

# Machine Learning

## Regression problems

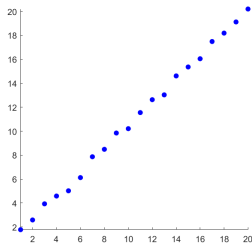
Emanuele Rodolà  
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2nd semester a.y. 2024/2025 · March 10, 2025

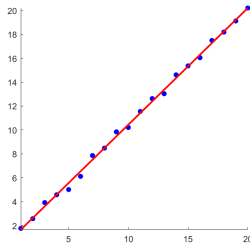
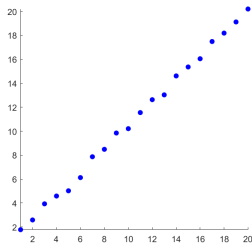
# Linear regression

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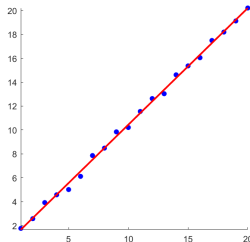
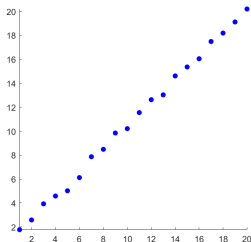
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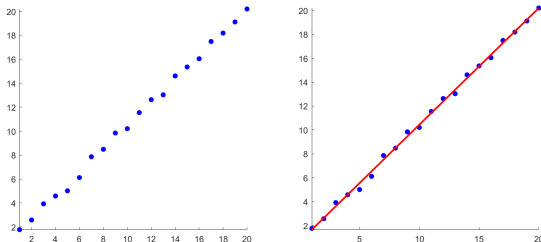
**Model:** linear + bias

**Parameters:**  $\Theta = \{a, b\}$

**Data:**  $n$  pairs  $(x_i, y_i)$ ; the  $x_i$  are called the **regressors**

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Given  $a$  and  $b$ , we have a **mapping** that gives new output from new input.

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The equations:

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$$\epsilon = \min_{a, b \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^n (y_i - f_{\Theta}(x_i))^2$$

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When  $f_{\Theta}$  is linear, this is called a **least-squares approximation** problem.

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The error criterion w.r.t. the parameters is also called a **loss** or **energy** function, usually denoted by  $\ell$ :

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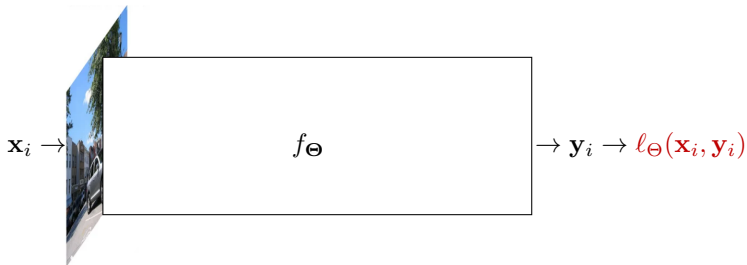
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**Remark:** We minimize the energy **w.r.t. the parameters  $\Theta$** , and **not** w.r.t. the **data**  $(x_i, y_i)$ .

# Linear regression

We are considering the following case:



where  $f_{\Theta}$  is linear, and  $\ell_{\Theta}$  is quadratic.

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Let's see what optimization problems we can solve **easily**!

# Convexity and gradients

# Convex functions

Jensen's inequality:

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y)$$

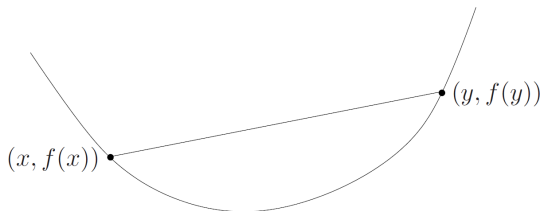
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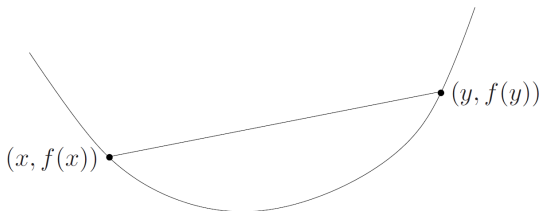


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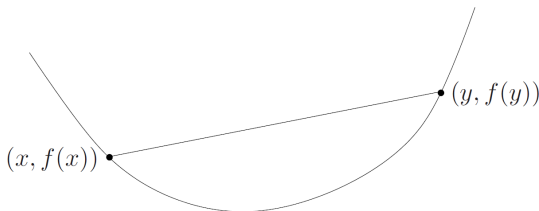
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Let us further assume that  $f$  is a **differentiable** function, so that we can compute its **derivative**  $\frac{df}{dx}$  at all points  $x$ .

**Theorem:** the **global** minimizer  $x$  is where  $\frac{df(x)}{dx} = 0$ .

## Convex functions on $\mathbb{R}^n$

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$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

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and we also have the **global optimality** condition:

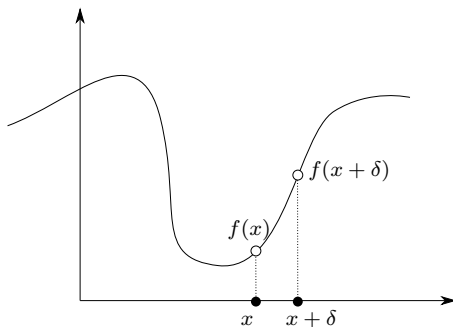
$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \mathbf{0} \implies f(\mathbf{x}) \leq f(\mathbf{y}) \text{ for all } \mathbf{y} \in \mathbb{R}^n$$

# The gradient

The gradient  $\nabla_{\mathbf{x}} f(\mathbf{x})$  encodes the **direction** of **steepest ascent** of  $f$  at point  $\mathbf{x}$ .

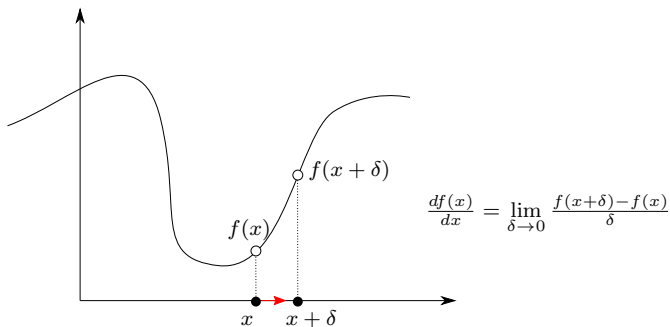
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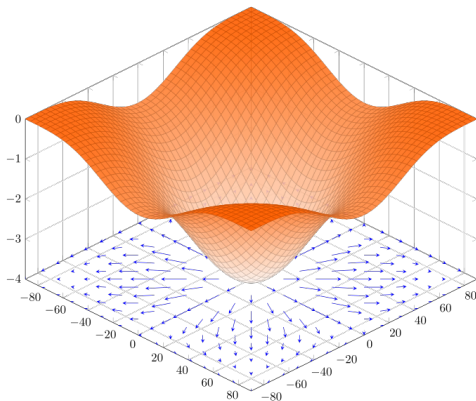
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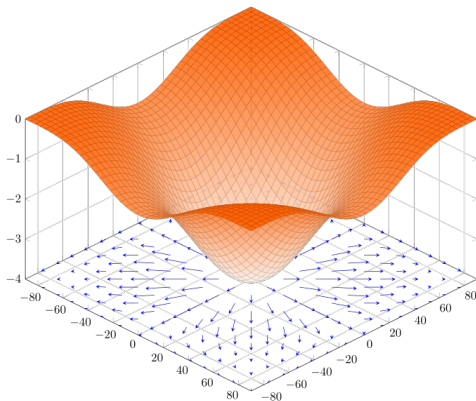
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The **length** of the gradient vector encodes its steepness.

## Convex functions: Global minima

To summarize:

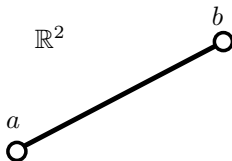
If  $f(x)$  is **convex**, then a **global minimizer** is found by setting  $\frac{df(x)}{dx} = 0$  and solving for  $x$ .

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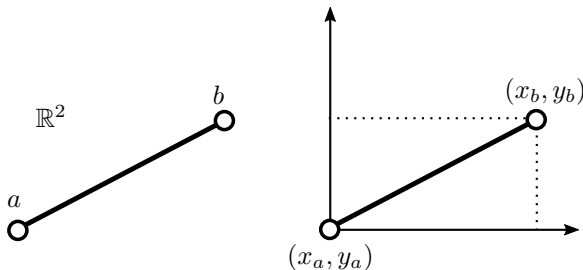
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How to measure the length of the gradient? Let's first start from the definition of **Euclidean distance**, which measures the length of any straight line connecting two points:



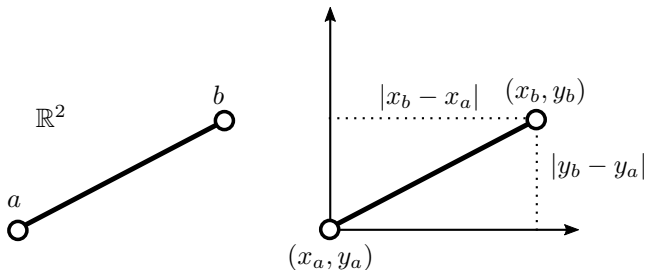
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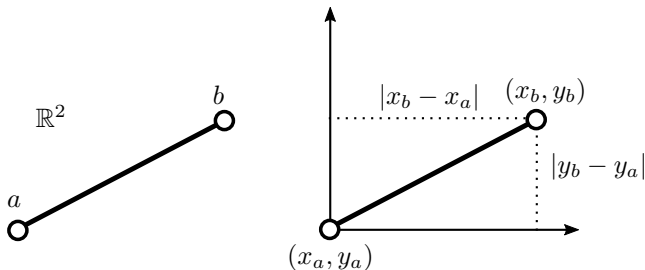
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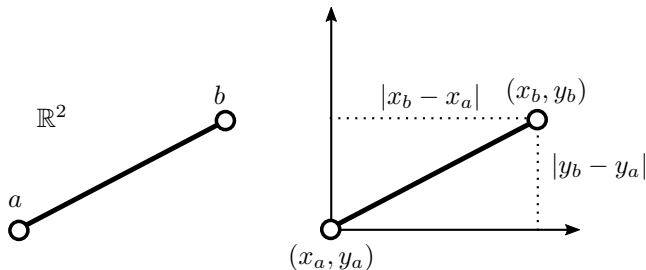
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In matrix notation:

$$d(\mathbf{a}, \mathbf{b}) = \|\mathbf{a} - \mathbf{b}\|_2$$

where  $\mathbf{a} = \begin{pmatrix} x_a \\ y_a \end{pmatrix}$  and  $\mathbf{b} = \begin{pmatrix} x_b \\ y_b \end{pmatrix}$

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One can generalize to different power coefficients  $p \geq 1$ :

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As well as generalize from  $\mathbb{R}^2$  to  $\mathbb{R}^k$ :

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The  $L_p$  length (or norm) of a vector is simply its distance from the origin:

$$\|\mathbf{x} - \mathbf{0}\|_2 = \|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^k |x_i|^2}$$

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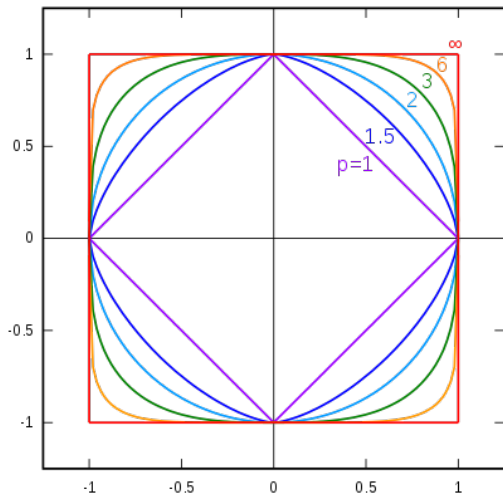
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$L_p$  unit balls in  $\mathbb{R}^2$



# Unit balls on manifolds

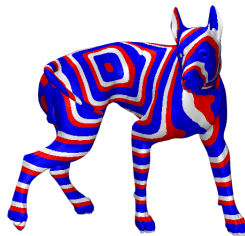
The notion of unit ball makes sense in any metric space, as it only depends on the presence of a [distance](#) function.



anisotropic



geodesic



$L_7$  in  $\mathbb{R}^3$

Each [isoline](#) identifies points at the same distance from the source

# Normal equation

## Linear regression: Finding a solution

$$\min_{a,b \in \mathbb{R}} \sum_{i=1}^n (y_i - ax_i - b)^2$$

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$$\Theta^* = \arg \min_{\Theta \in \mathbb{R}^2} \ell(\Theta)$$

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We get 2 linear equations in the 2 unknowns  $a, b$ :

$$\begin{pmatrix} \sum_{i=1}^n ax_i^2 + bx_i - x_iy_i \\ \sum_{i=1}^n ax_i + b - y_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

## Linear regression: Matrix notation

The learning model of linear regression is **linear in the parameters** (while it is **not** linear in  $x$ , due to the bias).

Therefore, in matrix notation the equations  $y_i = ax_i + b$  read:

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**Remark:** Deep learning frameworks frequently use the alternative expression with the bias encoded separately:

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## Linear regression: Matrix notation

Familiarize with matrix calculus.

When implementing a ML system, we manipulate matrices, vectors, and tensors.

## Linear regression: Matrix notation

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This expresses all the equations  $y_i = ax_i + b$  at once and makes the linearity w.r.t.  $a, b$  evident.

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Setting  $\nabla_{\boldsymbol{\theta}} \ell = \mathbf{0}$  we get:

$$\boldsymbol{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

We get a closed form solution to our problem (aka **normal equation**).

# Linear regression: Higher dimensions

Until now we have seen the case where:

$$y_i = ax_i + b \quad \text{for } i = 1, \dots, n$$

that is, each data point is one-dimensional (just one number).

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Defining the matrices  $\mathbf{X} = \begin{pmatrix} | & | & \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots \\ | & | & \\ 1 & 1 & \end{pmatrix}$ ,  $\mathbf{Y} = \begin{pmatrix} | & | & \\ \mathbf{y}_1 & \mathbf{y}_2 & \cdots \\ | & | & \end{pmatrix}$ ,  $\Theta = \begin{pmatrix} \mathbf{A} \\ \mathbf{b}^\top \end{pmatrix}$ ,

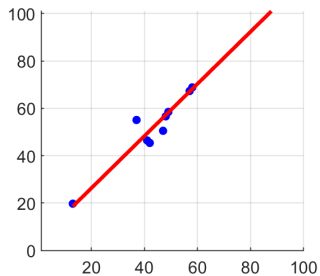
we get a closed-form solution to  $\nabla_{\Theta} \ell(\Theta) = \mathbf{0}$ :

$$\Theta = (\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{X}\mathbf{Y}^\top$$



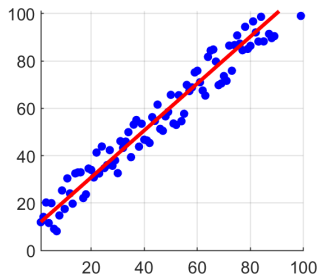
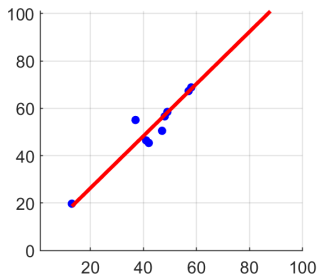
# Polynomial regression

# Data distribution



Assumption: **linear** model

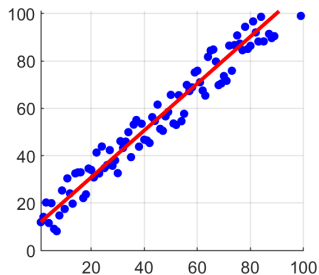
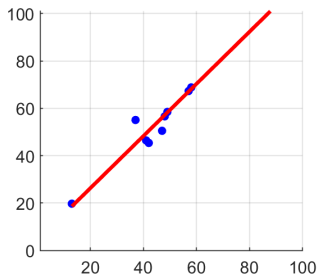
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Assumption: **linear** model

More data allows us to improve our prediction

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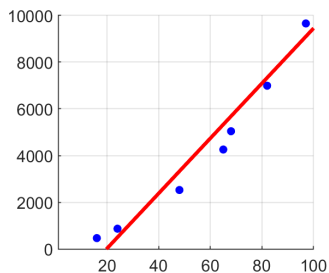


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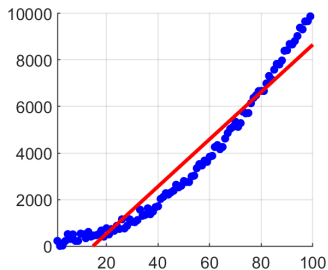
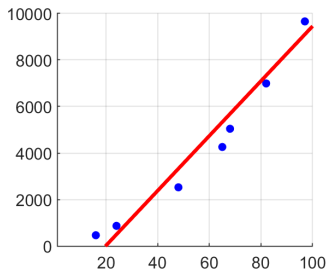
What if the assumption (i.e. linear prior here) is **wrong**?

# Data distribution



Assumption: linear model

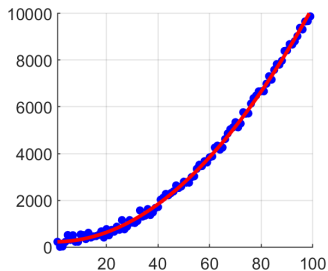
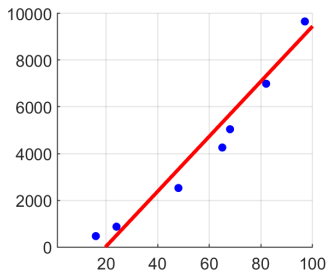
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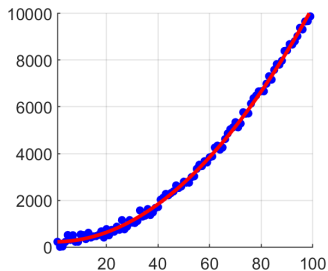
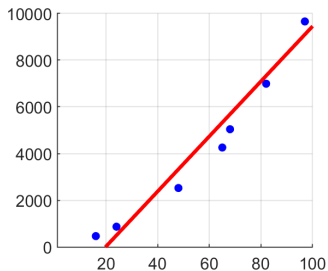
More data **confutes** our assumptions

# Data distribution



Assumption: quadratic model

# Data distribution



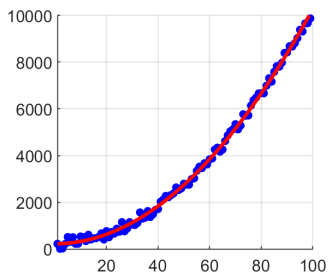
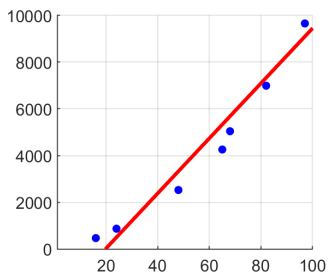
Assumption: **quadratic** model

Key questions:

- How to select the **correct distribution**?



# Data distribution

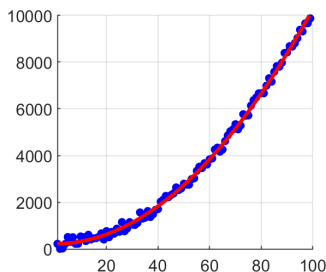
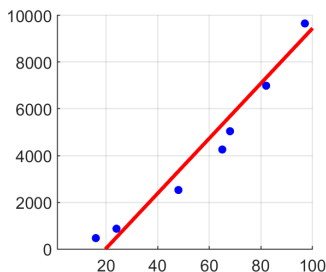


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# Data distribution



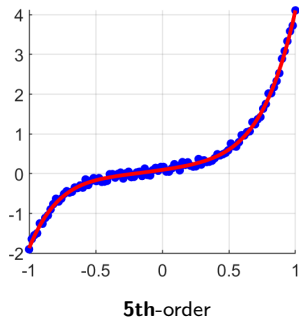
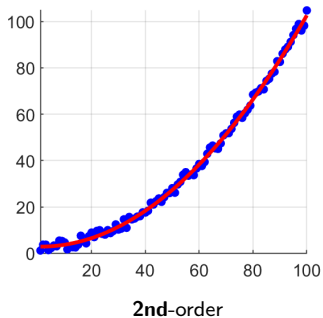
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Key questions:

- How to select the **correct distribution**?
- **How much data** do we need?
- What if the correct distribution does not admit a **simple expression**?

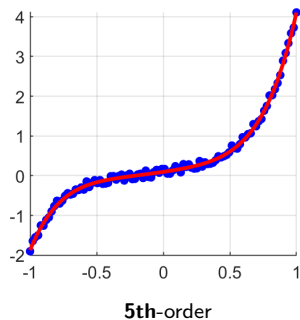
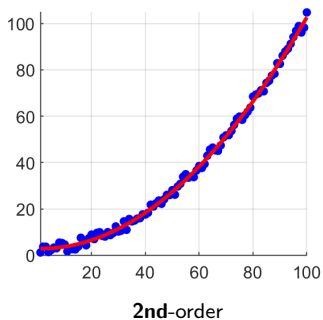
# Polynomial regression

After the linear model, the simplest thing is a **polynomial model**.



# Polynomial regression

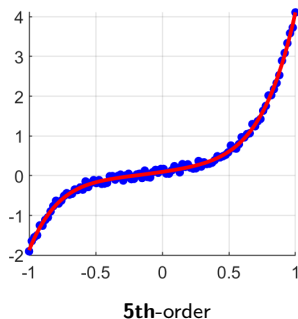
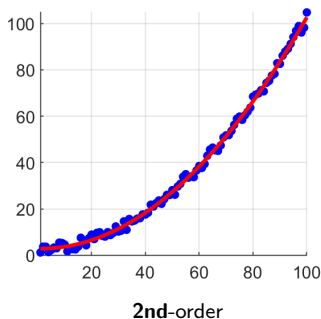
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**More data** are needed to make an informed decision on the order.

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**Remark:** Despite the name, polynomial regression is still **linear in the parameters**. It is polynomial with respect to the data.

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The same exact **least-squares** solution as with linear regression applies, with the requirement that  $k < n$ .

# Underfitting and overfitting

# Polynomial fitting

An application of the [Stone-Weierstrass theorem](#) tells us:

If  $f$  is continuous on the interval  $[a, b]$ , then for every  $\epsilon > 0$  [there exists a polynomial  \$p\$](#)  such that  $|f(x) - p(x)| < \epsilon$  for all  $x$ .

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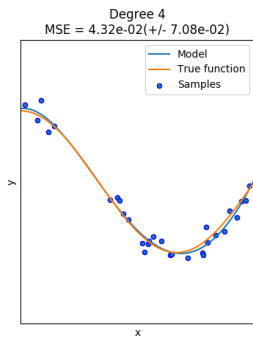
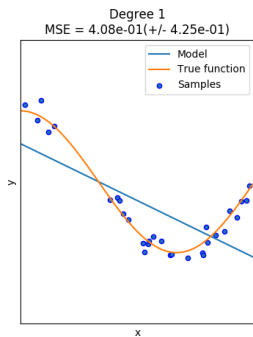
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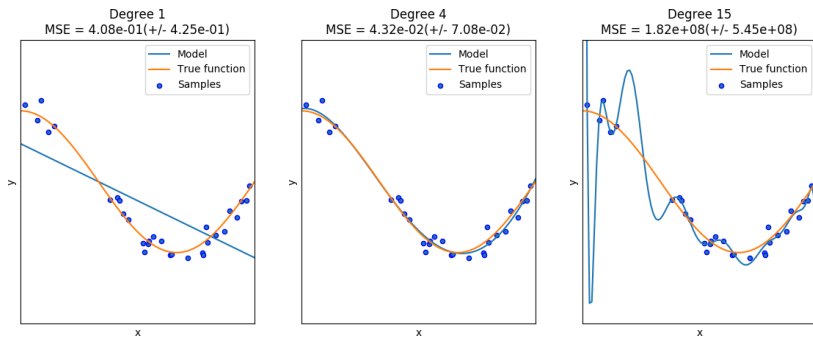


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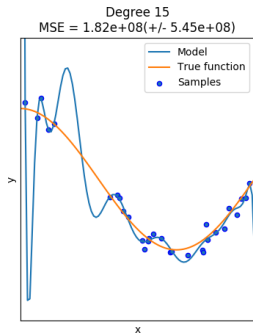
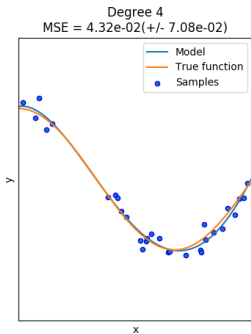
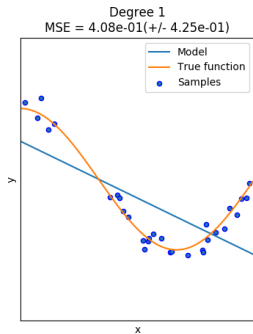
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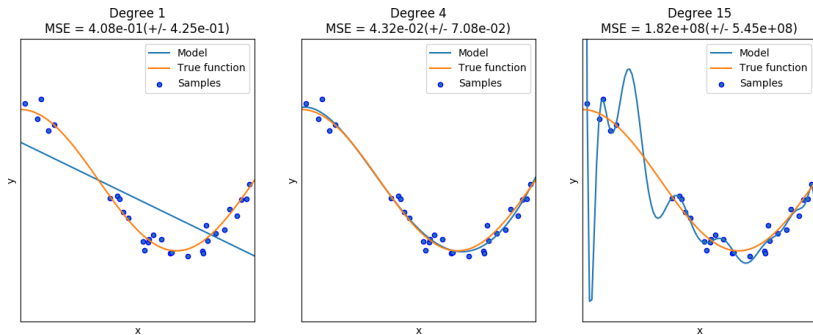
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# Underfitting vs. Overfitting

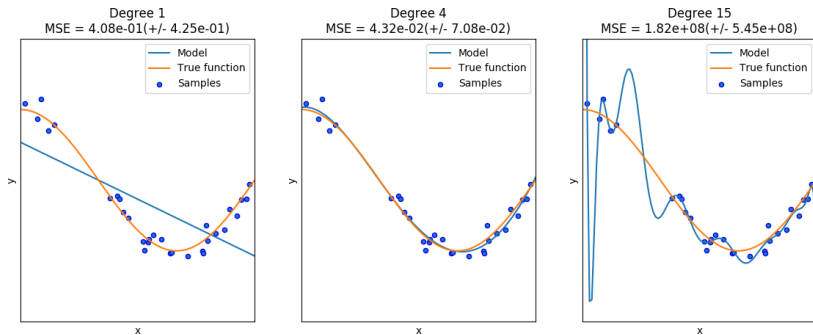


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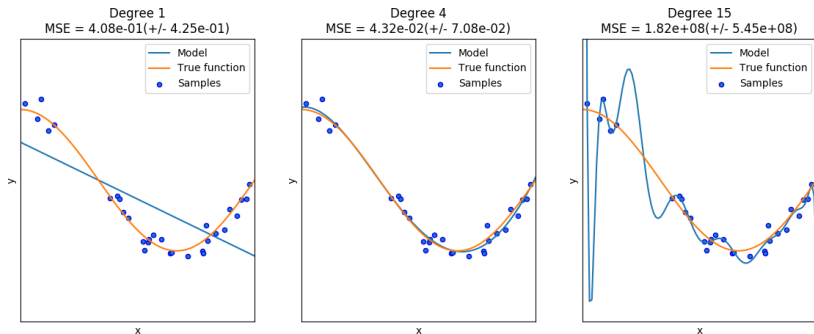
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Adding complexity can lead to **overfitting** and thus worse **generalization**.

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To recap, **overfitting** happens with small training error and large validation error

## $n$ -fold cross-validation

We do not want to overfit on the validation set either!

## $n$ -fold cross-validation

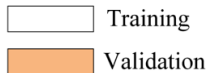
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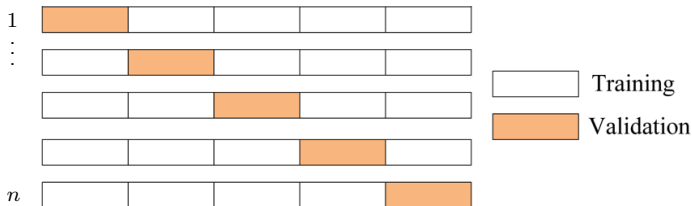
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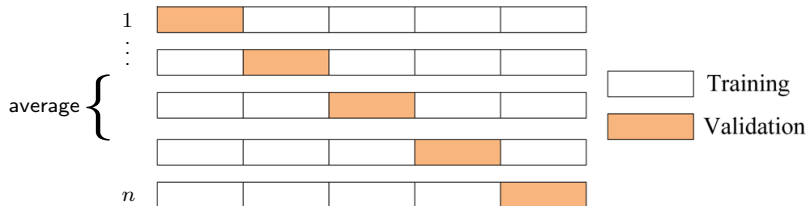
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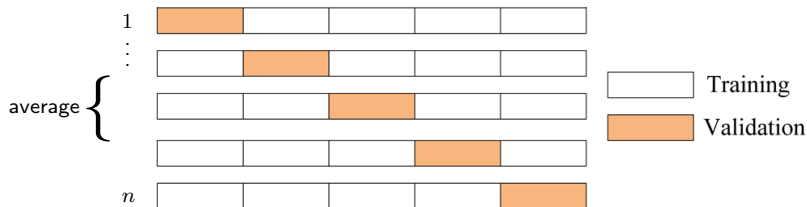


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**Example:** For polynomial regression, do the above many times with different degrees, choose the run with the smallest average MSE.

# Not done yet

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So is polynomial regression all we need?

Not really!

- Different loss than MSE
- Regularization
- Additional priors
- Intermediate features
- Flexibility
- Regression (predict a value) vs. classification (predict a category)

# Regularization penalties

Sometimes our prior knowledge can be expressed in terms of an **energy**.

For example, avoid **large** parameters to **counteract overfitting**:

$$\min_{\Theta} \underbrace{\ell_{\Theta}}_{\text{data term}} + \underbrace{\lambda}_{\text{trade-off}} \cdot \underbrace{\|\Theta\|_F^2}_{\text{regularizer}}$$

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# Logistic regression

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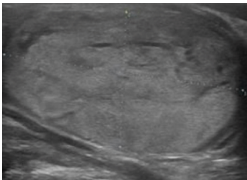
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⇒ The solution is not necessarily an optimum anymore.

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⇒ The solution is not necessarily an optimum anymore.

Instead: Modify the loss to minimize over **categorical values directly**.

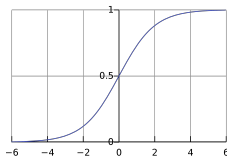
# Logistic regression

New loss:

$$\ell_{\Theta}(\{x_i, y_i\}) = \sum_{i=1}^n (y_i - \underbrace{\sigma(ax_i + b)}_{\text{linear}})^2$$

Here,  $\sigma$  is the nonlinear **logistic sigmoid**:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



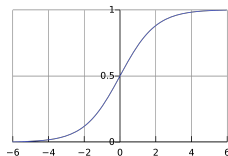
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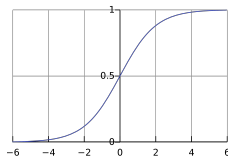
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New loss:

$$\ell_{\Theta}(\{x_i, y_i\}) = \sum_{i=1}^n (y_i - \underbrace{\sigma(ax_i + b)}_{\text{linear}})^2 \quad \text{non-convex in } a, b$$

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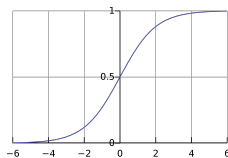
# Logistic regression

New loss:

$$\ell_{\Theta}(\{x_i, y_i\}) = \sum_{i=1}^n c(x_i, y_i), \quad \text{with}$$
$$c(x_i, y_i) = \begin{cases} -\ln(\sigma(ax_i + b)) & y_i = 1 \\ -\ln(1 - \sigma(ax_i + b)) & y_i = 0 \end{cases} \quad \text{convex}$$

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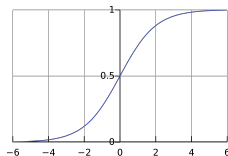
New loss:

$$\ell_{\Theta}(\{x_i, y_i\}) = \sum_{i=1}^n c(x_i, y_i), \quad \text{with}$$

$$c(x_i, y_i) = -y_i \ln(\sigma(ax_i + b)) - (1 - y_i) \ln(1 - \sigma(ax_i + b)) \quad \text{convex}$$

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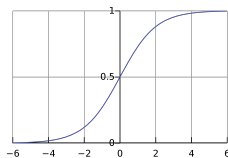
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New **convex** loss:

$$\ell_{\Theta}(\{x_i, y_i\}) = - \sum_{i=1}^n y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b))$$

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# Logistic regression: Finding a solution

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# Logistic regression: Finding a solution

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where  $\Theta = \{a, b\}$ .

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Consider the gradient of each term in the summation:

$$\nabla_{\Theta} (y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)))$$

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Apply the **chain rule** to each partial derivative:

$$\frac{\partial}{\partial \mathbf{a}} f(g(h(\mathbf{a}, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial \mathbf{a}}$$

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...and so on for the **second term** and for parameter  $b$ .

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By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a **nonlinear** way.

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model	loss	solution
linear regression linear regression + Tikhonov logistic regression		

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model	loss	solution
linear regression	convex	
linear regression + Tikhonov	convex	
logistic regression	convex	

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model	loss	solution
linear regression	convex	least squares
linear regression + Tikhonov	convex	
logistic regression	convex	

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model	loss	solution
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	



# Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a **nonlinear** way.

Thus:

- $\nabla \ell_{\Theta} = 0$  is **not a linear system** that we can solve easily.
- $\nabla \ell_{\Theta} = 0$  is a **transcendental equation**  $\Rightarrow$  no analytical solution.

model	loss	solution
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	<b>nonlinear optimization</b>

## Suggested reading

For convexity and optimality, read Sections 3.1.1 and 3.1.3 of the book:

S. Boyd & L. Vandenberghe, “Convex optimization”. Cambridge University Press, 2009

Public download link: [https://web.stanford.edu/~boyd/cvxbook/bv\\_cvxbook.pdf](https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf)

On polynomial regression vs. neural nets:

<https://arxiv.org/abs/1806.06850>

Proof that the logistic loss is convex:

<https://math.stackexchange.com/questions/1582452/logistic-regression-prove-that-the-cost-function-is-convex>