Simulated annealing

Nicolas & Sigurd

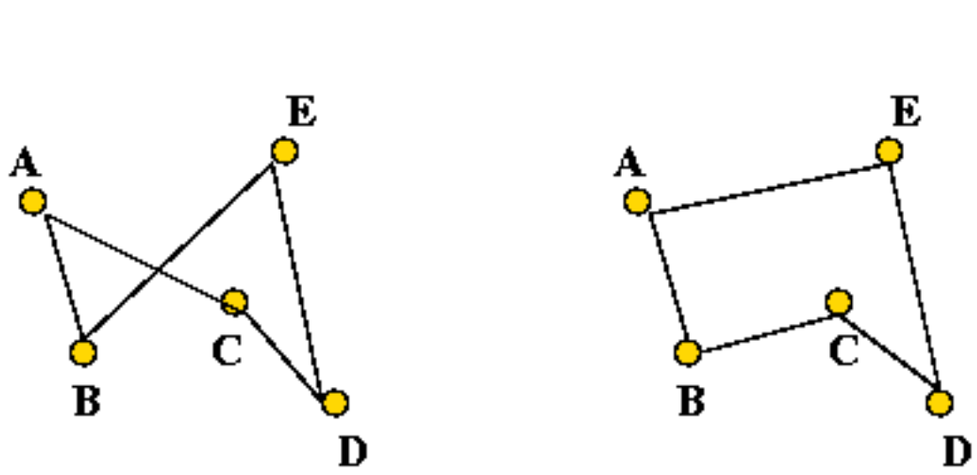
MCMC

Markov Chain Monte Carlo

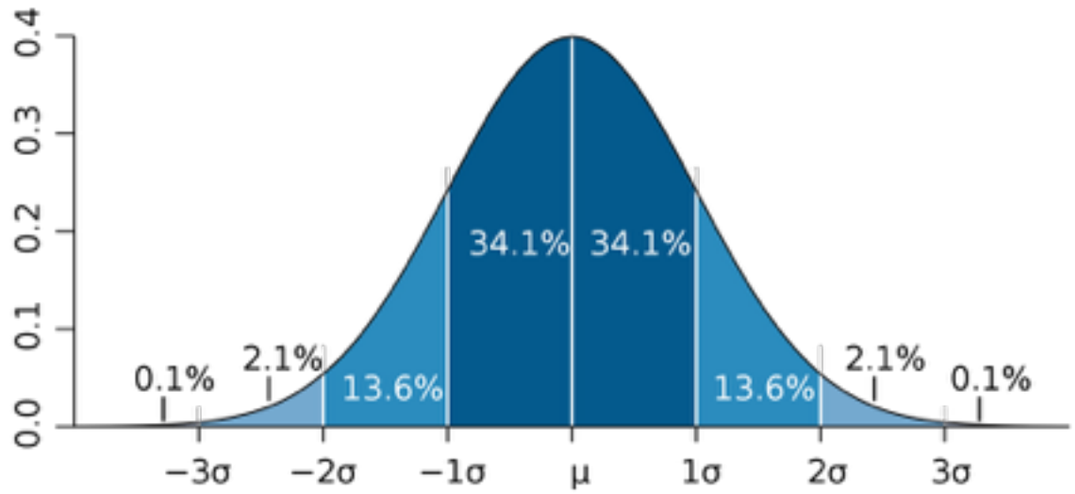
Metropolis algorithm

Able to accept states with higher energy, to avoid ending up in local minima

Define movement class

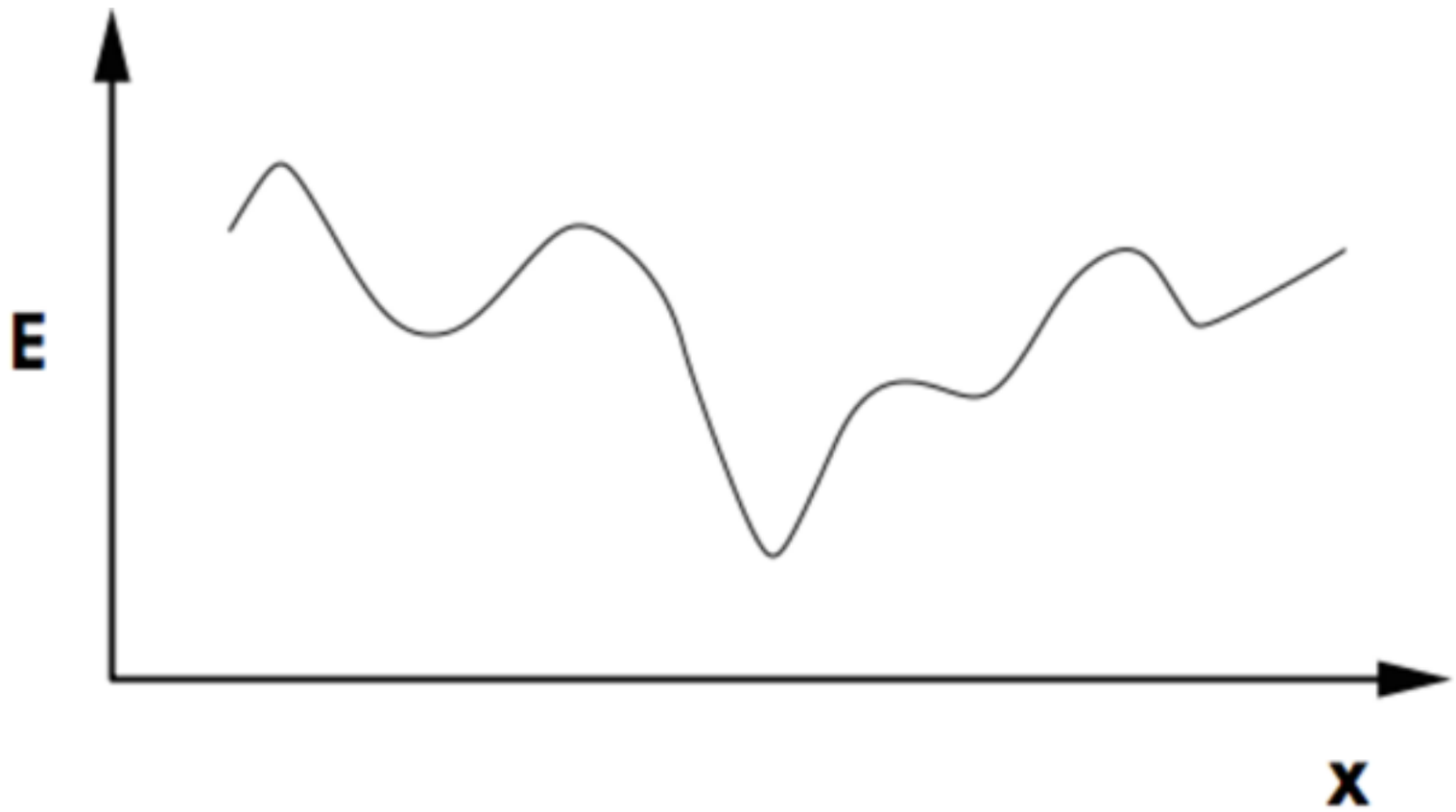


Traveling sales-man



Parameter dependent

Define energy function

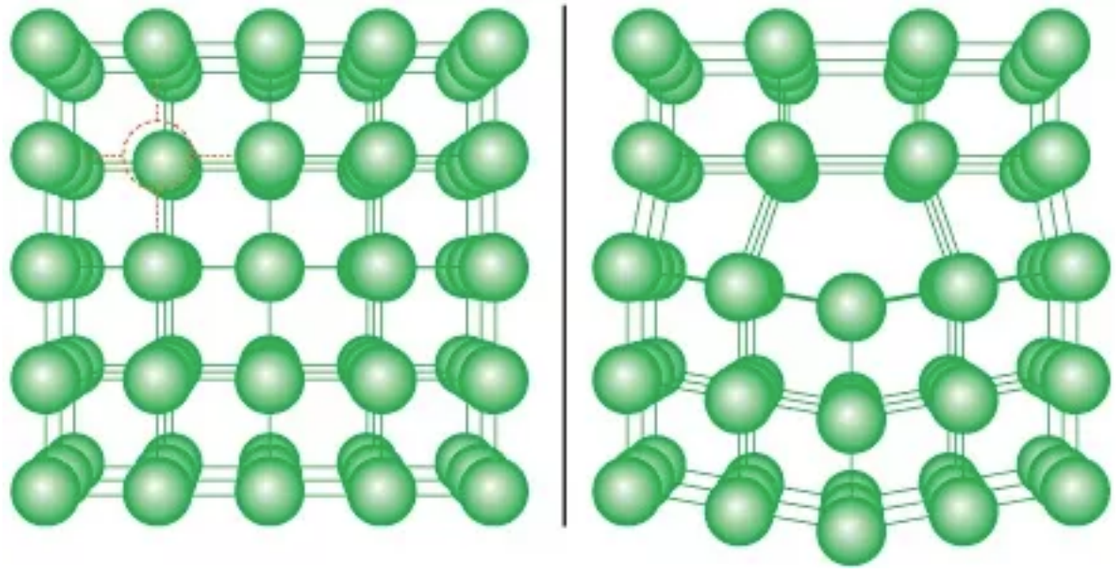


$$P_{accept} \begin{cases} 1 & \text{if } \Delta E \leq 0 \\ e^{-\Delta E/T_t} & \text{if } \Delta E > 0 \end{cases}$$

Boltzmann distribution

Physical Analogy

Cooling molecules to get crystal structure



Defects when cooled too fast

Ideas of how to vary temperature

$$T(t) = ae^{-t/b}$$ Exponential

$$T(t) = \frac{a}{log(b+t)}$$ Logarithmic

Ideas of how to vary temperature

$$T(t) = ae^{-t/b}$$ Exponential

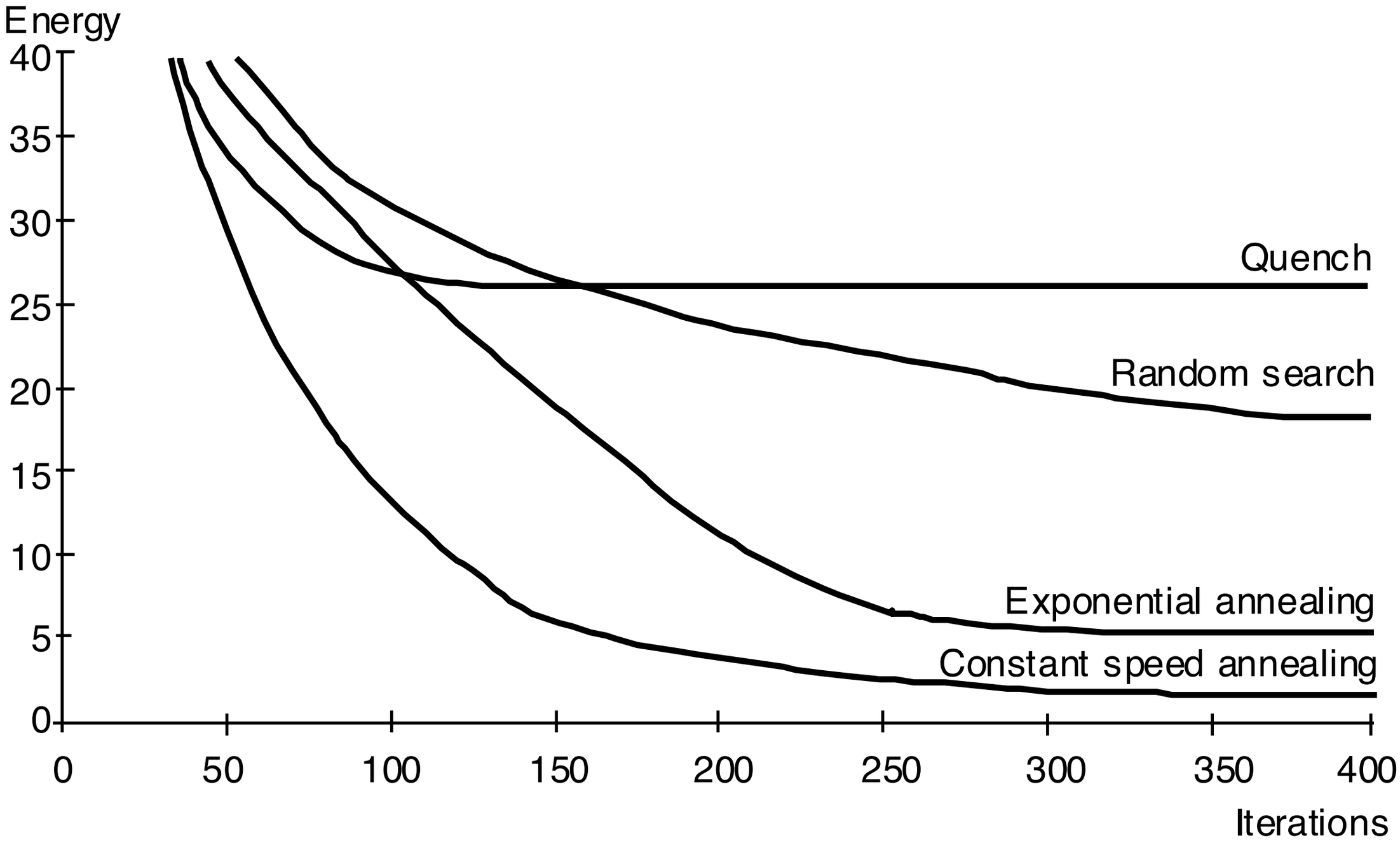
$$T(t) = \frac{a}{log(b+t)}$$ Logarithmic

Constant thermodynamic speed

$$\frac{dT}{dt} = -\frac{vT}{\epsilon\sqrt{C}}$$

$$\frac{\langle E \rangle - E_{\mathrm{eq}}(T)}{\sigma_E} = v$$

Comparing methods



Appendix

Calculation of partition function, energy,
heat capacity and relaxation constant during simulation

$$Z(T) = \sum_i p_i \exp(-E_i/T)$$

$$E(T) = T^2 \frac{d \ln Z}{dt}$$

$$C(T) = \frac{dE}{dT} = \frac{\langle (\Delta E)^2 \rangle}{T^2}$$

$$\varepsilon(T) = \frac{-1}{\ln \lambda_2} \approx \frac{T^2 C(T)}{\sum_i p_i \sum_{j>i} (E_j - E_i)^2 P_{ji} \exp(-E_i/T)}$$