

15-780 – Graduate Artificial Intelligence: Optimization

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Notations

→ Binary classification

→ "linear" classifier.

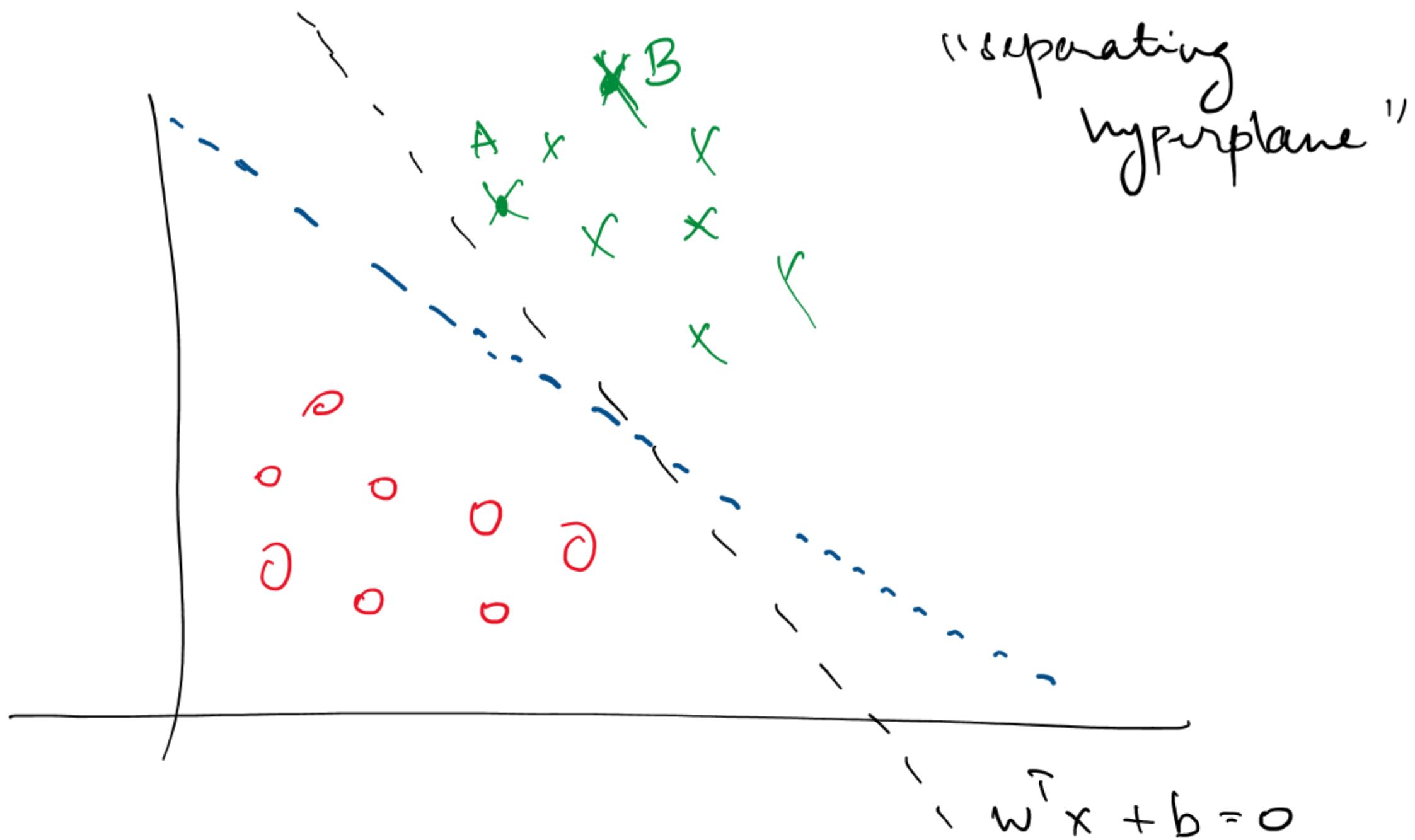
→ $h: \mathcal{X} \rightarrow \mathbb{R}$

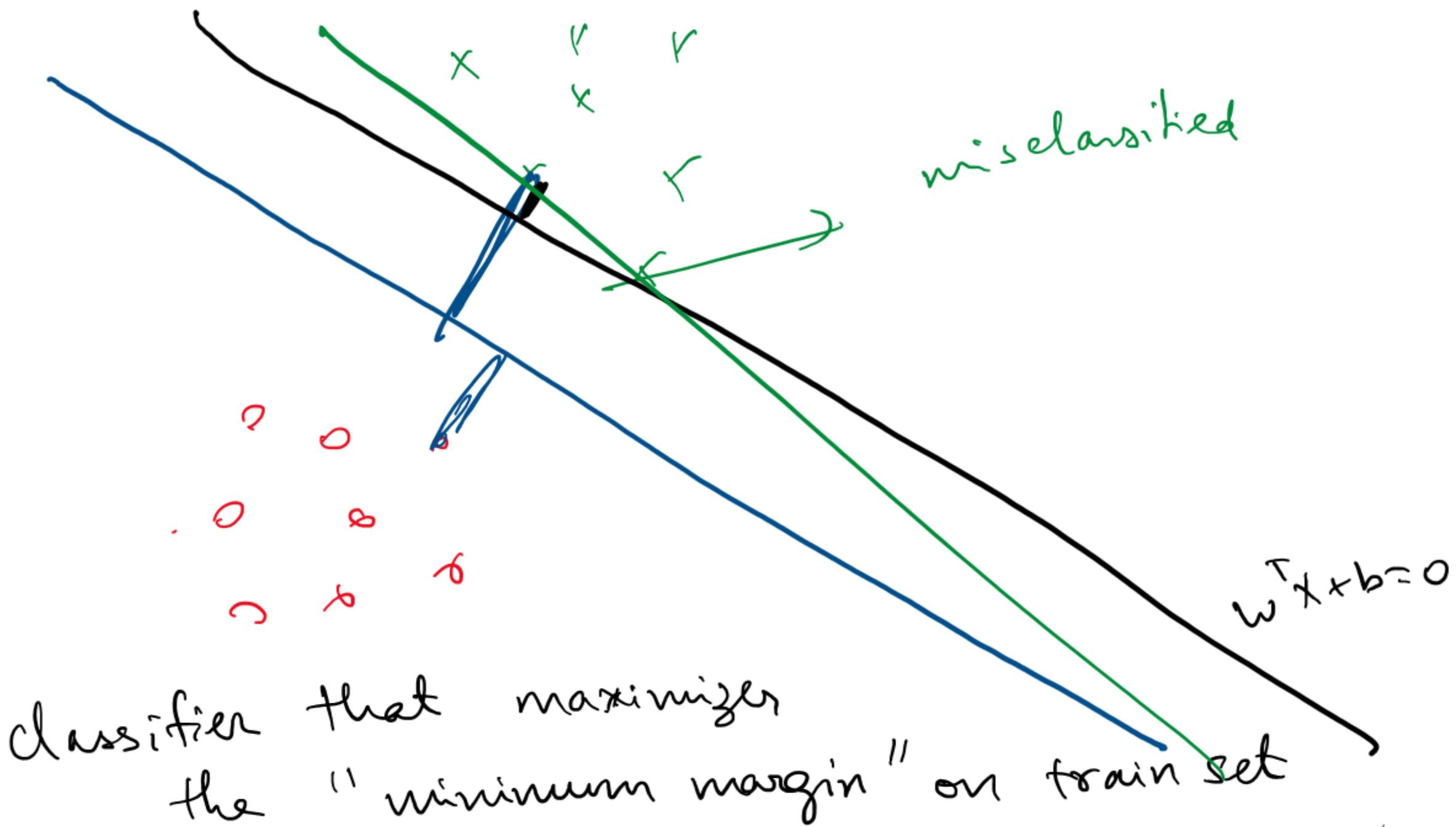
$$h(x) = w^T x + b$$

$$y = \text{sign}(h(x)) = \text{sign}(w^T x + b)$$

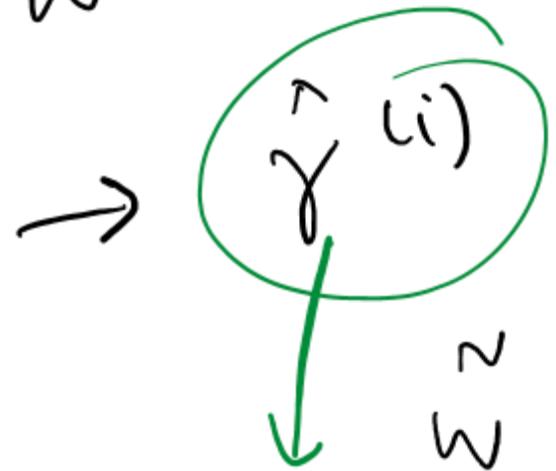
$$y \in \{-1, +1\}$$

$$\left. \begin{aligned} \theta^T x : & w^T x + b \\ \downarrow [x, 1] & \leftarrow \text{bias} \end{aligned} \right\} \begin{array}{l} \text{Classifier} \\ \text{need not} \\ \text{pass through} \\ \text{origin} \end{array}$$





What is "margin"?



$$= \hat{y}^{(i)} (\mathbf{w}^\top \mathbf{x}^{(i)} + b)$$

B is more
confident than A

$$\sim \mathbf{w}, b = 100 \times w, 100 \times b$$

functional
margin

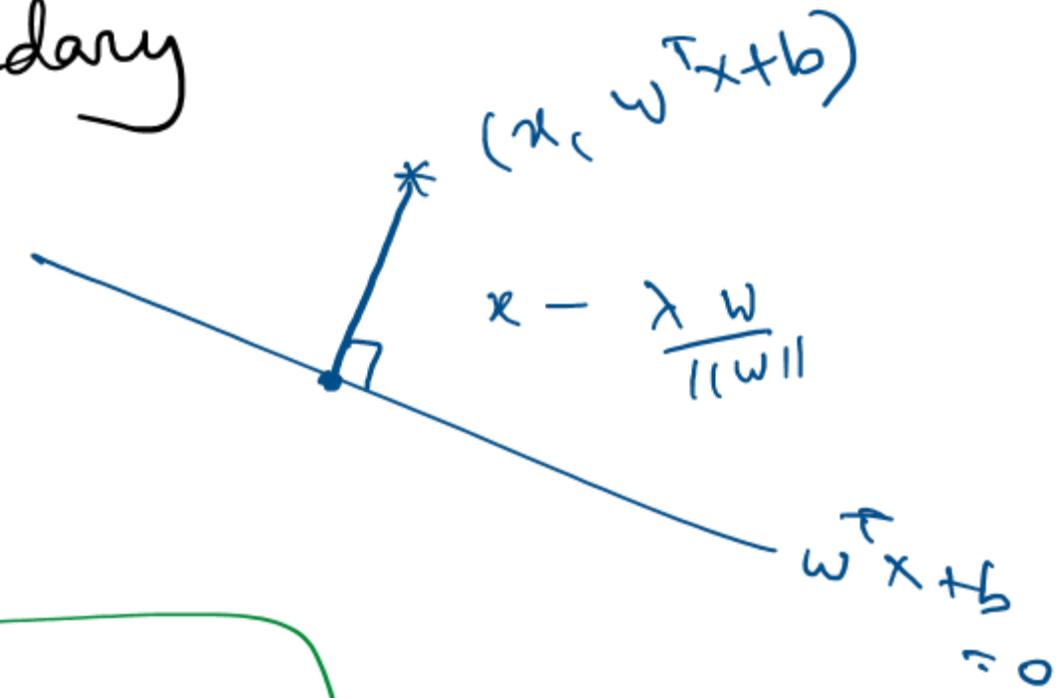
geometric margin

margin increases by 100

Geometric margin

Distance to decision boundary

$$\gamma^{(i)} = y^{(i)} \left(\frac{w^T x^{(i)} + b}{\|w\|} \right)$$



$$\boxed{\begin{array}{l} \max \gamma \\ \text{s.t.} \\ y^{(i)} \left(\frac{w^T (x^{(i)}) + b}{\|w\|} \right) \geq \gamma \end{array}}$$

$$\hat{\gamma} = \gamma \cdot \|w\|$$

$$\|w\|=1 : \max \gamma$$

$$\text{st. } y^{(i)}(w^T(x^{(i)}) + b) \geq \gamma$$

$$\|w\|=1$$

→ hard to optimize!

$$\max \frac{\gamma}{\|w\|} \rightarrow \text{functional margin}$$

in dr \Rightarrow not a nice fn to optimize

$$\text{st. } y^{(i)}(w^T(x^{(i)}) + b) \geq \gamma$$

$\gamma^* = 1$ (functional margin can be arbitrarily scaled)

$$\max \frac{1}{\|w\|} \equiv \min \frac{1}{2} \|w\|_2^2$$

$$\boxed{\begin{aligned} & \min \frac{1}{2} \|w\|_2^2 \\ \text{s.t. } & y^{(i)} (w^\top x^{(i)} + b) \geq 1 \end{aligned}}$$

"Non-separable case"

slack variable

$$y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i$$
$$\xi_i \geq 0$$

min

$$\frac{1}{2} \|w\|_2^2 + C \sum \xi_i$$

convex

s.t.

$$y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i$$

regularizer

$$\frac{1}{2} \|w\|_2^2$$

$$\xi_i \geq 0$$

+ Train loss $(y^{(i)}, x^{(i)})$

$$\max(1 - y^{(i)}(w^T x + b^{(i)}), 0)$$

Hinge-loss

Outline

Introduction to optimization

Types of optimization problems, convexity

Solving optimization problems

Opt: Train Loss + λ Regularizer

Outline

Introduction to optimization

Types of optimization problems, convexity

Solving optimization problems

Optimization definitions

We'll write optimization problems like this:

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

θ : min train loss
+ reg

which should be interpreted to mean: we want to find the value of x that achieves the smallest possible value of $f(x)$, out of all points in \mathcal{C}

Optimization definitions

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

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
- $x^* \equiv \operatorname{argmin}_{x \in \mathcal{C}} f(x)$ – optimal solution
- $f^* \equiv f(x^*) \equiv \min_{x \in \mathcal{C}} f(x)$ – optimal objective

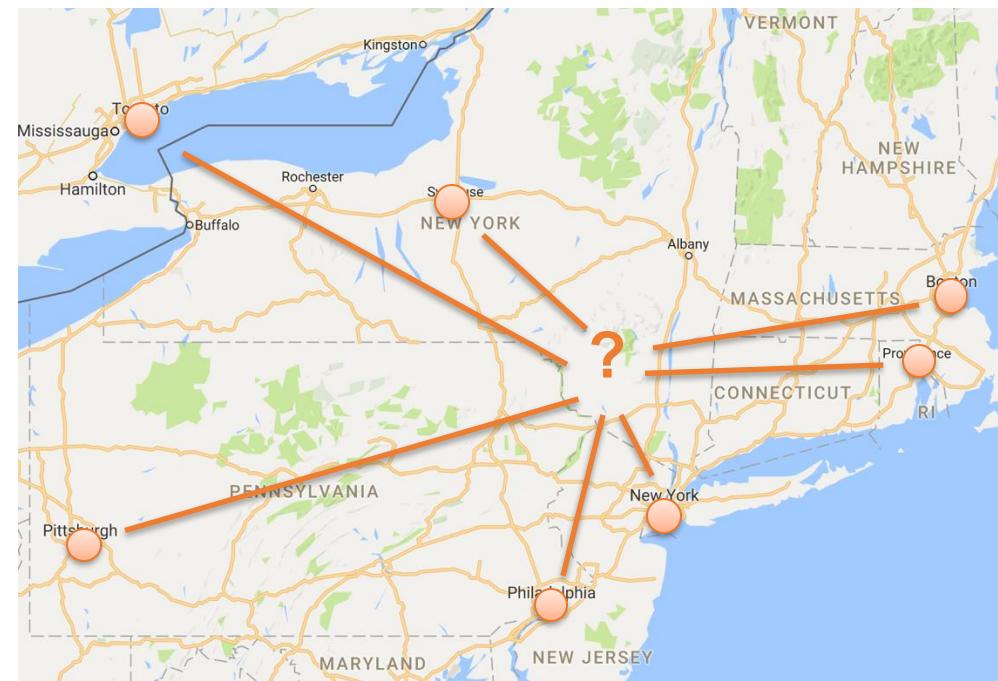
Example: Weber point

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

Write as the optimization problem:

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



Example: image deblurring



(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 image by solving problem:

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

where $K *$ denotes convolution with a blurring filter

Example: image deblurring

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

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Reverse image blurring "prior" on natural images: nearby pixels are similar

where $K *$ denotes convolution with a blurring filter

Total variation image deblurring

Example: robot trajectory planning

We want a sequence of control inputs that take a robot from start to goal

Why tricky? Some obstacles, and also can't simply move along any coordinate at will (joint limits)

One approach: model this as a search problem (sample points in the space, discard ones that hit obstacles and

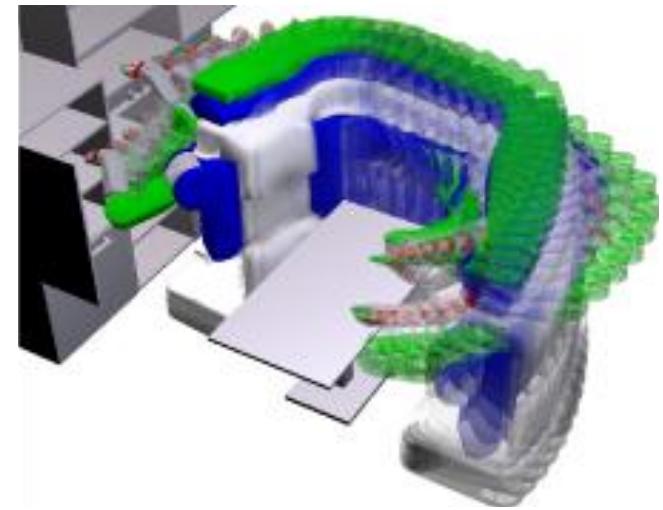


Figure from (Schulman et al., 2014)

Example: robot trajectory planning

Robot state x_t and control inputs u_t

$$\underset{x_{1:T}, u_{1:T-1}}{\text{minimize}} \sum_{i=1}^T \|u_t\|_2^2$$

$$\text{subject to } x_{t+1} = f_{\text{dynamics}}(x_t, u_t)$$

$$x_t \in \text{FreeSpace}, \forall t$$

$$x_1 = x_{\text{init}}, x_T = x_{\text{goal}}$$

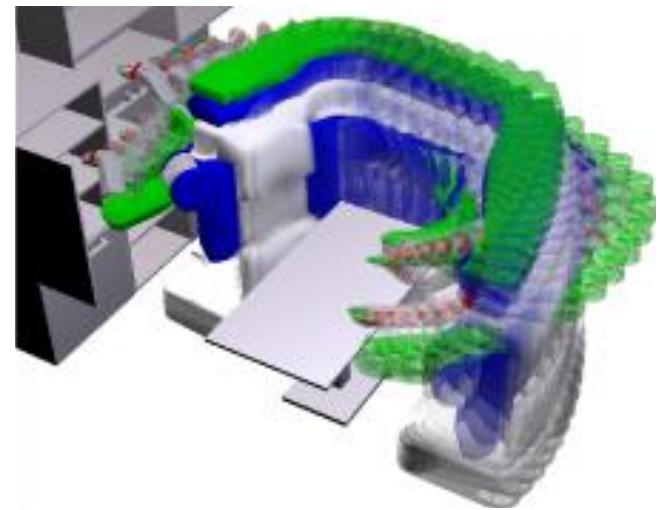


Figure from (Schulman et al., 2014)

Example: learning from examples

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

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

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

Find a model that best fits the observed data

Much more on this from next lecture...

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



Outline

Introduction to optimization

Types of optimization problems, convexity

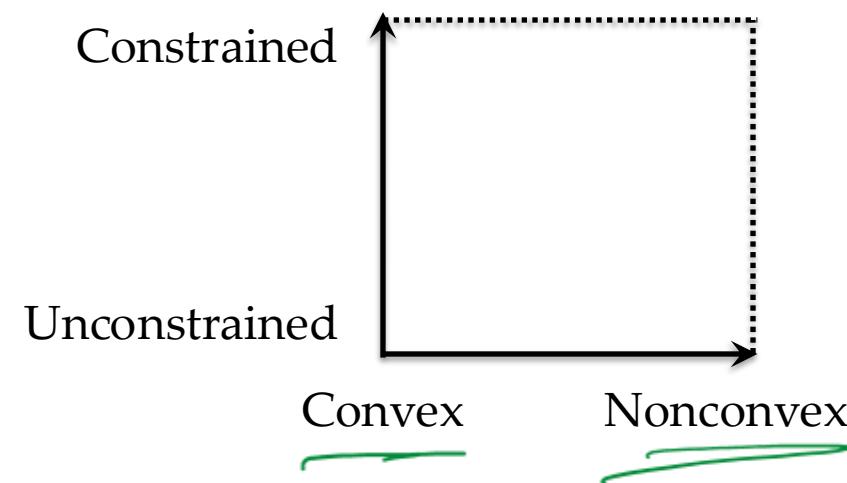
Solving optimization problems

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

We're instead going to focus on two dimensions: convex vs. nonconvex and constrained vs. unconstrained

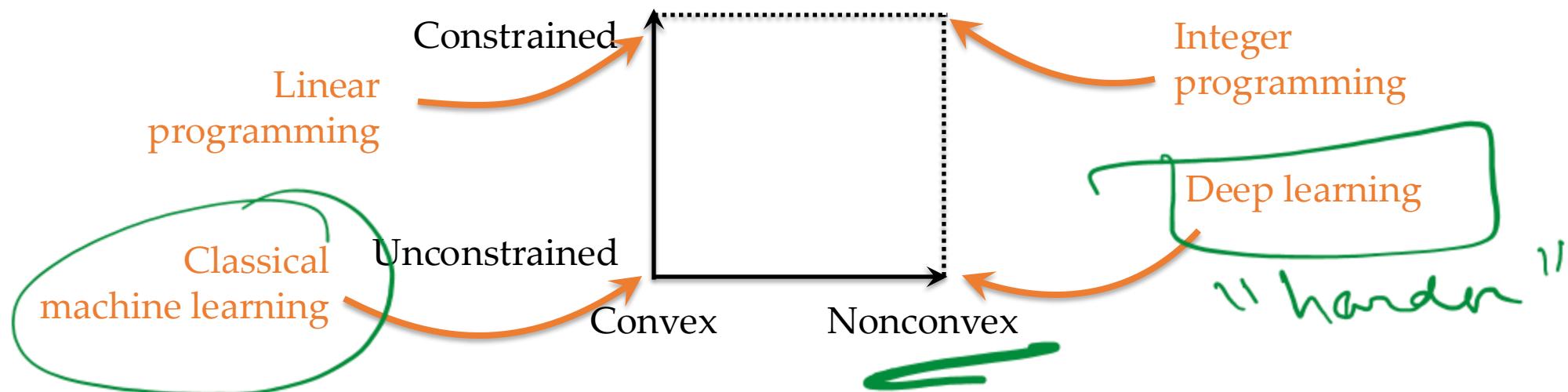
Which problems are easy?



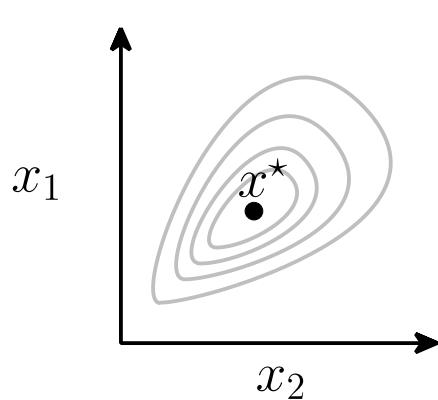
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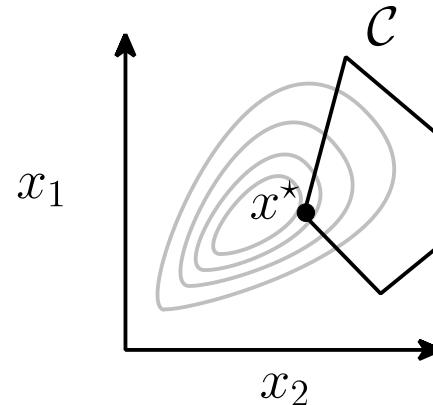
We're instead going to focus on two dimensions: convex vs. nonconvex and constrained vs. unconstrained



Constrained vs. unconstrained



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



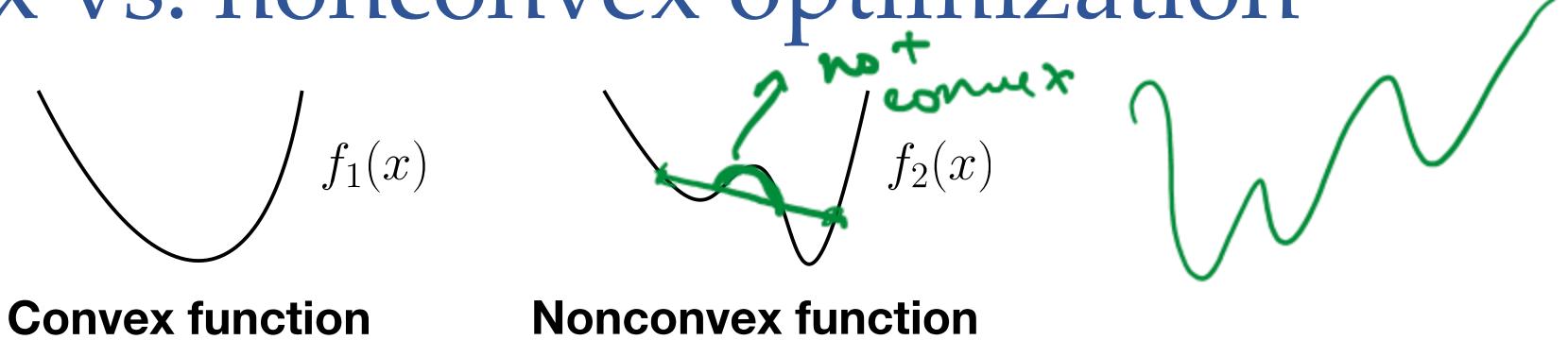
$\underset{x}{\text{minimize}} \ f(x)$
subject to $x \in \mathcal{C}$

↙ allowed

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 $x \in \mathcal{C}$

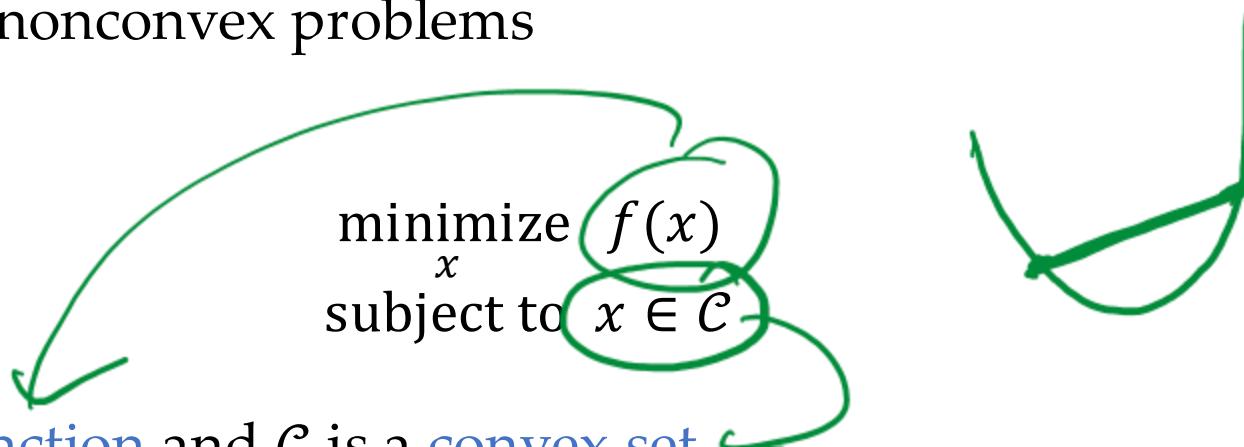
Convex vs. nonconvex optimization



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:

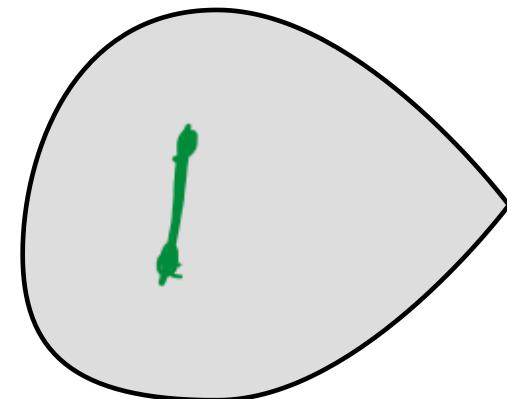


Where f is a **convex function** and \mathcal{C} is a **convex set**

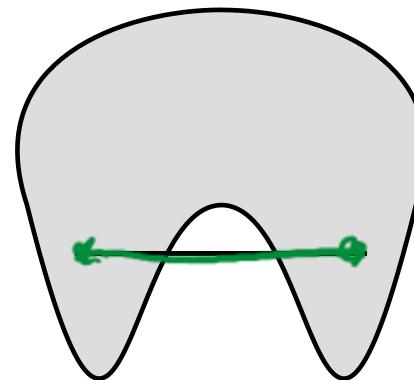
Convex sets

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

Line segment between two points
in the set is also in the set



Convex set



Nonconvex set

Convex sets

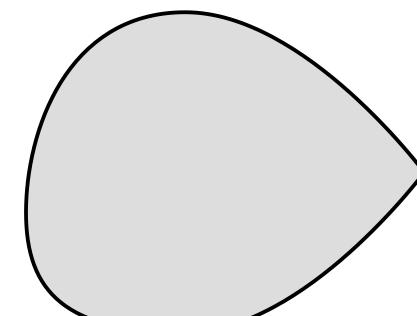
$$\begin{aligned} [x_1 \ x_2] & \quad \lambda x_1 + (1-\lambda) z_1 \\ [z_1 \ z_2] & \quad \lambda x_2 + (1-\lambda) z_2 \end{aligned}$$

Examples:

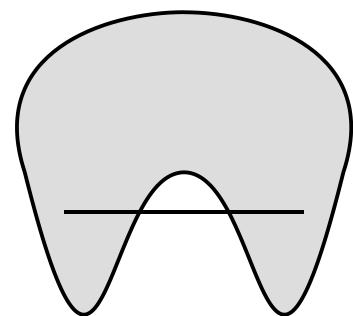
- All points $\mathcal{C} = \mathbb{R}^n$

~~Intervals~~ Intervals $\mathcal{C} = \{x \in \mathbb{R}^n \mid l \leq x \leq u\}$ (elementwise inequality)

- Linear equalities $\mathcal{C} = \{x \in \mathbb{R}^n \mid Ax = b\}$ (for $A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$)
- Norm balls
- Intersection of convex sets $\mathcal{C} = \bigcap_{i=1}^m \mathcal{C}_i$



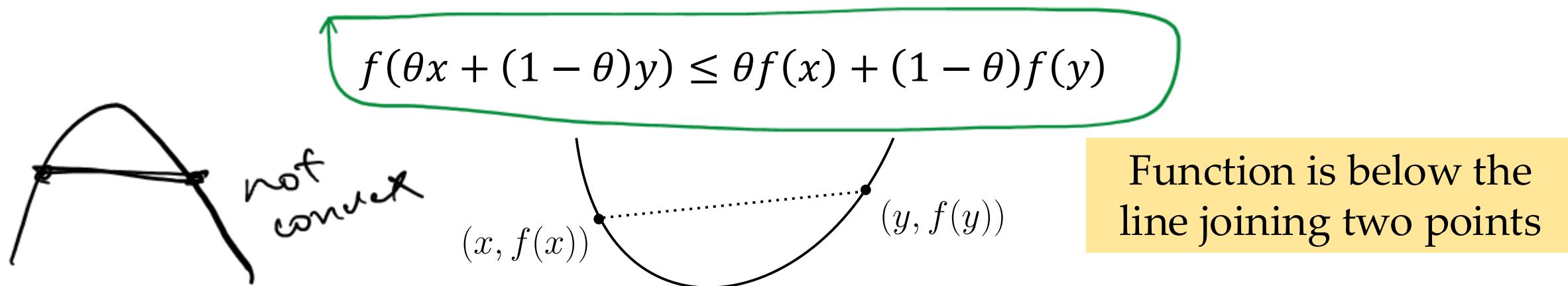
Convex set



Nonconvex set

Convex functions

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



Convex functions “curve upwards” (or at least not downwards)

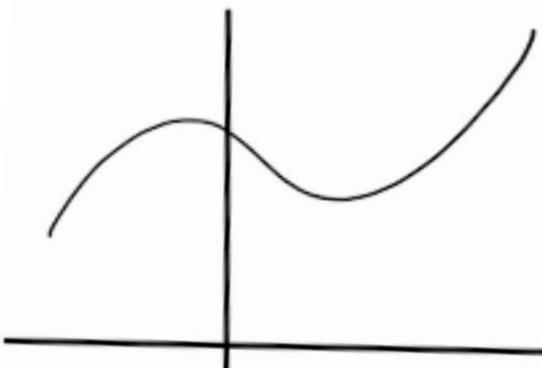


Convex functions

If f is convex then $-f$ is concave (*curves downwards now*)

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

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



Function can be neither convex nor concave

Examples of convex functions

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

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

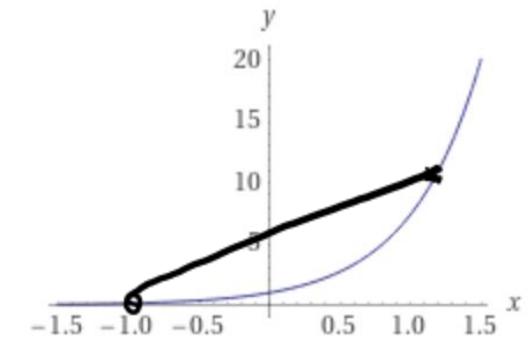
Squared Euclidean norm: $f(x) = \|x\|_2^2 \equiv x^T x \equiv \sum_{i=1}^n x_i^2$

Euclidean norm: $f(x) = \|\underline{x}\|_2$ $\frac{1}{2} \|\omega\|_2^2$

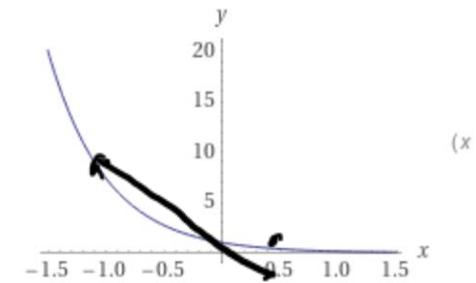
Convex function of affine function $f(x) = g(Ax + b)$, g convex

Non-negative weighted sum of convex functions

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



Exponential



Negative log

Examples of convex functions

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

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

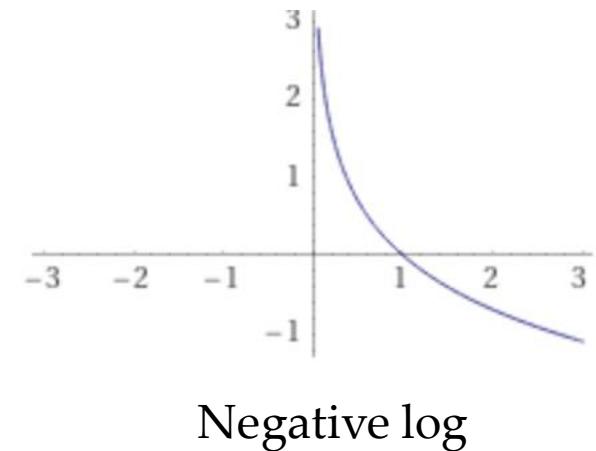
Squared Euclidean norm: $f(x) = \|x\|_2^2 \equiv x^T x \equiv \sum_{i=1}^n x_i^2$

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

Convex function of affine function $f(x) = g(Ax + b)$, g convex

Non-negative weighted sum of convex functions

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



Convex sets and functions: piazza

$$\theta x + (1-\theta)y \in C \quad \forall x, y \in C$$



~~1.~~ The union of two convex sets $C = C_1 \cup C_2$

~~2.~~ The set $\{x \in \mathbb{R}^2 \mid x \geq 0, x_1 x_2 \geq 1\}$

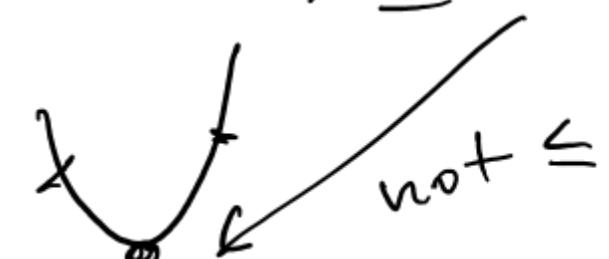
~~3.~~ The function $f: \mathbb{R}_+^2 \rightarrow \mathbb{R}$, $f(x) = x_1 x_2$ with domain $x > 0$

~~4.~~ The function $f: \mathbb{R}^2 \rightarrow \mathbb{R}$, $f(x) = x_1^2 + x_2^2 + x_1 x_2$

counter example

$$(2, 4) \quad (4, 1)$$

$$(3, 3) = 9$$



$$\frac{1}{2} (x_1 + x_2)^2$$

convex

$$\frac{1}{2} x_1^2 + \frac{1}{2} x_2^2$$

convex

Convex optimization

The key aspect of convex optimization problems that make them tractable
is that *all local optima are global optima*

Convex optimization

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 there is no feasible y with $\|x - y\|_2 \leq R$, $f(y) < f(x)$

Theorem: for a convex optimization problem all locally optimal points are globally optimal

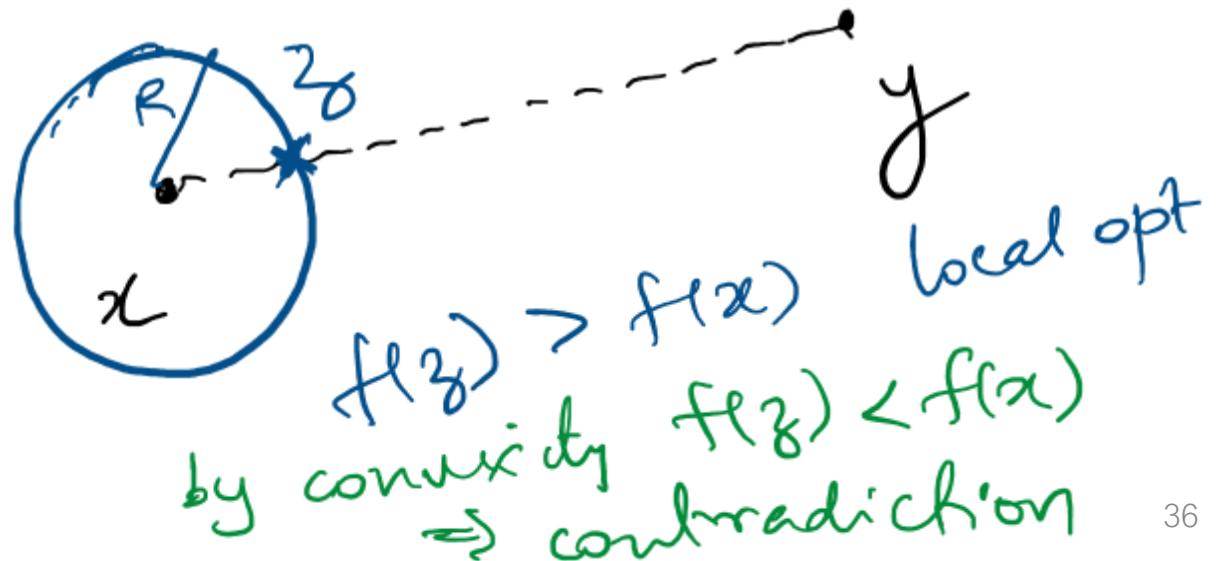
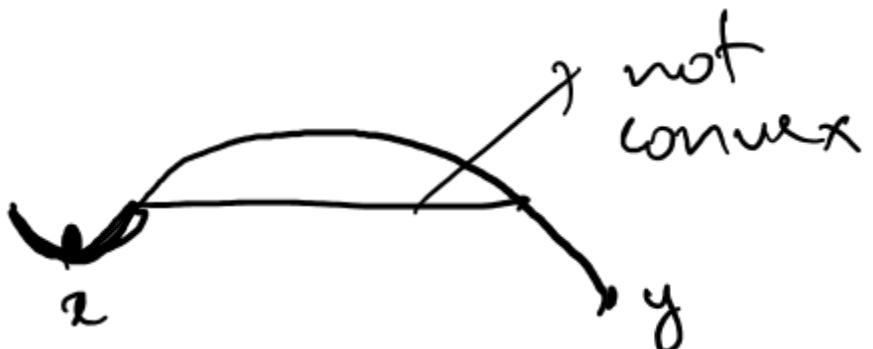
Picture proof

local optimality \Rightarrow global optimality
Suppose x is locally opt but not global

$x, f(x)$

$$f(y) < f(x)$$

$y, f(y)$



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

pt in the ball around x $\leftarrow z = \theta x + (1 - \theta)y, \quad \theta = 1 - \frac{R}{2\|x - y\|_2}$

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

Local optimality \Rightarrow global optimality

If you are not at the minima of a convex function, there is a direction that reduces your function value locally

We used both convexity of feasible set and convexity of objective

Outline

Introduction to optimization

Types of optimization problems, convexity

Solving optimization problems

The gradient

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

Derivative: $f'(x) = \lim_{h \rightarrow 0} \frac{f(x + h) - f(x)}{h}$



Partial derivative: A partial derivative of a function of several variables is derivative with respect to one of those variables with rest constant

$$\frac{\partial f}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x + he_i) - f(x)}{h}$$

only i^{th} coordinate
is changed by h ,
rest are unchanged

$$f(x_1, x_2) = x_1^2 + 2x_2^3$$

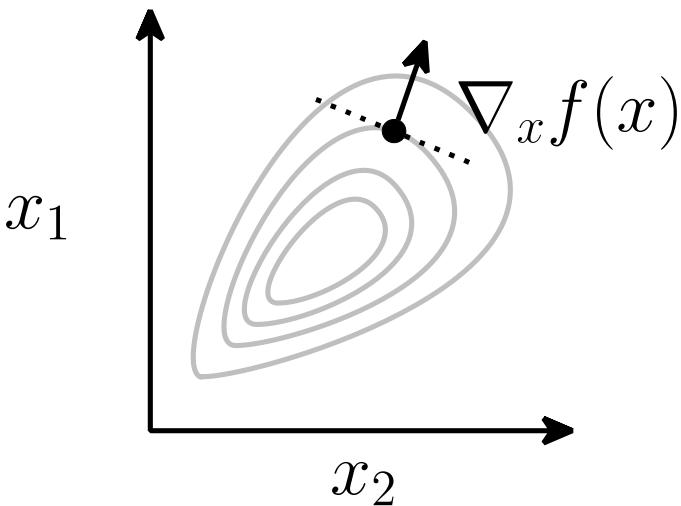
∇f at (1, 1)

The gradient

$$\nabla f = \begin{bmatrix} 2x_1 & = 2 \\ 6x_2 & = 6 \end{bmatrix}$$

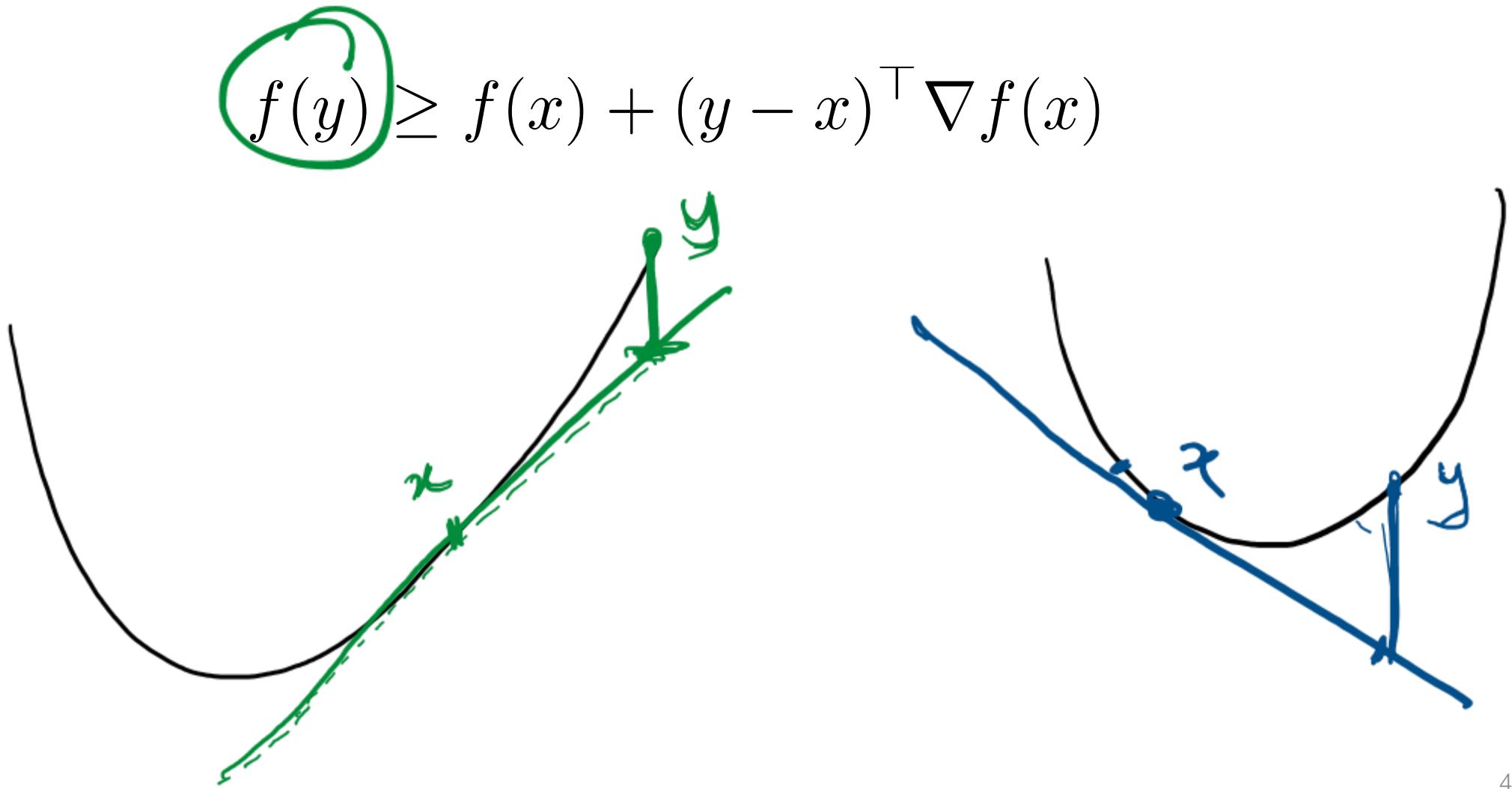
For $f: \mathbb{R}^n \rightarrow \mathbb{R}$, gradient is defined as vector of partial derivatives

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



Points in “steepest direction” of increase in function f

First-order condition for convexity



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 $\alpha > 0$

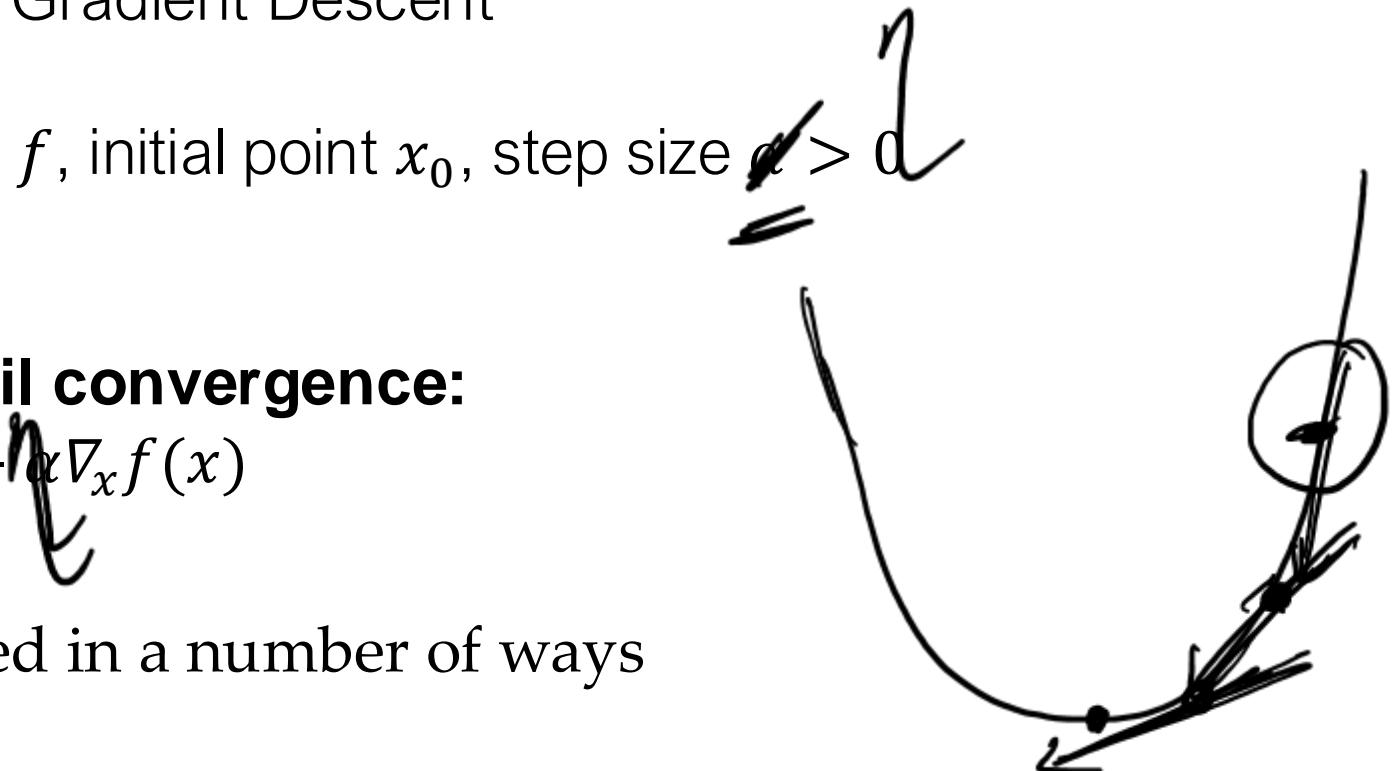
Initialize:

$x := x_0$

Repeat until convergence:

$x := x - \alpha \nabla_x f(x)$

“Convergence” can be defined in a number of ways



Why does gradient descent work?

Smooth function: Derivative exists everywhere, and gradient is L-Lipschitz

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

Taylor expansion: $f(y) \leq f(x) + (y - x)^T \nabla_x f(x)$

$$+ \frac{1}{2} \|\nabla^2 f(\xi)\|_2^2 \leq \frac{L}{2} \|y - x\|_2^2$$

x_{t+1}
 \uparrow
 x_t
 \uparrow

$$f(y) \leq f(x) + (y - x)^T \nabla_x f(x) + \frac{L}{2} \|y - x\|_2^2$$

Why does gradient descent work?

Smooth function: Derivative exists everywhere, and gradient is L-Lipschitz

$y = x + h$
 $x = x_t$ from prev slide

$$x_{t+1} = x_t - \eta \nabla f(x_t) \quad \eta = \frac{1}{L}$$
$$f(x_{t+1}) \leq f(x_t) - \eta \nabla f(x_t)^\top \nabla f(x_t) + \frac{L\eta^2}{2} \|\nabla f(x_t)\|_2^2$$

$$f(x_{t+1}) \leq f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|_2^2$$

Function value decreases

Why does gradient descent work?

Convexity: First-order condition $f(y) \geq f(x) + (y - x)^\top \nabla f(x)$

$$\left. \begin{aligned} f(x^*) &\geq f(x_t) + (x^* - x_t)^\top \nabla f(x_t) \\ f(x_{t+1}) &\leq f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|_2^2 \end{aligned} \right\} \begin{array}{c} \text{Convexity} \\ \text{Smoothness} \end{array}$$

χ^* : optimum
W

Why does gradient descent work?

Convexity: First-order condition $f(y) \geq f(x) + (y - x)^\top \nabla f(x)$

$$\begin{aligned} f(x^*) &\geq f(x_t) + (x^* - x_t)^\top \nabla f(x_t) \\ f(x_{t+1}) &\leq f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|_2^2 \end{aligned}$$

Convexity
Smoothness

$$\|x_{t+1} - x^*\|_2^2 = \|x_t - x^*\|_2^2 + \frac{1}{L^2} \|\nabla f(x_t)\|_2^2 + \frac{2}{L} (x^* - x_t)^\top \nabla f(x_t)$$

$u := x_t - x^*$
 $v := \eta \nabla f(x_t)$

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

$$= x_t - \frac{1}{L} \nabla f(x_t)$$

$\|u - v\|_2^2$
 $= \|u\|_2^2 + \|v\|_2^2$
 $+ 2 u^\top v$

$"no \text{magic}"$

Why does gradient descent work?

Convexity: First-order condition $f(y) \geq f(x) + (y - x)^\top \nabla f(x)$

$$f(x_{t+1}) \leq f(x^*) + \frac{L}{2} \left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right) \rightarrow \text{telescopic sums}$$

$$f(x_{t+1}) \leq f(x^*) + \frac{L}{2} \left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right)$$

summing over $t = 1$ to T

$$f(x_1) + f(x_2) \dots f(x_T)$$

$$\leq T f(x^*) + \frac{L}{2} \left(\|x_0 - x^*\|_2^2 - \|x_T - x^*\|_2^2 \right)$$

$$f(x_1) + f(x_2) \dots f(x_T)$$

$$\leq T f(x^*) + \frac{L}{2} \left(\|x_0 - x^*\|_2^2 \right)$$

$$f(x_T) \leq f(x_0) + t$$

$$\begin{array}{ccc} x_1 - x^* & & x_2 - x^* \\ \cancel{x_2 - x^*} & & \cancel{x_3 - x^*} \\ & & \end{array}$$

Why does gradient descent work?

Convexity: First-order condition $f(y) \geq f(x) + (y - x)^\top \nabla f(x)$

$$\left. \begin{aligned} f(x^*) &\geq f(x_t) + (x^* - x_t)^\top \nabla f(x_t) \\ f(x_{t+1}) &\leq f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|_2^2 \end{aligned} \right\} \begin{array}{c} \text{Convexity} \\ \text{Smoothness} \end{array}$$

$$\|x_{t+1} - x^\star\|_2^2 = \|x_t - x^\star\|_2^2 + \frac{1}{L^2} \|\nabla f(x_t)\|_2^2 + \frac{2}{L} (x^\star - x_t)^\top \nabla f(x_t)$$

$$f(x_{t+1}) \leq f(x^*) + \frac{L}{2} \left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right)$$

$$f(x_T) - f(x^*) \leq \frac{L}{2T}(\|x_0 - x^*\|_2^2)$$

as T increases
 $f(x_T)$ gets closer
to $f(x^*)$

Why does gradient descent work?

Function value decreases via smoothness assumption

Combining smoothness with convexity, with telescoping sums, we get

$$f(x_T) - f(x^*) \leq \frac{L}{2T}(\|x_0 - x^*\|_2^2)$$

When does gradient descent work?

Do you need smoothness?

What we really needed to show function value decreases:

$$f(y) \geq f(x) + (y - x)^T \nabla f(x)$$

When does gradient descent work?

Do you need smoothness?

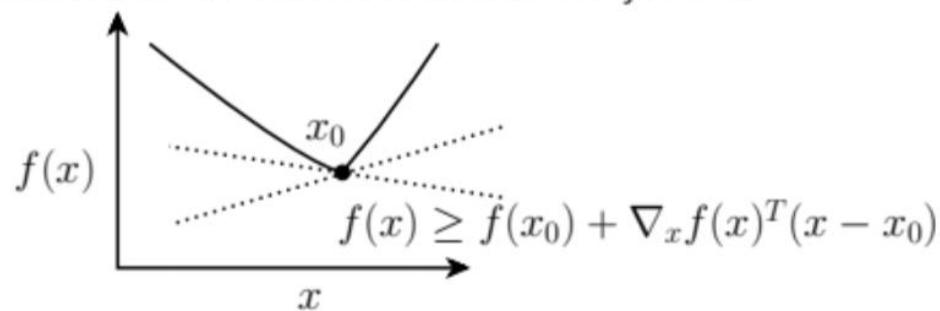
What we really needed to show function value decreases:

$$f(y) \geq f(x) + (y - x)^T \nabla f(x)$$

Can use subgradients instead

$$f(y) \geq f(x) + g^T(y - x)$$

A subgradient is something “like” a gradient, in that for a convex function it must lie below the function everywhere



Example: $f(x) = |x|$, subgradients are given by

$$\nabla_x f(x) = \begin{cases} -1 & x < 0 \\ 1 & x > 0 \\ g \in [0, 1] & x = 0 \end{cases}$$

When does gradient descent work?

Do you need smoothness?

What we really needed to show function value decreases:

$$f(y) \geq f(x) + (y - x)^\top \nabla f(x)$$

Can use subgradients instead

$$f(y) \geq f(x) + g^\top (y - x)$$

Method: subgradient “descent”

Need a decreasing sequence of step sizes...

Theory and practice of convergence is quite different

When does gradient descent work?

Do you need convexity?

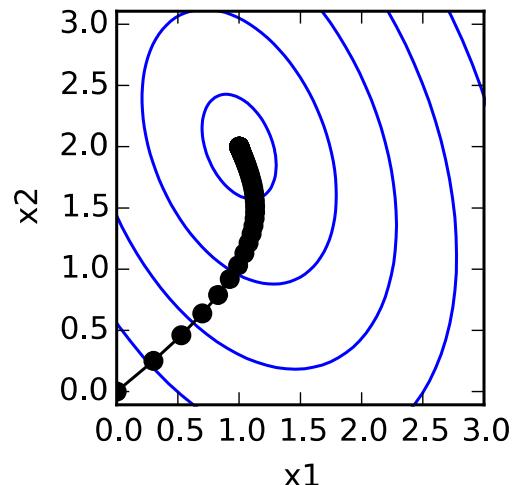
Local optimality no longer implies global optimality

Works surprisingly well in practice...

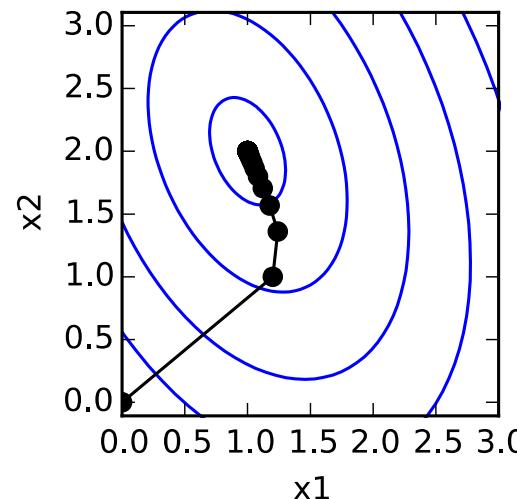
Gradient descent in practice

Choice of α matters a lot in practice:

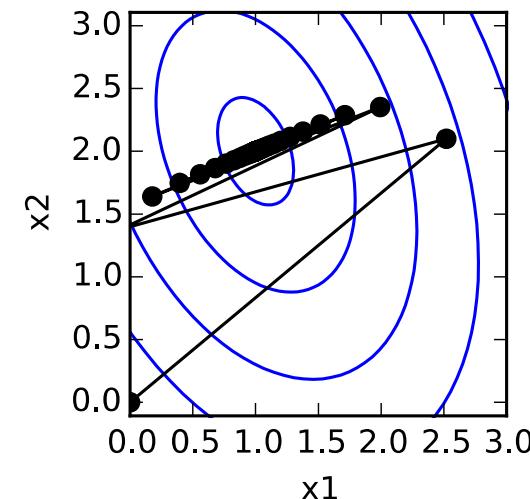
$$\underset{x}{\text{minimize}} \quad 2x_1^2 + x_2^2 + x_1x_2 - 6x_1 - 5x_2$$



$$\alpha = 0.05$$



$$\alpha = 0.2$$



$$\alpha = 0.42$$

Dealing with constraints

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

Repeat: $x := P_{\mathcal{C}}(x - \alpha \nabla_x f(x))$

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()
```