \dots, \theta_k)$$

$$= \int \underbrace{p(y_k \mid (\theta_0, \dots, \theta_{k-1}), (y_0, \dots, y_{k-1}), x_k)}_{= \text{(ex.) Law of } Y_k = C_k(\theta_k)x_k + V_k}$$

= (ex.) Law of $Y_k = C_k(\theta_k)x_k + V_k$

$$\times \underbrace{p(x_k \mid (\theta_0, \dots, \theta_{k-1}), (y_0, \dots, y_{k-1}))}_{= \text{Kalman-predictor} = \eta_{\theta, k}(dx_k)} dx_k$$

= Kalman-predictor = $\eta_{\theta, k}(dx_k)$

FK model with $\mathcal{X}_n = (\Theta_0, \dots, \Theta_n)$ (or $\mathcal{X}_n = (\Theta_n, \eta_{\Theta, n})$) \Rightarrow IKF

A dozen of examples

Laboratory examples

Particle-MCMC methodologies

7 Exercises with solutions

LAB-4 (SCILAB)



SCILAB :

- ▶ Polymer models.
Code : Non-intersecting-SRW.sce
- ▶ Confinements + top eigen values/vectors
Code : SRW-Tube.sce
- ▶ Interacting Simulated annealing (ISA) on TSP.
Code : ISA.sce
- ▶ Subset simulation (Level restrictions).
Code : RVLevel-restrictions.sce

A dozen of examples

Laboratory examples

Particle-MCMC methodologies

Independent Metropolis-Hastings scheme

Frozen particle path & Particle Gibbs sampler

7 Exercises with solutions

The independent Metropolis-Hastings

Boltzmann-Gibbs formulation

$$Q_n(dx) \propto \mathbb{H}_n(x) \mathbb{P}_n(dx)$$

with $\mathbb{P}_n = \text{Law}(X_0, \dots, X_n)$ and for any $x = (x_0, \dots, x_n)$

$$\mathbb{H}_n(x) = \prod_{0 \leq k < n} G_k(x_k)$$

Independent Metropolis-Hastings

$$x \rightsquigarrow y \sim \mathbb{P}_n \rightsquigarrow \bar{x} = \begin{cases} y & \text{proba. } a_n(x, y) := \min\left(1, \frac{\mathbb{H}_n(y)}{\mathbb{H}_n(x)}\right) \\ x & \text{proba. } 1 - a_n(x, y) \end{cases}$$

Problem

$$\frac{\mathbb{H}_n(y)}{\mathbb{H}_n(x)} = \prod_{0 \leq k < n} \frac{G_k(y_k)}{G_k(x_k)} \quad \text{mixing prop/degeneracy w.r.t. } n$$

Island type model

FK model $\sim (\chi_n, \mathcal{G}_n) \rightsquigarrow$ **N-IPS = Island particle models**

$$\mathbb{E} \left(\mathcal{F}_n(\chi_n) \prod_{0 \leq k < n} \mathcal{G}_k(\chi_k) \right) \stackrel{\forall N}{=} \mathbb{E} \left(f_n(X_n) \prod_{0 \leq k < n} G_k(X_k) \right)$$

with

$$\chi_n = \xi_n \quad \mathcal{F}_n(\chi_n) := \eta_n^N(f_n) \quad \text{and} \quad \mathcal{G}_n(\chi_n) := \eta_n^N(G_n)$$

\subset **FK** $\sim (\chi_n, \mathcal{G}_n)$ **on path space = Many body FK model**

$$Q_n(f) \propto \mathbb{E} \left(f(\chi_0, \dots, \chi_n) \left\{ \prod_{0 \leq k < n} \mathcal{G}_k(\chi_k) \right\} \right)$$

The independent Metropolis-Hastings

Boltzmann-Gibbs formulation

$$Q_n(d\chi) \propto \mathcal{H}_n(\chi) \mathcal{P}_n(d\chi)$$

with $\mathcal{P}_n = \text{Law}(\chi_0, \dots, \chi_n)$ and

$$\mathcal{H}_n(\chi) = \prod_{0 \leq k < n} \mathcal{G}_k(\chi_k) = \prod_{0 \leq k < n} \eta_k^N(G_k) \simeq_{N \uparrow \infty} \mathcal{Z}_n$$

Independent Metropolis-Hastings

$$\chi \rightsquigarrow \zeta \sim \mathcal{P}_n \rightsquigarrow \bar{\chi} = \begin{cases} \zeta & \text{proba. } a_n(\chi, \zeta) := \min\left(1, \frac{\mathcal{H}_n(\zeta)}{\mathcal{H}_n(\chi)}\right) \\ \chi & \text{proba. } 1 - a_n(\chi, \zeta) \end{cases}$$

Advantage/Drawback

$$\mathcal{H}_n(\zeta)/\mathcal{H}_n(\chi) \simeq_{N \uparrow \infty} 1 \quad \text{but } O(n)\text{-fluctuations (admitted)}$$

Frozen particle path & Particle Gibbs sampler

Algorithm

1. Run an N -IPS model with a frozen path $\mathbb{X} = x$ on $[0, n]$
2. Select one of the ancestral lines **or** sample a backward path $\bar{\mathbb{X}} = \bar{x}$

Theo

Both (Markov) transitions $\mathbb{X} \rightsquigarrow \bar{\mathbb{X}}$ are \mathbb{Q}_n -reversible

Advantage

$$\underbrace{\mathbb{X} = \bar{\mathbb{X}}_0 \rightsquigarrow \bar{\mathbb{X}}_1 \rightsquigarrow \dots \rightsquigarrow \bar{\mathbb{X}}_m}_{m\text{-th step transition}} \Rightarrow \text{Law}(\bar{\mathbb{X}}_m) = O((n/N)^m)$$

A dozen of examples

Laboratory examples

Particle-MCMC methodologies

7 Exercises with solutions



7 Exercises with solutions



Sol. Ex. 1 - Positioning/Radar obs.

Filtering model

$$\begin{cases} X_n^{(1)} &= X_{n-1}^{(1)} + \epsilon_n W_n \\ X_n^{(2)} &= (1 - \alpha \Delta) X_{n-1}^{(2)} + \beta \Delta X_n^{(1)} \\ X_n^{(3)} &= X_{n-1}^{(3)} + \Delta X_n^{(2)} \end{cases}$$

Gaussian W_n and ϵ_n i.i.d. Bernoulli $\sim p = \Delta$

$$Y_n = X_n^{(3)} + \Delta V_n \quad \text{with} \quad V_n \text{ i.i.d. } \sim N(0, \sigma_v^2)$$

Some questions:

- ▶ $\text{Law}(X_0, \dots, X_n \mid (Y_0, \dots, Y_{n-1} \text{ or } n))$?
- ▶ $p(y_0, \dots, y_n)$?

Solution

FK model:

$$X_n = \left(X_n^{(i)} \right)_{i=1,2,3} \oplus G_n(x_n) = p(y_n | x_n) \propto e^{-\frac{1}{2\Delta^2} (y_n - x_n^{(3)})^2}$$

Solution

FK model:

$$X_n = \left(X_n^{(i)} \right)_{i=1,2,3} \oplus G_n(x_n) = p(y_n | x_n) \propto e^{-\frac{1}{2\Delta^2} (y_n - x_n^{(3)})^2}$$

More developed solution ...

Solution

FK model:

$$X_n = \left(X_n^{(i)} \right)_{i=1,2,3} \oplus G_n(x_n) = p(y_n | x_n) \propto e^{-\frac{1}{2\Delta^2} (y_n - x_n^{(3)})^2}$$

More developed solution ...



↪ **Genetic algo. mutation as $X_{n-1} \rightsquigarrow X_n$, selection fitness G_n :**

$$\left(\xi_n^i \right)_{1 \leq i \leq N} \xrightarrow{\text{updating/selection}} \left(\widehat{\xi}_n^i \right)_{1 \leq i \leq N} \xrightarrow{\text{free exploration}} \left(\xi_{n+1}^i \right)_{1 \leq i \leq N}$$

Particle estimates

- ▶ *After the n -th mutation:*

$$\mathbb{E}(f(X_0, \dots, X_n) \mid (Y_0, \dots, Y_{n-1})) \simeq_{N \uparrow \infty} \frac{1}{N} \sum_{1 \leq i \leq N} f(\underbrace{\xi_{0,n}^i, \xi_{1,n}^i, \dots, \xi_{n,n}^i}_{i\text{-th ancestral line}})$$

- ▶ *After the n -th selection:*

$$\mathbb{E}(f(X_0, \dots, X_n) \mid (Y_0, \dots, Y_n)) \simeq_{N \uparrow \infty} \frac{1}{N} \sum_{1 \leq i \leq N} f(\underbrace{\widehat{\xi}_{0,n}^i, \widehat{\xi}_{1,n}^i, \dots, \widehat{\xi}_{n,n}^i}_{i\text{-th ancestral line}})$$

- ▶ **Normalizing constants:**

$$p(y_0, \dots, y_n) \simeq \prod_{0 \leq k \leq n} \frac{1}{N} \sum_{1 \leq i \leq N} G_k(\xi_k^i) \quad (\text{unbiased})$$

Sol. Ex. 2 - SRW/Brownian $\in [-1, 1]$

Markov chain model

$$X_n = X_{n-1} + \sqrt{\Delta} W_n \simeq dX_t = dW_t$$

Wiener/Brownian process W_t ($X_0 = 0$, $\Delta = 10^{-2}$)

↓

Some questions:

- ▶ Law($X_0, \dots, X_n \mid \forall 0 \leq k < n X_k \in [-1, 1]$) (two ways)?
- ▶ $\mathbb{P}(\forall 0 \leq k \leq n X_k \in [-1, 1])$?

Solution = FK: $G_n = 1_{[-1,1]}$

Solution = FK: $G_n = 1_{[-1,1]}$
More developed solution ...

Solution = FK: $G_n = 1_{[-1,1]}$

More developed solution ...

\rightsquigarrow Genetic algo. mutation as $X_{n-1} \rightsquigarrow X_n$, selection fitness G_n :

$(\xi_n^i)_{1 \leq i \leq N}$ $\xrightarrow{\text{updating/selection}}$ $(\widehat{\xi}_n^i)_{1 \leq i \leq N}$ $\xrightarrow{\text{free exploration}}$ $(\xi_{n+1}^i)_{1 \leq i \leq N}$

Solution = FK: $G_n = 1_{[-1,1]}$

More developed solution ...

\rightsquigarrow Genetic algo. mutation as $X_{n-1} \rightsquigarrow X_n$, selection fitness G_n :

$$(\xi_n^i)_{1 \leq i \leq N} \xrightarrow{\text{updating/selection}} (\widehat{\xi}_n^i)_{1 \leq i \leq N} \xrightarrow{\text{free exploration}} (\xi_{n+1}^i)_{1 \leq i \leq N}$$

Particle estimates

► After the n -th mutation:

$$\mathbb{E}(f(X_0, \dots, X_n) \mid \forall 0 \leq k < n X_k \in [-1, 1])$$

$$\simeq_{N \uparrow \infty} \frac{1}{N} \sum_{1 \leq i \leq N} f \left(\underbrace{(\xi_{0,n}^i, \xi_{1,n}^i, \dots, \xi_{n,n}^i)}_{i\text{-th ancestral line}} \right)$$

► Normalizing constants (unbiased):

$$\mathbb{P}(\forall 0 \leq k \leq n X_k \in [-1, 1]) \simeq \prod_{0 \leq k \leq n} \frac{1}{N} \sum_{1 \leq i \leq N} 1_{[-1,1]}(\xi_k^i)$$

Sol. Ex. 3 - Top spectrum

Matrix with positive entries

$$P = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{pmatrix}$$

↓

Some questions:

- ▶ To of the spectrum of $Q = P'P$?
- ▶ Corresponding eigenvector?

Solution = FK (G, M) (cf. example (5))

$$Q(i, j) = G(i) \times M(i, j) \quad \text{with} \quad G(i) = \sum_{1 \leq j \leq 4} Q(i, j)$$

FK ($\mu = \eta_0 = 1_{i_0}$, $f = 1_{i_n}$, and X_n Markov transition M)

$$Q^n(i_0, i_n) = \mathbb{E} \left(f(X_n) \prod_{0 \leq k < n} G_k(X_k) \right) \propto \eta_n(f)$$

Spectral theo \rightsquigarrow long time approx./power method

$$Q^n(i_0, i_n) = \sum_{0 \leq k < 4} \lambda_k^n \varphi_k(i_0) \varphi_k(i_n) \simeq_{n \uparrow \infty} \lambda_0^n \varphi_0(i_0) \varphi_0(i_n)$$

$$\sum_{1 \leq i_n \leq 4} Q^n(i_0, i_n) = \mathbb{E} \left(\prod_{0 \leq k < n} G_k(X_k) \right) = \mathcal{Z}_n \simeq_{n \uparrow \infty} \text{cte } \lambda_0^n$$

\Downarrow

$$\frac{1}{n} \log \mathcal{Z}_n \simeq_{n \uparrow \infty} \log \lambda_0 \quad \text{and} \quad \eta_n(f) = \frac{Q^n(i_0, i_n)}{\sum_{1 \leq j_n \leq 4} Q_n(i_0, j_n)} \simeq_{n \uparrow \infty} \frac{\varphi_0(i_n)}{\sum_{j_n} \varphi_0(j_n)}$$

Sol. Ex. 4 - Black-box/inverse pb

Input(X)/Output(Y) model

$X = (X^1, X^2) \sim$ uniform in the unit disk $\mapsto Y = V(X) = |X^1| + |X^2|$



Some questions:

- ▶ Law($X \mid V(X) \leq 1/10$) (MH+SMC)?
- ▶ $\mathbb{P}(V(X) \leq 1/10)$?
- ▶ When X is Gaussian?

FK-Proba. restrictions (example (8))

Notation

$$\text{Law}(X) = \lambda \text{ and } A_n = \{V(X) \leq \epsilon_n\} \text{ with } \epsilon_n \downarrow$$

\Downarrow

$$\begin{aligned} \mathbb{P}(X \in dx \mid V(X) \leq \epsilon_n) &= Z_{A_n}^{-1} 1_{A_n}(x) \lambda(dx) := \pi_n(dx) \\ Z_{A_n} &= \mathbb{P}(V(X) \leq \epsilon_n) \end{aligned}$$

FK model

$$G_n = 1_{A_{n+1}} \quad \text{and} \quad M_n \quad \text{s.t.} \quad \pi_n = \pi_n M_n \quad (A_n\text{-Shaker})$$

\Downarrow

$$\eta_n = \pi_n \quad \text{and} \quad Z_{A_n}/Z_{A_0} = \mathcal{Z}_n$$

Initialisation:

$$\epsilon_0 = \sqrt{2} \Rightarrow \{|x_1|^2 + |x_2|^2 \leq 1\} \subset \{|x_1| + |x_2| \leq \sqrt{2}\} \Rightarrow Z_{A_0} = \pi$$

On the shakers $\pi_n = \pi_n M_n$

Case $\lambda = \text{Uniform in the unit disk } D(\supset A_n)$

$$1) \quad x(\in A_n) \xrightarrow{\text{Gibbs move/proposal in } D} y \xrightarrow{\text{MH-accept/reject}} \bar{x} = \begin{cases} y & \text{if } y \in A_n \\ x & \text{if } y \notin A_n \end{cases}$$

$$2) \quad x(\in A_n) \xrightarrow{\text{local gauss. } p_\epsilon(x,y)} y_i = x_i + \epsilon \mathcal{N}(0,1), i = 1, 2$$

↓ MH-accept/reject

$$\bar{x} = \begin{cases} y & \text{proba } \min\left(1, \frac{1_{A_n}(y)p_\epsilon(y,x)}{1_{A_n}(x)p_\epsilon(x,y)}\right) = 1_{A_n}(y) \\ x & \text{otherwise } x \end{cases}$$

On the shakers $\pi_n = \pi_n M_n$

Case $\lambda = \text{Gaussian } \mathcal{N}(0, 1)$

$$x(\in A_n) \xrightarrow{\text{local reversible gauss. } p_\epsilon(x, y)} y_i = \sqrt{1 - \epsilon^2} x_i + \epsilon \mathcal{N}(0, 1), \quad i = 1, 2$$

↓ MH-accept/reject

$$\bar{x} = \begin{cases} y & \text{proba } \min\left(1, \frac{1_{A_n}(y)\lambda(dy)p_\epsilon(y, x)}{1_{A_n}(x)\lambda(dx)p_\epsilon(x, y)}\right) \\ x & \text{otherwise } x \end{cases} = 1_{A_n}(y)$$

Sol. Ex. 5 - Polymer models

Toy polymer model X_n SRW on \mathbb{Z}^2 starting at the origin



Some questions:

- ▶ Mean displacement given self-repulsion?

$$\mathbb{E} \left(\frac{1}{n} \sum_{1 \leq k \leq n} X_k^2 \mid \forall 0 \leq k \neq l \leq n, X_k \neq X_l \right)$$

- ▶ Probability of self-avoiding paths?

Solution = Example (4) with

$$f(X_0, \dots, X_n) = \frac{1}{n} \sum_{1 \leq k \leq n} X_k^2$$

Ex. 6 - Partially linear [HMM (X, W, V) Gauss]

$$(a) \quad \begin{cases} \Theta & \sim N(0, 1) & \text{Unknown parameter} \\ X_n & = \Theta X_{n-1} + W_n & \text{Signal} \\ Y_n & = X_n + V_n & \text{Observation} \end{cases}$$

$$(b) \quad X_n = X_{n-1} + W_n \quad \text{with} \quad W_n \sim N(0, \Theta^2)$$

$$(c) \quad Y_n = X_n + V_n \quad \text{with} \quad V_n \sim N(0, \Theta^2)$$

IN ALL CASES = HMM lin-Gauss \rightsquigarrow Sol. = Ex. (10)

Addition:

$$\begin{aligned} & \mathbb{P}(X_n \in dx \mid (Y_0, \dots, Y_n)) \\ &= \int \underbrace{\mathbb{P}(X_n \in dx \mid (Y_0, \dots, Y_n), \Theta = \theta)}_{\text{given by Kalman!}} \underbrace{p(d\theta \mid (y_0, \dots, y_n))}_{= \pi_n(d\theta) \text{ approx. particles ex. (10)}} \end{aligned}$$

Ex. 7 - general HMM

HMM model = positioning Radar problem

$$\left\{ \begin{array}{l} \Theta = (\Theta_1, \Theta_2, \Theta_3) \sim N(0, I_{3 \times 3}) \\ dX_t^{(1)} = \Theta_1 W_t dN_t \\ \frac{dX_t^{(2)}}{dt} = \Theta_2 X_t^{(2)} + \Theta_3 X_t^{(1)} \\ \frac{dX_t^{(3)}}{dt} = X_t^{(2)} \end{array} \right.$$

= Nonlinear/Non Gaussian HMM \rightsquigarrow Sol. = Ex. (11)

As above (same addition):

$$\begin{aligned} & \mathbb{P}(X_n \in dx \mid (Y_0, \dots, Y_n)) \\ &= \int \underbrace{\mathbb{P}(X_n \in dx \mid (Y_0, \dots, Y_n), \Theta = \theta)}_{\text{given by the particle filter!}} \underbrace{p(d\theta \mid (y_0, \dots, y_n))}_{= \pi_n(d\theta) \text{ approx. particles ex. (10)}} \end{aligned}$$