

Stochastic Processes

MATH5835, P. Del Moral

UNSW, School of Mathematics & Statistics

Lectures Notes No. 11

Consultations (RC 5112):

Wednesday 3.30 pm \rightsquigarrow 4.30 pm & Thursday 3.30 pm \rightsquigarrow 4.30 pm

References in the slides

- ▶ **Material for research projects** \rightsquigarrow Moodle
(*Stochastic Processes and Applications* \ni variety of applications)

I learned very early
the difference
between knowing the
name of something
and knowing
something.

Richard P. Feynman

meetville.com

– *Richard P. Feynman (1918-1988)* ⊕ [video](#)

Three objectives



Understanding & Solving

- ▶ Classical stochastic algorithms
- ▶ Some advanced Monte Carlo schemes
- ▶ Intro to computational physics/biology

Plan of the lecture

- ▶ **Stochastic algorithms**
 - ▶ Robbins Monro model
 - ▶ Simulated annealing



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- ▶ **Stochastic algorithms**
 - ▶ Robbins Monro model
 - ▶ Simulated annealing
- ▶ **Some advanced Monte Carlo models**
 - ▶ Interacting simulated annealing
 - ▶ Rare event sampling
 - ▶ Black box and inverse problems

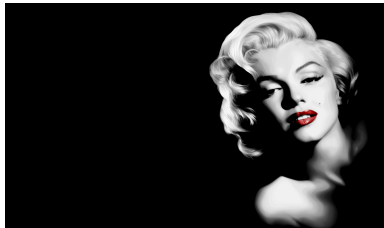


Plan of the lecture

- ▶ **Stochastic algorithms**
 - ▶ Robbins Monro model
 - ▶ Simulated annealing
- ▶ **Some advanced Monte Carlo models**
 - ▶ Interacting simulated annealing
 - ▶ Rare event sampling
 - ▶ Black box and inverse problems
- ▶ **Computational physics/biology**
 - ▶ Molecular dynamics
 - ▶ Schödinger ground states
 - ▶ Genetic type algorithms



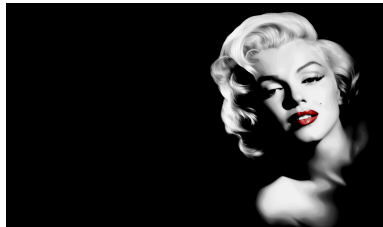
Robbins Monro model



Objectives

Given $U : \mathbb{R}^d \mapsto \mathbb{R}^d \ni a$ find $U_a = \{x \in \mathbb{R}^d : U(x) = a\}$

Robbins Monro model



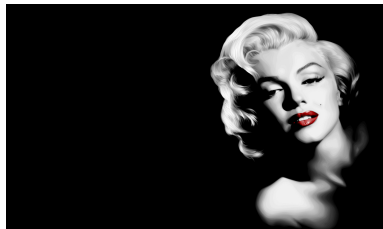
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Examples

- ▶ *Concentration of products (therapeutic,...):* $U(x) = \mathbb{E}(U(x, Y))$
 $U(x, Y) := \mathcal{U}(\text{"drug" dose } x, \text{"data" patients } Y) = \text{dosage effects}$

Robbins Monro model



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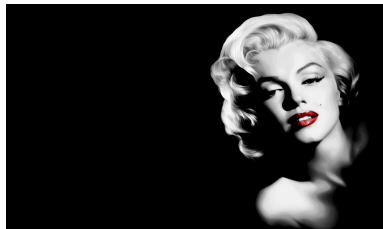
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- ▶ *Concentration of products (therapeutic,...):* $U(x) = \mathbb{E}(U(x, Y))$
 $U(x, Y) := \mathcal{U}$ ("drug" dose x , "data" patients Y) = dosage effects
- ▶ *Median and quantiles estimation*

$$U(x) = \mathbb{P}(Y \leq x) \rightsquigarrow \text{find } x_a \text{ s.t. } \mathbb{P}(Y \leq x_a) = a$$

Robbins Monro model



Objectives

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Examples

- ▶ *Concentration of products (therapeutic,...):* $U(x) = \mathbb{E}(U(x, Y))$
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$$U(x) = \mathbb{P}(Y \leq x) \rightsquigarrow \text{find } x_a \text{ s.t. } \mathbb{P}(Y \leq x_a) = a$$

- ▶ *Optimization problems* (V smooth & convex)

$$U(x) = \nabla V(x) \rightsquigarrow \text{find } x_0 \text{ s.t. } \nabla V(x_0) = 0$$

When U is known

Hypothesis

$$U_a = \{x_a\} \quad \& \quad \langle (x - x_a), U(x) - U(x_a) \rangle > 0$$



When U is known



Hypothesis

$$U_a = \{x_a\} \quad \& \quad \langle (x - x_a), U(x) - U(x_a) \rangle > 0$$

$$\Updownarrow d = 1$$

Same sign!

$$U(x) \geq U(x_a) \Rightarrow x \geq x_a$$

$$U(x) \leq U(x_a) \Rightarrow x \leq x_a$$

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Algorithm?

$$x_{n+1} = x_n + \gamma_n (U(x_a) - U(x_n))$$

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Algorithm?

$$x_{n+1} = x_n + \gamma_n (U(x_a) - U(x_n))$$

with some technical conditions

$$\sum_n \gamma_n = \infty \quad \text{and} \quad \sum_n \gamma_n^2 < \infty$$

When $U(x) = \mathbb{E}(\mathcal{U}(x, Y))$ is **unknown**



Examples

► Quantiles

$$U(x) = \mathbb{P}(Y \leq x) = \mathbb{E}(\mathcal{U}(x, Y)) \quad \mathcal{U}(x, Y) := 1_{]-\infty, x]}(Y)$$

When $U(x) = \mathbb{E}(\mathcal{U}(x, Y))$ is **unknown**



Examples

- ▶ **Quantiles**

$$U(x) = \mathbb{P}(Y \leq x) = \mathbb{E}(\mathcal{U}(x, Y)) \quad \mathcal{U}(x, Y) := 1_{]-\infty, x]}(Y)$$

- ▶ **Dosage effects** Y = absorption curves of drugs w.r.t. time

$$U(x) = \mathbb{E}(\mathcal{U}(x, Y))$$

When $U(x) = \mathbb{E}(\mathcal{U}(x, Y))$ is **unknown**



Examples

- ▶ **Quantiles**

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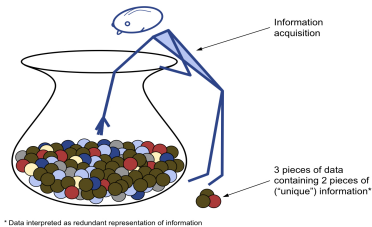
$$U(x) = \mathbb{E}(\mathcal{U}(x, Y))$$

- ▶ **Noisy measurements**

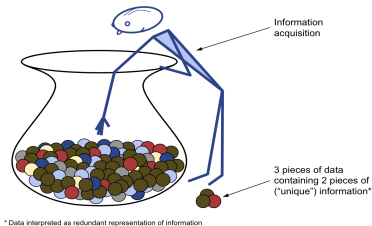
$$x \longrightarrow \boxed{\text{sensor/black box}} \longrightarrow \mathcal{U}(x, Y) := U(x) + Y$$

Unknown \rightsquigarrow Sampling

Ideal deterministic algorithm



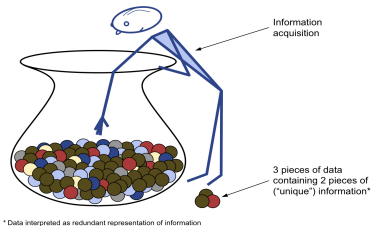
Unknown \rightsquigarrow Sampling



Ideal deterministic algorithm

$$x_{n+1} = x_n + \gamma_n (U(x_a) - U(x_n)) = x_n + \gamma_n (a - U(x_n))$$

Unknown \rightsquigarrow Sampling



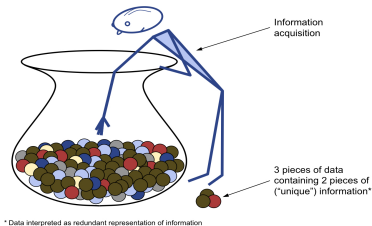
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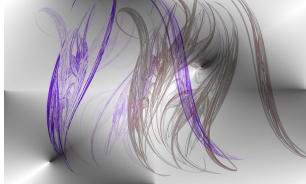
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Robbins Monro algorithm

$$X_{n+1} = X_n + \gamma_n (a - U(x_n, Y_n))$$

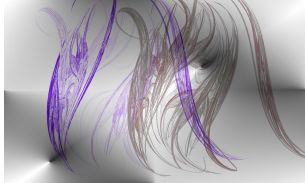
Stochastic gradient



Robbins Monro algorithm

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Stochastic gradient

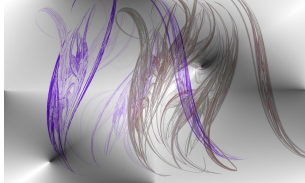


Robbins Monro algorithm

$$X_{n+1} = X_n + \gamma_n (a - U(x_n, Y_n))$$

$$\Downarrow a = 0 \quad \& \quad U(x, Y_n) = \nabla \mathcal{V}_x(x, Y_n) \quad (\rightsquigarrow U(x) = \nabla_x \mathbb{E}(\mathcal{V}_x(x, Y)))$$

Stochastic gradient



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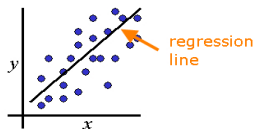
$$X_{n+1} = X_n - \underbrace{\gamma_n}_{\text{learning rate}} \nabla \mathcal{V}_x(X_n, Y_n)$$

Example (linear regression)

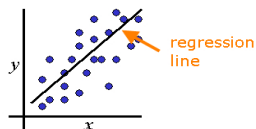
N data set $z^i \in \mathbb{R}^d \rightsquigarrow$ observation $y^i \in \mathbb{R}^{d'}$

Best $x \in \mathbb{R}^d$? such that

$$y^i \simeq h_x(z^i) + N(0, 1) \quad \text{with} \quad h_x(z) = \sum_{1 \leq i \leq d} x_i z_i$$



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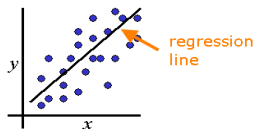
Averaging criteria

$$\mathcal{U}(x) = \mathbb{E}(\mathcal{V}(x, (y^I, z^I))) \stackrel{I \text{ unif} \in \{1, \dots, N\}}{=} \frac{1}{2N} \sum_{1 \leq i \leq N} (h_x(z^i) - y^i)^2$$

with

$$\mathcal{V}(x, (y^i, z^i)) = \frac{1}{2} (h_x(z^i) - y^i)^2 \Rightarrow \nabla_x \mathcal{V} = \begin{pmatrix} (h_x(z^i) - y^i) z_1^i \\ \dots \\ (h_x(z^i) - y^i) z_d^i \end{pmatrix}$$

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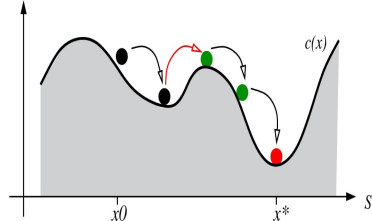
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Stochastic gradient process

$$X_{n+1} = X_n - \gamma_n \nabla_x \mathcal{V}(X_n, (Y^n, Z^n))$$

Simulated annealing

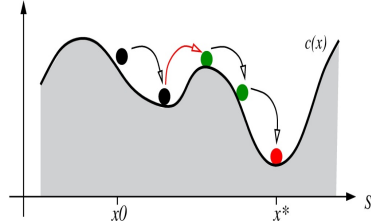
Objectives



given $V : S \mapsto \mathbb{R}$ find $V^* = \{x \in S : V(x) = \inf_y V(y)\}$

Simulated annealing

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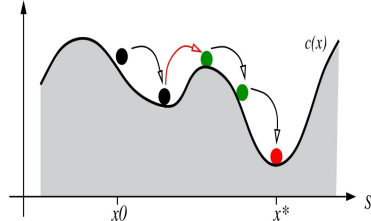


Probabilist viewpoint: \Leftrightarrow *Sampling the Boltzmann-Gibbs distribution*

$$\mu_\beta(dx) := \frac{1}{Z_\beta} e^{-\beta V(x)} \lambda(dx)$$

for some reference measure λ .

Simulated annealing



Objectives

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Probabilist viewpoint: \Leftrightarrow Sampling the Boltzmann-Gibbs distribution

$$\mu_\beta(dx) := \frac{1}{Z_\beta} e^{-\beta V(x)} \lambda(dx)$$

for some reference measure λ . **A couple of examples**

$$\begin{aligned} S &= \{x_1, \dots, x_k\} & \lambda(\{x_i\}) &:= \lambda(x_i) = \frac{1}{d} \\ S &= \mathbb{R}^k & \lambda(dx) &:= \prod_{1 \leq i \leq k} dx^i = \text{Lebesgue measure on } \mathbb{R}^k \end{aligned}$$

Optimization vs. Sampling



Finite state spaces $S = \{x_1, \dots, x_k\} \ni x_i$

$$\mu_\beta(x_i) := \frac{e^{-\beta V(x_i)} \lambda(x_i)}{\sum_{y \in S} e^{-\beta V(y)} \lambda(y)} = \frac{e^{-\beta V(x_i)}}{\sum_{1 \leq j \leq k} e^{-\beta V(x_j)}}$$

Optimization vs. Sampling



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Proposition

$$\mu_\beta(x_i) \xrightarrow{\beta \uparrow \infty} \mu_\infty(x_i) = \frac{1}{\text{Card}(V^*)} 1_{V^*}(x_i)$$

Proof:



Metropolis-Hastings transition



Reversible proposition w.r.t. λ (local moves/neighbors)

$$\lambda(x)P(x, y) = \lambda(y)P(y, x)$$

Metropolis-Hastings transition



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Acceptance/rejection transition

$$\begin{aligned} M_{\beta}(x, y) &= P(x, y) \min \left(1, \frac{\mu_{\beta}(y)P(y, x)}{\mu_{\beta}(x)P(x, y)} \right) + \dots \delta_x(dy) \\ &= P(x, y) e^{-\beta(V(y)-V(x))_+} + \dots \delta_x(dy) \end{aligned}$$

\Downarrow

Metropolis-Hastings transition



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Acceptance/rejection transition

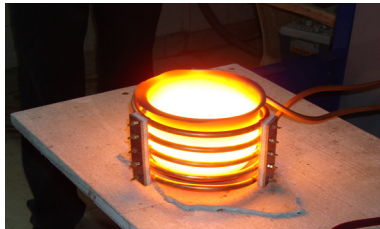
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\Downarrow

Balance/Reversibility equation

$$\mu_\beta(y)M_\beta(y, x) = \mu_\beta(x)M_\beta(x, y)$$

Simulated Annealing



$$X_0 \xrightarrow{M_{\beta_0}^{n_0}} X_{n_0} \xrightarrow{M_{\beta_1}^{n_1}} X_{n_0+n_1} \xrightarrow{M_{\beta_2}^{n_2}} X_{n_0+n_1+n_2} \dots / \dots$$

$\sim \mu_{\beta_0} \qquad \qquad \sim \mu_{\beta_1} \qquad \qquad \sim \mu_{\beta_2}$

Simulated Annealing



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You Tube illustrations

- ▶ SA and Travelling Salesman problem
- ▶ Automatic Label placement
- ▶ Ising model with SA
- ▶ Artist view of the SA & the Ising model

Interacting Simulated Annealing

$$e^{-\beta_1 V} = e^{-(\beta_1 - \beta_0)V} \times e^{-\beta_0 V}$$

Interacting Simulated Annealing

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⇔ **Bayes' type multiplication rule**

$$\mu_{\beta_1}(dx) \propto e^{-(\beta_1 - \beta_0)V(x)} \times \mu_{\beta_0}(dx)$$

Interacting Simulated Annealing

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$\forall i = 1, \dots, N \rightsquigarrow$ Interacting Simulated Annealing

$$\begin{array}{ccc} \widehat{X}_0^i & \xrightarrow{M_{\beta_0}^{n_0}} & X_{n_0}^i \\ \sim \mu_{\beta_0} & & \downarrow \\ \mu_{\beta_0}^N = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{X_{n_0}^i} & \sim & \mu_{\beta_0} \end{array}$$

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⇓

$$(*) \sum_{1 \leq i \leq N} \frac{e^{-(\beta_1 - \beta_0)V(X_{n_0}^i)}}{\sum_{1 \leq j \leq N} e^{-(\beta_1 - \beta_0)V(X_{n_0}^j)}} \delta_{X_{n_0}^i} \sim \mu_{\beta_1}$$

Interacting Simulated Annealing

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⇓

∀ i = 1, ..., N ⇔ Interacting Simulated Annealing

$$\begin{array}{ccc} \widehat{X}_0^i & \xrightarrow{M_{\beta_0}^{n_0}} & X_{n_0}^i & \xrightarrow{N \text{ samples from } (*)} & \widehat{X}_{n_1}^i \\ \sim \mu_{\beta_0} & & \downarrow & & \sim \mu_{\beta_1} \end{array}$$
$$\mu_{\beta_0}^N = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{X_{n_0}^i} \sim \mu_{\beta_0}$$

⇓

$$(*) \sum_{1 \leq i \leq N} \frac{e^{-(\beta_1 - \beta_0)V(X_{n_0}^i)}}{\sum_{1 \leq j \leq N} e^{-(\beta_1 - \beta_0)V(X_{n_0}^j)}} \delta_{X_{n_0}^i} \sim \mu_{\beta_1}$$

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$\forall i = 1, \dots, N \rightsquigarrow$ Interacting Simulated Annealing

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⇓

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Rare event sampling



$$\mu_A(dx) := \frac{1}{Z_A} \mathbf{1}_A(x) \lambda(dx)$$

Rare event sampling



$$\mu_A(dx) := \frac{1}{Z_A} 1_A(x) \lambda(dx)$$

Black box model

$$\begin{array}{l} A \ni X \\ \sim \lambda \end{array} \rightarrow \boxed{\text{Black-Box = Input/Output}} \rightarrow \begin{array}{l} Y = F(X) \\ \in \text{critical set B} \end{array}$$

Rare event sampling



$$\mu_A(dx) := \frac{1}{Z_A} 1_A(x) \lambda(dx)$$

Black box model

$$\begin{array}{l} A \ni X \\ \sim \lambda \end{array} \rightarrow \boxed{\text{Black-Box = Input/Output}} \rightarrow \begin{array}{l} Y = F(X) \\ \in \text{critical set } B \end{array}$$

\Downarrow

$$\mu_A = \text{Law}(X \mid Y \in B) = \text{Law}(X \mid X \in A)$$

Subset shakers



Reversible proposition w.r.t. λ (local moves/neighbors)

$$\lambda(x)P(x, dy) = \lambda(y)P(y, dx)$$

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Example:

$$\lambda = N(0, 1) \quad \text{and} \quad Y = \sqrt{\epsilon} x + \sqrt{1 - \epsilon} N(0, 1) \sim P(x, dy)$$

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Acceptance/rejection transition = A-Shaker

$$M_A(x, dy) = P(x, dy) 1_A(y) + (1 - P(x, A)) \delta_x(dy)$$

\Downarrow

$$\mu_A(dy)M_A(y, dx) = \mu_A(dx)M_A(x, dy)$$

Interacting Subset Sampling $A_n \downarrow$

$$1_{A_1} = 1_{A_1 \cap A_0} = 1_{A_1} \times 1_{A_0}$$

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$\forall i = 1, \dots, N \rightsquigarrow$ **Interacting Simulated Annealing**

$$\begin{array}{ccc} \widehat{X}_0^i & \xrightarrow{M_{A_0}^{n_0}} & X_{n_0}^i \\ \sim \mu_{A_0} & & \downarrow \\ \mu_{A_0}^N & = \frac{1}{N} \sum_{1 \leq i \leq N} & \delta_{X_{n_0}^i} \sim \mu_{A_0} \end{array}$$

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$$(*) \sum_{1 \leq i \leq N} \frac{1_{A_1}(X_{n_0}^i)}{\sum_{1 \leq j \leq N} 1_{A_1}(X_{n_0}^j)} \delta_{X_{n_0}^i} \sim \mu_{A_1}$$

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Interacting Subset Sampling $A_n \downarrow$

Local approximations

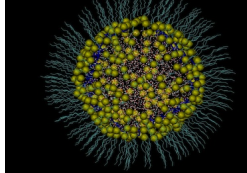
$$\begin{aligned}\mathbb{P}(X \in A_{p+1} \mid X \in A_p) &= \int 1_{A_{p+1}}(x) \mu_{A_p}(dx) \\ &\simeq \int 1_{A_{p+1}}(x) \mu_{A_p}^N(dx) = \frac{1}{N} \sum_{1 \leq j \leq N} 1_{A_{p+1}}(X_{n_0+\dots+n_p}^j)\end{aligned}$$

↓

Unbias estimate

$$\begin{aligned}\mathbb{P}(X \in A_n \mid X \in A_0) &= \mathbb{P}(X \in A_n \mid X \in A_{n-1}) \times \mathbb{P}(X \in A_{n-1} \mid X \in A_0) \\ &= \prod_{0 \leq p < n} \mathbb{P}(X \in A_{p+1} \mid X \in A_p) \\ &\simeq \prod_{0 \leq p < n} \frac{1}{N} \sum_{1 \leq j \leq N} 1_{A_{p+1}}(X_{n_0+\dots+n_p}^j)\end{aligned}$$

Molecular dynamics

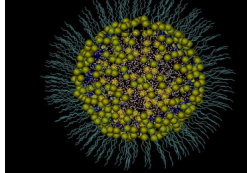


$q = (q_i)_{1 \leq i \leq k} = k$ atomic particles $\in \mathbb{R}^3$

$m = (m_i)_{1 \leq i \leq k} = k$ masses $\in \mathbb{R}_+$

$p = (p_i)_{1 \leq i \leq k} = k$ velocities $\in \mathbb{R}^3$

Molecular dynamics



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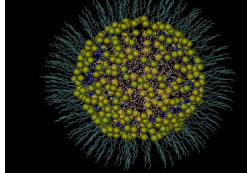
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Hamiltonian energy functional $x = (q, p)$ = phase vector

$$H(q, p) = \sum_{i=1}^k \underbrace{\frac{\|p_i\|^2}{2m_i}}_{\text{kinetic energy}} + \underbrace{V(q_1, \dots, q_k)}_{\text{interparticle potential}}$$

Molecular dynamics



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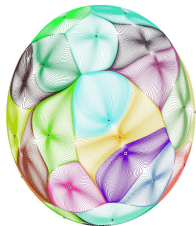
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Example: Lennard Jones potential

$$V(q_1, \dots, q_k) = \sum_{1 \leq i < j \leq k} V_{LJ}(\|q_j - q_i\|)$$

with weak van de Waals bonds energies

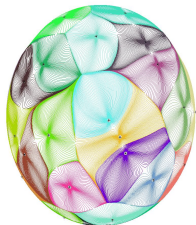
$$V_{LJ}(r) = 4\epsilon \left[\left(\frac{\tau}{r} \right)^{12} - \left(\frac{\tau}{r} \right)^6 \right]$$



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Dynamical gradient flow equations

$$\begin{cases} \frac{dq_i}{dt} = \frac{p_i}{m_i} = \frac{\partial H}{\partial p_i}(q, p) \\ \frac{dp_i}{dt} = -\frac{\partial V}{\partial q_i}(q) = -\frac{\partial H}{\partial q_i}(q, p) \end{cases}$$



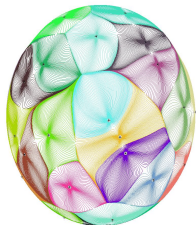
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Conservation properties

$$\frac{d}{dt} H(q, p) = \sum_{i=1}^k \left[\frac{\partial H}{\partial q_i}(q, p) \frac{dq_i}{dt} + \frac{\partial H}{\partial p_i}(q, p) \frac{dp_i}{dt} \right] = 0$$



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Time discretizations: Beeman, Leapfrog and Verlet schemes

Molecular dynamics

Boltzmann-Gibbs measures

$$H(x) = H(q, p) \rightsquigarrow \mu_\beta(dx) = \frac{1}{Z_\beta} e^{-\beta H(x)} dx \quad \text{with} \quad \beta = \frac{1}{\text{temperature}}$$

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= Invariant measures of the Langevin stochastic gradient process

$$\left\{ \begin{array}{l} dq_i = \beta \overbrace{\frac{\partial H}{\partial p_i}(q, p)}^{p_i/m_i} dt \\ dp_i = -\beta \underbrace{\left[\frac{\partial H}{\partial q_i}(q, p) + \sigma^2 \frac{\partial H}{\partial p_i}(q, p) \right]}_{= \frac{\partial V}{\partial q_i}(q) + \sigma^2 p_i/m_i} dt + \sigma \sqrt{2} \underbrace{dW_t^i}_{\text{iid Brownian}} \end{array} \right.$$

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(1 trillion simulation steps ($\sim O(\text{year})$) for 1millisecond...)

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Introduction to MD (a.k.a. the SPC water model).

Supercritical water by MDSimulator (YouTube).

Oil and water separation

Schrödinger ground states

Schrödinger equation

≈ Quantum type Newton law (De Broglie 1924)

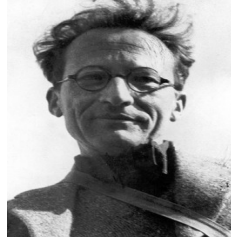
[“Physics reasoning”]

Wave function of a massive particle with:

- ▶ Velocity/momentum $p = k\hbar$
- ▶ Energy $E_c = p^2/(2m) = \hbar\omega \Rightarrow$ frequency $\omega = E_c/\hbar$

is given by

$$\psi(t, x) = \psi_0 e^{i(kx - \omega t)} \xrightarrow{\text{Bb}} i\hbar \frac{\partial \psi}{\partial t} = E_c \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$



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In a potential energy

$$E = E_c + V(x) \Rightarrow i\hbar \frac{\partial \psi}{\partial t} = E_c \psi + V \psi = \underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}}_{-L^V(\psi)} + V \psi$$

Schrödinger ground states

The wave function is the result of two traveling waves in the x and t directions.

Schrödinger ground states

Schrödinger eq. \simeq Quantum version of Newton law

$$i\hbar \frac{\partial \psi}{\partial t} = E_c \psi + V \psi = \underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}}_{-L^V(\psi)} + V \psi$$

$$\Downarrow \quad u(\tau, x) = \psi(-i\tau\hbar, x)$$

Feynman-Kac model/Heat equation

$$\frac{\partial u}{\partial \tau} = L^V(u) := \frac{\hbar^2}{2m} \frac{\partial^2 u}{\partial x^2} - Vu$$

Feynman-Kac/Heat equation

$$\frac{\partial u}{\partial \tau} = L^V(u) := \underbrace{\frac{\hbar^2}{2m} \frac{\partial^2 u}{\partial x^2}}_{:=L^0(u)} - Vu$$

Solution s.t. $u(0, x) = f(x) \rightsquigarrow$ **Feynman-Kac model**

$$\begin{aligned} u(\tau, x) &= Q_\tau(f)(x) \\ &:= \mathbb{E} \left(f(X_\tau) e^{-\int_0^\tau V(X_s) ds} \mid X_0 = x \right) \end{aligned}$$

with the diffusion:

$$dX_s = (\hbar/\sqrt{m}) \underbrace{dW_s}_{\text{Brownian}}$$

Proof:



Spectral decomposition of L^V

Reversibility

$$\begin{aligned}\int g(x) L^V(f)(x) dx &= \int g(x) \frac{\hbar^2}{2m} \frac{\partial^2 f}{\partial x} dx - \int g(x) V(x) f(x) dx \\ &= \int f(x) \frac{\hbar^2}{2m} \frac{\partial^2 g}{\partial x} dx - \int f(x) V(x) g(x) dx \\ &= \int f(x) L^V(g)(x) dx := \langle f, L^V(g) \rangle\end{aligned}$$

⇓

Spectral decomposition on $\mathbb{L}_2(\mathbb{R}^d)$ $\exists E_i \uparrow \in [0, \infty[$ and $\exists \psi_i$ orthonormal eigenfunctions s.t.

$$Q_t(f) = \sum_{i \geq 0} e^{-tE_i} \langle \varphi_i, f \rangle \varphi_i$$

Spectral decomposition of L^V

$$Q_t(f) = \sum_{i \geq 0} e^{-tE_i} \varphi_i \langle \varphi_i, f \rangle$$

Consequences:

$$\begin{aligned} \frac{dQ_t(f)}{dt} &= - \sum_{i \geq 0} E_i e^{-tE_i} \langle \varphi_i, f \rangle \varphi_i \\ &= \sum_{i \geq 0} e^{-tE_i} \langle \varphi_i, f \rangle L^V(\varphi_i) \Rightarrow L^V(\varphi_i) = -E_i \varphi_i \end{aligned}$$

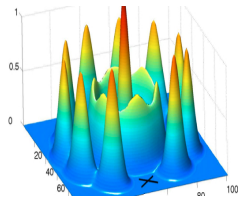
and for the "top" eigenvalue and its eigenvector φ_0 (ground state)

$$-\frac{1}{t} \log Q_t(1) \xrightarrow{t \uparrow \infty} E_0 \quad \text{and} \quad \frac{Q_t(f)}{Q_t(1)} \simeq_{t \uparrow \infty} \frac{\langle f, \varphi_0 \rangle}{\langle 1, \varphi_0 \rangle}$$

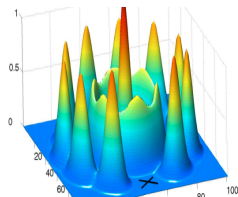
Quantum/Diffusion Monte Carlo methods

$$\mathbb{E} \left(f(X_\tau) e^{-\int_0^\tau V(X_s) ds} \right)$$

$$\simeq \mathbb{E} \left(f(X_{t_n}) \prod_{0 \leq t_k < t_n} e^{-V(X_{t_k})(t_k - t_{k-1})} \right)$$



Quantum/Diffusion Monte Carlo methods



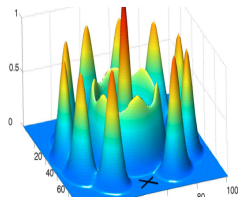
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N interacting walkers/replica evolving in two steps (toy model)

$$(X_{t_k}^i)_{1 \leq i \leq N} \xrightarrow{V\text{-reconfiguration}} (\hat{X}_{t_k}^i)_{1 \leq i \leq N} \xrightarrow{X\text{-exploration}} (X_{t_{k+1}}^i)_{1 \leq i \leq N}$$

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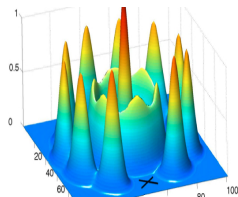
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► **Reconfigurations (selected of low energies)**

$$(\hat{X}_{t_k}^i)_{1 \leq i \leq N} \text{ iid } \sum_{1 \leq j \leq N} \frac{e^{-V(X_{t_k}^i)(t_k - t_{k-1})}}{\sum_{1 \leq j \leq N} e^{-V(X_{t_k}^j)(t_k - t_{k-1})}} \delta_{X_{t_k}^i}$$

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► **Explorations**

$$X_{t_{k+1}}^i := \hat{X}_{t_k}^i + (\hbar/\sqrt{m}) \underbrace{(W_{t_{k+1}}^i - W_{t_k}^i)}_{\text{iid Brownian}}$$

Some Monte Carlo estimates

$$\mathbb{E} \left(f(X_\tau) e^{-\int_0^\tau V(X_s) ds} \right)$$

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$$\begin{aligned} & \mathbb{E} \left(f(X_\tau) e^{-\int_0^\tau V(X_s) ds} \right) \\ & \simeq \mathbb{E} \left(f(X_{t_n}) \prod_{0 \leq t_k < t_n} e^{-V(X_{t_k})(t_k - t_{k-1})} \right) \\ & \simeq \left[\frac{1}{N} \sum_{1 \leq i \leq N} f(X_{t_n}^i) \right] \prod_{0 \leq t_k < t_n} \underbrace{\frac{1}{N} \sum_{1 \leq i \leq N} e^{-V(X_{t_k}^i)(t_k - t_{k-1})}} \end{aligned}$$

Some Monte Carlo estimates

$$\mathbb{E} \left(f(X_T) e^{-\int_0^T V(X_s) ds} \right)$$

$$\simeq \mathbb{E} \left(f(X_{t_n}) \prod_{0 \leq t_k < t_n} e^{-V(X_{t_k})(t_k - t_{k-1})} \right)$$

$$\simeq \left[\frac{1}{N} \sum_{1 \leq i \leq N} f(X_{t_n}^i) \right] \prod_{0 \leq t_k < t_n} \underbrace{\frac{1}{N} \sum_{1 \leq i \leq N} e^{-V(X_{t_k}^i)(t_k - t_{k-1})}}_{\sim 1 - \frac{1}{N} \sum_{1 \leq i \leq N} V(X_{t_k}^i)(t_k - t_{k-1})}$$

Some Monte Carlo estimates

$$\mathbb{E} \left(f(X_T) e^{-\int_0^T V(X_s) ds} \right)$$

$$\simeq \mathbb{E} \left(f(X_{t_n}) \prod_{0 \leq t_k < t_n} e^{-V(X_{t_k})(t_k - t_{k-1})} \right)$$

$$\simeq \left[\frac{1}{N} \sum_{1 \leq i \leq N} f(X_{t_n}^i) \right] \prod_{0 \leq t_k < t_n} \underbrace{\frac{1}{N} \sum_{1 \leq i \leq N} e^{-V(X_{t_k}^i)(t_k - t_{k-1})}}_{\sim 1 - \frac{1}{N} \sum_{1 \leq i \leq N} V(X_{t_k}^i)(t_k - t_{k-1})}$$

$$\simeq \left[\frac{1}{N} \sum_{1 \leq i \leq N} f(X_{t_n}^i) \right] e^{-\sum_{t_k < t_n} \frac{1}{N} \sum_{1 \leq i \leq N} V(X_{t_k}^i)(t_k - t_{k-1})}$$

Some Monte Carlo estimates

$$\mathbb{E} \left(f(X_\tau) e^{-\int_0^\tau V(X_s) ds} \right)$$

$$\simeq \mathbb{E} \left(f(X_{t_n}) \prod_{0 \leq t_k < t_n} e^{-V(X_{t_k})(t_k - t_{k-1})} \right)$$

$$\simeq \left[\frac{1}{N} \sum_{1 \leq i \leq N} f(X_{t_n}^i) \right] \prod_{0 \leq t_k < t_n} \underbrace{\frac{1}{N} \sum_{1 \leq i \leq N} e^{-V(X_{t_k}^i)(t_k - t_{k-1})}}_{\sim 1 - \frac{1}{N} \sum_{1 \leq i \leq N} V(X_{t_k}^i)(t_k - t_{k-1})}$$

$$\simeq \left[\frac{1}{N} \sum_{1 \leq i \leq N} f(X_{t_n}^i) \right] e^{-\sum_{t_k < t_n} \frac{1}{N} \sum_{1 \leq i \leq N} V(X_{t_k}^i)(t_k - t_{k-1})}$$

\rightsquigarrow **Log-Lyapunov exponent/top eigenvalue**

$$(f = 1) \Rightarrow -\frac{1}{t} \log \mathbb{E} \left(e^{-\int_0^\tau V(X_s) ds} \right) \simeq E_0 \simeq \frac{1}{t_n} \sum_{t_k < t_n} \frac{1}{N} \sum_{1 \leq i \leq N} V(X_{t_k}^i)(t_k - t_{k-1})$$

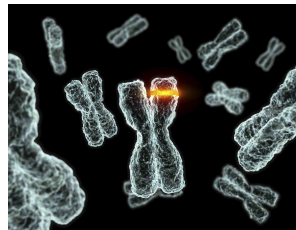
and the eigenvector/ground state energy

$$N^{-1} \sum_{1 \leq i \leq N} \delta_{X_{t_n}^i} \simeq_{t_n \uparrow \infty} \psi_0(x) dx / \langle 1, \psi_0 \rangle$$

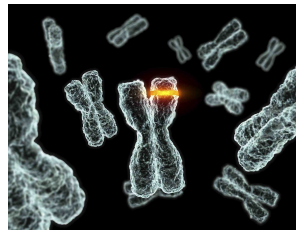
Genetic type algorithms

Population of N individuals

- ▶ Mutation (\sim some given Markov transition M_n)
- ▶ Selection w.r.t. some fitness functions $G_n(x)$



Genetic type algorithms



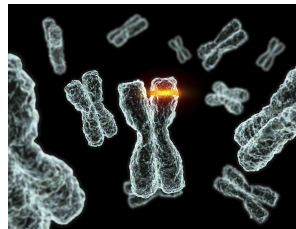
Population of N individuals

- ▶ Mutation (\sim some given Markov transition M_n)
- ▶ Selection w.r.t. some fitness functions $G_n(x)$

Synthetic picture

$$(X_0^i)_{1 \leq i \leq N} \xrightarrow{\text{selection} \sim G_0} (\hat{X}_0^i)_{1 \leq i \leq N} \xrightarrow{\text{mutation} \sim M_1} (X_1^i)_{1 \leq i \leq N}$$

Genetic type algorithms



Population of N individuals

- ▶ Mutation (\sim some given Markov transition M_n)
- ▶ Selection w.r.t. some fitness functions $G_n(x)$

Synthetic picture

$$\begin{array}{ccccc} (X_0^i)_{1 \leq i \leq N} & \xrightarrow{\text{selection } \sim G_0} & (\hat{X}_0^i)_{1 \leq i \leq N} & \xrightarrow{\text{mutation } \sim M_1} & (X_1^i)_{1 \leq i \leq N} \\ & & \xrightarrow{\text{selection } \sim G_1} & & \xrightarrow{\text{mutation } \sim M_2} \\ & & (\hat{X}_1^i)_{1 \leq i \leq N} & & (X_2^i)_{1 \leq i \leq N} \quad \dots / \dots \end{array}$$

Genetic type algorithms

$G_n = e^{-\beta_n V}$ & $M_n =$ Simulated annealing move \rightsquigarrow interacting SA (optimization)

More generally:

$N \uparrow \infty$ computational power $\Rightarrow \hat{X}_n^i$ almost iid with Feynman-Kac law

$$\frac{1}{N} \sum_{1 \leq i \leq N} f(X_n^i) \underset{N \uparrow \infty}{\propto} \mathbb{E}(f(X_n)) \prod_{0 \leq p < n} G_p(X_p)$$

Somme illustrations - Artificial Intelligence

- ▶ Painting Mona Lisa
- ▶ Darwin - Genetic programming
- ▶ GA robot controller
- ▶ Learning how to walk
- ▶ GA vs Tetris
- ▶ Evolutionary computation (Danubia 2011)