

Scientific Computing

March 21, 2025

Announcements

- Homework 4 assigned, see D2L
- Due Wednesday, April 2, 11:59pm

Today

- Introduction to Metaheuristics
- Hill Climbing

Office Hours:

Mon + Fri

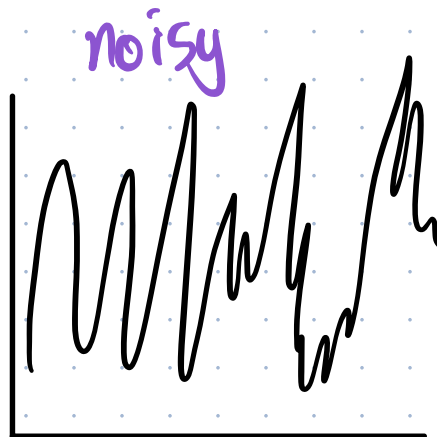
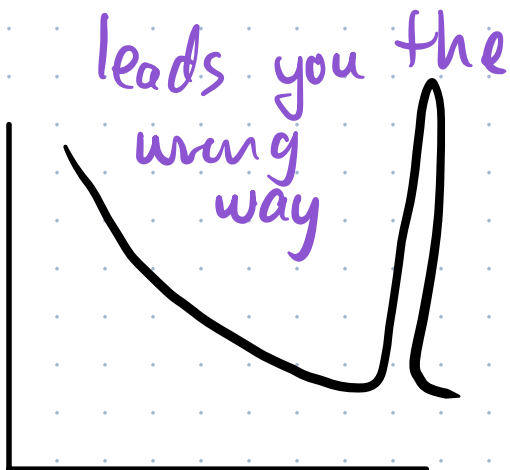
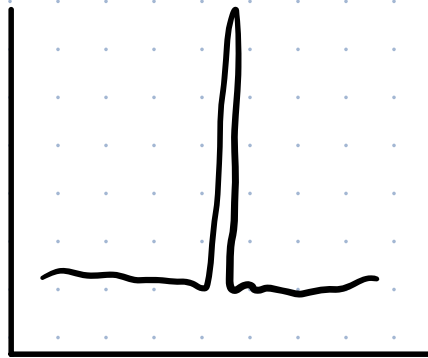
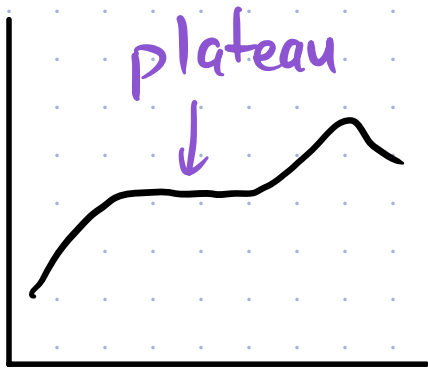
9:30am - 10:30am

Cudahy 307

Metaheuristics are all about exploring the search space in clever ways in the hopes of finding the global optimum.

Typical obstacles:

hard-to find



We can't see the landscape when we're on the mountain!

Topic 11 - Hill Climbing

With Gradient Ascent as our inspiration, we want to think about ways to search for global optima in cases where our search space is

- (1) discrete
- (2) cns, but can't compute a gradient

Problem Setup:

* Search space S full of candidates / possible solutions

* Scoring function: score(x), $x \in S$
(also called "fitness" w/ biological inspiration, or "quality")

* A way to generate either $x = \text{current candidate}$
= where you're standing in the mountains

- all the candidates "near" a candidate,
the "neighborhood" nbhd(x)

probably doesn't
make total
sense in
cns space

OR

one

- a random candidate near a candidate
(sometimes called a "tweak") tweak(x).
"nearby" is up for you to define, and
different definitions can totally change how
a metaheuristic behaves.

Two running examples in this section.

(1) TSP:

* discrete

* score = cost of tour, want to minimize

* nbhd(x): Suppose $x = C_1 \rightarrow C_2 \rightarrow \dots \rightarrow C_n \rightarrow C_1$

"n-1 choose 2" Define the neighborhood to be all ways of picking two cities and swapping them (excluding C_1). $\approx n^2$

$$\text{size} = \binom{n-1}{2} = \frac{1}{2}(n-1)(n-2) \quad (\text{big!})$$

* tweak(x): a random thing in the nbhd of x

(2) Optimizing a continuous function
in two variables $f(x,y)$.

* continuous

* score = value of the function

* $\text{nbhd}(x)$ = all points within some
fixed distance δ of x Small #

* tweak(x) = a random point in $\text{nbhd}(x)$

infinite

MH #1: Random Search

best = random element of S

while True: (quit whenever you want)

x = random element of S

if $\text{score}(x) > \text{score}(\text{best})$:

best = x

Possible stopping conditions:

- * best score does not improve for N iters
- * preset number of iters
- * you get impatient

This is not a good metaheuristic in most cases! It doesn't use any old information to guide future choices.

[2 Demos] { 01: TSP random
02: Contour 1-random

Gradient Ascent inspires this next one.

MH #2: Steepest Ascent Hill-Climbing (Discrete only)

$x = \text{random element of } S$

while True:

$N = \text{nbhd}(x)$

$s = \text{element of } N \text{ with the best score}$

if $\text{score}(s) > \text{score}(x)$:

$x = s$

else:

quit

Stopping conditions:

* run out of time

* no further improvement

What does this do? Climbs right up the hill you start on.

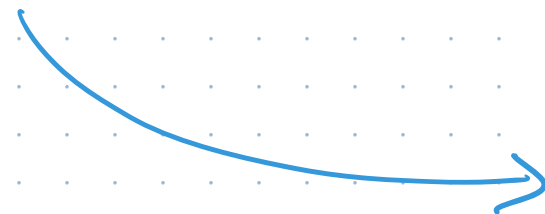
Pros

- * Finds a local optimum

Cons

- * Unlikely to find global optimum except in very nice spaces
- * very slow, especially if nbhds are big, like TSP.

why?



Only really doing two things:
(1) generating the neighborhood
(2) scoring each element of it

Scoring a tour with 300 cities is not
horrible - 300 distance calculations
(two subtractions, two squarings,
one addition, one square root)

But bad when you do it
 $\binom{299}{2} = 44,551$ times.

Often, you don't have to restore a solution from scratch because it only changes a little bit. More on this in a bit.

Demos: 03 - TSP St. Asc. 50
04 - TSP St. Asc. 300 slow!