Optimization

CE417: Introduction to Artificial Intelligence
Sharif University of Technology
Fall 2023

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Most slides have been adopted from J.Z. Kolter's slides, CMU 15-780 and some slides from CS188.

Local search in continuous spaces

Outline

- Introduction to optimization
- Convexity
- Gradient descent

Continuous optimization

- The problems we have seen so far (i.e., search) in class involve making decisions over a discrete space of choices
- An amazing property:

	Discrete search	(Convex) optimization
Variables	Discrete	Continuous
# Solutions	Finite	Infinite
Solution complexity	Exponential	Polynomial

- One of the most significant trends in AI in the past 15 years has been the integration of optimization methods throughout the field

Optimization definitions

- Optimization problems:

$$\min_{x} f(x)$$
$$\text{subject to } x \in \mathcal{C}$$

- It means that we want to find the value of x that achieves the smallest possible value of $f(x)$, out of all points in $\mathcal{C}$

- Important terms
  - $x \in \mathbb{R}^n$ – optimization variable(vector with n real-valued entries)
  - $f: \mathbb{R}^n \rightarrow \mathbb{R}$ – optimization objective
  - $\mathcal{C} \subseteq \mathbb{R}^n$ – constraint set
  - $x^* \equiv argmin\, f(x)$ – optimal objective
  - $f^* \equiv f(x^*) \equiv \min_{x \in \mathcal{C}} f(x)$ – optimal objective

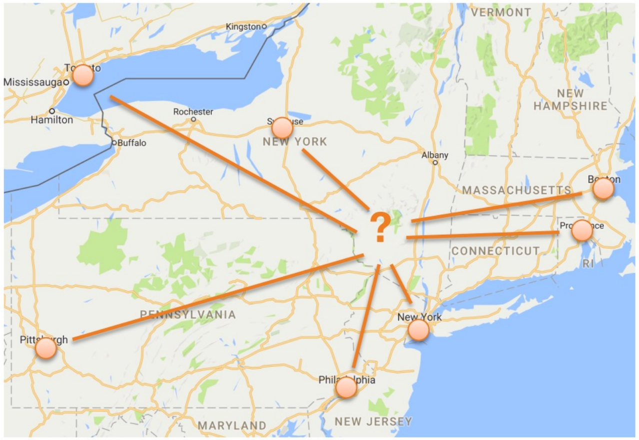
Handling a continuous state/action space

- Discretize it!!!
  - Define a grid with increment δ, use any of the discrete algorithms
- Choose random perturbations to the state
  - First-choice hill-climbing: keep trying until something improves the state
  - Simulated annealing
- Compute gradient of $f(\mathbf{x})$ analytically

Example: Weber point

- Given a collection of cities (assume on 2D plane) how can we find the location that minimizes the sum of distances to all cities?
- Denote the locations of the cities as $(x_1, y_1), \ldots, (x_C, y_C)$
- Write as the optimization problem:

$$\min_{(x,y)} \sum_{c=1}^{C} (x - x_c)^2 + (y - y_c)^2$$



How to solve?

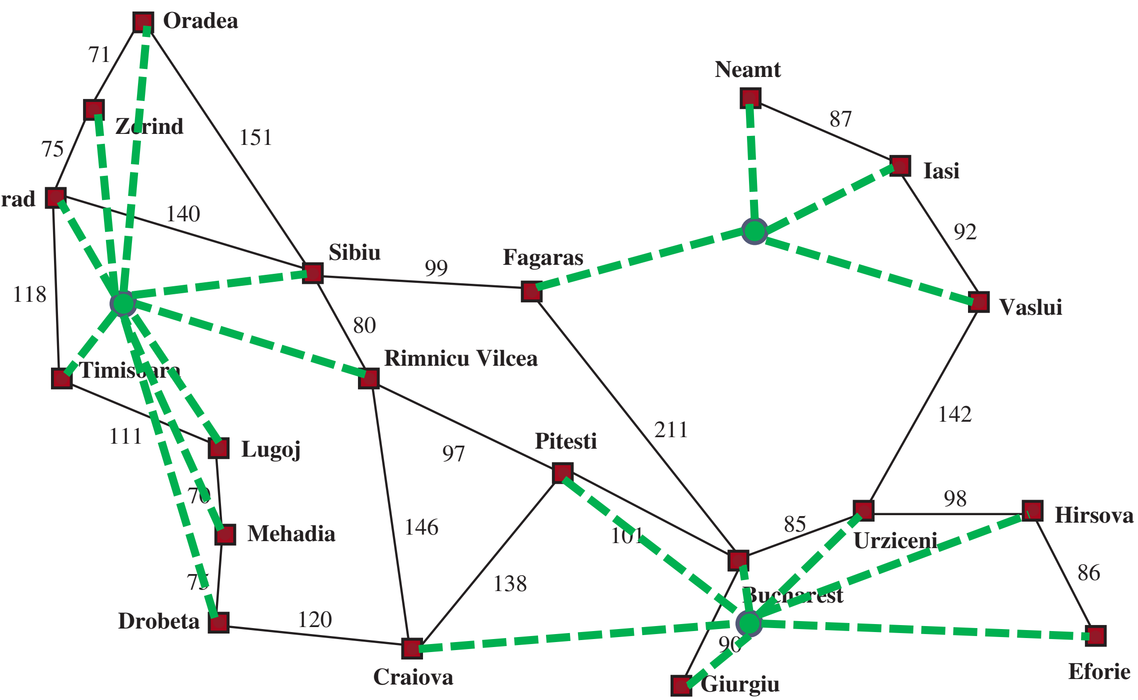
- $\nabla f = 0$ to find extremums
- only for simple cases

Example

- Select locations for 3 airports such that sum of squared distances from each city to its nearest airport is minimized
  - (x_1^a, y_1^a) , (x_2^a, y_2^a), (x_3^a, y_3^a)
  - $F(x_1^a, y_1^a, x_2^a, y_2^a, x_3^a, y_3^a) = \sum_{i=1}^{3} \sum_{c \in C_i} (x_i^a - x_c)^2 + (y_i^a - y_c)^2$

Example: Siting airports in Romania

Place 3 airports to minimize the sum of squared distances from each city to its nearest airport



Airport locations

$$x = (x_1^a, y_1^a), (x_2^a, y_2^a), (x_3^a, y_3^a)$$

City locations (x_c, y_c)

C_i = cities closest to airport *i*

Objective: minimize

$$f(\boldsymbol{x}) = \sum_{i=1}^{3} \sum_{c \in C_i} (x_i^a - x_c)^2 + (y_i^a - y_c)^2$$

Example: machine learning

- As we will see in much more detail shortly, virtually all (supervised) machine learning algorithms boil down to solving an optimization problem

$$\min_{\theta} \sum_{i=1}^{n} l(f_\theta(x^{(i)}), y^{(i)})$$

- $x^{(i)} \in \mathcal{X}$ are inputs
- $y^{(i)} \in \mathcal{Y}$ are outputs
- l is a loss function
- f_θ is a hypothesis function parameterized by θ, which are the parameters of the model we are optimizing over

Example: robot trajectory planning

- Many robotic planning tasks are more complex than shortest path, e.g. have robot dynamics, require "smooth" controls
- Common to formulate planning problem as an optimization task
- Robot state x_t and control inputs u_t

$$
\begin{aligned}
\underset{x_{1:T}, u_{1:T-1}}{\text{minimize}} \quad & \sum_{i=1}^{T} \|u_t\|_2^2 \\
\text{subject to} \quad & x_{t+1} = f_{\text{dynamics}}(x_t, u_t) \\
& x_t \in \text{FreeSpace}, \forall t \\
& x_1 = x_{\text{init}}, \; x_T = x_{\text{goal}}
\end{aligned}
$$

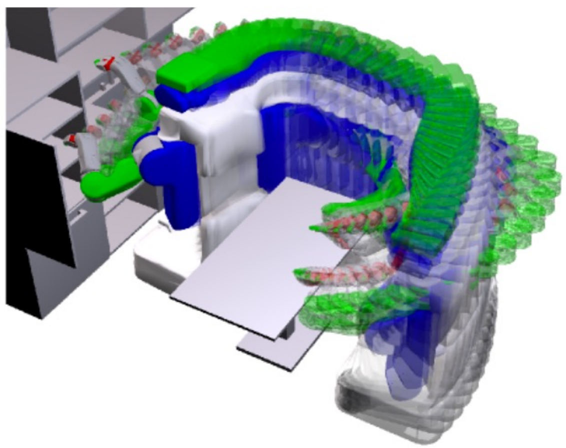
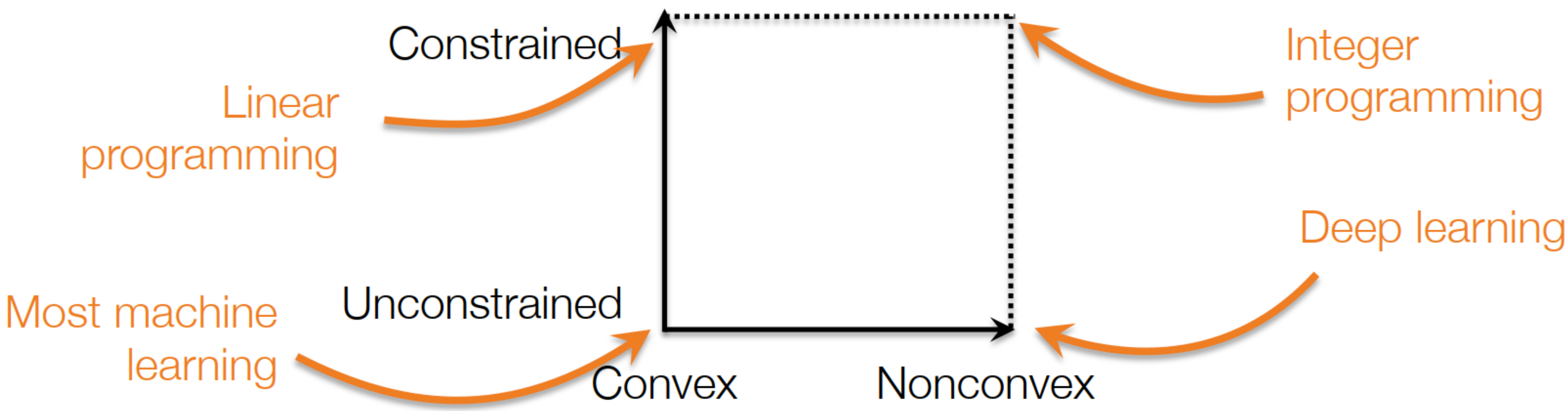


Figure from (Schulman et al., 2014)

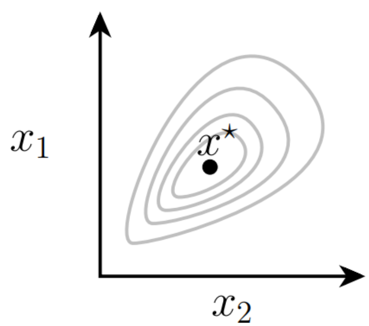
Classes of optimization problems

- Many different names for types of optimization problems: linear programming, quadratic programming, nonlinear programming, semidefinite programming, integer programming, geometric programming, mixed linear binary integer programming (the list goes on and on, can all get a bit confusing)
- We're instead going to focus on two dimensions: convex vs. nonconvex and constrained vs. unconstrained

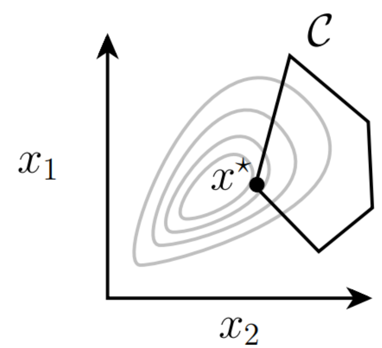


Constrained vs. unconstrained

- In unconstrained optimization, every point $x \in \mathbb{R}^n$ is feasible, so singular focus is on minimizing $f(x)$
- In contrast, for constrained optimization, may be hard to even find a point $x \in \mathcal{C}$
- Often leads to different methods for optimization

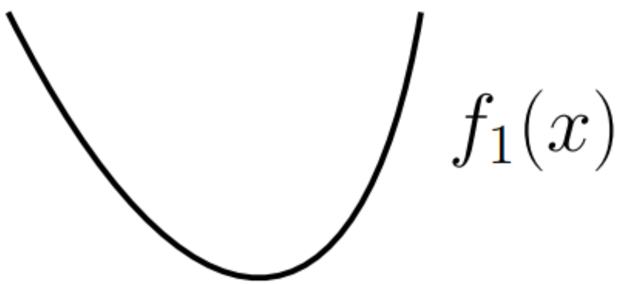


$$\underset{x}{\text{minimize}} \quad f(x)$$



$$\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to} & x \in \mathcal{C} \end{array}$$

Convex vs. nonconvex optimization



Convex function

Nonconvex function

Convex vs. nonconvex optimization

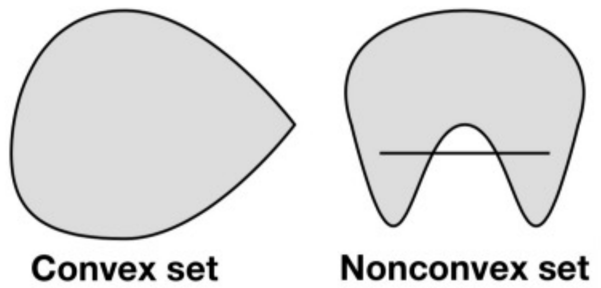
Convex function **Nonconvex function**

- Convex problem:

$$\min_{x} f(x)$$
$$\text{subject to } x \in \mathcal{C}$$

- Where f is a convex function and $\mathcal{C}$ is a convex set

Convex Sets



- A set $\mathcal{C}$ is convex if, for any $x, y \in \mathcal{C}$ and $0 \leq \theta \leq 1$:
  - $\theta x + (1 - \theta)y \in \mathcal{C}$

- Examples:
  - All points $\mathcal{C} = \mathbb{R}^n$
  - Intervals $C = \{x \in \mathbb{R}^n \mid l \leq x \leq u\}$ (elementwise inequality)
  - Linear equalities $C = \{x \in \mathbb{R}^n \mid Ax = \mathrm{b}\}$ (for $\mathrm{A} \in \mathbb{R}^{m*n}, b \in \mathbb{R}^m$)
  - Intersection of convex sets $C = \cap_{i=1}^{m} C_i$

Convex Functions

- A function $f\colon \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if, for any $x, y \in \mathbb{R}^n$ and $\theta \in [0,1]$:

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta)f(y)$$

- If f is convex then $-f$ is concave

- Convex functions "curve upwards" (or at least not downwards)

- f is affine if it is both convex and concave, must be of form:

$$f(x) = a^T x + b = \sum_{i=1}^{n} a_i x_i + b$$

for $a \in \mathbb{R}^n$, $b \in \mathbb{R}$

Examples of convex functions

- Exponential: $f(x) = \exp(ax), a \in \mathbb{R}$
- Negative logarithm: $f(x) = -\log x,\ with\ domain\ x > 0$
- Squared Euclidean norm: $f(x) = \|x\|_2^2 = x^T x = \sum_{i=1}^{n} x_i^2$
- Euclidean norm: $f(x) = \|x\|_2$
- Non-negative weighted sum of convex functions:

$$f(x) = \sum_{i=1}^{m} w_i f_i(x),\ w_i \geq 0,\ f_i\ convex$$

Poll: Convex sets and functions

Which of the following functions or sets are convex?

- A union of two convex sets $\mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2$
- The set $\{x \in \mathbb{R}^2 | x \geq 0, \; x_1 x_2 \geq 1\}$
- The function $f: \mathbb{R}^2 \rightarrow \mathbb{R}, f(x) = x_1 x_2$
- The function $f: \mathbb{R}^2 \rightarrow \mathbb{R}, f(x) = x_1^2 + x_2^2 + x_1 x_2$

Convex optimization

- The key aspect of convex optimization problems that make them tractable is that all local optima are global optima
- **Definition**: a point x is globally optimal (or global minimum) if x is feasible and there is no feasible y such that $f(y) < f(x)$
- **Definition**: a point x is locally optimal if x is feasible and there is some $R > 0$ such that for all feasible y with $\|x - y\|_2 \leq R, f(x) \leq f(y)$
- Theorem: for a convex optimization problem all locally optimal points are globally optimal

Proof of global optimality

Proof: Given a locally optimal x (with optimality radius R), and suppose there exists some feasible y such that $f(y) < f(x)$

Now consider the point

$$z = \theta x + (1-\theta) y, \qquad \theta = 1 - \frac{R}{2\|x-y\|_2}$$

1) Since $x, y \in \mathcal{C}$ (feasible set), we also have $z \in \mathcal{C}$ (by convexity of $\mathcal{C}$)

2) Furthermore, since f is convex:
$f(z) = f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y) < f(x)$
and $\|x - z\|_2 = \left\| x - \left(1 - \frac{R}{2\|x-y\|_2}\right) x + \frac{R}{2\|x-y\|_2} y \right\|_2 = \left\| \frac{R(x-y)}{2\|x-y\|_2} \right\|_2 = \frac{R}{2}$

Thus, z is feasible, within radius R of x, and has lower objective value, a contradiction of supposed local optimality of x ∎

The benefit of optimization

- One of the key benefits of looking at problems in AI as optimization problems: we separate out the definition of the problem from the method for solving it
- For many classes of problems, there are off-the-shelf solvers that will let you solve even large, complex problems, once you have put them in the right form

Optimization in practice

- We won't discuss this too much yet, but one of the beautiful properties of optimization problems is that there exists a wealth of tools that can solve them using very simple notation

- Example: solving Weber point problem using cvxpy (http://cvxpy.org)

```
import numpy as np
import cvxpy as cp

n,m = (5,10)
y = np.random.randn(n,m)
x = cp.Variable(n)
f = sum(cp.norm2(x - y[:,i]) for i in range(m))
cp.Problem(cp.Minimize(f), []).solve()
```

Outline

- Introduction to optimization
- Convexity
- Gradient descent (as an optimization method)

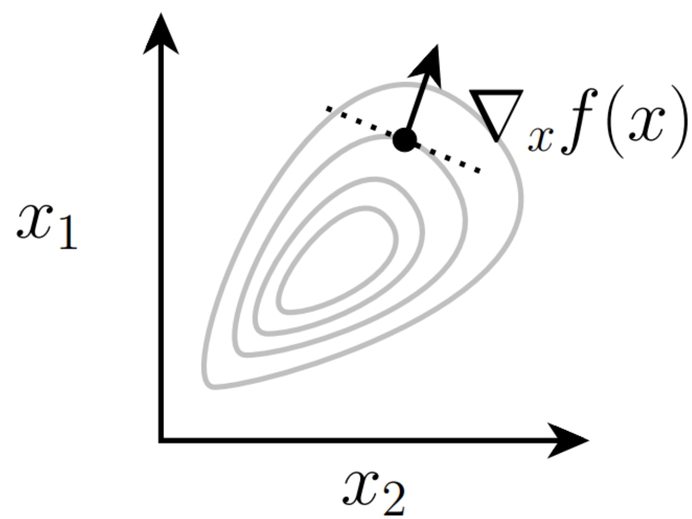
The gradient

- A key concept in solving optimization problems is the notation of the gradient of a function (multi-variate analogue of derivative)

- For $f\colon \mathbb{R}^n \rightarrow \mathbb{R}$, gradient is defined as vector of partial derivatives

- Points in "steepest direction" of increase in function f

$$\nabla_x f(x) \in \mathbb{R}^n = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$



Gradient descent

- Gradient motivates a simple algorithm for minimizing $f(x)$: take small steps in the direction of the negative gradient

- "Convergence" can be defined in a number of ways

Algorithm: Gradient Descent
Given:
Function f, initial point x_0, step size $\alpha > 0$
Initialize:
$x \leftarrow x_0$
Repeat until convergence:
$x \leftarrow x - \alpha \nabla_x f(x)$

Gradient descent works

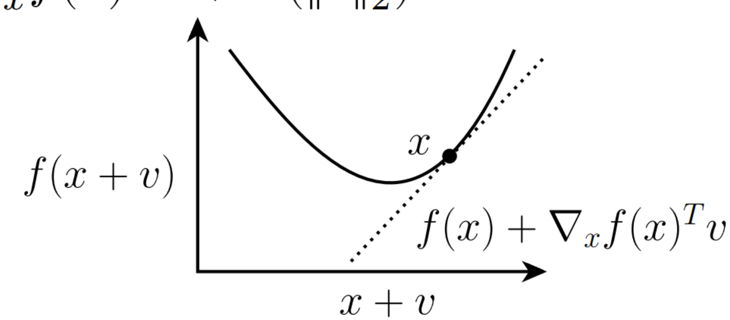
- Theorem: For differentiable f and small enough α, at any point x that is not a (local) minimum

$$f(x - \alpha \nabla_x f(x)) < f(x)$$

- i.e., gradient descent algorithm will decrease the objective

Proof: Any differentiable function f can be written in terms of its *Taylor expansion*

$$f(x + v) = f(x) + \nabla_x f(x)^T v + O(\|v\|_2^2)$$



Gradient descent works (cont)

Choosing $v = -\alpha \nabla_x f(x)$, we have

$$\begin{aligned} f\big(x - \alpha \nabla_x f(x)\big) &= f(x) - \alpha \nabla_x f(x)^T \nabla_x f(x) + O(\|\alpha \nabla_x f(x)\|_2^2) \\ &\leq f(x) - \alpha \|\nabla_x f(x)\|_2^2 + C\|\alpha \nabla_x f(x)\|_2^2 \\ &= \ f(x) - (\alpha - \alpha^2 C)\|\nabla_x f(x)\|_2^2 \\ &< f(x) \quad (\text{for } \alpha < 1/C \text{ and } \|\nabla_x f(x)\|_2^2 > 0) \end{aligned}$$

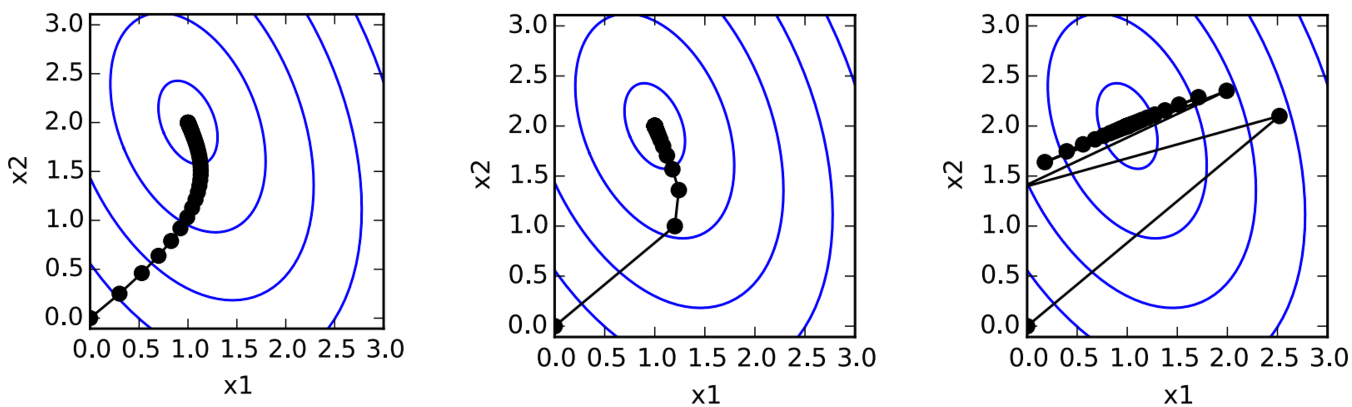
We are guaranteed to have $\|\nabla_x f(x)\|_2^2 > 0$ except at optima.

- Works for both convex and non-convex functions, but this doesn't actually prove that gradient descent converges, just that it decreases objective

Gradient descent in practice

Choice of α matters a lot in practice:

$$\underset{x}{\text{minimize}} \;\; 2x_1^2 + x_2^2 + x_1x_2 - 6x_1 - 5x_2$$



$\alpha = 0.05$ $\alpha = 0.2$ $\alpha = 0.42$

Poll: modified gradient descent

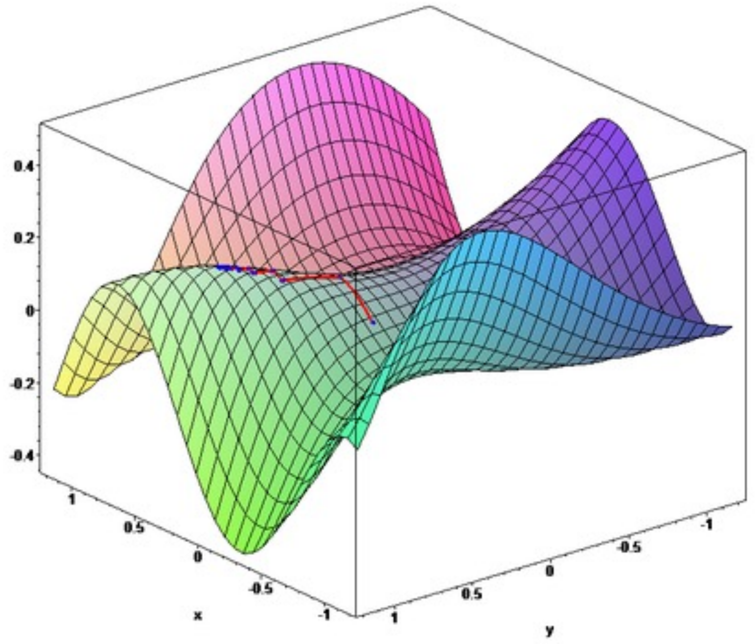
- Consider an alternative version of gradient descent, where instead of choosing an update $x - \alpha \nabla_x f(x)$

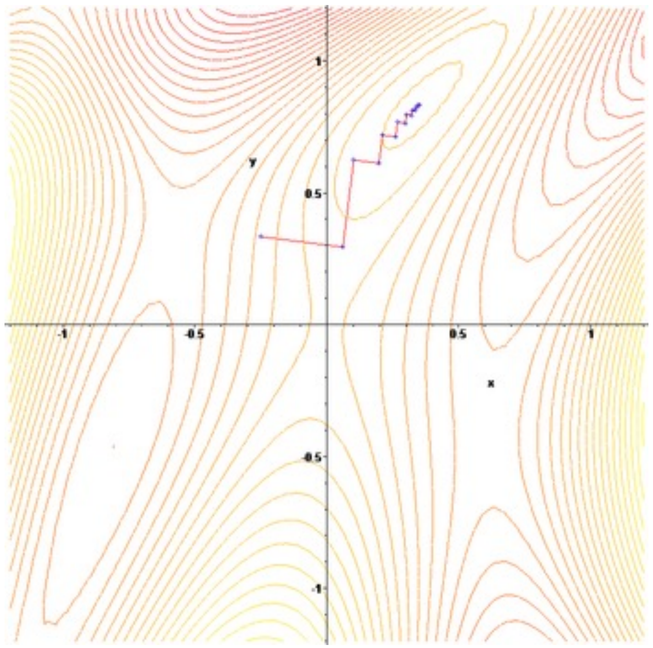
  we chose some other direction $x + \alpha v$ where v has a negative inner product with the gradient $\nabla_x f(x)^T v < 0$

- Will this update, for suitably chosen α, still decrease the objective?
  1) No, not necessarily (for either convex or nonconvex functions)
  2) Only for convex functions
  3) Only for nonconvex functions
  4) Yes, for both convex and nonconvex functions

Gradient ascent for maximization

$$\mathbf{x}^{t+1} \leftarrow \mathbf{x}^{t} + \alpha \nabla f\,(\mathbf{x}^{t})$$





Gradient ascent (step size)

- Adjusting α in gradient descent
  - Line search
  - Newton-Raphson

$$\mathbf{x}^{t+1} \leftarrow \mathbf{x}^{t} - \mathbf{H}_f^{-1}(\mathbf{x}^{t})\nabla f(\mathbf{x}^{t})$$

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

Dealing with constraints, non-differentiability

- For settings where we can easily project points onto the constraint set $\mathcal{C}$, can use a simple generalization called projected gradient descent

$$\text{Repeat: } x \leftarrow P_e\big(x - \alpha \nabla_x f(x)\big)$$

- If f is not differentiable, but continuous, it still has what is called a subgradient, can replace gradient with subgradient in all cases (but theory/practice of convergence is quite different)