Metodi Numerici dell'Informatica

Polynomial regression

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SAPIENZA
UNIVERSITÀ DI ROMA

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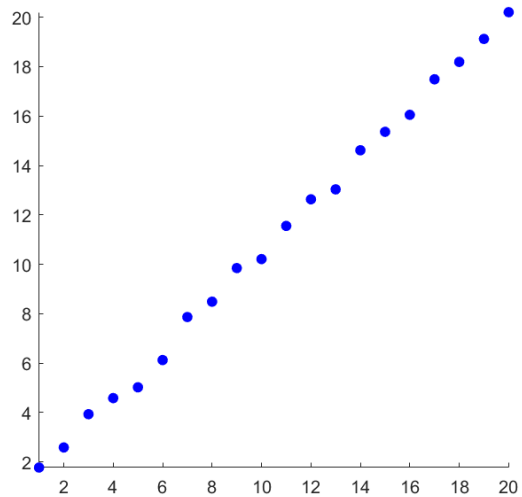
Motivation

Linear regression

Consider the following fitting problem:



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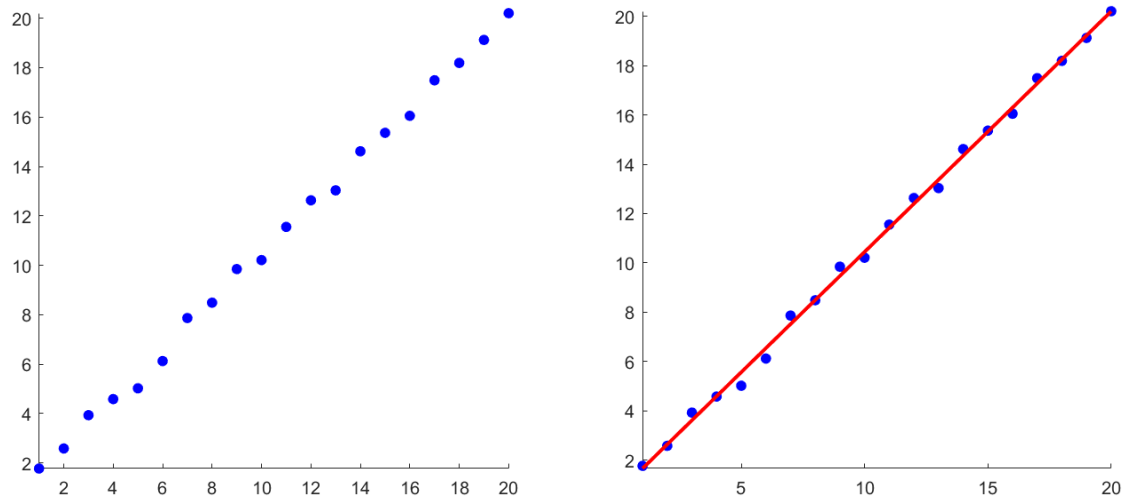

$$y_i = ax_i + b$$

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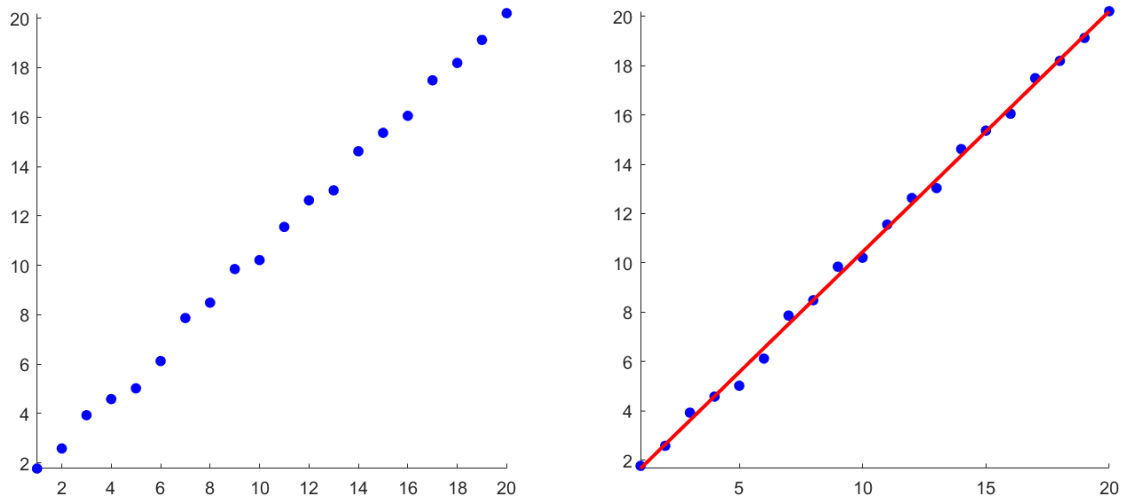

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Model: linear + bias

Unknown parameters: $\Theta = \{a, b\}$

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

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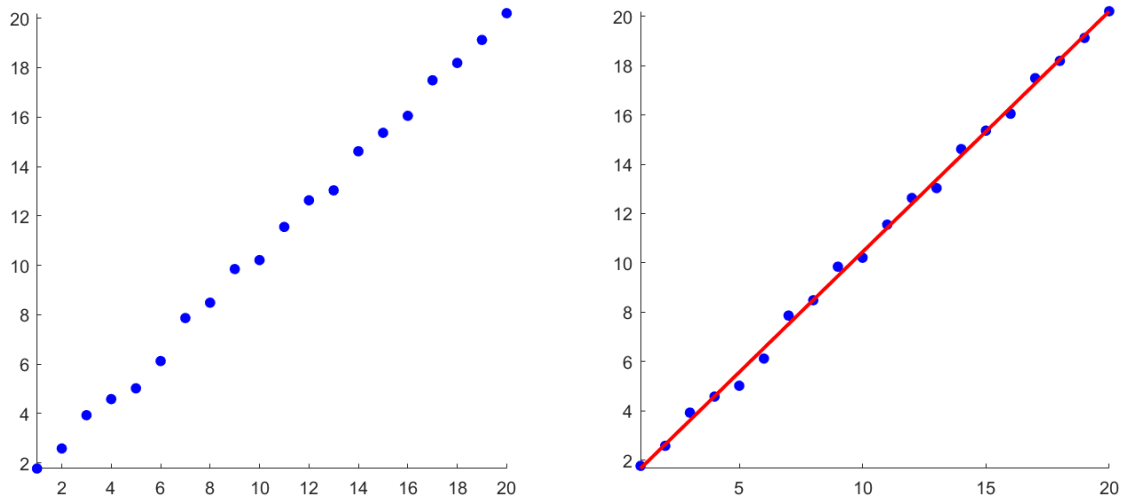

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Given a and b, we have a mapping that gives new output from new input.

Linear regression

The equations:

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must approximately hold for all $i = 1, \ldots, n$.

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vinyl scratch

What is this weird mathematical expression?

Optimization

We are looking at what is typically called a minimization problem.

The general form for a minimization problem is:

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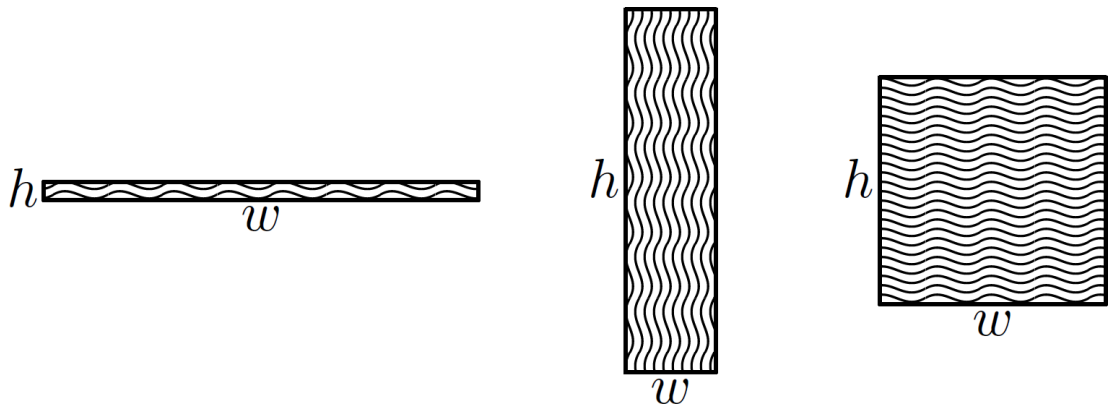
There are no general recipes that work well for all problems!

In general, the algorithm you choose depends on the properties of f.

The research area is broadly called optimization.

Example

Suppose a rectangle has width w and height h. A classic geometry problem is to maximize area with a fixed perimeter equal to 1:



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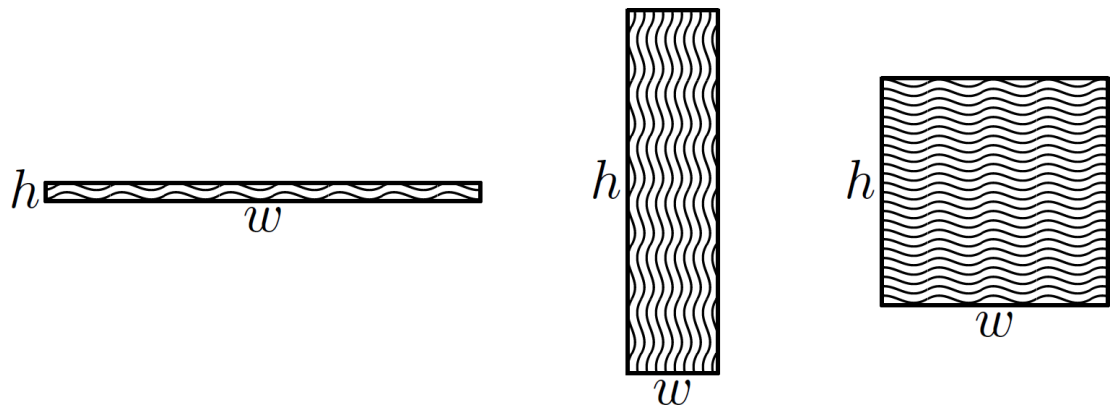

$$\begin{aligned} \max_{w,h \in \mathbb{R}} \quad & wh \\ \text{subject to} \quad & 2w + 2h = 1 \end{aligned}$$

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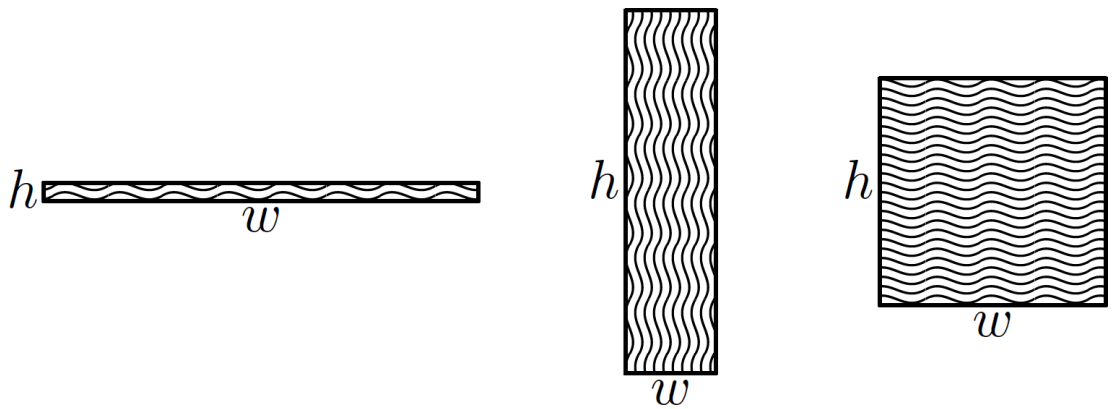

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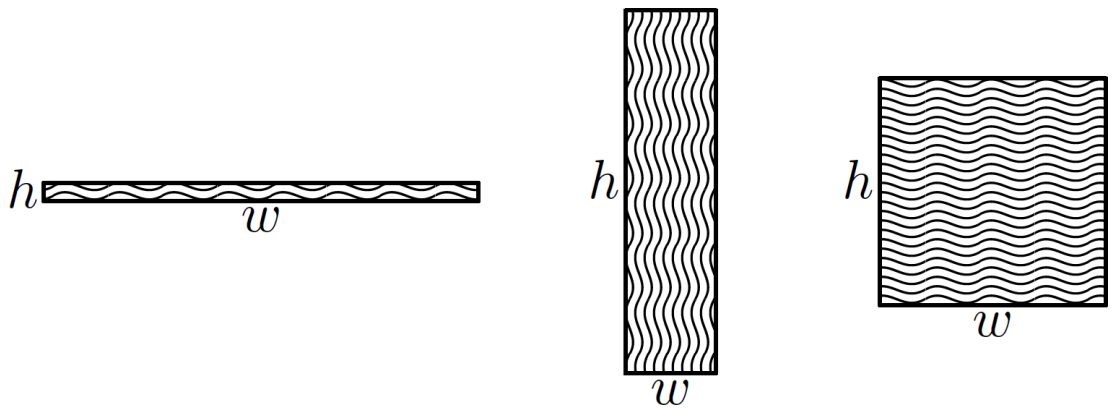

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This is an example of a constrained problem.

Linear regression

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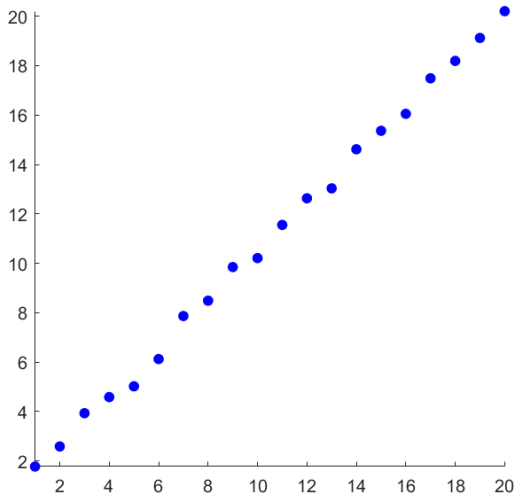

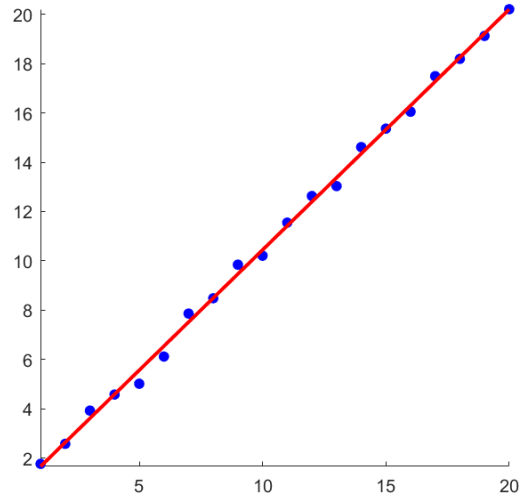

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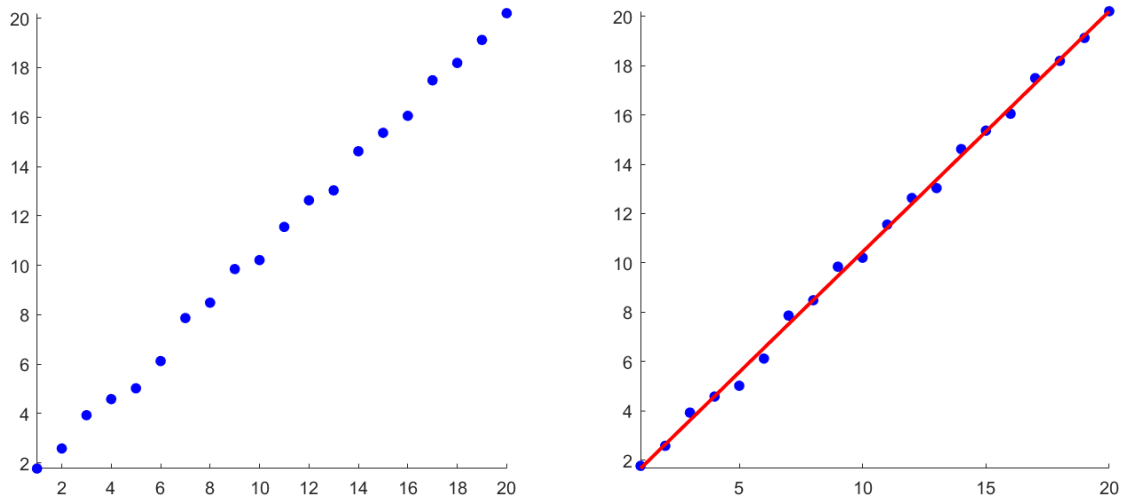

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For cleaner and more generic formulas, we simply wrote:

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This is called a least-squares approximation problem.

Finding a solution

To find a solution to the least-squares approximation problem that arises in linear regression, we need to introduce two more ingredients:

The notion of convexity

The definition of gradient

Convexity

Convex functions

Jensen's inequality:

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

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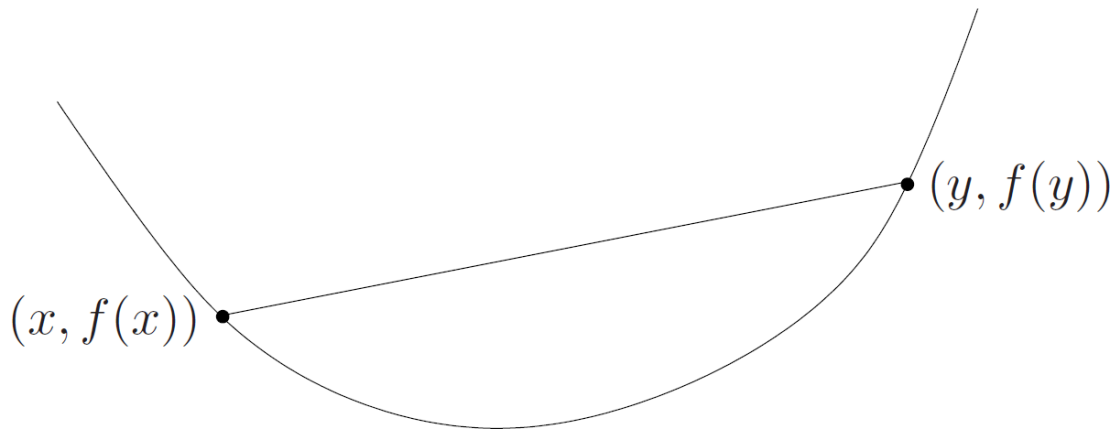

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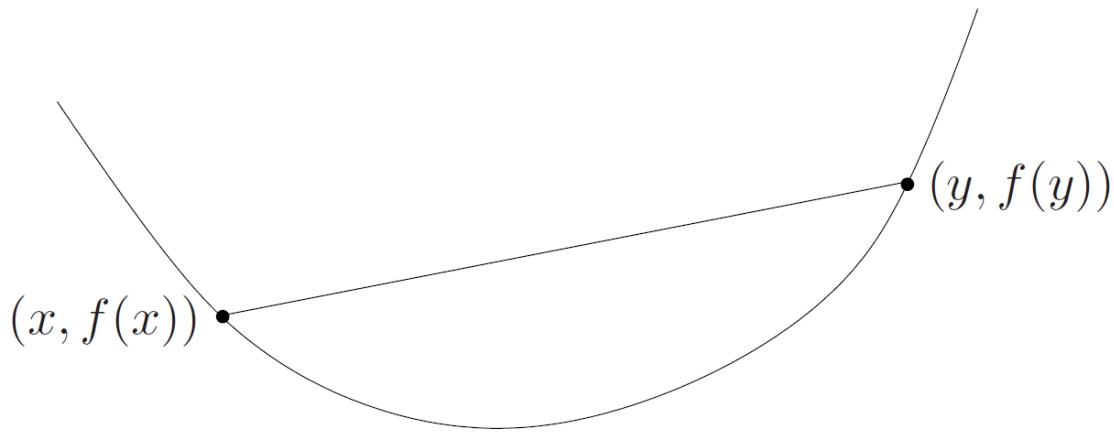

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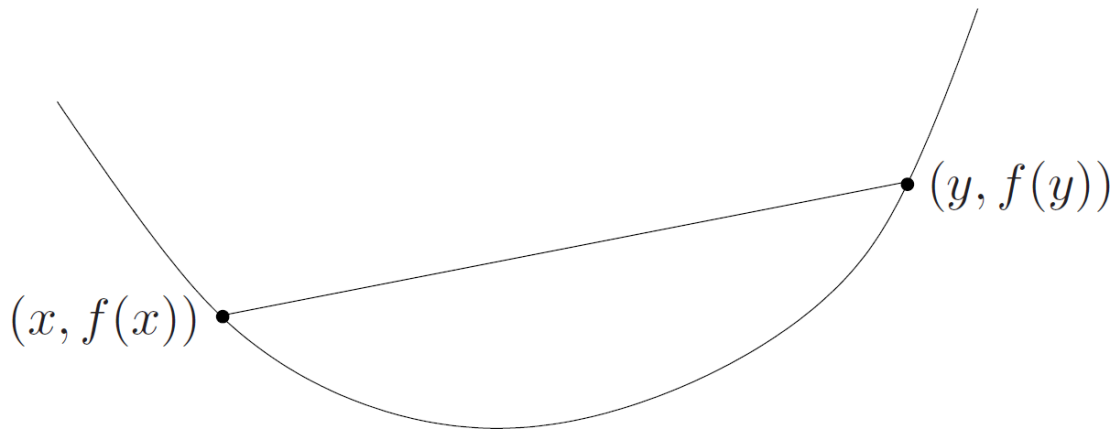

Let us further assume that f is a differentiable function, so that we can compute its derivative $\frac{df}{dx}$ at all points x.

Intuition tells us that the minimizer x is where $\frac{df(x)}{dx} = 0$.

Convex functions: Global minima

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

for all x, y and $\alpha \in (0, 1)$

Convex functions: Global minima

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

for all x, y and $\alpha \in (0, 1)$

Convex functions: Global minima

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

for all x, y and $\alpha \in (0,1)$

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

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

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$$\lim_{\alpha \to 0} \frac{f(x + \alpha(y - x)) - f(x)}{\alpha} + f(x) \leq f(y)$$

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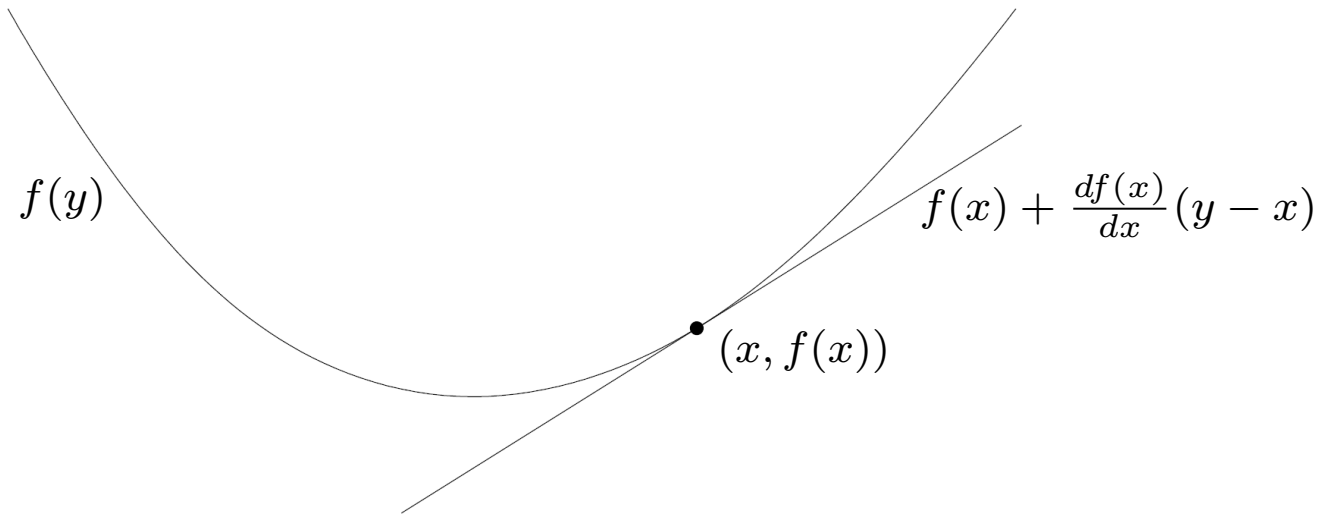
$$\underbrace{\frac{df(x)}{dx}(y-x)+f(x)}_{1\text{st}-\text{order Taylor of } f(y) \text{ at } x} \leq f(y)$$



Thus, if $\frac{df(x)}{dx} = 0$:

$$f(x) \leq f(y)$$

which means that x is a global minimizer of f.

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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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?

The gradient

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

In general we will deal with functions of $n \gg 1$ variables:

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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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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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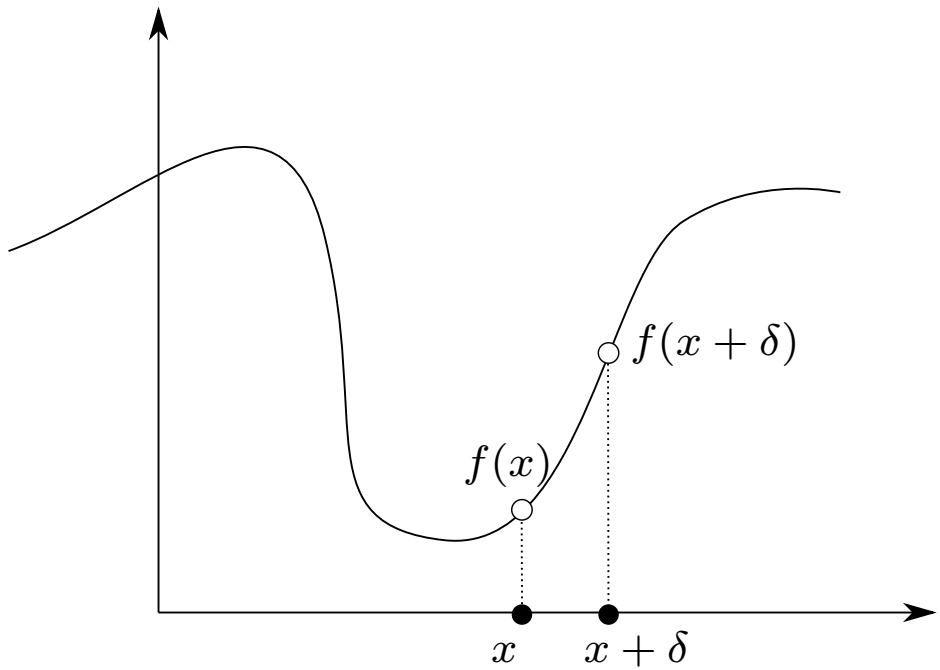

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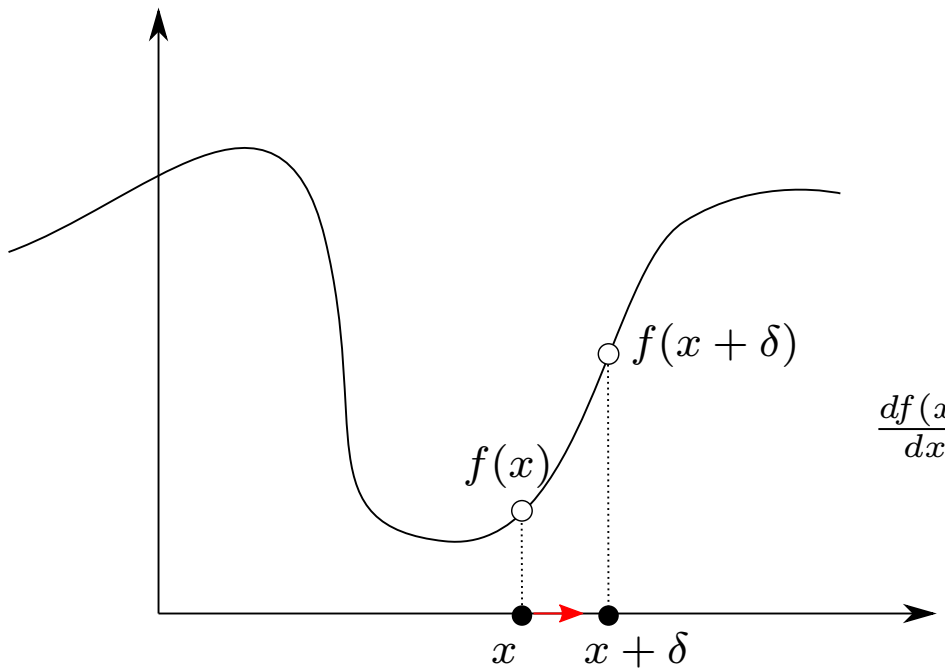

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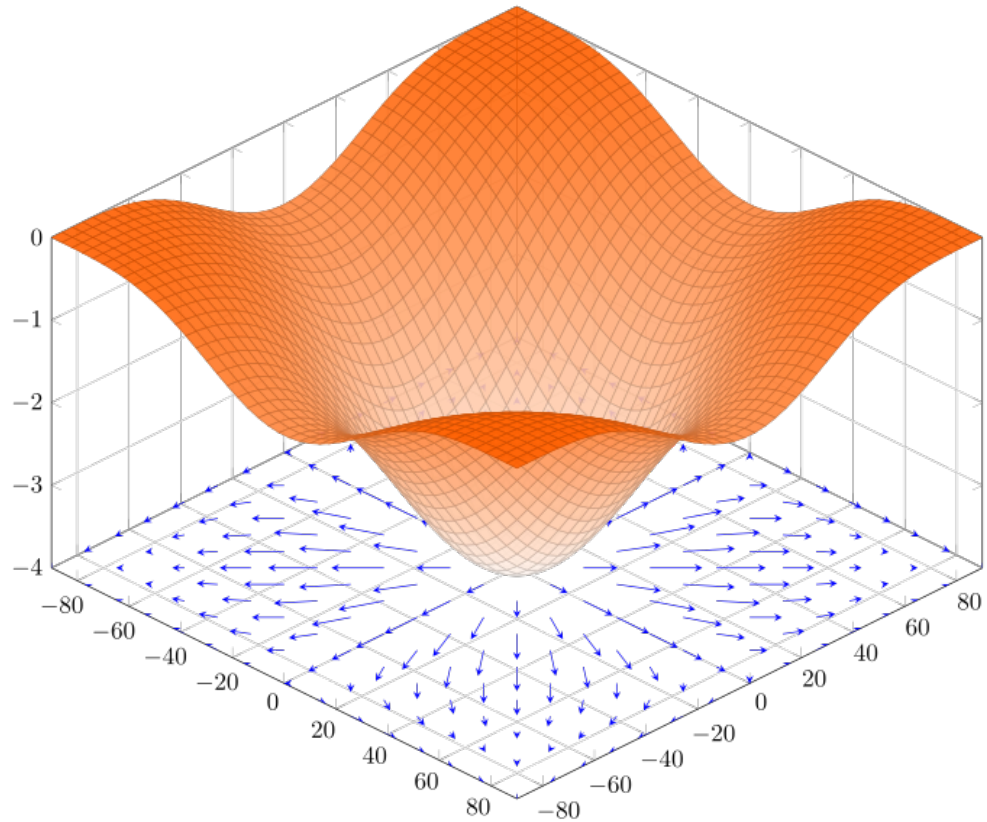

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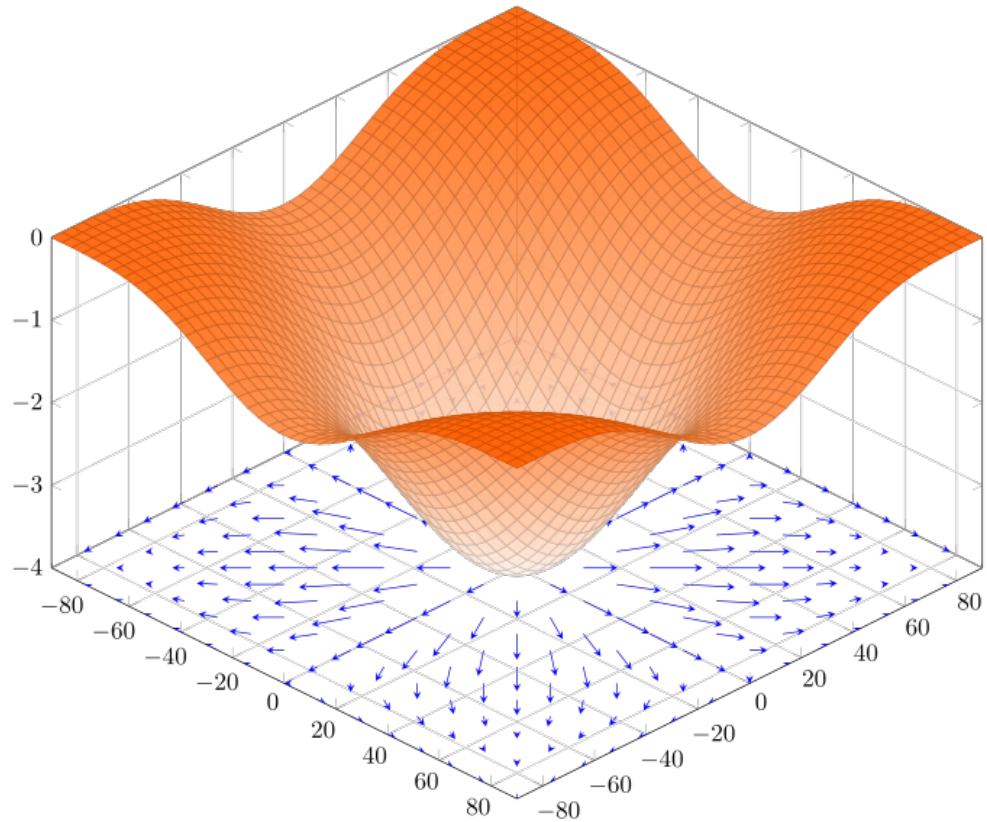

The length of the gradient vector encodes its steepness.

Convex functions: Global minima

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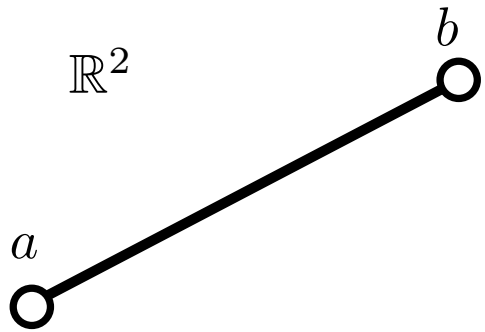
If $f(\mathbf{x})$ is convex, then a global minimizer is found by setting $\nabla_{\mathbf{x}} f(\mathbf{x}) = \mathbf{0}$ and solving for $\mathbf{x}$.

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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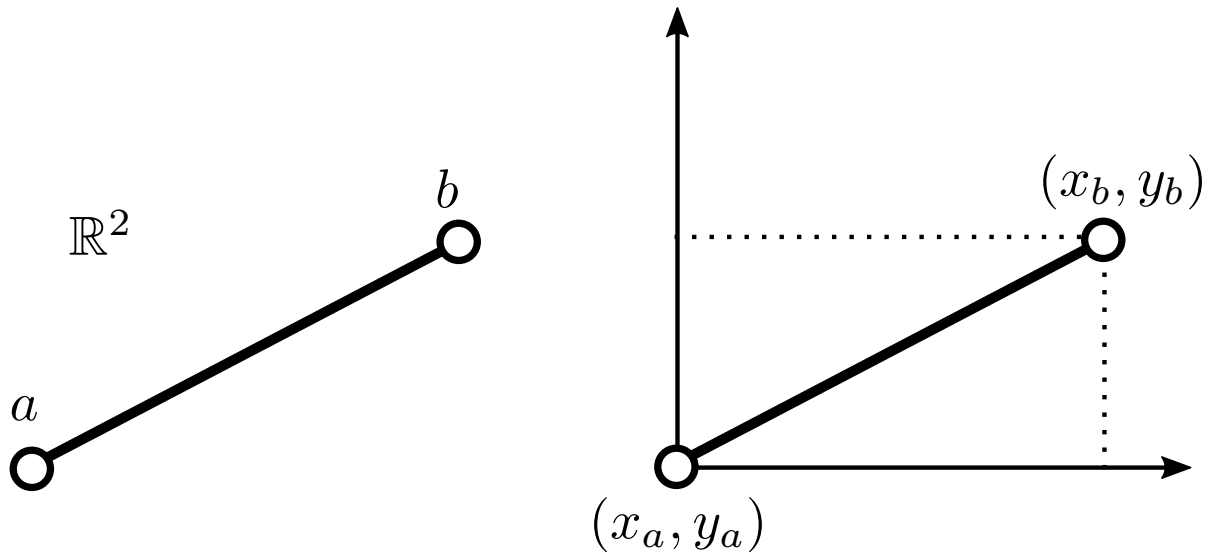

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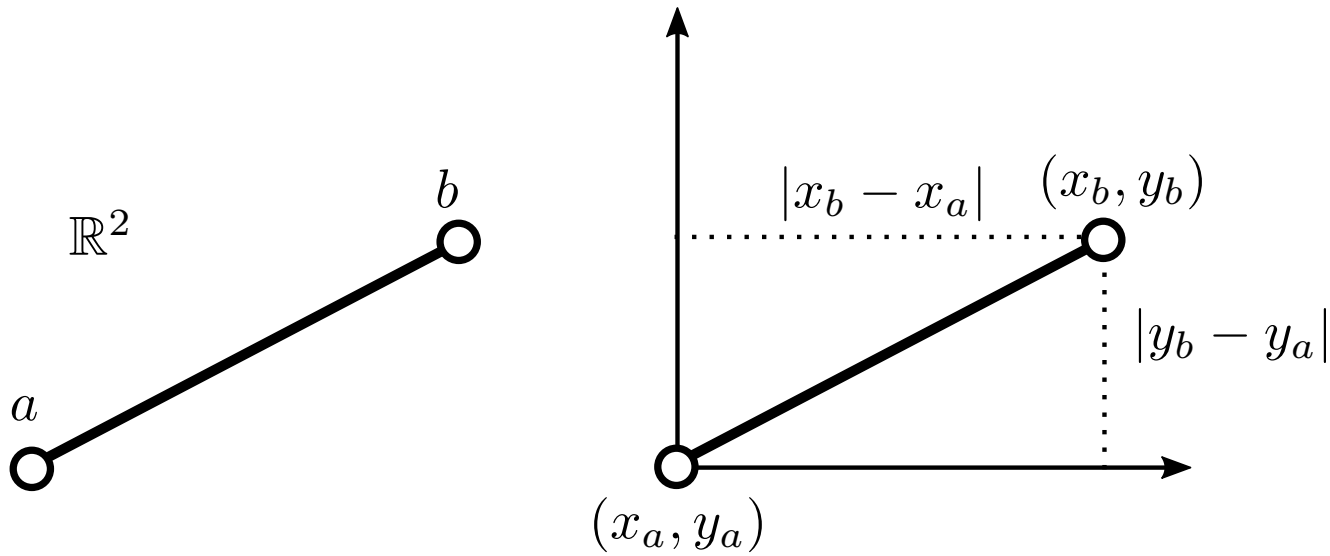

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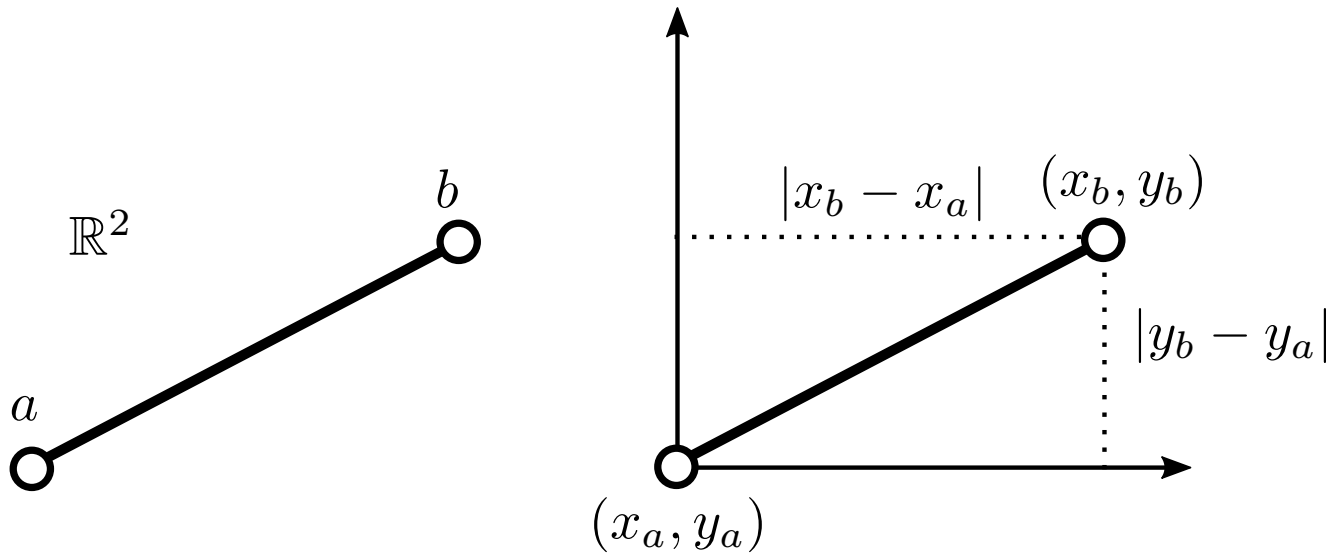

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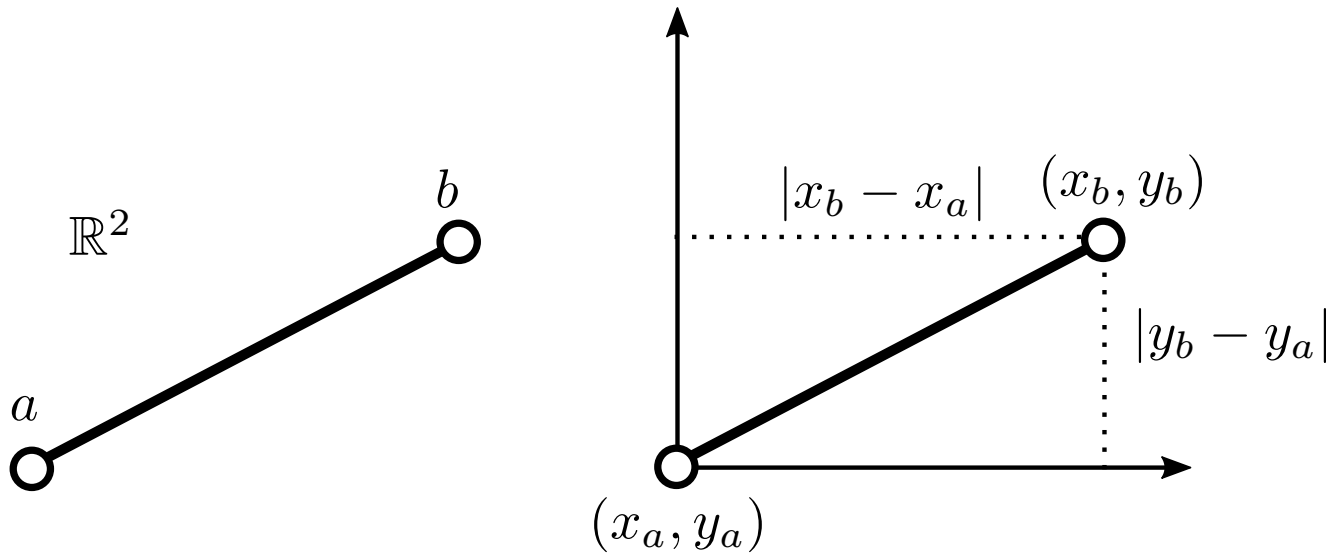

Apply Pythagoras' theorem: $d(a,b) = (|x_b - x_a|^2 + |y_b - y_a|^2)^{\frac{1}{2}}$

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 $\mathbf{b} = \begin{pmatrix} x_b \\ y_b \end{pmatrix}$

Vector lengths

Thus, with this definition of distance:

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

We can simply define the length of a vector $\mathbf{x}$ as the distance from the origin to $\mathbf{x}$:

$$\|\mathbf{x} - \mathbf{0}\|_2 = \|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^\top \mathbf{x}}$$

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Often, for simplicity and to avoid computing square roots, we will consider squared distances and norms:

$$\|\mathbf{x}\|_2^2 = \mathbf{x}^\top \mathbf{x}$$

Least squares

Linear regression: Finding a solution

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

Linear regression: Finding a solution

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

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:

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

Linear regression: Matrix notation

We need to familiarize with matrix calculus.

When we use a numerical method, we manipulate matrices and vectors.

Linear regression: Matrix notation

The linear regression problem is so called, because it is linear in the parameters a, b.

This is evident if we switch to matrix notation:

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{pmatrix}}_{\mathbf{X}} \underbrace{\begin{pmatrix} a \\ b \end{pmatrix}}_{\boldsymbol{\theta}}$$

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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.

The MSE is simply:

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

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Setting the gradient w.r.t. $\boldsymbol{\theta}$ to zero:

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

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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.

Linear regression: Higher dimensions

In the general case, the data points $(\mathbf{x}_i, \mathbf{y}_i)$ are vectors in $\mathbb{R}^d$:

$$\mathbf{y}_i = \mathbf{A}\mathbf{x}_i + \mathbf{b} \quad \text{for } i = 1, \ldots, n$$

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Stacking all data points into matrices $\tilde{\mathbf{X}} = \begin{pmatrix} | & | & \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots \\ | & | & \end{pmatrix}$ and $\mathbf{Y}$, we get:

$$\underbrace{\begin{pmatrix} y_{11} & \cdots & y_{1d} \\ y_{21} & \cdots & y_{2d} \\ \vdots & & \vdots \\ y_{n1} & \cdots & y_{nd} \end{pmatrix}}_{\mathbf{Y}^\top} = \underbrace{\begin{pmatrix} x_{11} & \cdots & x_{1d} & 1 \\ x_{21} & \cdots & x_{2d} & 1 \\ \vdots & & \vdots & \vdots \\ x_{n1} & \cdots & x_{nd} & 1 \end{pmatrix}}_{\mathbf{X}^\top := (\tilde{\mathbf{X}}^\top | \mathbf{1})} \underbrace{\begin{pmatrix} a_{11} & \cdots & a_{1d} \\ \vdots & & \vdots \\ a_{d1} & \cdots & a_{dd} \\ b_1 & \cdots & b_d \end{pmatrix}}_{\boldsymbol{\Theta}}$$

According to which, for each output data point $\mathbf{y}_i$ we have:

$$\underbrace{\begin{pmatrix} y_{i1} \\ \vdots \\ y_{id} \end{pmatrix}}_{\mathbf{y}_i} = \begin{pmatrix} \sum_{j=1}^d a_{j1} x_{ij} + b_1 \\ \vdots \\ \sum_{j=1}^d a_{jd} x_{ij} + b_d \end{pmatrix}$$

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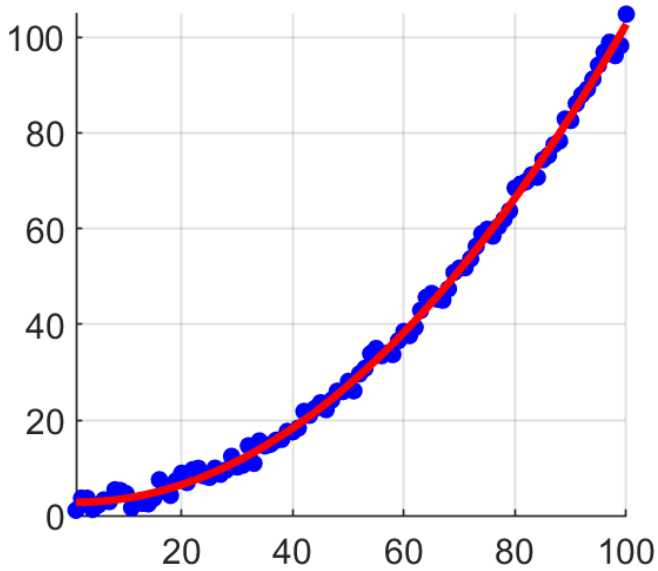
The closed form solution of $\nabla_{\boldsymbol{\Theta}} \ell(\boldsymbol{\Theta}) = \mathbf{0}$ is:

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

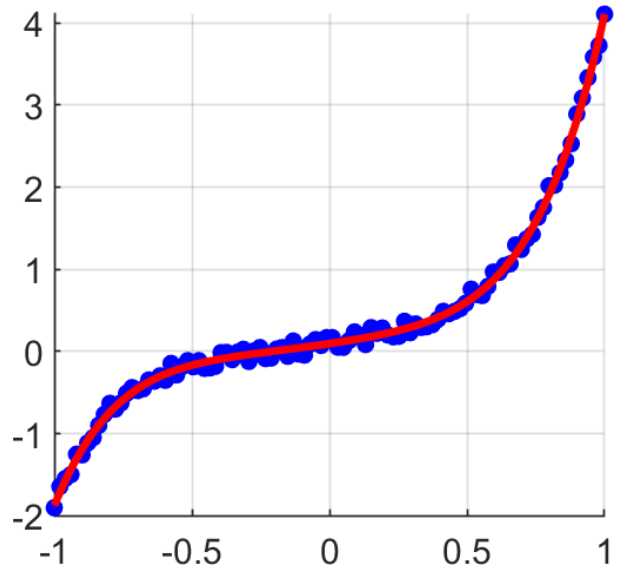
Fitting polynomials

Polynomial regression

Instead of linear functions, can we fit higher-order polynomials?



2nd-order



5th-order

Polynomial regression

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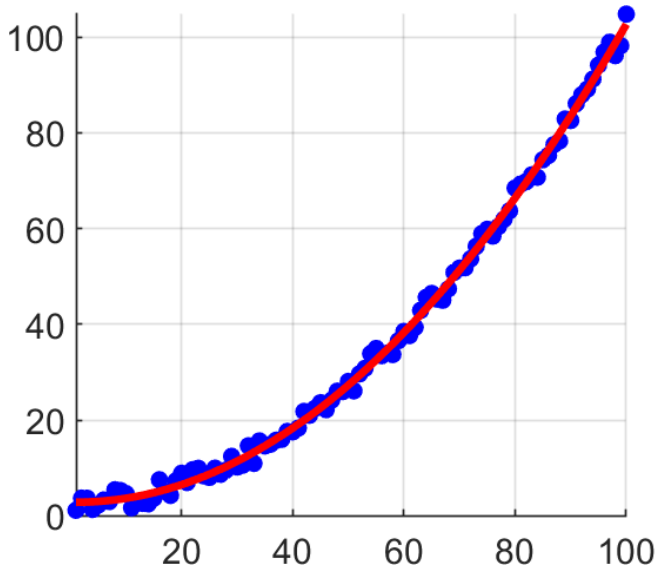

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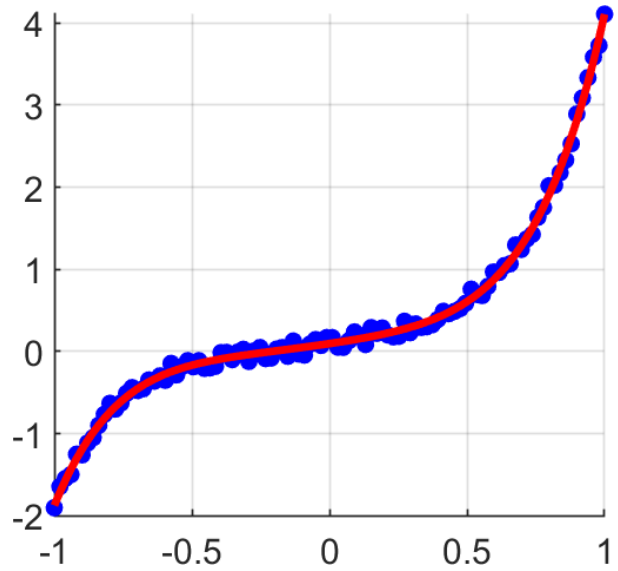

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The number of parameters grows with the order.

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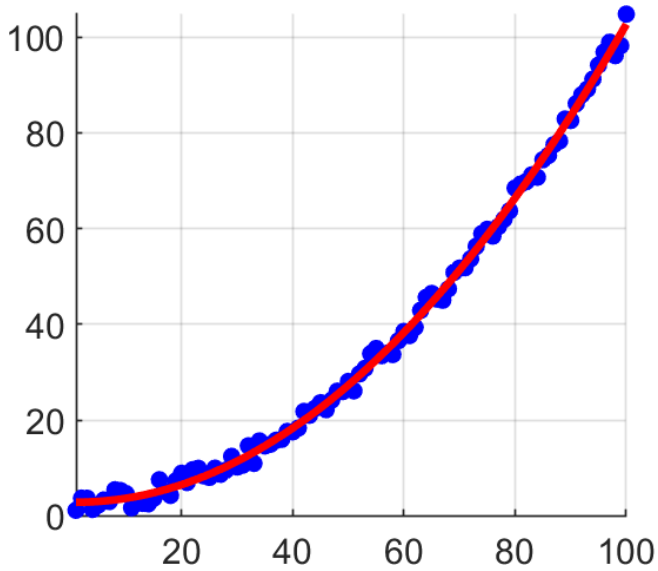

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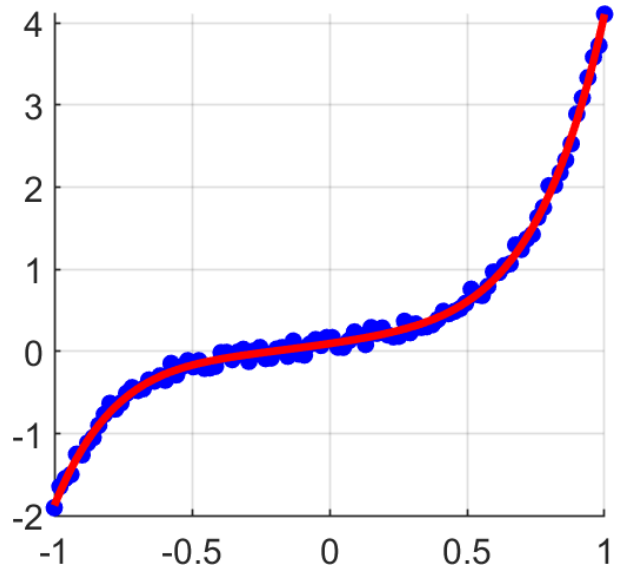

5th-order

The number of parameters grows with the order.

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

Polynomial regression

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Linear regression with polynomial features

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

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 $k < n$.

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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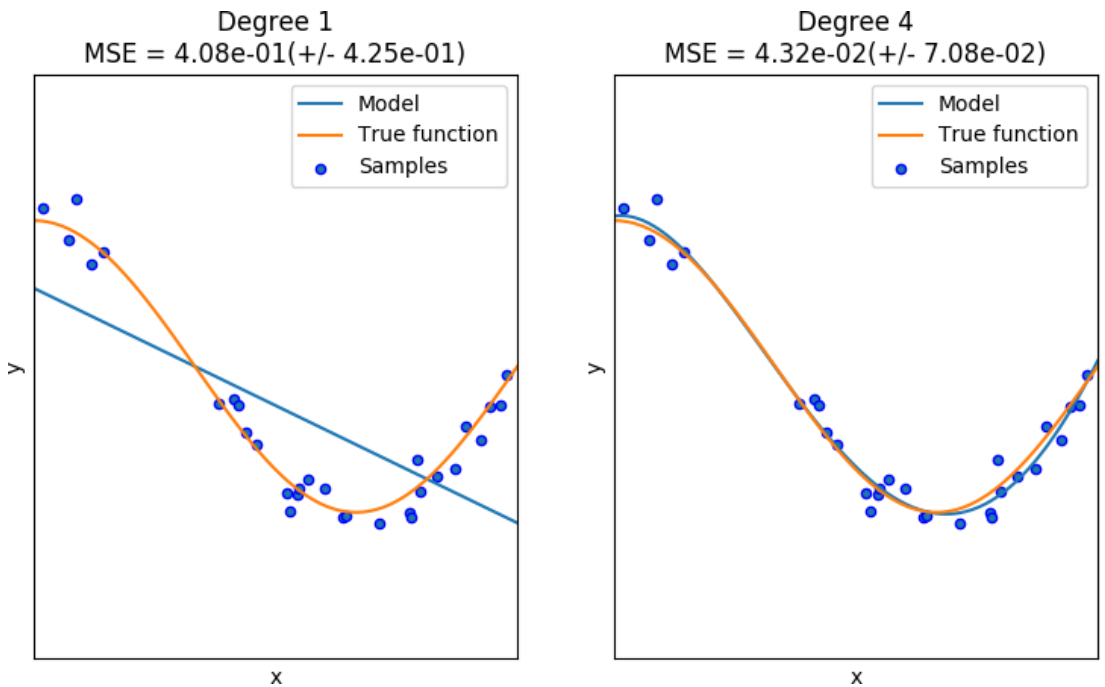

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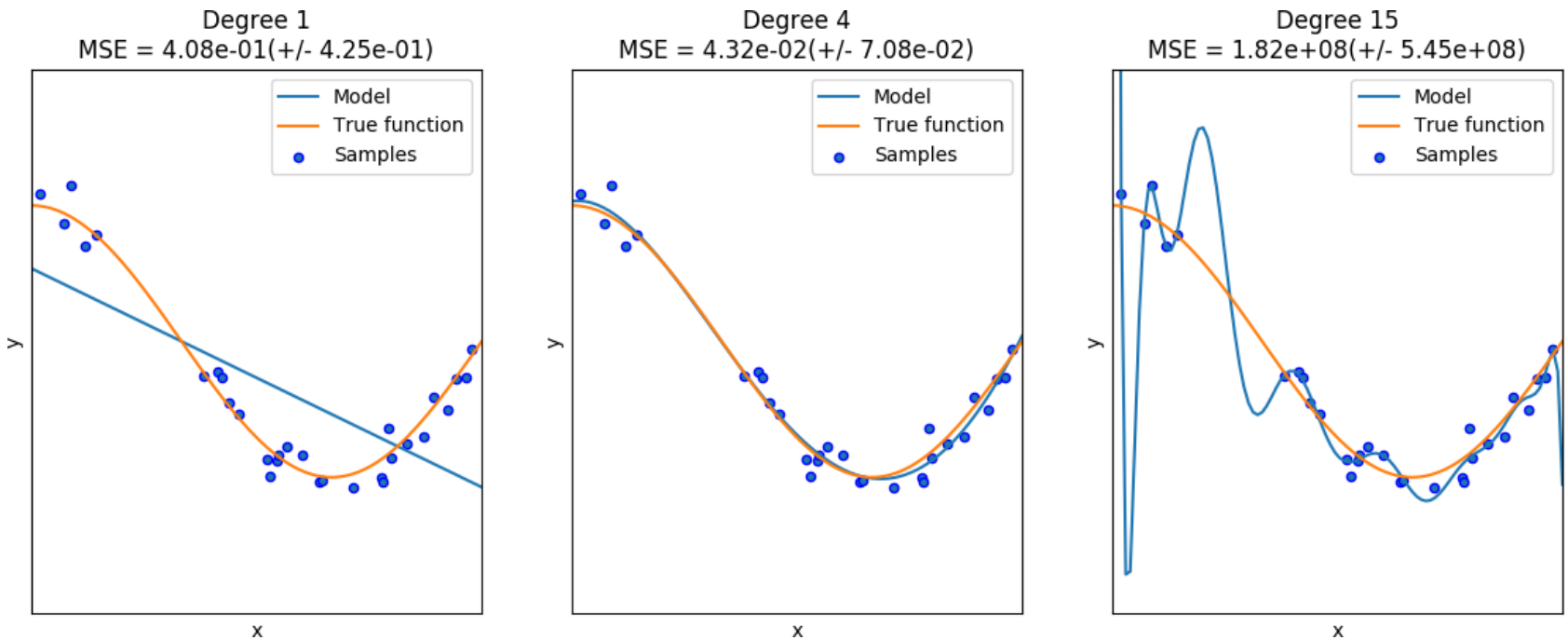

Suggested reading

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`