Stochastic methods for global optimization

Computational Methods in Optimization
CS 520, Purdue

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IMPORTANT

University class survey.
Please fill these out.
These are used to evaluate faculty members.

My class survey.
I use this to improve the class.
Do quizzes help you?
Does it help to discuss with peers for in-class questions?
Did you expect to cover additional material? (If so, what?)

Optimization and Sampling

Construct a probability distribution where the "most likely" point is a global max.

$$P(x) = 1/Z \exp(-f(x))\, Ind[c(x) = 0]\, Ind[x \geq \ell]$$

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Metropolis-Hastings Markov-Chain Monte Carlo

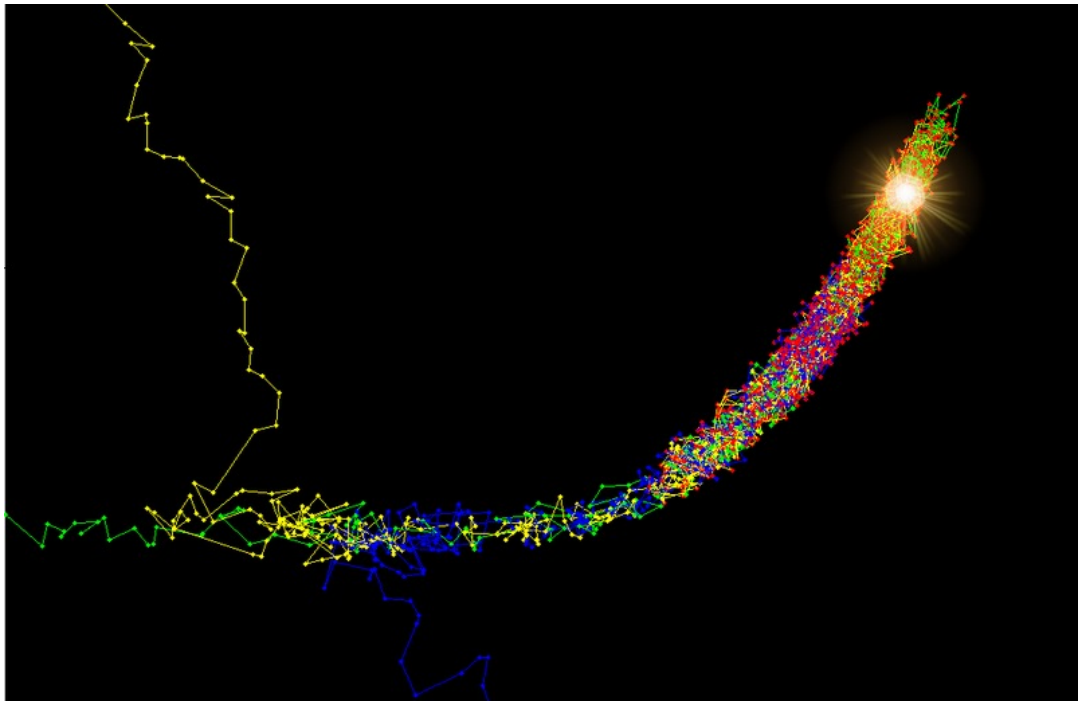
Given x_k, propose $x_{k+1} = x_k + N(0,\tau)$

Then compute $a = P(x_{k+1}) / P(x_k)$.
Accept if $a > 1$. Else accept with prob a.

Markov-Chain Monte Carlo

Sampling from the Rosenbrock function with a Markov-chain Monte Carlo sampler. The chain spends most of its time in regions where the objective function is large.

From wikipedia.



Show movie!

http://vimeo.com/22616409

Simulated Annealing (like M-H)

Let P(a,T) be the probability of accepting a move with a such that P(a,T) → Ind[a > 1] as T → 0. "T" is called the temperature. It's like a step-size parameter.

T going to zero called "cooling"

Improving these samplers

Abraham Flaxman has a great series of blog posts about improving these samplers.

http://healthyalgorithms.com/2011/01/28/mcmc-in-python-pymc-step-methods-and-their-pitfalls/

Goodman and Weare suggest multiple walks:

http://astrobites.com/2012/02/20/code-you-can-use-the-mcmc-hammer/

These improvements

All of these improvements seem to have the flavor of randomizing a deterministic derivative free method.

This can often be a very good idea.

Simulated annealing

Genetic algorithms

Ant colony optimization

“meta-heuristics”

The elephant in the room

What is the big issue with these methods?

MCMC for combinatorial problems

Instead of $x_{k+1} = x_k + N(0,\tau)$, consider a combinatorial structure:

- paths
- permutations
- graphs

And let x_{k+1} = random neighbor of x_k

Now… same procedure.

Discussion

These are all “randomized greedy” procedures in a combinatorial search space.

Difficult to trust the output for anything but improvements.

I'm not an expert on these things.

Avoid them if possible. Find a way to state your problem as an optimization problem and relax.

Look at Wikipedia for more details if you need to use them.