3D geoinformation
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GEO5017
Machine Learning for the Built Environment

https://3d.bk.tudelft.nl/courses/geo5017/

Linear Regression

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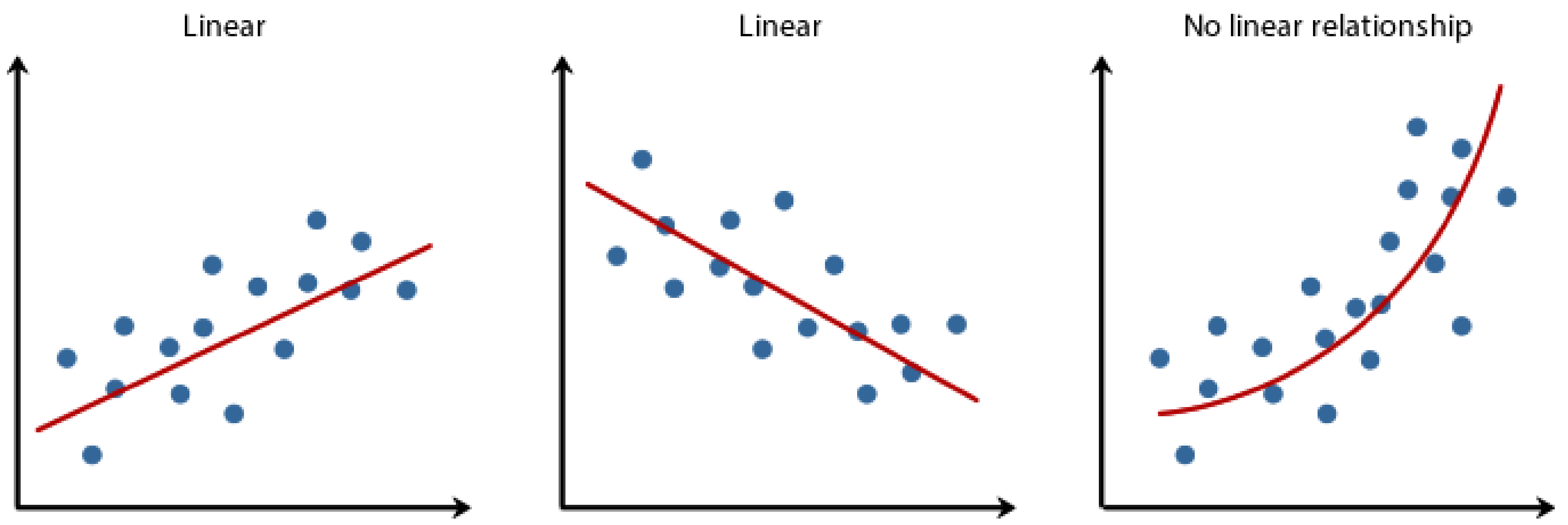
Agenda

- What is linear regression?
- The least-squares (closed-form) solution
  - Simple linear regression
  - Polynomial regression
  - Multivariate linear regression
- Solve linear regression by optimization
  - Gradient descent

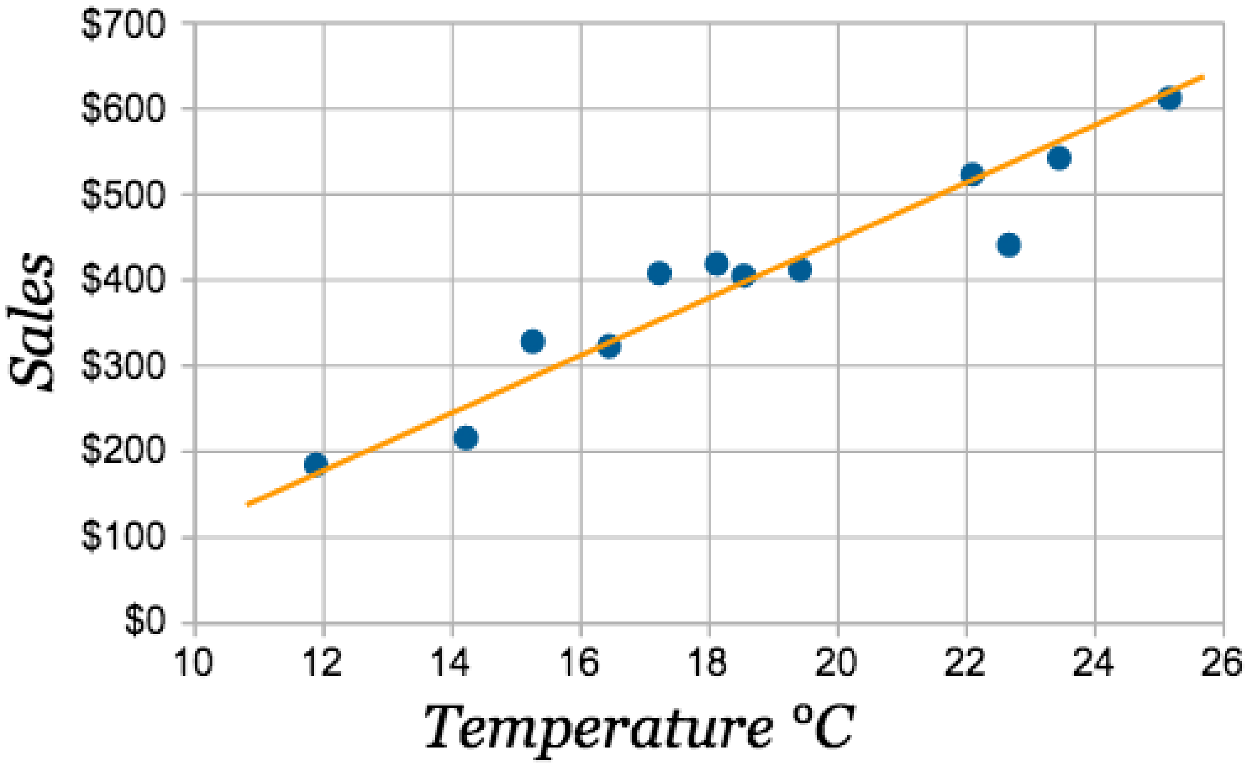
What is linear regression?

- Given a set of observed values of the **independent (input) variables** and the corresponding values of the **dependent (output) variable**, **determine a relation** between the independent variable(s) and a continuous output variable



Linear regression

- Examples



Linear regression

- Examples

Prices of used cars: example data for regression

Price (US$)	Age (years)	Distance (km)	Weight (pounds)
13500	23	46986	1165
13750	23	72937	1165
13950	24	41711	1165
14950	26	48000	1165
13750	30	38500	1170
12950	32	61000	1170
16900	27	94612	1245
18600	30	75889	1245
21500	27	19700	1185
12950	23	71138	1105

Linear regression

- General approach
  - Regression function

$$y = f(x, \theta)$$

  - Objective
    - Optimize θ such that the approximation error is minimized

$$E = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Example

$$\text{Price} = a_0 + a_1 \cdot \text{Age} + a_2 \cdot \text{Distance} + a_3 \cdot \text{Weight}$$

$$x = \{\text{Age}, \text{Distance}, \text{Weight}\}$$

$$\theta = \{a_0, a_1, a_2, a_3\}$$

Prices of used cars: example data for regression

Price (US$)	Age (years)	Distance (km)	Weight (pounds)
13500	23	46986	1165
13750	23	72937	1165
13950	24	41711	1165
14950	26	48000	1165
13750	30	38500	1170
12950	32	61000	1170
16900	27	94612	1245
18600	30	75889	1245
21500	27	19700	1185
12950	23	71138	1105

Different linear regression models

- Simple linear regression
  - Only one continuous independent variable

$$y = a + bx$$

- Polynomial regression
  - Only one continuous independent variable

$$y = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

- Multivariate linear regression
  - More than one independent variables

$$y = a_0 + a_1 x_1 + \ldots + a_n x_n$$

Agenda

- Linear regression
- The least-squares (closed-form) solution
  - Simple linear regression
  - Polynomial regression
  - Multivariate linear regression
- Gradient descent
  - Solve linear regression using optimization
  - Solve many other optimization problems

Simple linear regression

- Ordinary least squares

$$y = \alpha + \beta x$$

x	x_1	x_2	$\dots$	x_n
y	y_1	y_2	$\dots$	y_n

- Objective function

$$E = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$= \sum_{i=1}^{n} [y_i - (\alpha + \beta x_i)]^2$$

$$\frac{\partial E}{\partial \alpha} = 0 \qquad \sum_{i=1}^{n} y_i = n\alpha + \beta \sum_{i=1}^{n} x_i$$

$$\frac{\partial E}{\partial \beta} = 0 \qquad \sum_{i=1}^{n} x_i y_i = \alpha \sum_{i=1}^{n} x_i + \beta \sum_{i=1}^{n} x_i^2$$

Simple linear regression

- Ordinary least squares

$$y = \alpha + \beta x$$

Final solution:

$$\beta = \frac{\mathrm{Cov}(x, y)}{\mathrm{Var}(x)}$$

$$\alpha = \bar{y} - \beta \bar{x}$$

$$\bar{x} = \frac{1}{n} \sum x_i$$

$$\bar{y} = \frac{1}{n} \sum y_i$$

$$\mathrm{Var}(x) = \frac{1}{n-1} \sum (x_i - \bar{x}_i)^2$$

$$\mathrm{Cov}(x, y) = \frac{1}{n-1} \sum (x_i - \bar{x})(y_i - \bar{y})$$

Simple linear regression

- Example

$$y = \alpha + \beta x$$

$$n = 5$$

$$\bar{x} = \frac{1}{5}(1.0 + 2.0 + 3.0 + 4.0 + 5.0) = 3.0$$

$$\bar{y} = \frac{1}{5}(1.00 + 2.00 + 1.30 + 3.75 + 2.25) = 2.06$$

$$\mathrm{Cov}(x, y) = \frac{1}{4}[(1.0 - 3.0)(1.00 - 2.06) + \cdots + (5.0 - 3.0)(2.25 - 2.06)] = 1.0625$$

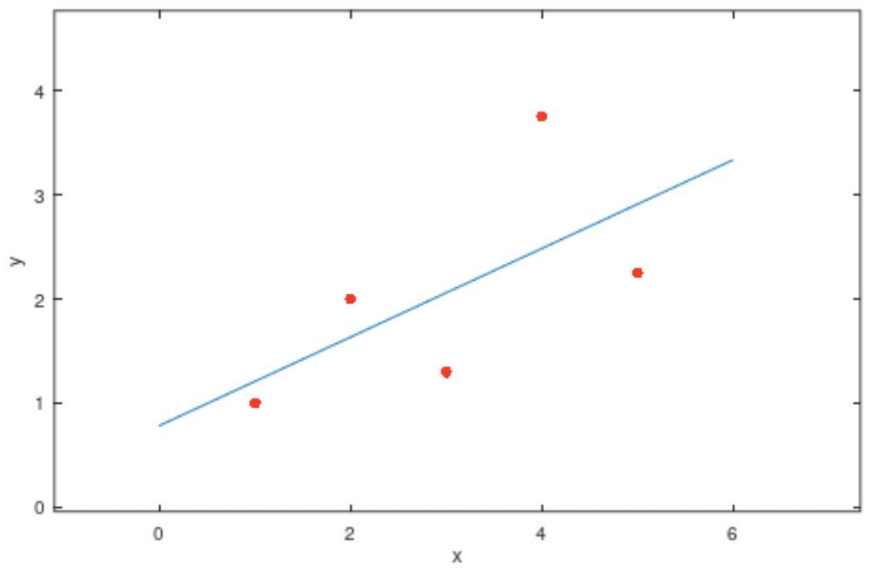
$$\mathrm{Var}(x) = \frac{1}{4}\left[(1.0 - 3.0)^2 + \cdots + (5.0 - 3.0)^2\right] = 2.5$$

$$b = \frac{1.0625}{2.5} = 0.425$$

$$a = 2.06 - 0.425 \times 3.0 = 0.785$$

$$y = 0.785 + 0.425x$$

x	1.0	2.0	3.0	4.0	5.0
y	1.00	2.00	1.30	3.75	2.25



Polynomial regression

- Model

$$y = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_k x^k$$

x	x_1	x_2	$\dots$	x_n
y	y_1	y_2	$\dots$	y_n

- Ordinary least squares
  - Objective

$$E = \sum_{i=1}^{n} \left[y_i - (\alpha_0 + \alpha_1 x_i + \alpha_2 x_i^2 + \cdots + \alpha_k x_i^k) \right]^2$$

  - Solution can be obtained by solving

$$\frac{\partial E}{\partial \alpha_i} = 0, \quad \forall i = 0, 1, \ldots, k.$$

Polynomial regression

- Ordinary least squares

$$y = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_k x^k$$

$$\frac{\partial E}{\partial \alpha_i} = 0, \quad \forall i = 0, 1, \ldots, k.$$

$$\begin{aligned}
\sum y_i &= \alpha_0 n + \alpha_1 \left(\sum x_i\right) + \cdots + \alpha_k \left(\sum x_i^k\right) \\
\sum y_i x_i &= \alpha_0 \left(\sum x_i\right) + \alpha_1 \left(\sum x_i^2\right) + \cdots + \alpha_k \left(\sum x_i^{k+1}\right) \\
\sum y_i x_i^2 &= \alpha_0 \left(\sum x_i^2\right) + \alpha_1 \left(\sum x_i^3\right) + \cdots + \alpha_k \left(\sum x_i^{k+2}\right) \\
&\vdots \\
\sum y_i x_i^k &= \alpha_0 \left(\sum x_i^k\right) + \alpha_1 \left(\sum x_i^{k+1}\right) + \cdots + \alpha_k \left(\sum x_i^{2k}\right)
\end{aligned}$$

Polynomial regression

- Ordinary least squares

$$y = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_k x^k$$

$$\frac{\partial E}{\partial \alpha_i} = 0, \quad \forall i = 0, 1, \ldots, k.$$

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\end{aligned}$$

$$\vec{y} = D\vec{\alpha}$$

$$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad D = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^k \\ 1 & x_2 & x_2^2 & \cdots & x_2^k \\ \vdots & & & & \\ 1 & x_n & x_n^2 & \cdots & x_n^k \end{bmatrix}, \text{ and } \vec{\alpha} = \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_k \end{bmatrix}$$

Polynomial regression

- Ordinary least squares

$$y = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_k x^k$$

$$\frac{\partial E}{\partial \alpha_i} = 0, \quad \forall i = 0, 1, \ldots, k.$$

$$\begin{aligned}
\sum y_i &= \alpha_0 n + \alpha_1 \left(\sum x_i\right) + \cdots + \alpha_k \left(\sum x_i^k\right) \\
\sum y_i x_i &= \alpha_0 \left(\sum x_i\right) + \alpha_1 \left(\sum x_i^2\right) + \cdots + \alpha_k \left(\sum x_i^{k+1}\right) \\
\sum y_i x_i^2 &= \alpha_0 \left(\sum x_i^2\right) + \alpha_1 \left(\sum x_i^3\right) + \cdots + \alpha_k \left(\sum x_i^{k+2}\right) \\
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$$\vec{\alpha} = \left(D^T D\right)^{-1} D^T \vec{y}$$

Polynomial regression

- Example

x	3.0	4.0	5.0	6.0	7.0
y	2.5	3.2	3.8	6.5	11.5

$$y = \alpha_0 + \alpha_1 x + \alpha_2 x^2$$

$$\sum y_i = n\alpha_0 + \alpha_1 \left(\sum x_i\right) + \alpha_2 \left(\sum x_i^2\right)$$
$$\sum y_i x_i = \alpha_0 \left(\sum x_i\right) + \alpha_1 \left(\sum x_i^2\right) + \alpha_2 \left(\sum x_i^3\right)$$
$$\sum y_i x_i^2 = \alpha_0 \left(\sum x_i^2\right) + \alpha_1 \left(\sum x_i^3\right) + \alpha_2 \left(\sum x_i^4\right)$$

$$27.5 = 5\alpha_0 + 25\alpha_1 + 135\alpha_2$$
$$158.8 = 25\alpha_0 + 135\alpha_1 + 775\alpha_2$$
$$966.2 = 135\alpha_0 + 775\alpha_1 + 4659\alpha_2$$

$$\alpha_0 = 12.4285714$$
$$\alpha_1 = -5.5128571$$
$$\alpha_2 = 0.7642857$$

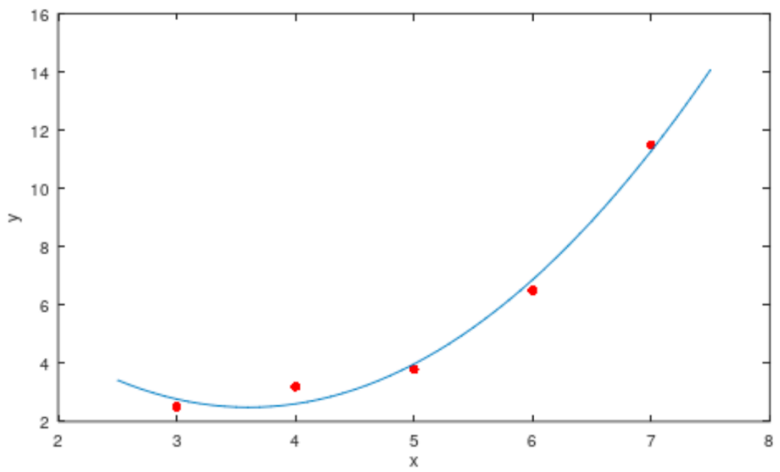
$$y = 12.4285714 - 5.5128571x + 0.7642857x^2$$

Polynomial regression

- Example

x	3.0	4.0	5.0	6.0	7.0
y	2.5	3.2	3.8	6.5	11.5

$$y = \alpha_0 + \alpha_1 x + \alpha_2 x^2$$



$$\sum y_i = n\alpha_0 + \alpha_1\left(\sum x_i\right) + \alpha_2\left(\sum x_i^2\right)$$
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$$\alpha_2 = 0.7642857$$

$$y = 12.4285714 - 5.5128571x + 0.7642857x^2$$

Multivariate linear regression

- Model

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_N x_N$$

- Ordinary least squares

Variables	Values (examples)			
	Example 1	Example 2	...	Example n
x_1	x_{11}	x_{12}	...	x_{1n}
x_1	x_{21}	x_{22}	...	x_{2n}
...				
x_N	x_{N1}	x_{N2}	...	x_{Nn}
y (outcomes)	y_1	y_2	...	y_n

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{N1} \\ 1 & x_{12} & x_{22} & \cdots & x_{N2} \\ \vdots & & & & \\ 1 & x_{1n} & x_{2n} & \cdots & x_{Nn} \end{bmatrix}, \text{ and } B = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_N \end{bmatrix}$$

$$B = \left(X^T X\right)^{-1} X^T Y.$$

Multivariate linear regression

- Example

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

x_1	1	1	2	0
x_2	1	2	2	1
y	3.25	6.5	3.5	5.0

Multivariate linear regression

- Example

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

x_1	1	1	2	0
x_2	1	2	2	1
y	3.25	6.5	3.5	5.0

$$B = (X^T X)^{-1} X^T Y$$

$$Y = \begin{bmatrix} 3.25 \\ 6.5 \\ 3.5 \\ 5.0 \end{bmatrix}, \quad X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \\ 1 & 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

$$y = 2.0625 - 2.3750 x_1 + 3.2500 x_2$$

$$X^T X = \begin{bmatrix} 4 & 4 & 6 \\ 4 & 6 & 7 \\ 6 & 7 & 10 \end{bmatrix} \Rightarrow (X^T X)^{-1} = \begin{bmatrix} \frac{11}{4} & \frac{1}{2} & -2 \\ \frac{1}{2} & 1 & -1 \\ -2 & -1 & 2 \end{bmatrix} \Rightarrow B = (X^T X)^{-1} X^T Y = \begin{bmatrix} 2.0625 \\ -2.3750 \\ 3.2500 \end{bmatrix}$$

Agenda

- Linear regression
- The least-squares (closed-form) solution
  - Simple linear regression
  - Polynomial regression
  - Multivariate linear regression
- Gradient descent
  - Solve linear regression using optimization
  - Solve many other optimization problems

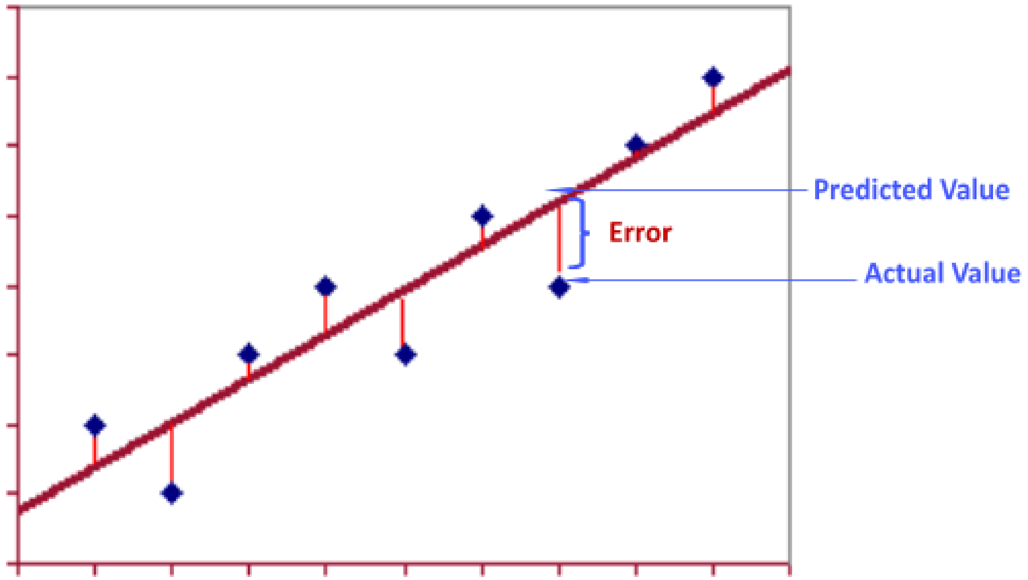
Objective function of linear regression

- Linear regression

$$y = f(x, \theta)$$

- Objective function
  - Sum of squared error

$$\boldsymbol{E} = \sum_{\boldsymbol{i}=\boldsymbol{0}}^{\boldsymbol{n}} (y_i - \widehat{y}_i)^2$$



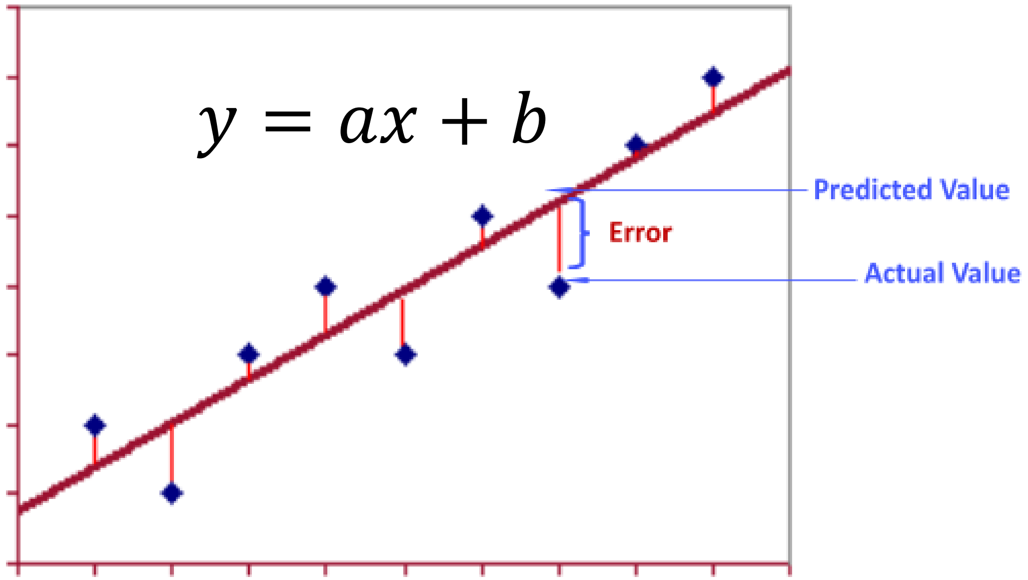
Objective function of linear regression

- Example
  - Objective function
    - Sum of squared error

$$E = \sum_{i=0}^{n} (y_i - (ax_i + b))^2$$

    - Solution

$$min \sum_{i=0}^{n} (y_i - (ax_i + b))^2$$



Objective function of linear regression

- Example
  - Objective function
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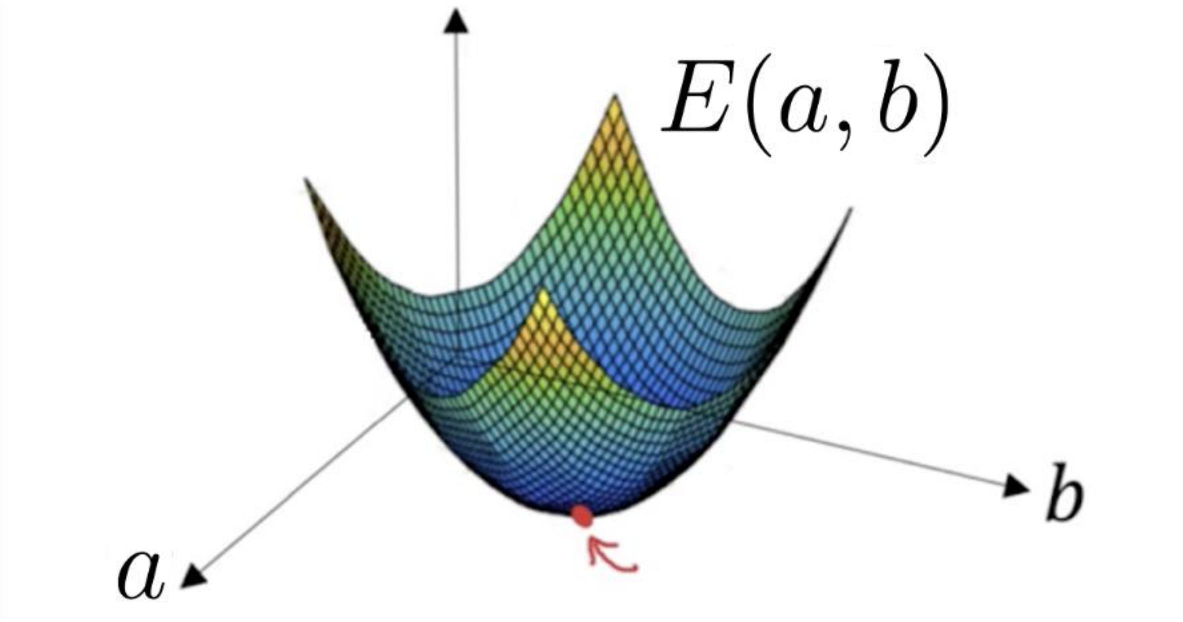
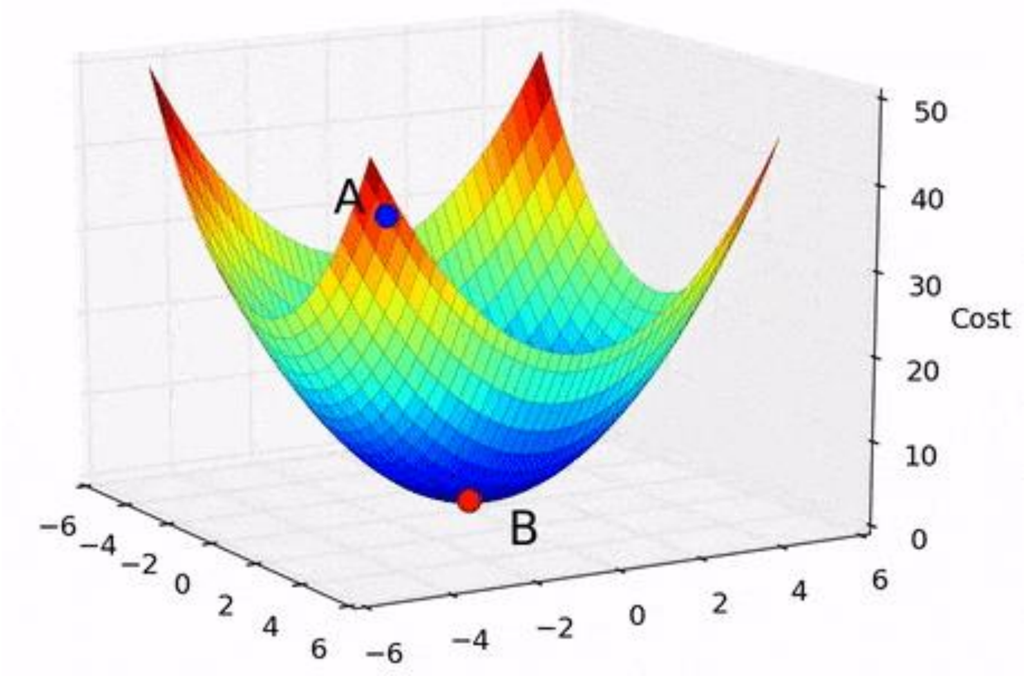


Gradient descent

- Basic idea
  - Take repeated steps in **steepest descent direction** until lowest point is reached
    - The **opposite** direction of the **gradient** of the function at the current point

$$\nabla f(\vec{p}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\vec{p}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\vec{p}) \end{bmatrix}$$



Gradient

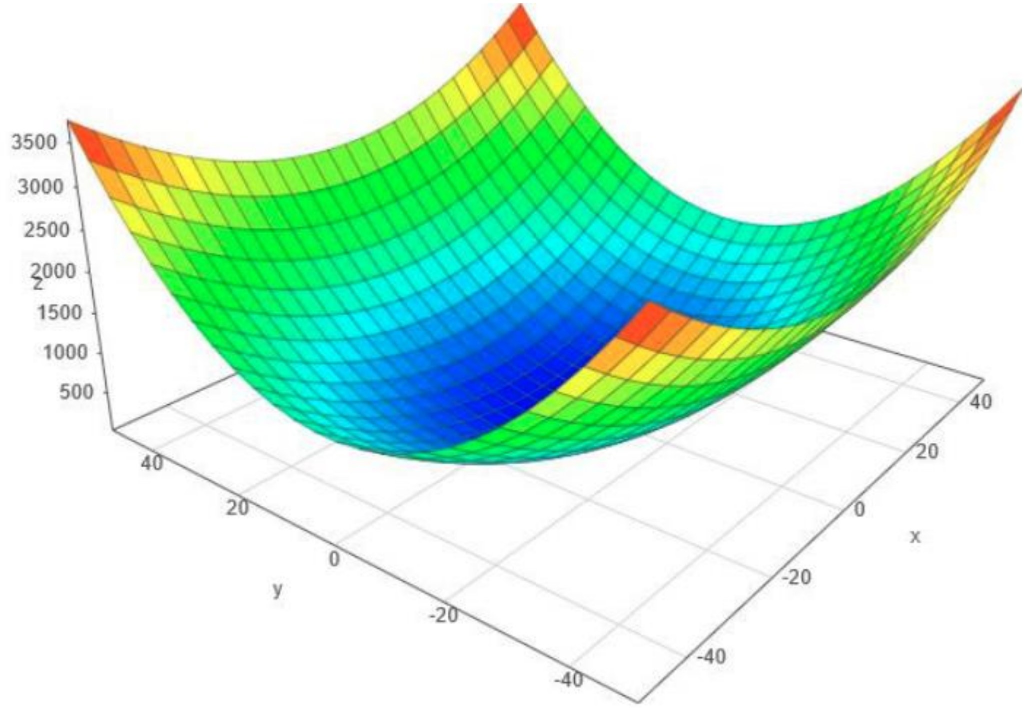
- Example

$$f(x, y) = 0.5x^2 + y^2$$

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

The gradient at point *p*(10, 10)

$$\nabla f(10, 10) = \begin{bmatrix} 10 \\ 20 \end{bmatrix}$$



Gradient descent algorithm

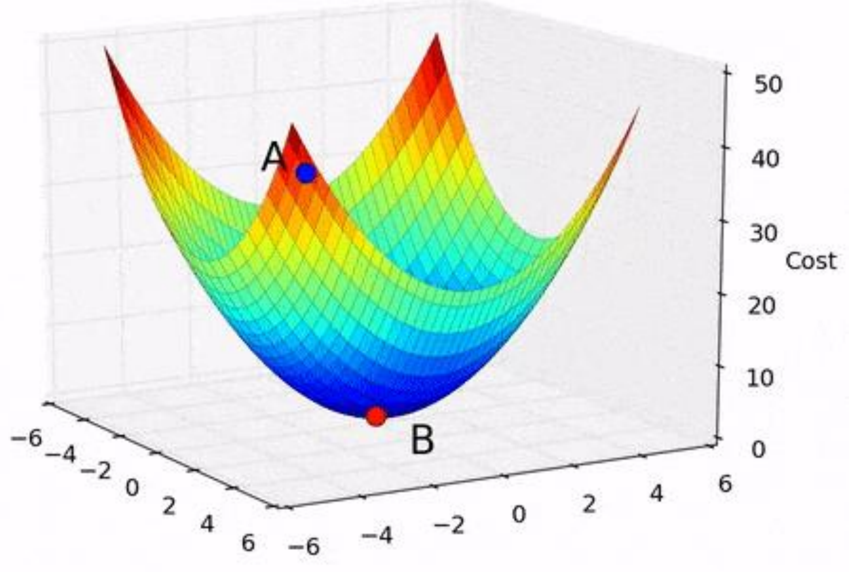
- Main steps
  1) Start from an initial guess (or even randomly)
  2) Calculate the the gradient of the function at current point
  3) Make a scaled step in the opposite direction to the gradient

$$\vec{p}_{n+1} = \vec{p}_n - \eta \nabla f\left(\vec{p}_n\right)$$

  4) Repeat 2) and 3) until one of the criteria is met

     -) maximum number of iterations reached

     -) step size (or the change of the function value) is smaller than a given tolerance



Gradient descent algorithm

- Example: a 1D function

$$f(x) = x^2 - 4x + 1$$

$$\frac{df(x)}{dx} = 2x - 4$$

$$\vec{p}_{n+1} = \vec{p}_n - \eta \nabla f(\vec{p}_n)$$

The first few steps

$$x_0 = 9, \qquad f(9) = 46$$

$$x_1 = 9 - 0.1 \times (2 \times 9 - 4) = 7.6, \qquad f(7.6) = 28.36$$

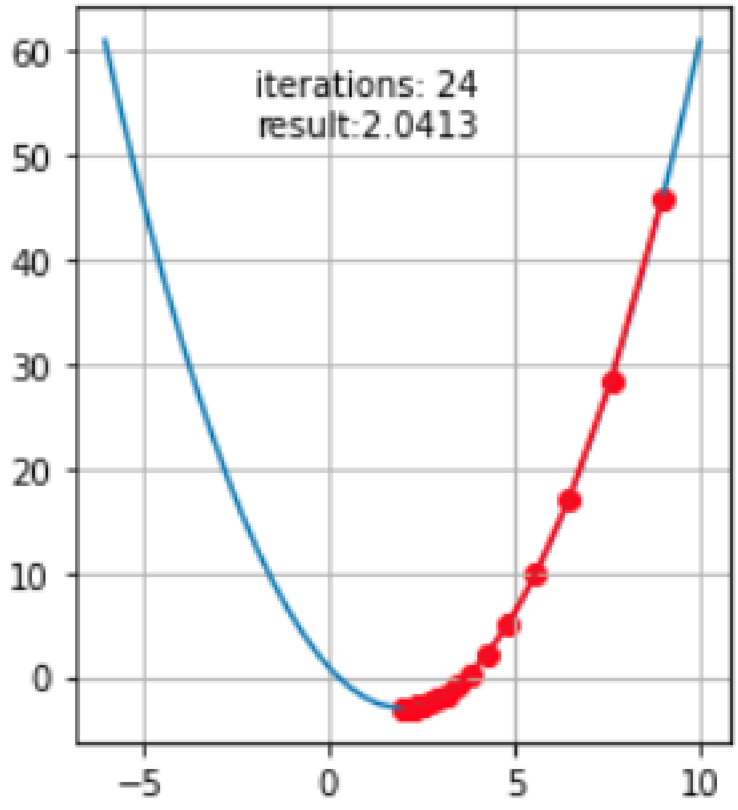
$$x_2 = 7.6 - 0.1 \times (2 \times 7.6 - 4) = 6.48, \qquad f(6.48) = 17.07$$

$$x_3 = 6.48 - 0.1 \times (2 \times 6.48 - 4) = 5.584, \qquad f(5.584) = 9.845$$

$$\ldots$$

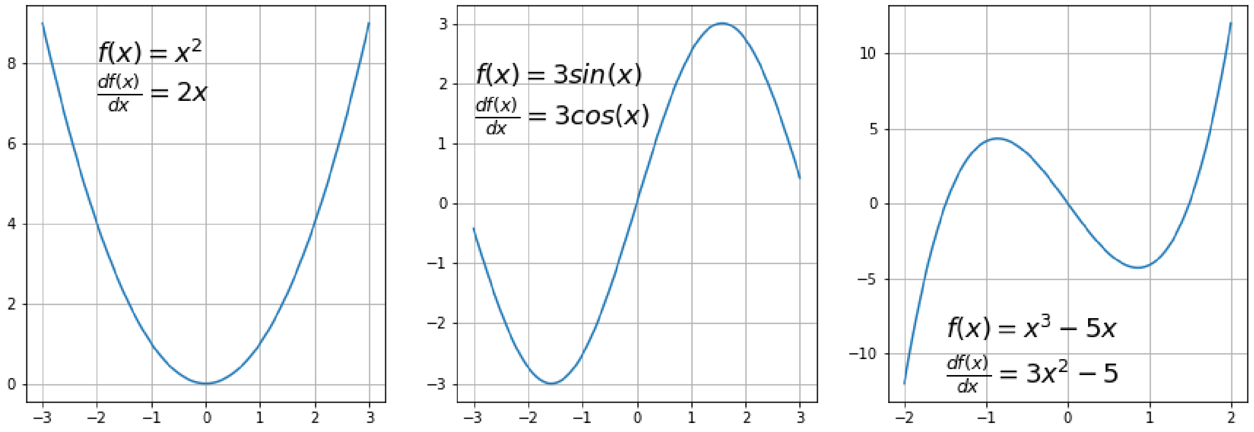
$$x_{21} = 2.065, \quad f(2.065) = -2.996$$

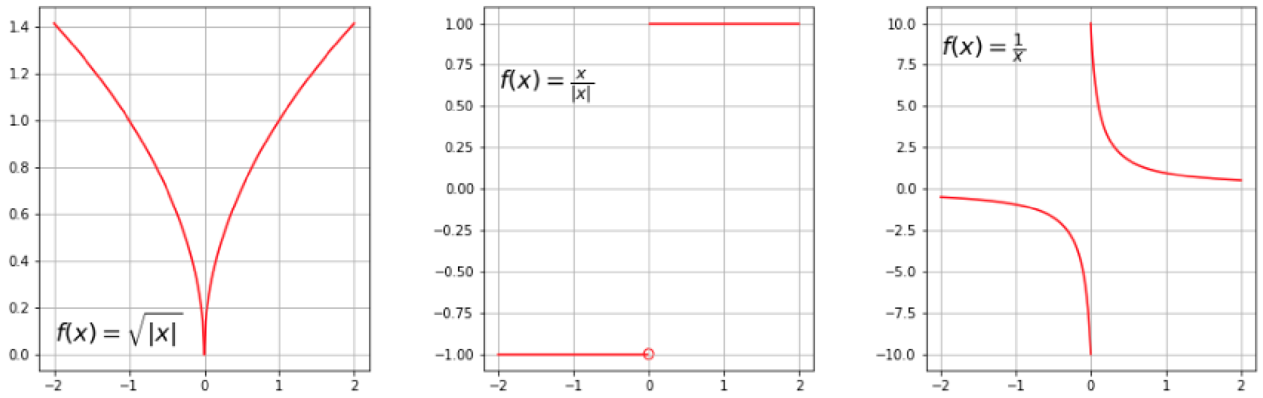
$$x_{22} = 2.052, \quad f(2.052) = -2.997$$



Function requirements

- Differentiable



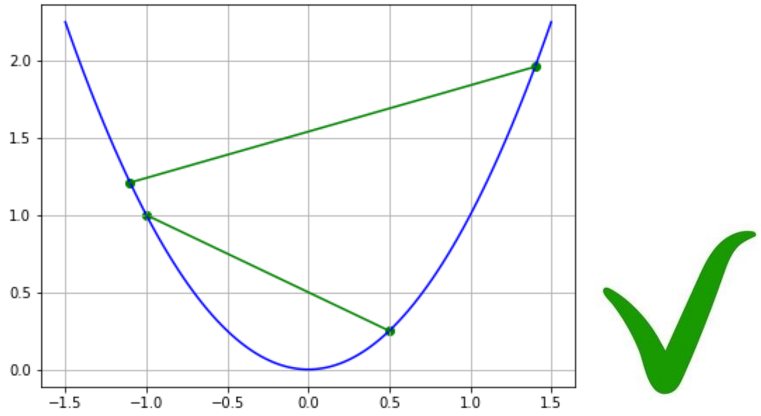


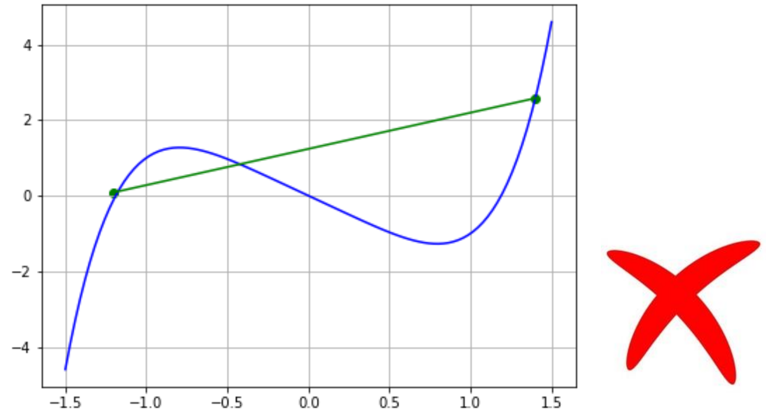
(a) Cusp (b) Jump discontinuity (c) Infinite discontinuity

Function requirements

- Differentiable
- Convex

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda)f(x_2)$$





Function requirements

- Example
  - Convex?

Example $f(x) = x^2 - x + 3$

Function requirements

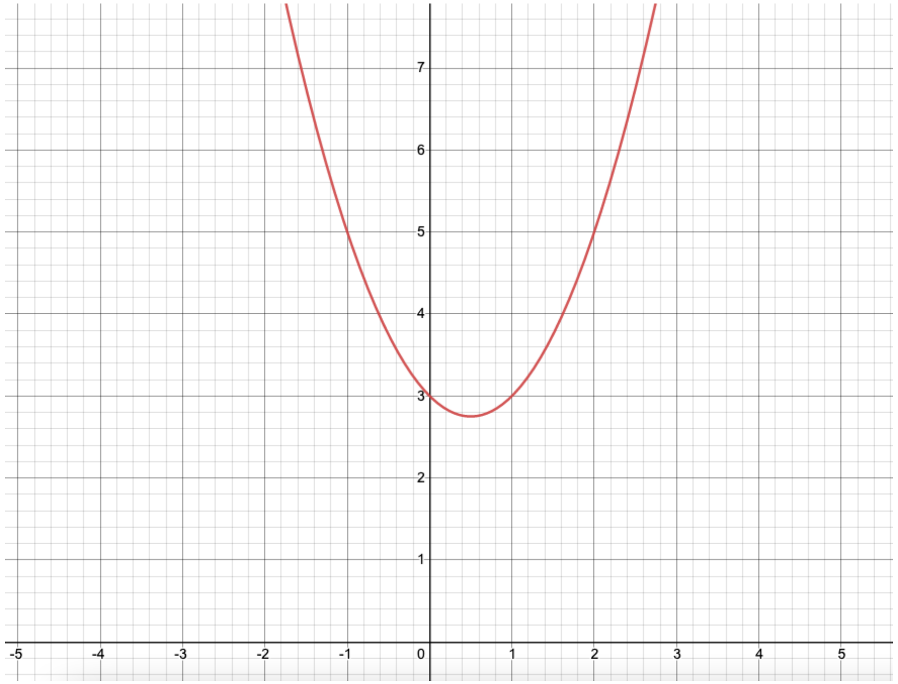
- Example
  - Convex?

Example $f(x) = x^2 - x + 3$

$$\frac{df(x)}{dx} = 2x - 1, \quad \frac{d^2 f(x)}{dx^2} = 2$$

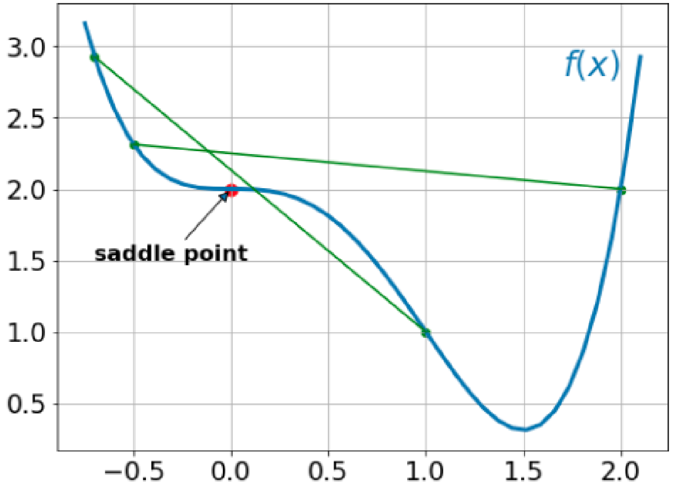
The function has derivative everywhere

The second derivative is always > 0



Function requirements

- Example
  - Differentiable
  - Convex?



Example of a semi-convex function with a saddle point

Example $f(x) = x^4 - 2x^3 + 2$

$$\frac{df(x)}{dx} = 4x^3 - 6x^2 = x^2(4x - 6)$$

$$\frac{d^2f(x)}{dx^2} = 12x^2 - 12x = 12x(x - 1)$$

- for $x < 0$: function is convex
- for $0 < x < 1$: function is concave
- for $x > 1$: function is convex again

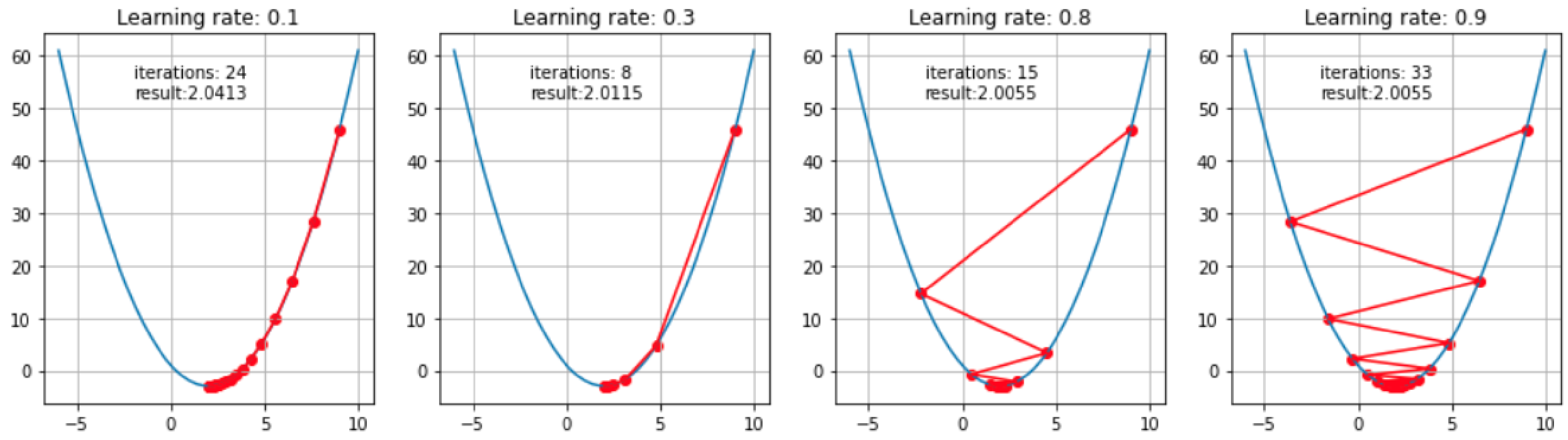
$x = 0$: saddle point

both first and second derivatives equal to zero

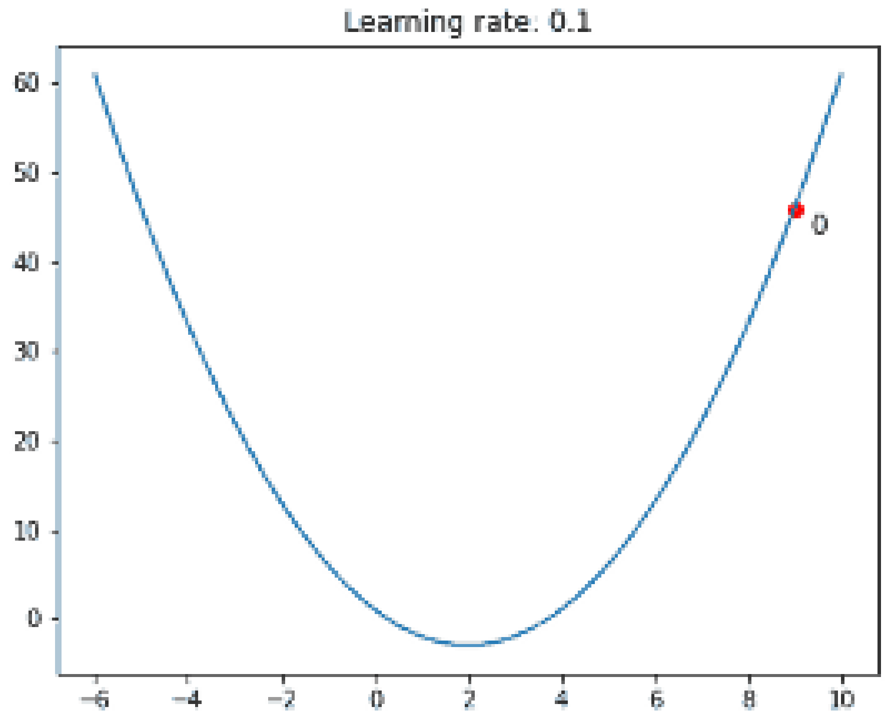
Challenges: learning rate

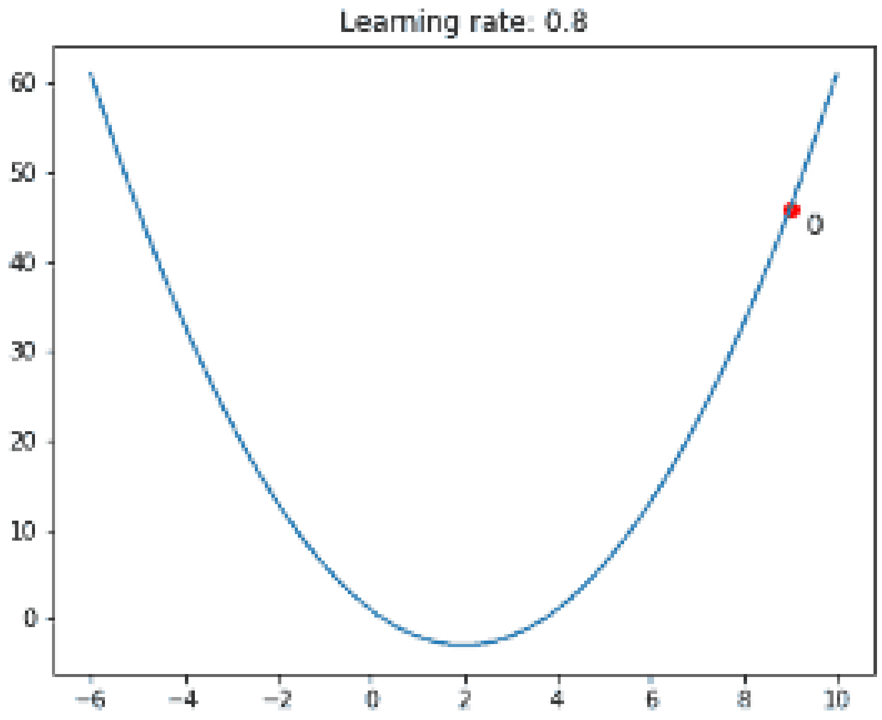
- Parameter update $\vec{p}_{n+1} = \vec{p}_n - \eta \nabla f\left(\vec{p}_n\right)$
- Learning rate $\boldsymbol{\eta}$: scales the gradient and thus controls the step size
  - Too small

    Too slow to converge; may reach maximum iteration before convergence
  - Too big
    - May not converge to the optimal point (jump around) or even to diverge completely



Challenges: learning rate



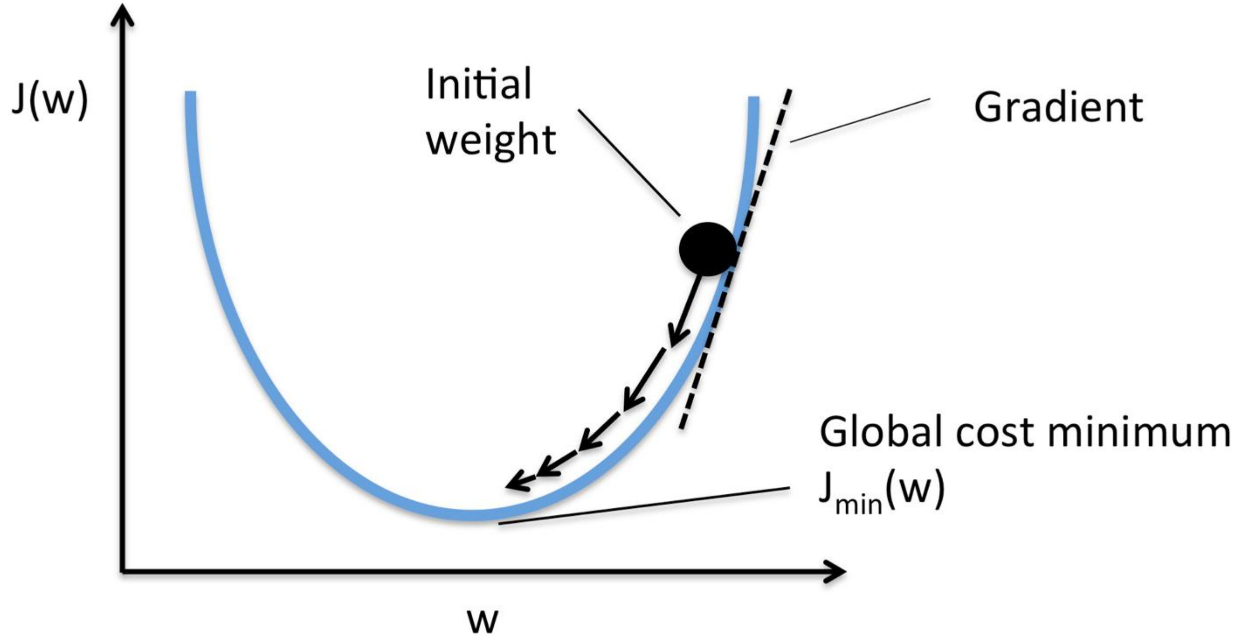


Challenges: learning rate

- Use a fixed learning rate $\vec{p}_{n+1} = \vec{p}_n - \eta \nabla f\left(\vec{p}_n\right)$
  - Try with a large value like 0.1
  - Try exponentially lower values: 0.01, 0.001, etc.

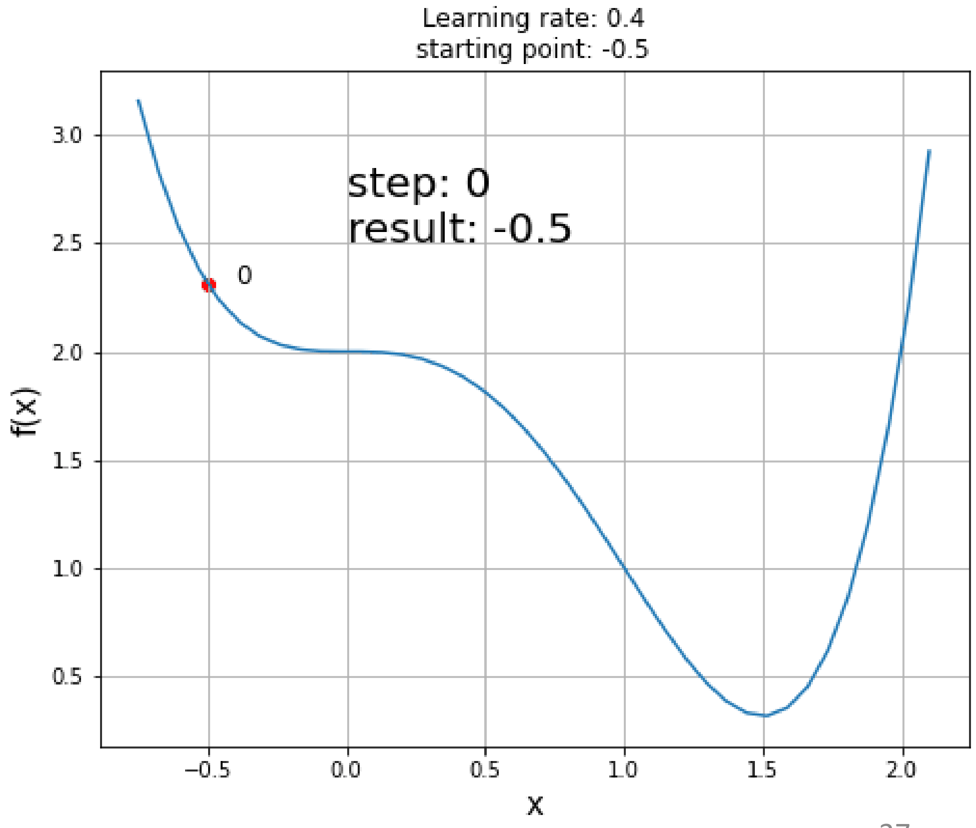
Challenges: learning rate

- Use a fixed learning rate $\vec{p}_{n+1} = \vec{p}_n - \eta \nabla f(\vec{p}_n)$
  - Try with a large value like 0.1
  - Try exponentially lower values: 0.01, 0.001, etc.
- Use an adaptive learning rate
  - Start with a larger value
  - Gradual decrease it



Challenges: saddle points

- Global minimum is not guaranteed
- Saddle point
  - Gradient = 0
  - Nether local minimum nor local maximum



Advanced methods

- Newton's method
  - Second-order derivative is used
  - Take a more direct route

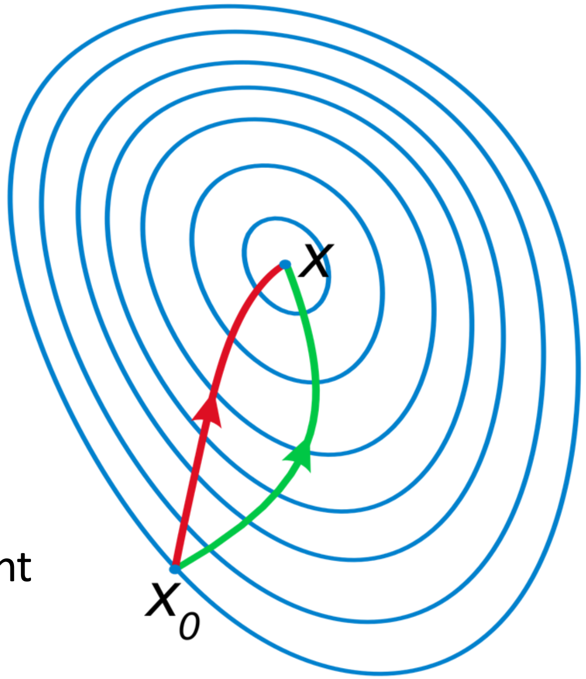
Gradient descent (linear approximation)

$$f(x_k + t) \approx f(x_k) + f'(x_k)t$$

Newton's method (quadratic approximation)

$$f(x_k + t) \approx f(x_k) + f'(x_k)t + \frac{1}{2}f''(x_k)t^2$$

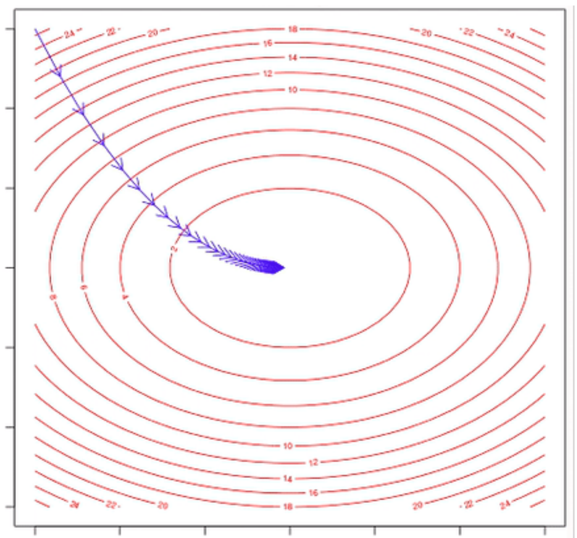
Green: Gradient descent
Red: Newton's method

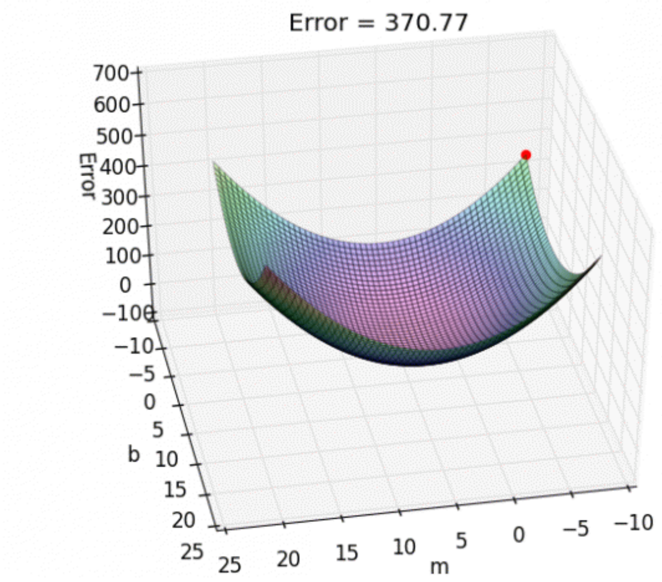


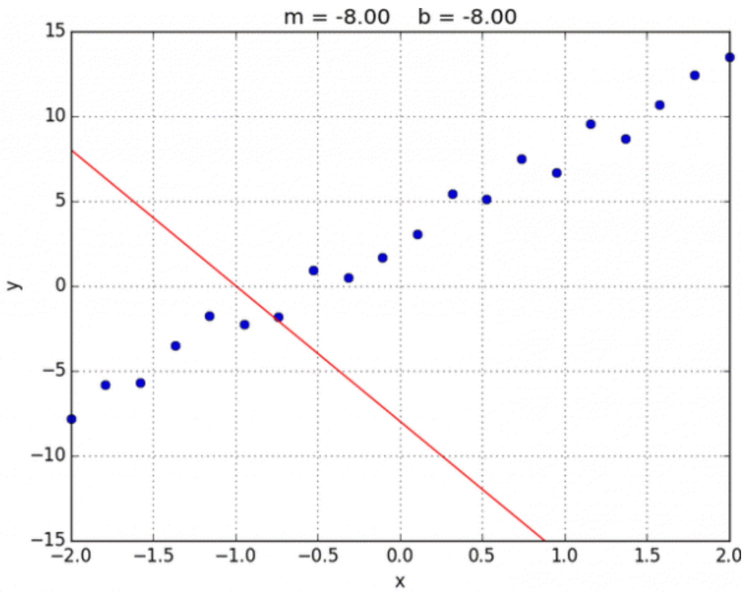
Solve linear regression using GD

- Objective function
  - Always convex

$$f(a,b) = \sum_{i=0}^{n} (y_i - (ax_i + b))^2$$







Next Lecture

- Clustering & Nearest Neighbor Classification