Deep Learning & Applied AI

Linear regression, convexity, and gradients

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SAPIENZA
UNIVERSITÀ DI ROMA

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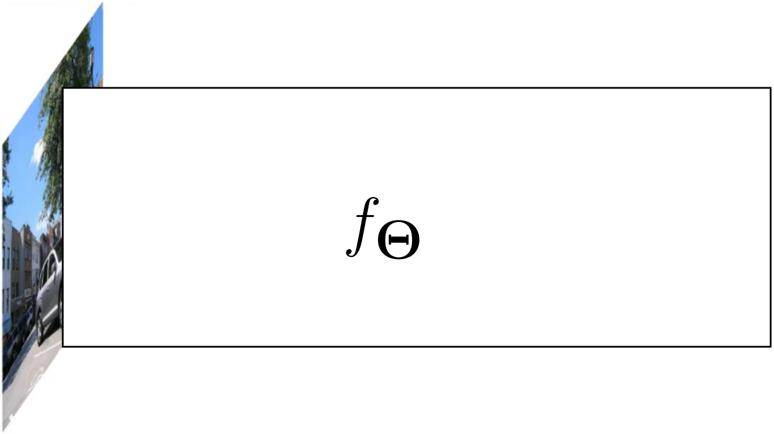
A glimpse into neural networks

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



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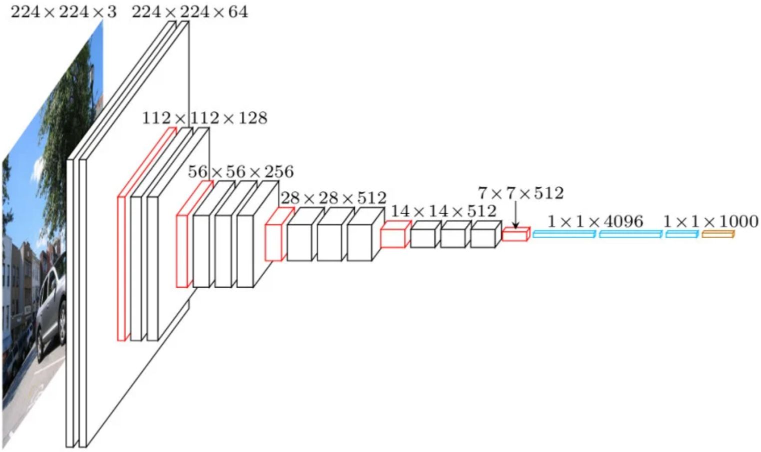

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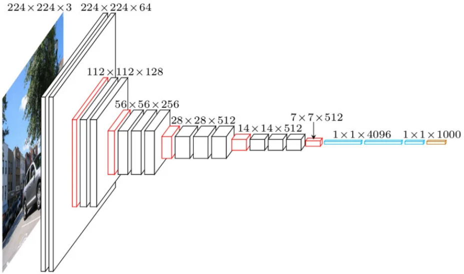

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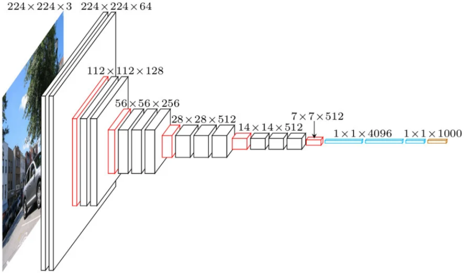

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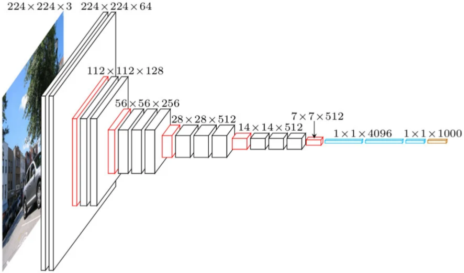

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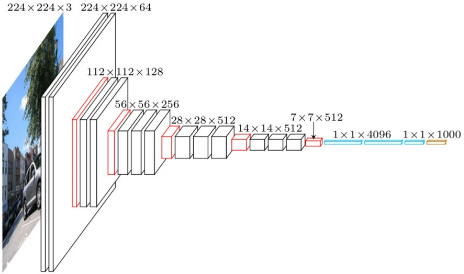

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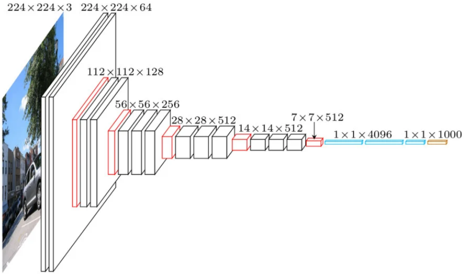

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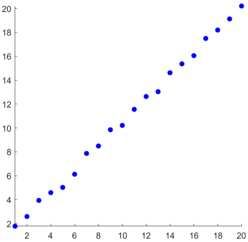
- ...which is done by minimizing a function called loss
- Minimization requires computing gradients, called backpropagation

Linear regression

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



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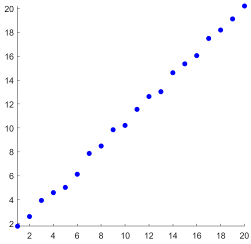

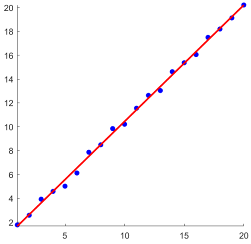

$$y_i = ax_i + b$$

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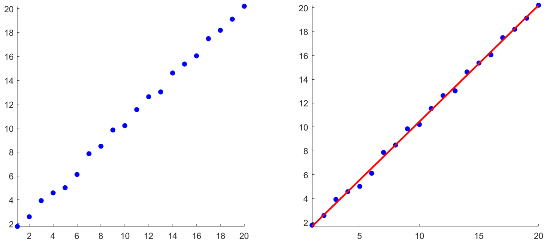

$$f_\Theta(x_i) = y_i$$

Model: linear + bias

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

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

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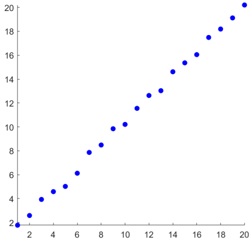

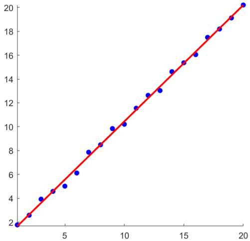

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Given a and b, we have a mapping that gives new output from new input.

Linear regression

The equations:

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

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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_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 function, usually denoted by ℓ:

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Remark: We minimize the loss w.r.t. the parameters Θ, 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:

$$\mathbf{x}_i \rightarrow \boxed{\quad f_{\boldsymbol{\Theta}} \quad} \rightarrow \mathbf{y}_i \rightarrow \color{red}{\ell_{\Theta}(\mathbf{x}_i, \mathbf{y}_i)}$$

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!

Convex functions

Jensen's inequality:

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

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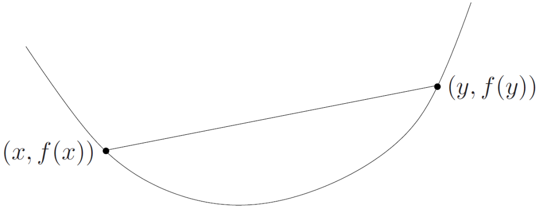

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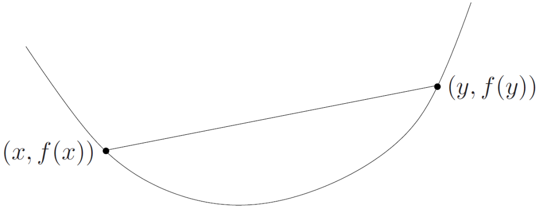

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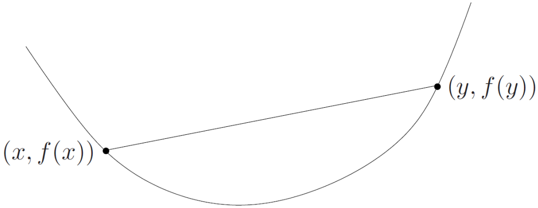

Let us further assume that f is a differentiable function, so that we can compute its derivative $\frac{df}{dx}$ at all points x.

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

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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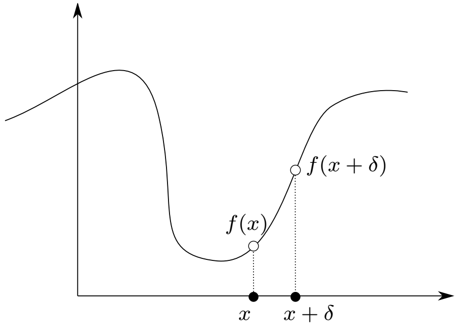

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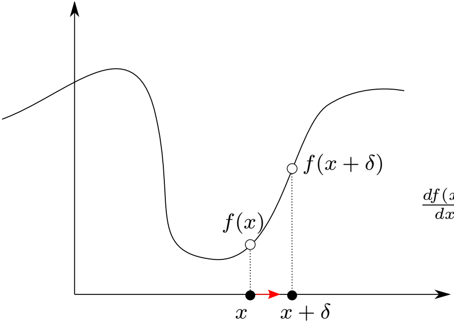

$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$

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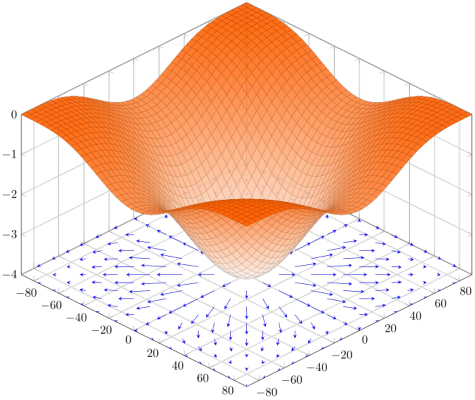

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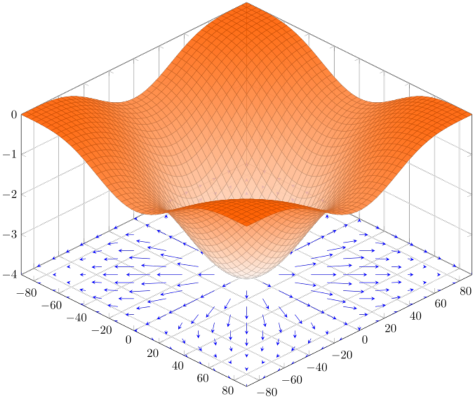
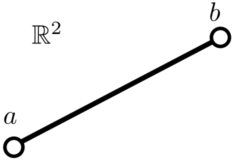


The length of the gradient vector encodes its steepness.

Vector lengths

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



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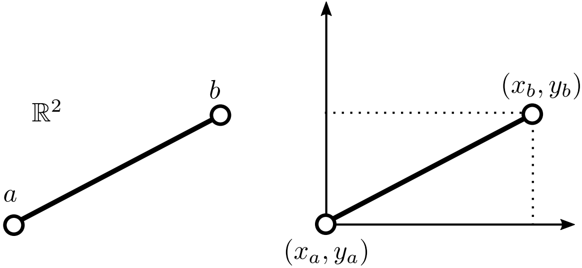

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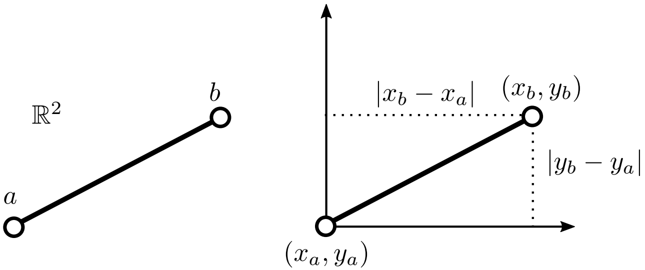

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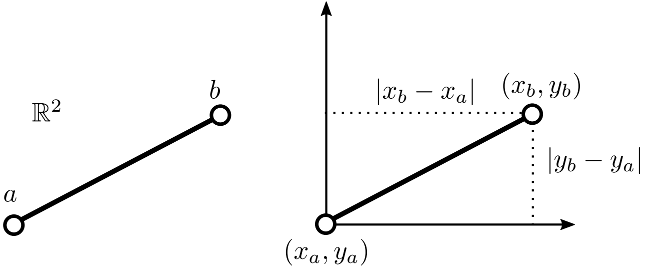

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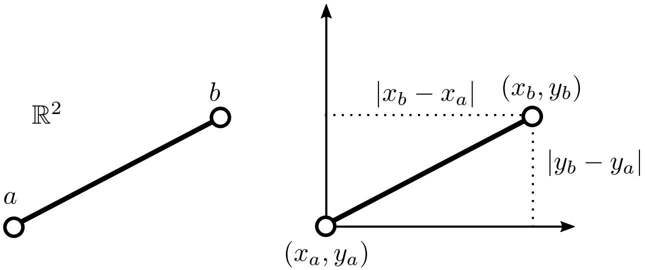

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In matrix notation:

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

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 $p \geq 1$:

$$\|\mathbf{x} - \mathbf{y}\|_2 = (|x_1 - y_1|^2 + |x_2 - y_2|^2)^{\frac{1}{2}}$$
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The length (or norm) of a vector is simply its distance from the origin:

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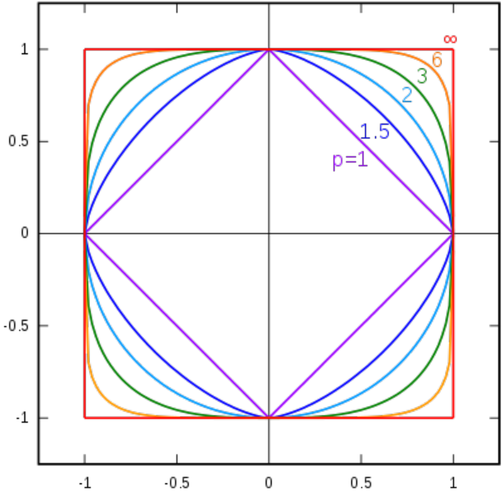
$$\|\mathbf{x} - \mathbf{0}\|_2 = \|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{k} |x_i|^2} = \sqrt{\mathbf{x}^\top \mathbf{x}}$$

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

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&= \sum_{i=1}^{n} \nabla_{\mathbf{\Theta}}(\cancel{y_i^2} + a^2x_i^2 + b^2 - 2ax_iy_i - 2by_i + 2abx_i)
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&= \sum_{i=1}^{n} \begin{pmatrix} 2ax_i^2 - 2x_i y_i + 2bx_i \\ 2b - 2y_i + 2ax_i \end{pmatrix}
\end{aligned}$$

Linear regression: Finding a solution

$$\mathbf{\Theta}^* = \operatorname{arg\,min}_{\mathbf{\Theta} \in \mathbb{R}^2} \ell(\mathbf{\Theta})$$

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

$$\ell(a, b) = \sum_{i=1}^{n} (y_i - a x_i - b)^2$$

A solution is found by setting $\nabla_{\mathbf{\Theta}} \ell(\mathbf{\Theta}) = \mathbf{0}$:

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&= \begin{pmatrix} \sum_{i=1}^{n} 2 a x_i^2 - 2 x_i y_i + 2 b x_i \\ \sum_{i=1}^{n} 2b - 2 y_i + 2 a x_i \end{pmatrix}
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$$\nabla_{\mathbf{\Theta}} \sum_{i=1}^{n} (y_i - a x_i - b)^2 = \begin{pmatrix} \sum_{i=1}^{n} 2a x_i^2 - 2 x_i y_i + 2 b x_i \\ \sum_{i=1}^{n} 2b - 2 y_i + 2 a x_i \end{pmatrix}$$

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:

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

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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:

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

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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.

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 #13/20, 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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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\theta_i\theta_j$$

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

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

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 $\nabla_{\mathbf{\Theta}} \ell(\mathbf{\Theta}) = \mathbf{0}$:

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

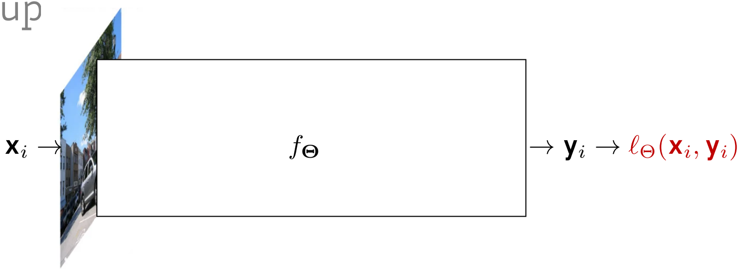
Wrap-up

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

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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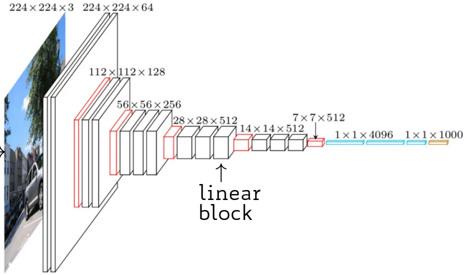

$\rightarrow \mathbf{y}_i \rightarrow \ell_\Theta(\mathbf{x}_i, \mathbf{y}_i)$

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- MLP: Linear blocks alternated with nonlinear functions

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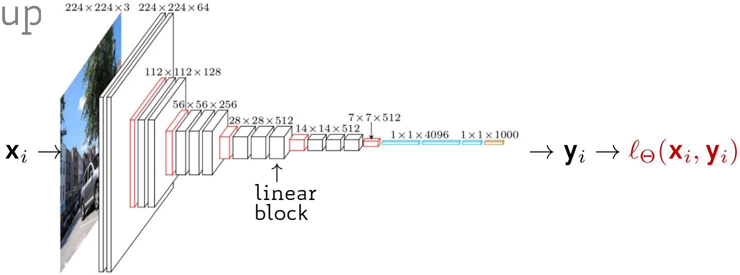

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- MLP: Linear blocks alternated with nonlinear functions
- Deep linear networks: Simple sequence of linear blocks

Saxe et al, Exact solutions to the nonlinear dynamics of learning in deep linear neural networks, 2013

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