# Nonconvex Optimization

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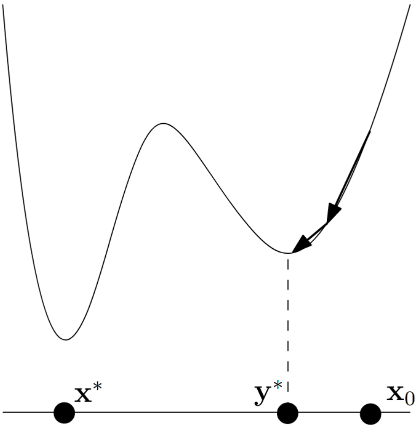
# Gradient Descent in the nonconvex world

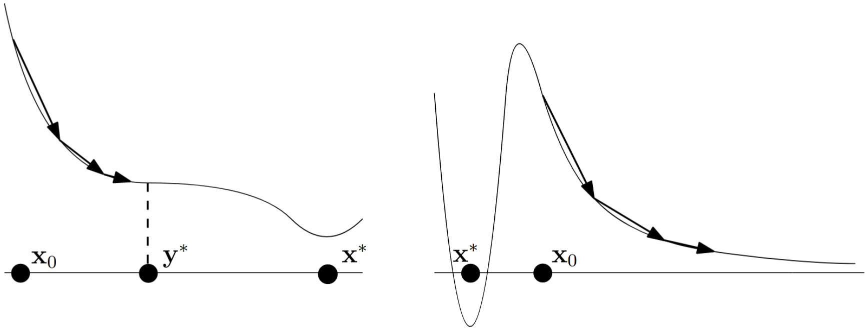
may get stuck in a local minimum and miss the global minimum



# 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.



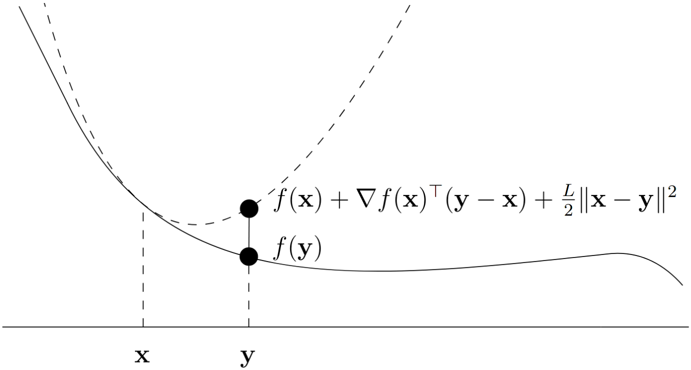
# Gradient Descent in the nonconvex world III

- 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 $f : \mathbb{R}^d \to \mathbb{R}$ 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 $f : \mathbb{R}^d \to \mathbb{R}$ be twice differentiable and*

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

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

Examples:

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

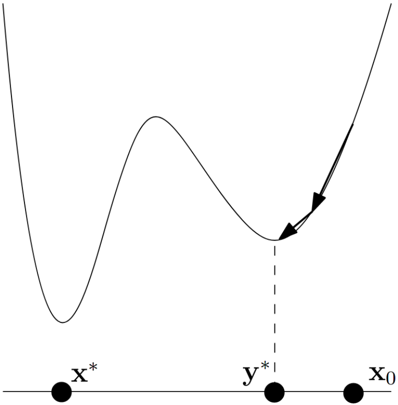
# Gradient descent on smooth functions

Will prove: $\|\nabla f(x_k)\|^2 \to 0 \ldots$

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

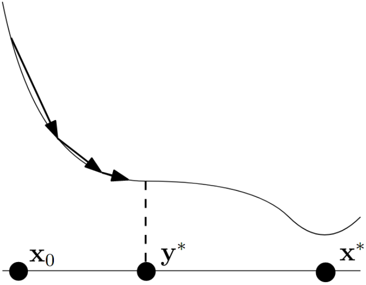
$f(x_k) - f(x^*) \to 0$ in the convex case.

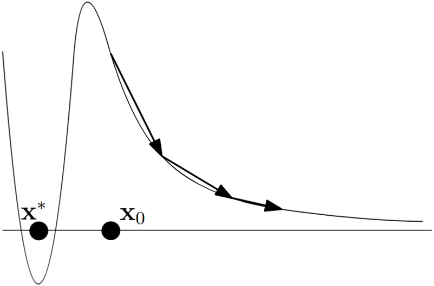
- $f(x_k) - f(x^*)$ itself may not converge to 0 in the nonconvex case:



# What does $\|\nabla f(x_k)\|^2 \to 0$ 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 $f : \mathbb{R}^d \to \mathbb{R}$ be $L$-smooth with a global minimum $x^*$. Choosing stepsize $\alpha := \frac{1}{L}$ gradient descent yields*

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

In particular, same bound hold for "best" iterate

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

and

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

# 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:**

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

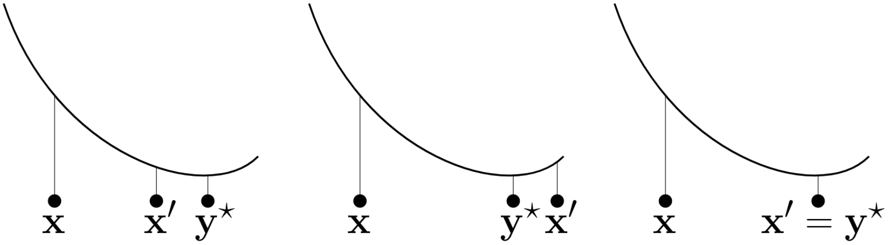
Sum up from $k = 0, 1, \ldots, K-1$ to get

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

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:




$\mathbf{x}' = \mathbf{x} - \gamma \nabla f(\mathbf{x}), \gamma < 1/L$ 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 $x_1, \ldots, x_n$, where each input $x_i \in \mathbb{R}^d$
- $n$ outputs $y_1, \ldots, y_n \in \mathbb{R}$
- Hypothesis (after centering / no bias):

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

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

Now more than one output value:

- $n$ outputs $y_1, \ldots, y_n$, 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

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

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

Then

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

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

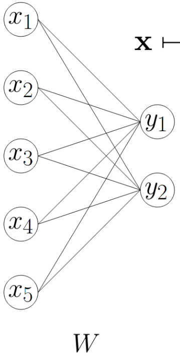
Frobenius norm of A = Euclidean norm of `vec(A)` (“flattening” of A).

# Minimizing the least squares error II

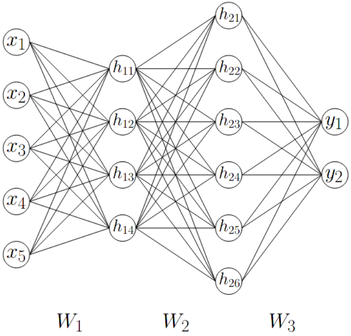
$$W^* = \underset{W \in \mathbb{R}^{m \times d}}{\arg\min} \|WX - Y\|_F^2$$

- 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.

$$\mathbf{x} \mapsto \mathbf{y} = W\mathbf{x}$$



# Deep linear neural networks




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

**Not more expressive**:

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

# Training deep linear neural networks

With $\ell$ layers:

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

**Nonconvex** function for $\ell > 1$.
Playground to understand why training deep neural networks with gradient descent works.
Here: all matrices are $1 \times 1$, $W_i = x_i$, $X = 1$, $Y = 1$, $\ell = d$
$\Rightarrow f : \mathbb{R}^d \to \mathbb{R}$,

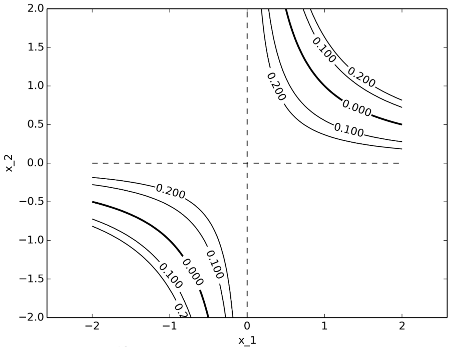
$$f(x) := \frac{1}{2}\left(\prod_{j=1}^{d} x_j - 1\right)^2.$$

Toy example in our simple playground

# A simple nonconvex function

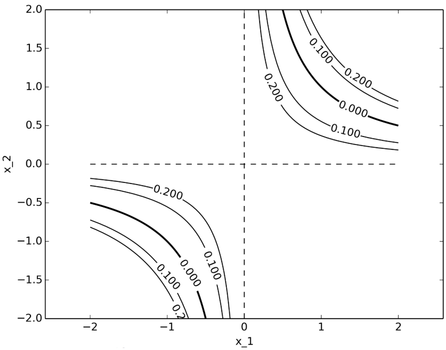
Nonconvex level sets: $f(x) = \frac{1}{2}\left(\prod_j x_j\right)$.

Dimensions is fixed so we ignore it.



# Gradient and critical points

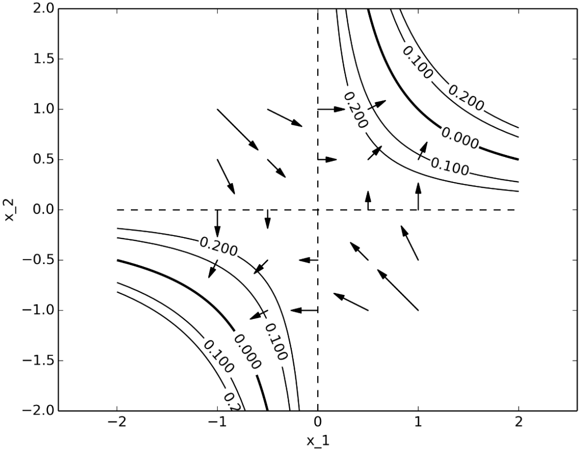
$$\nabla f(x) = \left(\prod_j x_j\right)\left(\prod_{j\neq 1} x_j, \cdots, \prod_{j\neq d} x_j\right).$$




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

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

- 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

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

- 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 $x_i \leq c x_j$ 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*

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

*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 $x^0 = (1/2, \ldots, 1/2)$. 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**

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

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

# Convex matrix completion

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

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

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

- 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: $QQ^T = \mathrm{Id}$

**No spurious local minima!**

Can often be efficiently solved by GD or alternating minimization.