Adding some memory in stochastic algorihms

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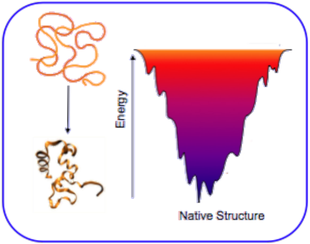
INRIA's Junior Seminar

High dimensional problems

Example: proteim folding, big data, path finding. . .

- Ω configuration space
- $x \in \Omega$ microscopic configuration
- $V(x)$: energy of x



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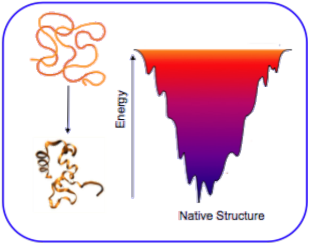

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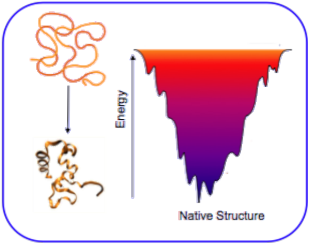

Two typical questions:

- Optimization: find x_0 such that $V(x_0) = \min_{\Omega} V$.
- Computing macroscopic quantities

$$\mathbb{E}\left(f(X)\right) = \frac{\int_\Omega f(x) e^{-\beta V(x)} \mathrm{d}x}{\int_\Omega e^{-\beta V(x)} \mathrm{d}x}$$

when X is random with Gibbs law at inverse temperature β.

Deterministic algorithms

Exhaustiveness: discretization (if necessary; Ω may already be discrete)

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- $d = 3 \times 100$ amino acid in a protein, $m = 10 \Rightarrow$ Crazy.
- $30! \simeq 10^{32}$ different paths to connect 30 nodes $\Rightarrow$ Crazy.

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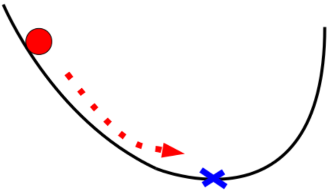
Gradient descent: Start from $x_0 \in \Omega$, then

$$x'(t) \;=\; -\nabla V\left(x(t)\right).$$



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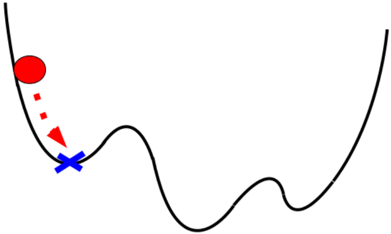
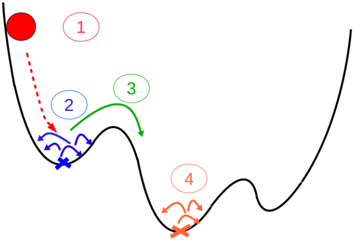


Problem: multi-modality.

Stochastic algorithms

Start from $x_0 \in \Omega$ and B a Brownian motion, then

$$x'(t) \;=\; -\nabla V\left(x(t)\right) + \sqrt{2\beta^{-1}}\mathrm{d}B_t.$$



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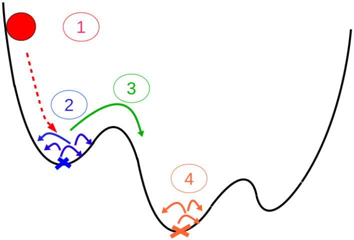

For large times t, $Law\left(x(t)\right) \simeq e^{-\beta V}$. The process is ergodic:

$$\frac{1}{t}\int_{s=0}^{t} f\left(x(s)\right)\mathrm{d}s \underset{t\to\infty}{\longrightarrow} \frac{\int_\Omega f(y)e^{-\beta V(y)}\mathrm{d}y}{\int_\Omega e^{-\beta V(y)}\mathrm{d}y}.$$

Markov Chain Monte Carlo (MCM) algorithms

Markov process/chain = no memory:

$$x'(t) \;=\; -\nabla V\left(x(t)\right) + \sqrt{2\beta^{-1}}\mathrm{d}B_t,$$

or, with a standard Gaussian variable G and a stepsize δ,

$$X_{n+1} \;=\; X_n - \delta\nabla V\left(X_n\right) + \sqrt{2\delta\beta^{-1}}G.$$

The past, $(X_k)_{k<n}$, is not needed (= is not used).

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Amnesic exploration of Ω :

Inefficient !

(metastability)

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Consider the velocity $y(t) = x'(t)$. Add some inertia.

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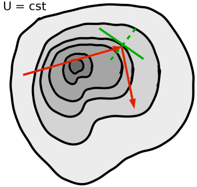

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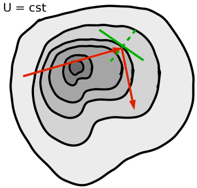

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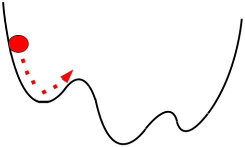

$$my'(t) = -\nabla V(x(t)) - \nu y(t) + \sqrt{2\beta^{-1}}\mathrm{d}B_t$$

(m = mass, ν = friction coefficient)

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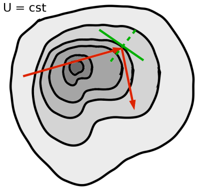

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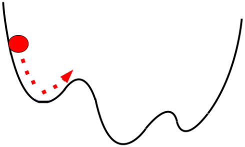

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So that in either case, again,

$$\frac{1}{t}\int_{s=0}^{t} f(x(s))\,\mathrm{d}s \underset{t\to\infty}{\longrightarrow} \frac{1}{\int_\Omega e^{-\beta V(y)}\mathrm{d}y}\int_\Omega f(y)e^{-\beta V(y)}\mathrm{d}y.$$

Degenerated Markov process

Example of the Langevin dynamics:

$$\begin{aligned} x'(t) &= y(t) \\ y'(t) &= -\nabla V\left(x(t)\right) - y(t) + \sqrt{2\beta^{-1}}\mathrm{d}B_t. \end{aligned}$$

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$$\partial_t \rho_t + v\nabla_u \rho_t = \nabla_v \cdot \left((V(u) + v)\rho \right) + \frac{1}{\beta}\Delta_v \rho$$

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"Degenerated" (linear) PDE : hypoelliptic, hypocoercive. Still, $\rho_t(u,v) \underset{t\to\infty}{\longrightarrow} e^{-V(u)-\frac{1}{2}|v|^2}$, but theory more difficult than

$$x'(t) = -\nabla V(x(t)) + \sqrt{2\beta^{-1}} \mathrm{d}B_t$$

(overdamped Langevin) for which $\rho_t(u)$ solves

$$\partial_t \rho_t = \nabla_u \cdot (V(u)\rho) + \frac{1}{\beta}\Delta_u \rho.$$

Adaptative Biasing Force (ABF) method

- Microscopic configuration: $x = (x_1, \ldots, x_d) \in \Omega = (\mathbb{T})^d$
- Reaction coordinates: (x_1, x_2)
- Free energy: $A(x_1, x_2) \;=\; \frac{1}{\beta} \ln \int e^{-\beta V(x)} \mathrm{d}x_3 \ldots \mathrm{d}x_d$

If X random with law $e^{-\beta V}$, then (X_1, X_2) with law $e^{-\beta A}$.

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Biased overdamped Langevin: sample $e^{-\beta(V-A)}$ with

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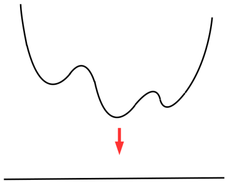
the metastability/multimodality disappeared !



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Un-biasing:

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- Benefit: the biased X converges faster to its equilibrium
- Drawback: ... A is unknown (precisely our aim in some cases)

Low dimensional, long-term memory

Solution: learn the bias ∇A on the fly, with:

$$\nabla A(x_1, x_2) = \frac{\int \nabla V(x) e^{-\beta V(x)} \mathrm{d}x_3 \ldots \mathrm{d}x_d}{\int e^{-\beta V(x)} \mathrm{d}x_3 \ldots \mathrm{d}x_d}$$

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&\simeq \frac{\sum_{s=1}^{t} \nabla V\left(X(s)\right) 1_{(X_1(s), X_2(s)) = (x_1, x_2)}}{\sum_{s=1}^{t} 1_{(X_1(s), X_2(s)) = (x_1, x_2)}}
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We keep a long-term memory: for all $(x_1,x_2) \in \{0, \frac{1}{m}, \frac{2}{m}, \dots, 1\}^2$,

$$\sum_{s=1}^t 1_{(X_1(s),X_2(s))=(x_1,x_2)} = \sharp\{\text{transit through cell } (x_1,x_2)\}$$

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The idea: A is a function of k variables. It can be approached (known greedy algorithms) by a sum of tensor products of functions of 1 variable:

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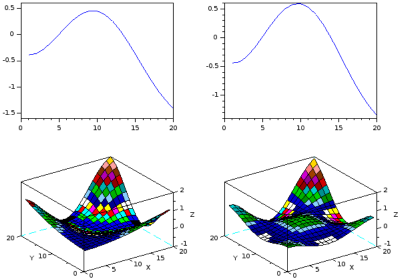
Example:

$$\begin{aligned} G(x,y) &= x^2 \cos(y) + y^2 \cos(x) \\ &\simeq r_1(x) r_2(y) \end{aligned}$$



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