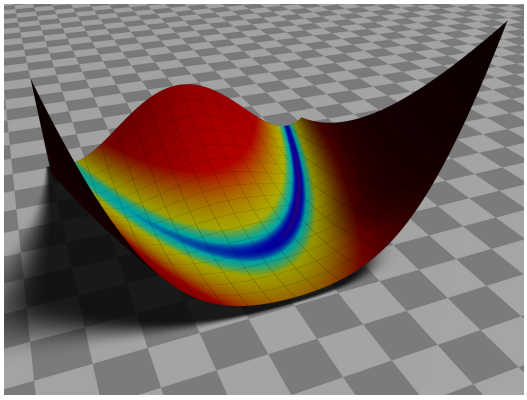
Nelder-Mead Simplex

Lecture 22



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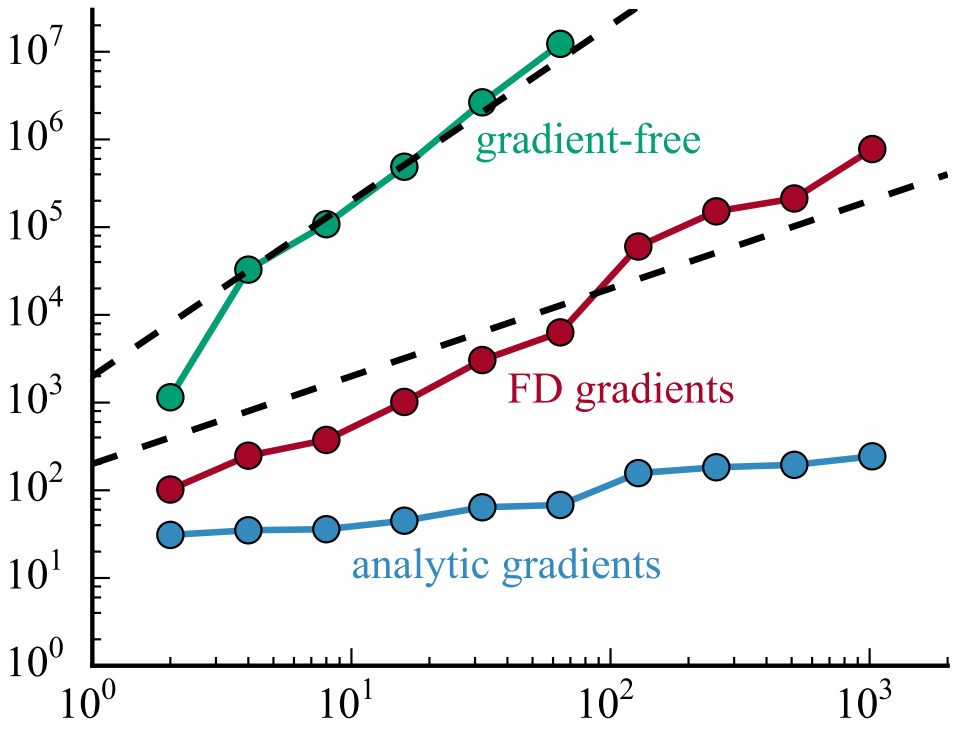
Outline

Gradient-Free Optimization

Nelder-Mead Simplex

Gradient-Free Optimization



Gradient-Free Optimization

When to use:

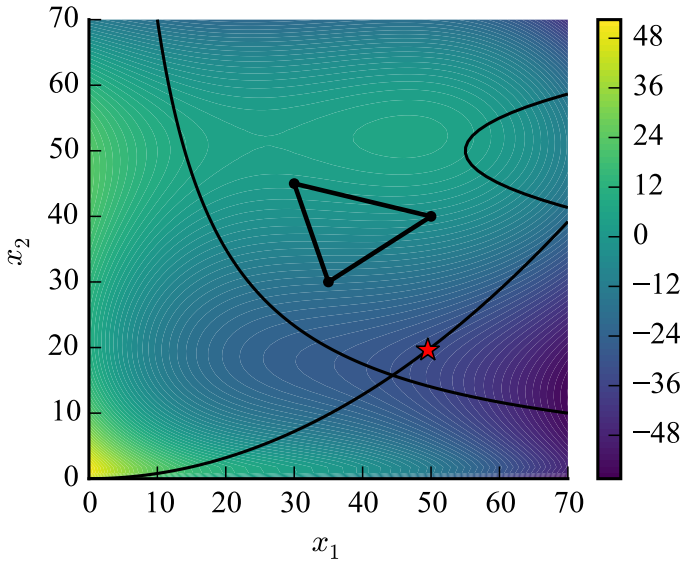
- The problem is low-dimensional (and the tradeoff in developer versus run time is not worth it).
- Your function space is *fundamentally* discontinuous or nondifferentiable.
- The function space is highly multi-modal.
- Your function produces unreliable gradients *and* is closed-source.
- You just need a good solution and don't really need "the optimum".

Nelder-Mead Simplex

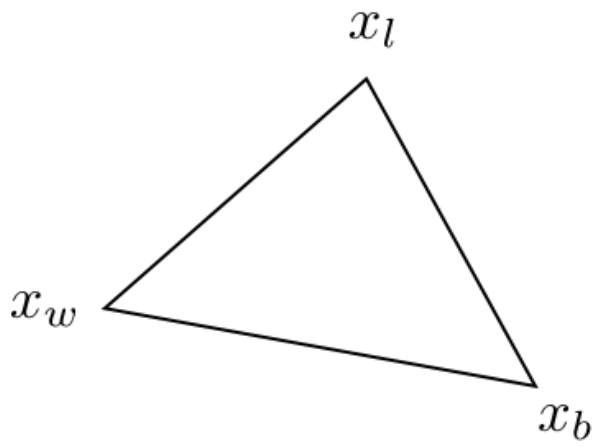
Nelder-Mead Simplex

- Does not require derivatives or smooth output.
- A local method, not a global method.
- Only effective for less than 10 dimensions.
- Cannot explicitly deal with constraints.

A simplex is a hypertetrahedron (with n+1 points).



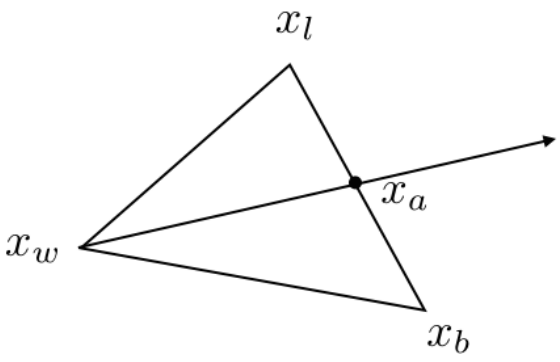
1. Rank the vertices: best, lousy (2nd worst), and worst



2. Find average of all points leaving out the worst

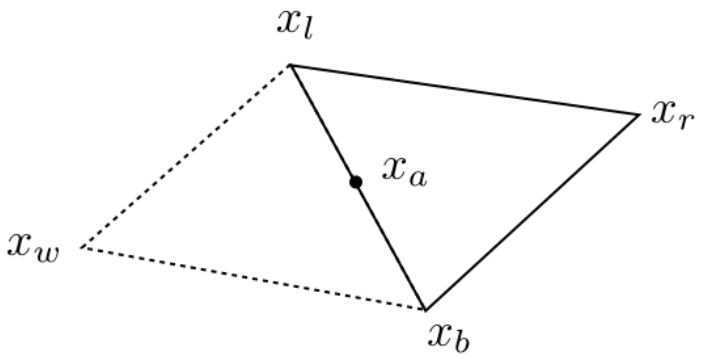
$$x_a = \frac{1}{n} \sum_{i=1, i \neq w}^{n+1} x_i$$

The line from x_w to x_a is probably a descent direction.



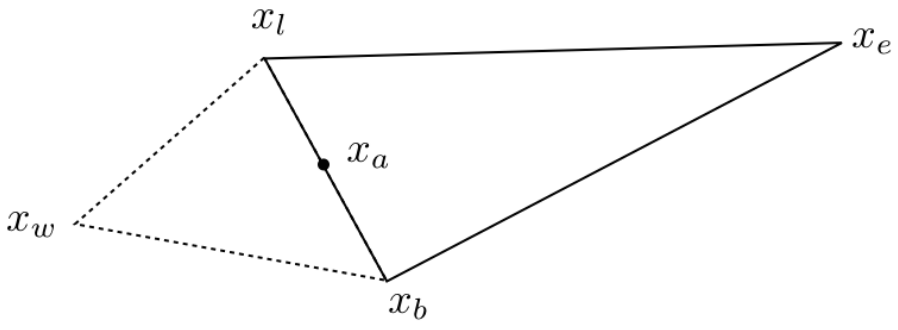
3. Reflection (α usually 1):

$$x_r = x_a + \alpha\left(x_a - x_w\right)$$



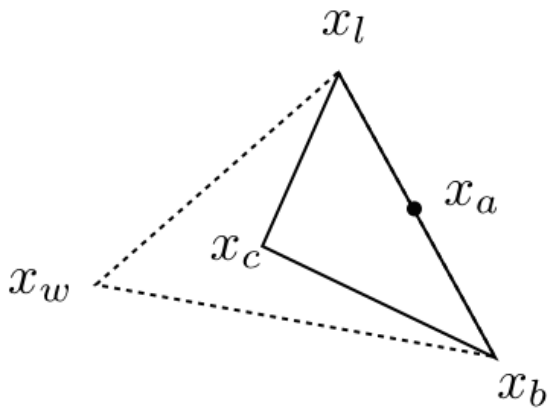
4. Is reflection better than best point? Keep going! Expansion (γ usually 1)

$$x_e = x_r + \gamma\left(x_r - x_a\right)$$



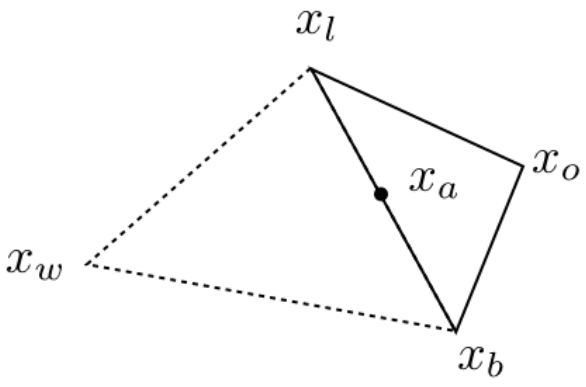
5. Or, is reflection worse than worst point? Inside contraction (β usually 0.5):

$$x_c = x_a - \beta\left(x_a - x_w\right)$$



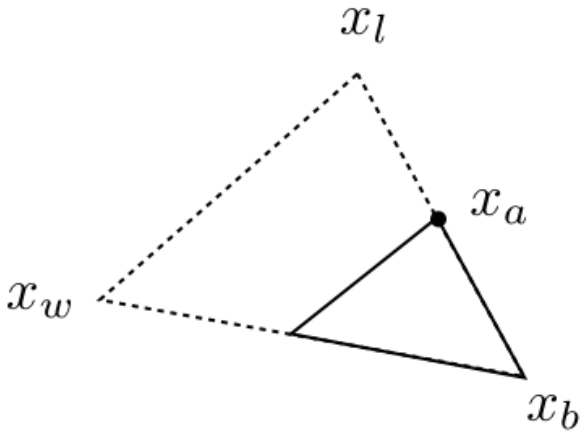
6. Or, is reflection better than worst, but worse than lousy point? Outside contraction:

$$x_o = x_a + \beta\left(x_a - x_w\right)$$



7. Is the contraction worse than reflection? Shrink (ρ usually 0.5):

$$x_i = x_b + \rho\left(x_i - x_b\right), \text{ for all } i \neq b$$



8. Repeat until convergence (function value not changing, size of simplex is small, etc.)

Implementations

Matlab: fminsearch

Python: minimize (method='Nelder-Mead')

Visual Examples:

https://youtu.be/HUqLxHfxWqU

https://youtu.be/D-VTab-pOTU