# CSE276C - Optimization





Computer Science and Engineering University of California, San Diego http://cri.ucsd.edu

October 2024

# Outline

- 1 Introduction
- 2 Bracket based methods
- 3 Downhill Simplex
- 4 Powell's Method
- 5 Conjugate Descent/Gradient
- 6 Stochastic Search
- Dynamic Programming
- 8 Summary

#### Introduction

- We have discussed approximation and root finding. We can leverage these methods to study optimization.
- Most of robotics is about optimization
- Best trajectory between two points
- Best fit of a model to a swarm of data
- Optimal coverage of an area for fire monitoring
- Energy efficient travel from San Diego to Hawaii by water

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#### Literature

• Numerical Recipes: Chapter 10

• Numerical Renaissance: Chap 14-16. (Part III)

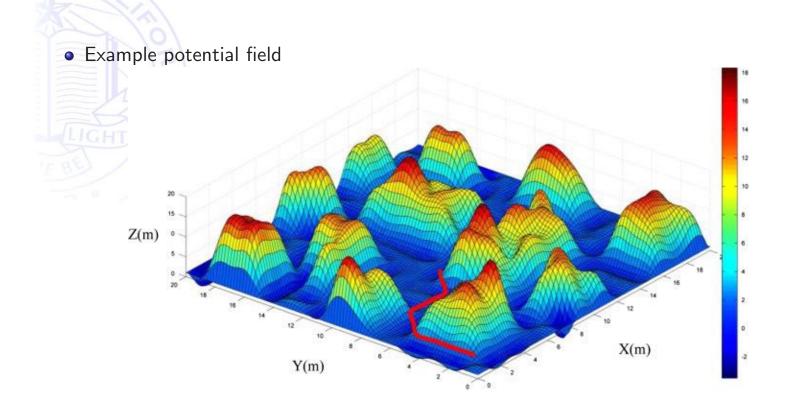
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# Example 1

• Optimization of trajectories at high speed

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# Path Planning



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# **Optimization**

- So what is optimization?
- Finding extrema for a function over a domain
- Minimum or maximum is immaterial as we can use f or -f
- In many cases we will have local and global extrema
- Consider both deterministic and stochastic approaches

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#### Golden section

- For bracketing of roots we use bi-section as a basis.
- We can use a similar technique to find an extremum
- We need two points to bracket a root!
- How many points do we need to bracket an extremum?
- We need three points to bracket.
- If we have a triplet a < b < c. Iff f(b) is smaller than f(a) and f(c), then we have a minimum within [a, c]

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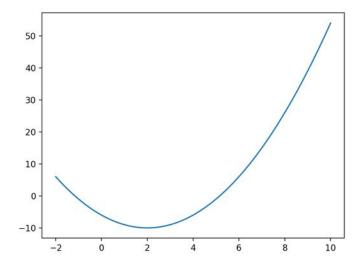
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#### Golden Section

- Pick a point between (a,b) or (b,c) and evaluate
- Suppose  $x \in (b, c)$  and f(x) < f(b) then our new triple is (b, x, c)
- Consider the function



• How would you choose a new value of x?

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#### Golden Section (cont.)

• Consider (a, b, c)

$$\frac{b-a}{c-a} = w \qquad \frac{c-b}{c-a} = 1 - w$$

• Lets assume  $x \in (b, c)$  and

$$\frac{x-b}{c-a}=z$$

- The next bracket is then w+z or 1-w
- If we want to make the intervals equal

$$z = 1 - 2w$$
 when  $w < \frac{1}{2}$ 

• z should be the same distance from b and c and b is from a and c

$$\frac{z}{1-w}=w$$

we can rewrite to replace z and get the equation

$$w^2 - 3w + 1 = 0 \Rightarrow w = \frac{3 - \sqrt{5}}{2} \approx 0.38197$$

Widely used to select iteration strategies

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#### Parabolic Interpolation

- We covered Brent's method in root finding and in interpolation
- If we have a triple (a, b, c) and the values f(a), f(b), f(c) we can generate a
   2nd order interpolation

$$x = b - \frac{1}{2} \frac{(b-a)^2 [f(b) - f(c)] - (b-c)^2 [f(b) - f(a)]}{(b-a) [f(b) - f(c)] - (b-c) [f(b) - f(a)]}$$

- When would this fail?
- When the triple pair is co-linear!
- The remedy is to use golden section for the co-linear case

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#### 1-D search w. derivative information



- If we have the triple (a, b, c) and f(a), f(b), f(c)
- In addition we have f'(b)
- You can use the sign of f'(b) to choose the next bracket

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#### Simplex Method

- Assume we have no gradient information or access to formal model.
- A simplex in N dimensions is composed of N+1 points. Connected by straight lines
  - A 2D simplex is a triangle
  - A 3D simplex is a tetrahedron.
- We have N+1 points  $x_1, \ldots, x_{N+1}$

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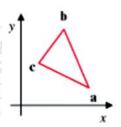
# Downhill Simplex Algorithm

- Initial simple
  - Order the values of the vertices:  $f(x_1) \le f(x_2) \le \ldots \le f(x_{N+1})$
- Compute  $x_0$ , the centroid of all points except  $x_{N+1}$
- Reflection compute  $x_r = x_0 + \alpha(x_0 x_{N+1})$ , with  $\alpha > 0$  if the reflection is better than  $f(x_{N-1})$  replace. Restart
- Expansion if  $f(x_r) < f(x_1)$  compute  $x_e = x_0 + \gamma(x_r x_0)$  if  $f(x_e) < f(x_r)$  replace  $x_{N+1}$  else replace  $x_{N+1}$  with  $x_r$ . Restart
- Contraction If  $f(x_r) > f(x_N)$  compute  $x_c = x_0 + \rho(x_{N+1} x_0)$  with  $\rho < .5$ . If  $f(x_c) < f(x_{N+1})$  replace and restart
- Shrink Replaces all points except  $x_1$  with  $x_i = x_1 + \sigma(x_i x_1)$  and restart
- Terminate when update is below a threshold.

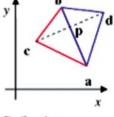
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# Simplex illustration

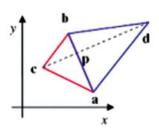
#### **Downhill Simplex Method**



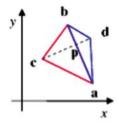
**Initial simplex** with vertices **a**, **b**, **c**, so that  $f(\mathbf{a}) < f(\mathbf{b}) < f(\mathbf{c})$ 



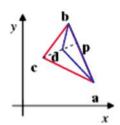
Reflection: d-p = -(c-p) with d-c perpendicular to b-a.



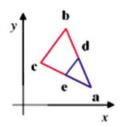
Reflection & expansion: d-p = -2(c-p) with d-c perpendicular to b-a.



Reflection & contraction:  $d-p = -\frac{1}{2}(c-p)$  with d-cperpendicular to b-a.



Contraction: d-p = ½(c-p) with d-c perpendicular to b-a.



Multiple contraction: (d-a)/(b-a) = (e-a)/(c-a)

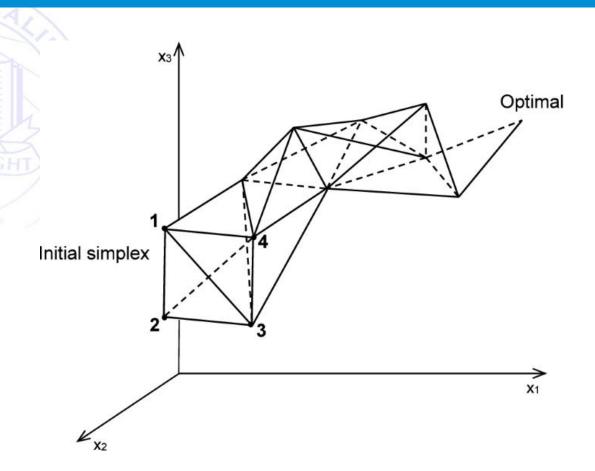
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# Simplex example



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#### Powell's Method

- Assume you have an n-dimensional function  $f(\vec{x})$  and a starting point  $P_0$ .
- We can use the local gradient to search for an extremum
- We can generate a new estimate

$$P_{new} = P_{old} + \lambda \vec{n}$$

Locally we can generate a Taylor expansion

$$f(x) = f(P) + \sum_{i} \frac{\partial f}{\partial x_{i}} x_{i} + \frac{1}{2} \sum_{ij} \frac{\partial^{2} f}{\partial x_{i} \partial x_{j}} x_{i} x_{j} + \dots$$

or

$$f(x) \approx \vec{c} - b\vec{x} + \frac{1}{2}\vec{x}^T A \vec{x}$$

where

$$\vec{c} = f(P)$$
 $b = -\nabla f_P$ 
 $A_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$  Hessian Matrix

Also remember

$$\nabla f = Ax - b$$

at an extremum

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#### Powell's Method

Initialize N unit vectors

$$u_i = e_i \ i \in 1...N$$

- Start at point  $P_0$
- For i=1 to N
- Move along  $P_i$  from  $P_{i-1}$  along  $u_i$
- **5** Set  $u_N = P_n P_0$
- Move  $P_n$  to minimum value
- $\bigcirc$  Make  $P_0 = P_n$
- Might generate linear degenerate solutions

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#### Conjugate gradient descent

If we have the gradient from

$$f(x) \approx \vec{c} - b\vec{x} + \frac{1}{2}\vec{x}^T A \vec{x}$$

- We can do a steepest descent
  - $\bullet$  Start at  $P_0$
  - **2** Compute  $\nabla f(P_i)$
  - $\odot$  move in the direction of gradient to point  $P_i$
  - 4 repeat
- We can construct a set of conjugate vectors

$$g_{i+1} = g_i - \lambda A h_i$$

$$h_{i+1} = g_{i+1} + \gamma_i h_i$$

$$\lambda_i = \frac{g_i g_j}{h_i A h_i}$$

$$\gamma_i = \frac{g_{i+1} g_{i+1}}{g_i g_i}$$

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#### Stochastic Search

- So far we have used direct functional values for optimization.
- The search has been deterministic
- Sometimes the search space is too large
- What if we use a sampling based approach?
- Some possible examples
  - Traveling salesman
  - Layout of silicon for chips
- Loosely based on Boltzmann distribution

$$P(E) = exp(-E/kT)$$

• where E is energy/entropy, T is temperature, and k is the Boltzmann constant.

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#### Metropolis Algorithm

- Transformed into an algorithm by 1953 by Metropolis
- Algorithm
- Let  $s = s_0$
- For k = 0 to  $k_{max}$ 
  - $T = temperature(k/k_{max})$
  - Pick random neighbor  $s_{new} = neighbor(T)$
  - If  $(P(S, T) \leq random(0, 1)$ 
    - $s = s_{new}$
- Return S

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# Simulated Annealing

- Description of possible configurations
- A way to generate random perturbation of a configuration
- An objective function whose minimization is the objective
- A control variable that is lowered over times.

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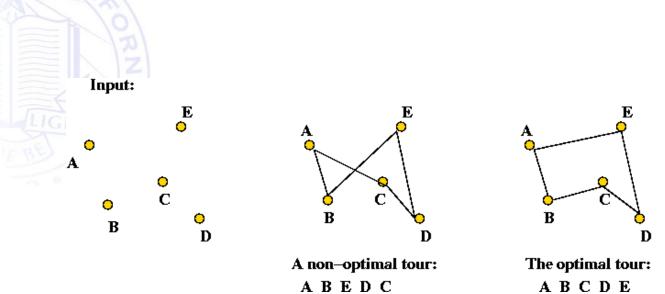
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#### Example - traveling salesman

- A salesman has to visit N cities at locations  $(x_i, y_i)$  returning to the original city
- Each city to be visited only once
- Minimize the travel route
- Problem in the optimal sense is known to be NP-hard.

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# Simple Example - Traveling Salesman



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# Vacation Planning

Going to Italy for vacations

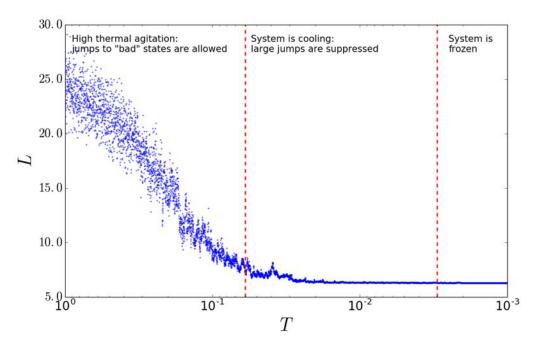


SRC https://mirkomiorelli.github.io/SA\_TSP/

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# Vacation Planning - Temperature

Going to Italy for vacations

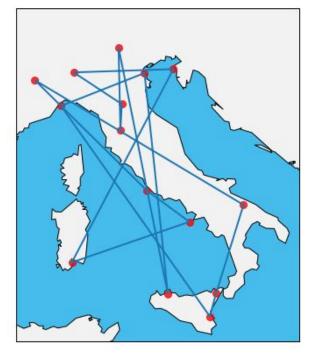


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# Vacation Planning - Random initialization

Going to Italy for vacations

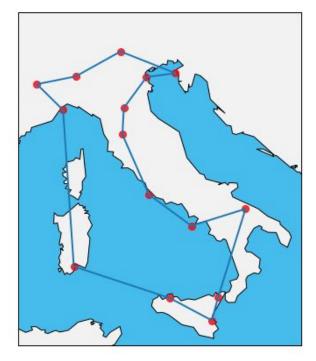


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# Vacation Planning - Random initialization

Going to Italy for vacations



SRC https://mirkomiorelli.github.io/SA\_TSP/

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#### Dynamic Programming

- So far we have considered functional optimization and stochastic optimization
- What if we have a limited set of action to optimize across?
- Say optimizing a set of actions to traverse a graph?
- A strategy to could be
  - Generate a cost-map across the state space
  - Backtrack to find the optimal set of actions

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# Dynamic programming

- A number of different names / approaches has been used
  - Bellman, Dijkstra, Viterbi, ...
- Selection a state space for optimization
- Identifying a set of possible actions
- Formulation of an objective function

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# Example navigation

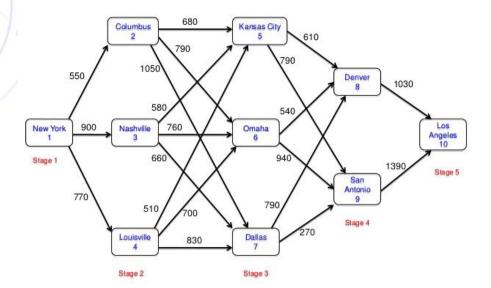




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# Example navigation

# Shortest Path: network figure



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#### Summary



- Robotics is many cases is about formulation of a graph
- Optimization of an objective function across the graph
- Considered deterministic and stochastic approaches to optimization
- Covered the basics and gave an impression of the fundamentals

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# Questions



# Questions

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