Scientific Computing

Friday, March 27

Announcements

* Homework 4 due tonight.
* Monday, April 6: No lecture, work from home day
* Homework 5 assigned later today, by email.
  Covers hill climbing and simulated annealing.

Office Hours:

Mon, 9:30-10:30

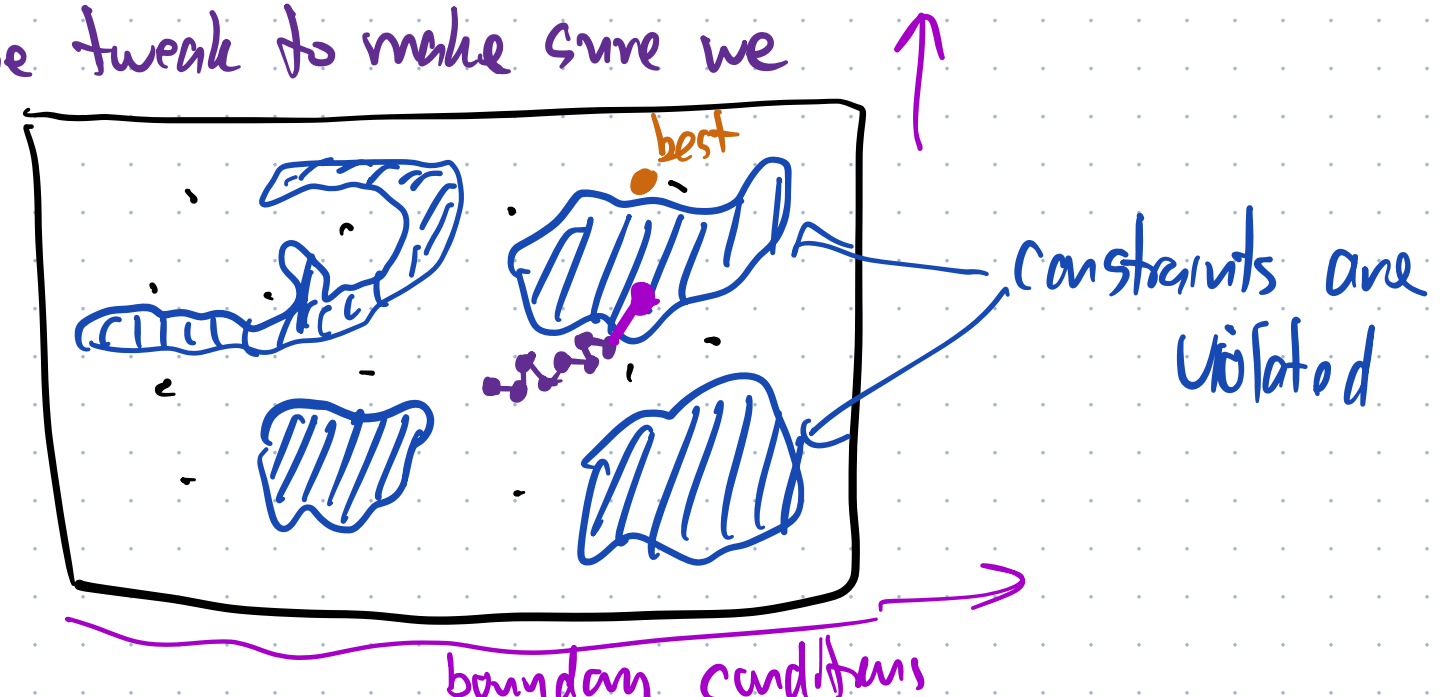
Fri, 2:00-3:00

Cudahy 307

* Spring Demo
  - staying within constraints by re-tweaking
  - playing with parameters

Metaphorical Picture of the search space

how do we tweak to make sure we satisfy constraints?



* Knapsack Demo

Sol: a subset of items

Tweak: Pick a random item out of all items
If it's in your set, remove.
If it's not, add it.

Hill Climbing: If the score must always go up, we can never remove an item — very badly

Starting solution: empty set, because picking a random valid solution is difficult

Better Tweak:

Idea: Pick 1 random item to remove
and 1 random item to add

Bad with H-C and S-A because you're forced to always have the same # of items

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Idea: Remove between 0 and 3 items at random
Add 1

* Knapsack Demo

Need to avoid overful solutions

How can we fix?

(1) retweak until solution is good

In this case, we need to start at an empty solution. Or a greedy one?

(2) Constraint penalty

$$score \rightarrow score \cdot \left(1 - \frac{10}{\mu} \cdot \frac{\text{excess weight}}{\text{capacity}}\right)$$

0.1 = % overweight

where μ can be tuned statically or dynamically

The constraint penalty idea lets us use simulated annealing on problems with only constraints, like Sudoku.

Score = [# of row conflicts]
+ [# of column conflicts]
+ [# of square conflicts]

Goal: Minimize score, hope to get to 0

Tweaks?

Parallel Tempering

An interesting related idea:

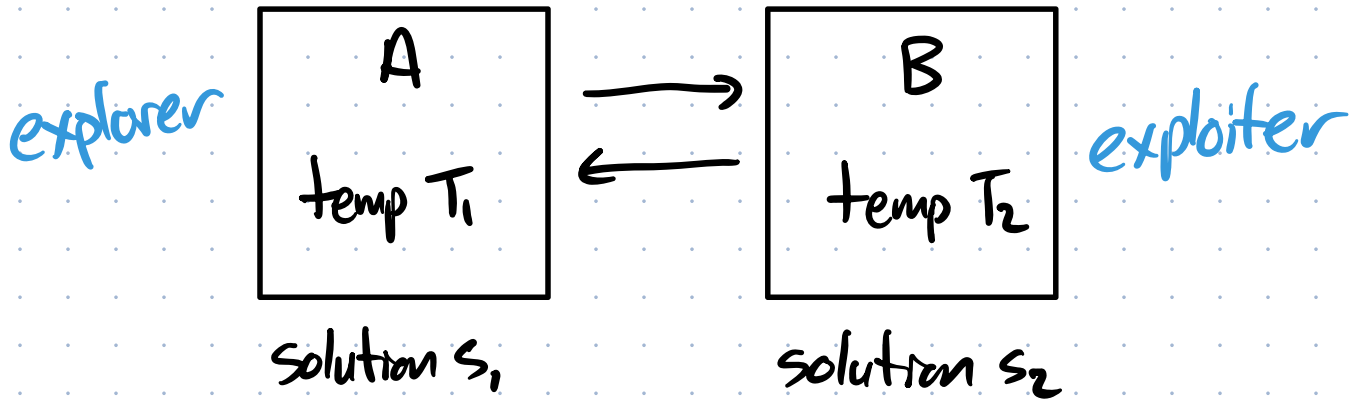
Instead of running one system that cools over time, run multiple systems each at constant, but different, temperatures that are allowed to swap solutions.

Intuition: Person A is very good at exploring

Person B is very good at exploiting

They both run for a while, until Person A says "Hey, I think I'm on a good hill, let's swap so you can exploit it."

$T_1 > T_2$



Should they swap solutions?

Let $E_i = \text{score}(s_i)$.

At any point in time, swap with probability

$$p = \min(1, e^{\Delta})$$

where

$$\Delta = (E_1 - E_2)\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

> 0 when the explorer is winning

always > 0

$$\Delta = (E_1 - E_2)\left(\frac{1}{\tau_2} - \frac{1}{\tau_1}\right)$$

>0 when the explorer is winning

always >0

When the explorer is winning, we should definitely swap, so the exploiter can improve it.

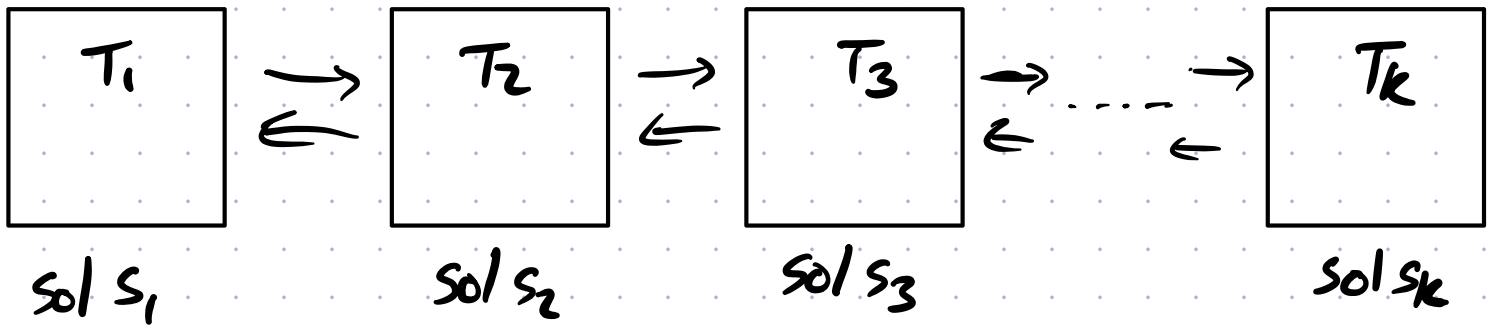
In this case, $\Delta > 0$ so $p = \min(1, e^{\Delta}) = 1$. ✓

Otherwise $E_1 - E_2 < 0$ and $p = e^{\frac{E_1 - E_2}{1/\tau_2 - 1/\tau_1}} < 1$.

The better the explorer is doing, the more likely they are to swap.

More generally:

k different explorers



$$\Delta_i = (E_i - E_{i+1})\left(\frac{1}{T_{i+1}} - \frac{1}{T_i}\right)$$

Swap s_i and s_{i+1} with prob $p_i = \min(1, e^{\Delta_i})$

Recap

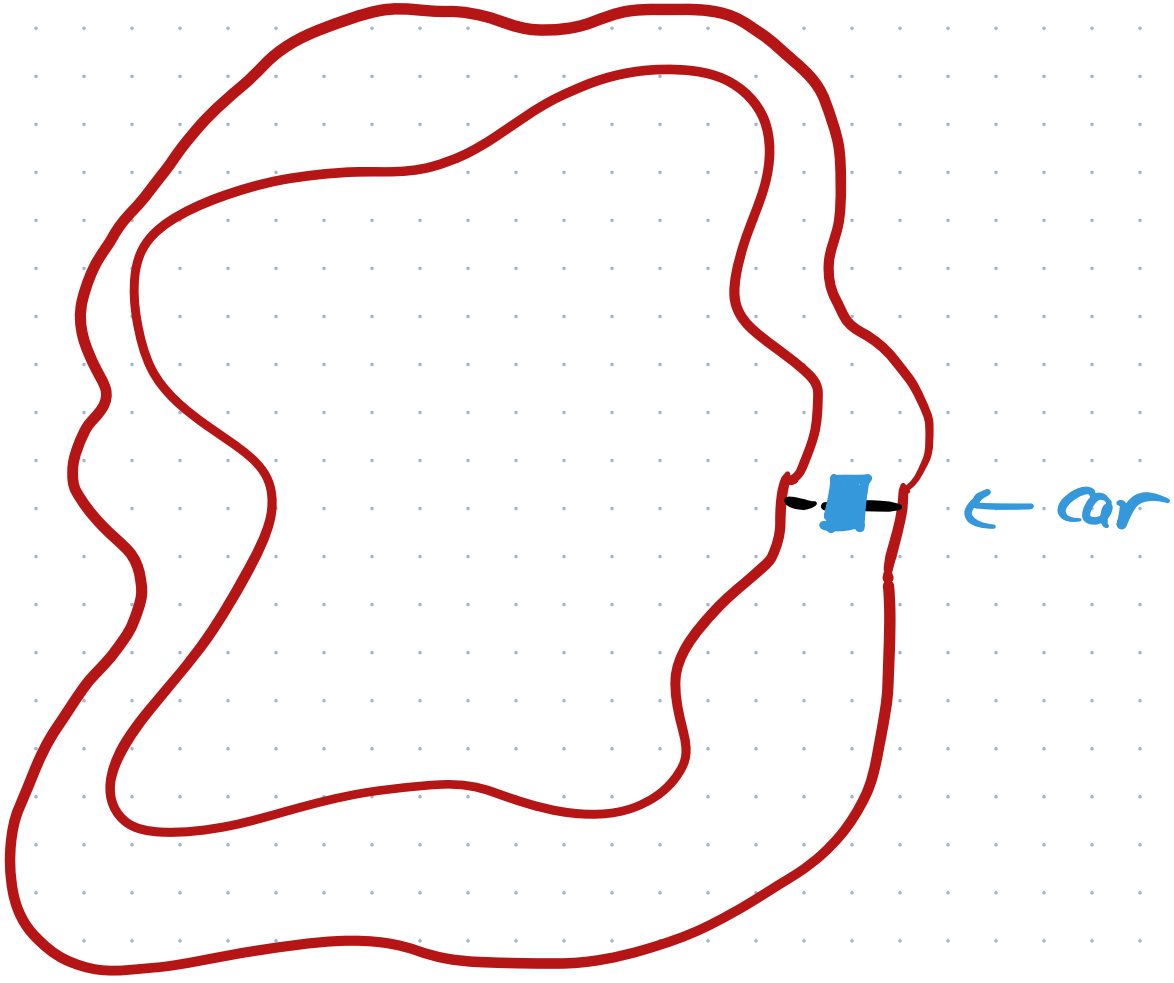
Want to use Hill Climbing or Simulated Annealing to solve a problem? You need:

* to understand the search space (or even need to rephrase the problem to have a search space)
* a scoring function that rates things in the search space as better or worse
* a "tweak" function that turns any solution into a very similar ("close") solution - and each solution should have many different tweaks possible
* a stopping condition

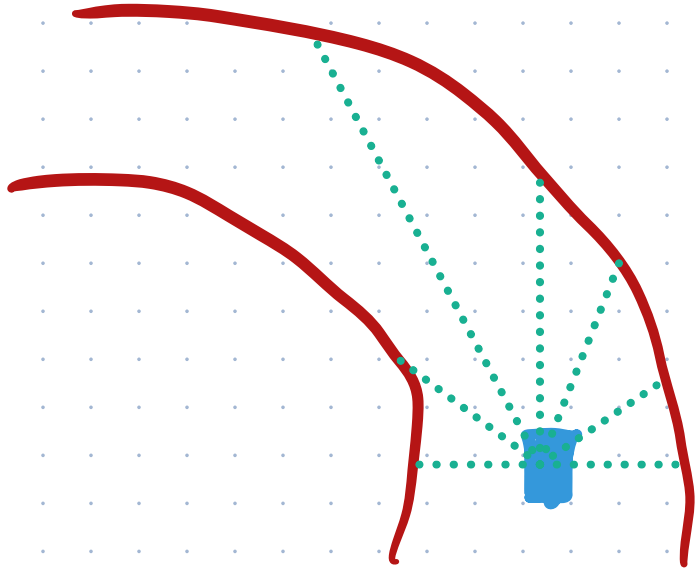
For SA: * an initial temp and a cooling schedule (how to cool and when to cool)

Crazy Example : Self-Driving Car

Problem: We want to teach a 2D car to drive around a track.



What data does the car have? Let's say it has 7 sensors that tell it the distance to the wall along that sensor direction.



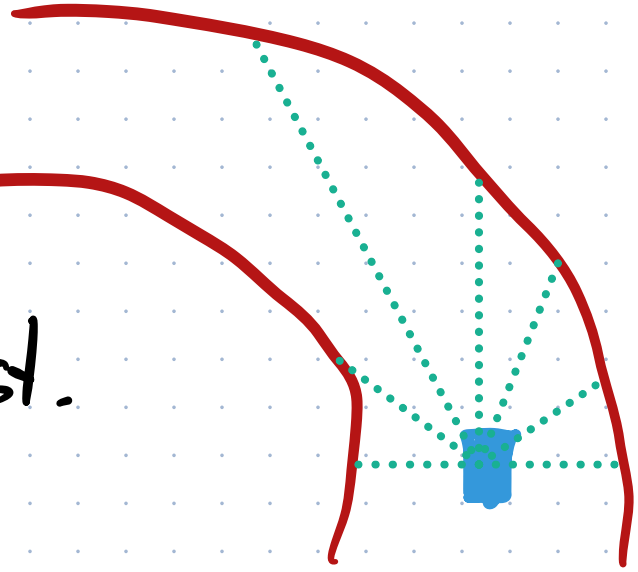
To drive, the car decides two things each step

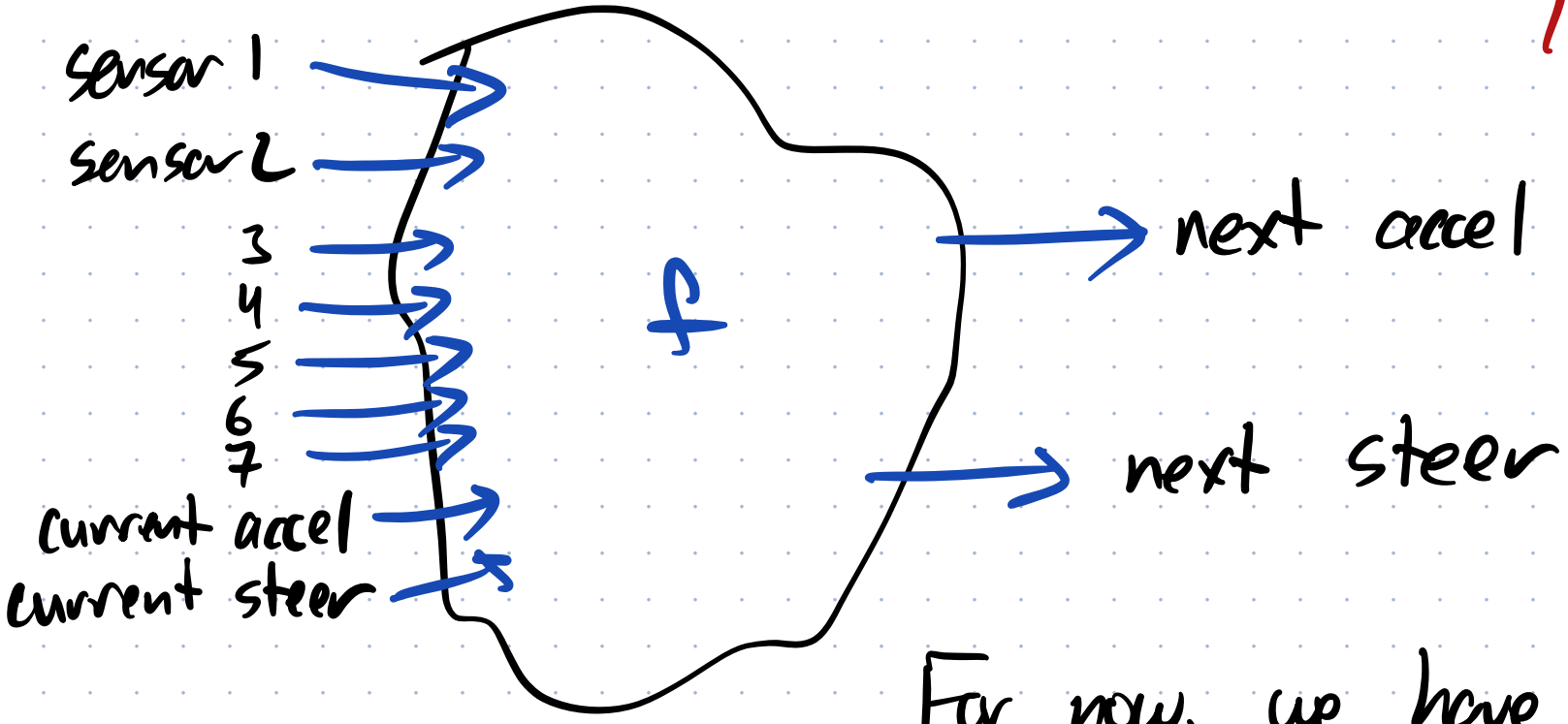
* acceleration (how much to change its speed)
* turning wheel (how much to change its steering angle)

[manual demo]

Conversion to an optimization problem:

Find the function f that makes the car drive the best.





For now, we have to pick a specific form for f.

$$f(s_1, s_2, \ldots, s_7, a_c, s_c) = (a_n, s_n)$$

One possibility: assume f is a <u>linear</u> function.

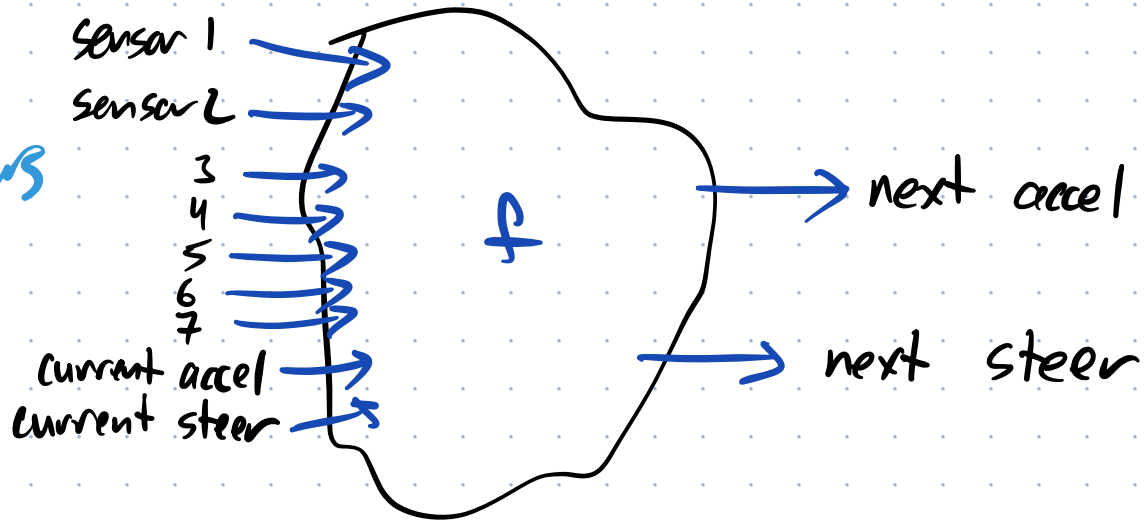
$$a_n = (?)s_1 + (?)s_2 + (?)s_3 + \cdots + (?)s_7 + (?)a_c + (?)s_c + (?)$$

$$s_n = (?)s_1 + (?)s_2 + (?)s_3 + \cdots + (?)s_7 + (?)a_c + (?)s_c + (?)$$

20 unknown coefficients that we get to choose.

Search space:

20-dimensional vectors of decimals, $\mathbb{R}^{20}$



Search space:

20-dimensional vectors of decimals, $\mathbb{R}^{20}$

tweak: change all (or some?) of the coefficients by a little bit (how much?)

Still need a scoring function! What do you want the car to do?

* Distance travelled without crashing?
* Incorporate average velocity?

Hill Climbing

Start with 20 random coefficients for f.

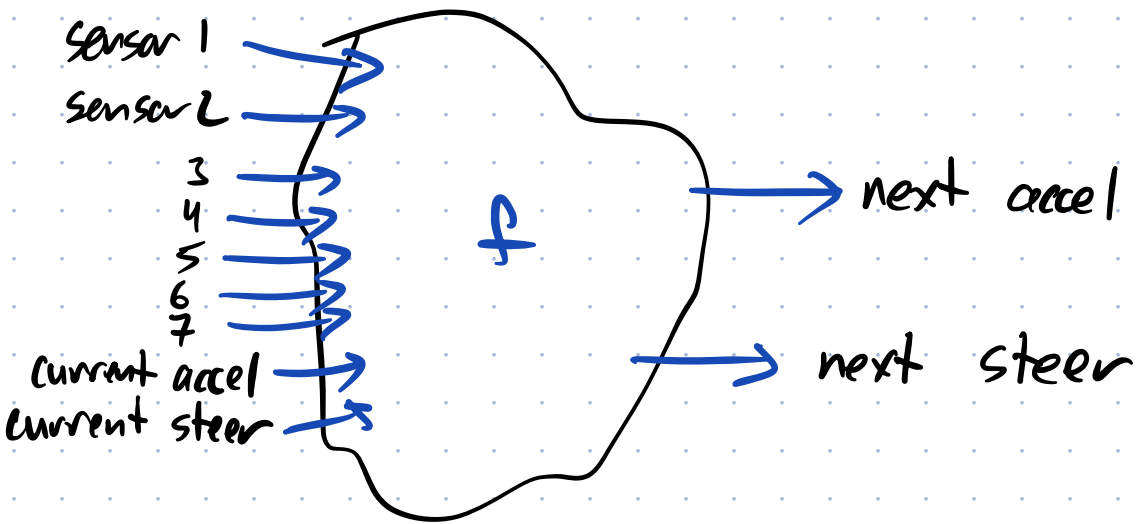
Put the car on a track and run it.

Each step, f decides how the car moves.

If the car scores better, that's your new "best". Tweak it and try again.

If the tweak is worse, throw it out.

Run for a long time!



Limitations:

* Slow scoring function!
* Maybe assuming self-driving is linear is very constraining - more complicated functions have more freedom to treat sensor input differently
* One car at a time doesn't give you a lot of diversity. Should try 100-trials steepest ascent or other metaheuristics like genetic algorithms

[demo]