Deep Learning & Applied AI

Linear regression, convexity, and gradients

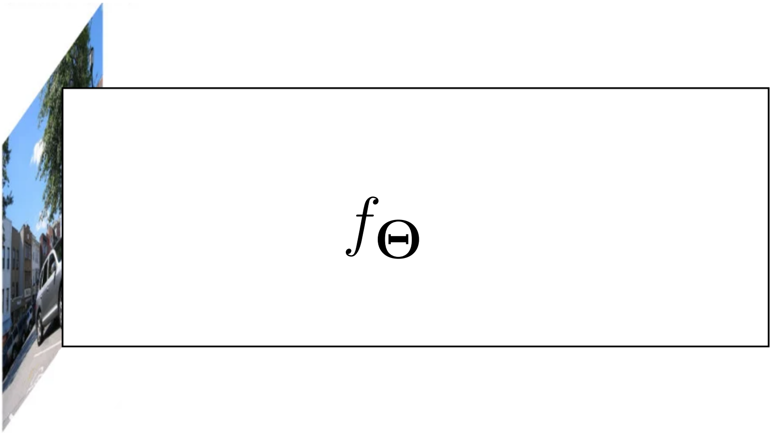
Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2022/2023 · March 08, 2023

A glimpse into neural networks

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



A glimpse into neural networks

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

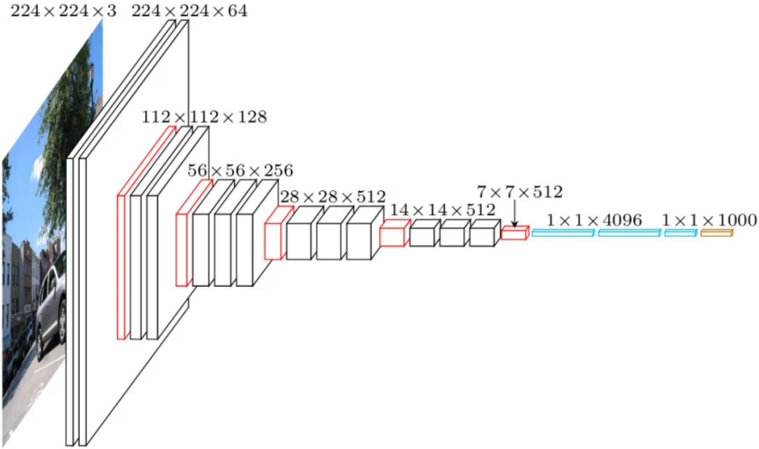
quindi una rete neurale può essere vista come una funzione che dipende dai parametri Θ

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

le lettere in grassetto servono per evidenziare oggetti che sono ad alte dimensioni (immagini, forme 3D, ecc...)

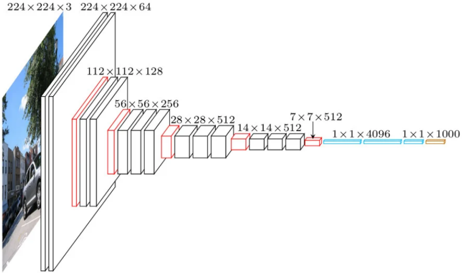
A glimpse into neural networks

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



A glimpse into neural networks

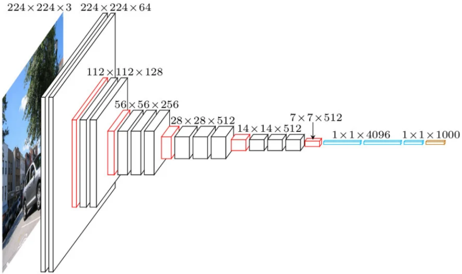
In deep learning, we deal with highly parametrized models called deep neural networks:



- Each block has a predefined structure (e.g., a linear map)

A glimpse into neural networks

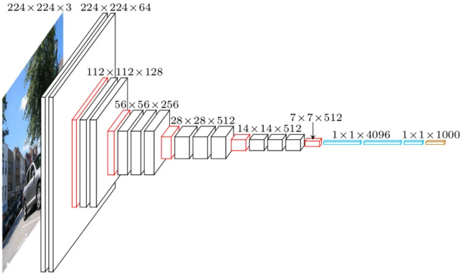
In deep learning, we deal with highly parametrized models called deep neural networks:



- Each block has a predefined structure (e.g., a linear map)
- Each block is defined in terms of unknown parameters θ

A glimpse into neural networks

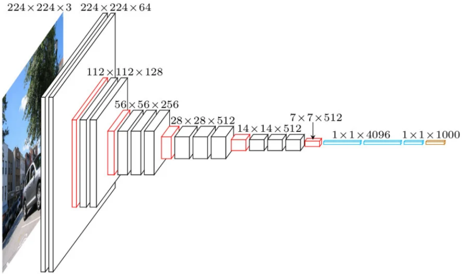
In deep learning, we deal with highly parametrized models called deep neural networks:



- Each block has a predefined structure (e.g., a linear map)
- Each block is defined in terms of unknown parameters θ
- Finding the parameter values is called training...

A glimpse into neural networks

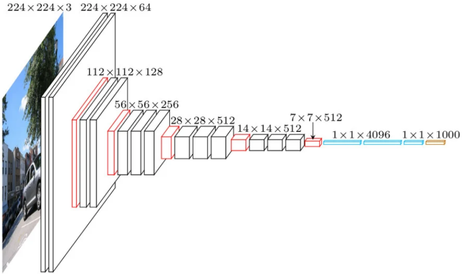
In deep learning, we deal with highly parametrized models called deep neural networks:



- Each block has a predefined structure (e.g., a linear map)
- Each block is defined in terms of unknown parameters θ
- Finding the parameter values is called training...
- ...which is done by minimizing a function called loss

A glimpse into neural networks

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

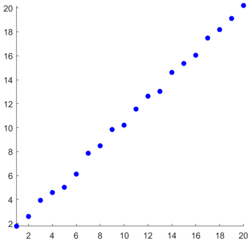


per esempio

- Each block has a predefined structure (e.g., a linear map)
- Each block is defined in terms of unknown parameters θ
- Finding the parameter values is called training...
- ...which is done by minimizing a function called loss
- Minimization requires computing gradients, called backpropagation

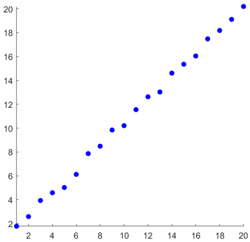
Linear regression

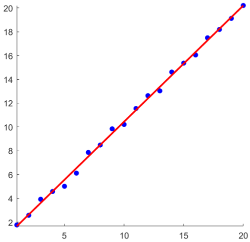
We start from the simplest non-trivial case for a learning model:



Linear regression

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



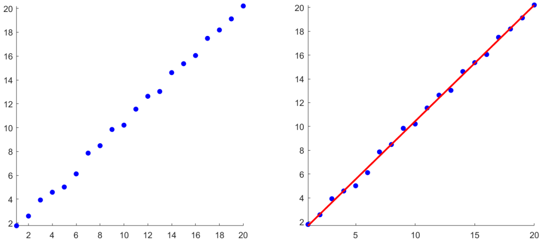


$$y_i = ax_i + b$$

questa funzione che descrive
il grafico della retta, può essere
parametrizzata così...

Linear regression

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



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

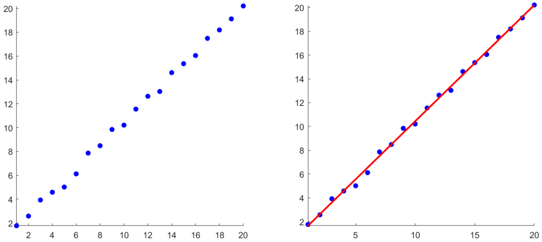
Model: linear + bias

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

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

Linear regression

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



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

rispetto ad x

Model: linear + bias

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

sia le x che le y sono scalari
perché parliamo di regressione

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

infatti questo è un compito
di regressione

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

quando si studiano le reti neurali, si stanno praticamente
analizzando modelli complessi di regressione lineare

Linear regression

The equations:

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

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

Linear regression

The equations:

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

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

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

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

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

Linear regression

The equations:

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

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

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

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

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

Spesso la media viene omessa, come in questo caso. Questo perché influenza i calcoli solo da un punto di vista numerico e non cambia il comportamento del risultato che cerchiamo (*a* e *b* in questo caso)

Linear regression

The equations:

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

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

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

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

questa formula può essere riscritta con...

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

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

Linear regression: Loss function

The equations:

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

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

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

$$\epsilon = \min_\Theta \ell_\Theta(\{x_i, y_i\})$$

...questa forma generica,
dove *l* è la loss function

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

$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} (y_i - f_\Theta(x_i))^2$$

Linear regression: Loss function

The equations:

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

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

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

$$\epsilon = \min_\Theta \ell_\Theta(\{x_i, y_i\})$$

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

$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} (y_i - f_\Theta(x_i))^2$$

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:

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

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

Optimization

We need to solve the general minimization problem:

$$\epsilon = \min_{\Theta} \ell(\Theta)$$

Optimization

We need to solve the general minimization problem:

$$\epsilon = \min_{\Theta} \ell(\Theta)$$

In particular, we are interested in the minimizer Θ.

Optimization

We need to solve the general minimization problem:

$$\epsilon = \min_{\Theta} \ell(\Theta)$$

In particular, we are interested in the minimizer Θ.

Finding minimizers for general ℓ is an open problem. The research area is broadly called optimization.

In general, the optimization method depends on the properties of ℓ.

Optimization

We need to solve the general minimization problem:

$$\epsilon = \min_{\Theta} \ell(\Theta)$$

In particular, we are interested in the minimizer Θ.

Finding minimizers for general ℓ is an open problem. The research area is broadly called optimization.

In general, the optimization method depends on the properties of ℓ.

We will mostly deal with unconstrained problems.

Optimization

We need to solve the general minimization problem:

$$\epsilon = \min_{\Theta} \ell(\Theta)$$

In particular, we are interested in the minimizer Θ.

Finding minimizers for general ℓ is an open problem. The research area is broadly called optimization.

In general, the optimization method depends on the properties of ℓ.

We will mostly deal with unconstrained problems.

ovvero problemi di ottimizzazione
che NON aggiungono vincoli
pesanti da rispettare

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

Convex functions

Jensen's inequality:

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

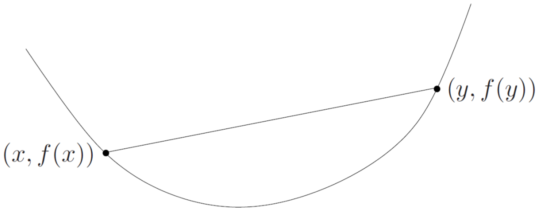
for all x, y and $\alpha \in (0,1)$

Convex functions

Jensen's inequality:

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

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

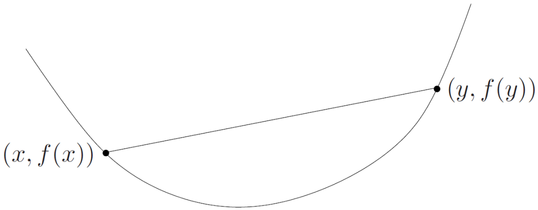


Convex functions

Jensen's inequality:

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

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



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

Convex functions

un esempio di ottimizzazione facile è quello delle funzioni convesse 2D

Jensen's inequality:

punti sulla curva sotto la retta

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

punti sulla retta di combinazione convessa

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

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 $\frac{df(x)}{dx} = 0$.

quindi le funzioni convesse hanno sempre un global minima (o più di uno con lo stesso valore)

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

In deep learning we deal with loss functions with $n \gg 1$ parameters:

$$f : \mathbb{R}^n \to \mathbb{R}$$

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

In deep learning we deal with loss functions with $n \gg 1$ parameters:

$$f : \mathbb{R}^n \to \mathbb{R}$$

The notion of derivative is replaced by the notion of gradient:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

which is the vector of partial derivatives of f.

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

In deep learning we deal with loss functions with $n \gg 1$ parameters:

$$f : \mathbb{R}^n \to \mathbb{R}$$

The notion of derivative is replaced by the notion of gradient:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

which is the vector of partial derivatives of f.

Convexity is defined as before:

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

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

quindi più dimensioni

In deep learning we deal with loss functions with $n \gg 1$ parameters:

$$f : \mathbb{R}^n \to \mathbb{R}$$

The notion of derivative is replaced by the notion of gradient:

f è la loss function ed *x* è il vettore dei parametri di *f*

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

vettore delle derivate parziali di *f* rispetto ai singoli parametri *x*

which is the vector of partial derivatives of f.

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:

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

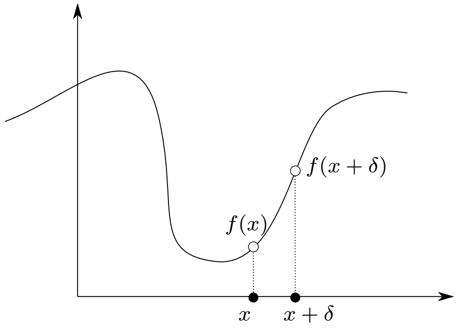
si legge: se il gradiente della f convessa con parametri x è = 0,
allora il punto x (ovvero i parametri) è un global optimum per f

The gradient

The gradient $\nabla_{\mathbf{x}} f(\mathbf{x})$ encodes the direction of steepest ascent of f at point $\mathbf{x}$.

The gradient

The gradient $\nabla_{\mathbf{x}} f(\mathbf{x})$ encodes the direction of steepest ascent of f at point $\mathbf{x}$. In the simple 1D case:

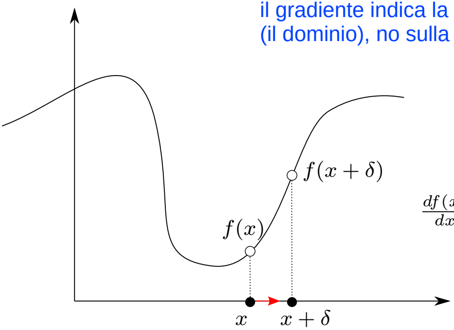


The gradient

la salita più ripida

The gradient $\nabla_{\mathbf{x}} f(\mathbf{x})$ encodes the direction of steepest ascent of f at point $\mathbf{x}$. In the simple 1D case:

il gradiente indica la direzione sul piano
(il dominio), no sulla funzione

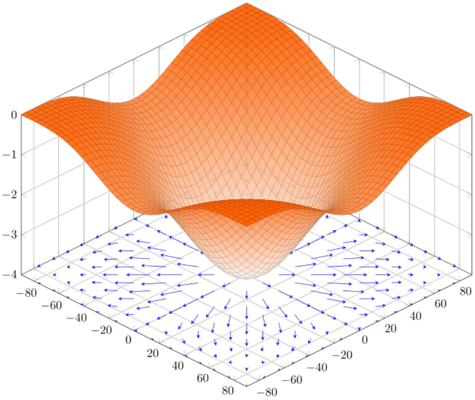


$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$

IMPORTANTE: il gradiente è un'operazione lineare

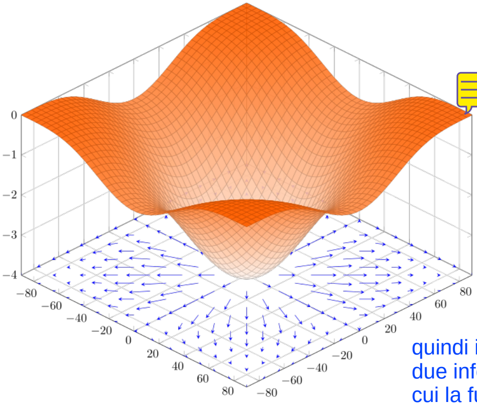
The gradient

The gradient $\nabla_{\mathbf{x}} f(\mathbf{x})$ encodes the direction of steepest ascent of f at point $\mathbf{x}$. In the more general case:



The gradient

The gradient $\nabla_{\mathbf{x}} f(\mathbf{x})$ encodes the direction of steepest ascent of f at point $\mathbf{x}$. In the more general case:

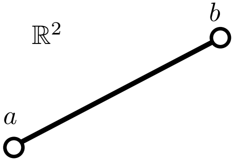


quindi il gradiente restituisce due informazioni: la direzione in cui la funzione cambia e la velocità con cui lo fa

The length of the gradient vector encodes its steepness.

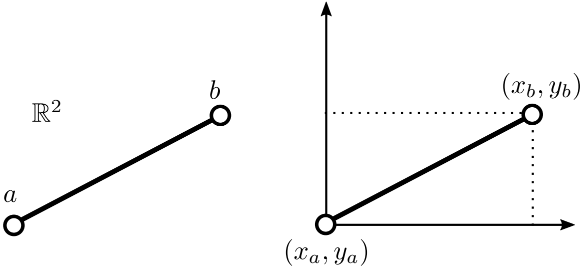
Vector lengths

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



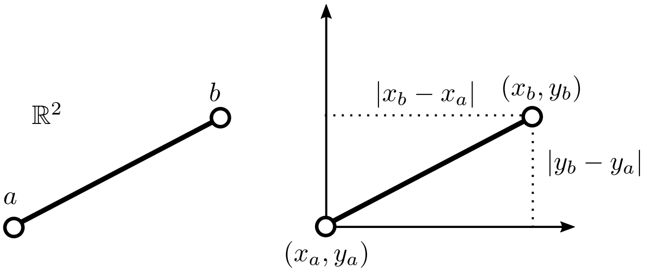
Vector lengths

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



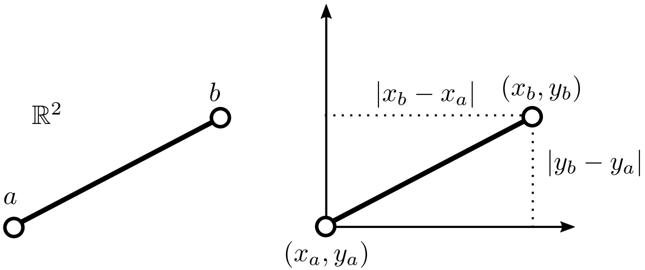
Vector lengths

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



Vector lengths

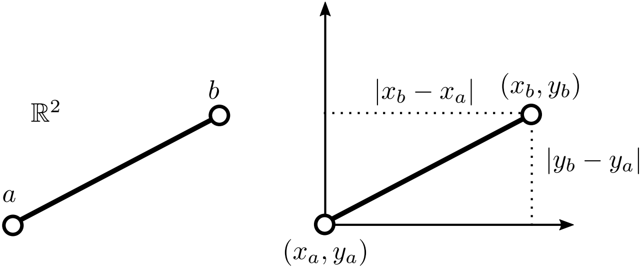
The Euclidean distance measures the length of a straight line connecting two points:



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

Vector lengths

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



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

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 $\mathbf{b} = \begin{pmatrix} x_b \\ y_b \end{pmatrix}$ sono i vettori che esprimono le coordinate di *a* e di *b*

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

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

$$\|\mathbf{x} - \mathbf{y}\|_2 = (|x_1 - y_1|^2 + |x_2 - y_2|^2)^{\frac{1}{2}}$$
$$\Downarrow$$
$$\|\mathbf{x} - \mathbf{y}\|_p = (|x_1 - y_1|^p + |x_2 - y_2|^p)^{\frac{1}{p}}$$

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

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

$$\|\mathbf{x} - \mathbf{y}\|_2 = (|x_1 - y_1|^2 + |x_2 - y_2|^2)^{\frac{1}{2}}$$
$$\Downarrow$$
$$\|\mathbf{x} - \mathbf{y}\|_p = (|x_1 - y_1|^p + |x_2 - y_2|^p)^{\frac{1}{p}}$$

As well as generalize from $\mathbb{R}^2$ to $\mathbb{R}^k$:

$$\|\mathbf{x} - \mathbf{y}\|_p = (\sum_{i=1}^k |x_i - y_i|^p)^{\frac{1}{p}}$$

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

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

$$\|\mathbf{x}-\mathbf{y}\|_2 = (|x_1 - y_1|^2 + |x_2 - y_2|^2)^{\frac{1}{2}}$$
$$\Downarrow$$
$$\|\mathbf{x}-\mathbf{y}\|_p = (|x_1 - y_1|^p + |x_2 - y_2|^p)^{\frac{1}{p}}$$

As well as generalize from $\mathbb{R}^2$ to $\mathbb{R}^k$:

$$\|\mathbf{x}-\mathbf{y}\|_p = (\sum_{i=1}^{k} |x_i - y_i|^p)^{\frac{1}{p}}$$

This definition gives us the L_p distance between vectors in $\mathbb{R}^k$.

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

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

$$\|\mathbf{x} - \mathbf{y}\|_2 = (|x_1 - y_1|^2 + |x_2 - y_2|^2)^{\frac{1}{2}}$$
$$\Downarrow$$
$$\|\mathbf{x} - \mathbf{y}\|_p = (|x_1 - y_1|^p + |x_2 - y_2|^p)^{\frac{1}{p}}$$

As well as generalize from $\mathbb{R}^2$ to $\mathbb{R}^k$:

$$\|\mathbf{x} - \mathbf{y}\|_p = \left(\sum_{i=1}^{k} |x_i - y_i|^p\right)^{\frac{1}{p}}$$

This definition gives us the L_p distance between vectors in $\mathbb{R}^k$.

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

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

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

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

$$\|\mathbf{x} - \mathbf{y}\|_2 = (|x_1 - y_1|^2 + |x_2 - y_2|^2)^{\frac{1}{2}}$$
$$\Downarrow$$
$$\|\mathbf{x} - \mathbf{y}\|_p = (|x_1 - y_1|^p + |x_2 - y_2|^p)^{\frac{1}{p}}$$

As well as generalize from $\mathbb{R}^2$ to $\mathbb{R}^k$:

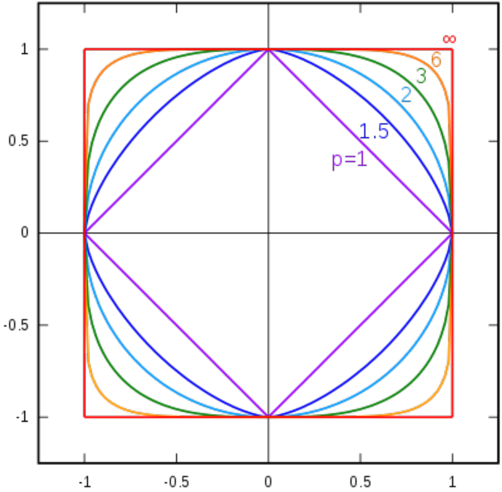
$$\|\mathbf{x} - \mathbf{y}\|_p = \left(\sum_{i=1}^{k} |x_i - y_i|^p\right)^{\frac{1}{p}}$$

This definition gives us the L_p distance between vectors in $\mathbb{R}^k$.

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

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

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



In questa immagine, le varie forme colorate indicano i punti distanti 1 dall'origine secondo le diverse norme

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

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

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

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

Linear regression: Finding a solution

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

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

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

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

$$\nabla_{\mathbf{\Theta}} \sum_{i=1}^{n} (y_i - ax_i - b)^2 = \sum_{i=1}^{n} \nabla_{\mathbf{\Theta}} (y_i - ax_i - b)^2$$

Linear regression: Finding a solution

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

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

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

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

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

Linear regression: Finding a solution

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

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

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

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

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

Linear regression: Finding a solution

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

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

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

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

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

Linear regression: Finding a solution

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

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

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

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

$$\nabla_{\mathbf{\Theta}}\sum_{i=1}^{n}(y_i - ax_i - b)^2 = \begin{pmatrix} \sum_{i=1}^{n} 2ax_i^2 - 2x_iy_i + 2bx_i \\ \sum_{i=1}^{n} 2b - 2y_i + 2ax_i \end{pmatrix}$$

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:

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

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:

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

questi sono i blocchetti che formano le reti neurali

Remark: Deep learning frameworks frequently use the alternative expression with the bias encoded separately:

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

questi sono i blocchetti che formano le reti neurali

Familiarize with matrix calculus.

When implementing deep nets, we manipulate matrices, vectors, and tensors.

Linear regression: Matrix notation

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

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:

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

Linear regression: Matrix notation

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

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:

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

Linear regression: Matrix notation

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

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:

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

Linear regression: Matrix notation

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

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:

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

ha calcolato il gradiente di questa

Setting $\nabla_{\boldsymbol{\theta}} \ell = \mathbf{0}$ we get:

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

Linear regression: Matrix notation

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

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:

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

Setting $\nabla_{\boldsymbol{\theta}} \ell = \mathbf{0}$ we get:

$$\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} = \mathbf{X}^\top \mathbf{y}$$

Linear regression: Matrix notation

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

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:

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

Setting $\nabla_{\boldsymbol{\theta}} \ell = \mathbf{0}$ we get:

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

ATTENZIONE: qui si parla di un problema supervisionato, perché si hanno i groundtruth

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.

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.

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

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

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.

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

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

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.

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

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial}{\partial \theta_1} \sum_{i=1}^n \sum_{j=1}^n a_{ij}\theta_i\theta_j \\ \vdots \\ \frac{\partial}{\partial \theta_n} \sum_{i=1}^n \sum_{j=1}^n a_{ij}\theta_i\theta_j \end{pmatrix}$$

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.

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

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \begin{pmatrix} \sum_j a_{1j}\theta_j + \sum_i a_{i1}\theta_i \\ \vdots \\ \sum_j a_{nj}\theta_j + \sum_i a_{in}\theta_i \end{pmatrix}$$

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.

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

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \begin{pmatrix} \sum_i (a_{1i} + a_{i1})\theta_i \\ \vdots \\ \sum_i (a_{ni} + a_{in})\theta_i \end{pmatrix}$$

A note on the gradient in matrix form

In the previous slide, for the differentiation step:

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

what we did is **exactly equivalent** to the element-by-element computation of slide $\#13/20$, but we did it directly in matrix form.

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

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

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.

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

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

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).

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).

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

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

Linear regression: Higher dimensions

ATTENZIONE: quindi qui si parla di regressione lineare dove sia gli input che gli output NON sono scalari, ma vettori

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).

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

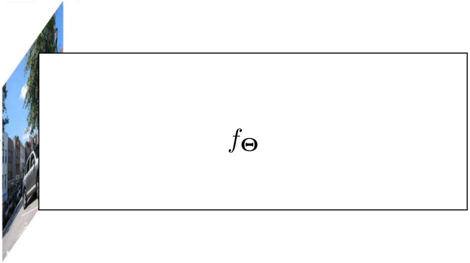
$$\mathbf{y}_i = \mathbf{A}\mathbf{x}_i + \mathbf{b} \quad \text{for } i = 1, \ldots, n$$

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

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

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

Wrap-up

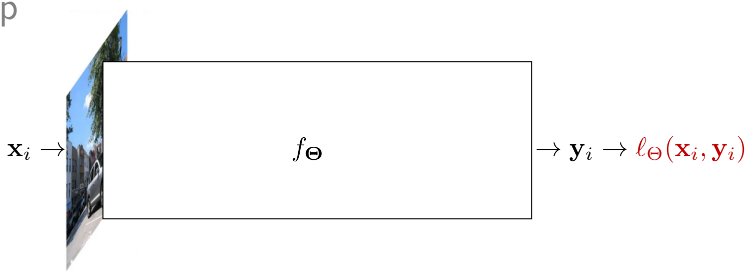


$$\mathbf{x}_i \rightarrow f_{\boldsymbol{\Theta}} \rightarrow \mathbf{y}_i \rightarrow \ell_{\Theta}(\mathbf{x}_i, \mathbf{y}_i)$$

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

This case can be solved in closed form.

Wrap-up

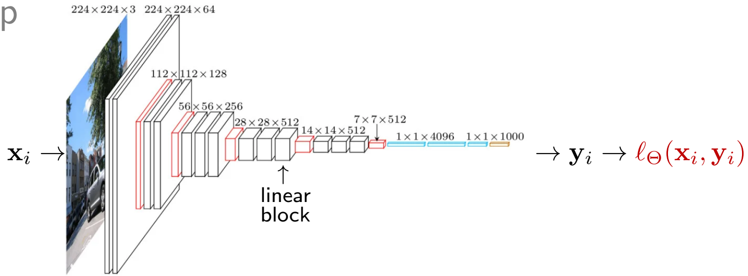


Sometimes, the learning model is linear and the loss is quadratic.

This case can be solved in closed form.

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

Wrap-up

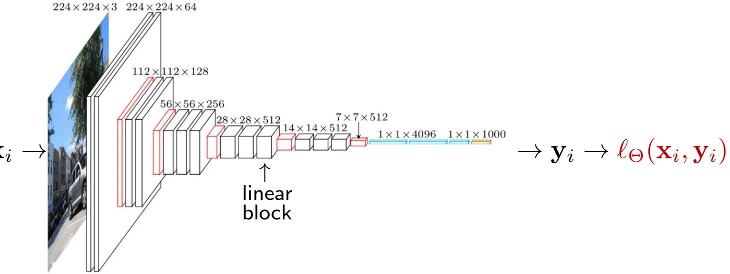


Sometimes, the learning model is linear and the loss is quadratic.
This case can be solved in closed form.

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

- MLP: Linear blocks alternated with nonlinear functions

Wrap-up



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

This case can be solved in closed form.

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

- 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`