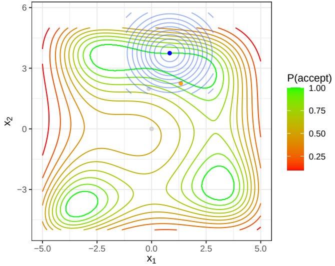
Optimization in Machine Learning

Simulated Annealing



Learning goals

- Motivation
- Metropolis algorithm
- Simulated Annealing

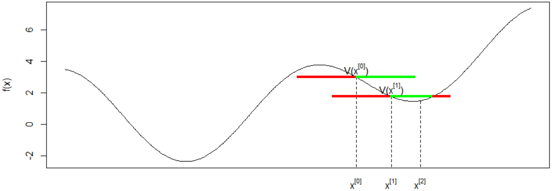
INTRODUCTION

Heuristics for the optimization of complex (multivariate, non-linear, non-convex) objective functions

- Procedure for finding good solutions to complex problems.
- Does not guarantee optimal/best result (global optimum), but usually good solutions.
- Goal for complex optimization problems: avoid “getting stuck” in local optima.
- Is often used for difficult discrete problems as well.
- Local search strategy with random option to accept worse values.

SIMPLE STOCHASTIC LOCAL SEARCH

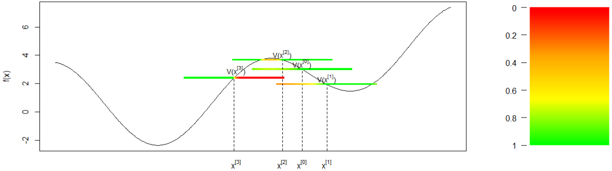
- Given is a multivariate objective function $f(\mathbf{x})$
- Define a local neighborhood area $V(\mathbf{x})$ for a given $\mathbf{x}$
- Sample proposal $\mathbf{x}^{[t+1]}$ uniformly at random from neighborhood $V(\mathbf{x}^{[t]})$
- Calculate $f(\mathbf{x}^{[t+1]})$
- If $\Delta f = f(\mathbf{x}^{[t+1]}) - f(\mathbf{x}^{[t]}) < 0$, $\mathbf{x}^{[t+1]}$ is accepted as new solution, otherwise a new proposal from neighborhood is sampled.



Simple stochastic local search: Acceptance (green) and rejection range (red)

METROPOLIS ALGORITHM

- Simple stochastic local search strongly depends on $\mathbf{x}^{[0]}$ and the neighborhood.
  $\Rightarrow$ Danger of ending up in local minima
- **Idea:** allow worse candidates with some probability
- **Metropolis:** accept candidates from previous rejection range ($\Delta f > 0$) with probability $\mathbb{P}(\text{accept} \,|\, \Delta f) = \exp(-\Delta f / T)$
- T denotes "temperature"

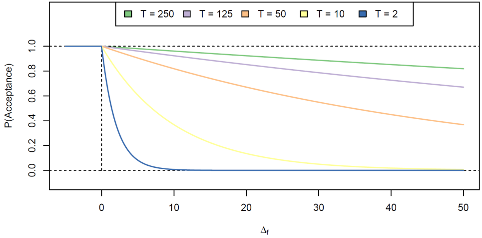


Simulated annealing: Colors correspond to $\mathbb{P}(\text{accept})$

METROPOLIS ALGORITHM

- Parameter T describes temperature/progress of the system
- High temperatures correspond to high probability of accepting worse $\mathbf{x}$
- Local minima can be escaped, but no convergence can be achieved at *constant* temperature
- We come across an important principle of optimization:

exploration (high T) vs. exploitation (low T)



SIMULATED ANNEALING

- Start with high temperature to **explore** whole space
- Slowly reduce temperature to converge
  $\Rightarrow$ Sequence of descending temperatures $T^{[t]}, t \in \mathbb{N}$
- Procedure is called **simulated annealing**
- Temperature is often kept constant several iterations in a row to explore the space, then multiplied by coefficient $0 < c < 1$:

$$T^{[t+1]} = c \cdot T^{[t]}$$

- Other strategies possible, for example:

$$T^{[t]} = T^{[0]} \left(1 - \frac{t}{t_{\text{max}}}\right)$$

Choosing neighborhood:

- Many different strategies. Strongly depends on objective function.

ANALOGY TO METALLURGY

- **Simulated annealing** draws analogy between a cooling process (e.g. a metal or liquid) and an optimization problem.
- If cooling of a liquid material (amount of atoms) is too fast, it solidifies in suboptimal configuration, slow cooling produces crystals with optimal structure (minimum energy stage).
- Consider atoms of the liquid as a system with many degrees of freedom, analogy to optimization problem of a multivariate function
- Minimum energy stage corresponds to optimum of objective function.