# Deep Learning & Applied AI

Overfitting and going nonlinear

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SAPIENZA
UNIVERSITÀ DI ROMA

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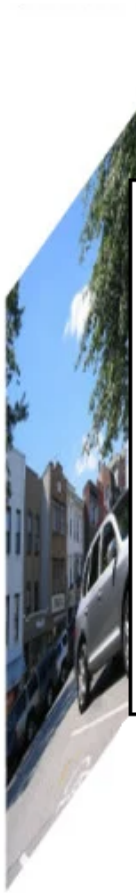
# A glimpse into neural networks

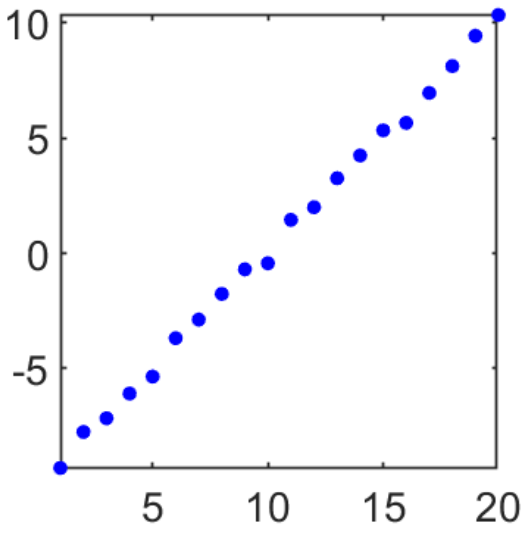
In deep learning, we deal with highly parametrized models called deep neural networks:



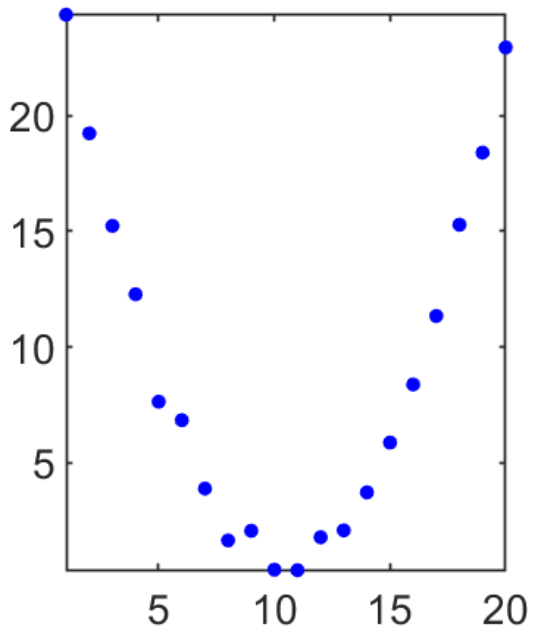
$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

# Parametrized models

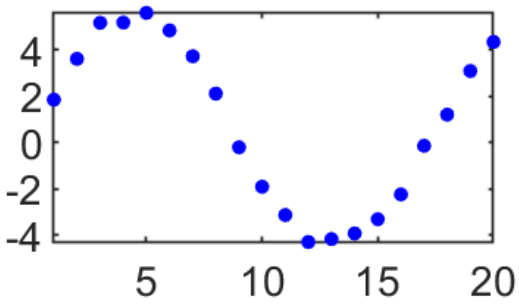
The parameters describe the behavior of the network, and must be solved for.




$y = ax + b$



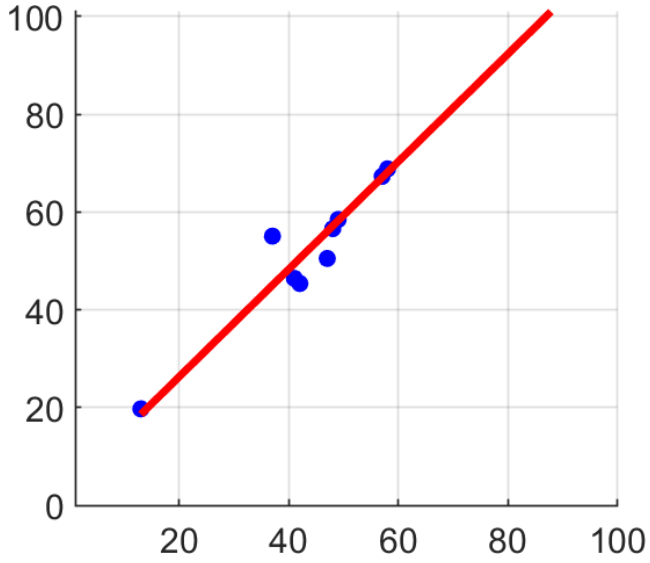

$y = ax^2 + bx + c$




$y = a\sin(x) + bx + c$

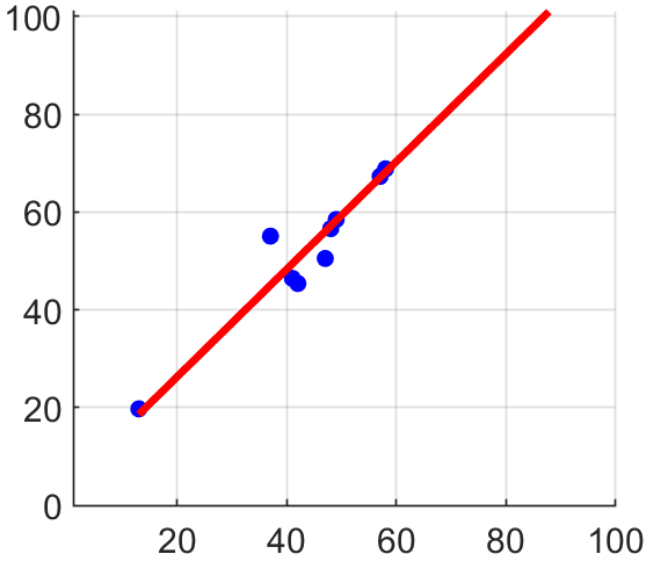
From a technical standpoint, our task is to determine the parameters $\Theta$.

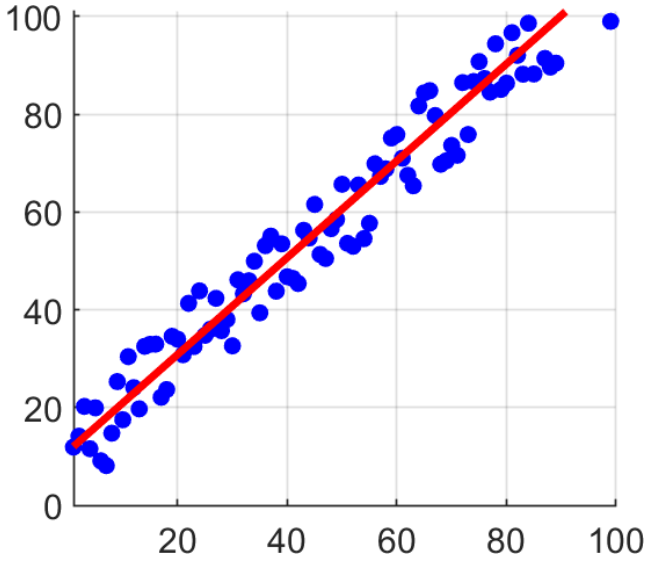
# Data distribution




Assumption: linear model

# Data distribution

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More data allows us to improve our prediction

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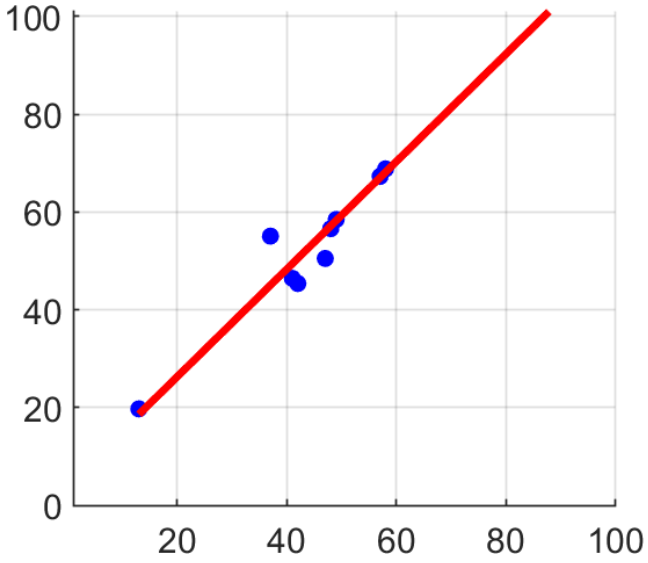


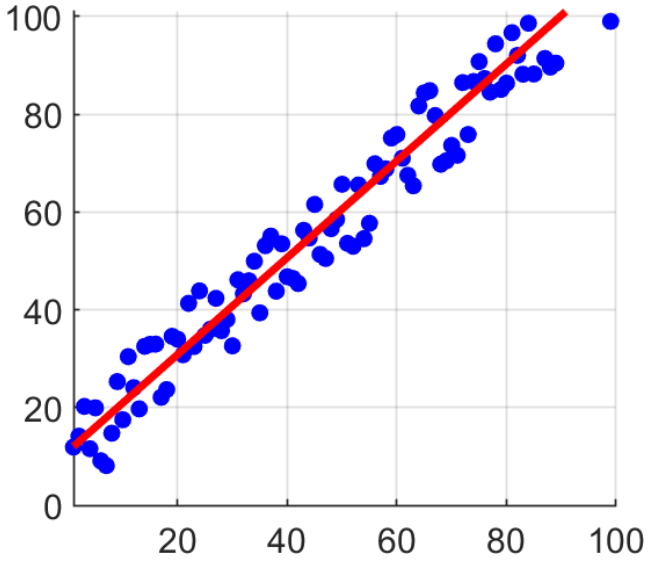


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What if the assumption (i.e. linear prior here) is **wrong**?

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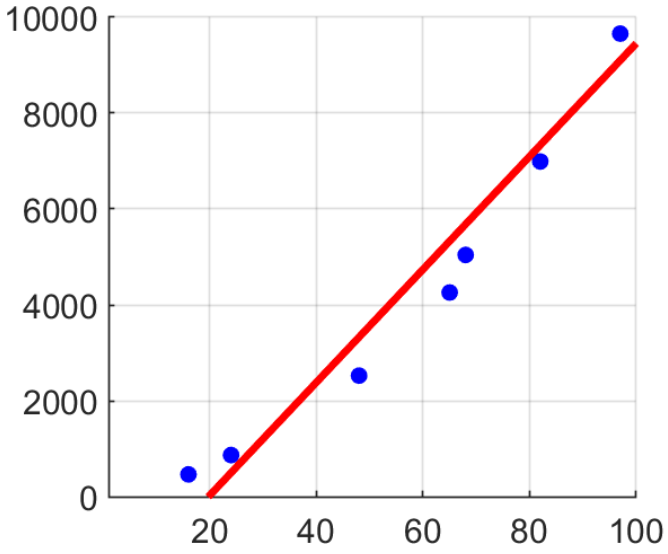


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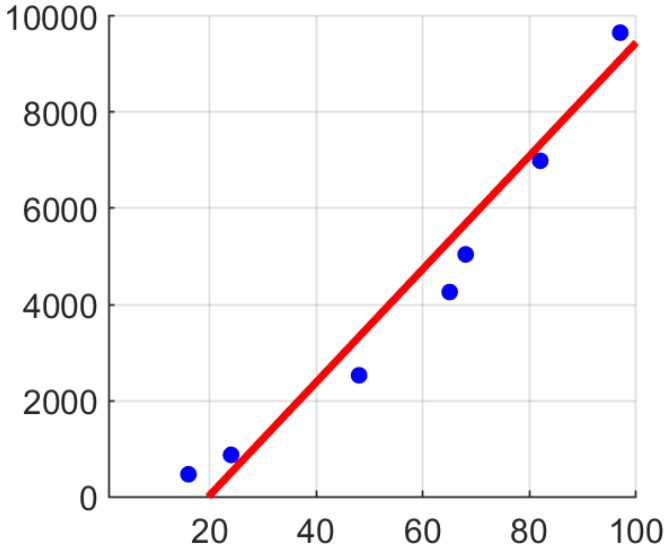


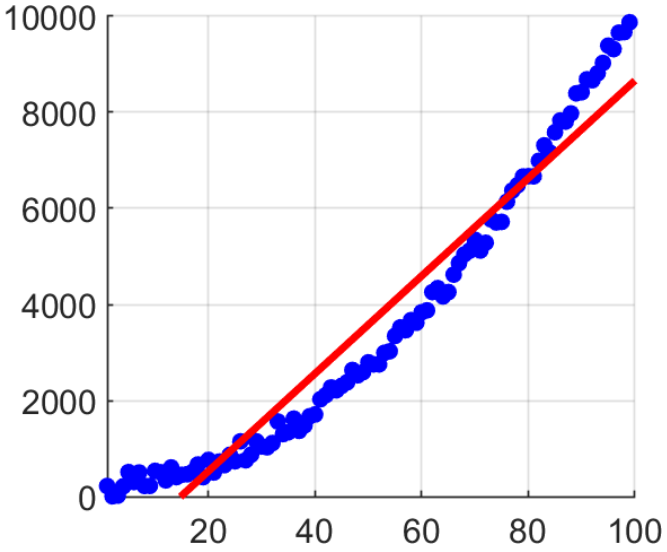


Assumption: linear model

More data confutes our assumptions

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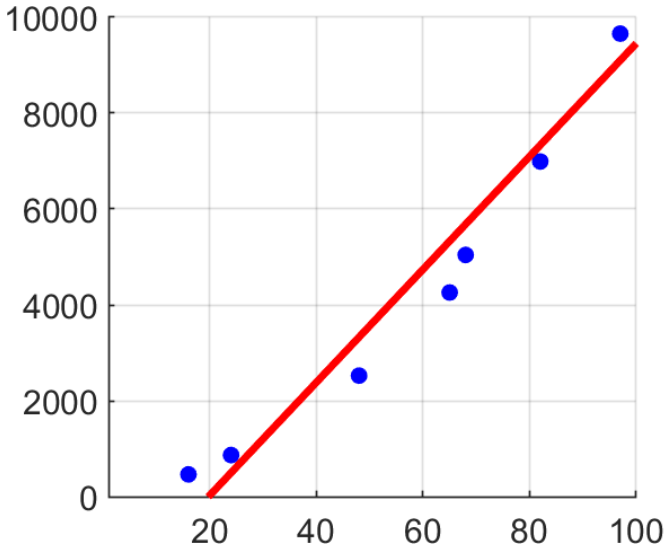


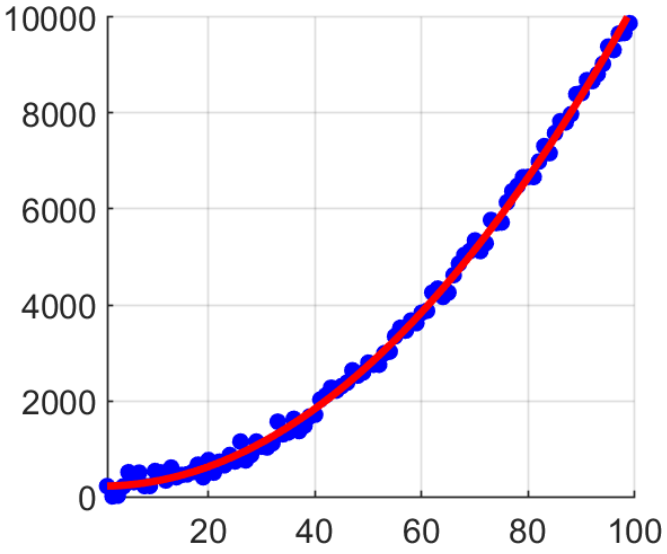


Assumption: quadratic model

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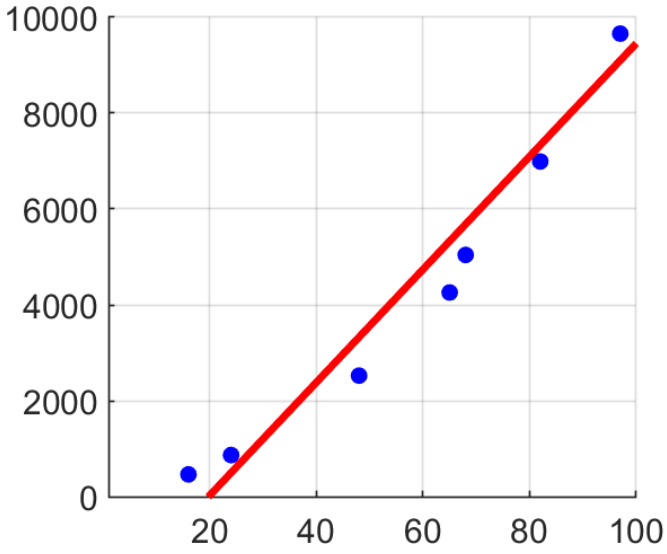


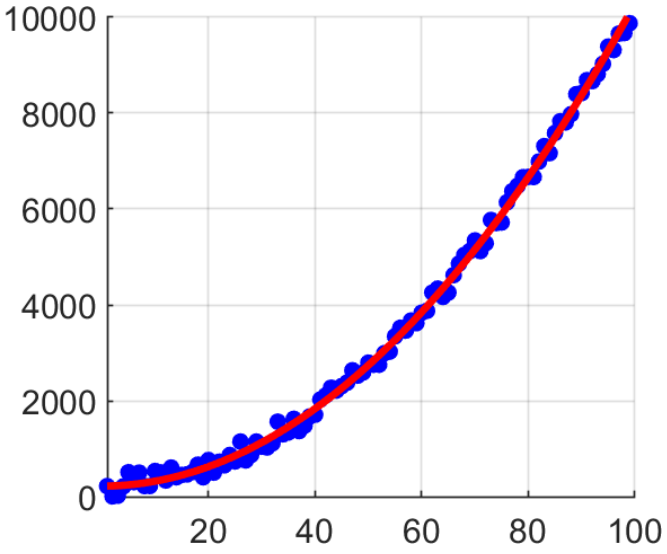


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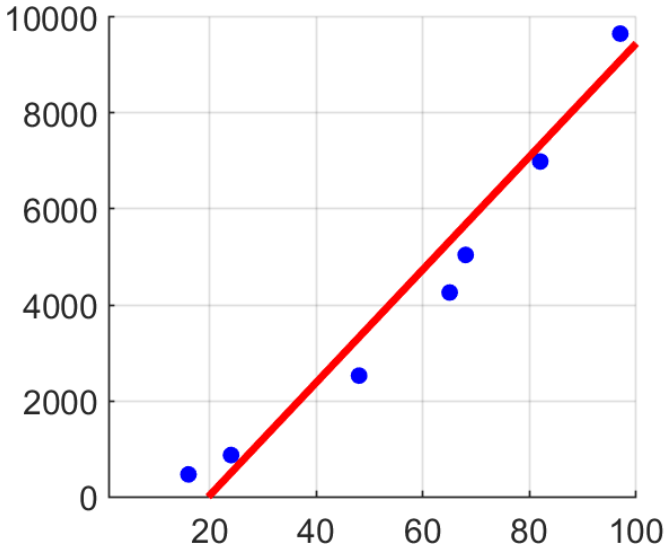


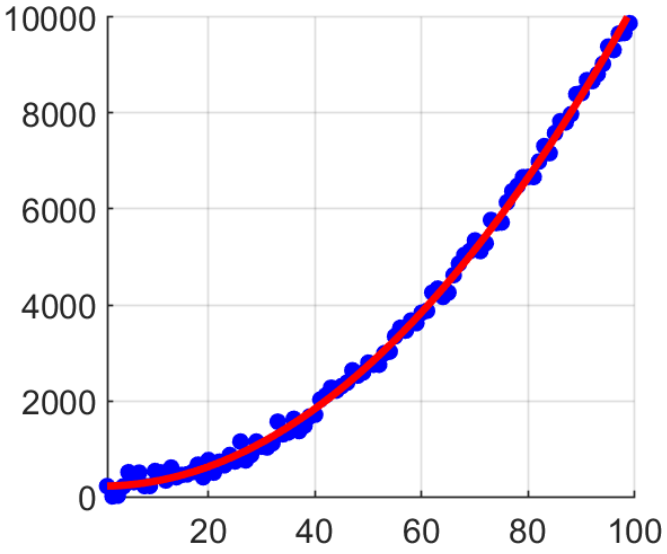


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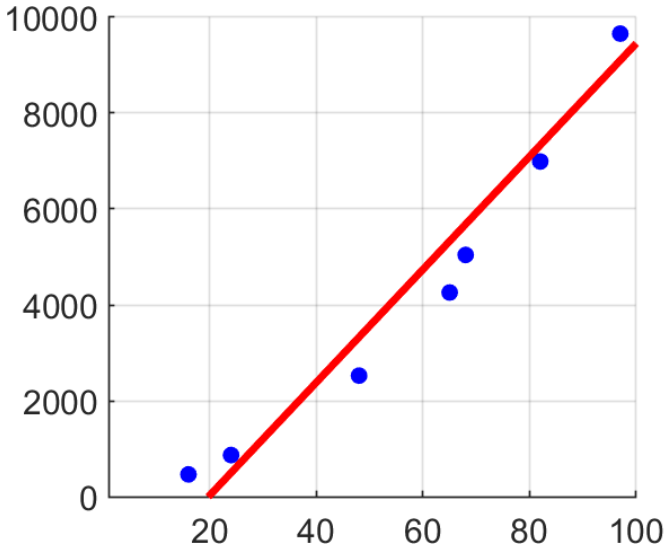


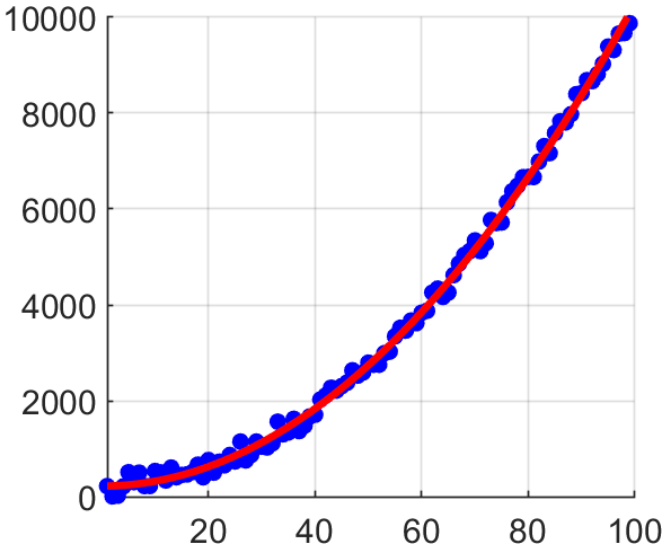


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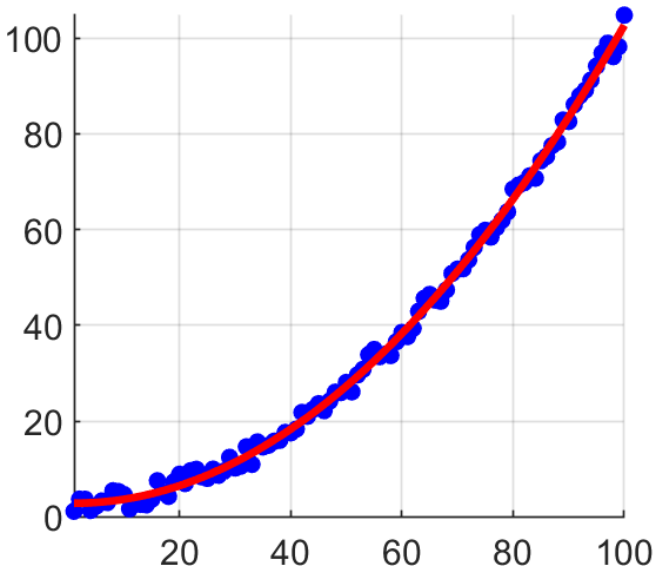
Key questions:

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

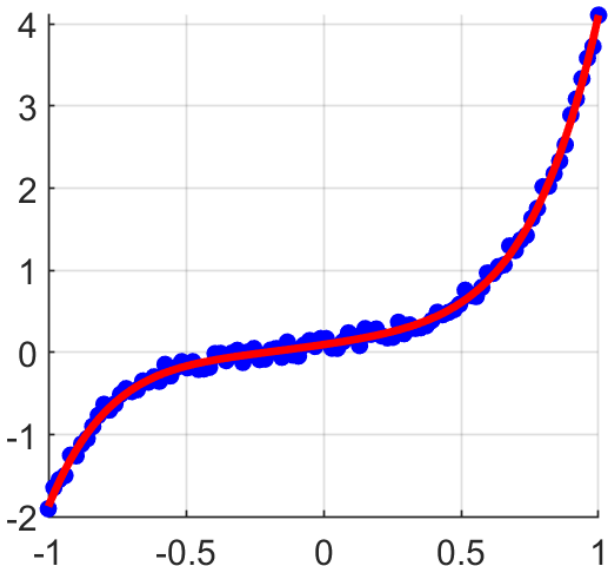
questo ultimo punto è riferito particolarmente al DL

# Polynomial regression

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




**2nd**-order

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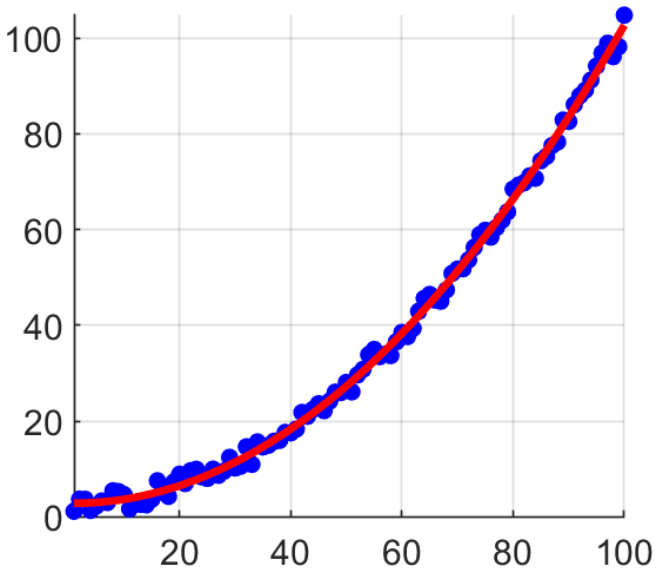


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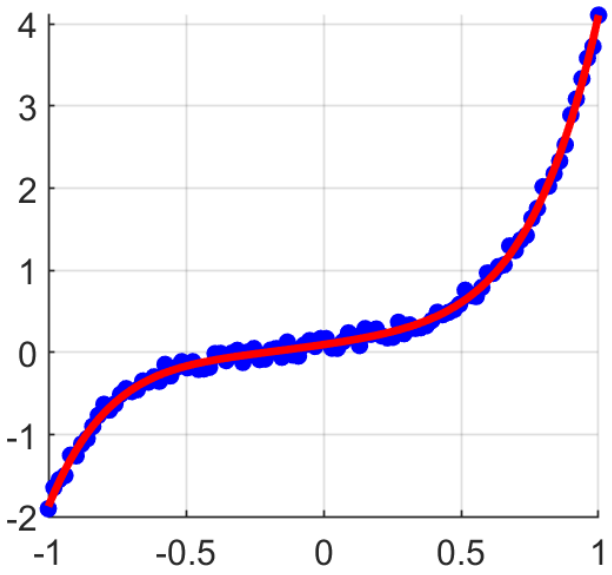


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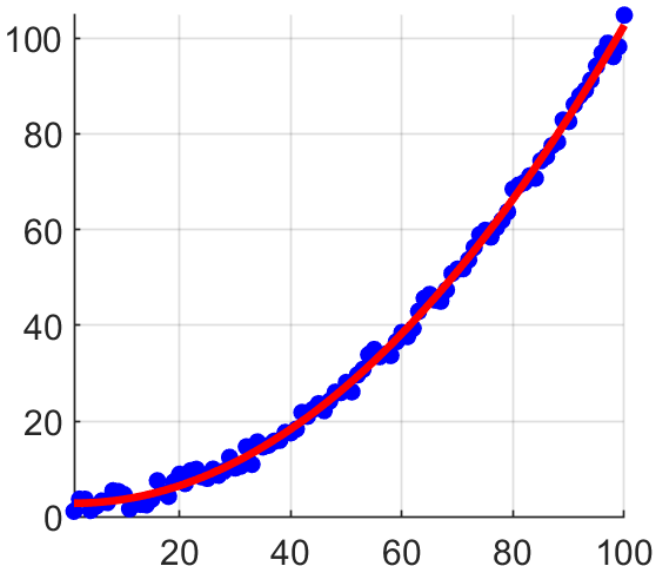


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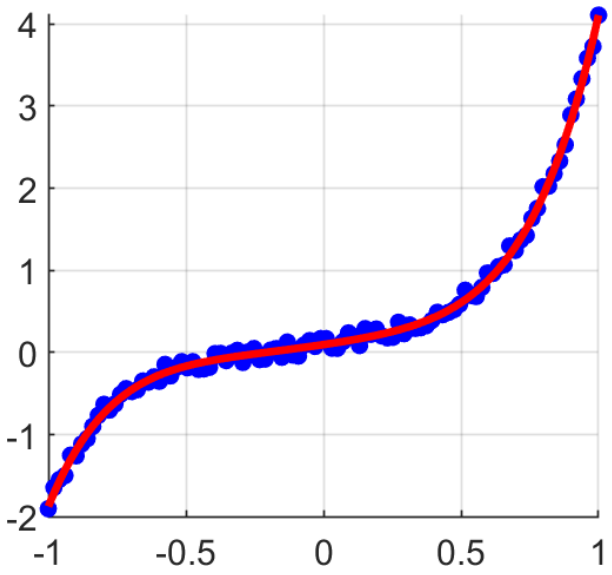


**5th**-order

The number of parameters grows with the order.

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

sembra che sia possibile trovare una curva polinomiale che si adatta bene a qualsiasi problema. In realtà questo è in parte vero, ma le curve polinomiali hanno alcune limitazioni...

# Polynomial regression

attenzione al nome: chiamata così sembra che la funzione non sia lineare, ma invece lo è! Per evitare confusione, si può chiamare...

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$$y_i = a_3 x_i^3 + a_2 x_i^2 + a_1 x_i + b \quad \text{for all data points } i = 1, \ldots, n$$

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In matrix notation:

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} x_1^k & x_1^{k-1} & \cdots & x_1 & 1 \\ x_2^k & x_2^{k-1} & \cdots & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^k & x_n^{k-1} & \cdots & x_n & 1 \end{pmatrix}}_{\mathbf{X}} \underbrace{\begin{pmatrix} a_k \\ a_{k-1} \\ \vdots \\ a_1 \\ b \end{pmatrix}}_{\boldsymbol{\theta}}$$

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The same exact least-squares solution as with linear regression applies, with the requirement that $k < n$. la condizione in specifica che bisogna avere sempre almeno più data points del grado della polinomiale

# 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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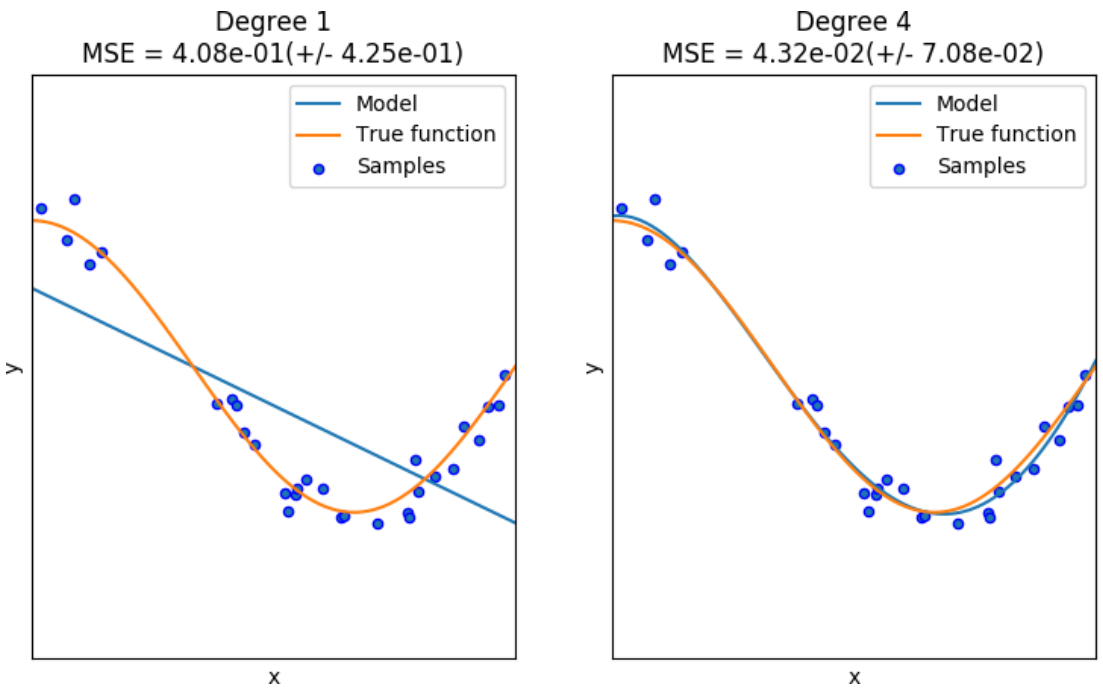

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teorema potentissimo

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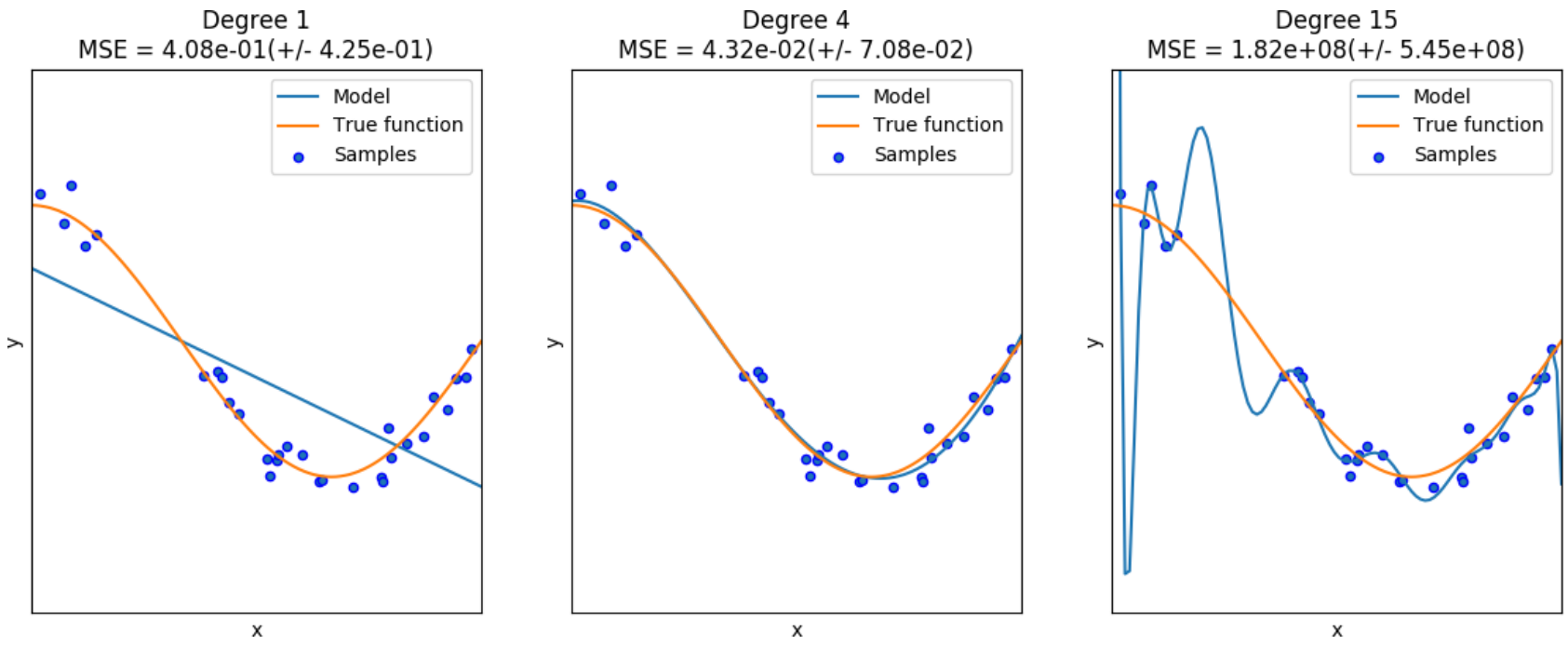

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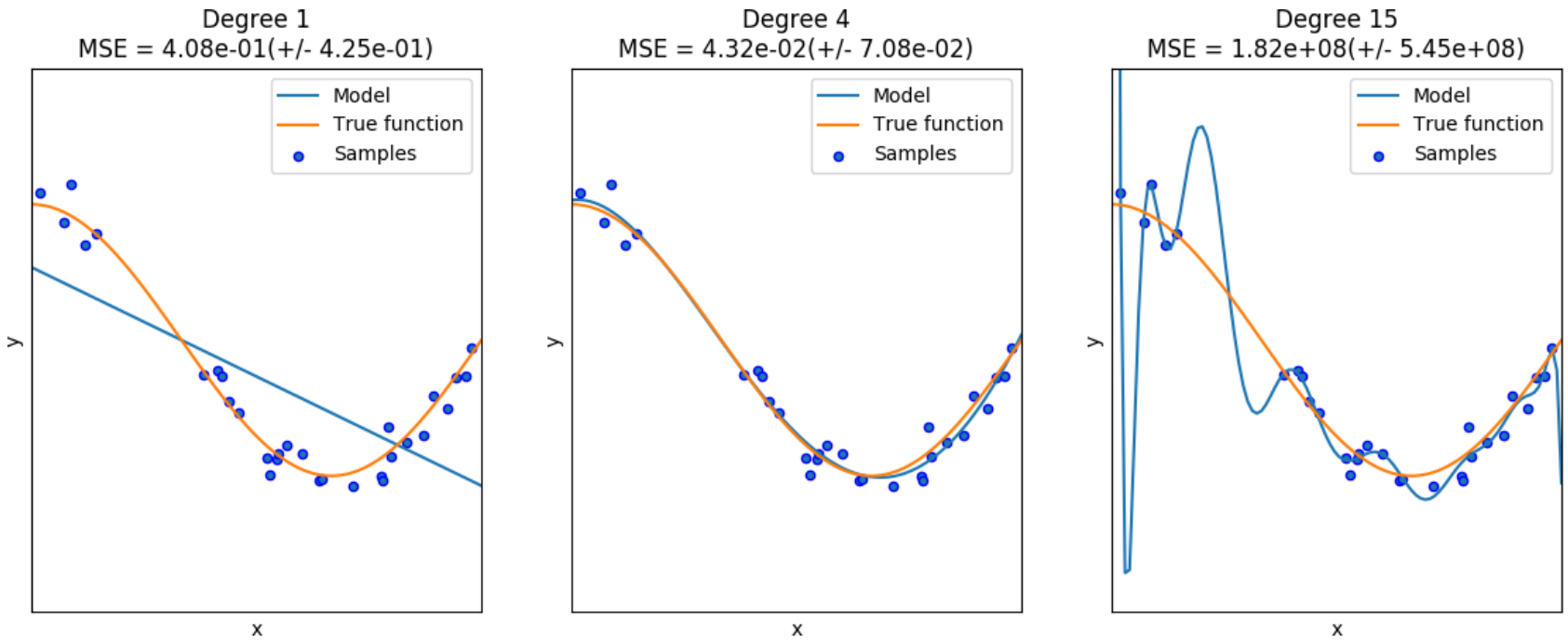

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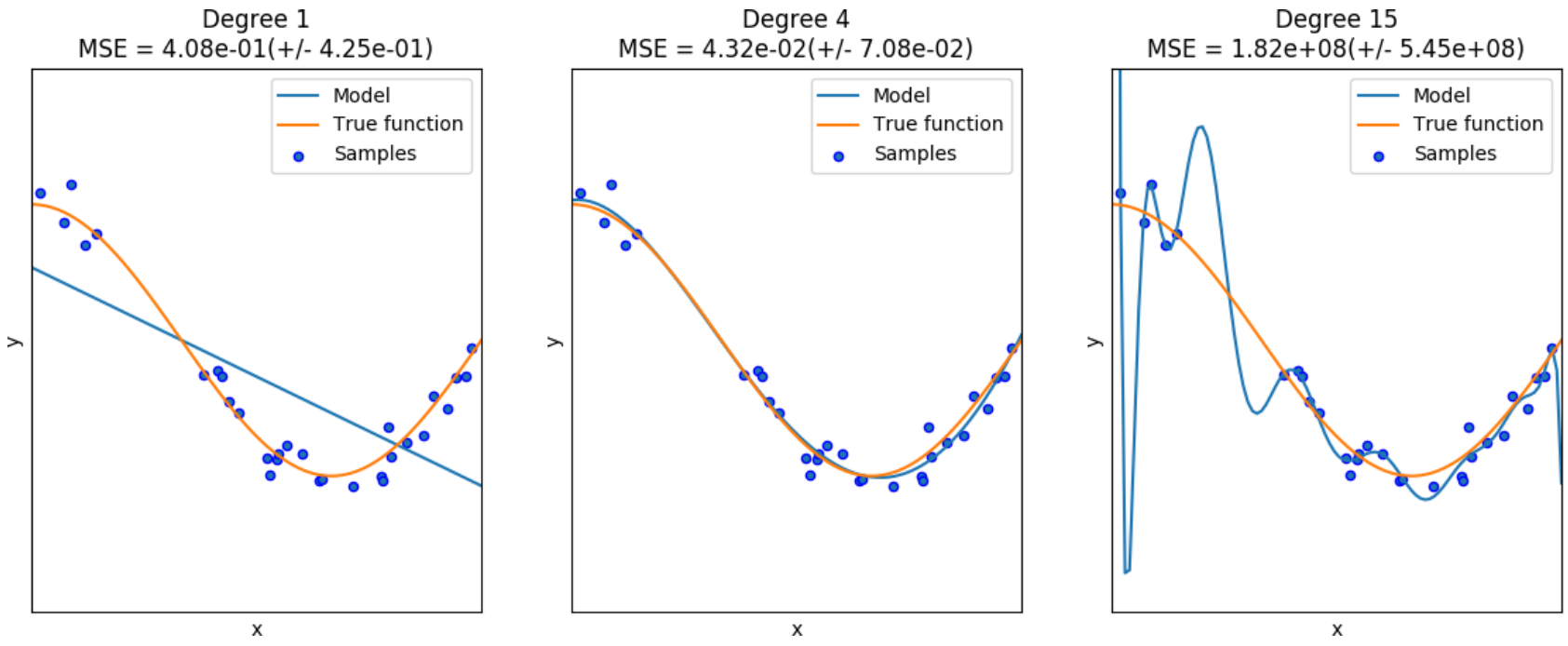


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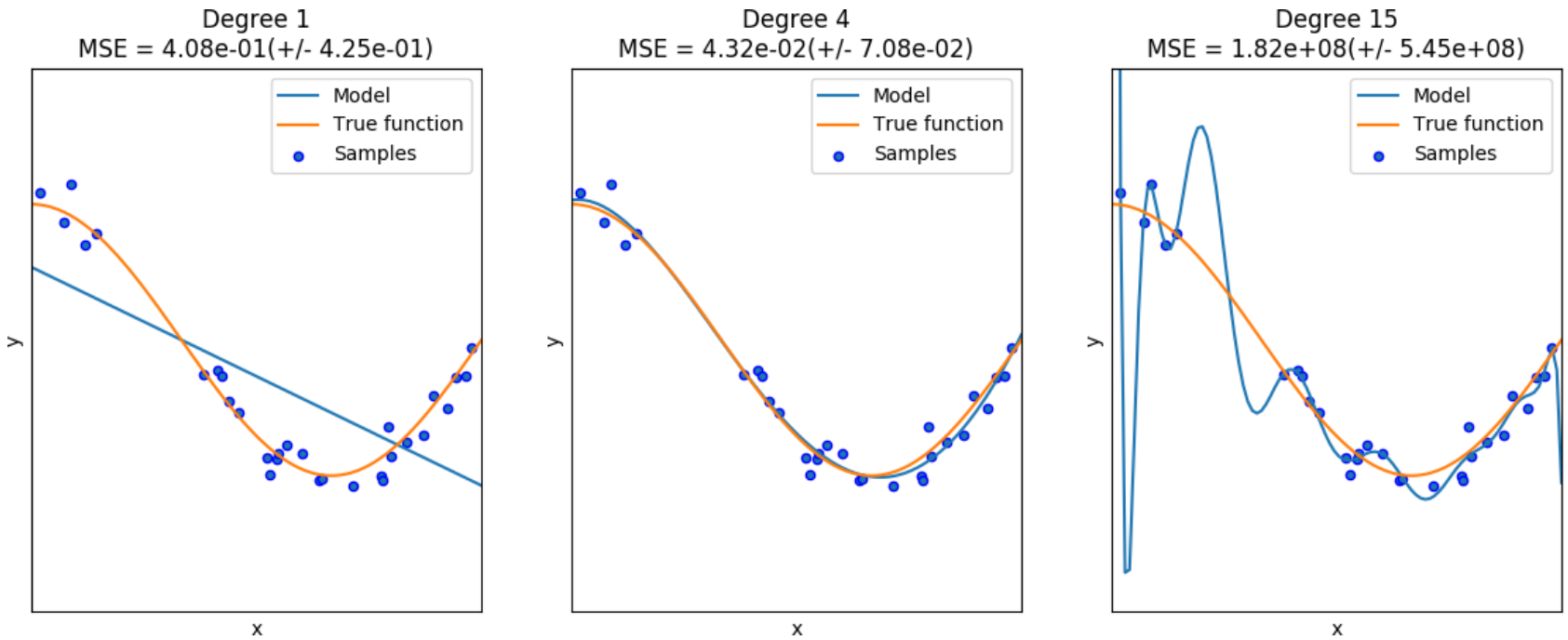


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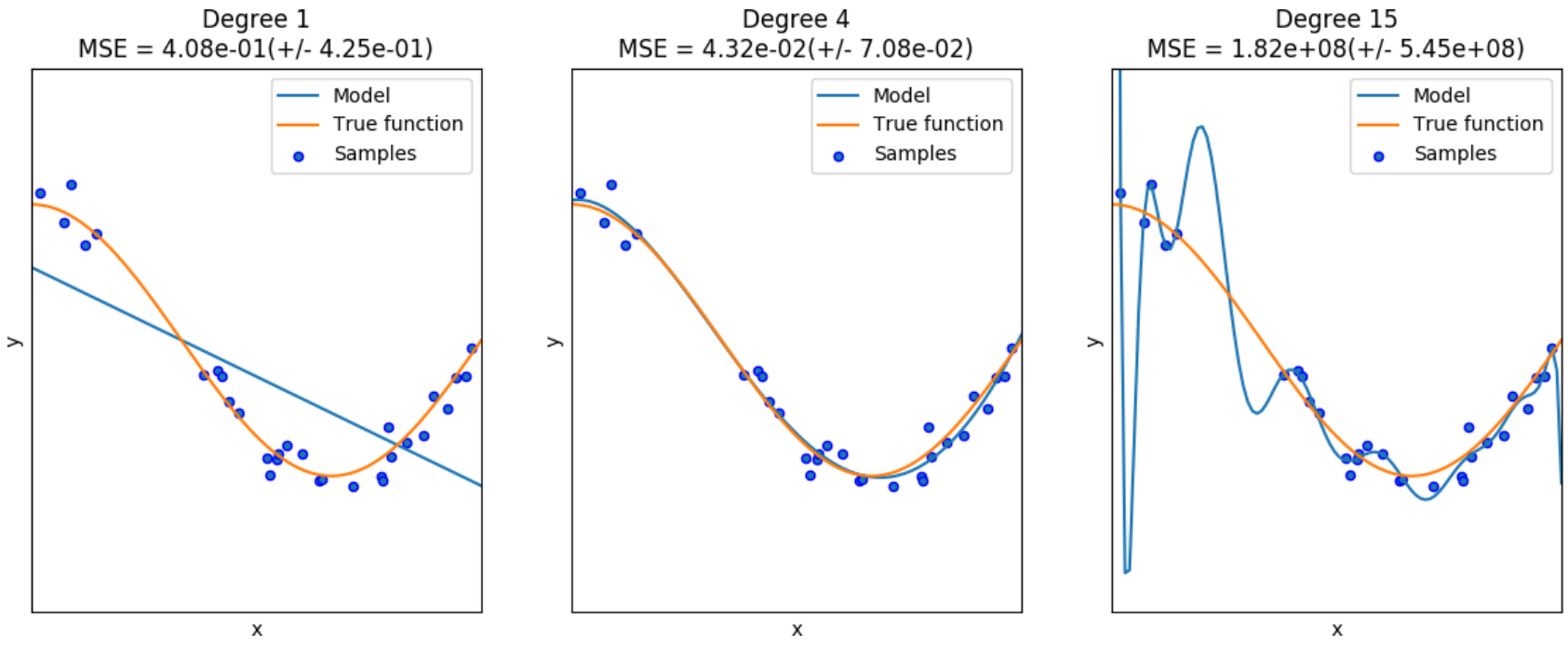


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Adding complexity can lead to overfitting and thus worse generalization.

# Underfitting vs. Overfitting

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Different mechanisms defend us from under- and overfitting.

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4. Large MSE on the validation $\Rightarrow$ overfitting $\Rightarrow$ bad generalization

# Underfitting vs. Overfitting

Underfitting:
large training error, large validation error

# Underfitting vs. Overfitting

Underfitting:
large training error, large validation error

Overfitting:
(very) small training error, large validation error

# Not done yet

"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 $x$."

So is polynomial regression all we need?

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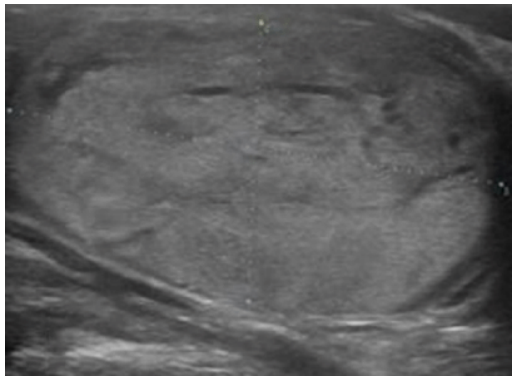
So is polynomial regression all we need?

Not really!

- Different loss than MSE
- Regularization
- Additional priors se si conoscono altre informazioni sui dati a priori, queste rendono difficile l'individuazione della soluzione polinomiale
- Intermediate features le reti neurali, durante il processo di allenamento producono le feature intermedie che sono molto utili. I modelli polinomiali non permettono ciò
- Flexibility
- Regression (predict a value) vs. classification (predict a category)

# Classification

What if we want to predict a category instead of a value?

$f_\Theta($  $) = \{0, 1\}$

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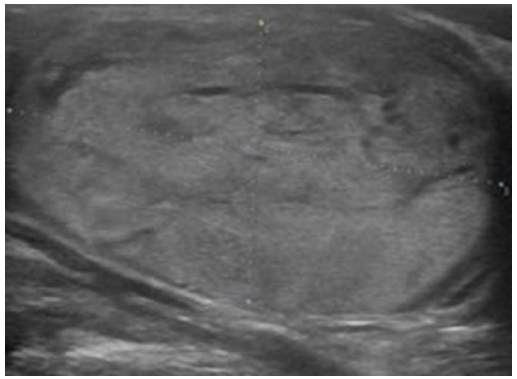
$f_\Theta($  $) = \{0, 1\}$

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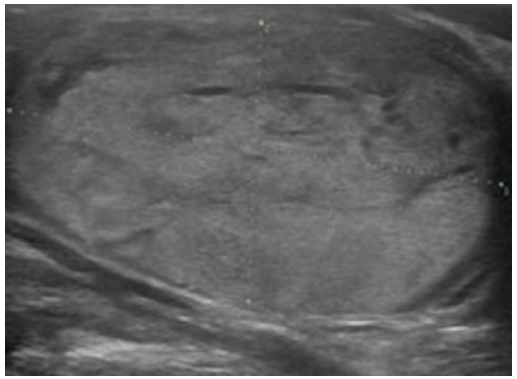
$f_\Theta($  $) = \{0, 1\}$

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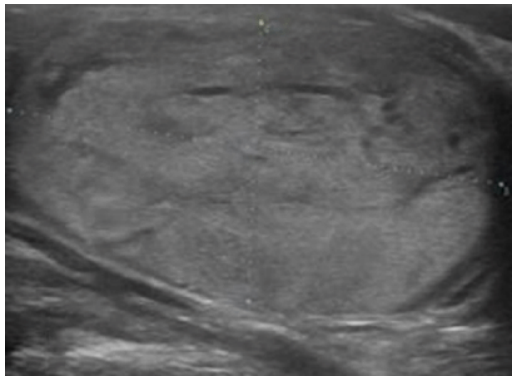
$f_\Theta($  $) = \{0, 1\}$

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$\Rightarrow$ The solution is not necessarily an optimum anymore.

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

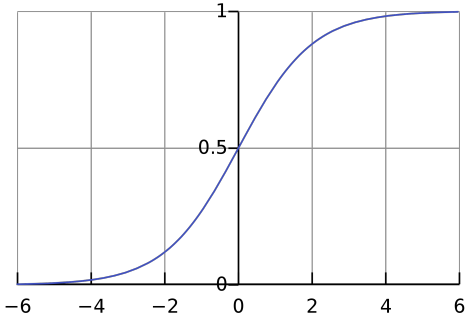
# Logistic regression

New loss:

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

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

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



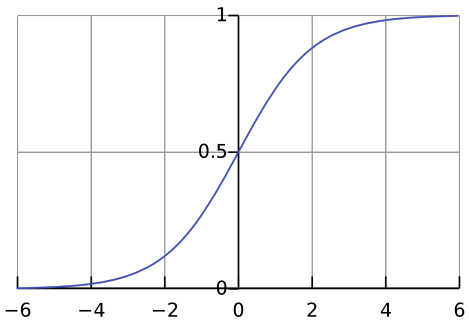
# Logistic regression

New loss:

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

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

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




$\sigma$ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

# Logistic regression

New loss:

in pratica applica il tresholding (dato dalla sigmoide)
all'interno della loss function stessa

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

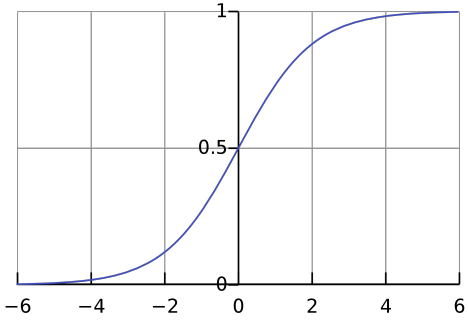
non-convex

anche detta **saturation function** o **equalizer**

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

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

se si moltiplica x per un coeff,
la curva diventa più ripida
(quindi cambia più in fretta)




$\sigma$ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

# Logistic regression

New loss: quindi ora la loss function è così

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

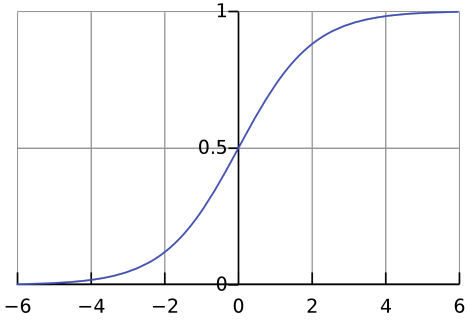
$$c(x_i, y_i) = \begin{cases} -\ln(\sigma(ax_i + b)) & y_i = 1 \\ -\ln(1 - \sigma(ax_i + b)) & y_i = 0 \end{cases}$$

convex

scritta in formula...

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

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




$\sigma$ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

# Logistic regression

New loss:

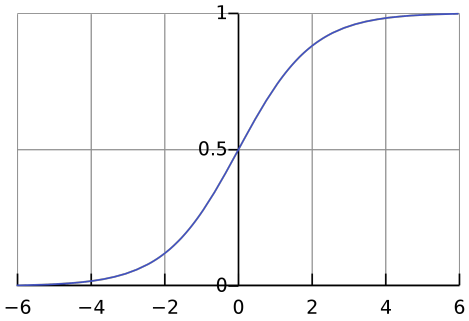
$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} c(x_i, y_i)\,, \quad \text{with}$$

$$c(x_i, y_i) = -y_i \ln(\sigma(ax_i + b)) - (1 - y_i)\ln(1 - \sigma(ax_i + b))$$ nvex

1 se giusto 0 se è giusto ...è così

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

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




$\sigma$ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

# Logistic regression

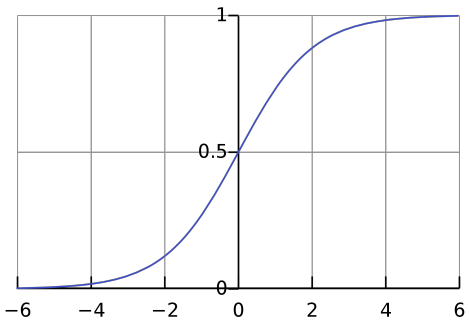
New convex loss:

è la **cross-entropy loss**

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

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

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




$\sigma$ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

# Logistic regression: Finding a solution

(taylor?)

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \ell_\Theta = 0$$

# Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

ci va il -

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

# Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

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

Consider the gradient of each term in the summation:

$$\nabla_\Theta \left( y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) \right)$$

# Logistic regression: Finding a solution

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

Consider the gradient of each term in the summation:

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

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Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

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Apply the chain rule to each partial derivative:

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

# Logistic regression: Finding a solution

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Apply the chain rule to each partial derivative:

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

# Logistic regression: Finding a solution

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial \sigma(ax_i + b)}{\partial (ax_i + b)} \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial}{\partial(ax_i + b)} \frac{1}{1 + e^{-(ax_i + b)}} \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{e^{-(ax_i + b)}}{(1 + e^{-(ax_i + b)})^2} \cdot x_i$$

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$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i + b)}} \frac{e^{-(ax_i + b)}}{1 + e^{-(ax_i + b)}} \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i + b)}} \frac{(1 + e^{-(ax_i + b)}) - 1}{1 + e^{-(ax_i + b)}} \cdot x_i$$

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Apply the chain rule to each partial derivative:

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Apply the chain rule to each partial derivative:

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

And similarly for the second term and for parameter $b$.

# 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.

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Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system that we can solve easily.

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| **model** | **loss** | **solution** |
|---|---|---|
| linear regression<br>linear regression + Tikhonov<br>logistic regression | | |

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|---|---|---|
| linear regression | convex | |
| linear regression + Tikhonov | convex | |
| logistic regression | convex | |

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|---|---|---|
| linear regression | convex | least squares |
| linear regression + Tikhonov | convex | |
| logistic regression | convex | |

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| linear regression | convex | least squares |
| linear regression + Tikhonov | convex | least squares |
| logistic regression | convex | |

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Thus:

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quindi non c'è una soluzione per a e b

| **model** | **loss** | **solution** |
|---|---|---|
| linear regression | convex | least squares |
| linear regression + Tikhonov | convex | least squares |
| logistic regression | convex | nonlinear optimization |

matrice di regolarizzazione nella minimizzazione del MSE (anche detta **ridge regression**)

che sarebbe GD

# Suggested reading

On polynomial regression vs. neural nets:
https://arxiv.org/pdf/1806.06850

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