Optimization Techniques

Programming for Data Science

Warm Up

Answer the following statements! Give reason for your answers.

1. What is the difference between global and local optimum?
2. What are ways to do random restarts?
3. How do you reference other functions as parameters in a function call?
4. How do you differentiate a function with several parameters?
5. How do you handle functions that are not differentiable?
6. How do you define a maximization problem?

https://amcs.website

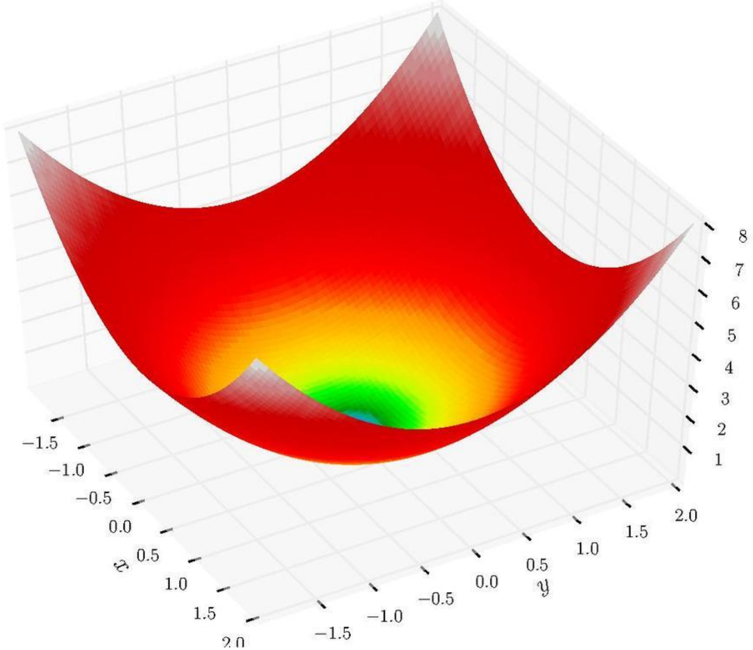
Model Estimation

Problem

- Find the parameters that minimize the costs
- For all data points

Example

- Cost function:
  - $f(x, y) = x^2 + \; y^2$
  - Return value of function: function value/cost
- Optimization problem:
  - $\underset{x,y}{\operatorname{argmin}} f(x, y) = \underset{x,y}{\operatorname{argmin}} x^2 + \; y^2$
- Parameter Estimator



Parameter Estimators

Overview on Optimization Methods (Not Complete!)

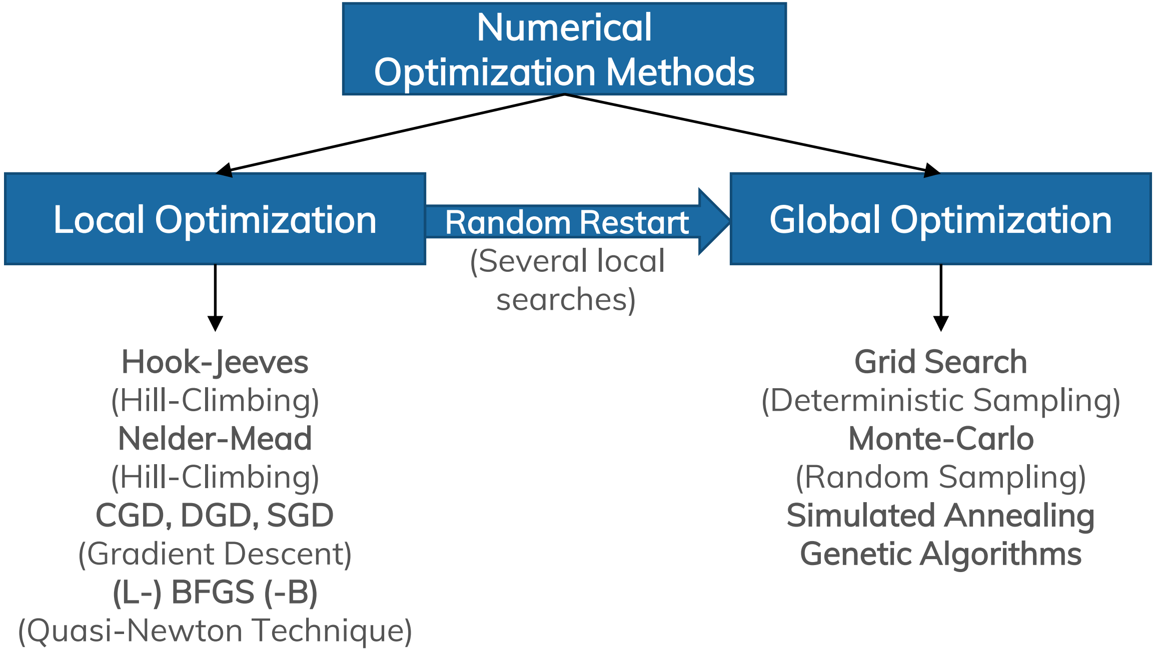
- Numerical general purpose optimization methods
- When there are no analytical solutions (system of linear equations)
- Or: No differentiable optimization target

Global Optimization

- Always find best solution

Local Optimization

- Always finds best solution in direct neighborhood



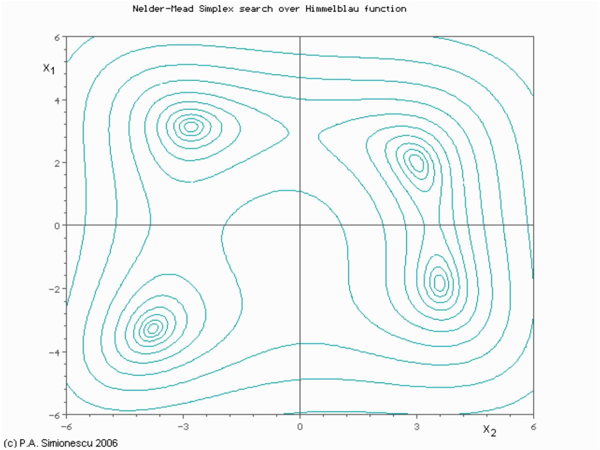
Nelder-Mead

Downhill-Simplex-Method

- Based on a simplex, most simple polygon with n+1 vertices in an n-dimensional space
  - One-dimensional: segment
  - Two-dimensional: triangle
  - Three-dimensional: rectangle
- Choose the worst point from the n+1 points
- In every Iteration the worst point is replaced by a new (hopefully better) point

Example

- Two dimensional parameter space with contour lines
- Triangle is approaching the optimum

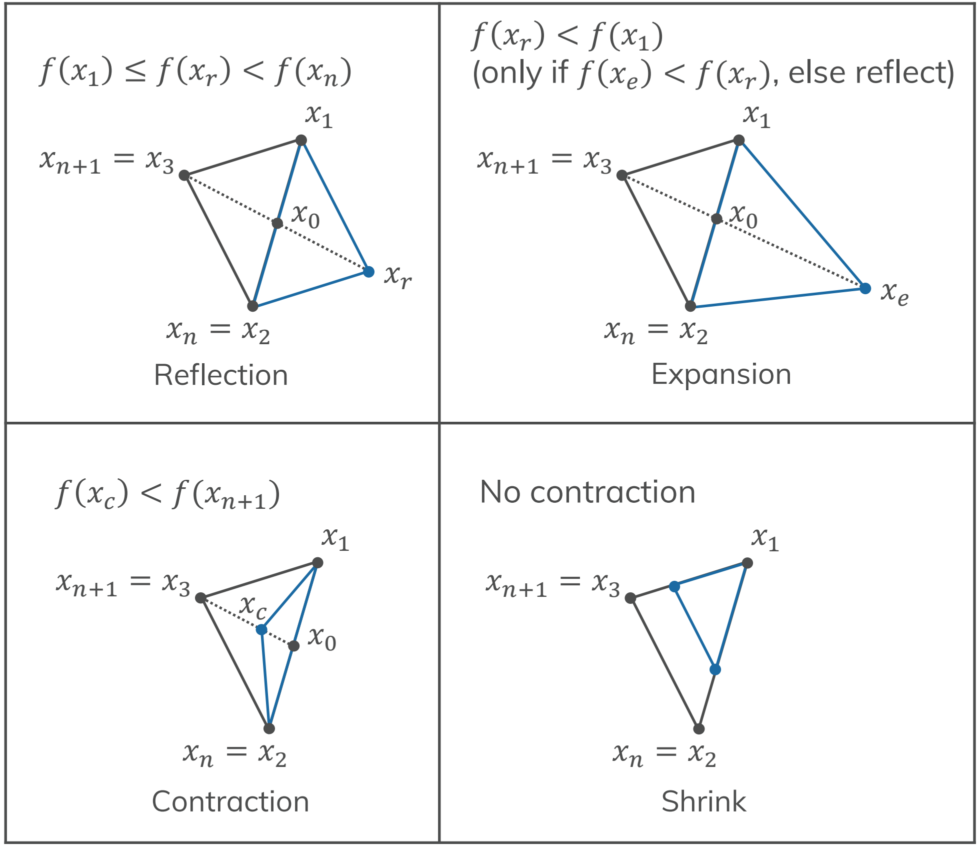


Nelder-Mead

4 strategies to calculate the new simplex

1. Sort the points in ascending order according to their costs f: $x_1, x_2, \dots, x_n, x_{n+1}$
2. Calculate the centroid x_0 with x_1 to x_n

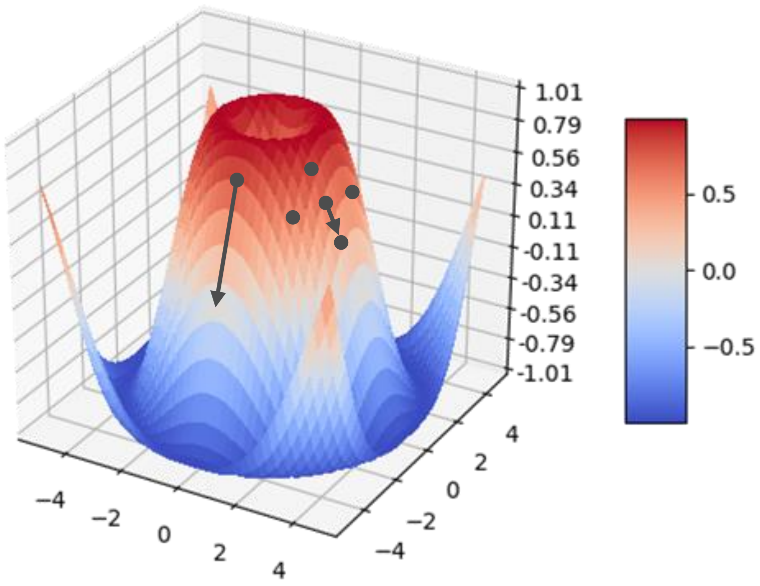
3. While $std(f(x_1), \dots, f(x_{n+1})) > t$:
   According to the given criteria,
   1. **Reflect** the worst point at the centroid
      $x_r = \mathrm{x}_0 + \alpha(x_0 - x_{n+1})$
   2. **Reflect & Expand** the worst point at the centroid
      $x_e = \mathrm{x}_0 + \gamma(x_r - x_0)$
   3. **Contract** the worst point towards the centroid
      $x_c = \mathrm{x}_0 + \rho(x_{n+1} - x_0)$
   4. **Shrink** all points (except x_1) towards x_1
      $x_i = \mathrm{x}_1 + \sigma(x_i - x_1)$



Internal optimizers

optim (R)/scipy.optimize.minimize (python)

- Takes a cost function and a starting configuration for all parameters.
- Supports several methods (Nelder-Mead, BFGS, L-BFGS-B, …).
- Some methods support pre-calculated gradient methods or Hessian matrices.



$$f'(x_i) = \frac{df}{dx_i}, \forall i$$

Task

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Step 0

- You will get a csv file from us. Load it in your language/environment.
- Explore the data in it.
- Write a cost function $f(x, y) \rightarrow z$.

Step 1

- Implement the Nelder-Mead simplex algorithm.* Use $\alpha = 1, \gamma = 2, \rho = 0.5, \sigma = 0.5$, and $t = 2$.
- Find the minimum in the data.

Step 2

- Use optim (minimize) to find the minimum with the conjugate gradient method:
$$f(x, y) = (1.5 - x + xy)^2 + (2.25 - x + xy^2)^2 + (2.625 - x + xy^3)^2$$
- Use your pre-calculated gradient $f'(x, y)$ to boost the calculation.
- Inspect the differences in run time.

*use your own implementation

Package suggestions

R

- -

python3

- numpy
- scipy
- (matplotlib.pyplot)

Exercise Appointment

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We compare and discuss the results

- Tuesday, 17.11.2020,
- Consultation: Please use the forum in Opal.
- Please prepare your solutions! Send us your code!

If you have questions, please mail us:

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