Machine Learning

Regression problems

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SAPIENZA
UNIVERSITÀ DI ROMA

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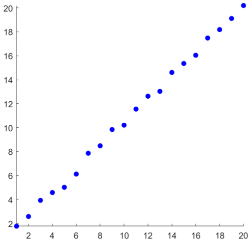
Linear regression

We start from the simplest non-trivial case for a learning model:



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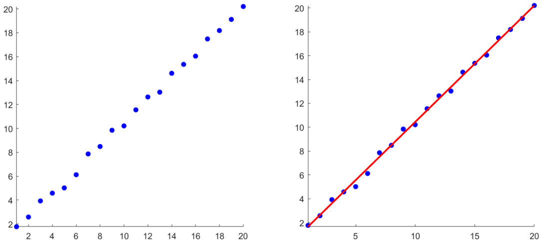

$$y_i = ax_i + b$$

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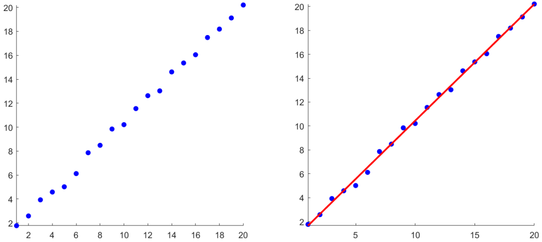

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Model: linear + bias

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

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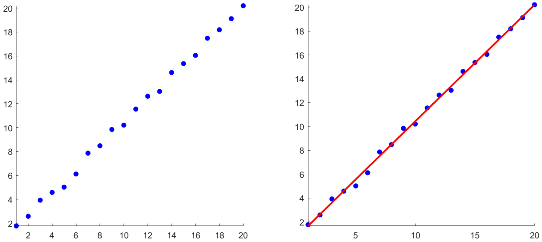

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Given a and b, we have a mapping that gives new output from new input.

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When f_Θ is linear, this is called a least-squares approximation problem.

Linear regression: Loss function

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

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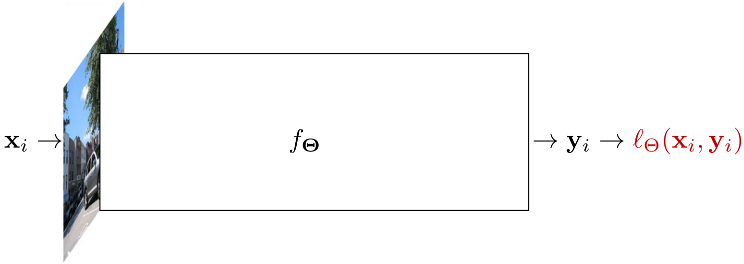
Remark: We minimize the energy w.r.t. the parameters Θ, and **not** w.r.t. the data (x_i, y_i). Also, the energy is defined on the entire dataset, not on just one data point.

Linear regression

We are considering the following case:



where $f_{\boldsymbol{\Theta}}$ is linear, and ℓ_{Θ} is quadratic.

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

Convexity and gradients

Convex functions

Jensen's inequality:

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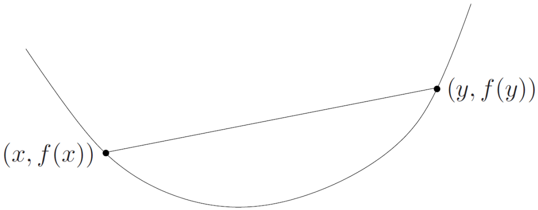

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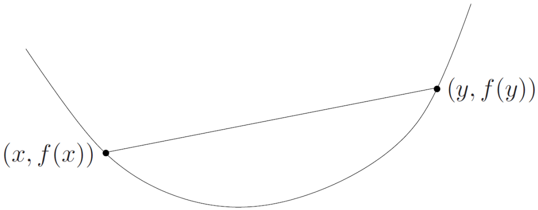

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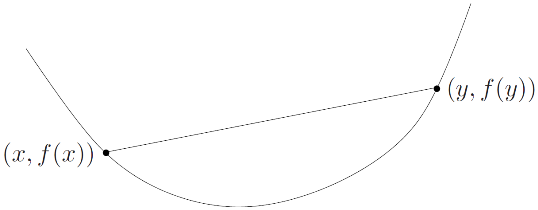

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Theorem: the global minimizer x is where $\frac{df(x)}{dx} = 0$.

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Convexity is defined as before:

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

and we also have the global optimality condition:

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

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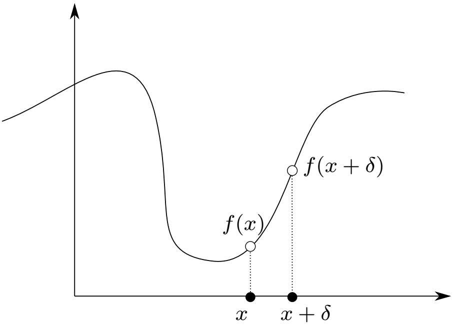

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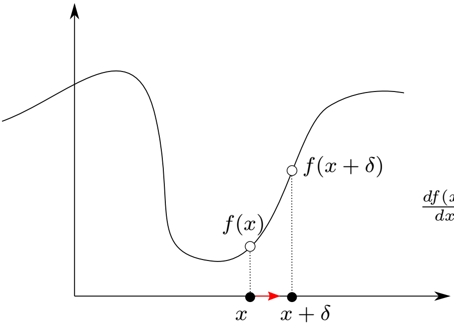

$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$

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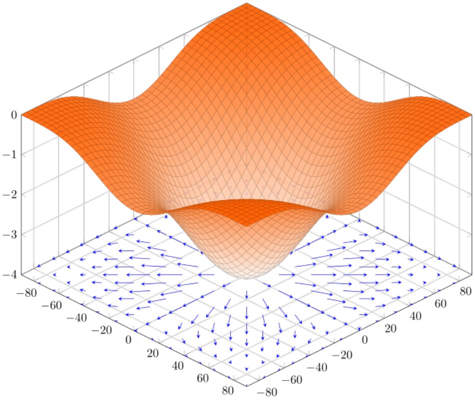

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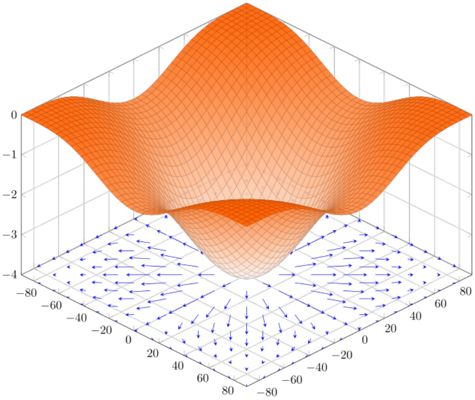

The length of the gradient vector encodes its steepness.

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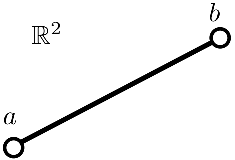
If $f(\mathbf{x})$ is multi-dimensional, i.e. $f : \mathbb{R}^n \to \mathbb{R}$, do we have a notion of convexity and derivative?

If yes, can we find global minimizers as easily as in the former case?

Vector lengths

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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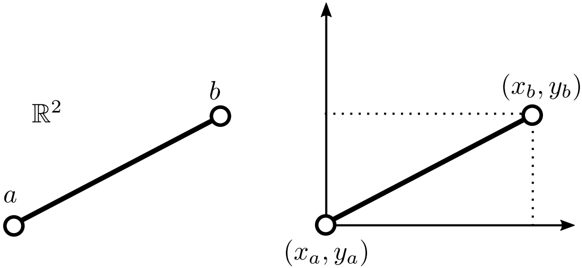

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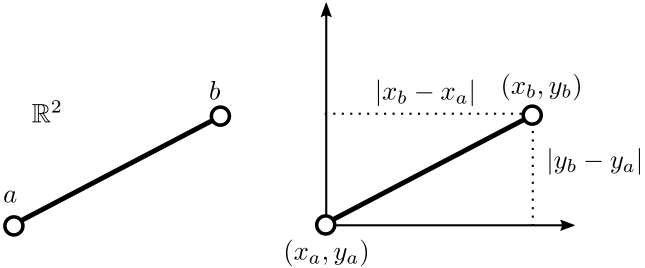

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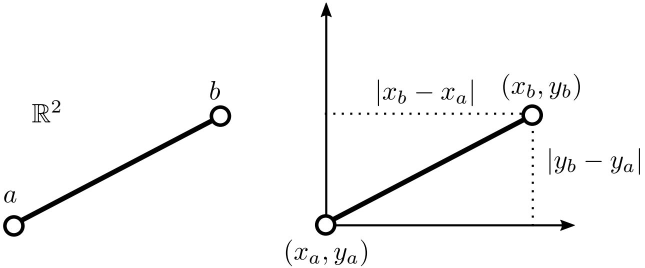

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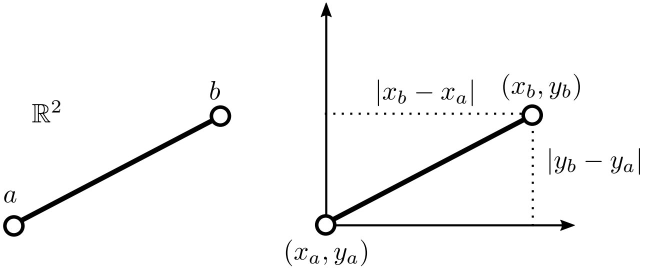

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In matrix notation:

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

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

L_p distance in $\mathbb{R}^k$

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

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

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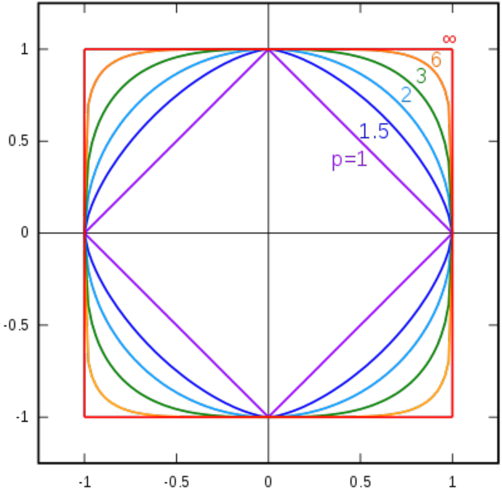
L_p unit balls in $\mathbb{R}^2$



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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where $\ell : \mathbb{R}^2 \to \mathbb{R}$ is defined as:

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

$$\begin{pmatrix} \sum_{i=1}^{n} a x_i^2 + b x_i - x_i y_i \\ \sum_{i=1}^{n} a x_i + b - y_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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:

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{\mathbf{y}} = a \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}}_{\mathbf{X}} + b$$

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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$$\ell(\boldsymbol{\theta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2$$

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$$-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} = \mathbf{0}$$

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

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

A note on the gradient in matrix form

In the previous slide, for the differentiation step:

$$\mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} \quad \xrightarrow{\nabla_{\boldsymbol{\theta}}} \quad -2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

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Example: $f(\boldsymbol{\theta}) = \boldsymbol{\theta}^\top\mathbf{A}\boldsymbol{\theta}$

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \begin{pmatrix}\theta_1 & \cdots & \theta_n\end{pmatrix} \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} \theta_1 \\ \cdots \\ \theta_n \end{pmatrix}$$

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If $\mathbf{A}$ is symmetric (e.g., $\mathbf{A} = \mathbf{X}^\top\mathbf{X}$), then:

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = 2\mathbf{A}\boldsymbol{\theta}$$

Linear regression: Higher dimensions

Until now we have seen the case where:

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

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

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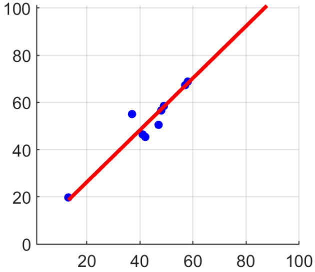
Defining the matrices $\mathbf{X} = \begin{pmatrix} | & | & \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots \\ | & | & \\ 1 & 1 & \end{pmatrix}, \mathbf{Y} = \begin{pmatrix} | & | & \\ \mathbf{y}_1 & \mathbf{y}_2 & \cdots \\ | & | & \end{pmatrix}, \mathbf{\Theta} = \begin{pmatrix} \mathbf{A} \\ \mathbf{b}^\top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

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

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

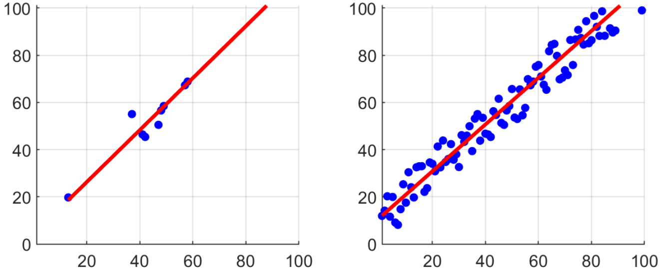
Polynomial regression

Data distribution



Assumption: linear model

Data distribution



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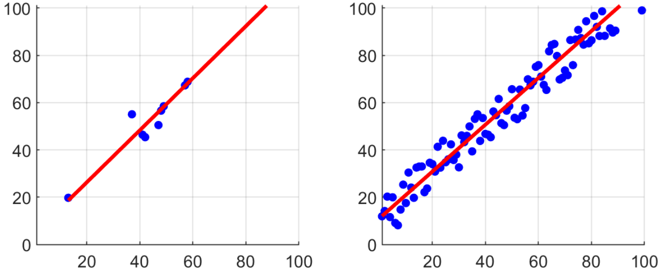
More data allows us to improve our prediction

Data distribution



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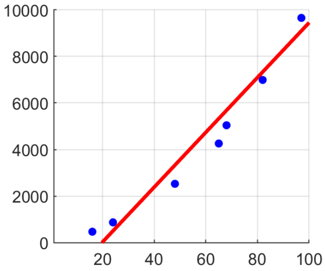
More data allows us to improve our prediction

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

Data distribution



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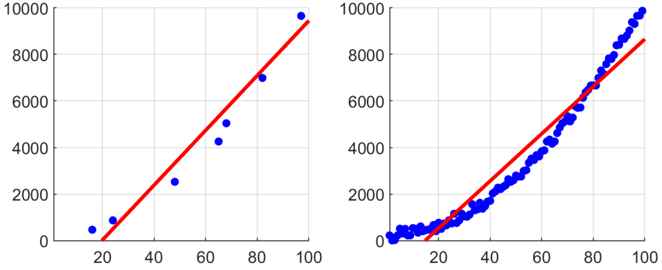

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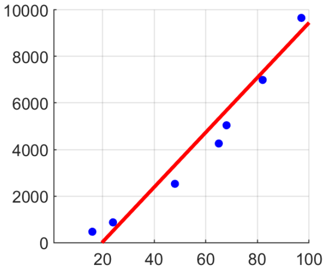
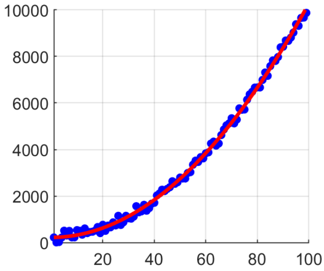
More data confutes our assumptions

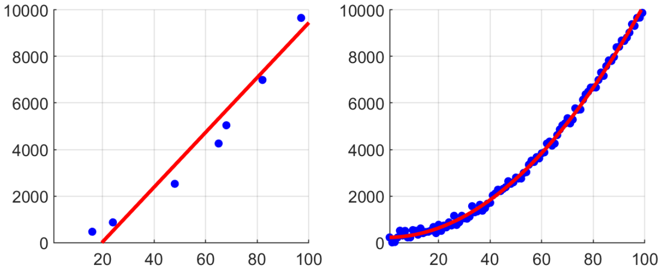
Data distribution





Assumption: quadratic model

Data distribution



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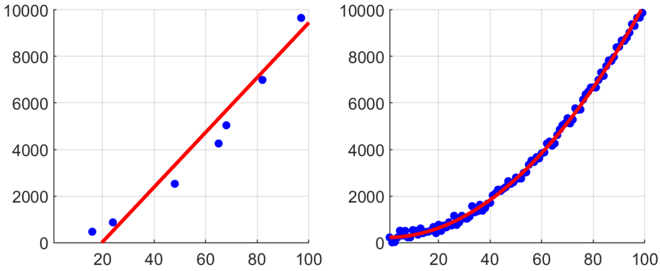
Key questions:

- How to select the correct distribution?

Data distribution



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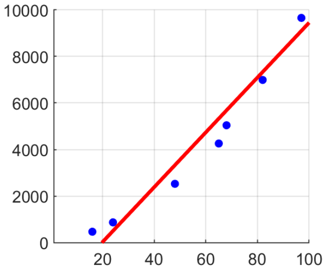
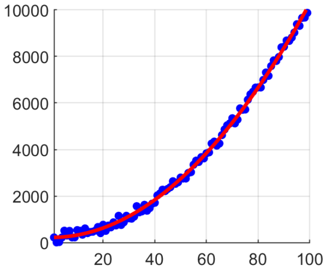




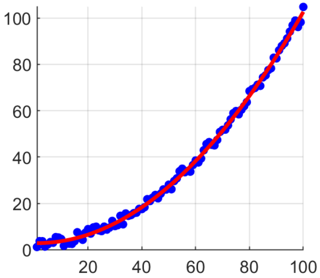
Assumption: quadratic model

Key questions:

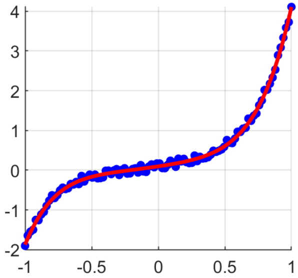
- How to select the correct distribution?
- How much data do we need?
- What if the correct distribution does not admit a simple expression?

Polynomial regression

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



2nd-order



5th-order

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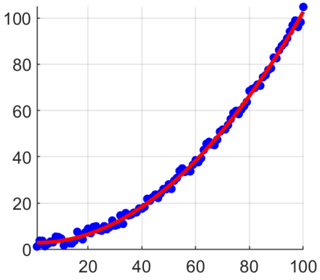

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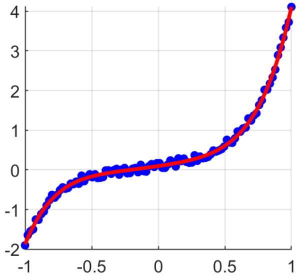

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The number of parameters grows with the order.

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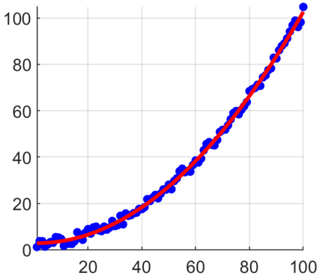

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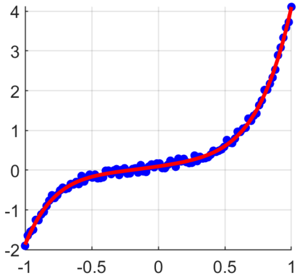

5th-order

The number of parameters grows with the order.

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

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

Linear regression with polynomial features

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Linear regression with polynomial features

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$$y_i = b + \sum_{j=1}^{k} a_j x_i^j \quad \text{for all data points } i = 1, \ldots, n$$

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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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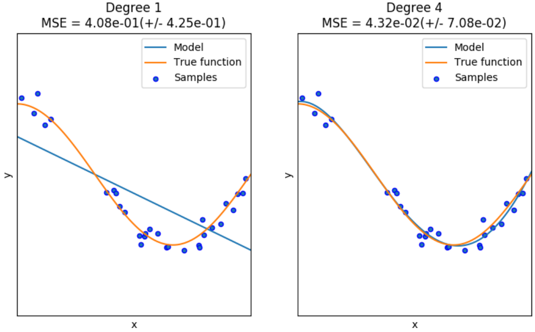

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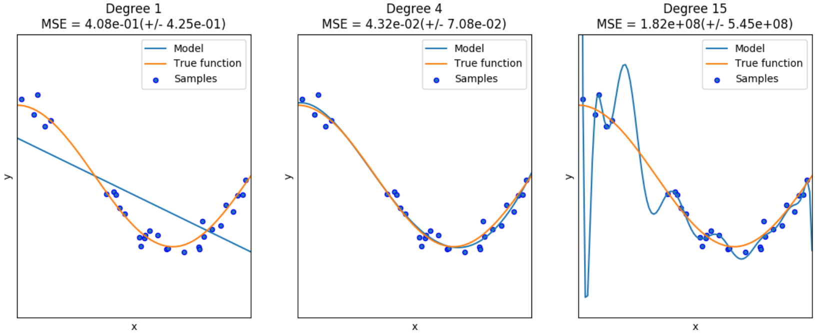
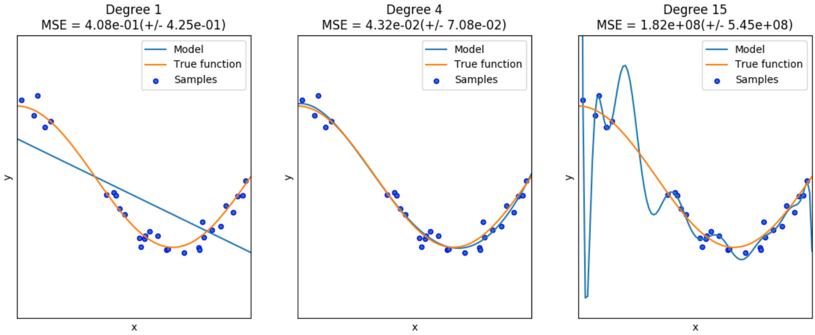


Underfitting vs. Overfitting



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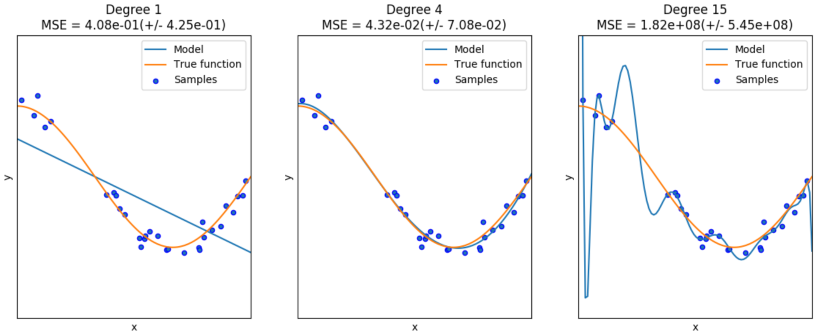

- Underfitting: Not sufficiently fitting the data (large MSE).

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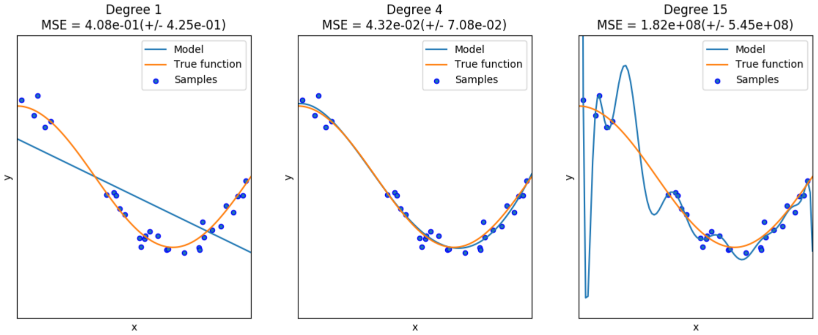
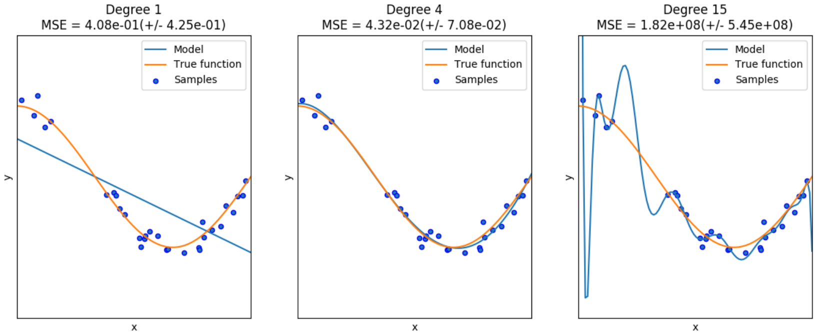


- Underfitting: Not sufficiently fitting the data (large MSE).
- Overfitting: We are "learning the noise" (small MSE).

Underfitting vs. Overfitting



- Underfitting: Not sufficiently fitting the data (large MSE).
- Overfitting: We are "learning the noise" (small MSE).

Adding complexity can lead to overfitting and thus worse generalization.

Underfitting vs. Overfitting

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Underfitting:
large training error, large validation error

Underfitting vs. Overfitting

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

n-fold cross-validation

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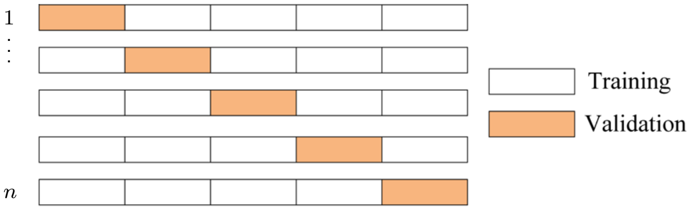

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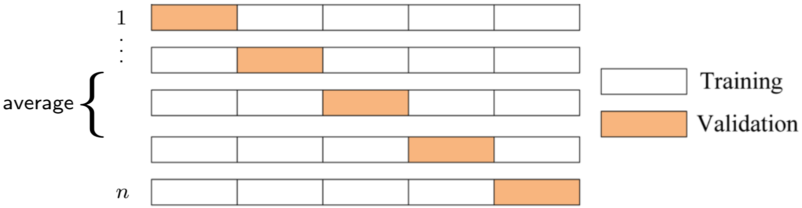

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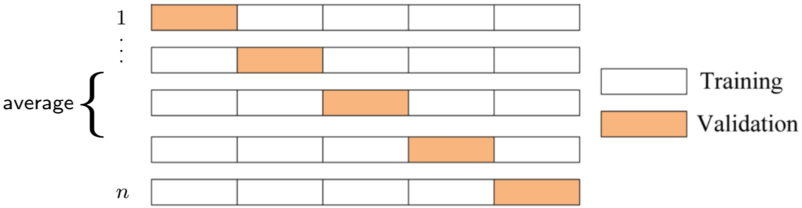

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Example: For polynomial regression, do the above many times with different degrees, choose the run with the smallest average MSE.

Not done yet

"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
- 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:

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

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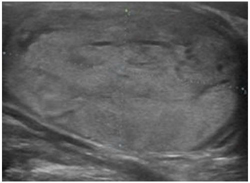
Logistic regression

Classification

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

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

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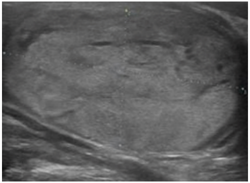
$f_\Theta($  $) = \{0, 1\}$

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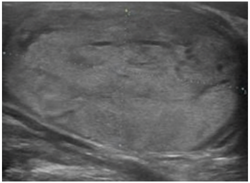
$f_\Theta($  $) = \{0, 1\}$

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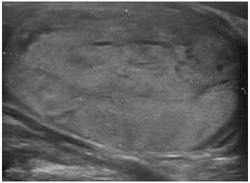
$f_\Theta($  $) = \{0, 1\}$

Possible solution: Do post-processing (e.g. thresholding) to convert linear regression to a binary output.

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

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

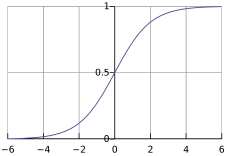
Logistic regression

New loss:

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

Here, σ is the nonlinear logistic sigmoid:

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



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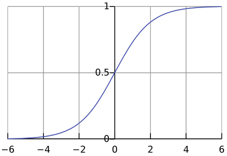

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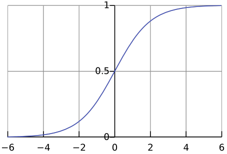

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Logistic regression

New loss:

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

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

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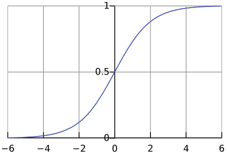

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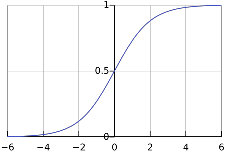

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Logistic regression

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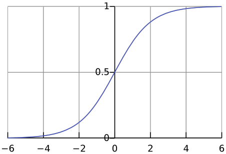

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Since the loss is convex, the first-order conditions apply:

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Consider the gradient of each term in the summation:

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Apply the chain rule to each partial derivative:

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Apply the chain rule to each partial derivative:

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

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:

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

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

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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 so on for the second term and for parameter b.

Logistic regression: Finding a solution

By looking at the partial derivative:

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

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

Logistic regression: Finding a solution

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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		
linear regression + Tikhonov		
logistic regression		

Logistic regression: Finding a solution

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

Logistic regression: Finding a solution

By looking at the partial derivative:

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

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

Logistic regression: Finding a solution

By looking at the partial derivative:

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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:

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

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`

On polynomial regression vs. neural nets:
`https://ar5iv.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`