Tutorial 8

COMP90014 Algorithm for Bioinformatics

Semester 2, 2025

Simulated Annealing

Use

The fitness landscape is not smooth.
Eg discrete problems, such as evolutionary tree building.

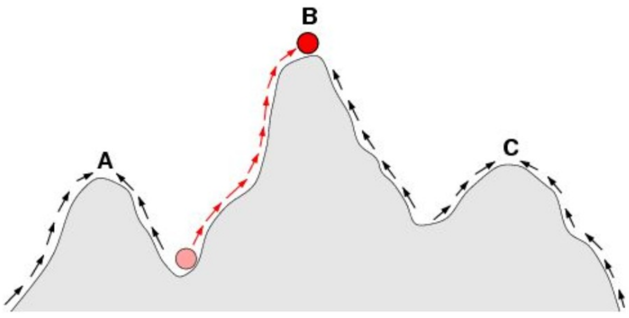
Main process

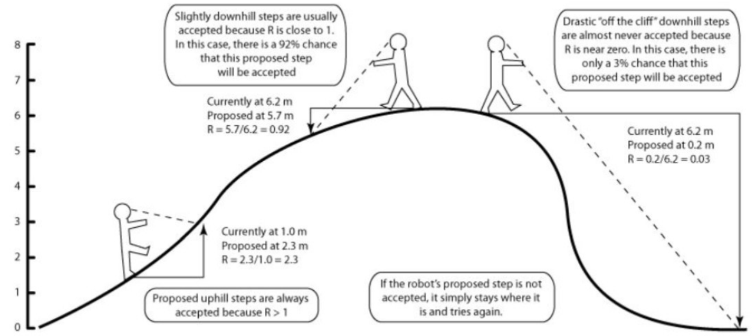
Start by generating a random solution. Score ***this*** solution.

Repeat

1. Generate ***next*** solution by randomly altering ***this*** solution.
2. Score the ***next*** solution.
3. If the ***next*** solution is better, jump to it.
4. Stop if the budget has been reached, else go to 1.

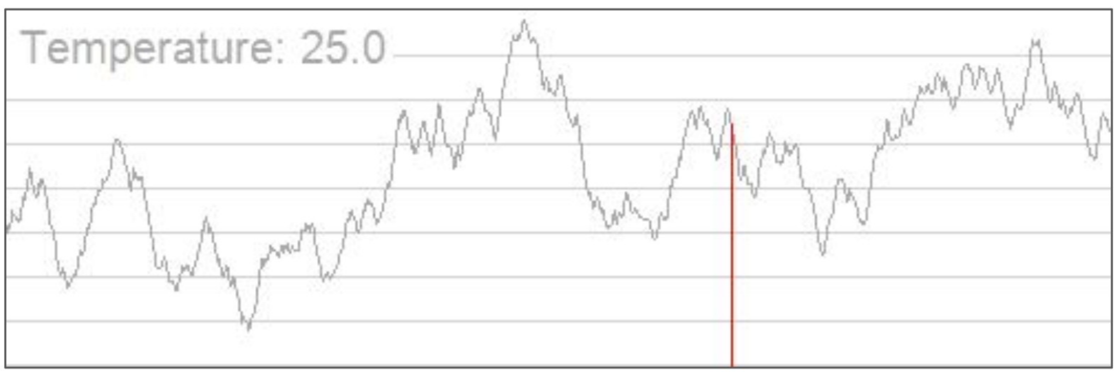
Naively, this would be prone to getting ‘stuck’ in local optima.
To remedy, let’s sometimes jump to worse solutions, hoping they eventual
lead to better solutions.





Simulated Annealing

- Let $s = s_0$ — # Start with any solution
- For $k = 0$ through k_{max} (exclusive): — # Steps
  - $T \leftarrow$ temperature($1 - (k+1)/k_{max}$) — # New temperature
  - Pick a random neighbour, $s_{new} \leftarrow$ neighbour(s) — # Generate a neighbour solution
  - If $P(E(s), E(s_{new}), T) \geq$ random(0, 1): — # Jump to neighbour or stay here
    - $s \leftarrow s_{new}$
- Output: the final state s



Neighbour

Generate new solution by making small change to current solution.
Eg change single edge in evolutionary tree.

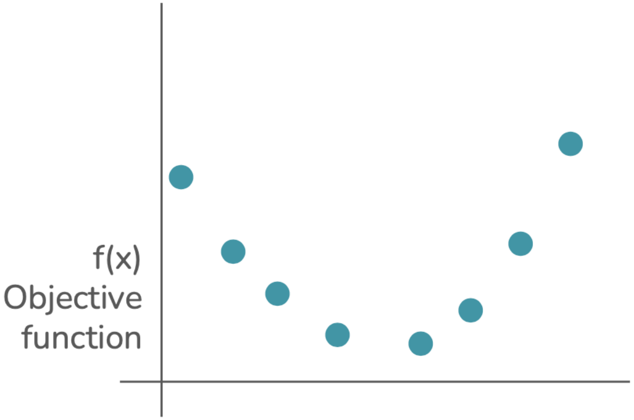
Randomness

Allows us to jump to a ‘worse’ solution occasionally.
Enables us to break out of local maxima!

Temperature

Reduces over time.
Near the end of our run, we’re less likely to jump to ‘worse’ solutions.
Ensures convergence at (hopefully) global maxima.

Gradient Descent

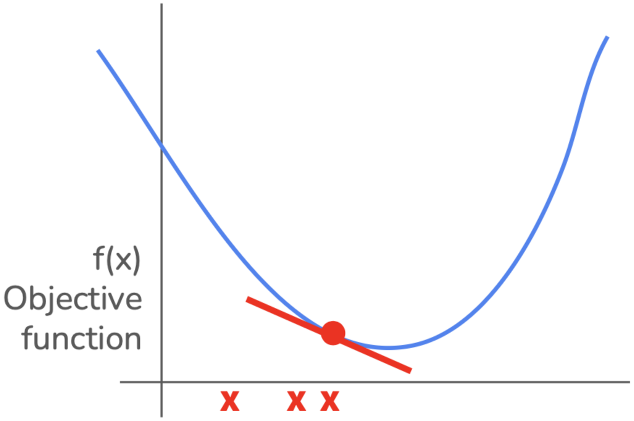


Step 1

- Use a sample of possible solutions (values) to get scores.
- Values and scores derive an equation for fitness landscape.

Step 2

- Start at any value. Repeat the following:
- Calculate the derivative of our equation at this point.
- Slope is negative: move to the right
- Slope is positive: move to the left
- The gradient tells us how much to move.
    - Big steps when we're far from the optimal.
    - Small steps when we're close.



Note

- We're not solving for derivative = 0.
- Sometimes it's not possible to solve the above, making gradient descent widely applicable.