Heuristic Optimization

Lecture 1

Algorithm Engineering Group
Hasso Plattner Institute, University of Potsdam

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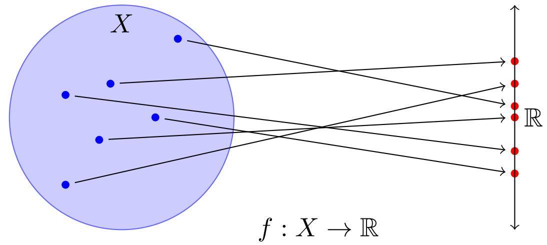
HPI Hasso Plattner Institut

Optimization



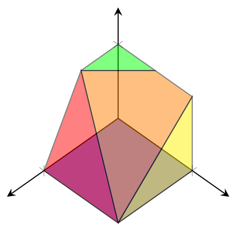
Goal:

- Find $z \in X$ such that $f(z) \leq f(x)$ for all $x \in X$ (minimization)
- Find $z \in X$ such that $f(z) \geq f(x)$ for all $x \in X$ (maximization)

Optimization examples

Linear programming

- X is the set of all vectors $x \in \mathbb{R}^n$ with $Ax \leq b$ and $x \geq 0$,
- $f(x) = c^\top x$.
- **Goal:** find $x \in X$ such that $f(x)$ is minimal



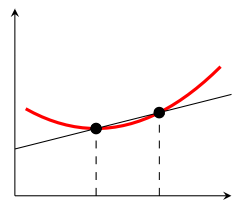
Example: Schedule production levels of a product to minimize total cost subject to resource constraints.

- Simplex algorithm
- Interior point methods

Optimization examples

Convex optimization

- X is the set of all vectors $x \in \mathbb{R}^n$ with some constraints,
- $f(tx + (1-t)y) \leq tf(x) + (1-t)f(y)$ for all $0 \leq t \leq 1$.
- **Goal:** find $x \in X$ such that $f(x)$ is minimal



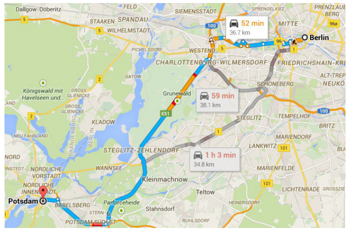
Example: Find the receiver location among a set of interfering transmitters that maximizes signal to noise ratio.

- Subgradient method
- Cutting plane method

Optimization examples

Find the shortest route between two cities

- X is the set of feasible paths
- f measures the length of a path
- **Goal:** find $x \in X$ such that $f(x)$ is minimal



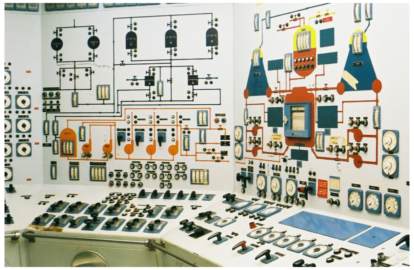
Example: Navigation software.

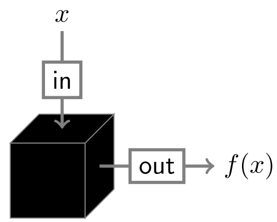
- Dijkstra's algorithm
- Bellman-Ford

The black-box scenario

Suppose we know nothing (or almost nothing) about the function

- $f(x)$ measures some complex (e.g., industrial) process
- $f(x)$ value depends on the result of an expensive simulation
- process of assigning f-values to X is noisy/unpredictable





How should we approach these problems?

Heuristic Optimization

Approaches

- Take a best guess at a good solution and "live with it"
- Try each possible solution and keep the best
- **Start with a good guess and then try to improve it iteratively**

Heuristic Optimization

- Can be inspired by *human problem solving*
  - Common sense, rules of thumb, experience
- Can be inspired by *natural processes*
  - Evolution, annealing, swarming behavior
- Typically rely on a source of *randomness* to make decisions
- General purpose, robust methods
- Easy to implement
- **Can be challenging to analyze and prove rigorous results**

Some success stories

NASA

- communication antennas on ST-5 mission (evolutionary algorithm)
- deployed on spacecraft in 2006

REFERENCE: Jason D. Lohn, Gregory S. Hornby and Derek S. Linden, "Human-competitive evolved antennas", *Artificial Intelligence for Engineering Design, Analysis and Manufacturing*, volume 22, issue 3, pages 235–247 (2008).

Some success stories

Boeing

- 777 GE engine: turbine geometry evolved with a genetic algorithm

REFERENCE: Charles W. Petit, "Touched by nature: putting evolution to work on the assembly line." *US News & World Report*, volume 125, issue 4, pages 43–45 (1998).

Some success stories

Oral B

- cross-action toothbrush design optimized by Creativity Machine (evolutionary algorithm)

REFERENCE: Robert Plotnick, "The Genie in the Machine: How Computer-Automated Inventing Is Revolutionizing Law and Business", Stanford Law Books, (2009)

Some success stories

Nutech Solutions

- improved car frame for GM (genetic algorithms, neural networks, simulated annealing, swarm intelligence)

BMW

- optimized acoustic and safety parameters in car bodies (simulated annealing, genetic and evolutionary algorithms)

REFERENCE: Fabian Duddeck, "Multidisciplinary Optimization of Car Bodies", *Structural and Multidisciplinary Optimization*, volume 35, pages 375–389 (2008).

Some success stories

Hitachi

- improved nose cone for N700 bullet train (genetic algorithm)

REFERENCE: Takenori Wajima, Masakazu Matsumoto and Shinichi Sekino, "Latest System Technologies for Railway Electric Cars", *Hitachi Review* volume 54, issue 4, pages 161–168 (2005).

Some success stories

Merck Pharmaceutical Company

- discovered first clinically-approved antiviral drug for HIV (Isentress) using AutoDock software (uses a genetic algorithm)

REFERENCE:
`http://autodock.scripps.edu/news/autodocks-role-in-developing-the-first-clinically-approved-hiv-integrase-inhibitor`

Heuristics

Assumptions

1. Solutions encoded as length-n bitstrings (elements of $\{0,1\}^n$),
2. want to maximize some $f\colon \{0,1\}^n \to \mathbb{R}$.

Random Search

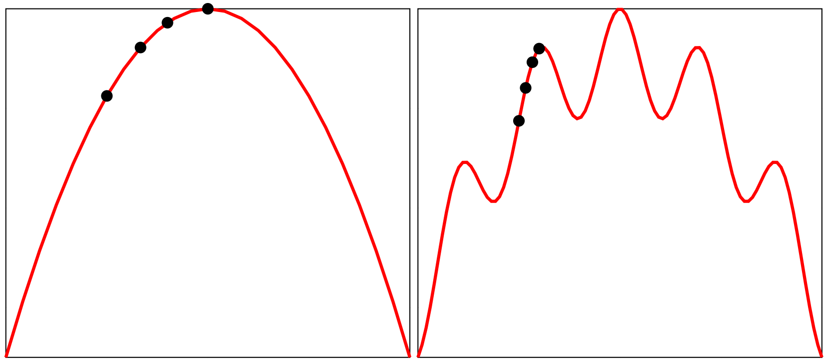
Choose x uniformly at random from $\{0,1\}^n$;
while *stopping criterion not met* **do**
    Choose y uniformly at random from $\{0,1\}^n$;
    if $f(y) \geq f(x)$ **then** $x \leftarrow y$;
end

Heuristics

Random(ized) Local Search (RLS)

Choose x uniformly at random from $\{0,1\}^n$;
while *stopping criterion not met* **do**
    $y \leftarrow x$;
    Choose i uniformly at random from $\{1,\ldots,n\}$;
    $y_i \leftarrow (1 - y_i)$;
    if $f(y) \geq f(x)$ **then** $x \leftarrow y$;
end

Local Optima



How to deal with local optima?

- Restart the process when it becomes trapped (ILS)
- Accept disimproving moves (MA, SA)
- Take larger steps (EA, GA)

Simple Randomized Search Heuristics

Metropolis Algorithm

Choose x uniformly at random from $\{0,1\}^n$;
while *stopping criterion not met* **do**
  $y \leftarrow x$;
  Choose i uniformly at random from $\{1,\ldots,n\}$;
  $y_i \leftarrow (1 - y_i)$;
  if $f(y) \geq f(x)$ **then** $x \leftarrow y$;
  else $x \leftarrow y$ with probability $e^{(f(x)-f(y))/T}$;
end

- Method developed for generating sample states of a thermodynamic system (1953)
- T is **fixed** over the iterations

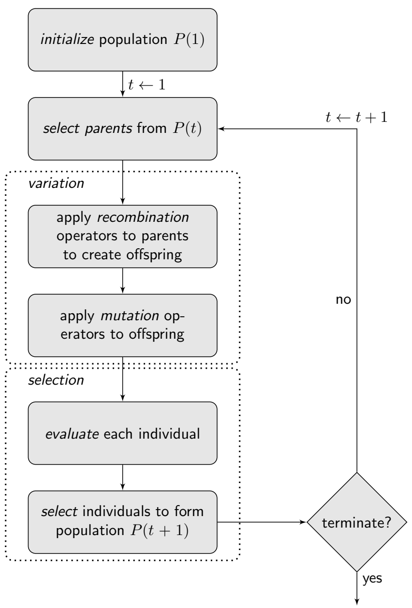
Simple Randomized Search Heuristics

Simulated Annealing

Choose x uniformly at random from $\{0,1\}^n$;
while *stopping criterion not met* **do**
  $y \leftarrow x, t \leftarrow 0$;
  Choose i uniformly at random from $\{1,\ldots,n\}$;
  $y_i \leftarrow (1 - y_i)$;
  if $f(y) \geq f(x)$ **then** $x \leftarrow y$;
  else $x \leftarrow y$ with probability $e^{(f(x)-f(y))/T_t}$;
  $t \leftarrow t + 1$;
end

- Heating and controlled cooling of a material to increase crystal size and reduce their defects.
- High temperature $\Rightarrow$ many random state changes
- Low temperature $\Rightarrow$ system prefers "low energy" states (high fitness)
- Idea is to carefully settle the system down over time to its lowest energy state (highest fitness) by **cooling**
- T_t is **dependent on** t, typically decreasing.

Evolutionary Algorithms



Evolutionary Algorithms

- Allow larger jumps
- Long (destructive) jumps should be rare

(1+1) EA

Choose x uniformly at random from $\{0,1\}^n$;
while *stopping criterion not met* **do**
  $y \leftarrow x$;
  foreach $i \in \{1,\ldots,n\}$ **do**
    With probability $1/n$, $y_i \leftarrow (1 - y_i)$;
  end
  if $f(y) \geq f(x)$ **then** $x \leftarrow y$;
end