Artificial Intelligence
CE-417, Group 1
Computer Eng. Department
Sharif University of Technology

Spring 2024

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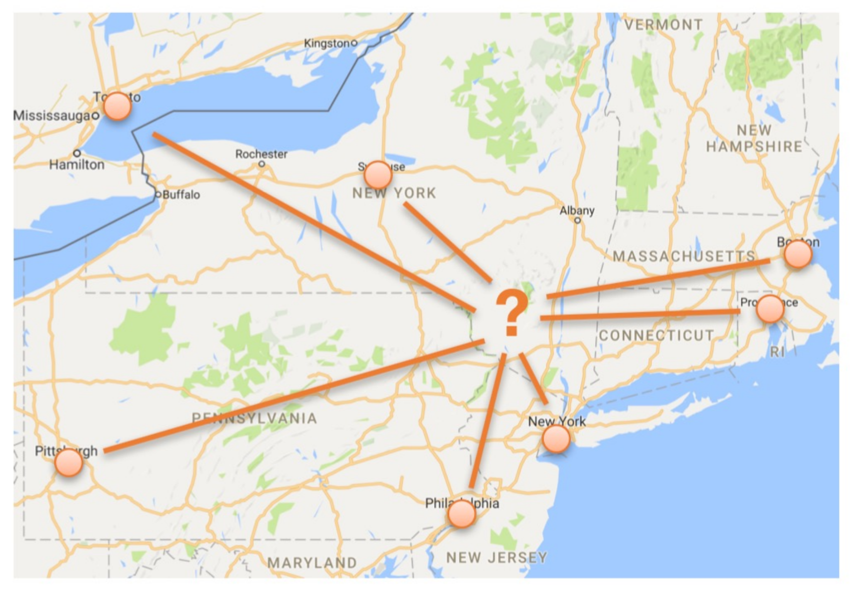
Courtesy: Most slides are adopted from **15-780** course at CMU.

Continuous Optimization

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 $y^{(1)}, \ldots, y^{(m)}$



- Write as the optimization problem:

$$\underset{x}{\text{minimize}} \sum_{i=1}^{m} \|x - y^{(m)}\|_2$$

Example: Image deblurring and denoising

(a) Original image. (b) Blurry, noisy image. (c) Restored image.

Figure from (O'Connor and Vandenberghe, 2014)

- Given corrupted image $Y \in \mathbb{R}^{m \times n}$, reconstruct the image by solving the optimization:

$$\underset{X}{\text{minimize}} \sum_{i,j} \left| Y_{ij} - (K * X)_{ij} \right| + \lambda \sum_{i,j} \left((X_{ij} - X_{i,j+1})^2 + (X_{i+1,j} - X_{ij})^2 \right)^{\frac{1}{2}}$$

- where K * denotes convolution with a blurring filter

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 inputs u_t:

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

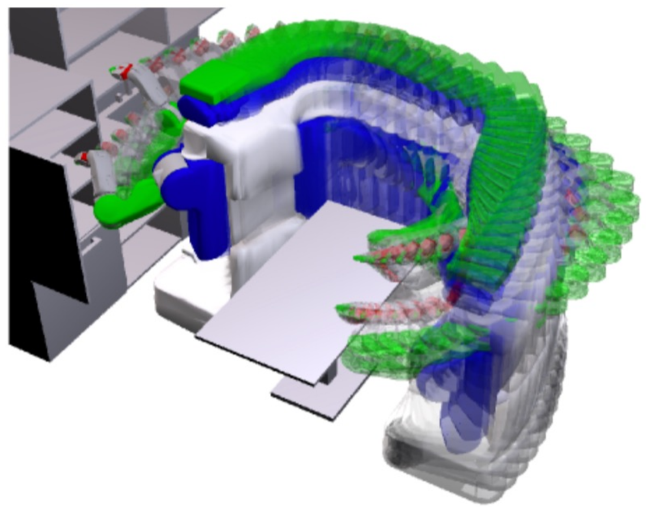


Figure from (Schulman et al., 2014)

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

$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{m} \ell(h_\theta(x^{(i)}), y^{(i)})$$

where

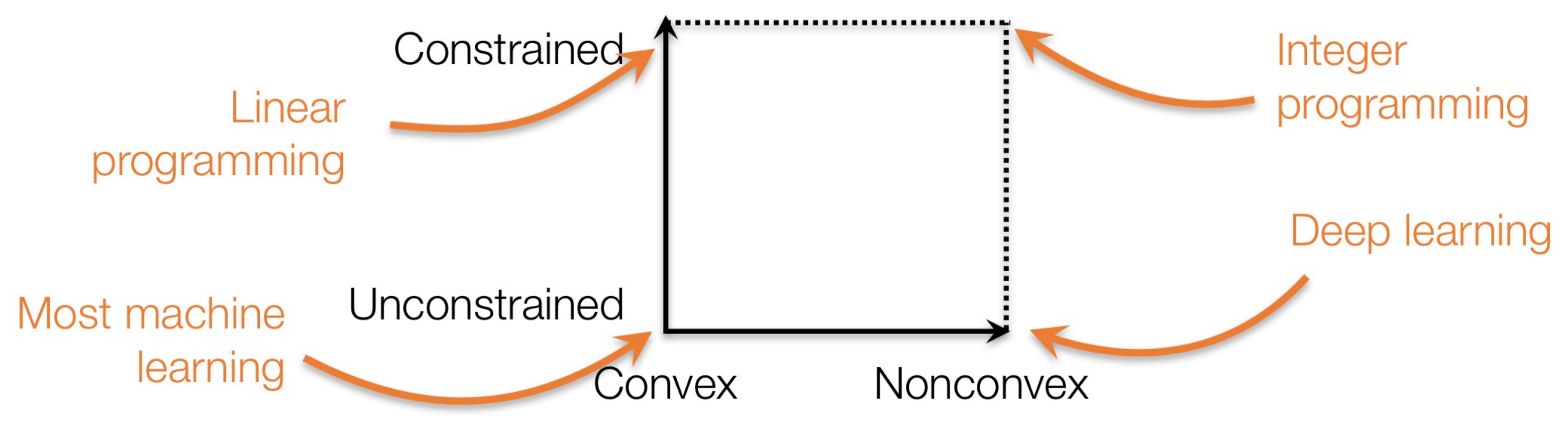
- $x^{(i)} \in \mathcal{X}$ are inputs
- $y^{(i)} \in \mathcal{Y}$ are outputs
- ℓ is a loss function
- h_θ is a hypothesis function parameterized by θ

The benefit of optimization

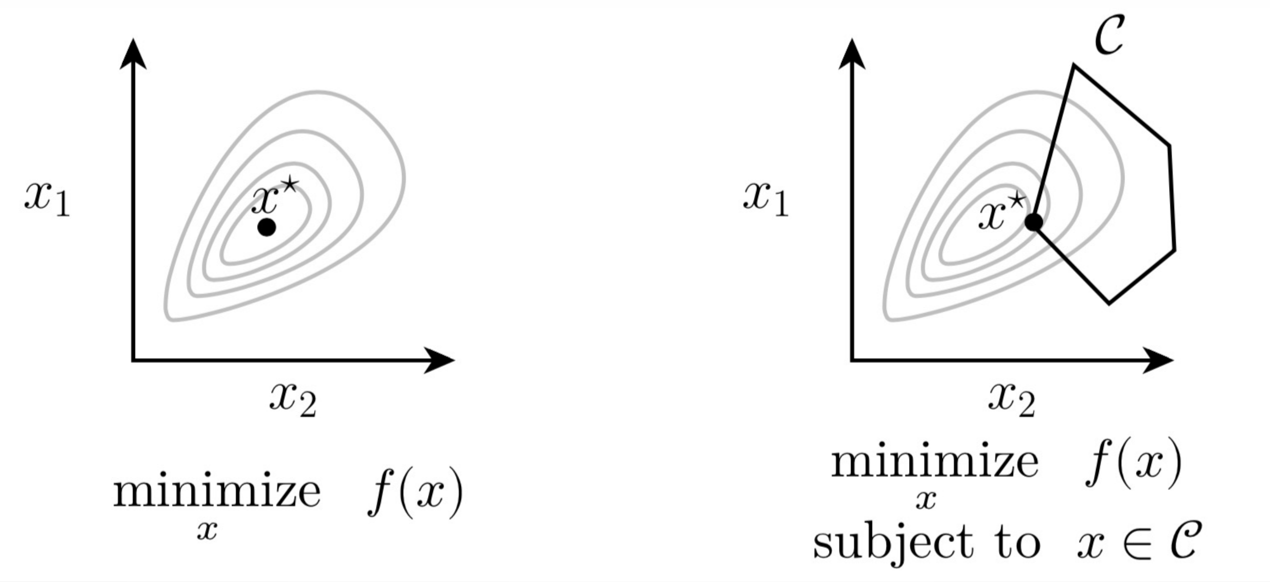
- One of the key benefits of looking at problems in AI as optimization problems: we separate out the *definition* of the problem from the *method for solving it*.
- For many classes of problems, there are off-the-shelf solvers that will let you solve even large, complex problems, once you have put them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

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

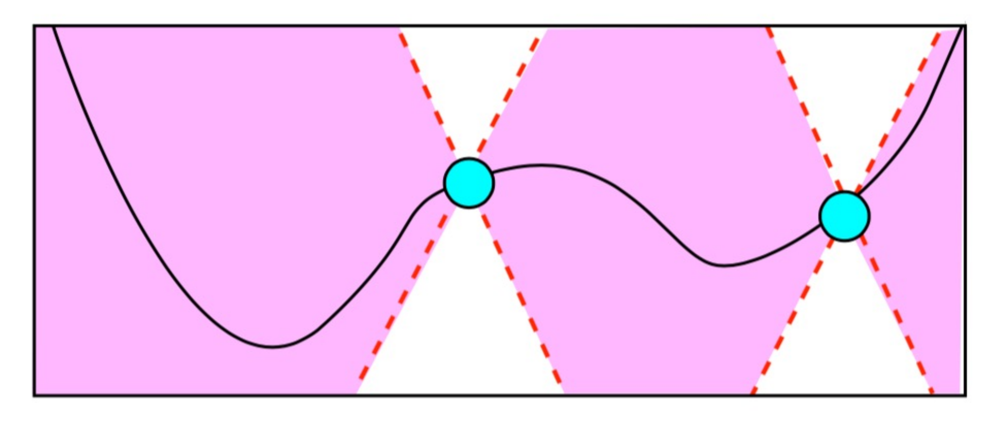
How hard is real-valued optimization?

- How long does it take to find an ε-optimal minimizer of a real-valued function?

  General function: impossible! $\min_{x \in \mathbb{R}^n} f(x).$

- We need to make some assumptions about the function:
  - Assume f is **Lipschitz-continuous**: (can not change too quickly)

$$|f(x) - f(y)| \leq L\|x - y\|.$$

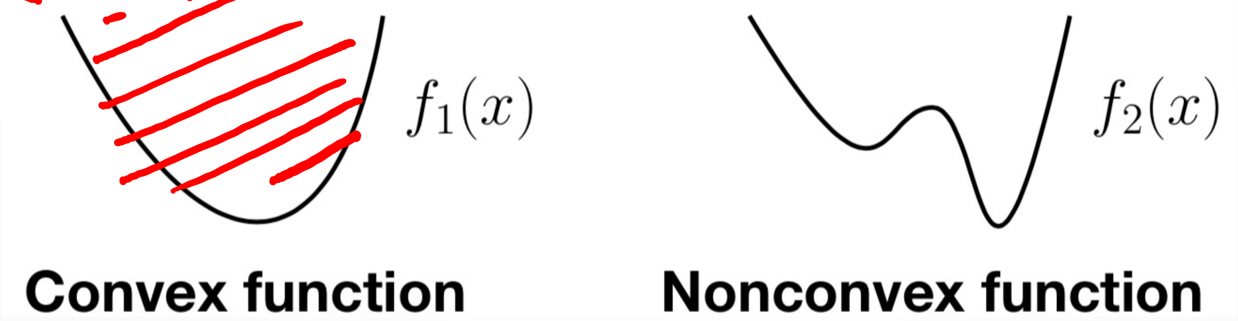


How hard is real-valued optimization? (cont.)

- After t iterations, the error of any algorithm is $\Omega\left(\frac{1}{t^{1/n}}\right)$.
  - Any grid-search is nearly optimal
- Optimization is hard, but assumptions make a big difference.
  - we went from impossible to very slow

f is convex $\Longleftrightarrow \{(x, y) \mid f(x) \leq y\}$ is convex

Convex vs. nonconvex optimization

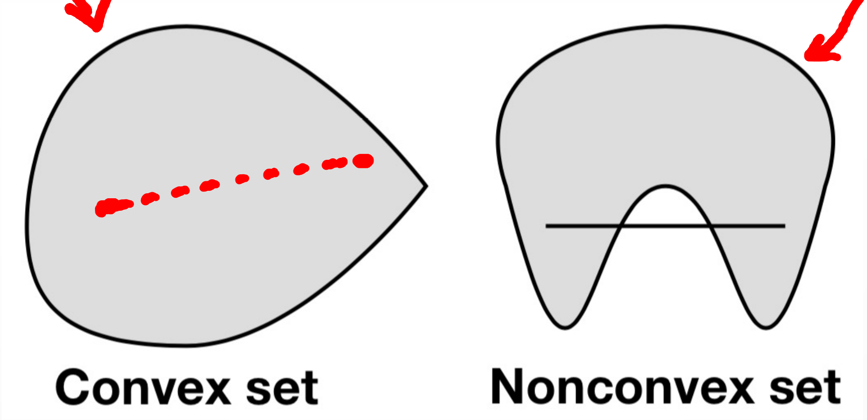


- Originally, researchers distinguished between linear (easy) and nonlinear (hard) problems
- But in 80s and 90s, it became clear that this wasn't the right distinction, key difference is between convex and nonconvex problems
- Convex problem:

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

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

Convex sets

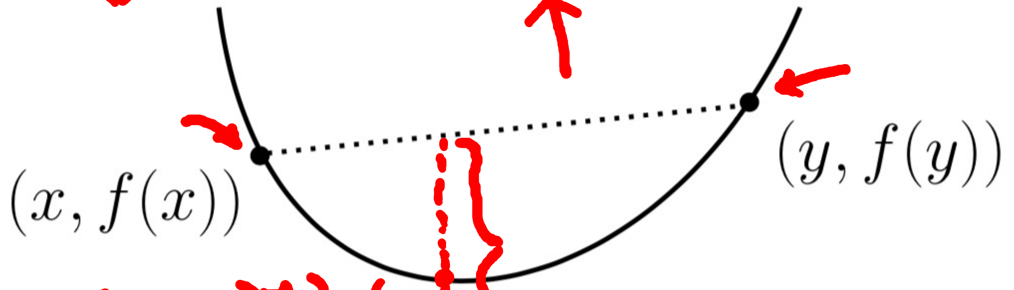


- A set $\mathcal{C}$ is convex if, for any $x, y \in \mathcal{C}$ and $0 \leq \theta \leq 1$
  - $\theta x + (1 - \theta)\, y \in \mathcal{C}$
- Examples:
  - All points $\mathcal{C} = \mathrm{R}^n$
  - Intervals $\mathcal{C} = \{x \in \mathrm{R}^n \mid l \leq x \leq u\}$ (elementwise inequality)
  - Linear equalities $\mathcal{C} = \{x \in \mathrm{R}^n \mid Ax = b\}$ (for $A \in \mathrm{R}^{m*n}$, $b \in \mathrm{R}^m$)
  - Intersection of convex sets $\mathcal{C} = \bigcap_{i=1}^{m} \mathcal{C}_i$

Convex functions

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

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



- Convex functions "curve upwards" (or at least not downwards)
- If f is convex then $-f$ is concave
- If f is both convex and concave, it is affine, must be of form:

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

2^{nd} derivative being positive iff convexity (one dimensional)

if part

From convexity, $f(ta + (1-t)b) \leqslant t f(a) + (1-t) f(b)$.

Let $t = 1/2$, $a = x - h$, and $b = x + h$.

Then

$$f(x) \leqslant \frac{1}{2} f(x-h) + \frac{1}{2} f(x+h)$$
$$\implies f(x+h) - 2f(x) + f(x-h) \geqslant 0$$

Only if part

Proof: We use the Taylor series expansion of the function around x_0:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x^*)}{2}(x - x_0)^2, \qquad (2.73)$$

where x^* lies between x_0 and x. By hypothesis, $f''(x^*) \geq 0$, and thus the last term is nonnegative for all x.

We let $x_0 = \lambda x_1 + (1 - \lambda) x_2$ and take $x = x_1$, to obtain

$$f(x_1) \geq f(x_0) + f'(x_0)((1 - \lambda)(x_1 - x_2)). \qquad (2.74)$$

Similarly, taking $x = x_2$, we obtain

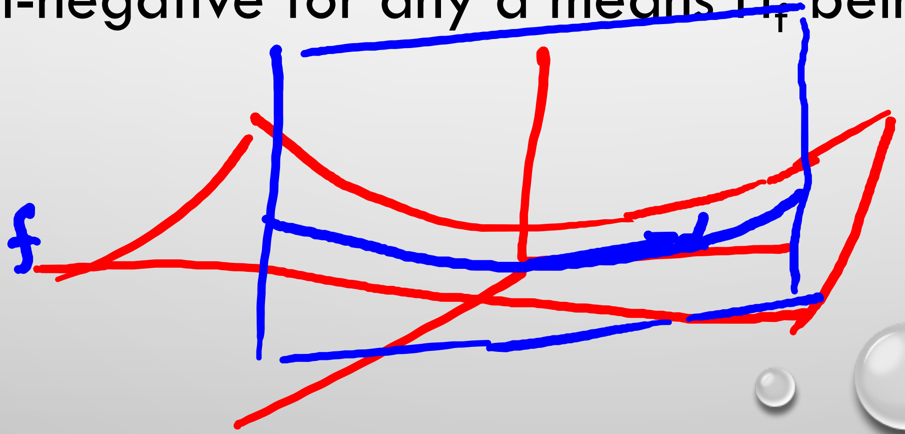
$$f(x_2) \geq f(x_0) + f'(x_0)(\lambda(x_2 - x_1)). \qquad (2.75)$$

Multiplying (2.74) by λ and (2.75) by $1 - \lambda$ and adding, we obtain (2.72). The proof for strict convexity proceeds along the same lines. □

Hessian being positive semi-definite iff convexity (multi-dimensional)

$$\forall d: \quad \frac{d^2}{dt^2} f(x+td) = \underset{1\times n}{d^T} \underset{n\times n}{H_f} \underset{n\times 1}{d} \geq 0 \longleftrightarrow H_f \succeq 0 \ \text{(PSD)}$$

- Function f(.) is convex iff its one-dimensional projection along ***any*** direction d, g(t) = f(.+td) is convex.
- Note that the 2nd derivative of g is $d^T H_f d$, where H_f is the hessian of the function f.
- $d^T H_f d$ being non-negative for any d means H_f being positive semi-definite.



Examples of convex functions

$f'' = a^2 \exp(ax)$

Exponential: $f(x) = \exp(ax)$, $a \in \mathbb{R}$

Negative logarithm: $f(x) = -\log x$, with domain $x > 0$

Squared Euclidean norm: $f(x) = \|x\|_2^2 \equiv x^T x \equiv \sum_{i=1}^{n} x_i^2$

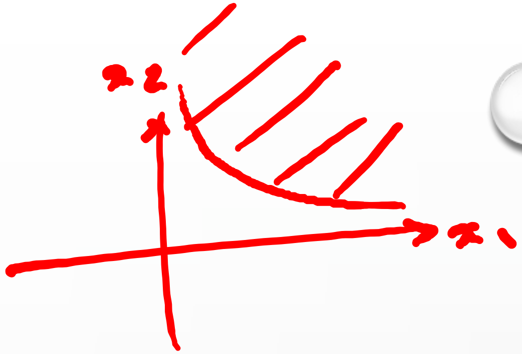
Euclidean norm: $f(x) = \|x\|_2$

$\|\alpha x + (1-\alpha)y\|_2 \leq \|\alpha x\|_2 + \|(1-\alpha)x\|_2$

Non-negative weighted sum of convex functions

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

Poll: convex sets and functions



Which of the following functions or sets are convex?

1. A union of two convex sets $\mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2$
2. The set $\{x \in \mathbb{R}^2 | x \geq 0, x_1 x_2 \geq 1\}$
3. The function $f: \mathbb{R}^2 \rightarrow \mathbb{R}, f(x) = x_1 x_2$
4. 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 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:

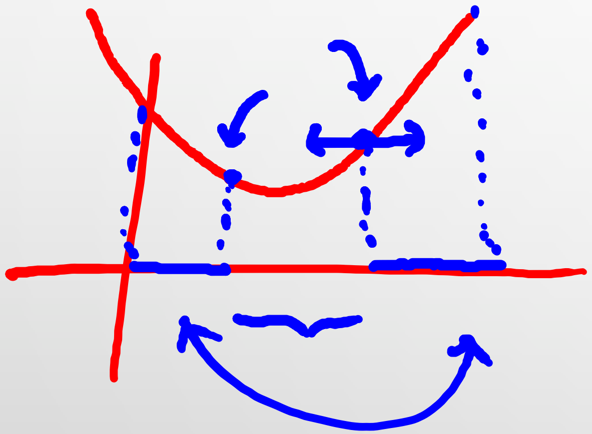
$$f(z) = f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y) < f(x) \quad \text{and}$$

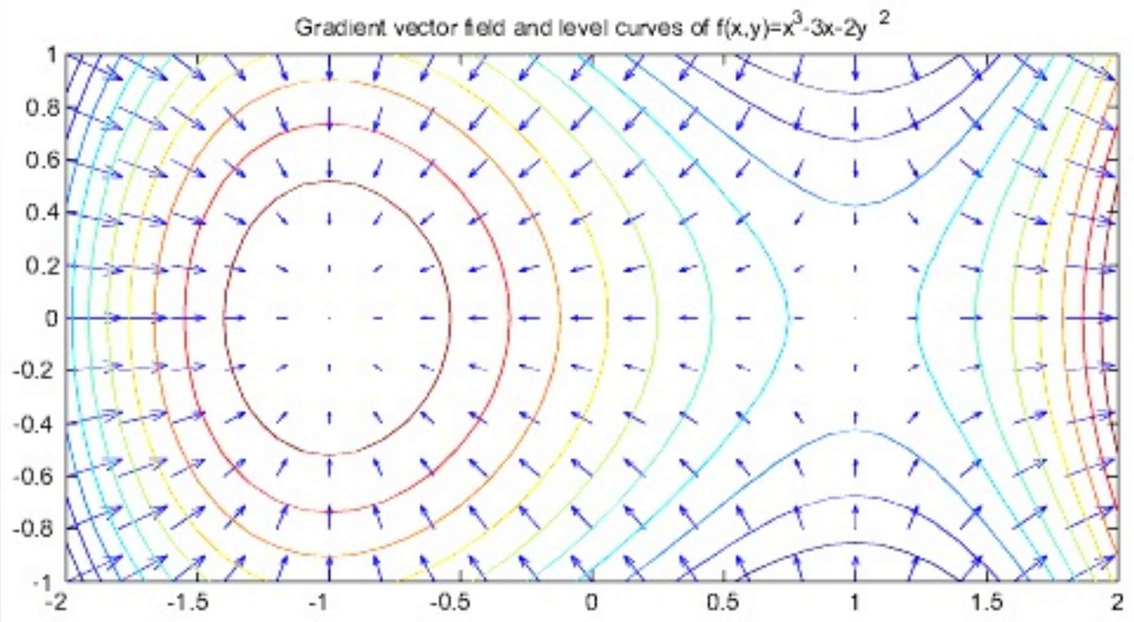
$$\|x - z\|_2 = \left\| x - \left(1 - \frac{R}{2\|x-y\|_2}\right) x + \frac{R}{2\|x-y\|_2} y \right\|_2 = \left\| \frac{R(x-y)}{2\|x-y\|_2} \right\|_2 = \frac{R}{2}$$

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

The gradient

- A key concept in solving optimization problems is the notation of the gradient of a function (multi-variate analogue of derivative)
- For $f : R^n \longrightarrow R$, gradient is defined as vector of partial derivatives





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

Gradient descent

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

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

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

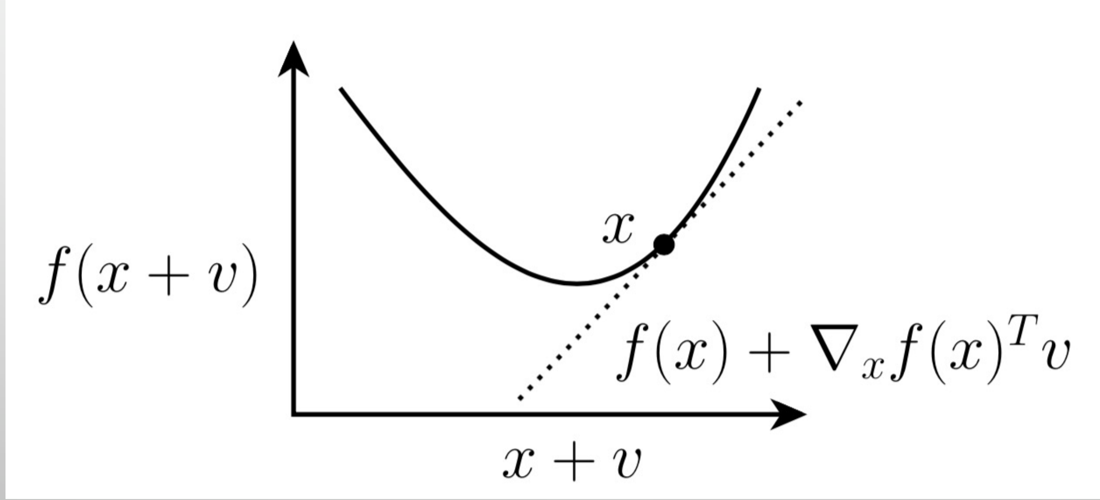
Gradient descent works

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

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

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

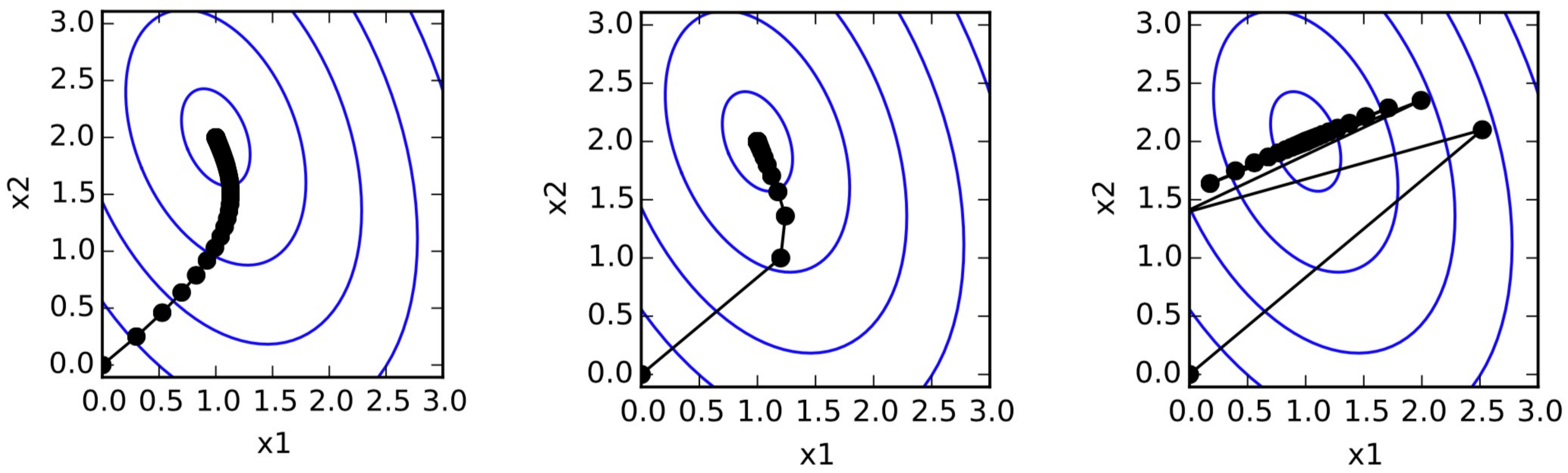
$$
\begin{aligned}
f\big(x - \alpha \nabla_x f(x)\big) &= f(x) - \alpha \nabla_x f(x)^T \nabla_x f(x) + O(\|\alpha \nabla_x f(x)\|_2^2) \\
&\leq f(x) - \alpha \|\nabla_x f(x)\|_2^2 + C\|\alpha \nabla_x f(x)\|_2^2 \\
&= \ f(x) - (\alpha - \alpha^2 C)\|\nabla_x f(x)\|_2^2 \\
&< f(x) \quad (\text{for }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

- (Watch out: a bit of subtlety of this line, only holds for small $\alpha \nabla_x f(x)$)
- We are guaranteed to have $\|\nabla_x f(x)\|_2^2 > 0$ except at optima
- Works for both convex and non-convex functions, but with convex functions guaranteed to find global optimum

Gradient descent in practice

- Choice of α matters a lot in practice:

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



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