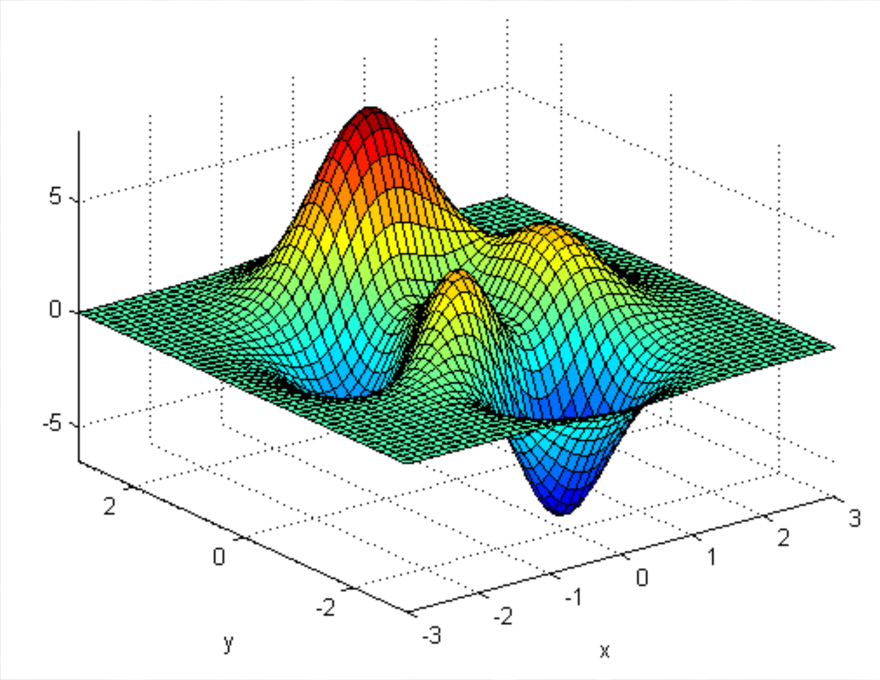
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0
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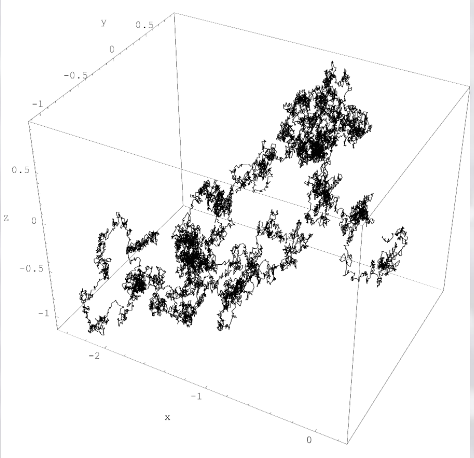
Trivial Algorithms



- Random Sampling
  - Generate a state randomly
- Random Walk
  - Randomly pick a neighbor of the current state
- Both algorithms asymptotically complete.

Overview

- **Previously** we addressed a single category of problems: **<u>observable, deterministic, known environments</u>** where the solution is a sequence of actions.
- Now we consider what happens when these assumptions are **relaxed**.
- First we look at purely **local search** strategies, including methods inspired by statistical physics (**simulated annealing**) and evolutionary biology (**genetic algorithms**).
- Later, we examine what happens when we relax the assumptions of determinism and observability. The key idea is that the agent cannot predict exactly what percept it will receive, so it considers a **contingency** plan.
- Lastly, we discuss online search.

Local Search for Optimization

- Note that for many types of problems, the path to a goal is irrelevant (we simply want the solution – consider the 8-queens).
- If the path to the goal does not matter, we might consider a class of algorithms that don't concern themselves with paths at all.

- **Local search algorithms** operate using a single current node (rather than multiple paths) and generally move only to neighbors of that node.

- Typically, the paths followed by the search are not retained (the benefit being a potentially substantial memory savings).

Local Search for Optimization

- Local search
  - Keep track of single current state
  - Move only to neighboring states
  - Ignore paths

- Advantages:
  - Use very little memory
  - Can often find reasonable solutions in large or infinite (continuous) state spaces.

- "Pure optimization" problems
  - All states have an objective function
  - Goal is to find state with max (or min) objective value
  - Does not quite fit into path-cost/goal-state formulation
  - Local search can do quite well on these problems.

Local Search for Optimization

- In addition to finding goals, local search algorithms are useful for solving **pure optimization problems**, in which we aim to find the best state according to an **objective function**.

- Nature, for example, provides an objective function – *reproductive fitness*.

- To understand local search, we consider **state-space landscapes**, as shown next.

Optimization

- So what is optimization?

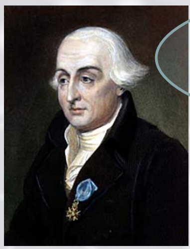
- Find the minimum or maximum of an objective function (usually: given a set of constraints):

$$\arg\min_x f_0(x)$$
$$\text{s.t.}\, f_i(x) \leq 0, i = \{1, \ldots, k\}$$
$$h_j(x) = 0, j = \{1, \ldots l\}$$

Aside: Optimization Paradigms

- Two of the most common optimization paradigms in ML include:

(1) **Optimization with equality constraints.**

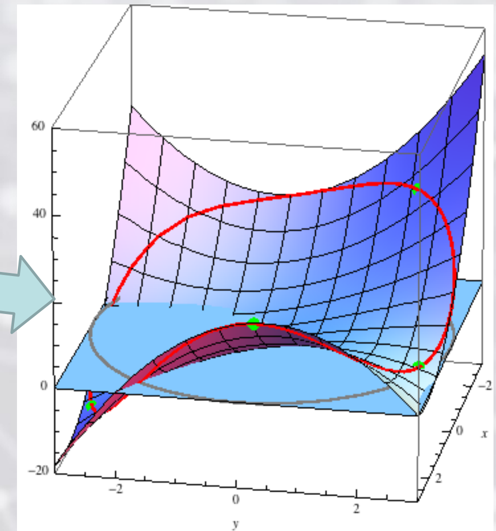


Lagrange

$$\text{maximize } f(x,y,z)$$
$$\text{subject to } g(x,y,z)=0,\ h(x,y,z)=0$$

$$\nabla f(x,y,z) = \lambda \nabla g(x,y,z) + \mu \nabla h(x,y,z)$$

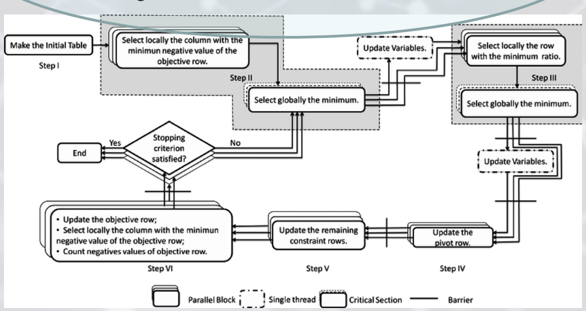
Method of Lagrange Multipliers



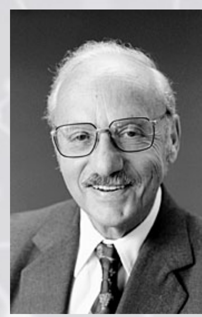
(2) **Optimization with inequality constraints.**

von Neumann

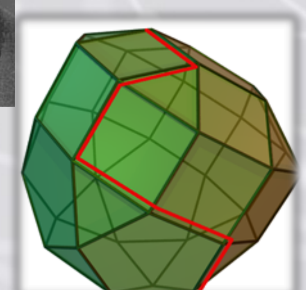
$$\text{maximize } c^T x$$
$$\text{subject to } Ax \le b \text{ and } x \ge 0$$



Linear Programming: Simplex Method

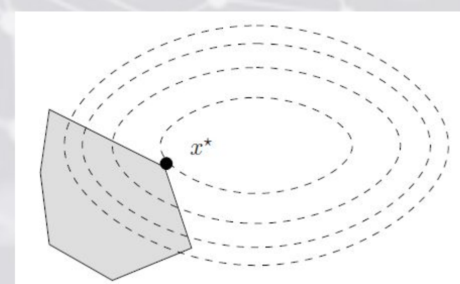


Dantzig



$$\text{maximize } \frac{1}{2} x^T Q x + c^T x$$
$$\text{subject to } Ax \le b$$

Quadratic Programming



Why Do We Care?

Linear Classification

$$\arg\min_{w} \sum_{i=1}^{n} ||w||^2 + C \sum_{i=1}^{n} \xi_i$$
$$\text{s.t. } 1 - y_i x_i^T w \leq \xi_i$$
$$\xi_i \geq 0$$

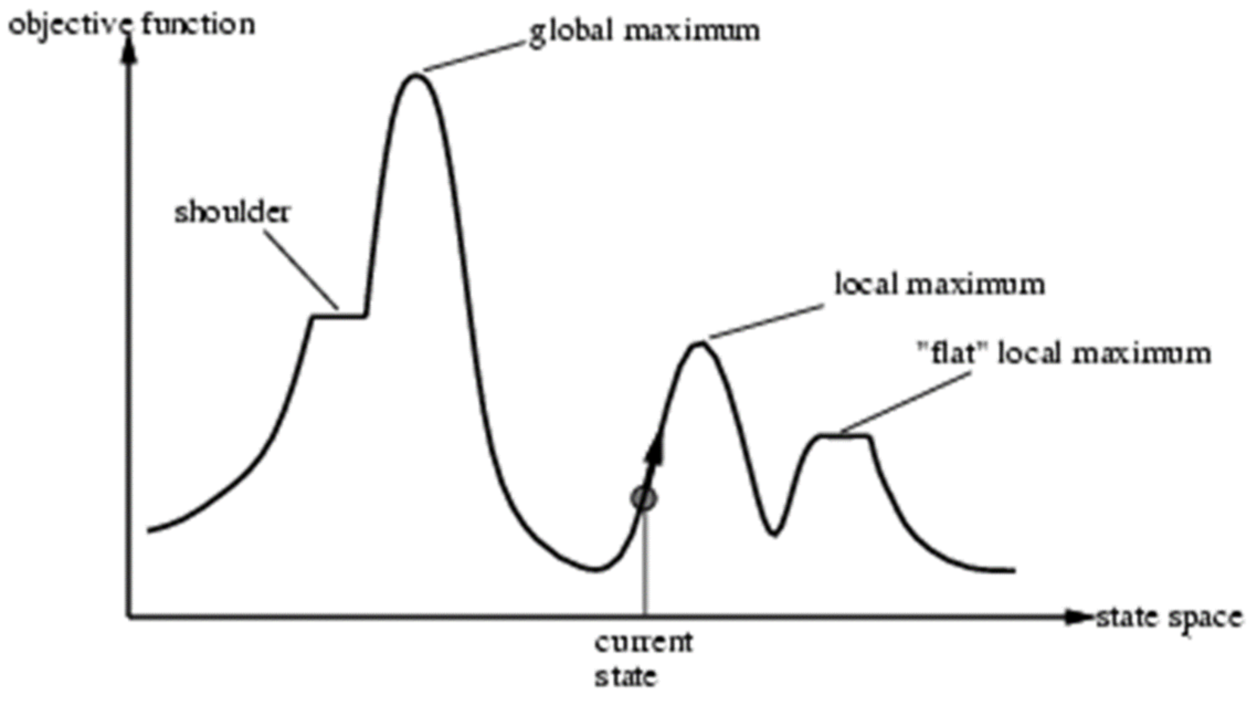
Maximum Likelihood

$$\arg\max_{\theta} \sum_{i=1}^{n} \log\, p_\theta(x_i)$$

K-Means

$$\arg \min_{\mu_1, \mu_2, \ldots, \mu_k} J(\mu) = \sum_{j=1}^{k} \sum_{i \in C_j} ||x_i - \mu_j||^2$$

Local Search for Optimization



State-Space Landscape

- If elevation corresponds with cost, then the aim is to find the lowest valley – **a global minimum**; if elevation corresponds to an objective function, then the aim is to find the highest peak – **a global maximum**.
- A **complete** local search algorithm always finds a goal (if one exists); an **optimal** algorithm always finds a global minimum/maximum.

Hill-Climbing (Greedy Local Search)

function HILL-CLIMBING(*problem*) **return** a state that is a local maximum
  input: *problem*, a problem
  local variables: *current*, **a node.**
          neighbor, **a node.**

  current ← MAKE-NODE(INITIAL-STATE[*problem*])
  loop do
    neighbor ← a highest valued successor of *current*
    if VALUE [*neighbor*] ≤ VALUE[*current*] **then return** STATE[*current*]
    current ← *neighbor*

Minimum version will reverse inequalities and look for lowest valued successor

Hill-Climbing

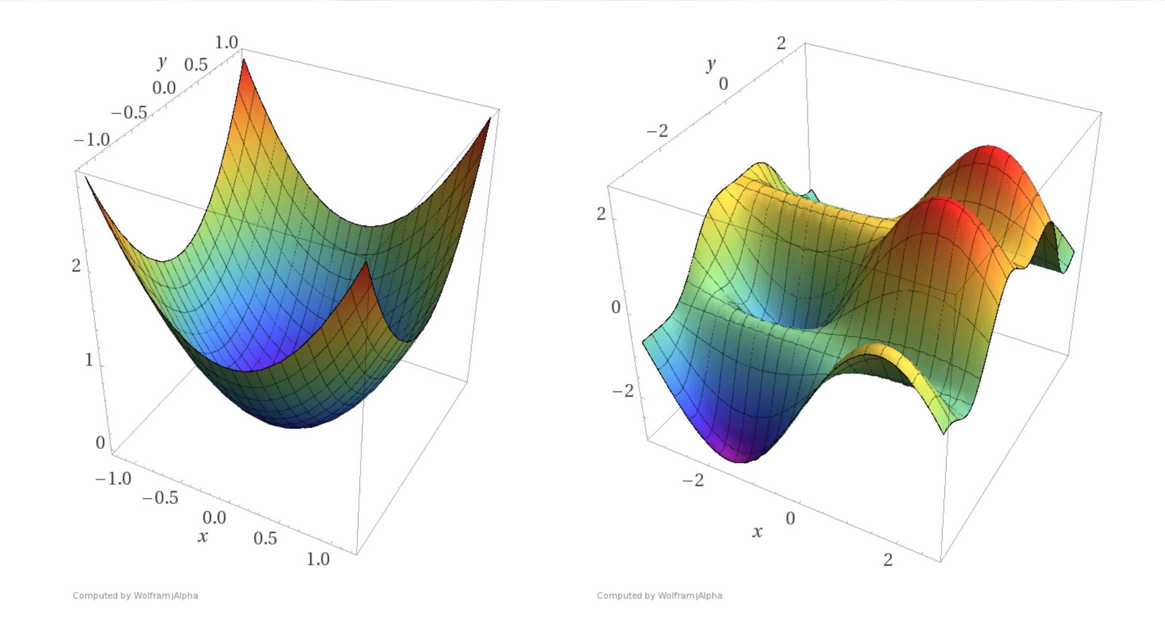
- "A loop that continuously moves towards increasing value"
  - terminates when a peak is reached
  - Aka greedy local search
- Value can be either
  - Objective function value
  - Heuristic function value (minimized)

- Hill climbing does not look ahead of the immediate neighbors
- Can randomly choose among the set of best successors
  - if multiple have the best value

- "Climbing Mount Everest in a thick fog with amnesia"

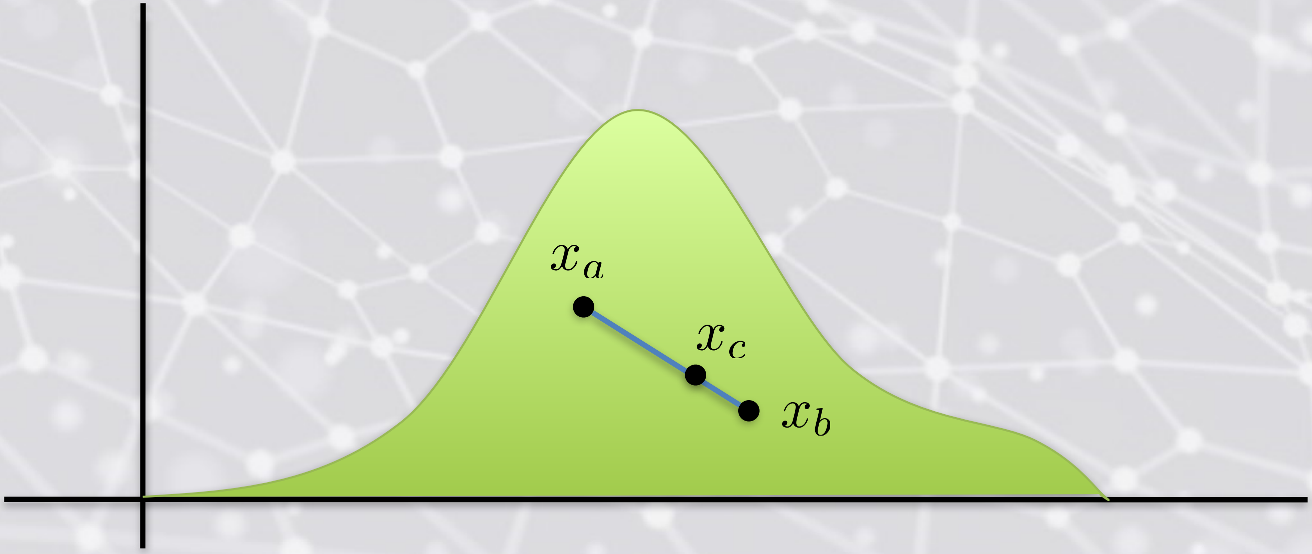
Convexity

- We prefer convex problems.



Aside: Convex Functions

- Convex: for any pair of points x_a and x_b within a region, every point x_c on a line between x_a and x_b is in the region



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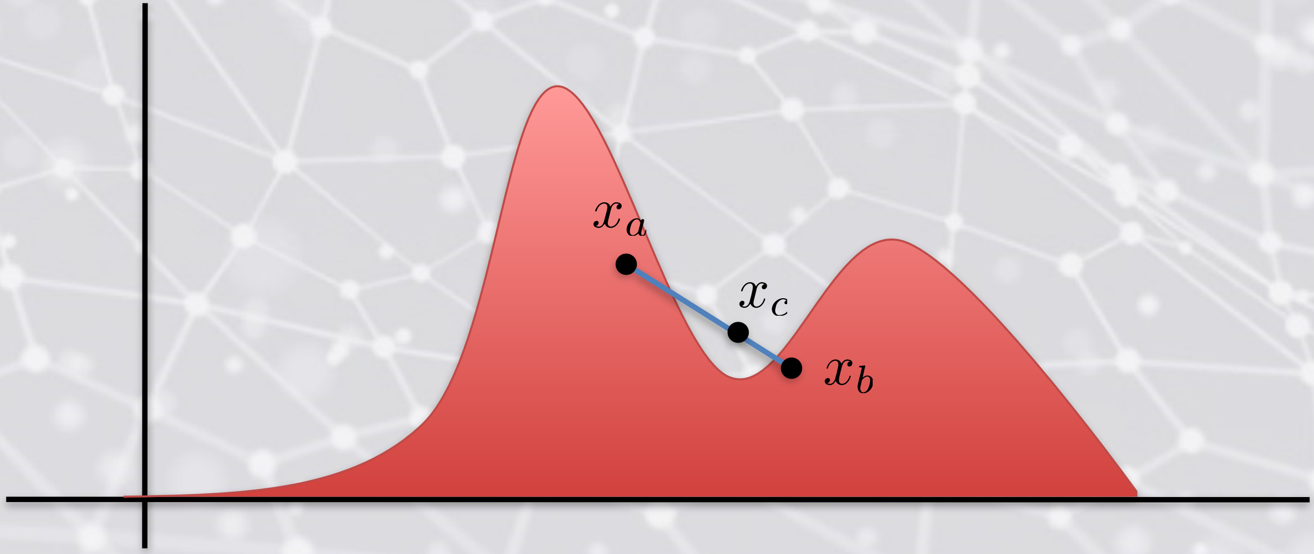
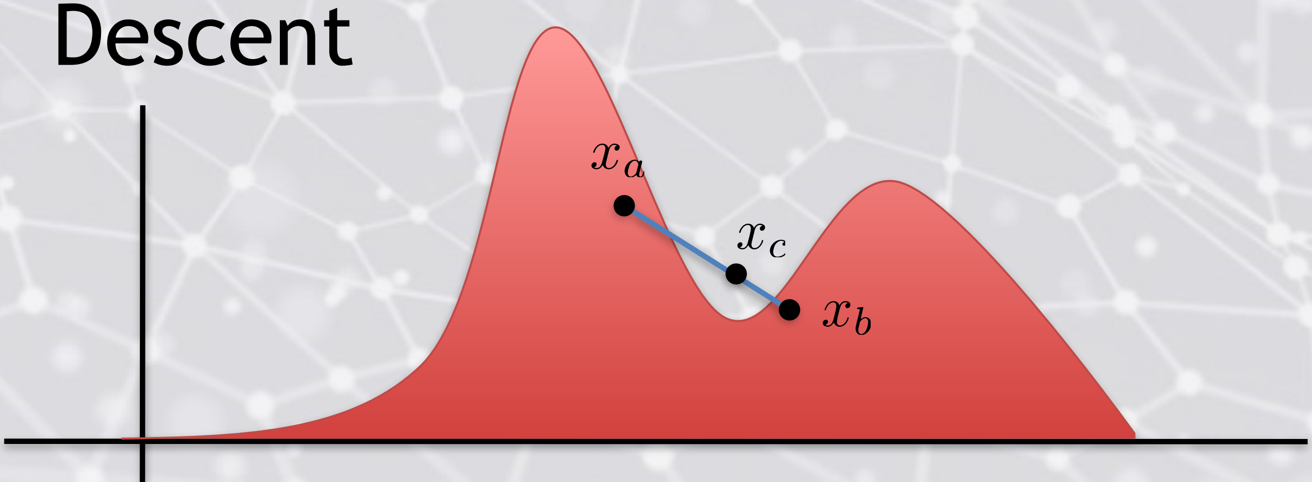


Aside: Convex Functions

- Convex functions have a single maximum and minimum!
- How does this help us?
- (nearly) Guaranteed optimality of Gradient Descent

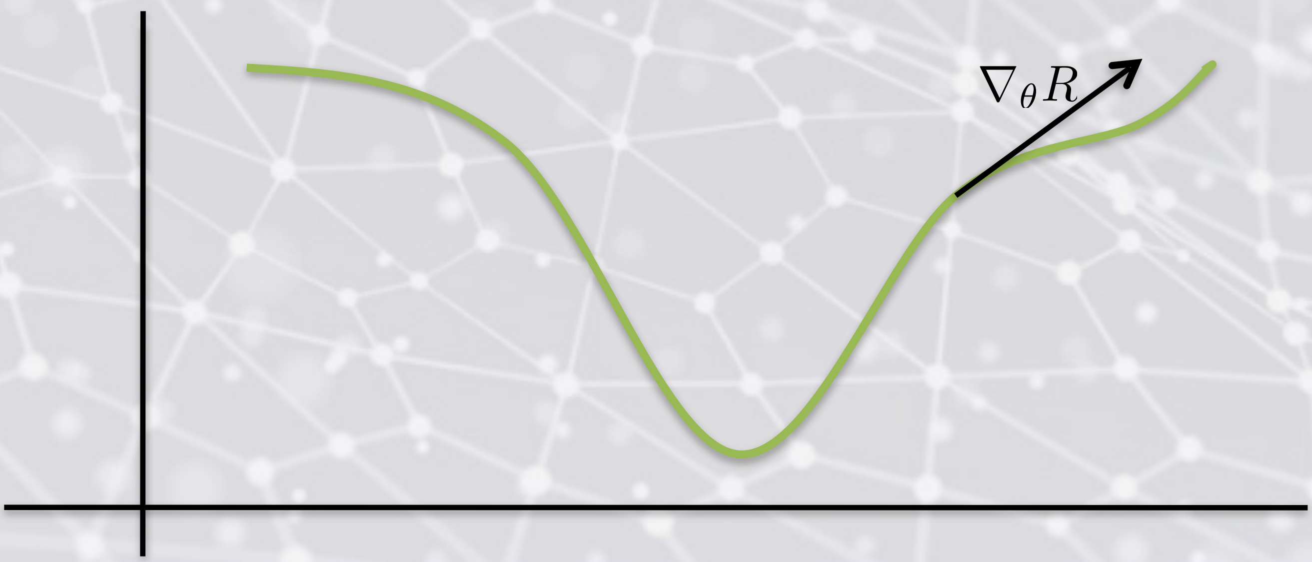


Gradient Descent

- The Gradient is defined (though we can't solve directly)

$$\nabla_\theta R = \frac{1}{2N}\sum_{i=0}^{N-1} 2(t_i - g(\theta^T x_i))(-1)g'(\theta^T x_i)x_i = 0$$

- Points in the direction of fastest increase

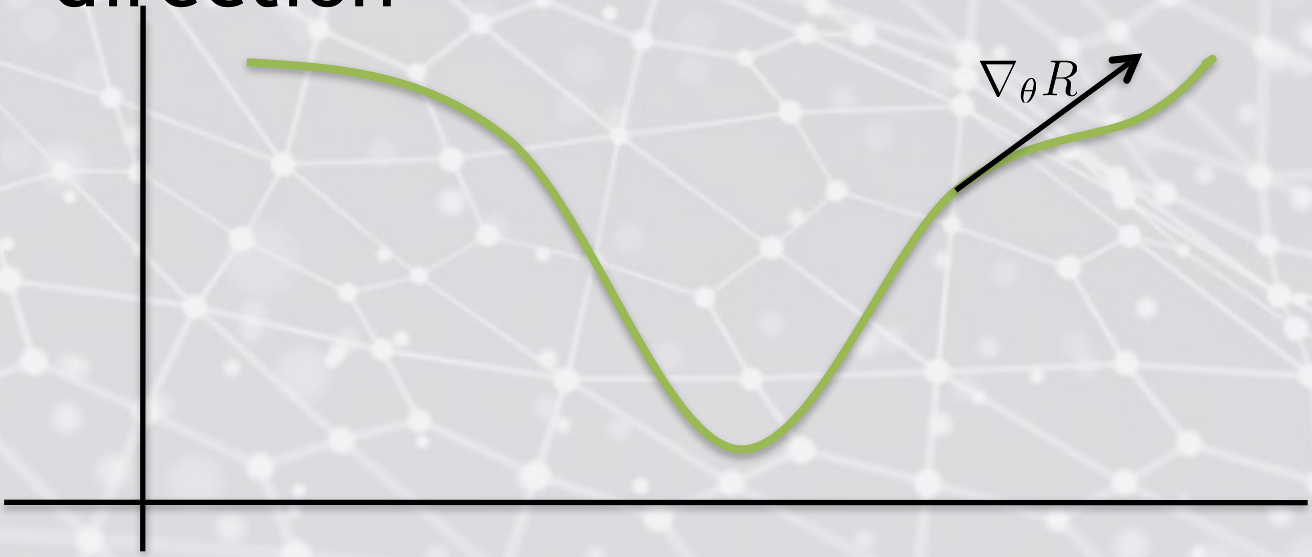


Gradient Descent

- Gradient points in the direction of fastest increase

$$\nabla_\theta R = \frac{1}{2N}\sum_{i=0}^{N-1} 2(t_i - g(\theta^T x_i))(-1)g'(\theta^T x_i)x_i = 0$$

- To minimize R, move in the opposite direction



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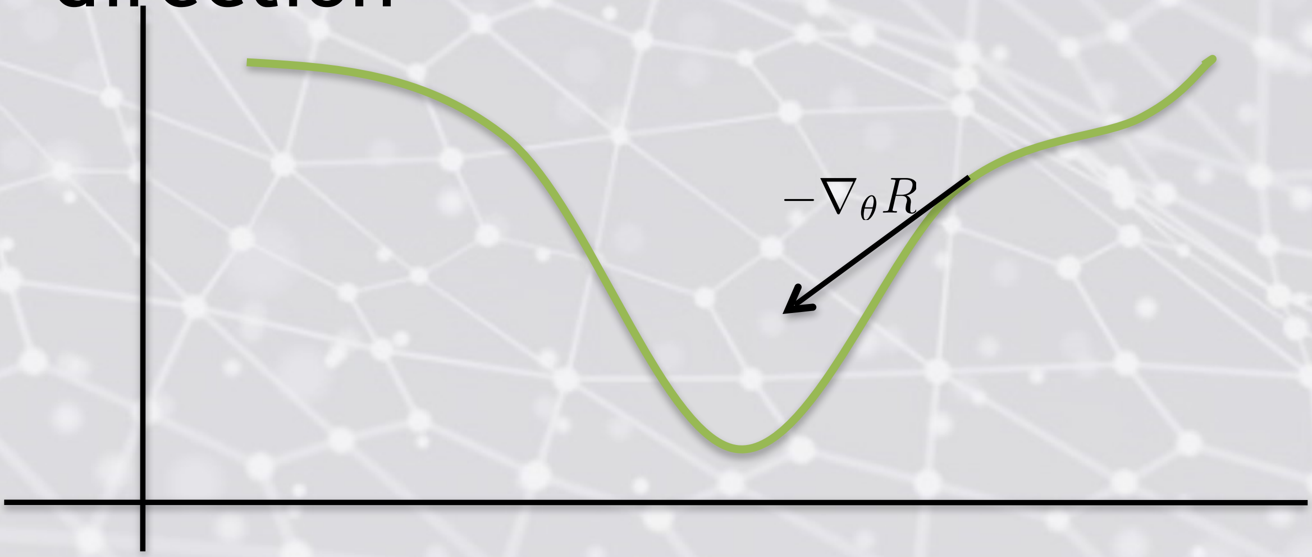
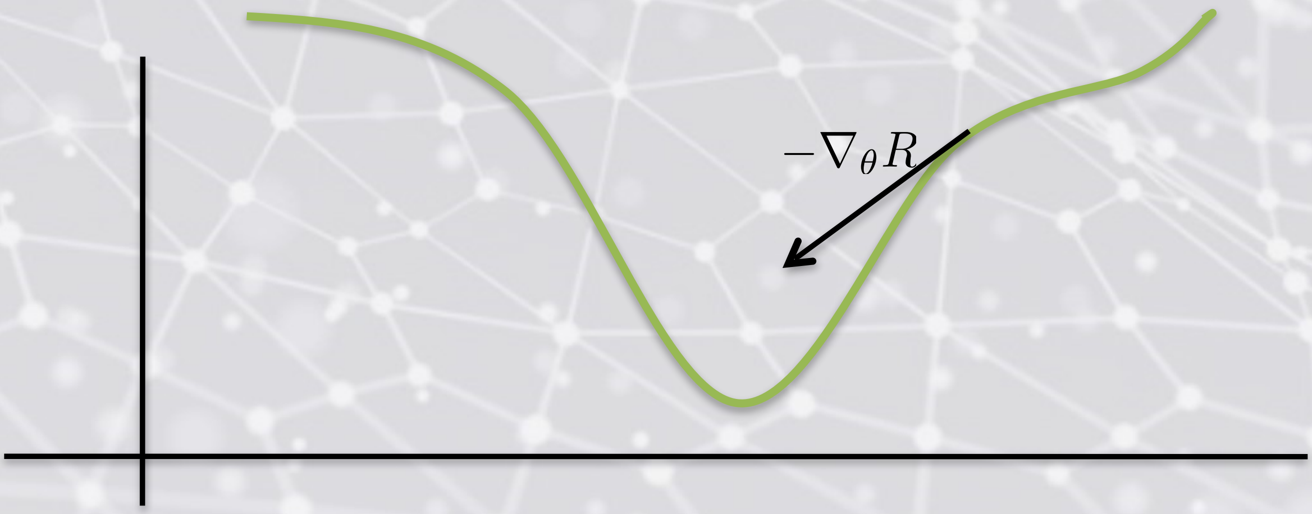


Gradient Descent

- Initialize Randomly $\theta_0 = random$
- Update with small steps $\theta_{t+1} = \theta_t - \eta \nabla_\theta R|_{\theta_t}$
- (nearly) guaranteed to converge to the minimum



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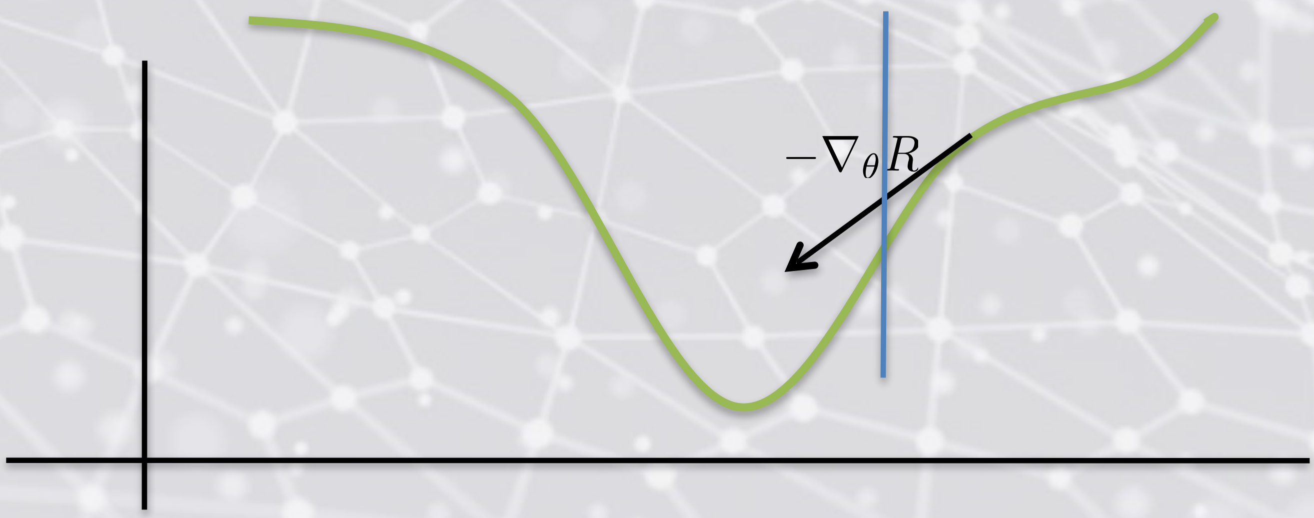

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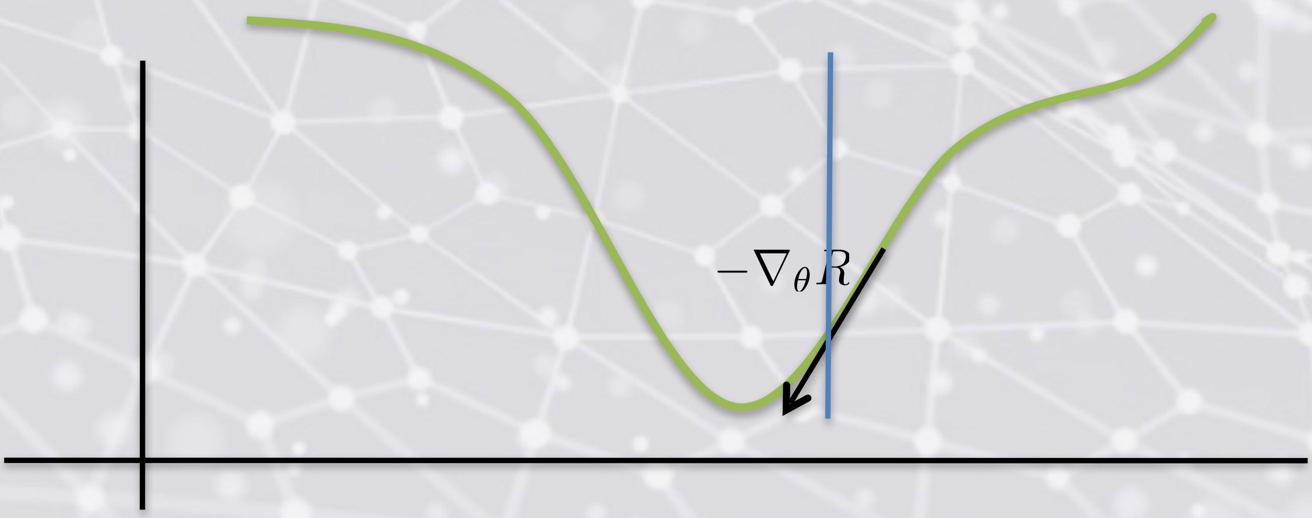

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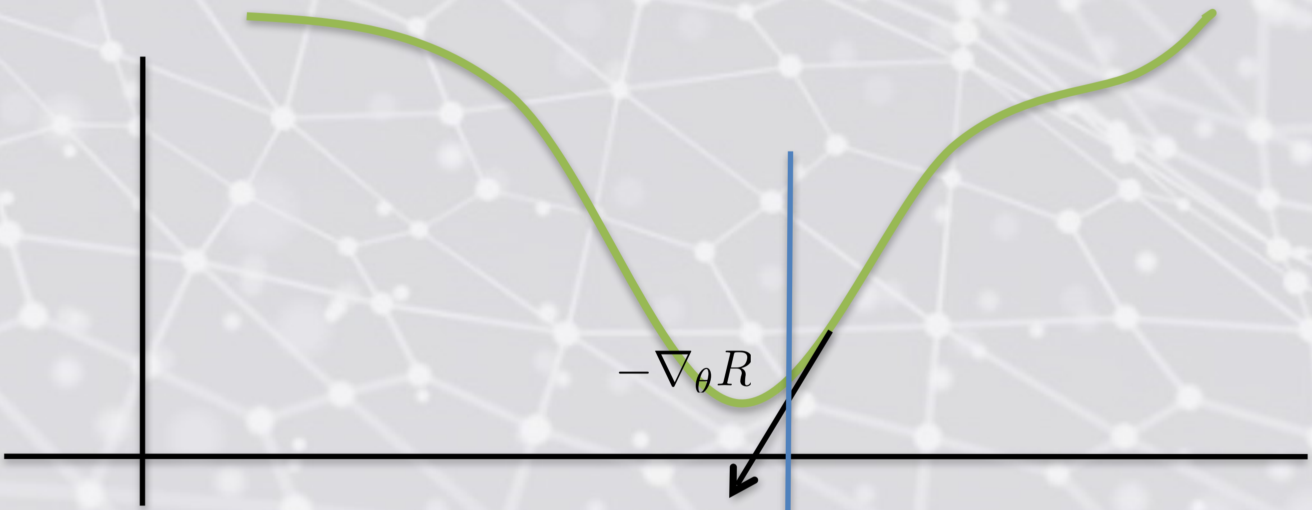

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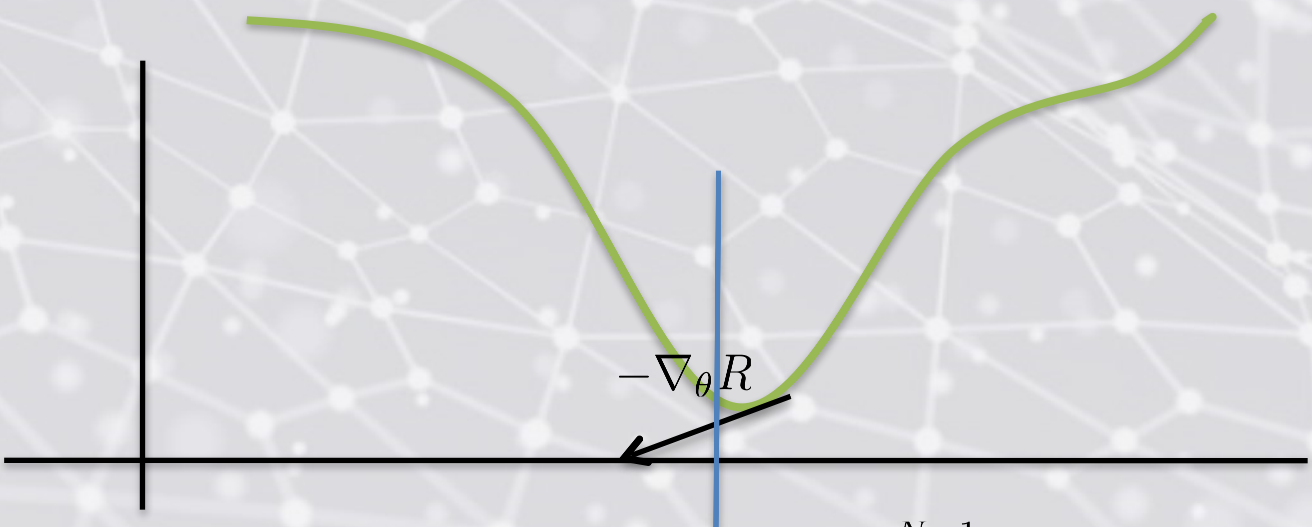

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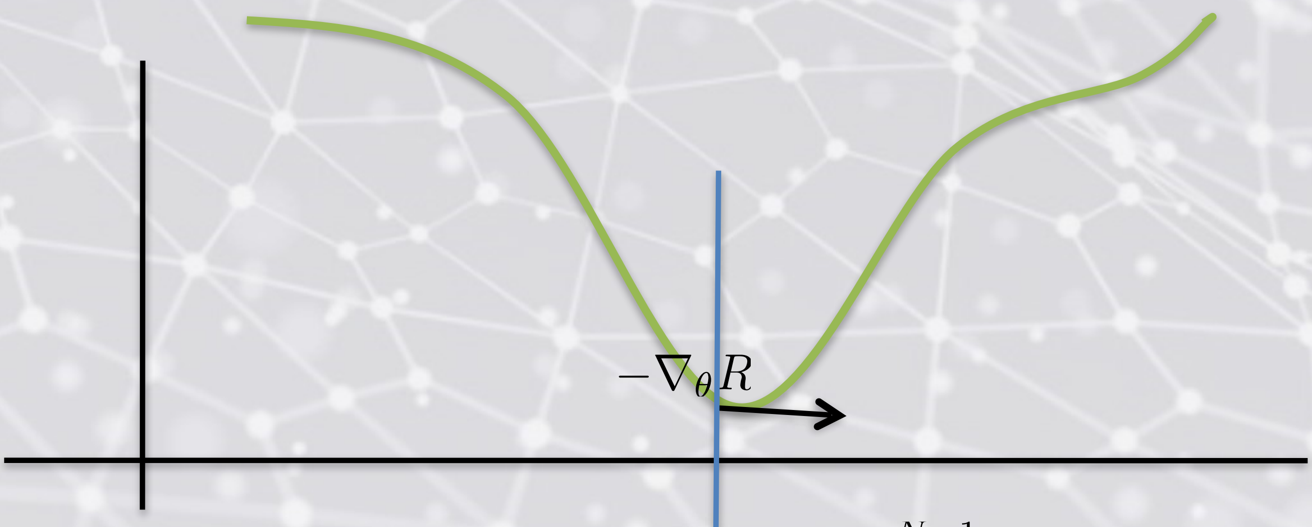

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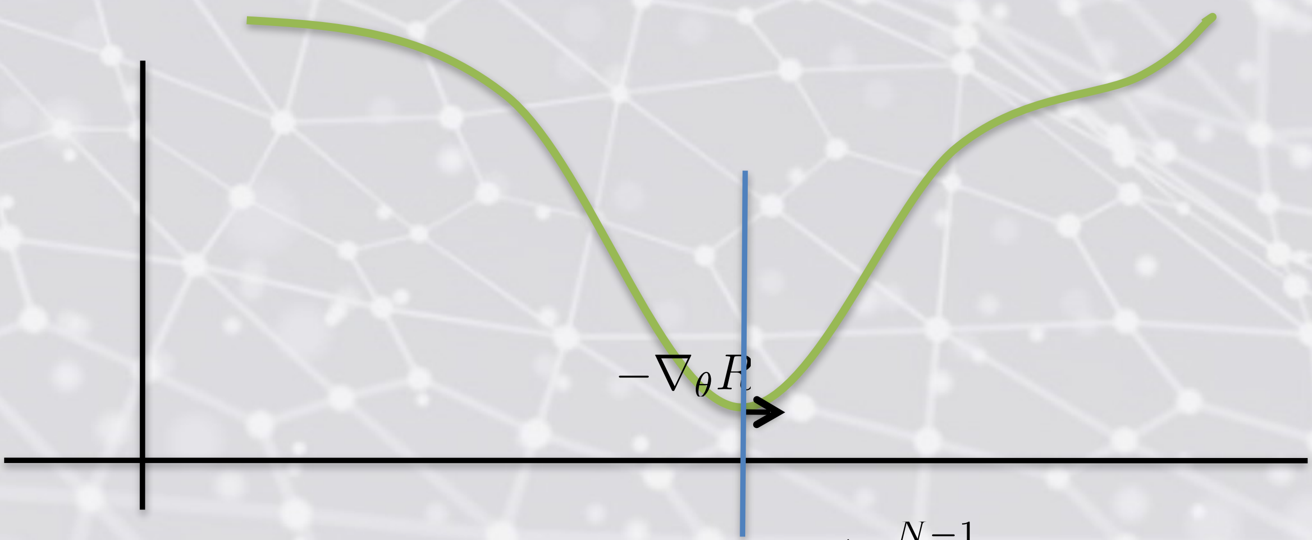

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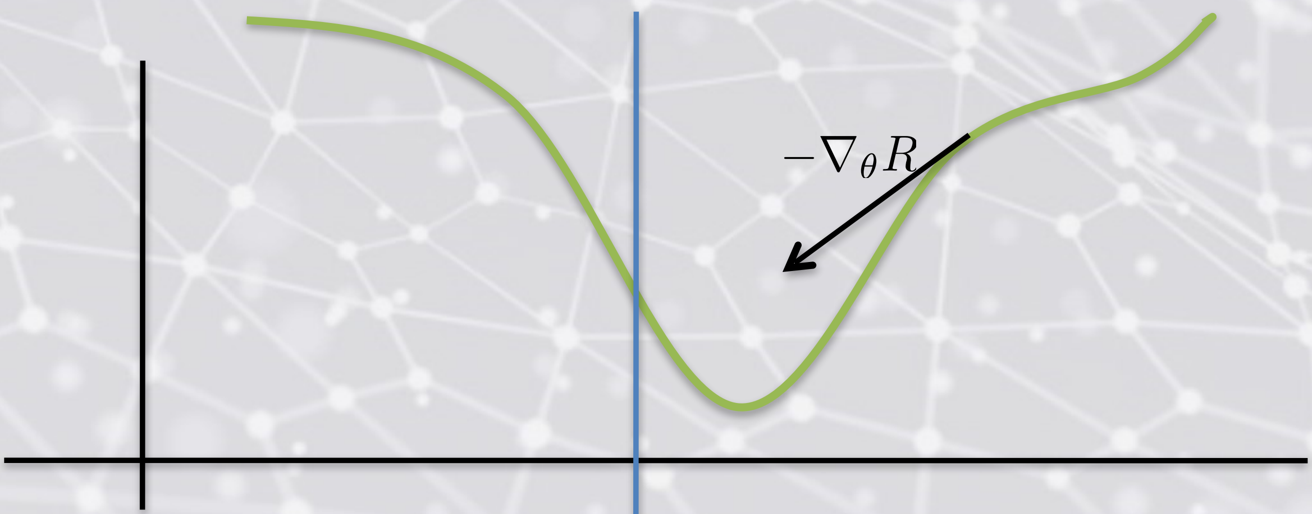
Gradient Descent

- Initialize Randomly $\theta_0 = random$
- Update with small steps $\theta_{t+1} = \theta_t - \eta \nabla_\theta R|_{\theta_t}$
- Can oscillate if η is too large



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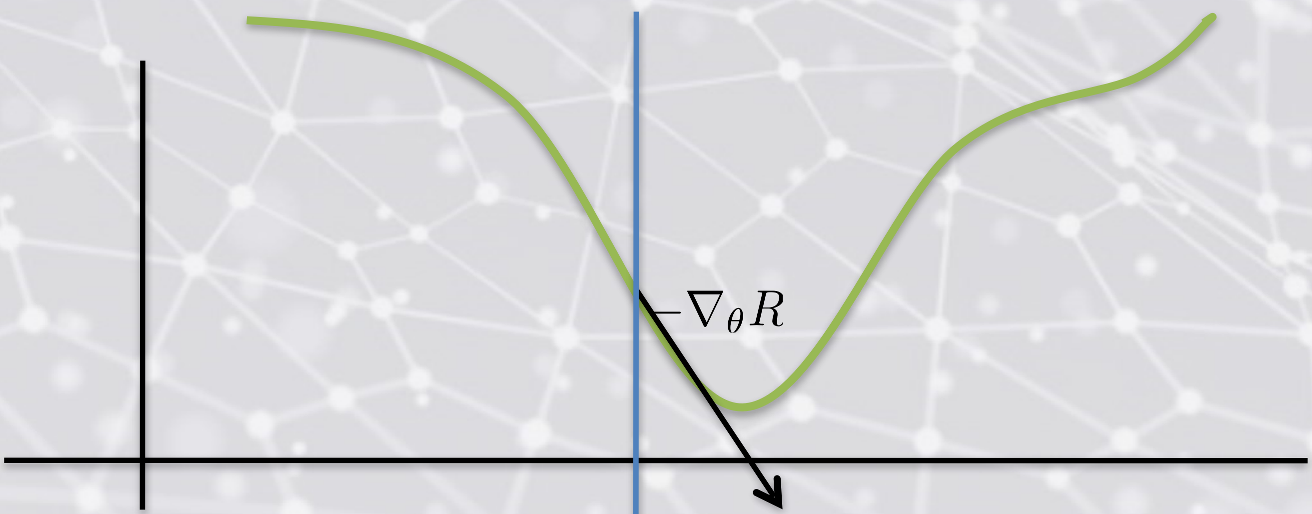

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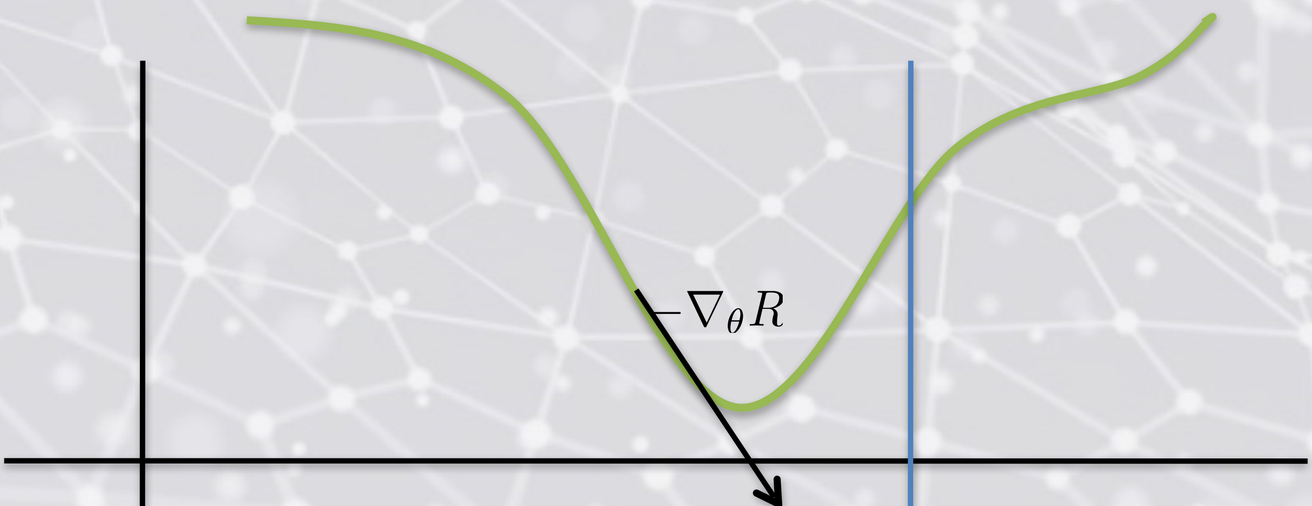

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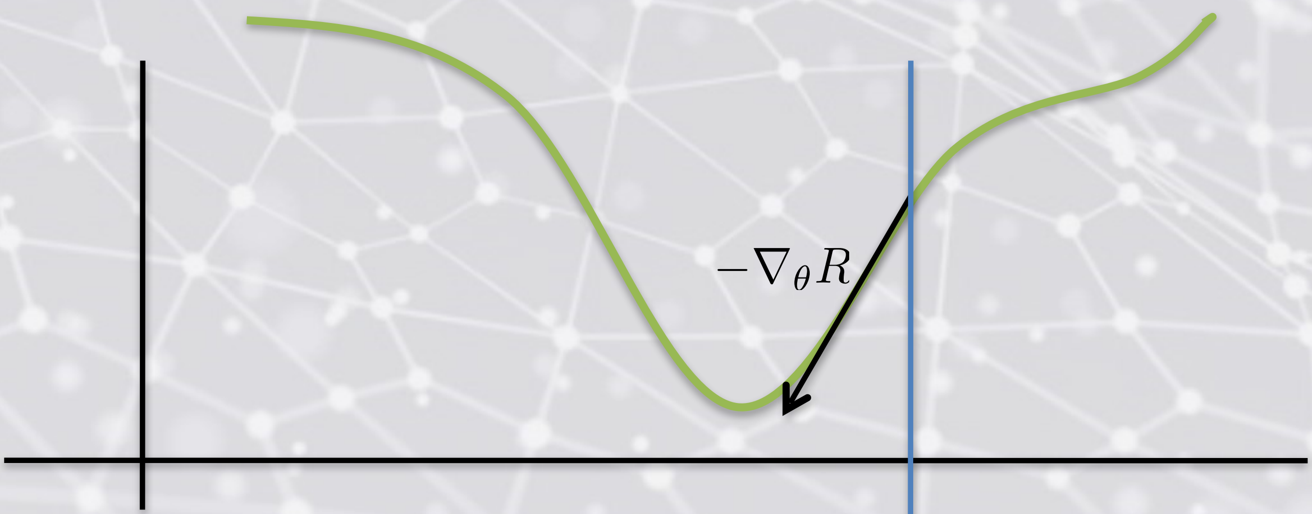

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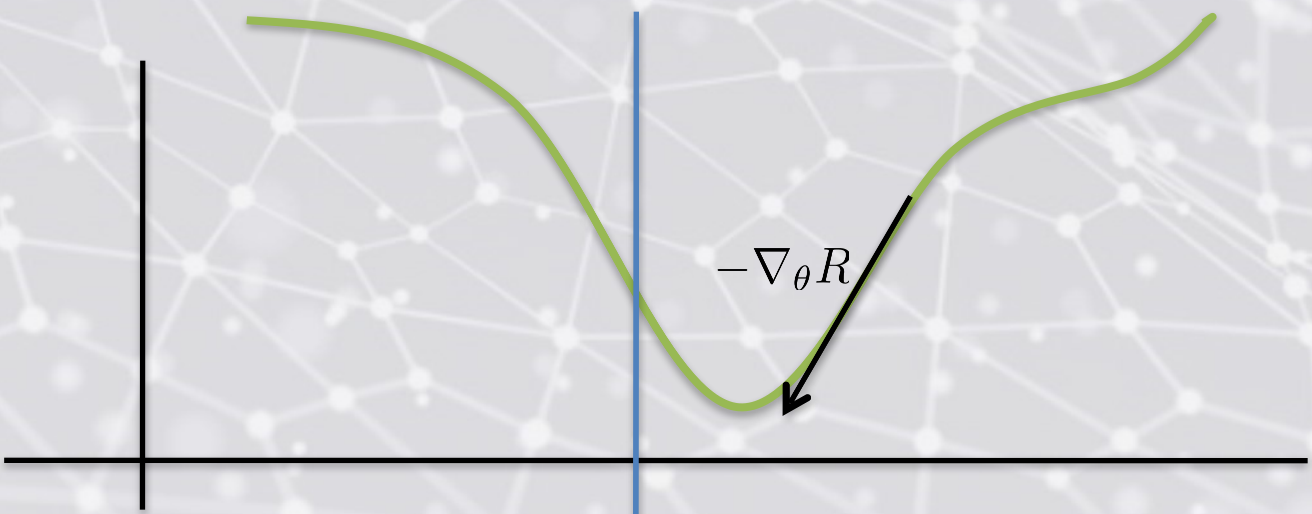

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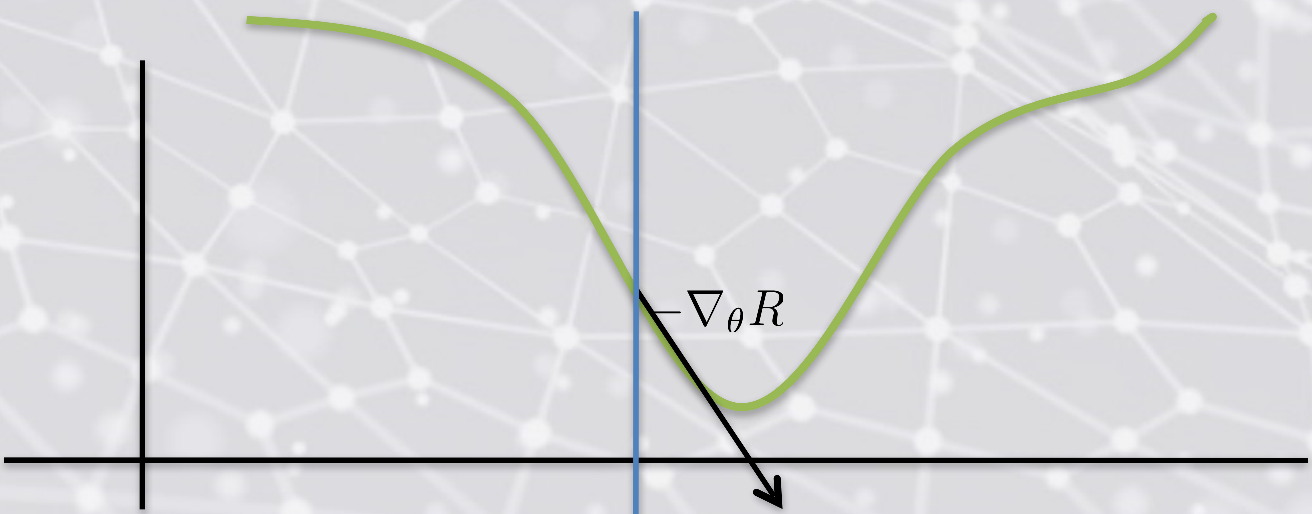

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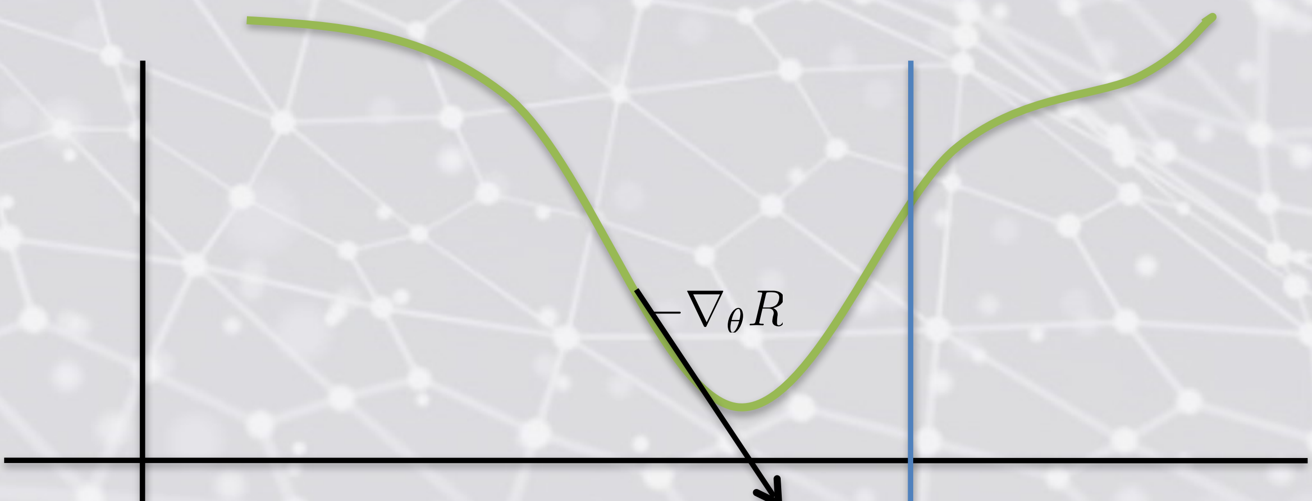

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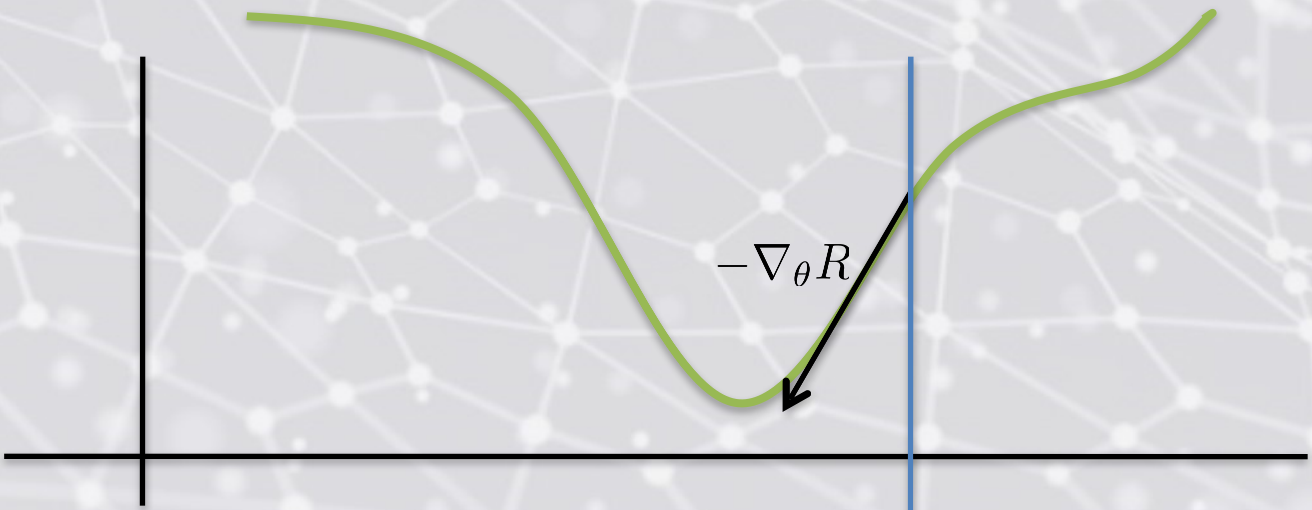

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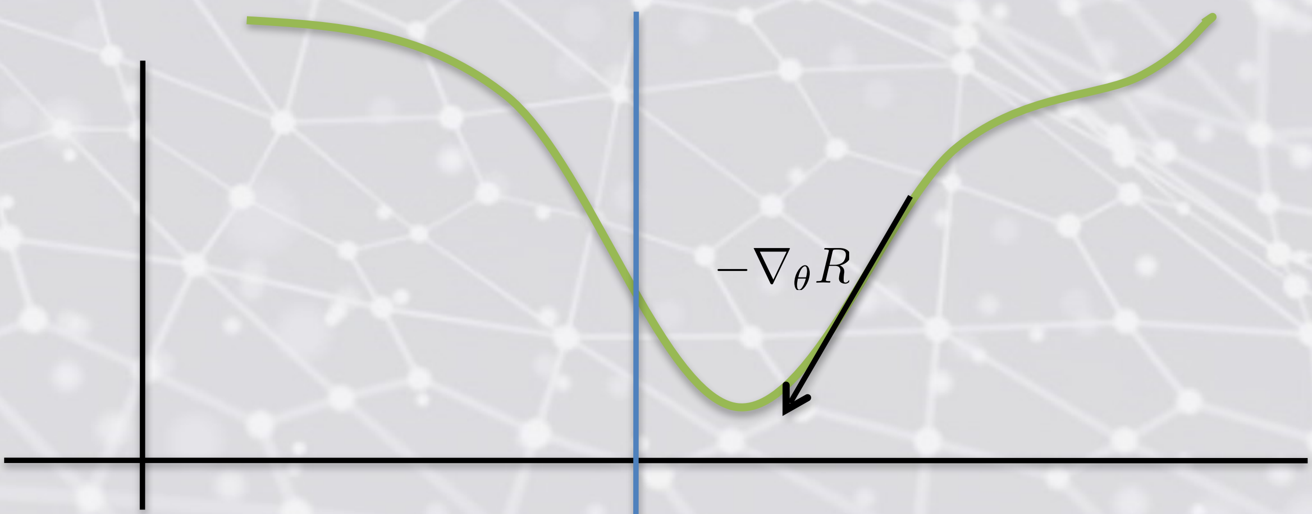

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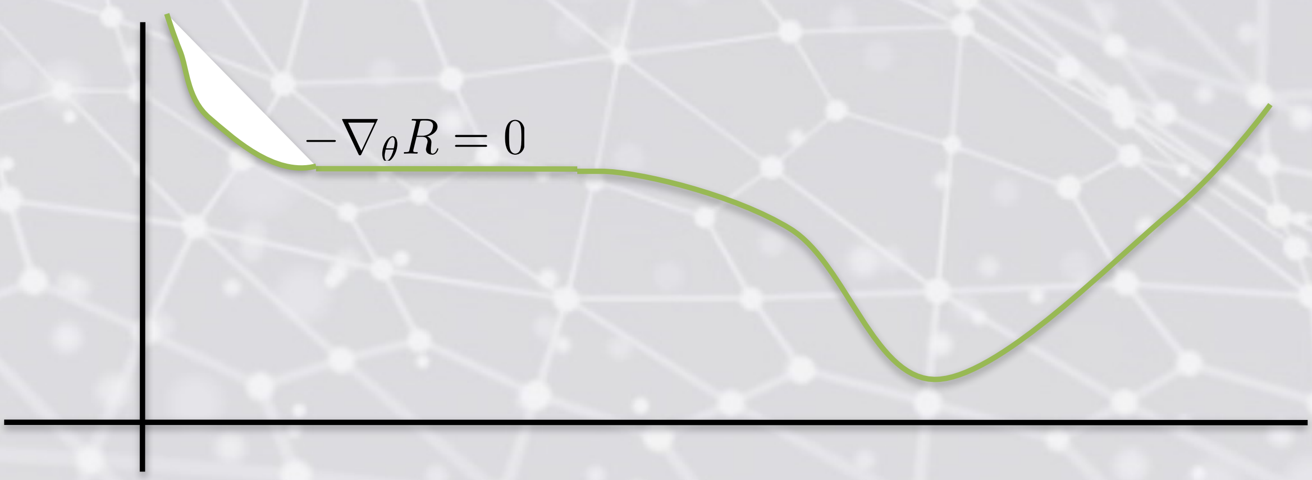
Gradient Descent

- Initialize Randomly $\theta_0 = random$
- Update with small steps $\theta_{t+1} = \theta_t - \eta \nabla_\theta R|_{\theta_t}$
- Can stall if $\nabla_\theta R$ is ever 0 not at the minimum



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Perceptron Learning

- Find **w** that minimizes average "loss":

$$J(\mathbf{w}) = \frac{1}{M}\sum_{k=1}^{M} L(\mathbf{w}, \mathbf{x}^k, t^k)$$

where M is number of training examples and L is a "loss" function.

- Here, define the loss function as follows:

$$\text{Let } y = a(\mathbf{w}\cdot\mathbf{x})$$

$$L(\mathbf{w}, \mathbf{x}^k, t^k) = \frac{1}{2}\left(t^k - y\right)^2 \quad \text{"squared loss"}$$

How to solve this minimization problem? **Gradient descent.**

Gradient descent

- To find direction of steepest descent, take the derivative of $J(\mathbf{w})$ with respect to $\mathbf{w}$.

- A vector derivative is called a "gradient": $\nabla J(\mathbf{w})$

$$\nabla J(\mathbf{w}) = \left[\frac{\partial J}{\partial w_0}, \frac{\partial J}{\partial w_1}, \ldots, \frac{\partial J}{\partial w_n} \right]$$

- Here is how we change each weight:

For $i = 0$ to n:

$$w_i \leftarrow w_i + \Delta w_i$$

where

$$\Delta w_i = -\eta \frac{\partial J}{\partial w_i}$$

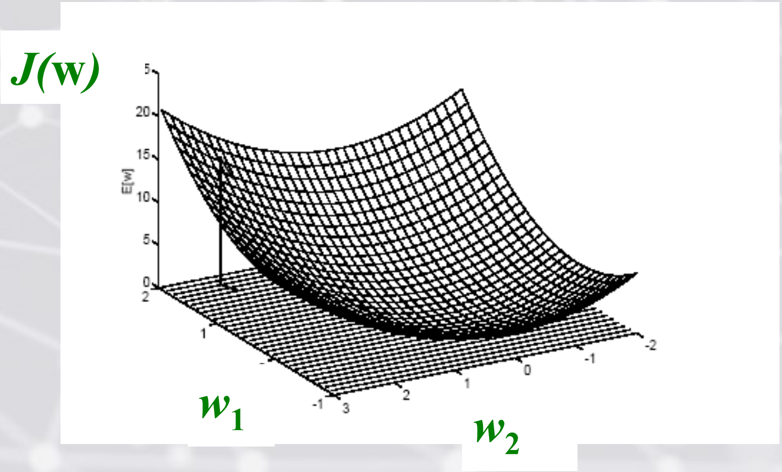
and η is the *learning rate* (i.e., size of step to take downhill).

"True" (or "batch") gradient descent

- One *epoch* = one iteration through the training data.
- After each epoch, compute average loss over the training set:

$$J(\mathbf{w}) = \frac{1}{M}\sum_{k=1}^{M} L(\mathbf{w}, \mathbf{x}^k, t^k) = \frac{1}{M}\sum_{k=1}^{M} \frac{1}{2}\left(t^k - y\right)^2$$

- Change the weights to move in direction of steepest descent in the average-loss surface:



From T. M. Mitchell, *Machine Learning*

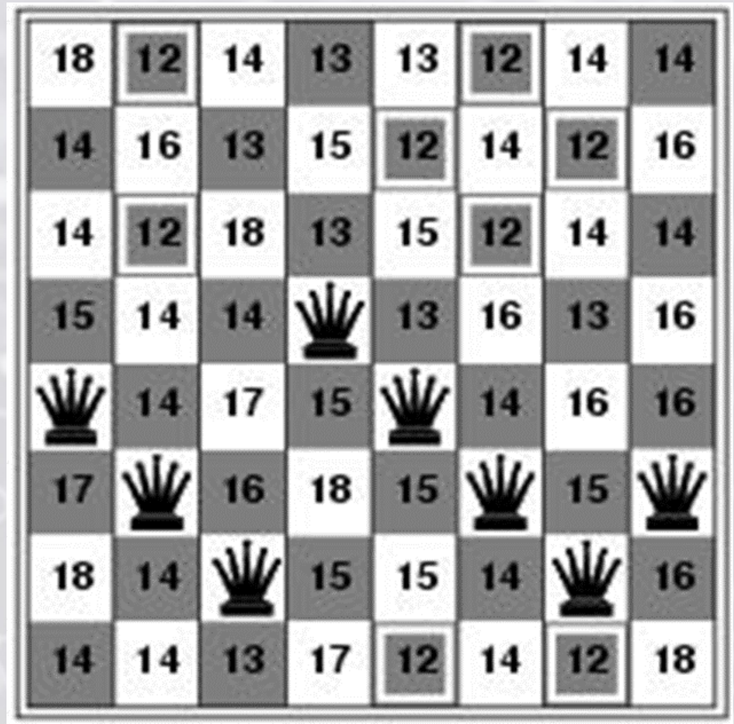
- Problem with ***true gradient descent***:

  Training process is slow.

  Training process can land in local optimum.

- Common approach to this: use ***stochastic gradient descent***:
  - Instead of doing weight update after all training examples have been processed, do weight update after each training example has been processed (i.e., perceptron output has been calculated).
  - Stochastic gradient descent approximates true gradient descent increasingly well as $\eta \rightarrow 1/\infty$.

Hill-Climbing (8-queens)

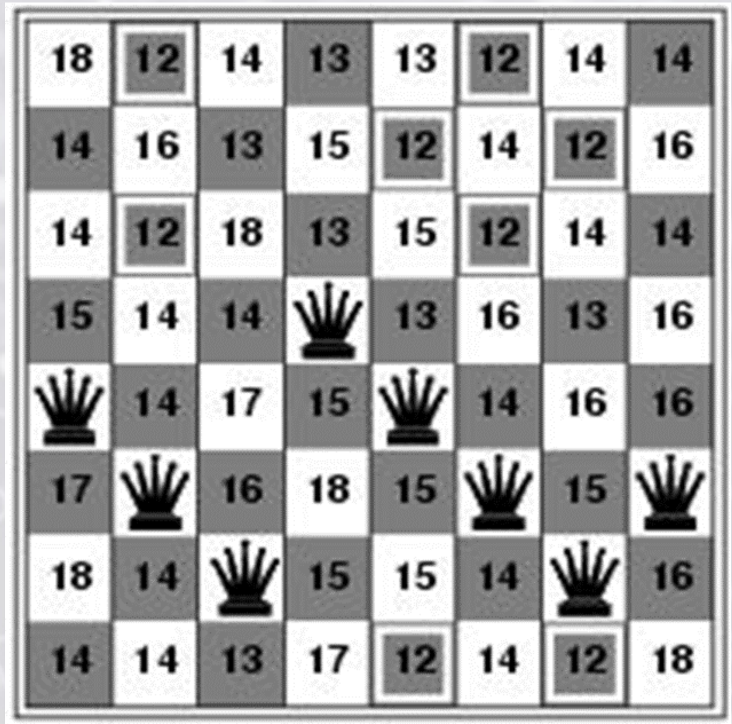


- Need to convert to an optimization problem!

Hill-Climbing (8-queens)

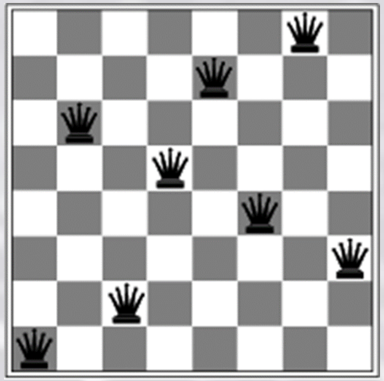
- State
  - All 8 queens on the board in some configuration
- Successor function
  - move a single queen to another square in the same column.
- Example of a heuristic function *h(n)*:
  - the number of pairs of queens that are attacking each other
  - (so we want to minimize this)

Hill-Climbing (8-queens)



- h = number of pairs of queens that are attacking each other
- $h = 17$ for the above state

Hill-Climbing (8-queens)

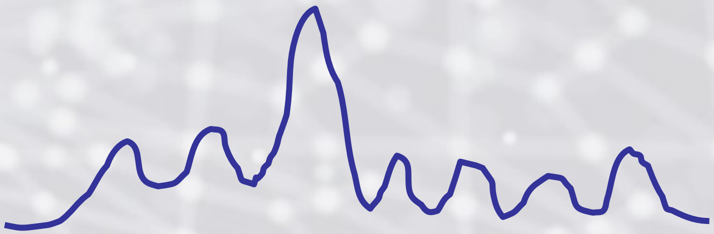


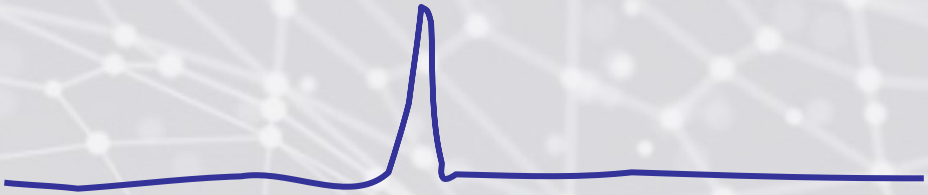
- Randomly generated 8-queens starting states…
- 14% the time it solves the problem
- 86% of the time it get stuck at a local minimum

- However…
  - Takes only 4 steps on average when it succeeds
  - And 3 on average when it gets stuck
  - (for a state space with 8^8 =~17 million states)

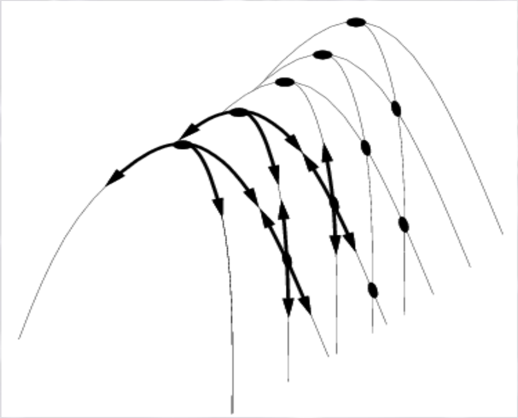
Hill Climbing Drawbacks

- Local maxima





- Plateaus



- Diagonal ridges

Escaping Shoulders: Sideways Move

- If no downhill (uphill) moves, allow sideways moves in hope that algorithm can escape
  - Need to place a limit on the possible number of sideways moves to avoid infinite loops
- For 8-queens
  - Now allow sideways moves with a limit of 100
  - Raises percentage of problem instances solved from 14 to 94%
  - However….
    - 21 steps for every successful solution
    - 64 for each failure

Tabu Search

- Prevent returning quickly to the same state
- Keep fixed length queue ("tabu list")
- Add most recent state to queue; drop oldest
- Never make the step that is currently tabu'ed

- Properties:
  - As the size of the tabu list grows, hill-climbing will asymptotically become "non-redundant" (won't look at the same state twice)
  - In practice, a reasonable sized tabu list (say 100 or so) improves the performance of hill climbing in many problems

Escaping Shoulders/local Optima Enforced Hill Climbing

- Perform breadth first search from a local optima
  - to find the next state with better h function
- Typically,
  - prolonged periods of exhaustive search
  - bridged by relatively quick periods of hill-climbing
- Middle ground b/w local and systematic search

Hill-climbing: stochastic variations

- Stochastic hill-climbing
  - Random selection among the uphill moves.
  - The selection probability can vary with the steepness of the uphill move.

- To avoid getting stuck in local minima
  - Random-walk hill-climbing
  - Random-restart hill-climbing
  - Hill-climbing with both

Hill Climbing: stochastic variations

→When the state-space landscape has local minima, any search that moves only in the greedy direction cannot be complete

→Random walk, on the other hand, is asymptotically complete

Idea: Put random walk into greedy hill-climbing

Hill-climbing with random restarts

- If at first you don't succeed, try, try again!
- Different variations
  - For each restart: run until termination vs. run for a fixed time
  - Run a fixed number of restarts or run indefinitely
- Analysis
  - Say each search has probability p of success
    - E.g., for 8-queens, $p = 0.14$ with no sideways moves
  - Expected number of restarts?
  - Expected number of steps taken?
- If you want to pick one local search algorithm, learn this one!!

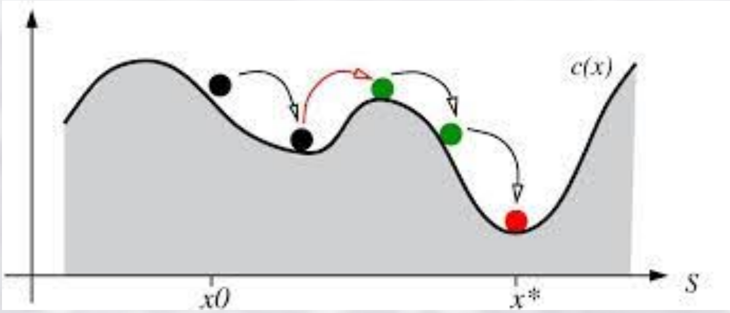
Hill-climbing with random walk

- At each step do one of the two
  - Greedy: With prob p move to the neighbor with largest value
  - Random: With prob 1-p move to a random neighbor

Hill-climbing with both

- At each step do one of the three
  - Greedy: move to the neighbor with largest value
  - Random Walk: move to a random neighbor
  - Random Restart: Resample a new current state

Simulated Annealing



- Simulated Annealing = physics inspired twist on random walk
- Basic ideas:
  - like hill-climbing identify the quality of the local improvements
  - instead of picking the best move, pick one randomly
  - say the change in objective function is d
  - if d is positive, then move to that state
  - otherwise:
    - move to this state with probability proportional to d
    - thus: worse moves (very large negative d) are executed less often
  - however, there is always a chance of escaping from local maxima
  - over time, make it less likely to accept locally bad moves
  - (Can also make the size of the move random as well, i.e., allow “large” steps in state space)

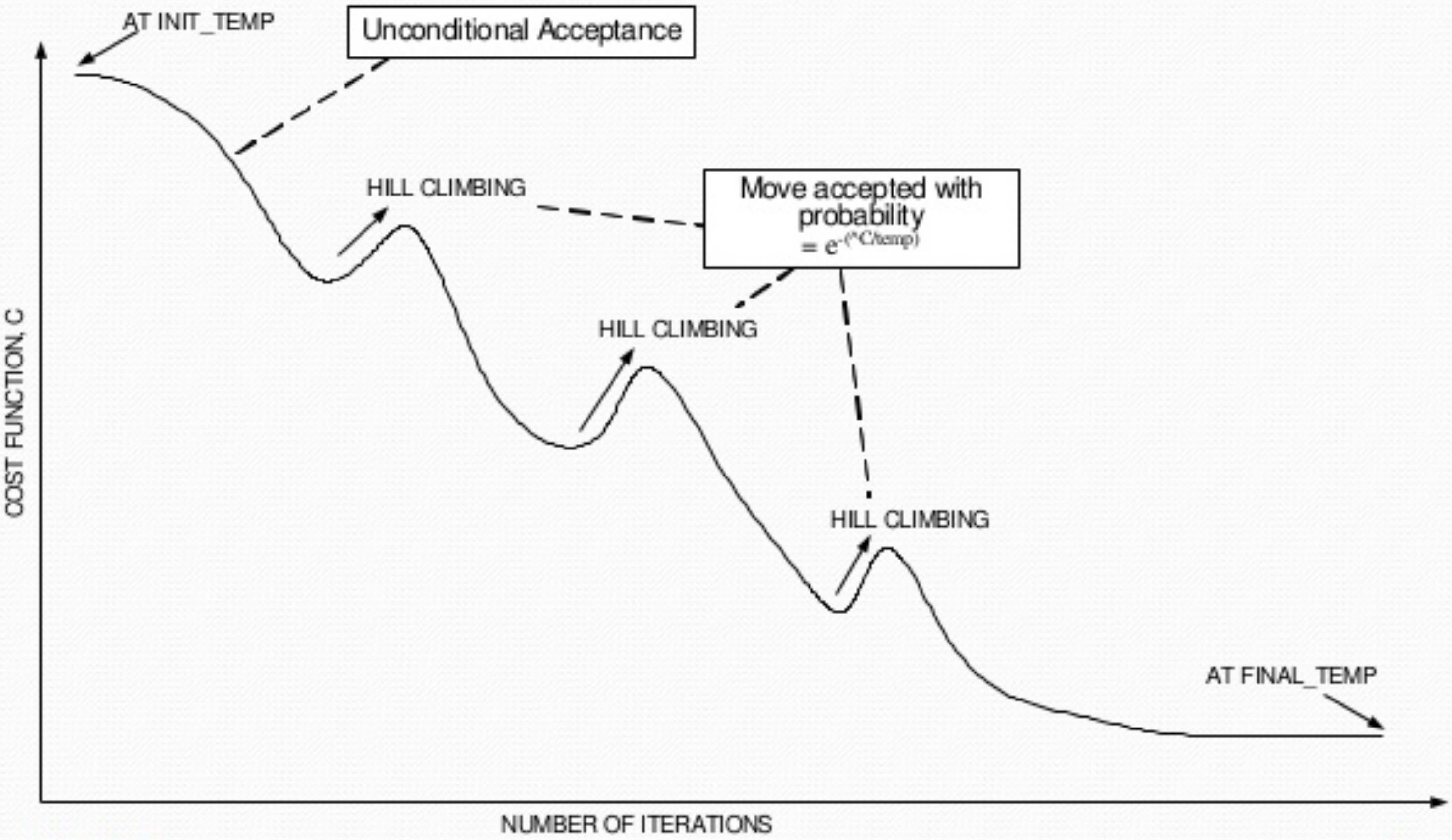
Physical Interpretation of Simulated Annealing

- A Physical Analogy:
    - imagine letting a ball roll downhill on the function surface
        - this is like hill-climbing (for minimization)
    - now imagine shaking the surface, while the ball rolls, gradually reducing the amount of shaking
        - this is like simulated annealing

- Annealing = physical process of cooling a liquid or metal until particles achieve a certain frozen crystal state
    - simulated annealing:
        - free variables are like particles
        - seek "low energy" (high quality) configuration
        - slowly reducing temp. T with particles moving around randomly

Simulated Annealing

Convergence of simulated annealing



Simulated annealing

function SIMULATED-ANNEALING(*problem, schedule*) **return** a solution state
  input: *problem*, a problem
    schedule, a mapping from time to temperature
  local variables: *current***,** a node.
      *next***,** a node.
      *T***,** a “temperature” controlling the prob. of downward steps

  current ← MAKE-NODE(INITIAL-STATE[*problem*])
  for t ← 1 to ∞ do
    T ← *schedule*[*t*]
    if *T = 0* **then return** *current*
    next ← a randomly selected successor of *current*
    ΔE ← VALUE[*next*] - VALUE[*current*]
    if $\Delta E > 0$ **then** *current* ← *next*
    else *current* ← *next* only with probability $e^{\Delta E / T}$

Temperature T

- High T: probability of "locally bad" move is higher.
- Low T: probability of "locally bad" move is lower.
- Typically, T is decreased as the algorithm runs longer, i.e., there is a "temperature schedule".

- In statistical mechanics, the **Boltzmann distribution** is a probability distribution that gives the probability of a certain state as a function of that state's energy and temperature of the system to which the distribution is applied. It is given as:

$$p_i = \frac{e^{-\varepsilon_i / kT}}{\sum_{j=1}^{M} e^{-\varepsilon_j / kT}}$$

Simulated Annealing in Practice

- method proposed in 1983 by IBM researchers for solving VLSI layout problems (Kirkpatrick et al, *Science*, 220:671-680, 1983).
  - theoretically will always find the global optimum

- Other applications: Traveling salesman, Graph partitioning, Graph coloring, Scheduling, Facility Layout, Image Processing, …

- useful for some problems, but can be very slow
  - slowness comes about because T must be decreased very gradually to retain optimality

Local beam search

- Idea: Keeping only one node in memory is an extreme reaction to memory problems.

- Keep track of *k* states instead of one
  - Initially: *k* randomly selected states
  - Next: determine all successors of *k* states
  - If any of successors is goal → finished
  - Else select *k* best from successors and repeat

Local Beam Search (contd)

- Not the same as *k random-start searches run in parallel!*
- Searches that find good states recruit other searches to join them

- Problem: quite often, all *k states end up on same local hill*
- Idea: Stochastic beam search
  - Choose *k successors randomly, biased towards good ones*

- Observe the close analogy to natural selection!

Genetic algorithms

- Twist on Local Search: successor is generated by combining two parent states

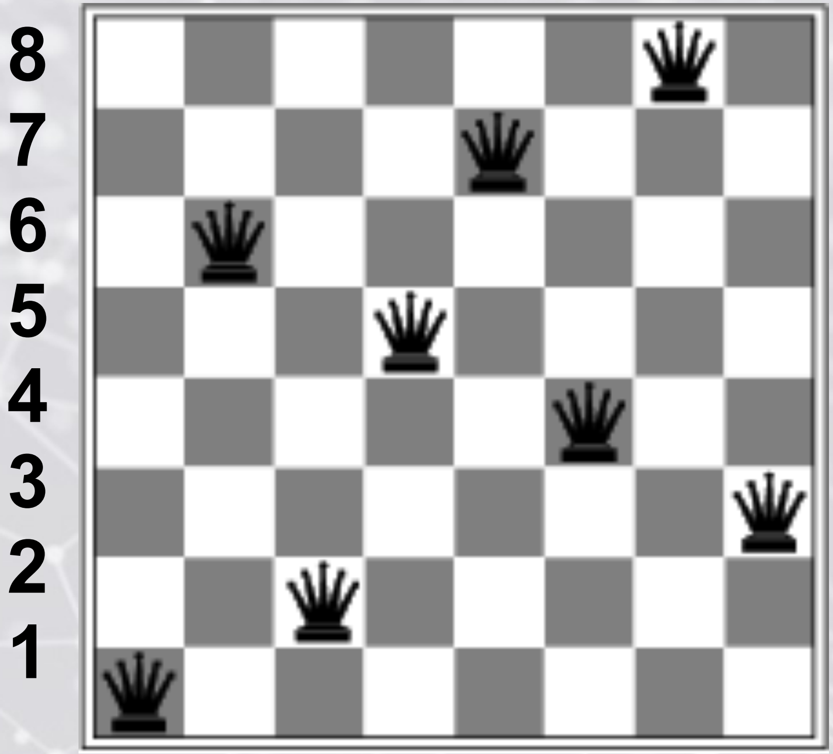
- A state is represented as a string over a finite alphabet (e.g. binary)
  - 8-queens
    - State = position of 8 queens each in a column

- Start with *k* randomly generated states (population)

- Evaluation function (fitness function):
  - Higher values for better states.
  - Opposite to heuristic function, e.g., # non-attacking pairs in 8-queens

- Produce the next generation of states by "simulated evolution"
  - Random selection
  - Crossover
  - Random mutation

Genetic algorithms & 8-queens



String representation
16257483

Can we evolve 8-queens through genetic algorithms?

Genetic algorithms

4 states for 8-queens problem

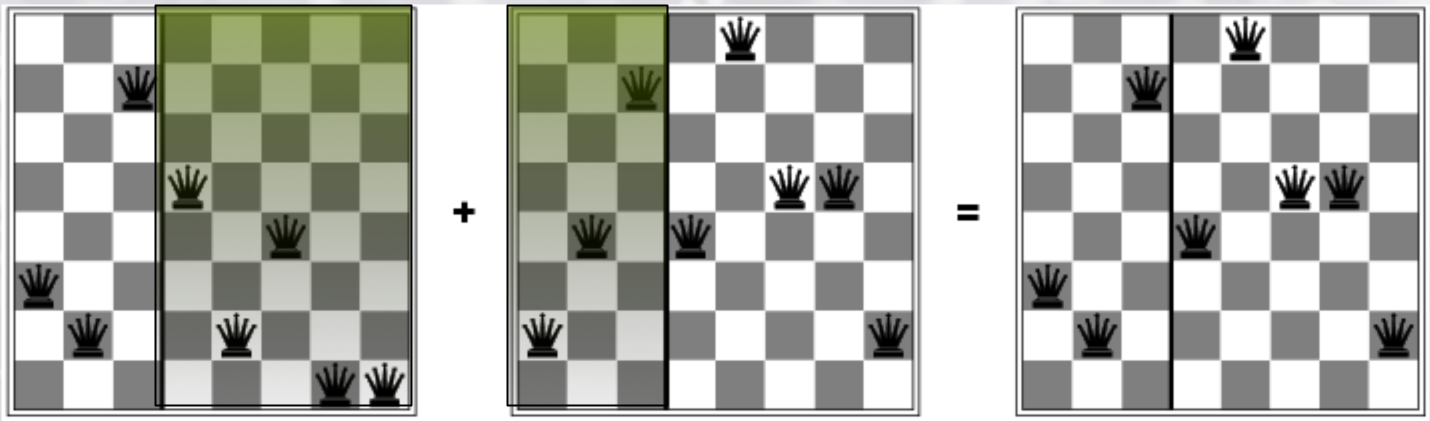
2 pairs of 2 states randomly selected based on fitness. Random crossover points selected

New states after crossover

Random mutation applied

- Fitness function: number of non-attacking pairs of queens (min = 0, max = $8 \times 7/2 = 28$)
- $24/(24+23+20+11) = 31\%$
- $23/(24+23+20+11) = 29\%$ etc

Genetic algorithms



Has the effect of "jumping" to a completely different new part of the search space (quite non-local)

Comments on Genetic Algorithms

- Genetic algorithm is a variant of "stochastic beam search"

- Positive points
  - Random exploration can find solutions that local search can't
    - (via crossover primarily)
  - Appealing connection to human evolution
    - "neural" networks, and "genetic" algorithms are **metaphors**!

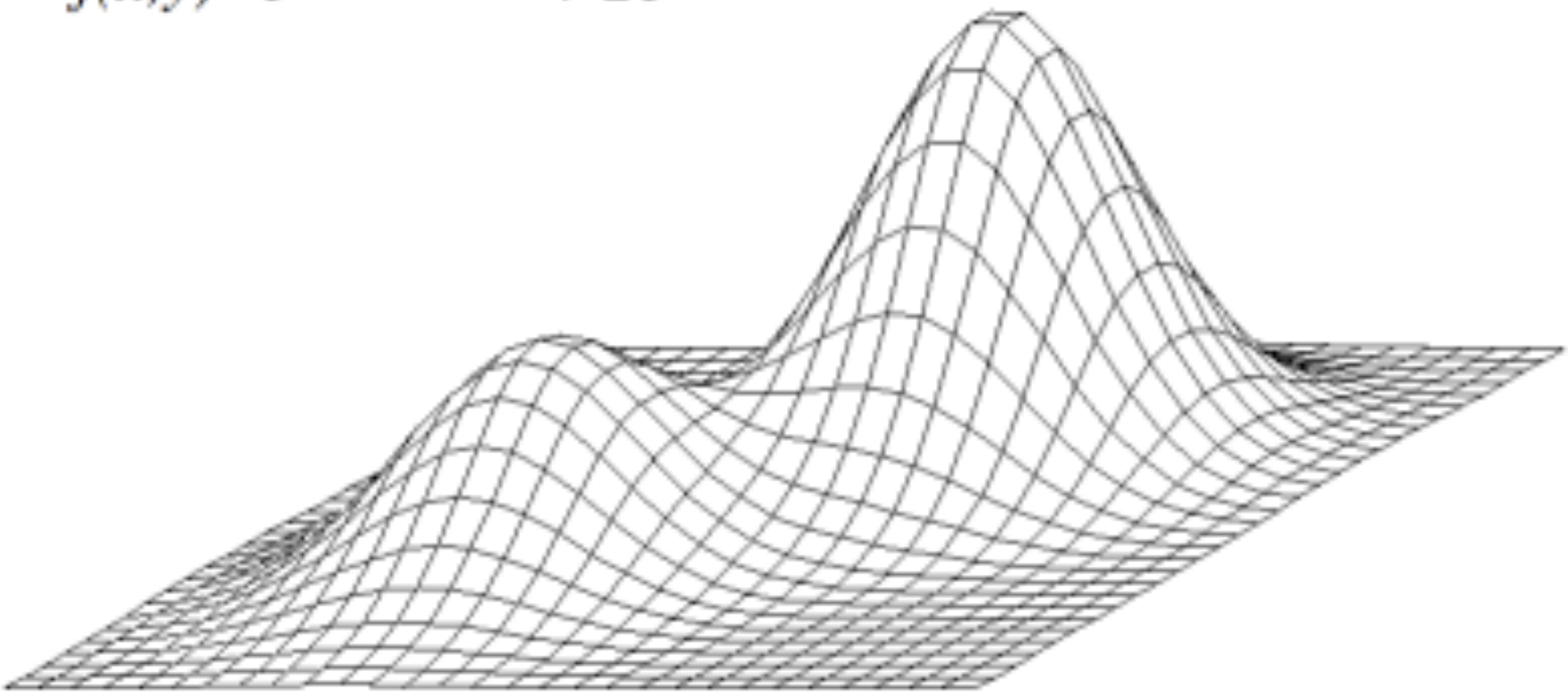
- Negative points
  - Large number of "tunable" parameters
    - Difficult to replicate performance from one problem to another
  - Lack of good empirical studies comparing to simpler methods
  - Useful on some (small?) set of problems but no convincing evidence that GAs are better than hill-climbing w/random restarts in general

Optimization of Continuous Functions

- Discretization
  - use hill-climbing
- Gradient descent
  - make a move in the direction of the gradient
    - gradients: closed form or empirical

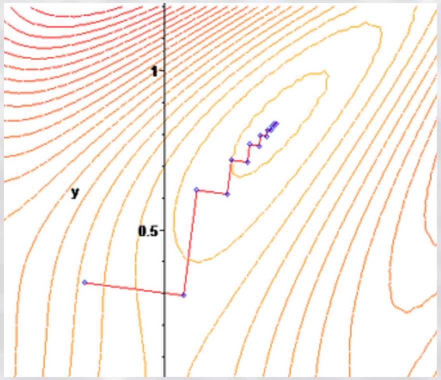
Objective Function in Continuous Search Space

$$f(x,y)=e^{-(x^2+y^2)} + 2e^{-((x-1.7)^2+(y-1.7)^2)}$$



Gradient Descent

Assume we have a continuous function: $f(x_1,x_2,\ldots,x_N)$
and we want minimize over continuous variables X1,X2,..,Xn



1. Compute the *gradients* for all *i*: $\partial f(x_1,x_2,\ldots,x_N) / \partial x_i$

2. Take a small step downhill in the direction of the gradient:

$$x_i \leftarrow x_i - \lambda \partial f(x_1,x_2,\ldots,x_N) / \partial x_i$$

3. Repeat.

- How to select λ
  - Line search: successively double
    - until *f* starts to increase again