

# NUMERICAL ANALYSIS FOR ARTIFICIAL INTELLIGENCE, WEEK 2

UCSD Summer session II 2018

CSE 190

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# Derivatives 1 (univariate)

## What is the derivative ?

Measures the rate of change of a function  
(**negative** when function is **decreasing**  
and **positive** when function is **increasing**)

[Mathematica 1d gradient presentation](#)

# Numerical vs symbolic derivatives

Derivative of function  $f$

Derivative symbol

at  $x$

with respect to  $x$

Limit as  $h$  approaches 0

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

Numerical derivative

Estimate of the rate  
change of  $f$  for fixed (small)  $h$

$$\frac{f(x+h) - f(x)}{h}$$

# Numerical vs symbolic derivatives

## *Computation of derivatives symbolically using the rules of differentiation*

$$\bullet \frac{d}{d(x)}(a) = 0 \quad \bullet \frac{d}{d(x)}(x) = 1 \quad \bullet \frac{d}{d(x)}(x^n) = n(x)^{n-1}$$

$$\bullet \frac{d}{d(x)}[f(x) \pm g(x)] = f'(x) \pm g'(x) \quad \bullet \frac{d}{d(x)}[c f(x)] = c f'(x)$$

$$\bullet \frac{d}{d(x)}[f(x) \cdot g(x)] = f'(x)g(x) + g'(x)f(x) \quad \text{Product rule}$$

$$\bullet \frac{d}{d(x)}\left[\frac{f(x)}{g(x)}\right] = \frac{f'(x)g(x) - g'(x)f(x)}{[g(x)]^2} \quad \text{Quotient rule}$$

$$\bullet \frac{d}{d(x)} f[g(x)] = f'[g(x)]g'(x) \quad \text{Chain rule}$$

$$\bullet \frac{d}{d(x)} f(x)^n = n f(x)^{n-1} \cdot f'(x) \quad \text{Power rule}$$

$$\bullet \frac{d}{d(x)} f(kx + e) = k f'(kx + e)$$

$$\bullet \frac{d}{d(x)} \ln[f(x)] = \frac{f'(x)}{f(x)}$$

smtutor.com

$$[x^a]' = a \cdot x^{a-1}, \quad x \in \mathbb{R} \text{ for } a \in \mathbb{N}, \quad x \in \mathbb{R} - \{0\} \text{ for } a \in \mathbb{Z}, \\ x \in \mathbb{R}^+ \text{ for } a \in \mathbb{R}.$$

$$[e^x]' = e^x, \quad x \in \mathbb{R};$$

$$[a^x]' = \ln(a)a^x, \quad x \in \mathbb{R}.$$

$$[\ln(x)]' = \frac{1}{x}, \quad x > 0;$$

$$[\log_a(x)]' = \frac{1}{\ln(a)} \frac{1}{x}, \quad x > 0.$$

$$[\sin(x)]' = \cos(x), \quad x \in \mathbb{R};$$

$$[\cos(x)]' = -\sin(x), \quad x \in \mathbb{R};$$

$$[\tan(x)]' = \frac{1}{\cos^2(x)}, \quad x \neq \frac{\pi}{2} + k\pi;$$

$$[\cot(x)]' = \frac{-1}{\sin^2(x)}, \quad x \neq k\pi.$$

$$[\arcsin(x)]' = \frac{1}{\sqrt{1-x^2}}, \quad x \in (-1, 1);$$

$$[\arccos(x)]' = \frac{-1}{\sqrt{1-x^2}}, \quad x \in (-1, 1);$$

$$[\arctan(x)]' = \frac{1}{x^2+1}, \quad x \in \mathbb{R};$$

$$[\operatorname{arccot}(x)]' = \frac{-1}{x^2+1}, \quad x \in \mathbb{R}.$$

$$[\sinh(x)]' = \cosh(x), \quad x \in \mathbb{R};$$

$$[\cosh(x)]' = \sinh(x), \quad x \in \mathbb{R};$$

$$[\tanh(x)]' = \frac{1}{\cosh^2(x)}, \quad x \in \mathbb{R};$$

$$[\operatorname{coth}(x)]' = \frac{-1}{\sinh^2(x)}, \quad x \neq 0.$$

$$[\operatorname{argsinh}(x)]' = \frac{1}{\sqrt{x^2+1}}, \quad x \in \mathbb{R};$$

$$[\operatorname{argcosh}(x)]' = \frac{1}{\sqrt{x^2-1}}, \quad x \in (1, \infty);$$

$$[\operatorname{argtanh}(x)]' = \frac{1}{1-x^2}, \quad x \in (-1, 1);$$

$$[\operatorname{argcoth}(x)]' = \frac{1}{1-x^2}, \quad x \in (-\infty, -1) \cup (1, \infty).$$

See the comparison of numerical and symbolic derivatives in [week1\\_2.ipynb](#)

# Chain rule

The rule for differentiating compositions of functions

inner function

If  $f = g(h)$  and  $h = h(x)$ , then  $\frac{df}{dx} = \frac{dg}{dh} \times \frac{dh}{dx}$

$f$  is a composed function

outer function

Derivative of the outer function

Derivative of the inner function

# Example for the chain rule in practice

$$f(x) = \arctan x^3$$

1. Decomposition of  $f$  into the outer ( $g$ ) / inner ( $h$ ) functions.

$$f(x) = g(h(x))$$

$g(h) = \arctan h$
$h(x) = x^3$

2. Differentiate  $g$  and  $h$ .

$\frac{d}{dx} \arctan x = \frac{1}{1+x^2}$	<table border="1"><tr><td><math>g(h) = \arctan h</math></td><td><math>g'(h) = \frac{1}{1+h^2}</math></td></tr><tr><td><math>h(x) = x^3</math></td><td><math>h'(x) = 3x^2</math></td></tr></table>	$g(h) = \arctan h$	$g'(h) = \frac{1}{1+h^2}$	$h(x) = x^3$	$h'(x) = 3x^2$
$g(h) = \arctan h$	$g'(h) = \frac{1}{1+h^2}$				
$h(x) = x^3$	$h'(x) = 3x^2$				
$\frac{d}{dx} x^3 = 3x^2$					

3. Compose the final result

$$\frac{df}{dx} = \frac{dg}{dh} \times \frac{dh}{dx} = \frac{1}{1+h^2} \cdot 3x^2 = \frac{1}{1+x^6} \cdot 3x^2.$$

See the comparison of this derivative with symbolic in [week1 2.ipynb](#)

# Partial derivatives and gradients

Partial derivative with respect to  $x$   $\longrightarrow \frac{\partial f}{\partial x}(x, y)$  When computing, treat  $y$  as a constant

Partial derivative with respect to  $y$   $\longrightarrow \frac{\partial f}{\partial y}(x, y)$  When computing, treat  $x$  as a constant

gradient  $\nabla f(x, y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix}$

[Mathematica 2d gradient presentation](#)

# Computing partial derivatives analytically

$$f(x, y) = \sin xy$$

Compute  $\frac{\partial f}{\partial x}$  applying the univariate chain rule (treating  $y$  as constant)  
we have  $f(x, y) = g(h)$ ,  $h = h(x)$

$g(h) = \sin h$	$g'(h) = \cos h$
$h(x) = xy$	$h'(x) = y$

$$\frac{\partial f}{\partial x} = \frac{dg}{dh} \times \frac{dh}{dx} = \cos(xy) \cdot y.$$

And analogously

$$\frac{\partial f}{\partial y} = \frac{dg}{dh} \times \frac{dh}{dy} = \cos(xy) \cdot x.$$



# Computing 2D gradients numerically

Estimate the rate of change of  $f(x, y)$   
for fixed (small)  $h$  in  $x$  and  $y$  direction

$$\frac{f(x + h, y) - f(x, y)}{h}$$

$$\frac{f(x, y + h) - f(x, y)}{h}$$

Those two quantities form a numerical gradient of  $f(x, y)$

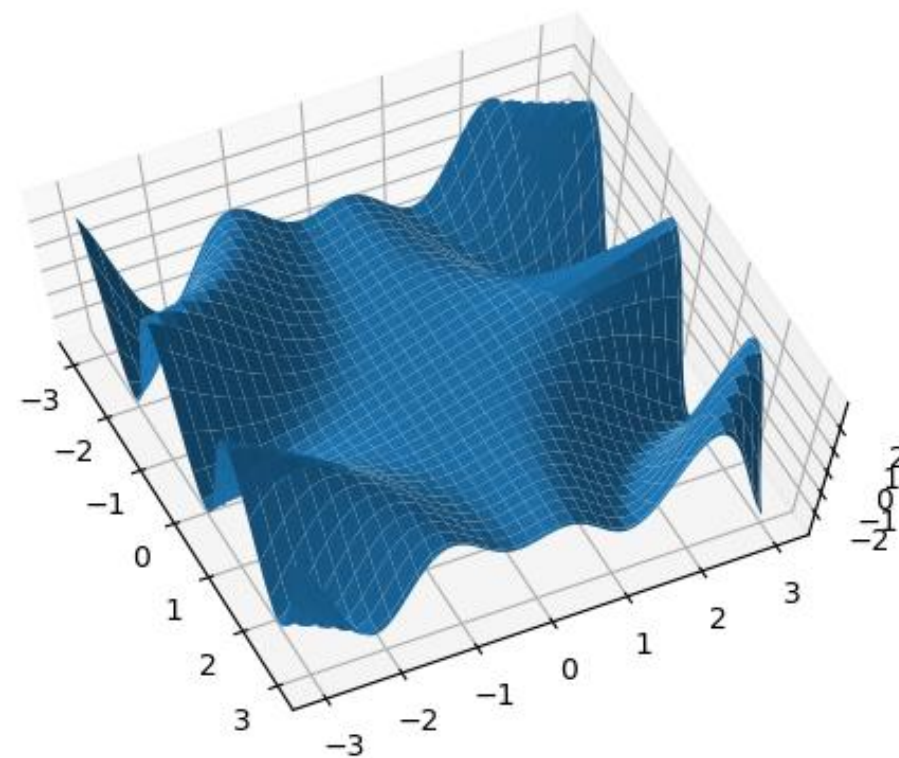
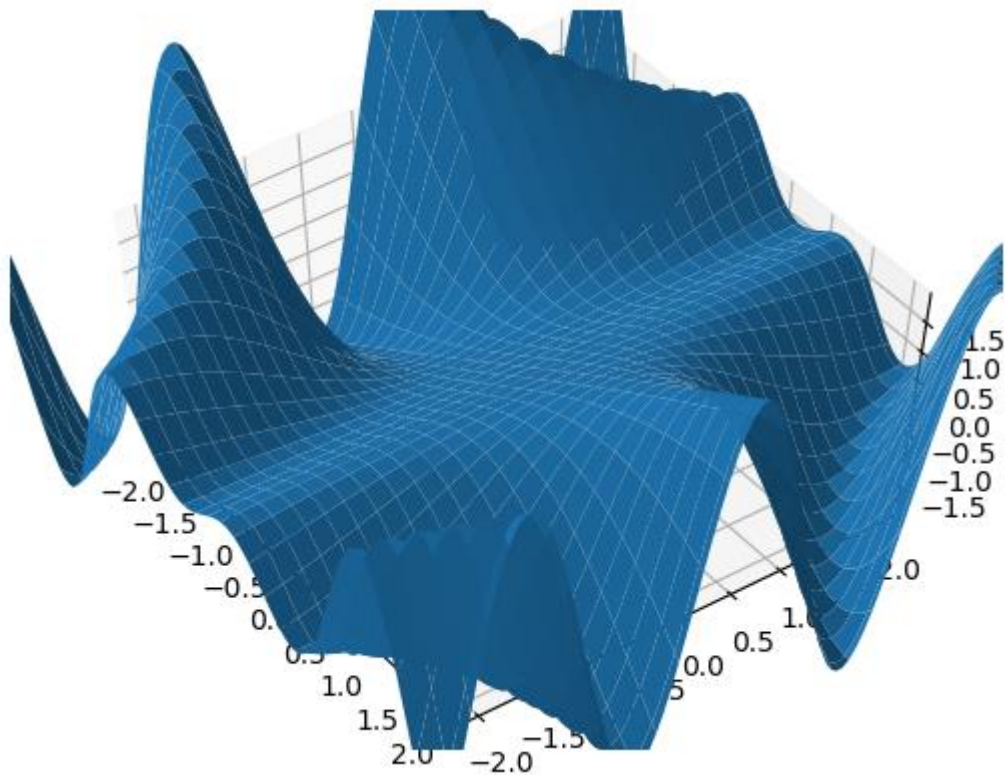
# Differentiating the sigmoid function

...Show on the blackboard...

# Plotting gradient components

```
#import matplotlib 3d plotting
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
```

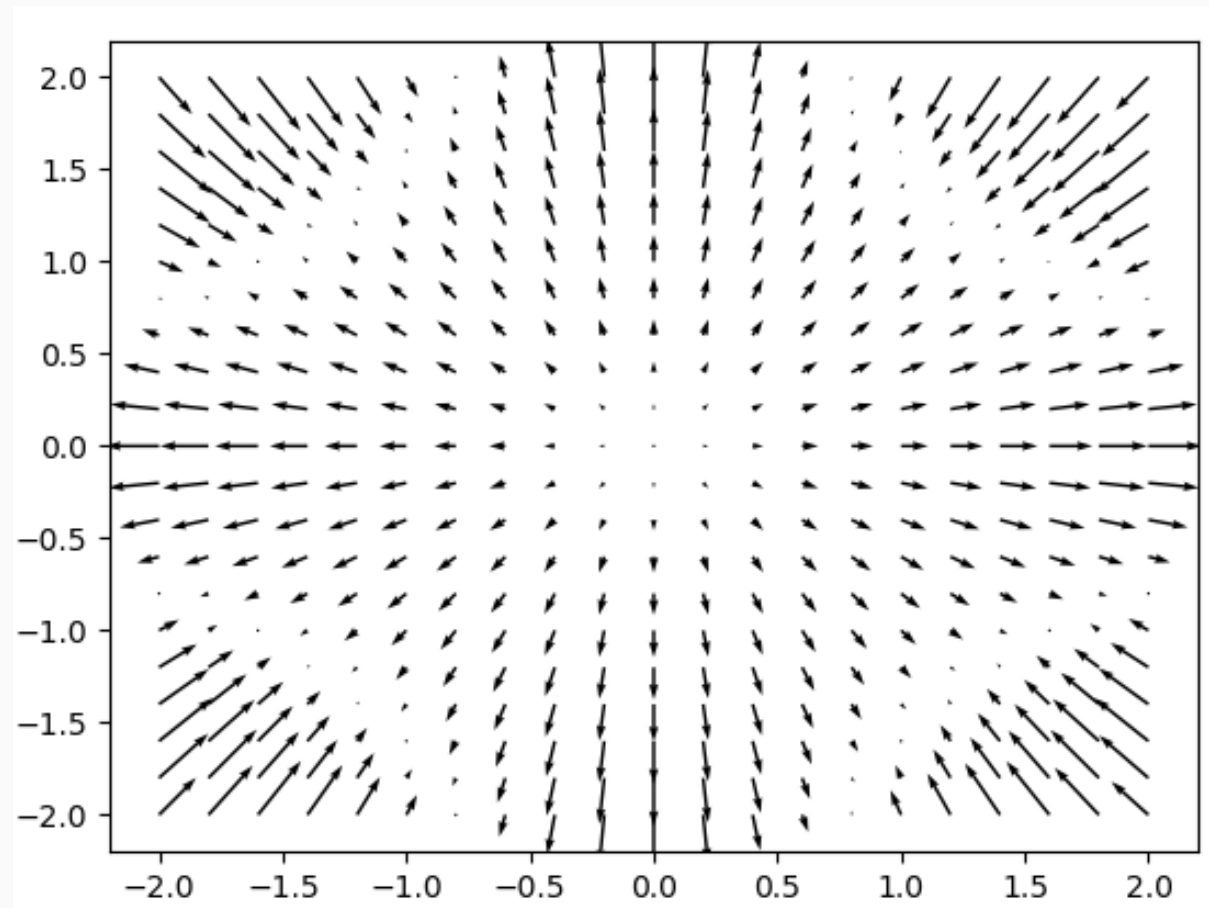
```
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.plot_surface(xsf, ysf, gradx)
plt.show()
```



See 3d plotting in [week2 1.ipynb](#)

# Plotting gradients as a vector field

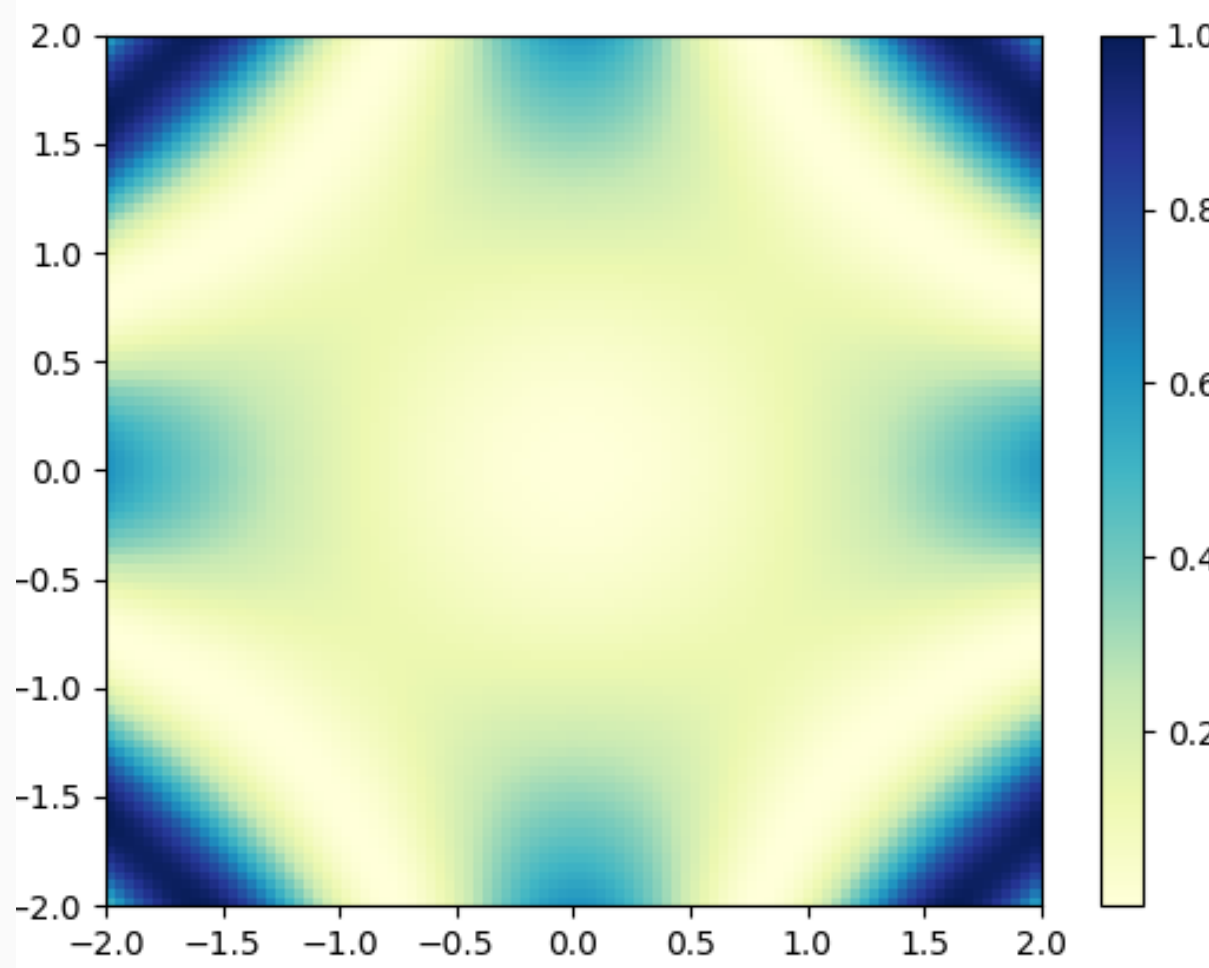
Two components of the gradient can be plotted on a single figure as a so-called **vector field**



See the gradient vector field plotting in [week2 1.ipynb](#)

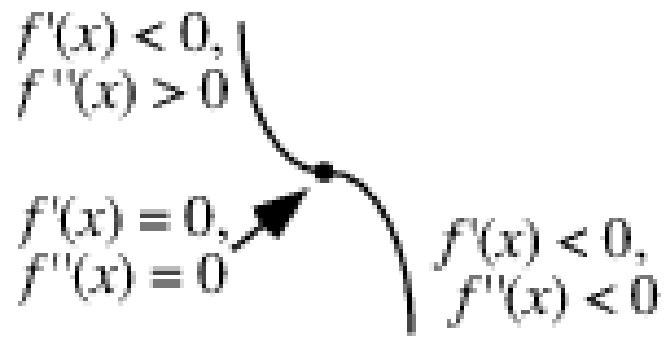
# Yet another way of plotting the gradient

## Heat map

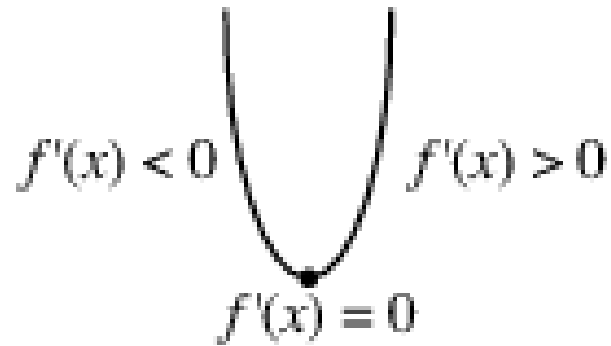


See the gradient heatmap plotting in [week2 1.ipynb](#)

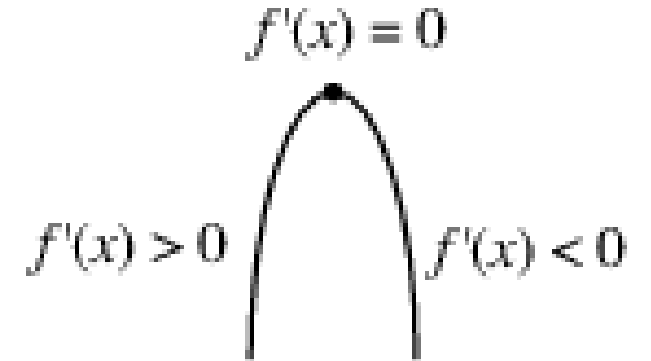
# Critical points in 1D



*inflection point*



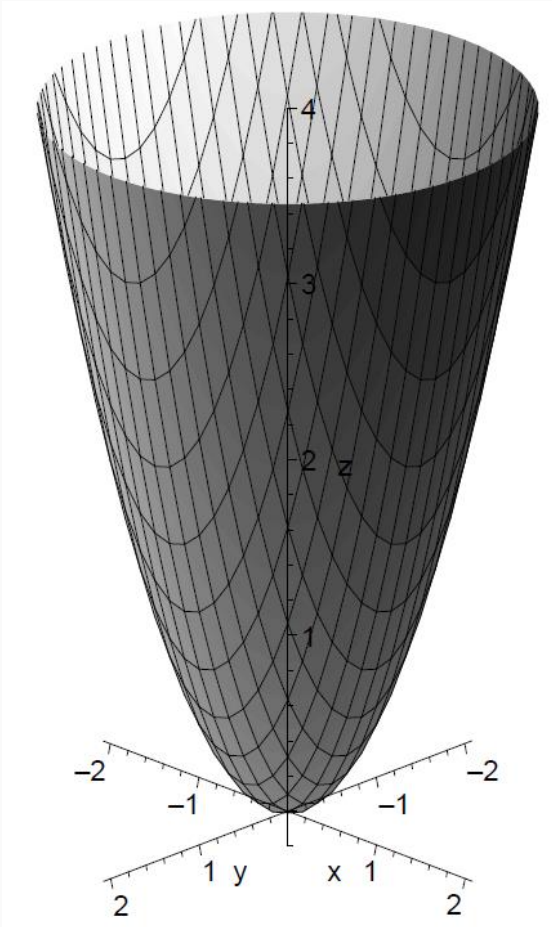
*minimum*



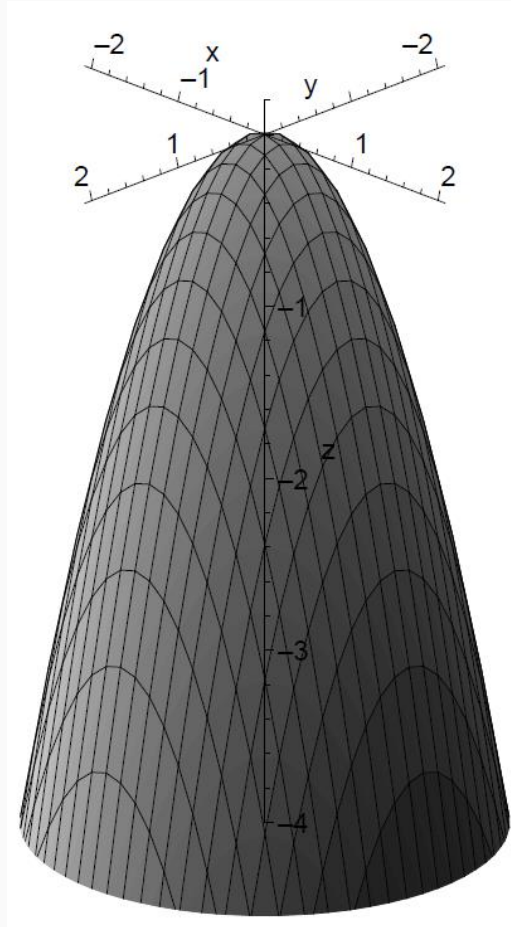
*maximum*

[Mathematica 1d derivative presentation](#)

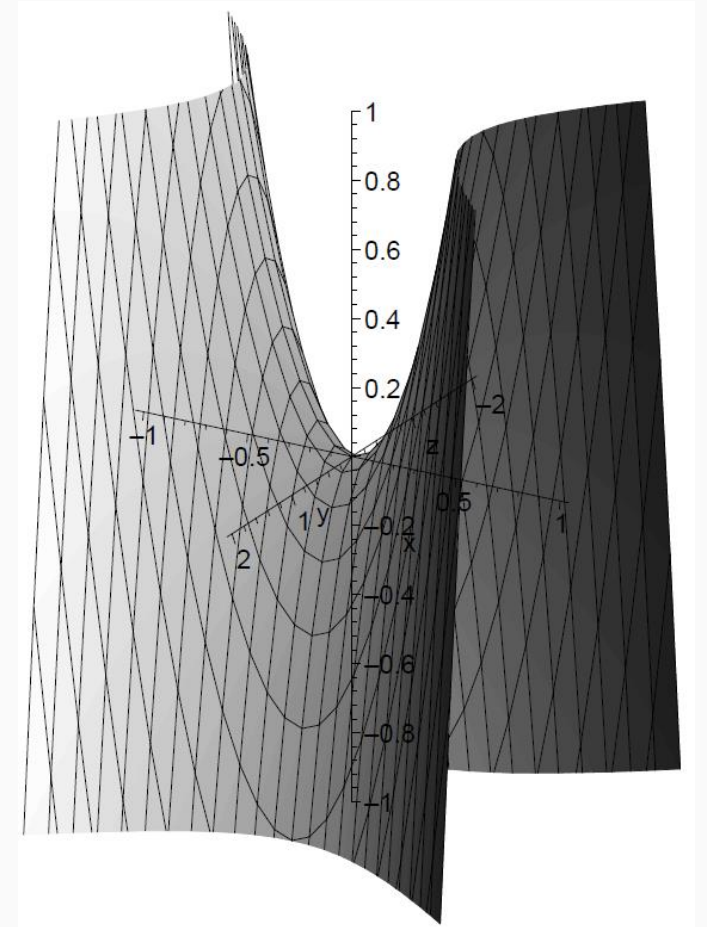
# Critical points in multi-D



$$f(x, y) = x^2 + 3y^2$$



$$f(x, y) = -(x^2 + y^2)$$



$$f(x, y) = -x^2 + 3y^2$$

$(x, y)$  is a critical point iff  $\nabla f(x, y) = 0$  (in the sense the gradient is zero vector)

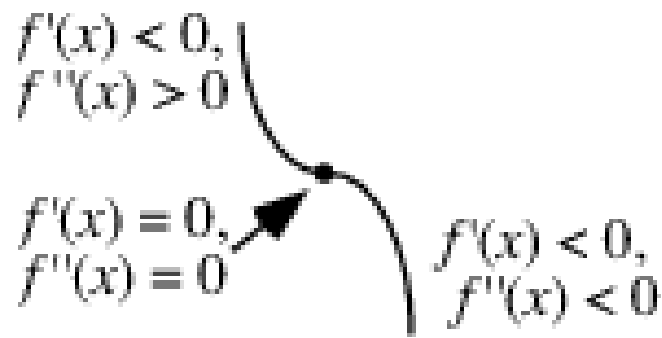
# Characterization of critical points in 1D

**Question:** how to characterize a critical point as **min / max / saddle ???**

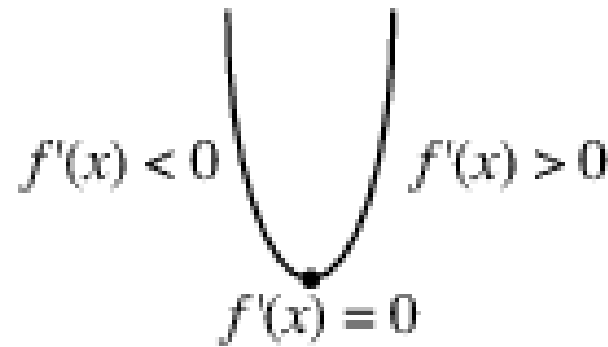
Apply calculus methods !!!



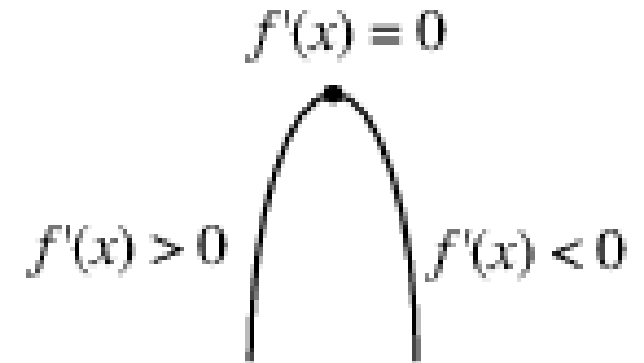
# The first derivative test for critical points in 1D



*inflection point*



*minimum*



*maximum*

**Algorithm for finding and classifying critical points of a 1D function using the 1<sup>st</sup> derivative test**

**IN:** function  $f$ , search interval  $[min, max]$ ,  $h$  'resolution parameter',  $\epsilon$  'precision parameter'

**OUT:** set of  $n$  critical points locations  $\{x_i\}_1^n$  and their characterization as min/max/saddle.

1. Compute the numerical derivative (with resolution  $h$  in interval  $[min, max]$  ).
2. Find critical points locations , i.e.  $x$  values for which  $|f'(x)| < \epsilon$ .
3. Check the sign of the derivative on the left-hand and right-hand side of the found  $x$  values.
4. If  $-$ ,  $-$  or  $+$ ,  $+$  then classify as inflection point, if  $-$ ,  $+$  then classify as minimum, and if  $+$ ,  $-$  then classify as maximum.

# Computing the second derivative numerically

The second derivative of function  $f$

$$f''(x) = \frac{d^2 f}{dx^2}(x)$$

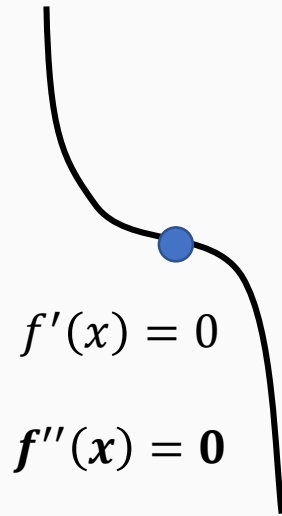
taken twice with respect to  $x$

*Interpretation:* 1<sup>st</sup> derivative measures the rate of change, 2<sup>nd</sup> derivative measures convexity(when+)/concavity(when-)

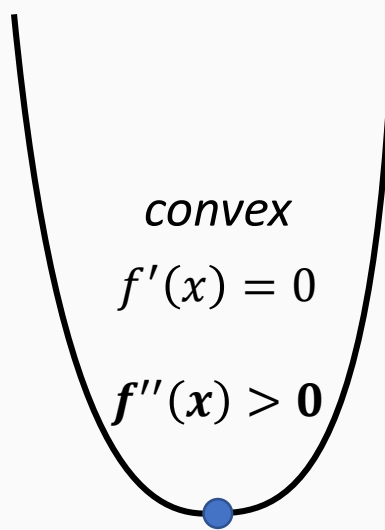
*Numerical formula for the second derivative in 1D*

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

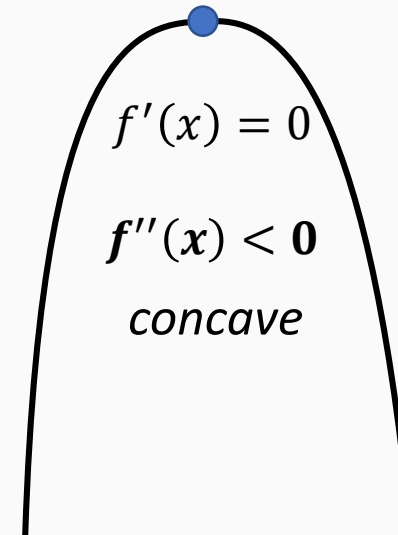
# The second derivative test for critical points in 1D



*Inflection point*



*minimum*



*maximum*

**Algorithm for finding and classifying critical points of a 1D function using the 2<sup>nd</sup> derivative test**

**IN:** function  $f$ , search interval  $[min, max]$ ,  $h$  'resolution parameter',  $\varepsilon$  'precision parameter'

**OUT:** set of  $n$  critical points locations  $\{x_i\}_1^n$  and their characterization as min/max/saddle.

1. Compute the numerical derivative ( with resolution  $h$  in interval  $[min, max]$  ).
2. Find critical points locations , i.e.  $x$  values for which  $|f'(x)| < \varepsilon$ .
3. Compute the second derivative at the found  $x$  values.
4. If 2<sup>nd</sup> derivative has value  $< \varepsilon$  then classify as inflection point, if  $-$  then classify as maximum, if  $+$  then classify as minimum.

# Second order partial derivatives

The second derivative of  $f$

$$\frac{\partial f^2}{\partial x \partial x}(x, y) \quad \frac{\partial f^2}{\partial x \partial y}(x, y) \quad = \quad \frac{\partial f^2}{\partial y \partial x}(x, y) \quad \frac{\partial f^2}{\partial y \partial y}(x, y)$$

↓ usually same

↑ ↑ taken first with respect to  $y$  and then w.r.t.  $x$

taken first with respect to  $y$  and then w.r.t.  $x$

*Altogether they form the so-called 'Hessian' matrix*

$$f''(x, y) = \begin{bmatrix} \frac{\partial f^2}{\partial x \partial x}(x, y) & \frac{\partial f^2}{\partial x \partial y}(x, y) \\ \frac{\partial f^2}{\partial y \partial x}(x, y) & \frac{\partial f^2}{\partial y \partial y}(x, y) \end{bmatrix}$$

*Also use a different notation*

$$\partial_{xx} f(x, y) \quad \partial_{xy} f(x, y) \quad \partial_{yx} f(x, y) \quad \partial_{yy} f(x, y)$$

# Eigenvalues and Eigenvectors

## Eigenvalues and Eigenvectors

For an  $n \times n$  matrix  $\mathbf{A}$ , scalars  $\lambda$  and vectors  $\mathbf{x}_{n \times 1} \neq \mathbf{0}$  satisfying  $\mathbf{Ax} = \lambda\mathbf{x}$  are called *eigenvalues* and *eigenvectors* of  $\mathbf{A}$ , respectively, and any such pair,  $(\lambda, \mathbf{x})$ , is called an *eigenpair* for  $\mathbf{A}$ . The set of *distinct* eigenvalues, denoted by  $\sigma(\mathbf{A})$ , is called the *spectrum* of  $\mathbf{A}$ .

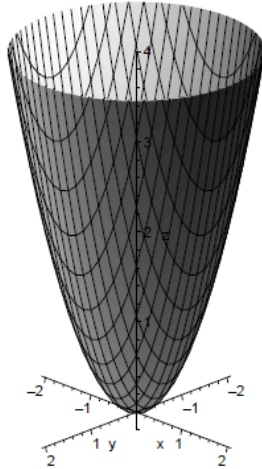
# Positive/negative definiteness of a symmetric matrix

Given symmetric matrix  $M \in \mathbb{R}^{n \times n}$  is

- **Positive-definite** if all its eigenvalues are positive (strictly) or equivalently  $x^T \cdot M \cdot x > 0$  for all vectors  $x \neq 0$ ,
- **Negative-definite** if all its eigenvalues are negative (strictly) or equivalently  $x^T \cdot M \cdot x < 0$  for all vectors  $x \neq 0$ ,
- Otherwise, it is *undefined*,

# Characterization of 2D (and multiD) critical points

EXAMPLE: **Standard minimum**  $f(x,y) = x^2 + 3y^2$



Find critical points:

$$\partial_x f(x,y) = 2x, \quad \partial_y f(x,y) = 6y$$

so the only critical point is the origin,  $(0,0)$ .

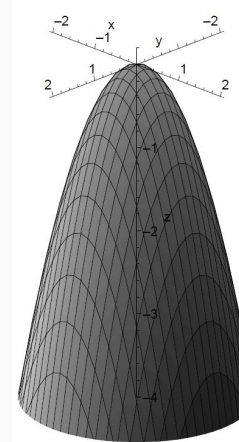
Second derivative test:

$$\partial_{xx} f(x,y) = 2, \quad \partial_{xy} f(x,y) = 0, \quad \partial_{yy} f(x,y) = 6$$

$f''(0,0)$  is the diagonal matrix

$$f''(0,0) = \begin{pmatrix} 2 & 0 \\ 0 & 6 \end{pmatrix}.$$

This is *positive definite* so the origin is a local minimum.



$$f(x,y) = -(x^2 + y^2)$$

$$\partial_x f(x,y) = -2x, \quad \partial_y f(x,y) = -2y,$$

The critical point is  $(0,0)$ ,

Second derivative test:

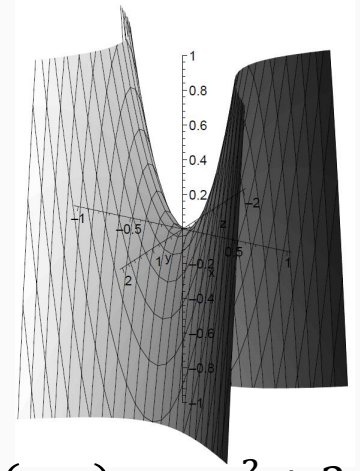
$$\partial_{xx} f(x,y) = -2,$$

$$\partial_{yy} f(x,y) = -2,$$

$$\partial_{xy} f(x,y) = 0.$$

$$f''(0,0) = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}$$

This is *negative-definite*,  
so  $(0,0)$  is a *local maximum*.



$$f(x,y) = -x^2 + 3y^2$$

$$\partial_x f(x,y) = -2x, \quad \partial_y f(x,y) = 6y,$$

The critical point is  $(0,0)$ ,

Second derivative test:

$$\partial_{xx} f(x,y) = -2,$$

$$\partial_{yy} f(x,y) = 6,$$

$$\partial_{xy} f(x,y) = 0.$$

$$f''(0,0) = \begin{bmatrix} -2 & 0 \\ 0 & 6 \end{bmatrix}$$

This is *undefined*,  
and no zero eigenvalues,  
so  $(0,0)$  is a *saddle*.

# Computing 2<sup>nd</sup> order derivatives numerically

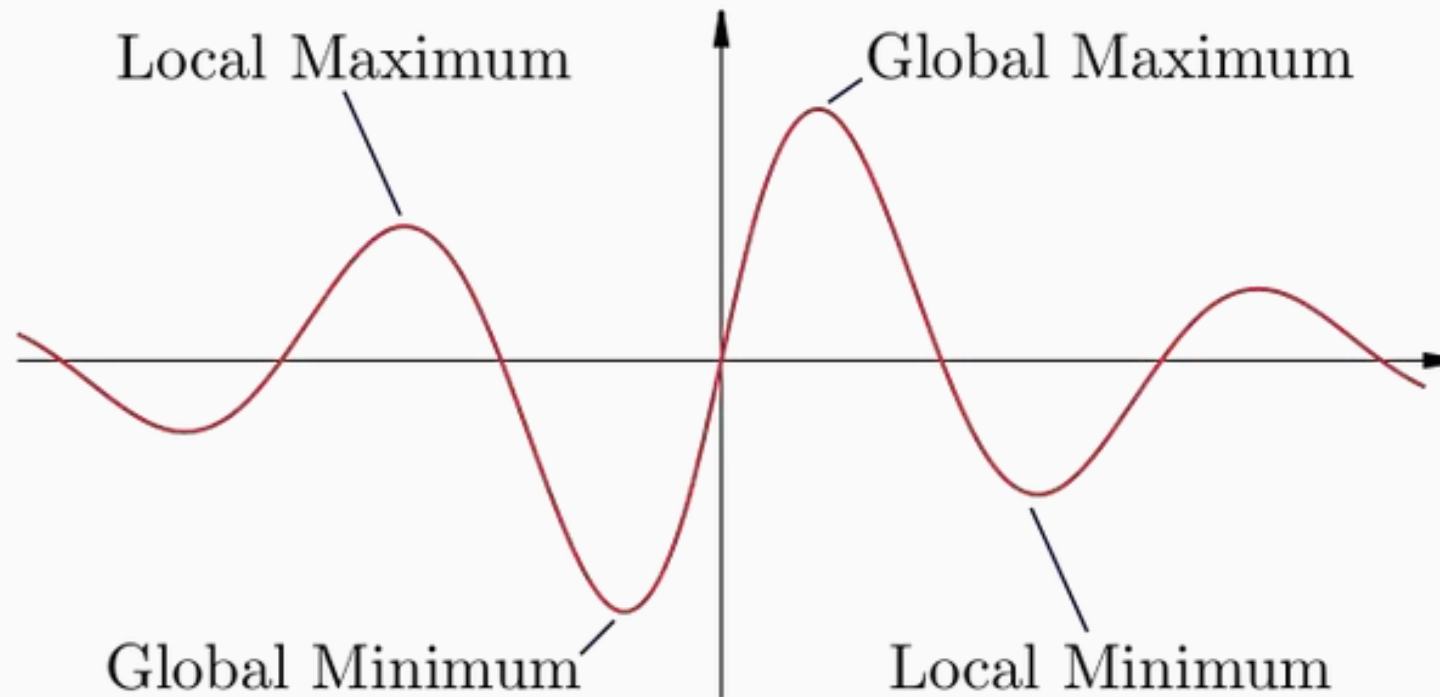
$$f_{xx}(x, y) \approx \frac{f(x + h, y) - f(x, y) + f(x - h, y)}{h^2},$$

$$f_{yy}(x, y) \approx \frac{f(x, y + h) - 2f(x, y) + f(x, y - h)}{h^2},$$

$$f_{xy}(x, y) \approx \frac{f(x + h, y + h) - f(x + h, y - h) - f(x - h, y + h) + f(x - h, y - h)}{4h^2}$$



# Global / local minima

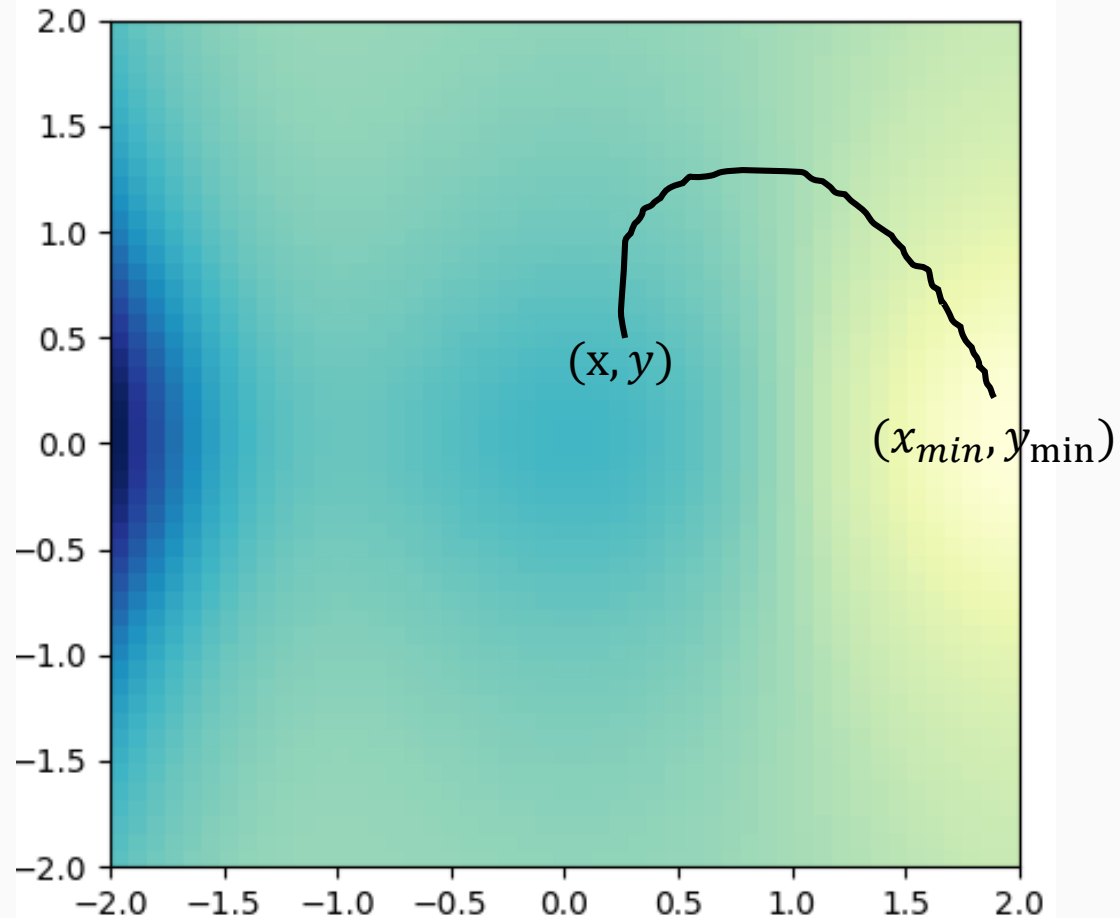


- Maximum = local maximum or global maximum,
- Minimum = local minimum or global minimum,
- There is only one global max and global min,
- There can be a lot of local min and local max.

# How to find a minimum of a 2D function?

**Big question:** How to find minima of a multiD function, without checking the numerical derivative of all points on a multiD grid ???  
(The first optimization algorithm)

# Algorithm for descent without gradient method

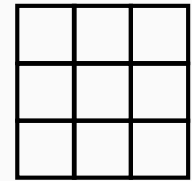


## Algorithm for descent without gradient method

**IN:** function  $f$ , search box  $[min, max]x[min, max]$ ,  $h$  'resolution parameter'

**OUT:** a minimum position  $(x_{min}, y_{min})$

1. Choose the initial point  $(x, y)$  by random,
2. Considering the current point  $(x, y)$ , investigate  $f$  values for all nodes in the neighborhood  
 $(x + h, y)$ ,  $(x, y + h)$ ,  
 $(x + h, y + h)$ ,  $(x - h, y - h)$ ,  
 $(x + h, y - h)$ ,  $(x - h, y + h)$ ,  
 $(x - h, y)$ ,  $(x, y - h)$
3. Set new  $(x, y)$  to the point in the neighborhood attaining the lowest  $f$  value (also lower than current  $f(x, y)$ )
4. If there is no such point terminate, otherwise go to Step 2.



### WARNING:

This Optimization method is impractical,  
We are implementing it to see advantages of  
the gradient descent method.

# Introduction to the gradient descent algorithm

## Gradient descent of a 2D function

The diagram shows the update equations for the gradient descent algorithm with several annotations:

- NEW  $x$** : Points to the new value of  $x$  in the first equation.
- OLD  $x$** : Points to the old value of  $x$  in the first equation.
- LEARNING RATE**: Points to the parameter  $\alpha$  in both equations.
- OLD  $x$** : Points to the  $x$  variable in the partial derivative of the first equation.
- OLD  $y$** : Points to the  $y$  variable in the partial derivative of the first equation.
- GRADIENT**: Two arrows point from this label to the partial derivative terms  $\frac{\partial}{\partial x} f(x, y)$  and  $\frac{\partial}{\partial y} f(x, y)$ .

$$x := x - \alpha \frac{\partial}{\partial x} f(x, y),$$
$$y := y - \alpha \frac{\partial}{\partial y} f(x, y)$$

Update simultaneously  $x$  and  $y$ .  
 $\alpha > 0$  – *learning rate* parameter.  
Repeat until convergence

Problem when using numerical derivatives ,  
they generate error at each step.  
Better to use analytic derivatives of  
backprop algorithm for computing gradients.

# Simultaneous update

```
temp0 :=  $x - \alpha \frac{\partial}{\partial x} f(x, y)$   
temp1 :=  $y - \alpha \frac{\partial}{\partial y} f(x, y)$   
 $x$  := temp0  
 $y$  := temp1
```

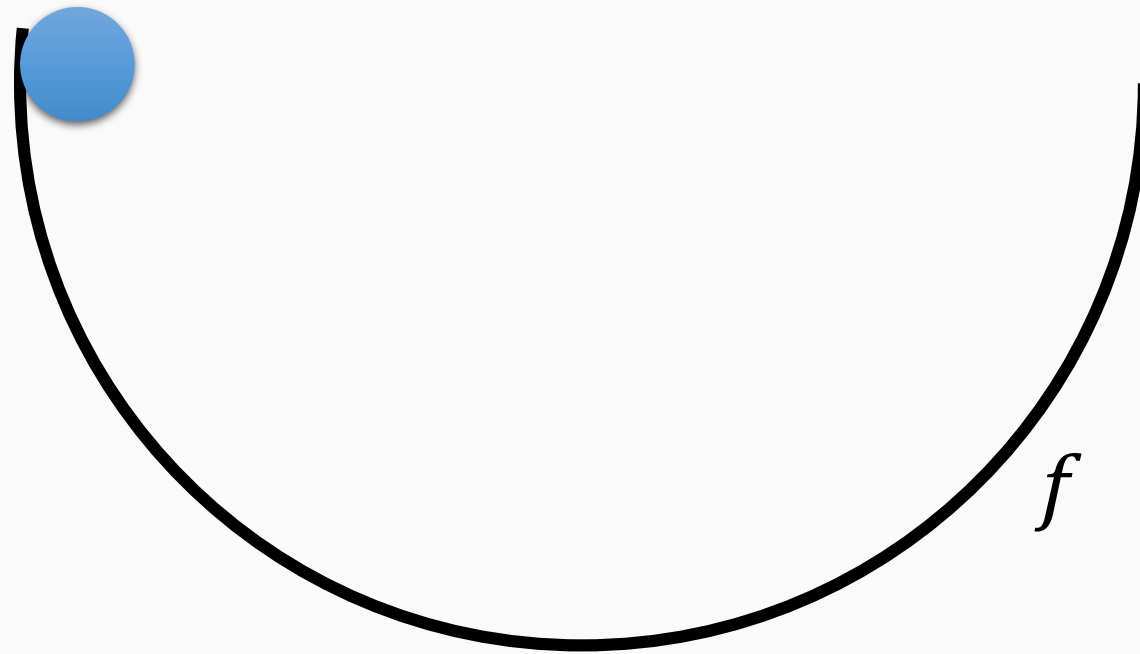
INCORRECT !

```
 $x$  :=  $x - \alpha \frac{\partial}{\partial x} f(x, y)$   
 $y$  :=  $y - \alpha \frac{\partial}{\partial y} f(x, y)$ 
```

# Convex Optimization

Show optimization using  
gradient descent of a  
quadratic function

[mathematica\\_demonstrations\ConvergenceOfMinimizationMethods.cdf](#)



1. Given a convex function  $f$
2. Locate the minimizer by following the descent

It follows that there is a unique minimizer

# The first convex optimization problem

Minimizing a quadratic function, where  $Q$  is a square symmetric positive definite matrix, and  $b$  is a vector

$$f(x) = \frac{1}{2}x^T \cdot Q \cdot x + b^T \cdot x$$

Observe that now  $x$  denotes a vector  $x \in R^n$ , we use interchangeably  $x$  as a vector and a number ( $x$  is a number on slide 30)

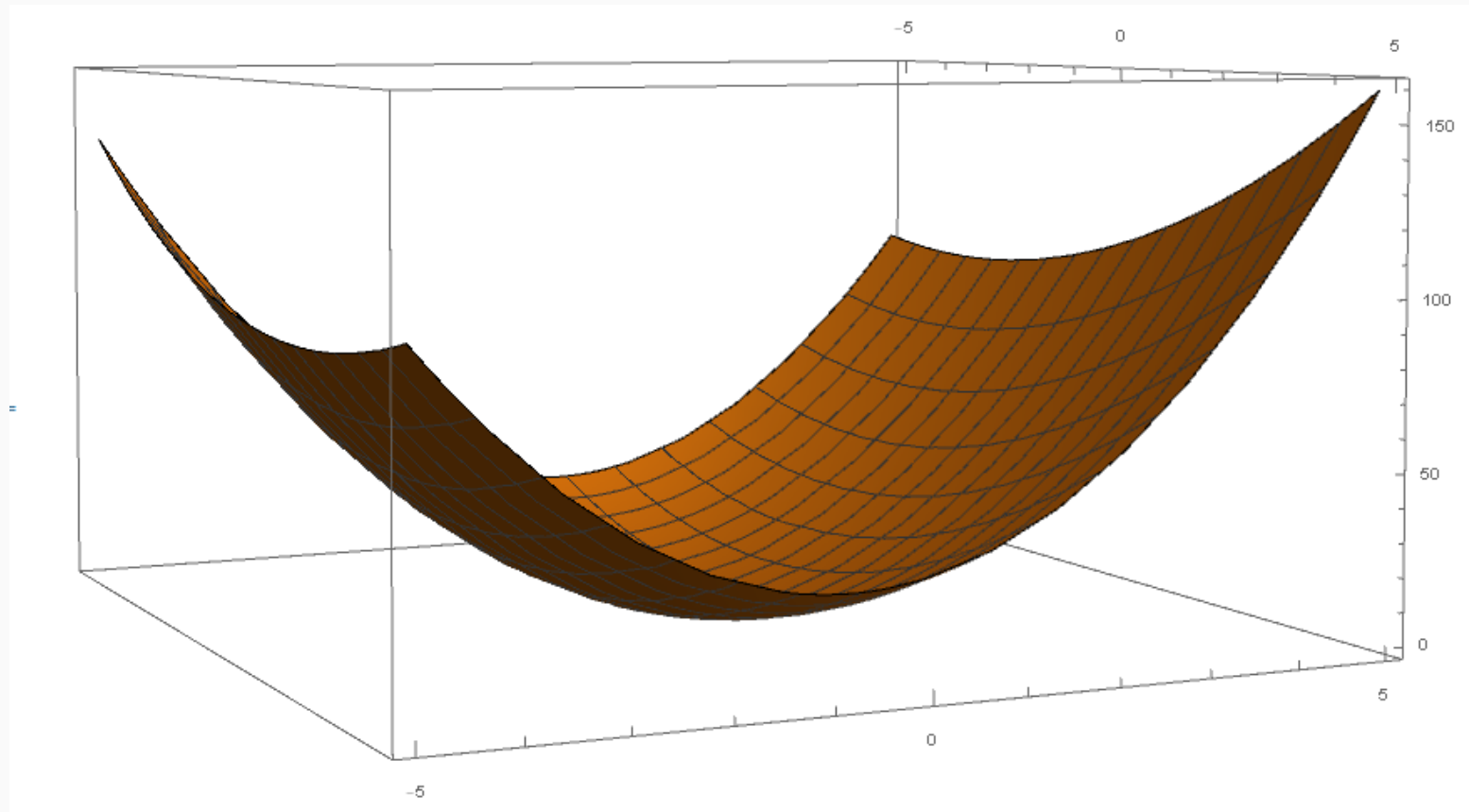
Symmetric matrix satisfies  $Q = Q^T$

The minimal point can be computed analytically by the formula  $x_{min} = -b^T \cdot Q^{-1}$

The formula for the gradient  $\nabla_x f(x)$  is simple  $\nabla_x f(x) = x^T Q + b^T$

# Example of a quadratic function

For example take  $Q = \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 2 \end{bmatrix}$ , and  $b = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ .





# Gradient descent for a quadratic function

Consider example  $Q = \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 2 \end{bmatrix}$ ,  $b = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$$x^* = [-0.85714286, -0.28571429]$$

$$f(x) = \frac{1}{2}x^T \cdot Q \cdot x + b^T \cdot x$$

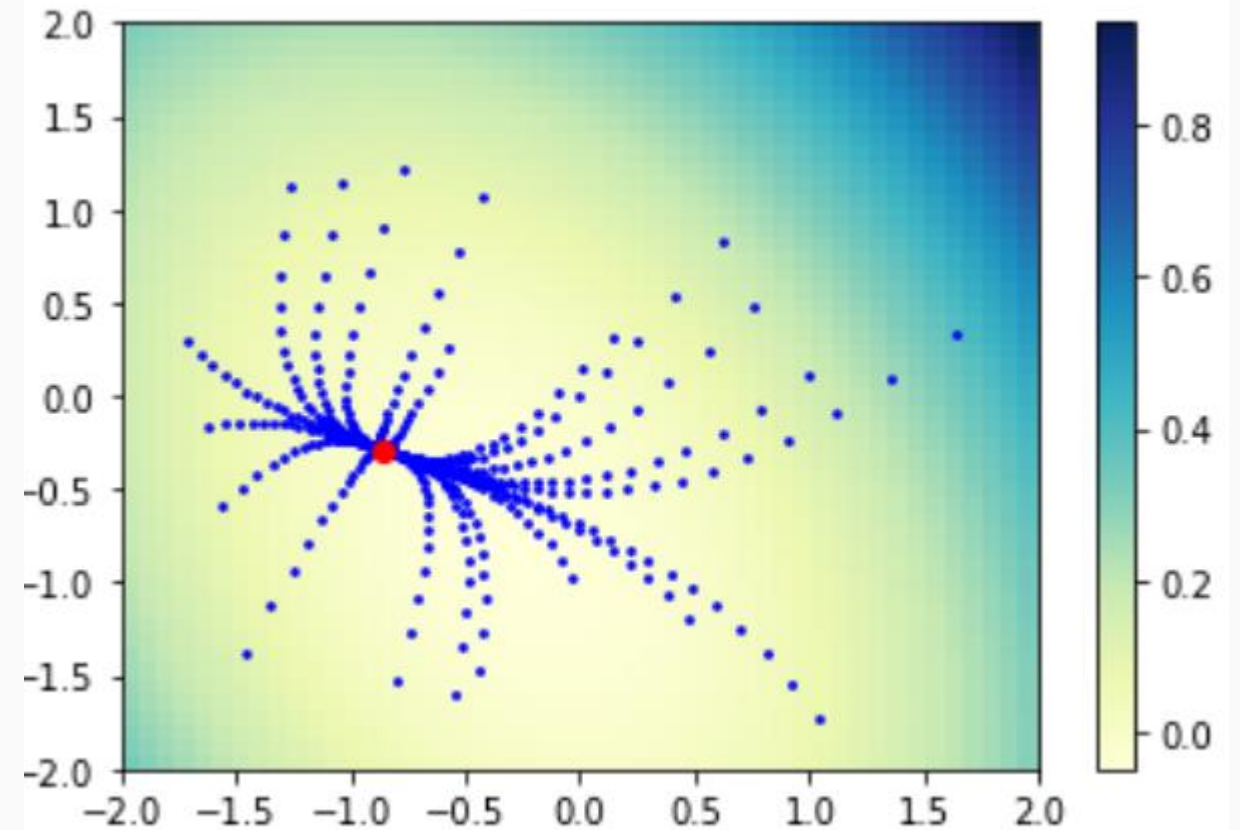
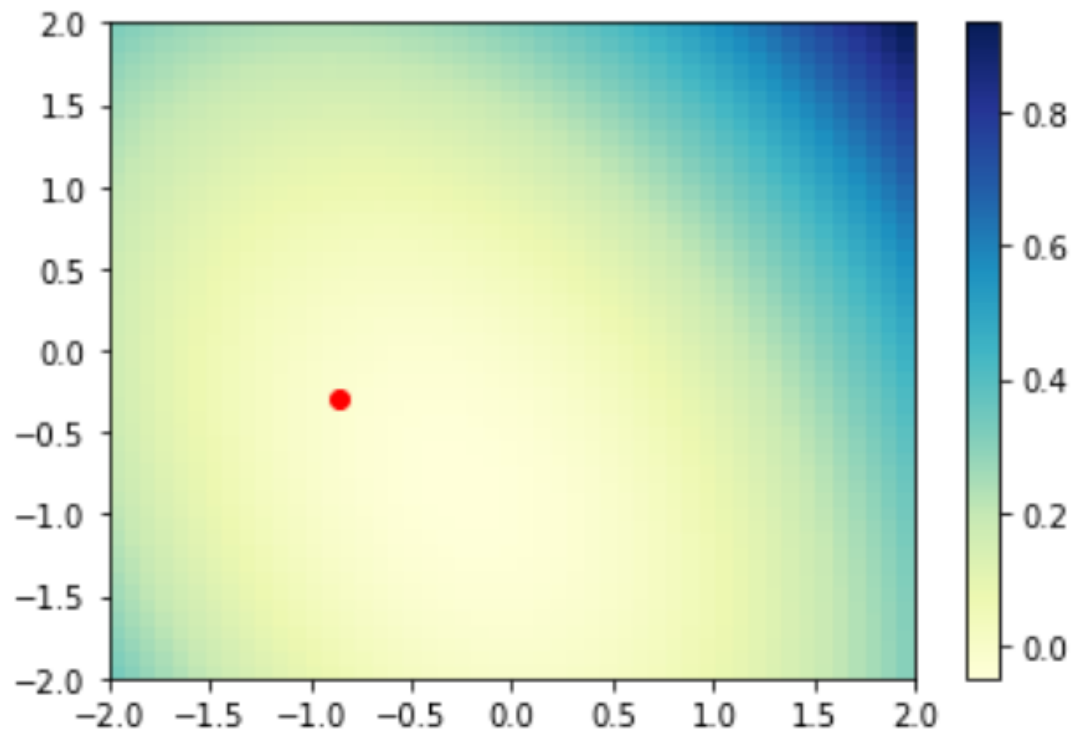
Gradient descent  $x := x - \alpha \nabla f(x)$   
(compactified notation)

$x \in \mathbb{R}^2$  is a two-dimensional vector,  
 $x_t$  denotes the  $t$ -th iteration.

See example computations and plots in [jupyter notebooks\week2 2.ipynb](#)

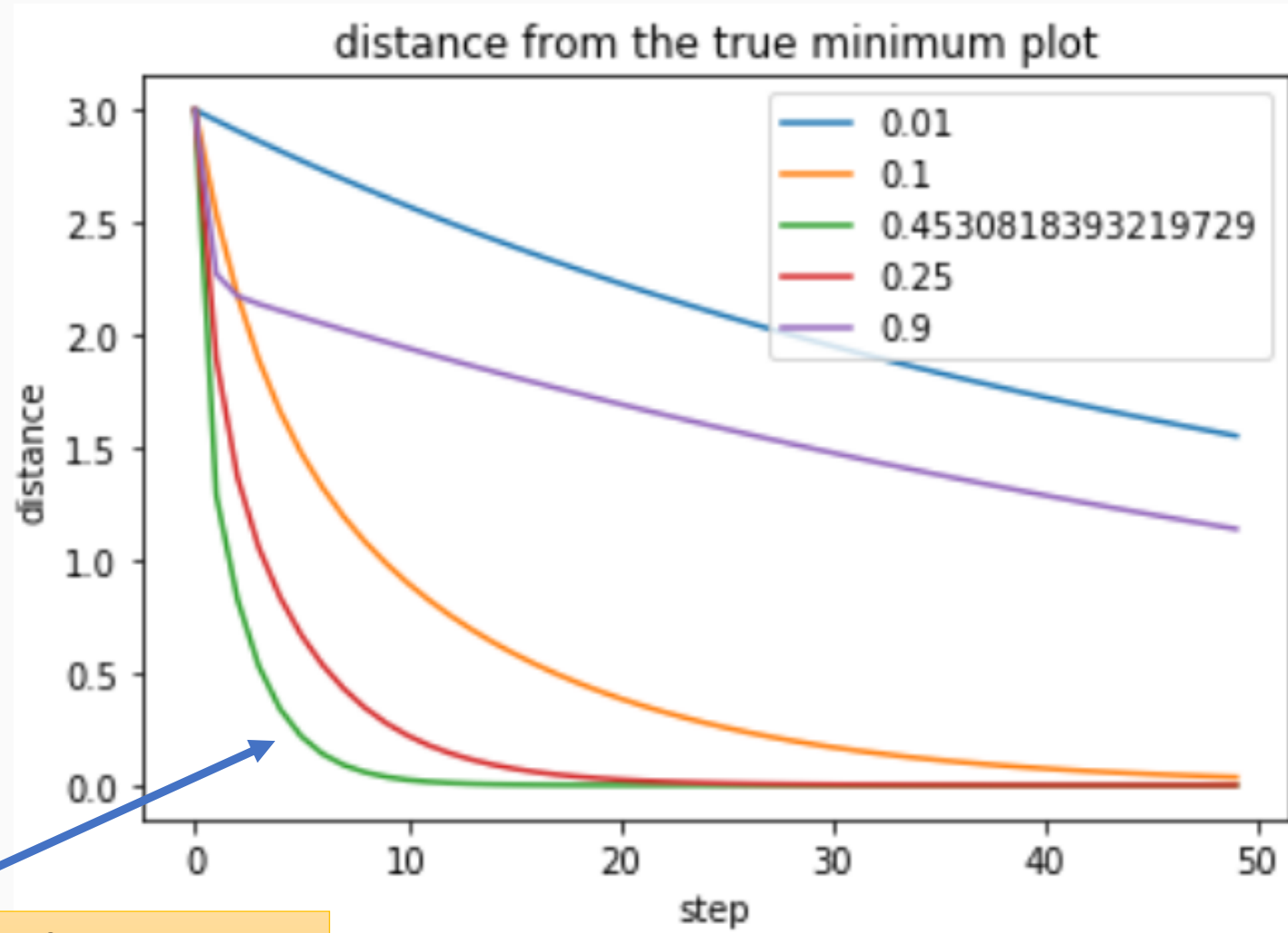
# Gradient descent for the quadratic function

`[-0.85714286 -0.28571429]`



# Behavior for different learning rates

the plot shows  
 $dist = ||x^* - x_t||$



We observe the fastest convergence for  $\alpha = 0.453 \dots$  **Why ?**

# A Glimpse at gradient descent convergence theory

Let  $L > 0$  be the *Lipschitz constant* of the gradient, i.e.

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\| \text{ for all } x, y \in \mathbb{R}^d.$$

The following theorem holds (informal statement below)

**Theorem 1.** *Let  $x^*$  be a global minimum of  $f$ .  $\nabla f$  is Lipschitz with a constant  $L > 0$  (see above). Choosing*

$$\alpha = \frac{1}{L}.$$

*Then, gradient descent with any  $x_0$  satisfies*

*1. Function values are monotone decreasing*

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

*2.*

$$\|f(x_T) - f(x^*)\| \leq \frac{L}{2T} \|x_0 - x^*\|^2, \quad T > 0.$$

# Remark on the Theorem

The Theorem provides us with a good guess for the learning rate.

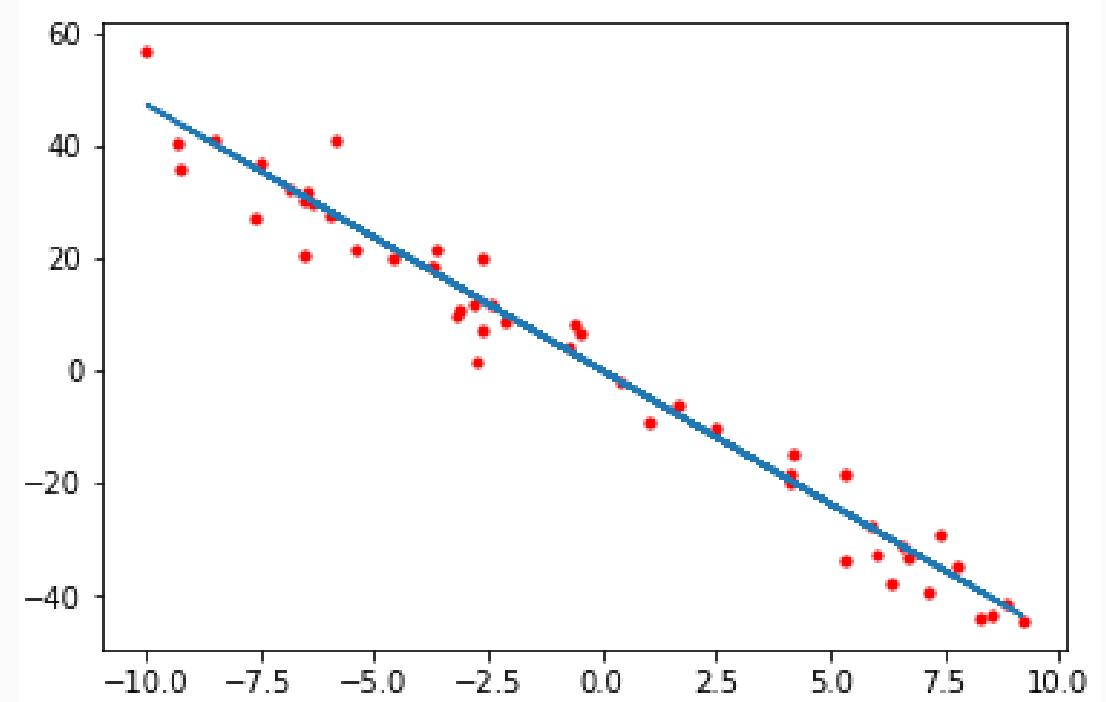
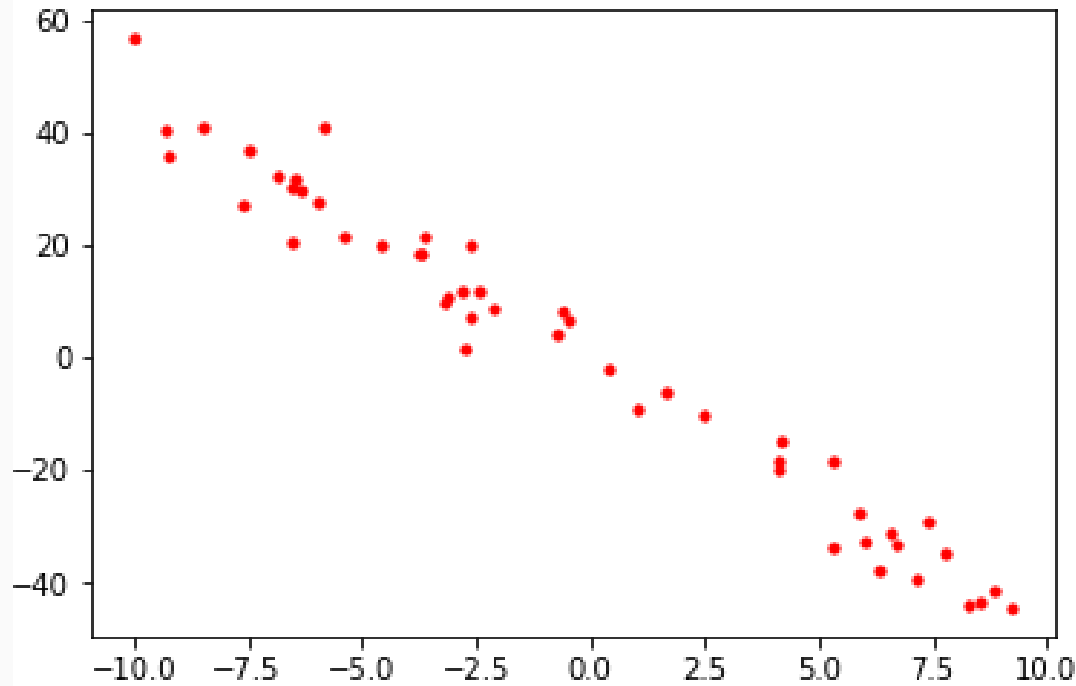
Informally, it guarantees that for the given choice of learning rate the function value along the gradient descent path is decreasing at least like  $\frac{1}{T}$ . It is provided as an example of mathematical statement about gradient descent applied to convex problems.

However, for most practical problems Theorem cannot be applied literally, it serves as a guide exclusively

- There is no global Lipschitz constant, only local, so the learning rate is usually being adapted from step to step,
- Lipschitz constant is computationally expensive to estimate,
- Practical optimization problems are nonconvex.

# Linear Regression

Statement of the *linear regression problem*:  
given data , find a linear function which is the best approximator



Given a set of  $N$  data-points  $\{(x_i, y_i)\}$

Best approximator = the line  $mx + b$  that minimizes  $\frac{1}{N} \sum (y_i - (mx_i + b))^2$

# Linear regression using gradient descent

**The task is**

**Find  $m, b$**  that minimize the '*mean square error*'  $MSE = \frac{1}{N} \sum (y_i - (mx_i + b))^2$

1. Compute the gradient  $\frac{\partial MSE}{\partial m} = \frac{2}{N} \sum_{i=1}^N -x_i(y_i - (mx_i + b)),$

$$\frac{\partial MSE}{\partial b} = \frac{2}{N} \sum_{i=1}^N -(y_i - (mx_i + b)),$$

It can be written using vectors (NumPy way)

$$\frac{\partial MSE}{\partial m} = \frac{2}{N} \left( -x^T y + m x^T x + x^T \hat{b} \right),$$

$$\frac{\partial MSE}{\partial b} = \frac{2}{N} (-1^T y + m 1^T x + 1^T \hat{b}),$$

where  $1 = [1, 1, \dots, 1]$ , i.e. is a vector of ones, and  $\hat{b} = [b, b, \dots, b]$  is a vector of  $b$ 's.

# Linear regression using gradient descent

2. Perform the simultaneous update

$$\text{temp0} := m - \alpha \frac{\partial}{\partial m} \text{MSE}(m, b)$$

$$\text{temp1} := b - \alpha \frac{\partial}{\partial b} \text{MSE}(m, b)$$

$$m := \text{temp0}$$

$$b := \text{temp1}$$

3. Until convergence

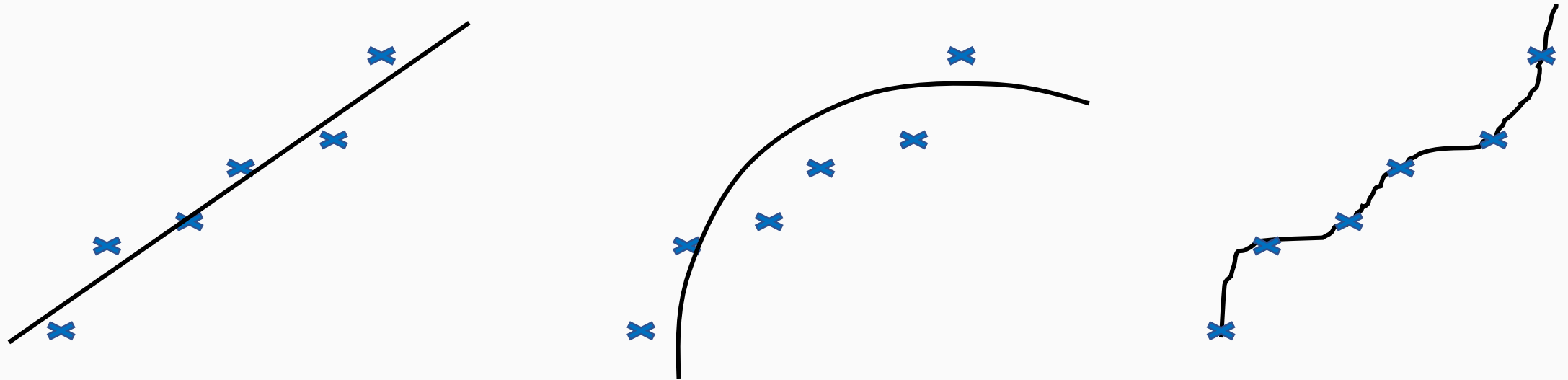
The analytic solution is given by

$$mx^T x - x^T y + x^T \hat{b} = 0,$$

$$m1^T x - 1^T y + 1^T \hat{b} = 0,$$



# Nonlinear polynomial regression – fitting a curve



**The task is of nonlinear regression for 2D datapoints**

**Find  $b, \{m_i\}_{i=1}^p$  that minimize the ‘mean square error’  
(fit a curve that approximates the data the best)**

MSE for the nonlinear regression  
using  $p$ -th order polynomials

$$MSE = \frac{1}{N} \sum (y_i - (m_1 x_i^1 + m_2 x_i^2 + \dots + m_p x_i^p + b))^2$$

# Nonlinear polynomial regression cont.

## Nonlinear regression for 2D datapoints

Using the compact polynomial notation

$$m_1 x_i^1 + m_2 x_i^2 + \cdots + m_p x_i^p + b = \sum_{j=1}^p m_j x_i^j + b$$

$$MSE = \frac{1}{N} \sum_{i=1}^N \left( y_i - \left( \sum_{j=1}^p m_j x_i^j + b \right) \right)^2$$

# Solving nonlinear regression using gradient descent

*We can solve nonlinear regression using gradient descent like we solved linear regression*

For the quadratic regression we have the following gradients

$$\frac{\partial MSE}{\partial m_1} = \frac{2}{N} \sum_{i=1}^N -x_i(y_i - (m_1x_i + m_2x_i^2 + b)),$$

$$\frac{\partial MSE}{\partial m_2} = \frac{2}{N} \sum_{i=1}^N -x_i^2(y_i - (m_1x_i + m_2x_i^2 + b)),$$

$$\frac{\partial MSE}{\partial b} = \frac{2}{N} \sum_{i=1}^N -(y_i - (m_1x_i + m_2x_i^2 + b)),$$

And perform simultaneous update (like on slide 41) of the three parameters  $m_1, m_2, b$

# Nonlinear regression of a general polynomial

*We can solve nonlinear regression for a arbitrary polynomial*

For the quadratic regression we have the following gradients

$$\frac{\partial MSE}{\partial m_1} = \frac{2}{N} \sum_{i=1}^N -x_i \left( y_i - \left( \sum_{j=1}^p m_j x_i^j + b \right) \right),$$

$$\frac{\partial MSE}{\partial m_2} = \frac{2}{N} \sum_{i=1}^N -x_i^2 \left( y_i - \left( \sum_{j=1}^p m_j x_i^j + b \right) \right),$$

...

$$\frac{\partial MSE}{\partial m_j} = \frac{2}{N} \sum_{i=1}^N -x_i^j \left( y_i - \left( \sum_{j=1}^p m_j x_i^j + b \right) \right),$$

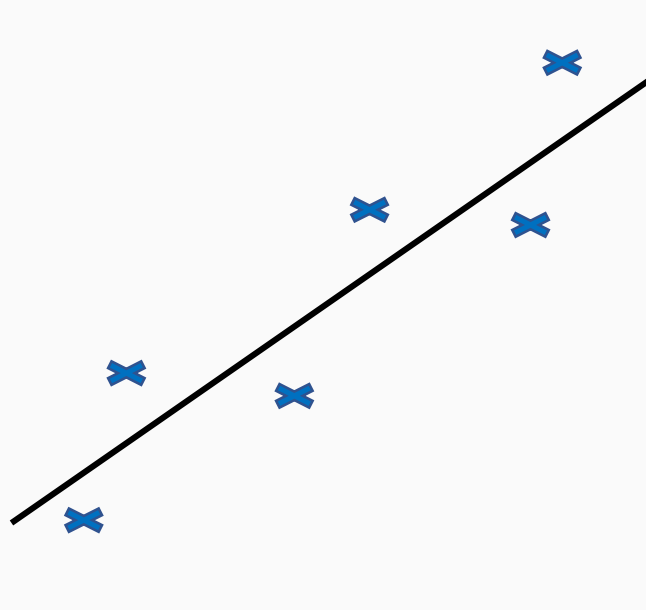
...

$$\frac{\partial MSE}{\partial b} = \frac{2}{N} \sum_{i=1}^N -(y_i - (\sum_{j=1}^p m_j x_i^j + b)),$$

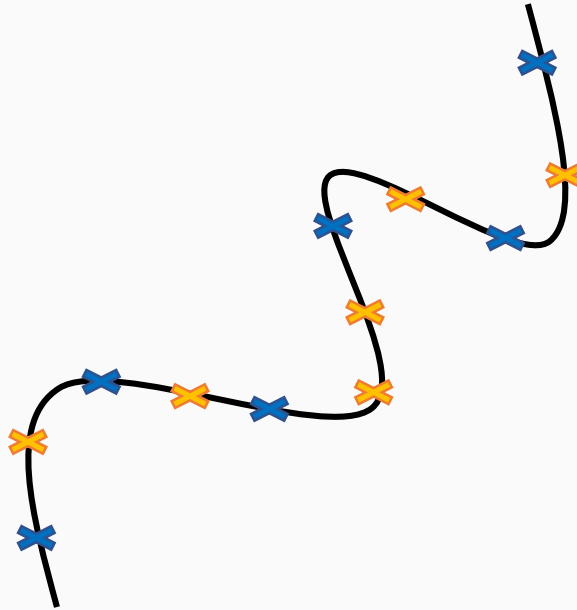
If doing nonlinear regression with a  $p$ -th order polynomial, then there are  $p + 1$  parameters for gradient descent (can store them in a vector).

# Overfitting / Underfitting

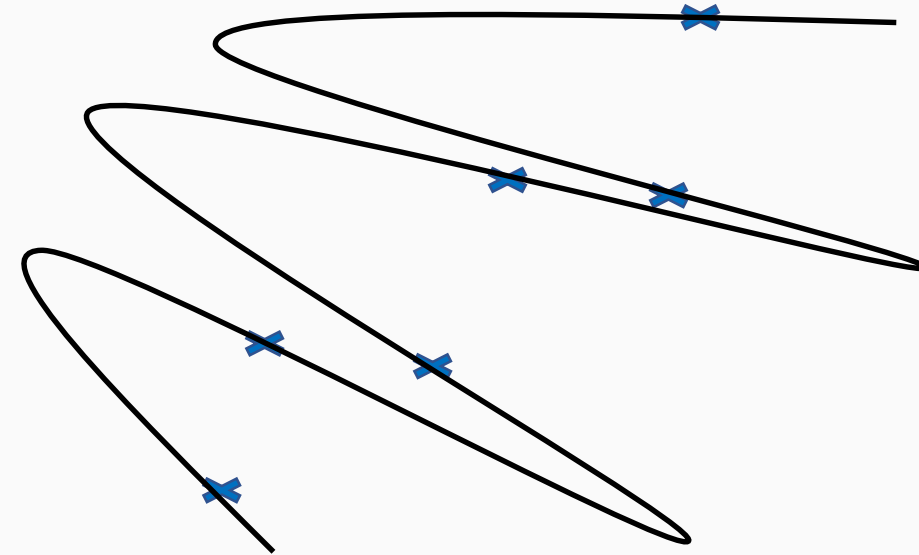
There is no a general recipe of choosing appropriate polynomials for nonlinear regression



Underfitted  
(order too low)



Good generalization  
order fits data well  
Test datapoints



Overfitted  
(order too large)

# Glimpse of the modern machine learning research



Generalization of Deep Neural Networks is an open problem of machine learning research.

*Why DNN seem to generalize well despite having enormous number of parameters???*