10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #29: Global Optimization. Multiple Minima.

Convex vs. Non-Convex

Convex – only one minimum

Non-convex – multiple relative minima

$\min_{\underline{x}} f(\underline{x})$

Global Optimization (Deterministic)

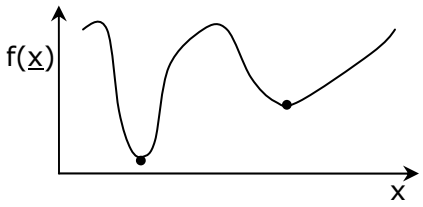
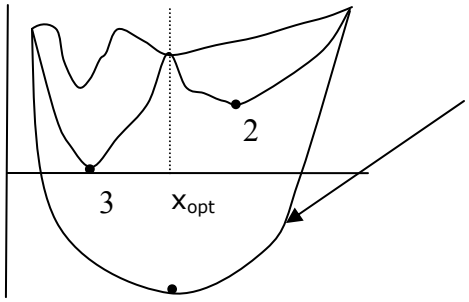


Figure 1. A function with relative minima.

Convex Underestimator



By looking at 2nd derivatives, find parabola that is lower than other minimum.

Figure 2. Convex underestimator.

Choose a f(x), upper bound. Divide domain. Underestimate the lower bound with a parabola. Find minimum of parabola. Bound again. If new upper bound is lower than lower bound in other region, can stop considering that section.

To converge – lower bound rises at a certain rate; upper bound decreases at a certain rate.

Going several zones deep, creates many divisions: $2^{N\text{divisions}}$(1-D)

Proteins: 100 dimensional space or more: 100^N or more

Current papers: can solve 4-5 dimensions

Method guarantees global optimum (if you care about the global optimum)

If you have 20 variables, use heuristics that often find the global optimum, but there is no guarantee.

Multi-start

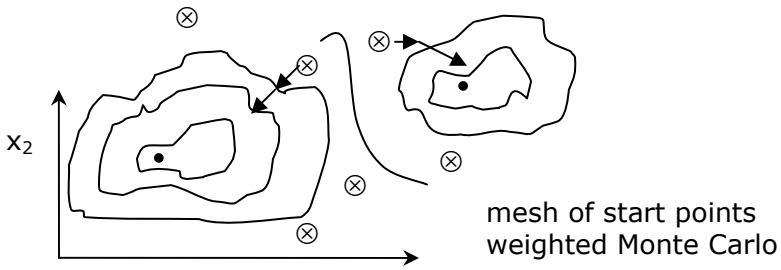


Figure 3. Begin in multiple locations and then run minimization.

In low dimension, draw map. One method, do different starts. Run a local minimization on each, then compare values. With enough points, can make a space. Can use mesh. Can use Monte Carlo – random guess. If there are 100 points and 6 variables, 100^6 calculations.

Simulated Annealing

Can use when there are lots of global minimum

$f(\underline{x}) \leftrightarrow kT$

Figure 4. The molecule is heated and then cooled slowly so that conformational changes taking place will lead to a local minimum. This process is repeated many times until several closely related, low energy, conformations are obtained.

$f(\underline{x}, \underline{z})$ mixed integer hybrid

Genetic Algorithms

➔ discretize everything

"DNA" (z_1, z_2, z_3, …)

mutate $z_n \rightarrow z_n'$

reproduction (exchange of DNA fragments)

replication

death

give everything probabilities to make it mirror evolution

Non-determinate methods ➔ do not exactly know when you are done