# Deep Learning & Applied AI

Linear regression, convexity, and gradients

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SAPIENZA
UNIVERSITÀ DI ROMA

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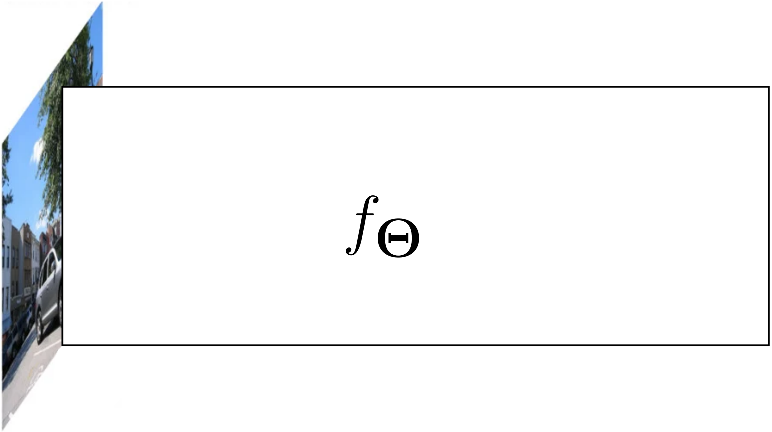
# A glimpse into neural networks

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



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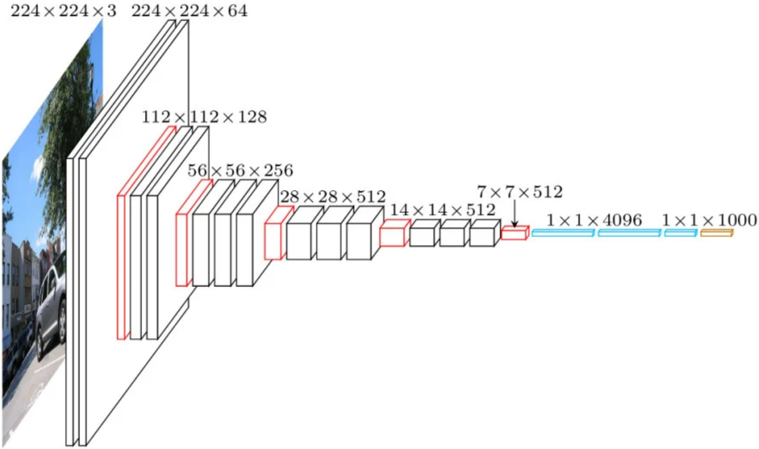

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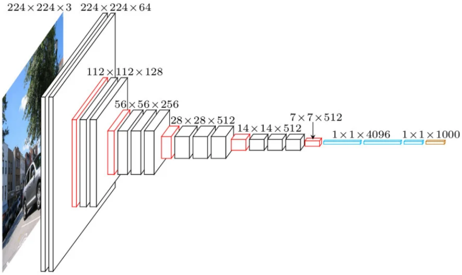


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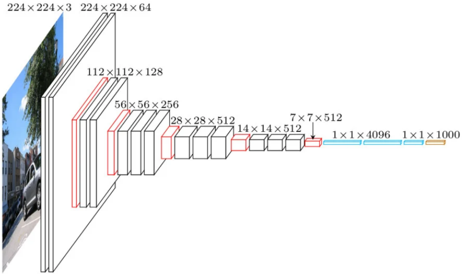


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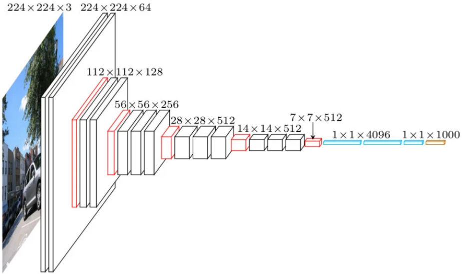


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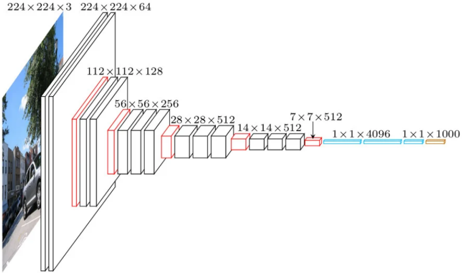


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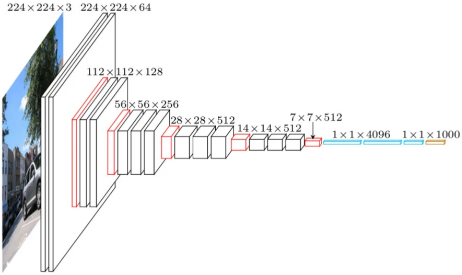


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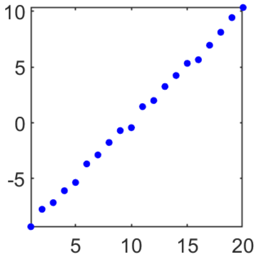
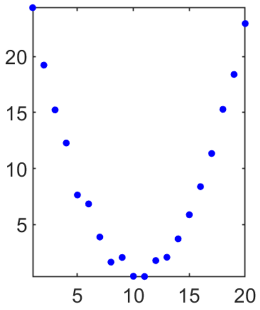
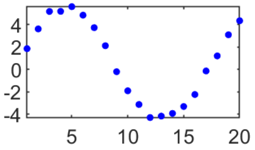
- ...which is done by minimizing a function called loss
- Minimization requires computing gradients, called backpropagation

# Parametrized models

The parameters determine the network's behavior and must be solved for.




$y = ax + b$

$y = ax^2 + bx + c$

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

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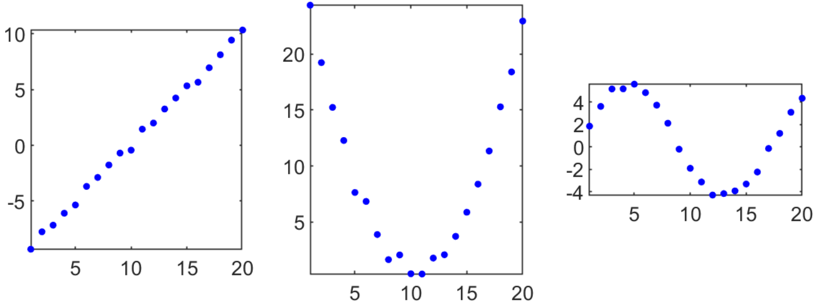


$$f_{a,b}(x) = ax + b$$

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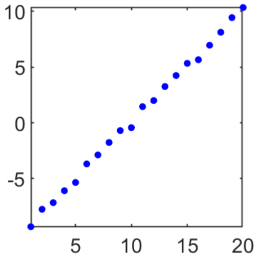
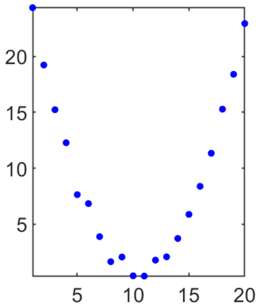
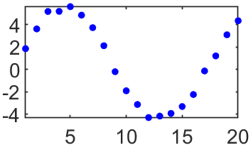



$f_{\Theta_f}(x)$

$\Theta_f \equiv \{a, b\}$




$g_{\Theta_g}(x)$

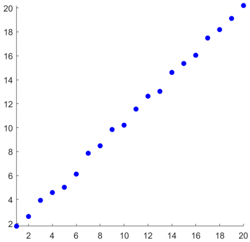



$h_{\Theta_h}(x)$

Our task is to find the parameters $\Theta$.

# Linear regression

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



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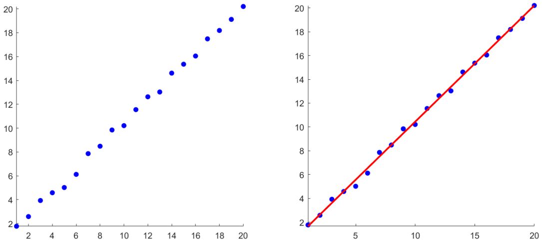


$$y_i = ax_i + b$$

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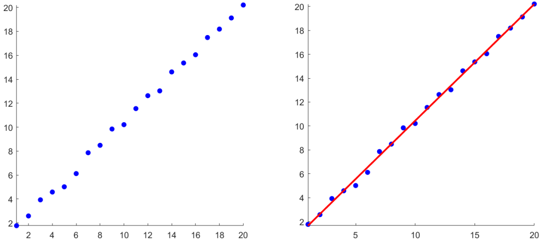


$$f_\Theta(x_i) = y_i$$

**Model**: linear + bias

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

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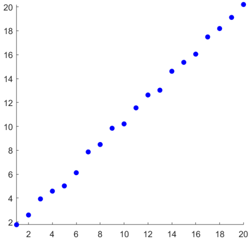


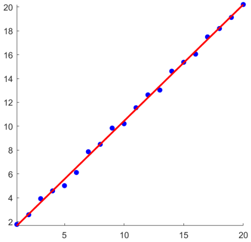


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**Model**: linear + bias

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

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

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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**Problem:** Choose $a$ and $b$ that minimize the mean squared error (MSE) between input and predicted output:

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

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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 function, usually denoted by $\ell$:

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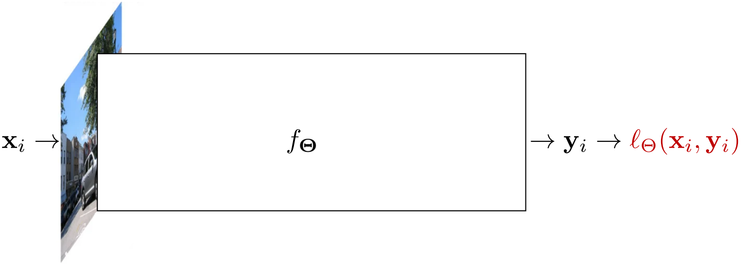
**Remark:** We minimize the loss w.r.t. the parameters $\Theta$, and **not** w.r.t. the data $(x_i, y_i)$. Also, the loss is defined on the entire dataset, not on just one data point.

# Linear regression

We are considering the following case:




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

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

# Convex functions

Jensen's inequality:

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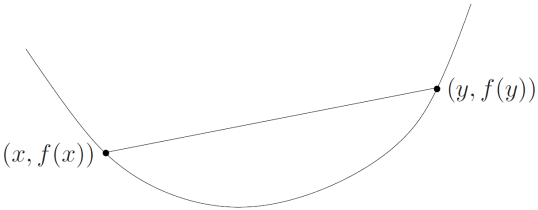

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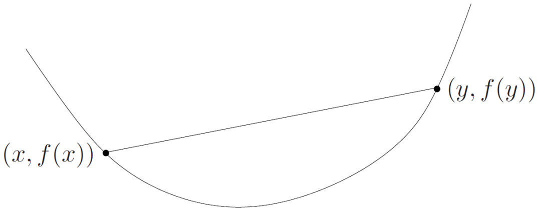


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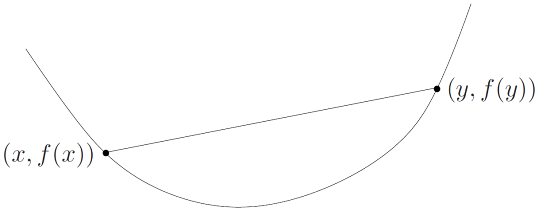


Let us further assume that $f$ is a differentiable function, so that we can compute its derivative $\frac{df}{dx}$ at all points $x$.

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

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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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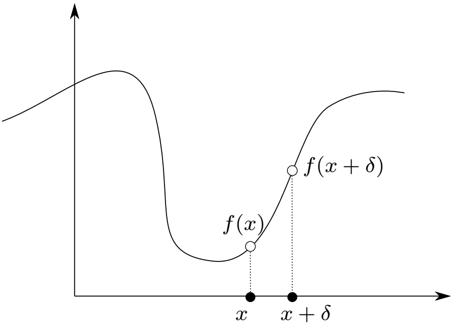

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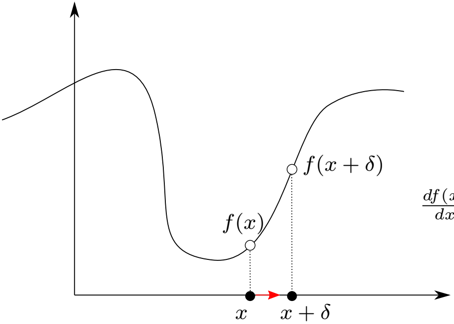


$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$

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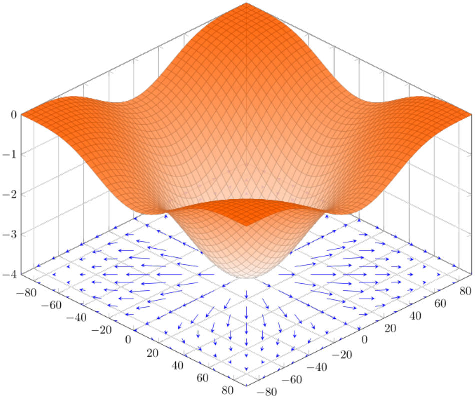

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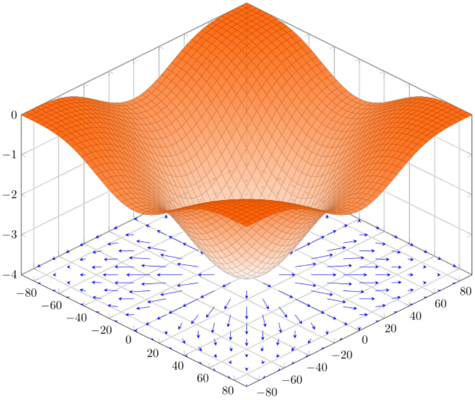
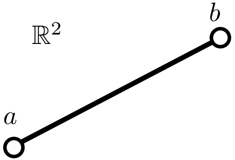



The length of the gradient vector encodes its steepness.

# Vector lengths

The Euclidean distance measures the length of a straight line connecting two points:



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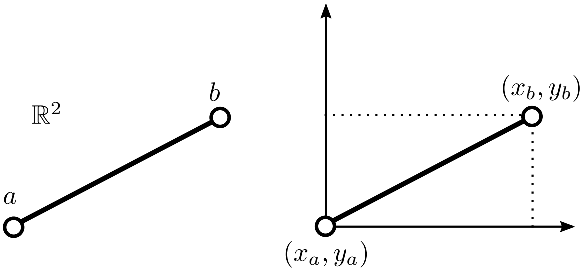

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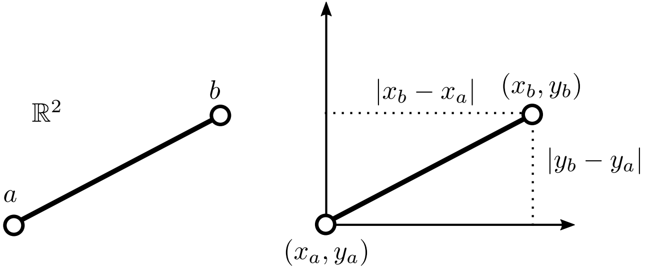

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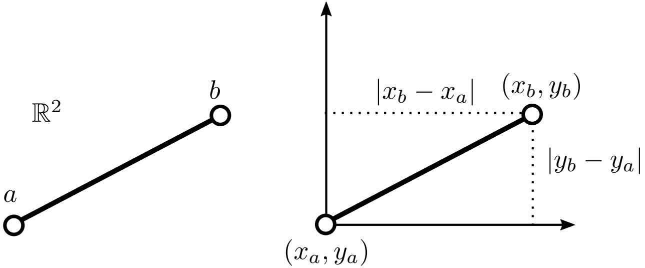


Apply Pythagoras' theorem: $d(a,b) = (|x_b - x_a|^2 + |y_b - y_a|^2)^{\frac{1}{2}}$

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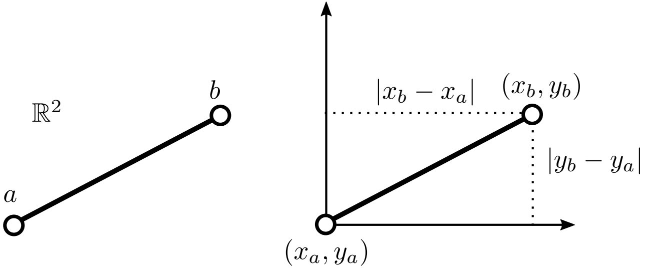


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In matrix notation:

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

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:

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

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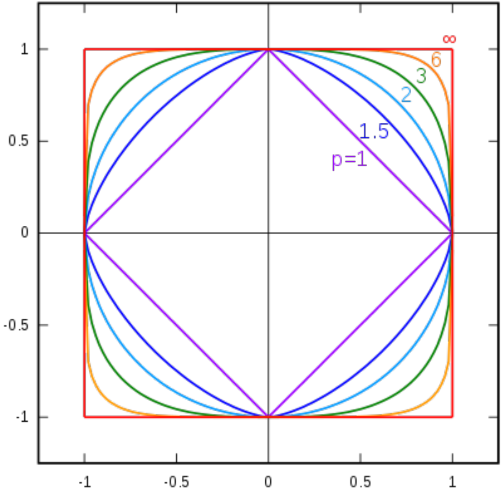
$$\|\mathbf{x} - \mathbf{0}\|_2 = \|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^k |x_i|^2} = \sqrt{\mathbf{x}^\top \mathbf{x}}$$

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



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

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

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&= \sum_{i=1}^{n} \nabla_{\mathbf{\Theta}} (\cancel{y_i^2} + a^2 x_i^2 + b^2 - 2ax_i y_i - 2by_i + 2abx_i)
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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:

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

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**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 deep nets, 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.

The MSE is simply:

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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.

# A note on the gradient in matrix form

In the previous slide, for the differentiation step:

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

what we did is **exactly equivalent** to the element-by-element computation of slide #14, but we did it directly in matrix form.

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

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\theta_i\theta_j$$

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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = (\mathbf{A} + \mathbf{A}^\top)\boldsymbol{\theta}$$

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

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = (\mathbf{A} + \mathbf{A}^\top)\boldsymbol{\theta}$$

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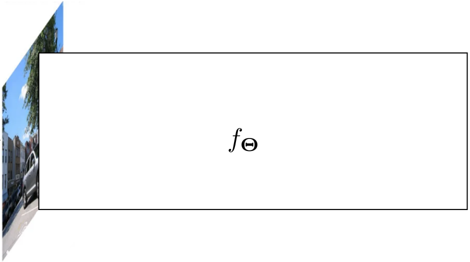
Defining the matrices $\mathbf{X} = \begin{pmatrix} | & | & \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots \\ | & | & \\ 1 & 1 & \end{pmatrix}, \mathbf{Y} = \begin{pmatrix} | & | & \\ \mathbf{y}_1 & \mathbf{y}_2 & \cdots \\ | & | & \end{pmatrix}, \mathbf{\Theta} = \begin{pmatrix} \mathbf{A} \\ \mathbf{b}^\top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

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

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

# Wrap-up

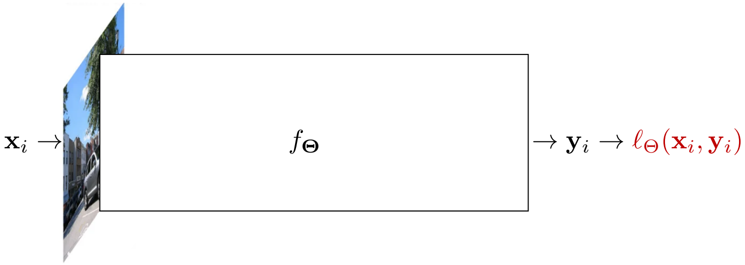
$\mathbf{x}_i \rightarrow$  $\rightarrow \mathbf{y}_i \rightarrow \ell_\Theta(\mathbf{x}_i, \mathbf{y}_i)$



Sometimes, the learning model is linear and the loss is quadratic.

This case can be solved in closed form.

# Wrap-up

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The more data points $(\mathbf{x}_i, \mathbf{y}_i)$ we have, the better.

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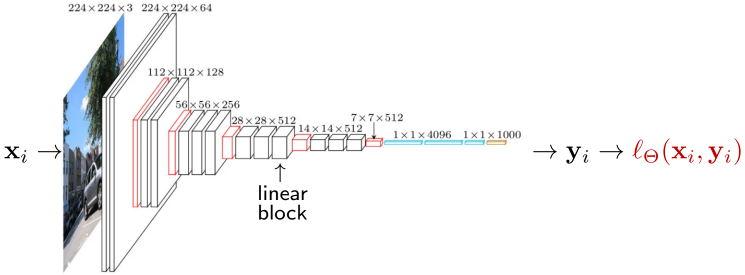


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The more data points $(\mathbf{x}_i, \mathbf{y}_i)$ we have, the better.

In deep learning, linear models usually appear as "pieces" within more complicated nonlinear models.

# 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`