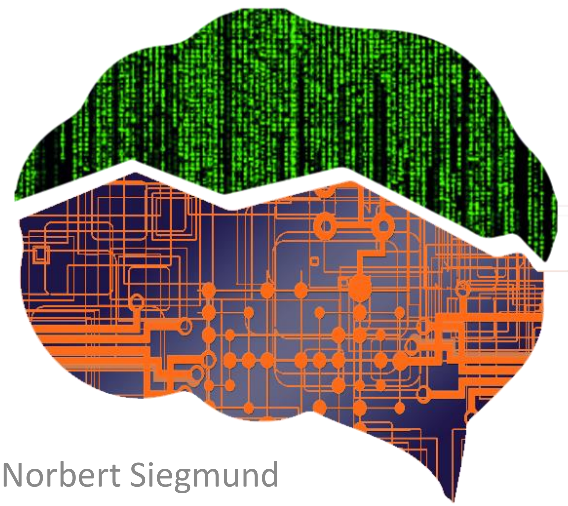
Search-Based Software Engineering

Single-State Meta-Heuristics



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Recap: Goal is to Find the Optimum

- Challenges of general optimization problems (not combinatorial for the moment):
  - Search space is too big
  - Too many solutions to compute
  - Even good heuristics for a *systematic* search are too costly in terms of performance and memory consumption
  - Note that we consider combinatorial optimization problems in later lectures based on the optimization approaches we learn next

- But, how to do optimization in a good-case scenario?

Gradient-based Optimization

- Given a cost function f(x), we can find the optimum via gradient ascent as long as we can compute the first derivative f'(x)
- Idea: Compute the slope at any given x and move up

$$x \leftarrow x + \alpha f'(x)$$

- With: α is a very small positive number controlling the extent of the change

- Generalization with $\vec{x}$ as the input vector:

$$\vec{x} \leftarrow \vec{x} + \alpha \nabla f(\vec{x})$$

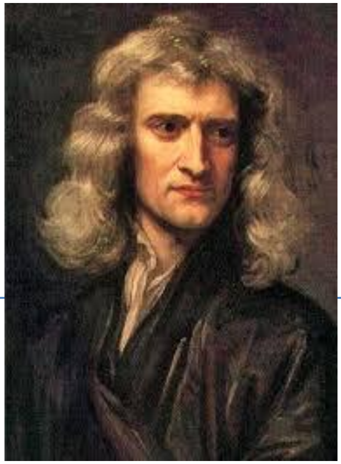
The gradient ∇ is a vector containing the derivative of each element of that dimension

Algorithm and Problems

$\vec{x} \leftarrow \text{random initial vector}$
repeat
  $\vec{x} \leftarrow \vec{x} + \alpha \nabla f(\vec{x})$
until $\vec{x}$ *is optimum or out of time*
return $\vec{x}$

- When do we know $\vec{x}$ is the optimum?
  - Slope is 0
  - Be ware of saddle points and minima!
- What is the convergence time?
  - Tuning α for convergence and against overshooting
- What else can we do?
  - Newton's Method: Directly compute extreme points with f''(x)

Newton's Method I

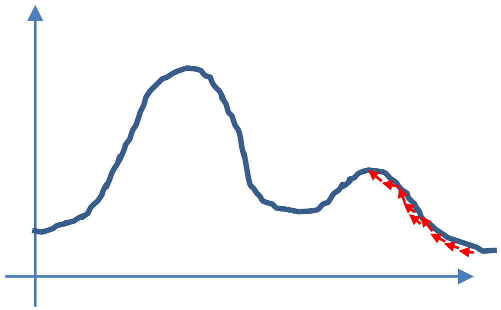


- One-dimensional case: $\vec{x} \leftarrow \vec{x} - \alpha \dfrac{f'(\vec{x})}{f''(\vec{x})}$
  - Dampens α as we get closer to zero slope
  - But, heads to any kind of zero slope (minima, maxima, saddle)
- Multi-dimensional version of the f''(x) is more complex:
  - Called: **Hessian** $H_f(\vec{x}) = \begin{bmatrix} \frac{\delta}{\delta x_1}\frac{\delta f}{\delta x_1} & \cdots & \frac{\delta}{\delta x_1}\frac{\delta f}{\delta x_n} \\ \vdots & \ddots & \vdots \\ \frac{\delta}{\delta x_n}\frac{\delta f}{\delta x_1} & \cdots & \frac{\delta}{\delta x_n}\frac{\delta f}{\delta x_n} \end{bmatrix}$
  - Partial second derivative along each dimension

Newton's Method II

$\vec{x} \leftarrow$ random initial vector
repeat
$\quad \vec{x} \leftarrow \vec{x} - \alpha \left[H_f(\vec{x})\right]^{-1} \nabla f(\vec{x})$
until $\vec{x}$ *is optimum or out of time*
return $\vec{x}$

- Converges faster than regular gradient ascent
- Problems:
  - Caught in local optima, but goal is global optima



Local optimization algorithm!

Toward Global Optimization

- Two options: increase α or repeat gradient ascent in a loop and always start from a different random position

$\vec{x} \leftarrow$ random initial vector
$\vec{x}^* \leftarrow \vec{x}$
repeat
  repeat
    $\vec{x} \leftarrow \vec{x} + \alpha \nabla f(\vec{x})$
  until $|| \nabla f(\vec{x}) || = 0$
  if $f(\vec{x}) > f(\vec{x}^*)$ **then**
    $\vec{x}^* \leftarrow \vec{x}$
  $\vec{x} \leftarrow$ random vector
until *out of time*
return $\vec{x}^*$

Finds local optimum

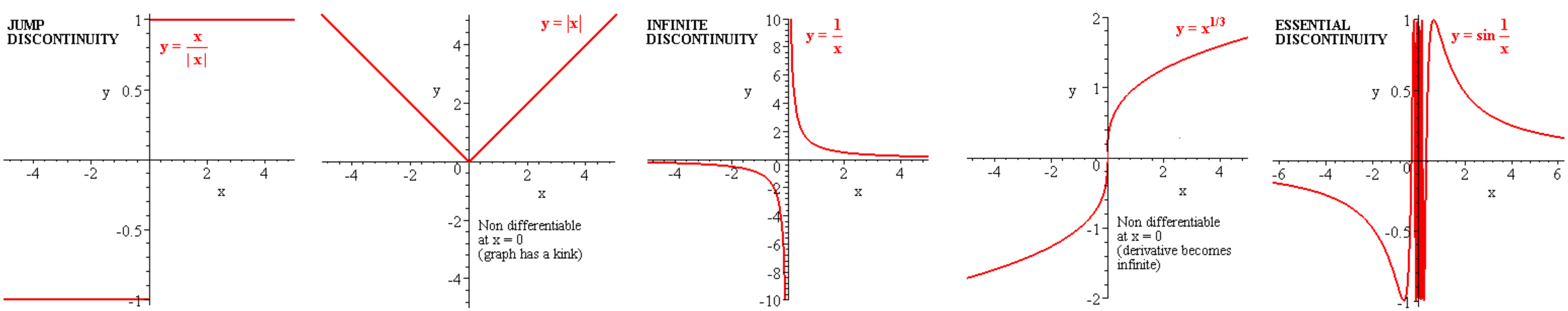
Finds the best local optimum, which is hopefully the global optimum

- Problem: $||\nabla f(\vec{x})|| = 0$ might never be exactly 0, so use a threshold: $-\epsilon < ||\nabla f(\vec{x})|| < \epsilon$

Shortcomings of Gradient Ascent

- Assumptions:
  - Ability to compute the first derivative
  - Often, we even don't know the function (e.g., in black-box scenarios)!
  - We only know how to create, modify, and test a solution

- Does not work for non-differentiable functions



Solution: Thoughtfull Random Probing

- Idea: Randomly select a starting point in the search space and search based on a *given strategy* for the optimal solution
- The given strategy represents the *meta-heuristic*

- This lecture:
  - Know pros and cons of gradient-based optimization
  - Learn about *single-state* meta-heuristics
    - Local search
    - Global search
    - Hill climbing, simulated annealing, etc.

Heuristics

- Heuristic (greek: to find)
  - “involving or serving as an aid to learning, discovery, or problem-solving by experimental and especially trial-and-error methods” Merriam-Webster dicitionary
- Why heuristics?
  - NP-hard problems including decision variables with many interdependencies
  - Nonlinear cost functions and constraints, even no mathematical functions (e.g., a cost function might be the execution of a program or asking an expert)
  - So, near-optimal solution might be just good enough

Meta-Heuristic

- Algorithms employing some degree of randomness to find "optimal" solutions to hard problems

- Applied to: "I know it when I see it" problems
  - In case when:
    - You don't know beforehand how the optimal solution looks like
    - You don't know how to find the optimal solution
    - The search space is too large and there is no domain heuristic
    - You can quantify the quality of a solution when you see it
- Two extremes:

Random search Hill climbing

Assumptions of Meta-Heuristic Optimization

- We need to be able to do four steps:
  - **Initialization procedure**: Provide one or more initial candidate solutions
  - **Assessment procedure**: Assess the *quality* of a candidate solution
  - Make a *copy* of a candidate solution
  - **Modification procedure**: *Tweak* a candidate solution to produce a randomly slightly different candidate solution
- A **selection procedure** decides, which candidate solution to retain

Hill Climbing (Local Search)

- Idea:
  - Use only your local solution and evaluate your *neighbors* to find a better one
  - Repeat this step until no better neighbor exists
  - Similar to gradient ascent, but does not compute gradient
- Pros:
  - Requires few resources (current state and neighbors)
  - Finds local optimum (global is possible)
  - Useful if the search space is huge (even unlimited)

Hill-Climbing Algorithm

$S \leftarrow$ random initial *solution* ← Initialization procedure
repeat
  $R \leftarrow Tweak(Copy(S))$ ← Modification procedure
  if $Quality(R) > Quality(S)$ **then** ← Assessment and selection procedure
    $S \leftarrow R$
until S is optimum or out of time
return S

- Observations:
  - Hill climbing is more general than gradient ascent
  - *Tweak* operation must rely on a stochastic/random process to find better candidate solutions
  - Strongly depends on “good” initialization

Variant: Steepest Ascent Hill Climbing

- Idea: Be more aggressive and parallelize by creating n tweaks to a candidate solution (like sampling the gradient)

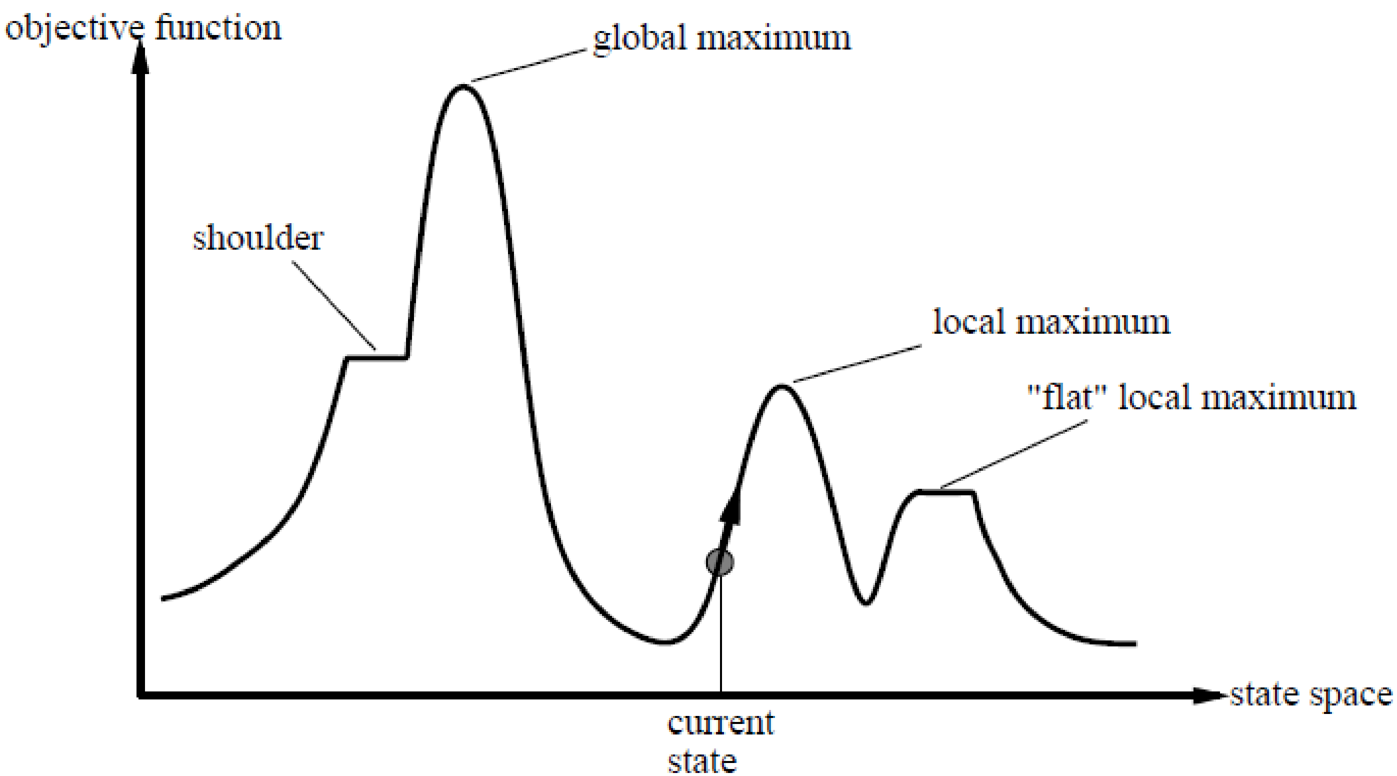
$n \leftarrow$ number of tweaks
$S \leftarrow$ random initial *solution*
repeat
  $R \leftarrow Tweak(Copy(S))$
  for n-1 times **do**
    $W \leftarrow Tweak(Copy(S))$
    if $(Quality(W) > Quality(R))$ **then**
      $R \leftarrow W$
  if $(Quality(R) > Quality(S))$ **then**
    $S \leftarrow R$
until S is optimum or out of time
return S

With replacement:

$n \leftarrow$ number of tweaks
$S \leftarrow$ random initial *solution*
$Best \leftarrow S$
repeat
  $R \leftarrow Tweak(Copy(S))$
  for n-1 times **do**
    $W \leftarrow Tweak(Copy(S))$
    if $(Quality(W) > Quality(R))$ **then**
      $R \leftarrow W$
  $S \leftarrow R$
  if $(Quality(S) > Quality(Best))$ **then**
    $Best \leftarrow S$
until *Best* is optimum or out of time
return $Best$

Problems with Hill Climbing

- Local optimum: usually won’t find global optimum
- Plateaus: algorithm gets stuck



How to Realize the Operations?

- Find a suitable representation of a candidate solution
  - Vector of numbers, list or set of objects, a tree, a graph, etc.
  - Representation must allow for implementing the operations for *Initialization*, *Tweak*, *Copy*, and *Quality*
- Example: fixed-length vector of real numbers as candidate solution
- Initialization operation:

$min \leftarrow$ minimum desired vector element value
$max \leftarrow$ maximum desired vector element value
$\vec{x} \leftarrow$ a new vector $\langle x_1, \ldots, x_l \rangle$
for i from 1 to l **do**
  $x_i \leftarrow$ random number taken uniformly between min and max
return $\vec{x}$

How to Realize the Operations? (Cont.)

- Idea of Tweak operation:
  - Add random noise as small value to each number in the vector
  - But only for a given probability (often, we set $p \leftarrow 1$)

$\vec{x} \leftarrow$ vector $\langle x_1, \dots, x_l \rangle$ to be convolved
$p \leftarrow$ probability of adding noise to an element in the vector
$r \leftarrow$ half range of uniform noise
$min \leftarrow$ minimum desired vector element value
$max \leftarrow$ maximum desired vector element value

for i from 1 to l **do**
  if $p \geq$ random number chosen uniformly from 0.0 to 1.0 **then**
    repeat
      $n \leftarrow$ random number chosen uniformly from $-r$ to r *inclusive*
    until $min \leq x_i + n \leq max$
    $x_i \leftarrow x_i + n$
return $\vec{x}$

Exploration vs. Exploitation

- Exploration:
  - Explore the search space and avoid being trapped in a local maximum (very fast to find a locally good solution)
- Exploitation:
  - Exploiting local information to reliably move to (local) maximum (very important if the search space has many local optima)

- How to balance or even manipulate both aspects?
  - Parameter r allows as to tweak exploration vs. exploitation
  - Small r will fully exploit the locality to reach the local optimum
  - Large r will result in bounces through the search space (random search in the extreme case)

Single-State Global Optimization Algorithms

About Global Optimization

- An algorithm is guaranteed to find the global optimum, at least in theory
  - Often requires running the algorithm an infinite amount of time
  - Realized by having a chance to visit every possible solution in the solution space

- Why are the aforementioned approaches not global?
  - Tweak operation is bounded so that it stays in a local area

Random Search

- Concept: full explorative and no exploitation
- Idea: Randomly select a candidate solution

$Best \leftarrow$ random initial candidate solution
repeat
  $S \leftarrow$ a random candidate solution
  if $Quality(S) > Quality(Best)$ **then**
    $Best \leftarrow S$
until $Best$ *is optimum or out of time*
return $Best$

Global

Random Search

Hill Climbing with
random restarts (global)

Hill Climbing with small r

Local

Exploration

Exploitation

Hill Climbing with Random Restarts

- Idea: Do Hill Climbing for some time and then start all over again from a different initial candidate solution

$T \leftarrow$ distribution of possible time intervals
$S \leftarrow$ random initial candidate solution
$Best \leftarrow S$
repeat
  $time \leftarrow$ random time in the near future, chosen from T
  repeat
    $S \leftarrow Tweak(Copy(S))$
    if $Quality(R) > Quality(S)$ **then**
      $S \leftarrow R$
  until S is optimum or *time* is up or out of time
  if $Quality(S) > Quality(Best)$ **then**
      $Best \leftarrow S$
  $S \leftarrow$ some random candidate solution
until $Best$ is optimum or out of time
return $Best$

Best Practices I

- Adjust the **modification procedure**
  - Tweak makes large, random changes
  - Global, because if long running, randomness will cause Tweak to try every solution
  - The more large, random changes, the more exploration
- Adjust the **selection procedure**
  - Change the algorithm so that you go *<u>down</u>*hills at least some time
  - Global, because if long running, you'll go down enough hills so that you can go up again at the global optimum hill
  - The more often going down hills, the more exploration

Best Practices II

- Jump to something new
  - Start from a new location every once in a while
  - Global, because if trying enough new locations, the optimum hill will be visited
  - The more frequent restarts, the more exploration
- Use a large sample
  - Try many candidate solutions in parallel
  - Global, because if enough parallel candidate solutions, one of them will be the optimum hill
  - More parallel candidate solutions, the more exploration

Currently: Single state optimization -> very small sample

Next Lecture & Literature

- Multi-State optimization algorithms (population methods)
  - Evolution strategies
  - Genetic algorithms
  - Differential Evolution