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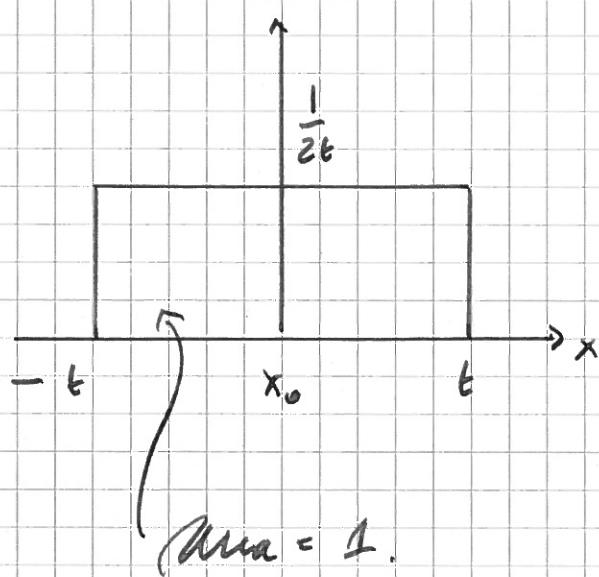
Basic idea: It is easier to ski when there is snow on the ground.

The version we will discuss here:

"Bad derivatives" clothoid

Define a smoothing function

$$I_\epsilon(x, x_0) = \frac{1}{2\epsilon} \left\{ \Theta(x - (x_0 - \epsilon)) - \Theta(x - (x_0 + \epsilon)) \right\}$$



Function to be minimized:  $U(x)$

Smoothed function.

$$U_\epsilon(x_0) = \int_{-\infty}^{+\infty} U(x) I_\epsilon(x, x_0) dx$$

$$= \frac{1}{2\epsilon} \int_{x_0 - \epsilon}^{x_0 + \epsilon} U(x) dx$$

Gradient of Smoothed function:

$$\frac{d}{dx_0} U_\epsilon(x_0) = \underline{\frac{1}{2\epsilon} [U(x_0 + \epsilon) - U(x_0 - \epsilon)]}$$

looks like a finite-difference approximation  
to non-smoothed function derivative:

Hence, the name.

optimize the smoothed  
function  $H_t(x)$ .

Then reduce  $t$  and minimize  
again starting from the  
minimum at the previous  
level. Continuum until solution  
is not improved.

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### Quantum annealing:

Basic idea:

Quantum particle is everywhere  
there is a wave function.

Particle sees entire energy  
landscape simultaneously.

Method consists in estimating ground state wave function and then let  $\hbar \rightarrow 0$ .

Wave function will then localize in global minimum of energy function.

Imaginary time Schrödinger equation:

$$\frac{\partial}{\partial \tau} \psi_m(\vec{r}, \tau) = \frac{\hbar^2}{2m} \nabla^2 \psi_m(\vec{r}, \tau)$$

$$-U(\vec{r}) \psi_m(\vec{r}, \tau)$$

↗

Function to be minimized.

$$\tau = \frac{it}{\hbar} \leftarrow \text{Imaginary time.}$$

Integration with respect to  $\tau$ :

$$\underline{\psi}_m(\vec{r}, \tau) = e^{-E_m \tau} \underline{\psi}_m(\vec{r})$$

Eigenfunction

$$H \underline{\psi}_m(\vec{r}) = E_m \underline{\psi}_m(\vec{r})$$

Random wave function:

$$\underline{\psi}(\vec{r}, \tau) = \sum_m a_m e^{-E_m \tau} \underline{\psi}_m(\vec{r})$$

When  $\tau \rightarrow \infty$ :

$$\underline{\psi}(\vec{r}, \tau) \sim e^{-E_0 \tau} \underline{\psi}_0(\vec{r})$$

Since  $E_0 < E_m$  for  $m > 0$ .

(A)

Write Schrödinger equation as

$$\frac{\partial}{\partial \tau} \psi_0(\vec{r}, \tau) = \underbrace{\frac{\hbar^2}{2m} \nabla^2 \psi_0(\vec{r}, \tau)}_{\text{diffusion equation}} - \underbrace{(U(r^2) - E_0) \psi_0(\vec{r}, \tau)}_{\text{Sources and sinks}}$$

Sinks term  
(when  $U > 0$ )      Sources term.

Start with some arbitrary  $\psi(\vec{r}, \tau)$ .

Model the system as an ensemble

of random walkers.

(Fokker-Planck equation  $\Rightarrow$  Langevin equation).

Adjust  $E_0$  iteratively so that  
a stationary process is achieved.

This is diffusion Monte Carlo.

How to do it in practice:

First suggested by  
Mark Kac in the '50ies.

Rediscovered by Leyendecker and Alder  
in the '80ies.

Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \nabla^2 + (U(\vec{r}) - E_T)$$

$\uparrow$   
last energy —  
a parameter.

Physics is not influenced  
by the choice of  $E_T$ .

Diffusion equation with unperturbative  
term.

$$\frac{\partial \psi}{\partial z} = D \nabla^2 \psi - (U(z) - E_T) \psi$$

$\frac{\hbar^2}{2m}$ .

If  $E_T = E_0$  (ground state), then

$$\lim_{z \rightarrow \infty} \psi \rightarrow \psi_0$$

↑  
ground state  
wave function.

\* If  $E_T > E_0$ , the integral

$$I = \int |Y(z, \tau)|^2 dz$$

will grow exponentially with  $\tau$ .

\* If  $E_T < E_0$ , the integral I  
will vanish exponentially with  $T$ .

$N$  random walks

$$\vec{r}_i(\tau_{n+1}) = \vec{r}_i(\tau_n) + \vec{s}_i$$

$i=1, \dots, N$

Gaussian with mean  
 $= 0$  and  $\sigma^2 = 20 \text{ st.}$

Assume an ensemble of  $M$  copies of  
the system, each with  $N$  random  
walks.

$i^{\text{th}}$  random walker in  $l^{\text{th}}$   
sample:

$$\vec{r}_{i,l}(\tau).$$

Diffusion problem alone:

$$\frac{\partial p}{\partial \tau} = D \nabla^2 p$$

$$p(\vec{r}, \tau) = \frac{1}{M} \frac{1}{N} \sum_{l=1}^M \sum_{i=1}^N \delta(\vec{r}_{i,l}(\tau) - \vec{r})$$

Autocatalytic problem alone:

$$\frac{\partial p}{\partial \tau} = f(\vec{r}) p$$

$$f(\vec{r}) = -(M(\vec{r}) - E_T).$$

General solution:

$$p(\vec{r}, \tau) = p(\vec{r}_0) e^{f(\vec{r}) \tau}$$

M samples: We let M become  
a variable:

$$M \rightarrow M(\tau).$$

1) For each of the  $M(\tau_n)$  samples,  
determine the multiplicity:

$$K_l = e^{\sum_{i=1}^N f(\vec{r}_{i;l}) \Delta t}$$

$$l = 1, \dots, M(\tau_n).$$

2) Generate  $\text{int}(K_l)$  copies of  
sample  $l$ .

With probability  $K_l - \text{int}(K_l)$   
generate an extra copy.

If  $K_l < 1$ , this  
corresponds to removing  
sample  $l$  from ensemble  
with probability  
 $1 + \text{int}(K_l) - K_l$ .

This procedure leads to an average of  $K_c$  copies of sample  $l$  in the ensemble.

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We now combine the diffusion steps based on Langevin and the autocatalytic steps.

We adjust  $E_T$  until a stationary system is achieved.

$\rightarrow \underline{\gamma_0}$  and  $\underline{E_0}$ .

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A note: We only find  $\gamma_0$  that is positive everywhere (since we interpret it as a probability).

This problem has been solved in  
the literature...

If  $\psi_0$  is negative at places, there  
are two procedures that can be  
followed:

- (A) Fixed node approximation and
- (B) Relaxed node approximation.

(A) If the  $\psi = 0$ -curves are known.  
(e.g. through symmetries), each  
region with constant sign may  
be treated separately.

(B) Vary the  $\psi = 0$  curves until a  
minimum value for  $E_T$  is found.

(A and B) : Distribute signs afterwards.

References for quantum annealing:

J. Chem. Phys. 97, 6715 (1993).

Chem. Phys. Lett. 219, 343 (1994).

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General reference for optimization  
in computational physics:

Andricom and Shaub:

Computers in Physics  
10, 449 (1996).

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Optimal paths

Suppose a network of tubes: