

# Nonconvex Optimization

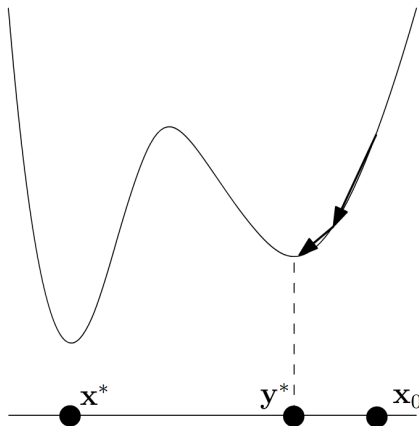
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# Gradient Descent in the nonconvex world

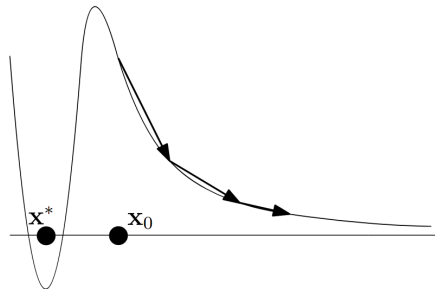
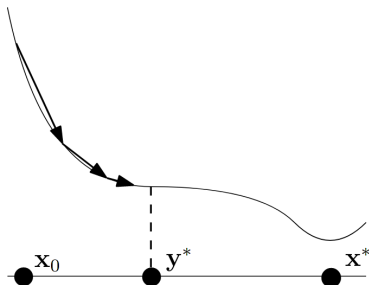
may get stuck in a **local** minimum and miss the global minimum



# Gradient Descent in the nonconvex world II

Even if there is a unique **local** minimum (equal to the global minimum), we

- ◇ may get stuck in a saddle point;
- ◇ run off to infinity;
- ◇ possibly encounter other bad behaviors.



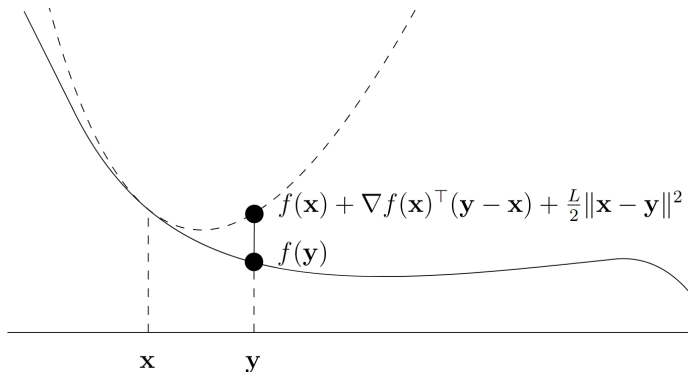
# Gradient Descent in the nonconvex world III

- ◇ Often, we observe good behavior in practice.
- ◇ Theoretical explanations many times missing.
- ◇ Under favorable conditions, we sometimes can say something useful about the behavior of GD.

# Smooth (but not necessarily convex) functions

**Recall:** A differentiable  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  is  $L$ -smooth over a convex set  $X$  if

$$f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} \|y - x\|^2, \quad \forall x, y \in X.$$



# Bounded Hessians $\Rightarrow$ smooth

## Lemma

Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  be twice differentiable and

$$\|\nabla^2 f(x)\| \leq L$$

where  $\|\cdot\|$  is spectral norm. Then  $f$  is  $L$ -smooth

Examples:

- ◇ all quadratic functions  $f(x) = x^T A x + b^T x + c$
- ◇  $f(x) = \sin(x)$  (many global minima)

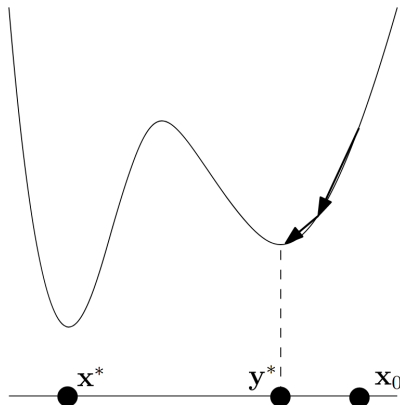
# Gradient descent on smooth functions

Will prove:  $\|\nabla f(x_k)\|^2 \rightarrow 0 \dots$

$\dots$  at the **same rate** as

$f(x_k) - f(x^*) \rightarrow 0$  in the convex case.

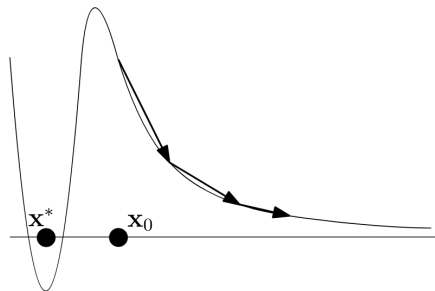
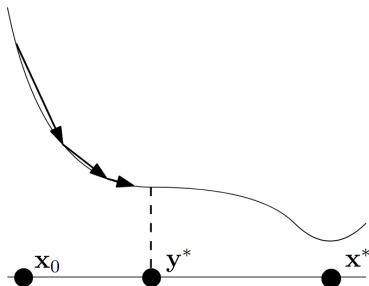
- ◇  $f(x_k) - f(x^*)$  itself may not converge to 0 in the nonconvex case:





# What does $\|\nabla f(x_k)\|^2 \rightarrow 0$ mean?

- ◇ May or **may not** mean convergence to a critical point  $\nabla f(y^*) = 0$
- ◇ critical point might not be even local minimum



# Gradient descent on smooth (not necessarily convex) functions

## Theorem

Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  be  $L$ -smooth with a global minimum  $x^*$ .  
Choosing stepsize  $\alpha := \frac{1}{L}$  gradient descent yields

$$\frac{1}{K} \sum_{k=0}^{K-1} \|\nabla f(x_k)\|^2 \leq \frac{2L}{K} (f(x_0) - f(x^*)).$$

In particular, same bound hold for “best” iterate

$$\min_{0 \leq k \leq K-1} \|\nabla f(x_k)\|^2 \leq \frac{2L}{K} (f(x_0) - f(x^*))$$

and (prove this — see exercises)

$$\lim_{k \rightarrow \infty} \|\nabla f(x_k)\|^2 = 0.$$

# Gradient descent on smooth functions II: Proof

Smoothness gives:

$$f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} \|y - x\|^2.$$

Use  $y = x_{k+1}$  and  $x = x_k$  to obtain

$$f(x_{k+1}) \leq f(x_k) + \langle \nabla f(x_k), -\alpha \nabla f(x_k) \rangle + \frac{L\alpha^2}{2} \|\nabla f(x_k)\|^2.$$

to obtain **sufficient decrease**:

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2L} \|\nabla f(x_k)\|^2.$$

# Proof II

**Sufficient decrease:**

$$\frac{1}{2L} \|\nabla f(x_k)\|^2 \leq f(x_k) - f(x_{k+1}).$$

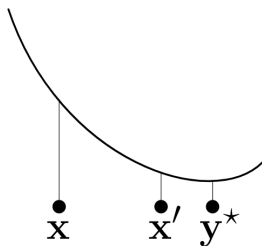
Sum up from  $k = 0, 1, \dots, K - 1$  to get

$$\frac{1}{2L} \sum_{k=0}^{K-1} \|\nabla f(x_k)\|^2 \leq f(x_0) - f(x_K) \leq f(x_0) - f(x^*).$$

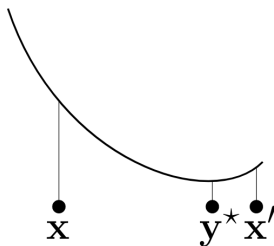
Multiply by  $2L/K$  to get the statement of the theorem.

# No overshooting

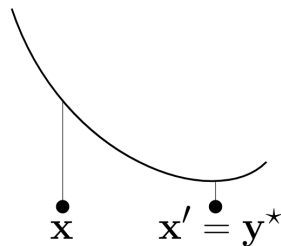
Under the **smoothness** assumption and **appropriate stepsize**  $\alpha \leq 1/L$ , GD cannot pass a critical point:



$$x' = x - \gamma \nabla f(x), \gamma < 1/L$$



overshooting



may happen with  $\gamma = 1/L$

# Trajectory Analysis

Even if the “landscape” (graph) of a nonconvex function has local minima, saddle points, and flat parts, gradient descent may avoid them and still converge to a global minimum.

For this, one needs a **good starting point** and some theoretical understanding of what happens when we start there — this is trajectory analysis.

# Linear models with several outputs

Recall: Learning linear models

- ◇  $n$  inputs  $x_1, \dots, x_n$ , where each input  $x_i \in \mathbb{R}^d$
- ◇  $n$  outputs  $y_1, \dots, y_n \in \mathbb{R}$
- ◇ Hypothesis (after centering / no bias):

$$y_i \approx w^T x_i,$$

for a weight vector  $w = (w_1, \dots, w_d) \in \mathbb{R}^d$  to be learned.

Now more than one output value:

- ◇  $n$  outputs  $y_1, \dots, y_n$ , where each output  $y_i \in \mathbb{R}^m$
- ◇ Hypothesis:

$$y_i \approx W x_i,$$

for a weight matrix  $W \in \mathbb{R}^{m \times d}$  to be learned.

# Minimizing the least squares error

Compute

$$W^* = \arg \min_{W \in \mathbb{R}^{m \times d}} \sum_{i=1}^n \|Wx_i - y_i\|^2.$$

- ◇  $X \in \mathbb{R}^{d \times n}$ : matrix whose columns are the  $x_i$
- ◇  $Y \in \mathbb{R}^{m \times n}$ : matrix whose columns are the  $y_i$

Then, equivalently

$$W^* = \arg \min_{W \in \mathbb{R}^{m \times d}} \|Wx - y\|_F^2.$$

where  $\|A\|_F = \sqrt{\sum_{i,j} a_{i,j}^2}$  is the Frobenius norm of a matrix  $A$ .

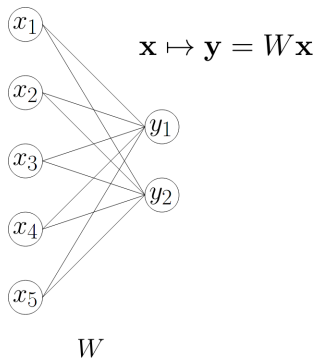
Frobenius norm of  $A$  = Euclidean norm of  $\text{vec}(A)$  ("flattening" of  $A$ ).



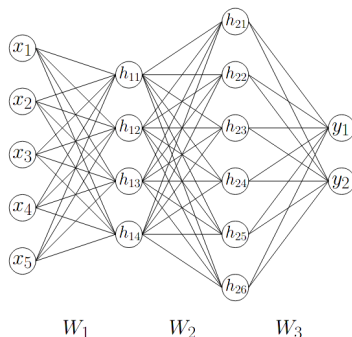
# Minimizing the least squares error II

$$W^* = \arg \min_{W \in \mathbb{R}^{m \times d}} \|WX - Y\|_F^2$$

- ◇ global minimum of a convex quadratic function  $f(W)$ .
- ◇ To find  $W^*$ , solve  $\nabla f(W) = 0$  (system of linear equations)
- ◇  $\Leftrightarrow$  training a linear neural network with **one layer** under least squares loss.



# Deep linear neural networks



$$\mathbf{x} \mapsto \mathbf{y} = W_3 W_2 W_1 \mathbf{x}$$

Not more expressive:

$$\mathbf{x} \mapsto W_3 W_2 W_1 \mathbf{x} \Leftrightarrow \mathbf{x} \mapsto W \mathbf{x}, \quad \text{for } W := W_3 W_2 W_1$$

# Training deep linear neural networks

With  $\ell$  layers:

$$W^* = \arg \min_{W_1, W_2, \dots, W_\ell} \|W_1 W_2 \cdots W_\ell X - Y\|_F^2$$

**Nonconvex** function for  $\ell > 1$ .

Playground to understand why training deep neural networks with gradient descent works.

Here: all matrices are  $1 \times 1$ ,  $W_i = x_i$ ,  $X = 1$ ,  $Y = 1$ ,  $\ell = d$

$\Rightarrow f : \mathbb{R}^d \rightarrow \mathbb{R}$ ,

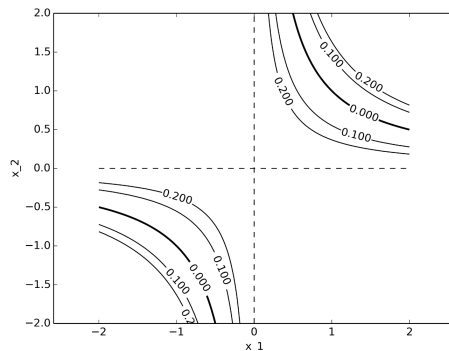
$$f(x) := \frac{1}{2} \left( \prod_{j=1}^d x_j - 1 \right)^2.$$

Toy example in our simple playground

# A simple nonconvex function

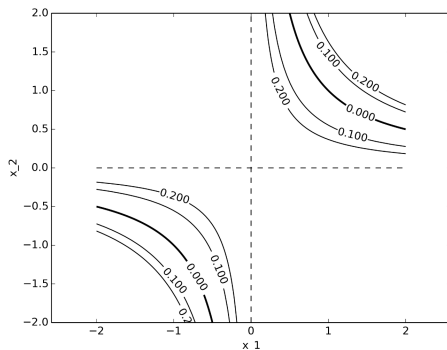
Nonconvex level sets:  $f(x) = \frac{1}{2} \left( \prod_j x_j - 1 \right)^2$ .

Dimensions is fixed so we ignore it.



# Gradient and critical points

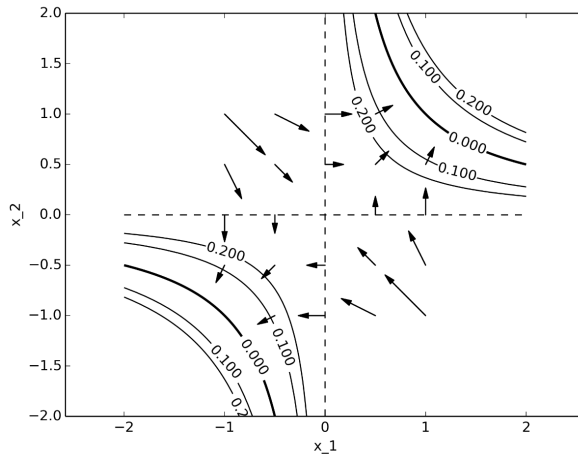
$$\nabla f(x) = \left( \prod_j x_j - 1 \right) \left( \prod_{j \neq 1} x_j, \dots, \prod_{j \neq d} x_j \right).$$



Critical points ( $\nabla f(x) = 0$ ) are either:

- ◇ global minima: if  $\prod_j x_j = 1$ 
  - ▶  $d = 2$ : hyperbola
- ◇ saddle point: if at least two of  $x_j$  are zero
  - ▶  $d = 2$ : only the origin  $(0, 0)$

# Negative gradient directions



Convergence to global minimum from almost everywhere.

# Convergence analysis: Overview

Convergence of GD holds for any  $d > 1$  and from anywhere in  $X = \{x : x > 0, \prod_j x_j \leq 1\}$ .

- ◇  $f$  is not smooth over  $X$ . But is smooth along the trajectory: For suitable  $L$  we still get

$$f(x_{k+1}) = f(x_k) - \frac{1}{2L} \|\nabla f(x_k)\|^2. \quad (\text{SD})$$

- ◇ saddle points have (at least two) zero entries  $\Rightarrow$  function value  $\geq 1/2$ .
- ◇ any starting point  $x_0 \in X$  has  $f(x_0) < 1/2$
- ◇ cannot converge to saddle points through (SD)

Still does not imply convergence to global minimum:

- ◇ Sublevel sets are unbounded: GD can run off to  $\infty$

## Convergence analysis: Overview II

For  $x > 0$ ,  $\prod_j x_j \geq 1$ , we can also show convergence:

$\Rightarrow$  convergence anywhere in the interior of the positive orthant  $\{x : x > 0\}$ .

For this, recall that

$$\nabla f(x) = \left( \prod_j x_j - 1 \right) \left( \prod_{j \neq 1} x_j, \dots, \prod_{j \neq d} x_j \right).$$

- ◇ since  $\prod_j x_j \geq 1$  then  $\nabla f(x) \geq 0$
- ◇ which implies that  $x_1 \leq x_0$  (componentwise)
- ◇ iterates remain in a bounded set  $\Rightarrow$  smoothness on this set



## Definition

Let  $x > 0$  (componentwise), and let  $c \geq 1$ .  $x$  is called  $c$ -balanced if  $x_i \leq cx_j$  for all  $1 \leq i, j \leq d$ .

## Theorem

Let  $c \geq 1$  and  $\delta > 0$  such that  $x^0 > 0$  is  $c$ -balanced with  $\delta \leq \prod_j x_j^0 < 1$ .  
Choosing the stepsize

$$\alpha = \frac{1}{3dc^2}$$

*gradient descent satisfies*

$$f(x^k) \leq \left(1 - \frac{\delta^2}{3c^4}\right)^k f(x^0).$$

# Discussion

- ◇ Error converges to 0 exponentially fast.
- ◇ But there's a catch: Consider  $x^0 = (1/2, \dots, 1/2)$ . Then  $\delta \leq \prod_j x_j^0 = 2^{-d}$
- ◇ Decrease in function value per step by factor

$$\left(1 - \frac{1}{34^d}\right).$$

- ◇ Contraction coefficient depends *exponentially bad on dimension*
- ◇ polynomial runtime: must start at distance  $\mathcal{O}(1/\sqrt{d})$  from optimality.

# Matrix completion

is the problem of recovering a **low rank** ( $r \ll d$ ) matrix  $M \in \mathbb{R}^{d \times d}$  from **partially observed entries**:

**Application: Netflix problem**

$$\begin{aligned} \min_{X \in \mathbb{R}^{d \times d}} \quad & \text{rank}(X) \\ \text{subject to} \quad & X_{i,j} = M_{i,j}, \quad \forall i, j \in \Omega \end{aligned}$$

But rank is **not continuous**...

# Convex matrix completion

Typically **convex** reformulations are considered via the **Nuclear norm** (sum of singular values)

$$\min_{X \in \mathbb{R}^{d \times d}} \|X\|_* := \sum_j \sigma_j(X)$$

subject to  $X_{i,j} = M_{i,j}, \quad \forall i, j \in \Omega$

- ◇ strong theoretical guarantees
- ◇ can be expensive
  - ▶  $\mathcal{O}(d^3)$  running time
  - ▶  $\mathcal{O}(d^2)$  memory.

# Nonconvex matrix completion

Can be cast in the bilinear  $X \approx UV^T$  form which gives:

$$\min_{U, V \in \mathbb{R}^{d \times r}} \sum_{i, j \in \Omega} \|(UV^T)_{i, j} - M_{i, j}\|^2.$$

- ◇ many global minima
- ◇ if  $UV^T = M$  then  $(UQ)(VQ)^T = M$  for any orthonormal matrix  $Q$   
orthonormal:  $QQ^T = \text{Id}$

No spurious local minima!

Can often be efficiently solved by GD or alternating minimization.