Stochastic Tunneling and Time Series Analysis for Global Optimization Techniques

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Preview

- Motivation – Heuristics, Randomized Algorithms
- Test Functions
  - 1D
  - Spin Glasses
- Metropolis-based Search
  - Simulated Annealing
  - Stochastic Tunneling
- Search as a Stochastic Process
  - Analysis: Detrended Fluctuation Analysis (DFA)
  - Guidance via DFA
- Application: Protein Structure Prediction of GvpA

Test Functions

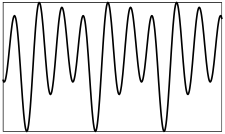
Ideas for Algorithms?

Need to Evaluate Performance

$\rightarrow$ test functions

- known minima
- combinatorial vs. continuous problems
- "tune-able" parameters
- not too hard but also not to easy

Test Functions – 1D



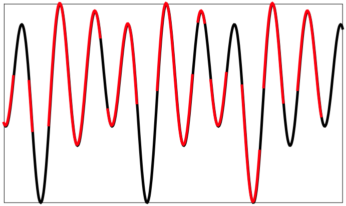
Problem!

Stochastic Search $\rightarrow$ Sampling

for general dynamics:
density of bins visited $\rho_s \sim n^{\alpha}$ for single walker with $\alpha < 1$

what happens, if

- we place m many walkers randomly
- and let them run each n/m many steps?



Test Functions – 1D

density of bins covered $\rho_m(n)$ (success rate), for small m:

$$\begin{aligned}
\rho_m(n) &= m \cdot \rho_1\left(\frac{n}{m}\right) \\
&= \frac{1}{N} \cdot m \cdot \langle\delta\rangle \cdot \left(\frac{n}{m}\right)^{\alpha} \\
&= \frac{1}{N} \cdot \langle\delta\rangle \, \underbrace{m^{1-\alpha}}_{>1} \cdot n^{\alpha} \\
&\boxed{>} \frac{1}{N} \cdot \langle\delta\rangle \cdot n^{\alpha} = \rho_1(n) = \rho_s
\end{aligned}$$

N: no. of bins

ρ_s : success rate of a single walk

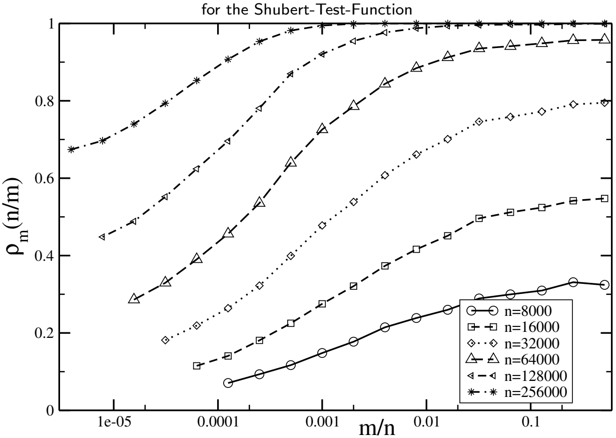
$\langle\delta\rangle$ expected jump length

for larger m

$$\boxed{\Longrightarrow \rho_n(1) = 1 - \gamma^n}$$

with $\gamma := 1 - 1/N$

Test Functions – 1D



K. Hamacher. *On Stochastic Global Optimization of one-dimensional functions*. **Physica A 354:547-557, 2005.**

$\Longrightarrow$ 1D test functions are useless

Test Functions – Spin Glasses

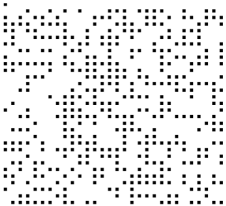
Combinatorial problem in discrete variables $\hat{s}_i \in [-1; +1]$

$$H = \frac{1}{2} \sum_{<i,j>} J_{ij} \hat{s}_i \hat{s}_j$$

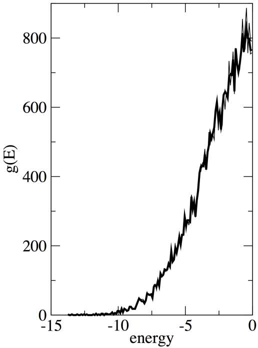
and $J_{ij} \in \mathcal{N}(0, 1)$

reference ground states from

`http://www.informatik.uni-koeln.de/spinglass`

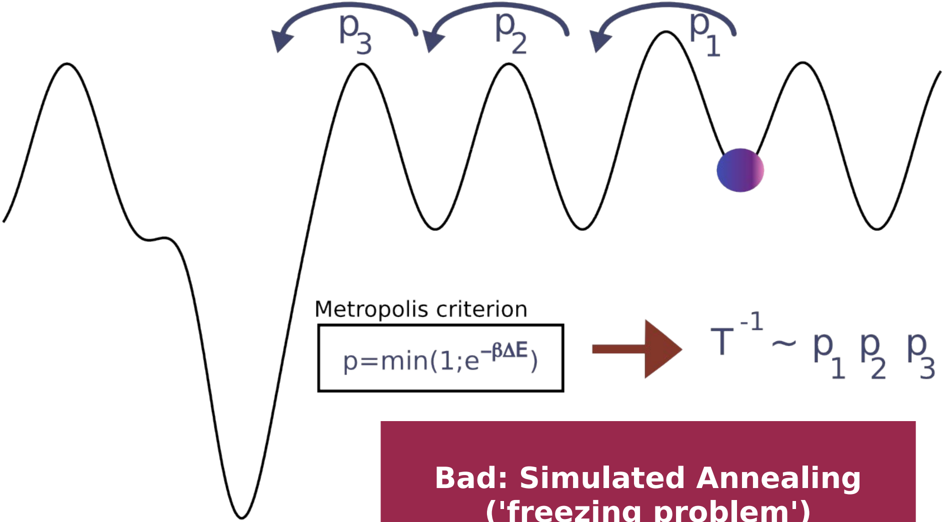


Density of State:



Heilmann, Hoffmann. Europhys. Lett. 70(2005):155

Sampling a PES (Potential Energy Surface) by Monte-Carlo



Metropolis criterion

$$\boxed{p=\min(1;e^{-\beta\Delta E})}$$

$\rightarrow$ $T^{-1} \sim p_1\ p_2\ p_3$

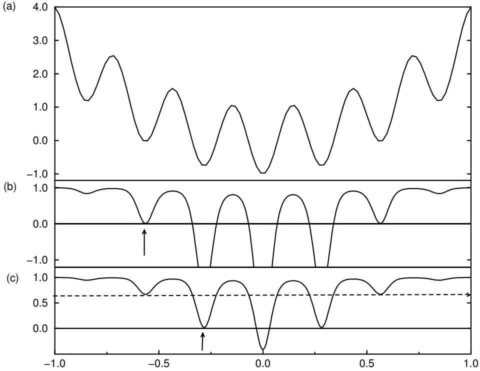
Bad: Simulated Annealing ('freezing problem')

Metropolis-based Search – Stochastic Tunneling

<u>Idea:</u>
do not care about
"high" regions

$$f_{\mathrm{STUN}}(\vec{x}) := 1 - e^{-\gamma \cdot (f(\vec{x}) - f_{\mathrm{best}})}$$

where f_{best} is the best value encountered so far



Metropolis-based Search – Stochastic Tunneling – It works!

Application to a spin model

Wenzel, Hamacher.
Phys. Rev. Lett.
82(15):3003-3007, 1999

$n_{\mathrm{iter}}/10^3$	SA	STUN
	N = 49	
10	212.48 / 176	185.12 / 136
50	196.64 / 164	168.72 / 136
100	191.68 / 144	161.60 / 136
500	177.68 / 136	151.76 / 136
1,000	175.52 / 136	139.44 / 136
	N = 101	
10	987.44 / 914	918.08 / 810
50	946.44 / 854	880.08 / 790
100	927.84 / 846	865.76 / 766
500	894.32 / 822	
1,000	891.68 / 818	

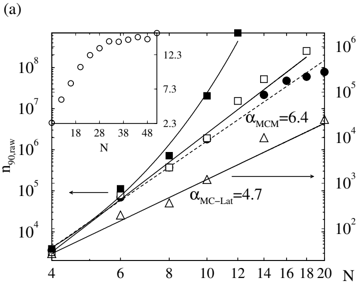
Average and best ground state

Metropolis-based Search – Stochastic Tunneling – It works!

Application to a “demixing” Lennard-Jones model

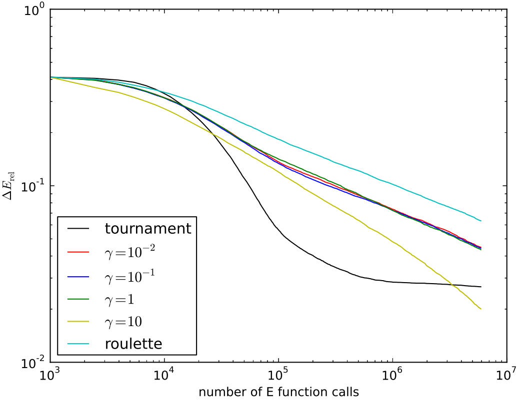
(toy model for protein folding)

Hamacher, Wenzel.
Phys. Rev. E
59(1):938-941, 1999



Stochastic Tunneling – It even works for GAs!

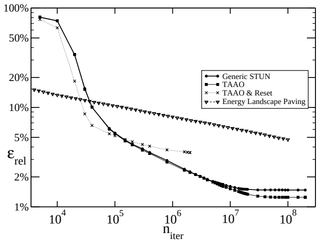
Based on a GA, we solve spin glasses, again

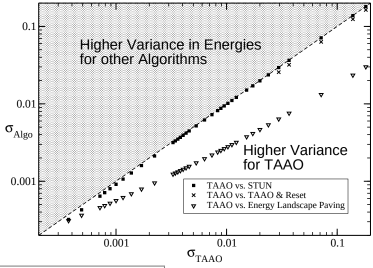


Mayer,
Hamacher.
GECCO'14
accepted, 2014

Stochastic Tunneling – Combined with Energy-Landscape-Paving

$$f_{\mathrm{TAAO}}(\vec{x}) := \underbrace{1 - e^{-\gamma\cdot(f(\vec{x})-f_{\mathrm{best}})}}_{\mathrm{STUN}} + \underbrace{\kappa \cdot H(q)}_{ELP}$$

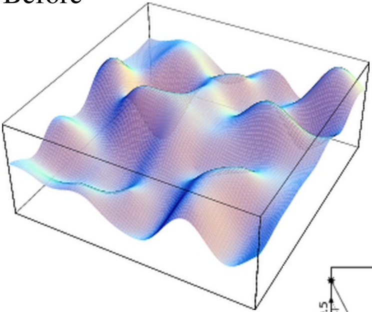




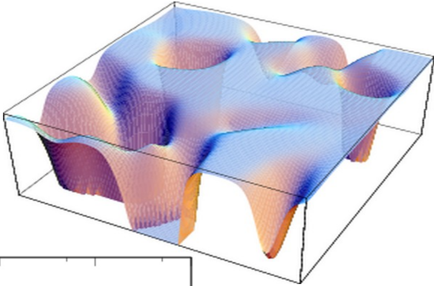
Hamacher. **Lecture Notes in Computer Science (LNCS 7919)** 107-117, 2013

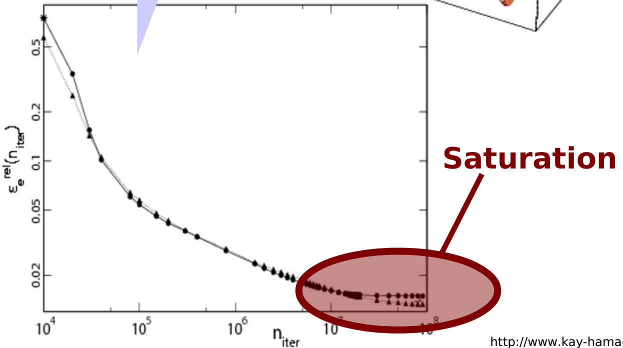
What happens under an STUN-Transformation?

Before



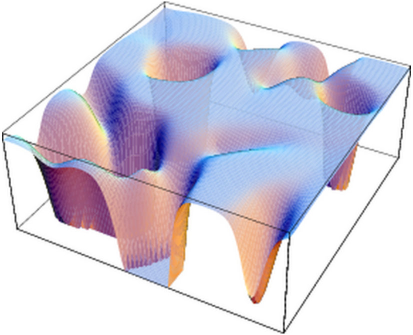
After





Search as a Stochastic Process

- can regard the iterative process as search dynamics evolving in time t
- visited objective function values E_t becomes time series
- can apply powerful methods of time series analysis



"forgotten too much"

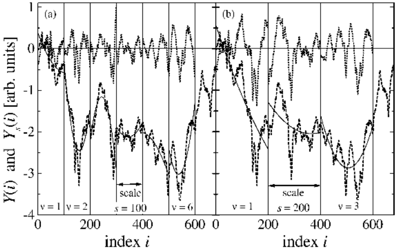
E_t is a random walk in original E-values, aka "wild guessing"

Random-Walk of E_t is indicator of poor performance!

Time Series Analysis

Detended Fluctuation Analysis

- within time windows τ delete (polynomial) trend $\to E_t^{(\tau)}$
- determine fluctuations $F^2(\tau)$ in $E_t^{(\tau)}$
- find scaling law $F^2(\tau) \sim \tau^{2-\gamma}$
- but auto-correlation function $C(\tau) \sim \tau^{-\gamma}$
- $\gamma \approx 1 \Longrightarrow$ Random-Walk !
- $\boxed{\gamma \text{ is an online signal}}$



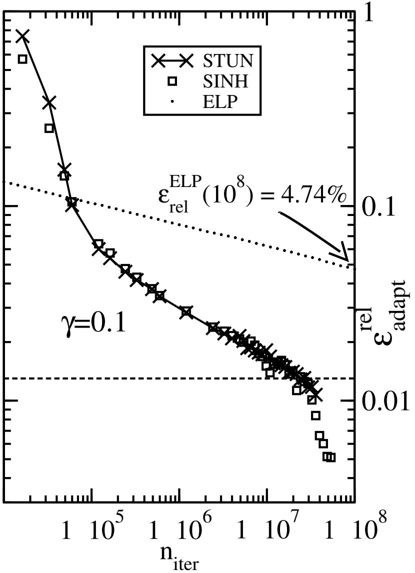
Kantelhard *et al.* **Physica A** 295(2001)441

DFA & STUN – Steering the Search

Idea:

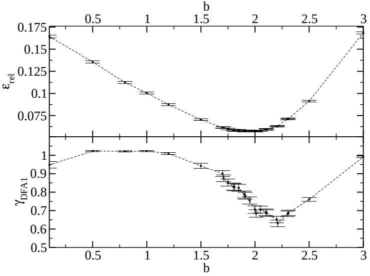
- whenever γ approaches 1 $\rightarrow$ saturation begins
- eventually, RW in E_t
- just start from scratch (keep f_{best})

Hamacher. **Europhys. Lett.** 74:944â950, 2006



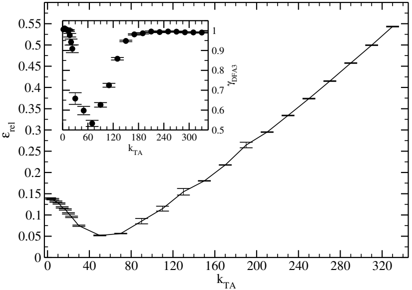
DFA & Other Stochastic Optimization Methods

Basin Hopping



Hamacher. **Lecture Notes in Computer Science (LNCS 8457)** *accepted*, 2014

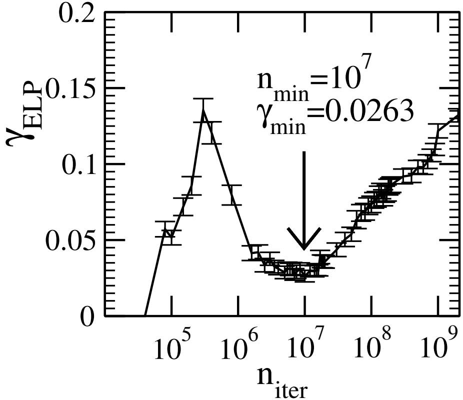
Extremal Optimization



Hamacher. **J. Comp. Phys.** 227:1500-1509, 2007

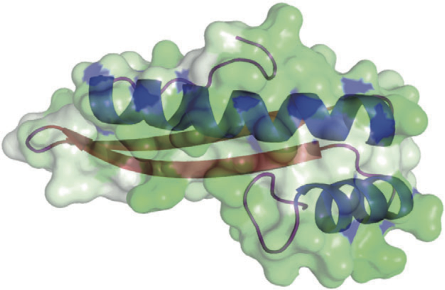
DFA & Other Stochastic Optimization Methods

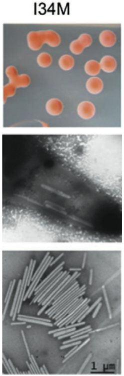
Energy Landscape Paving



Hamacher. **Physics A** 378:307-314, 2007

Application : Protein Structure Prediction





Strunk, Hamacher, *et al.* **Mol. Microbiol.** 1500-1509, 2007

Summary

- Heuristics solve *pragmatically* GO problems
- traditional approaches (like SA) suffer from problems
- STUN one way to address these issues $\rightarrow$ other problems
- Time Series Analysis, DFA in particular, leads to insight and thus *empirical algorithm design*
- Real world problems can be addressed

Shameless Advertisement

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co-editor in chiefs: C. Klingenberg & K. Hamacher

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