Deep Learning & Applied AI

Linear regression, convexity, and gradients

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SAPIENZA
UNIVERSITÀ DI ROMA

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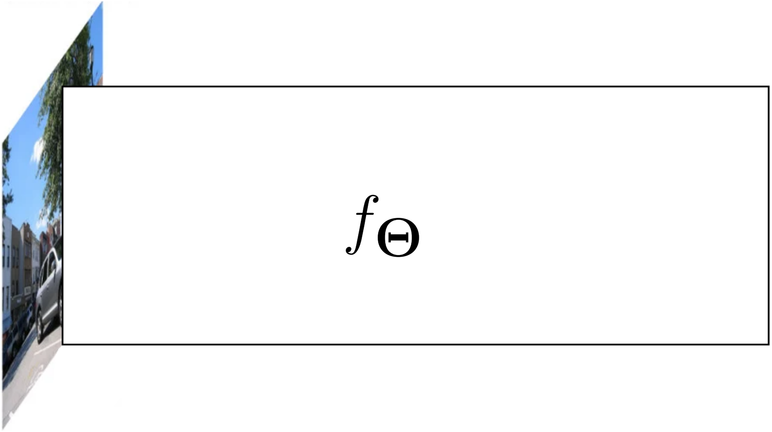
A glimpse into neural networks

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



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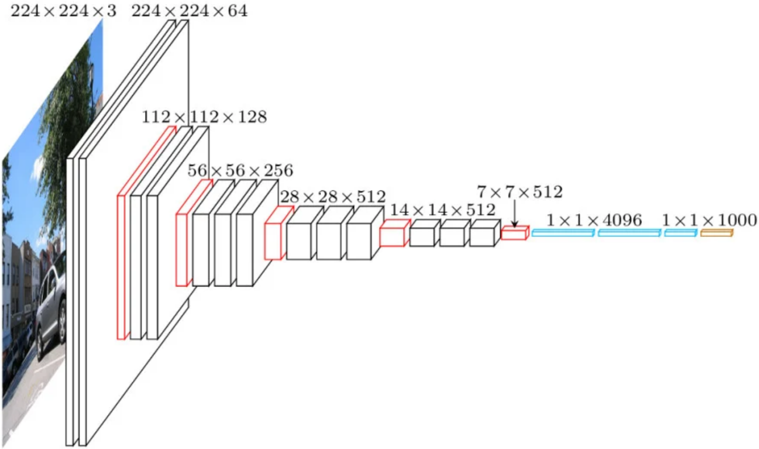

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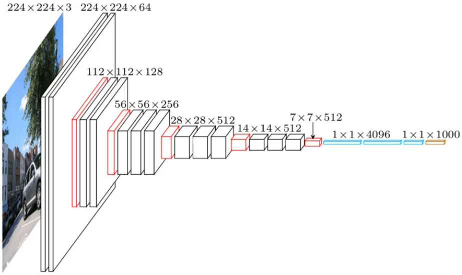

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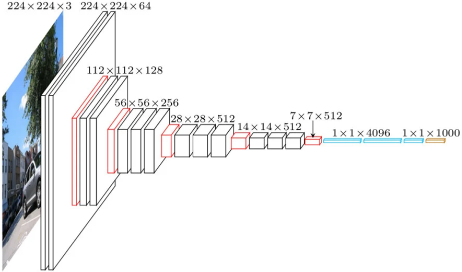

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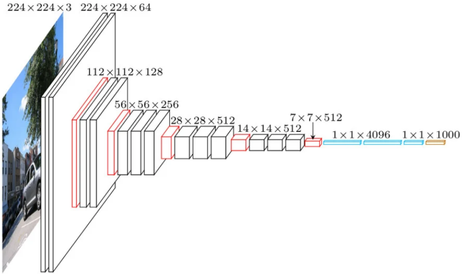

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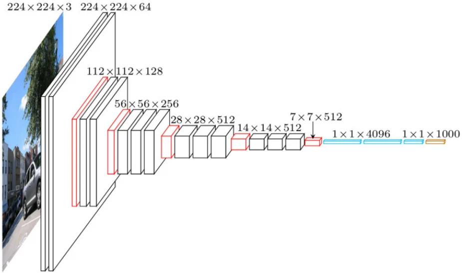

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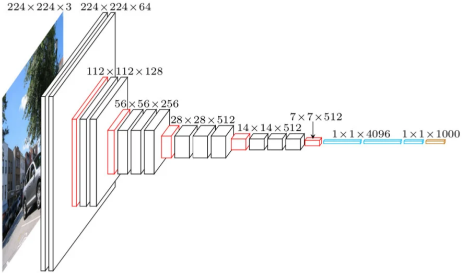

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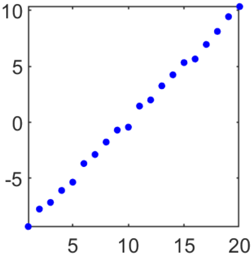
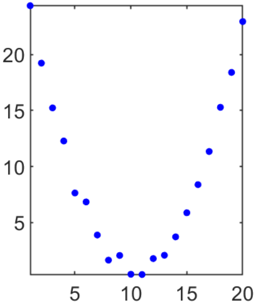
- ...which is done by minimizing a function called loss
- Minimization requires computing gradients, called backpropagation

Parametrized models

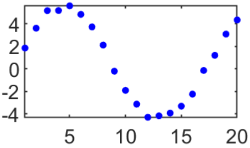
The parameters describe the behavior of the network, and must be solved for.



$$y = ax + b$$



$$y = ax^2 + bx + c$$



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

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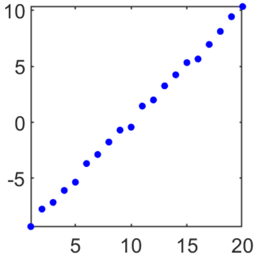

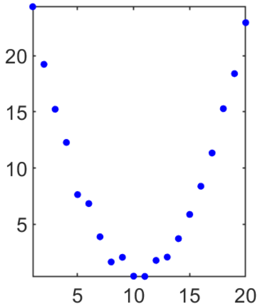

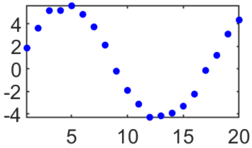

$$f_{a,b}(x) = ax + b$$

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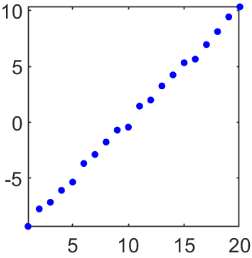
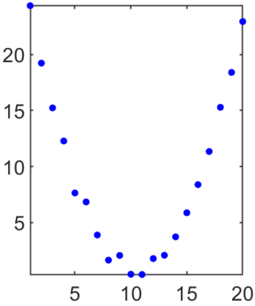
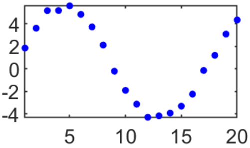






$f_{\Theta_f}(x)$
$\Theta_f \equiv \{a, b\}$

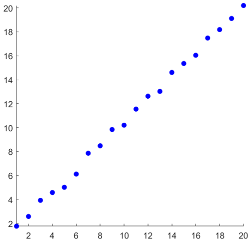
$g_{\Theta_g}(x)$

$h_{\Theta_h}(x)$

From a technical standpoint, our task is to determine the parameters Θ.

Linear regression

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



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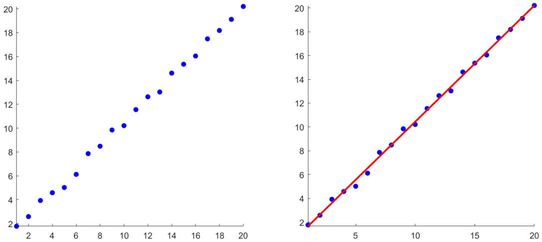

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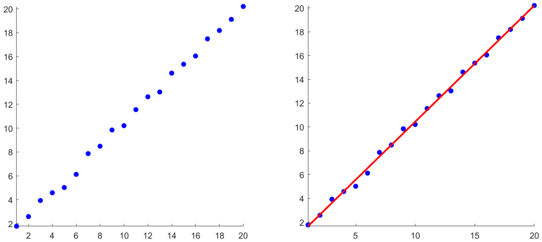

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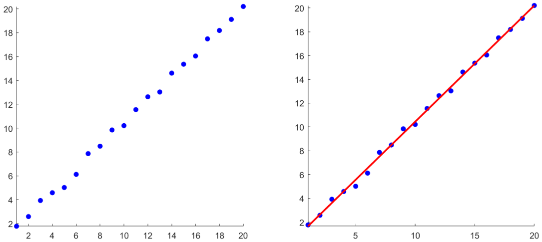

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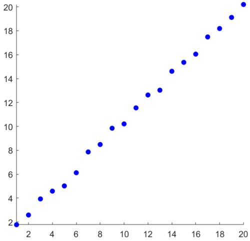

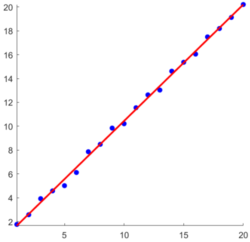

$$f_\Theta(x_i) = y_i$$

Model: linear + bias (we ignore the noise)

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

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

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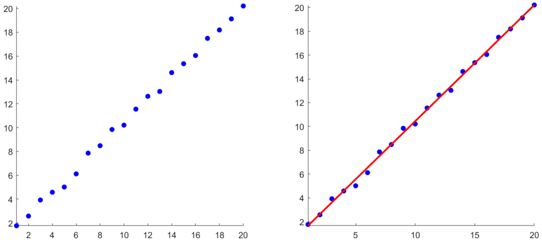

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Given a and b, we have a mapping that gives new output from new input.

Linear regression

The equations:

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Problem: Choose a and b minimizing 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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$$\epsilon = \min_\Theta \ell_\Theta(\{x_i, y_i\})$$

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

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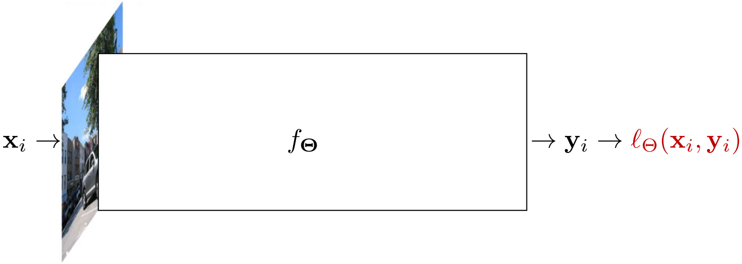
Remark: We minimize the loss w.r.t. the parameters Θ, and **not** w.r.t. the data (x_i, y_i). Also, the loss is defined on the entire dataset, not on just one data point.

Linear regression

We are considering the following case:



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

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We will mostly deal with unconstrained problems.

Convex functions

Jensen's inequality:

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for all x, y and $\alpha \in [0, 1]$

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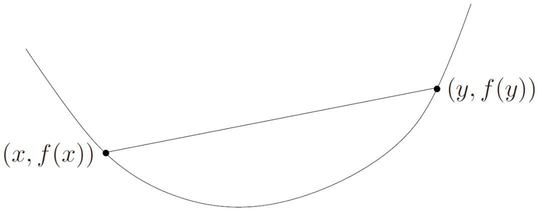

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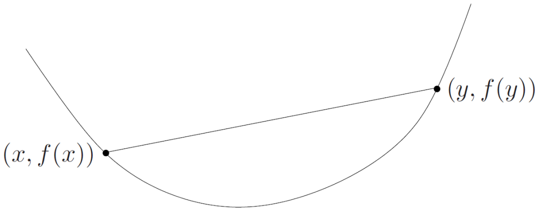

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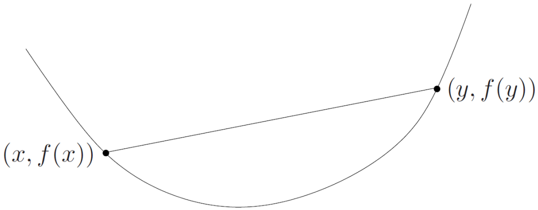

Let us further assume that f is a differentiable function, so that we can compute its derivative $\frac{df}{dx}$ at all points x.

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

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

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Convex functions: Global minima

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

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

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

Convex functions: Global minima

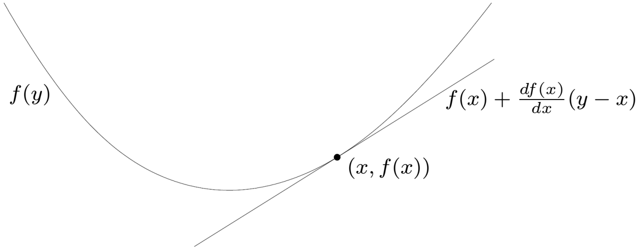
$$\lim_{\alpha \to 0} \frac{f(x + \alpha(y - x)) - f(x)}{\alpha(y - x)}(y - x) + f(x) \leq f(y)$$

Convex functions: Global minima

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

Convex functions: Global minima

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



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

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

and x is a global minimizer of f.

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

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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:

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

The gradient

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

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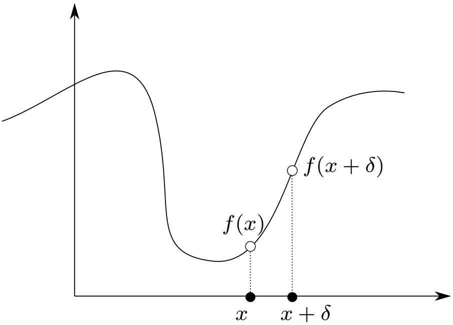

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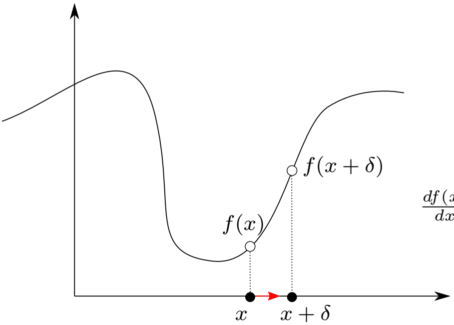

$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$

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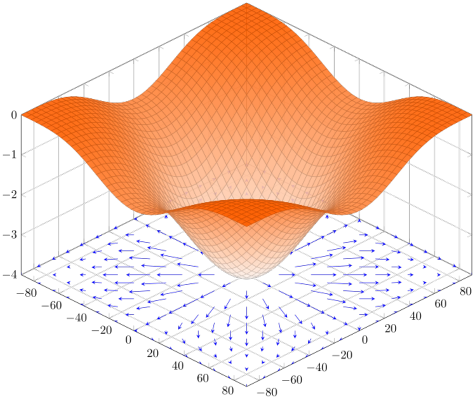

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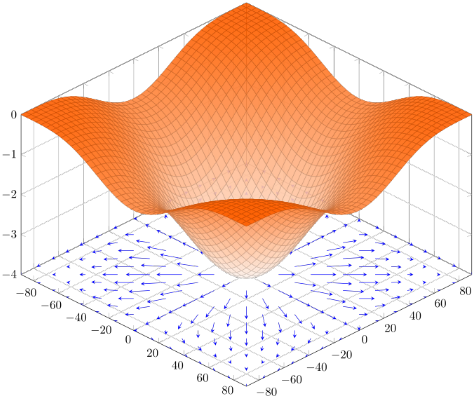
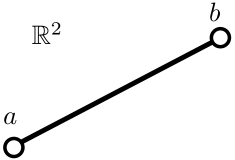


The length of the gradient vector encodes its strength.

Vector lengths

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



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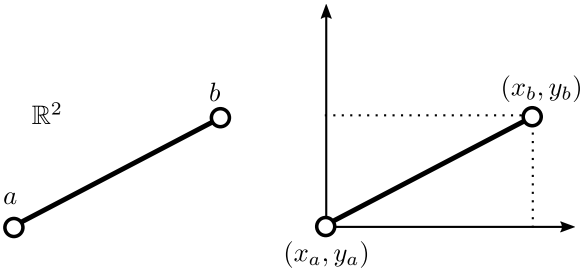

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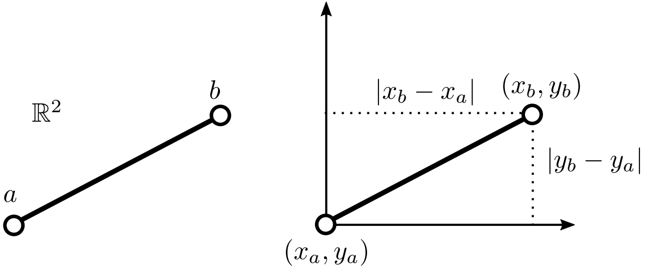

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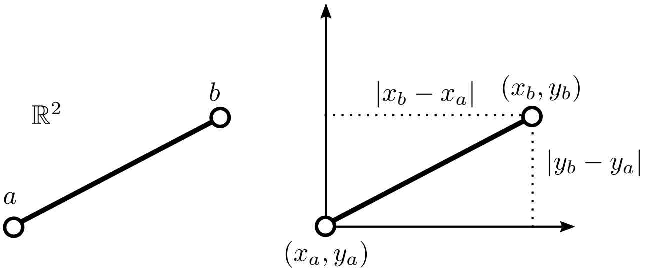

Apply Pythagoras' theorem: $d(a,b) = (|x_b - x_a|^2 + |y_b - y_a|^2)^{\frac{1}{2}}$

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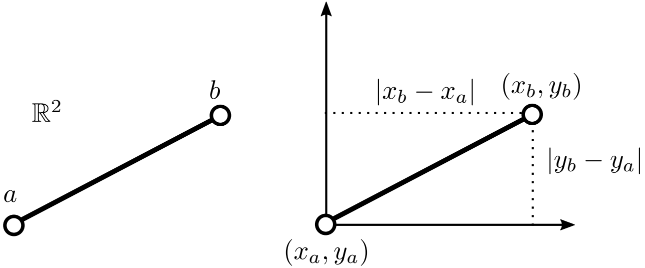

Apply Pythagoras' theorem: $d(a, b) = (|x_b - x_a|^2 + |y_b - y_a|^2)^{\frac{1}{2}}$

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

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

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

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

$$\Downarrow$$

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

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

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

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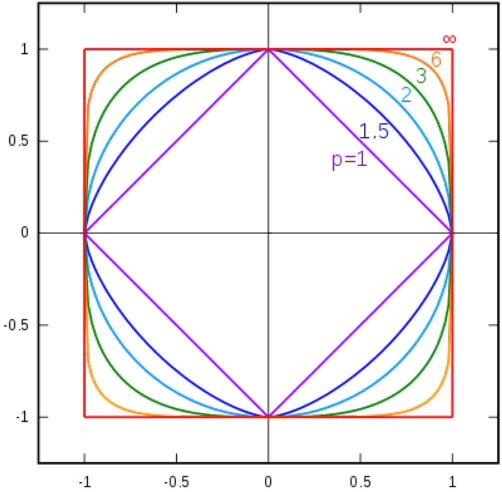
L_p unit balls in $\mathbb{R}^2$



Convex functions: Examples

So, for convex functions $f(\mathbf{x})$, a global minimizer $\mathbf{x}$ is found by setting:

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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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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, we can use 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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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.

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(if you need it: brief lecture on matrix manipulation tricks?)

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

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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:

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

what we did is **exactly equivalent** to the element-by-element computation of slide $\#16$, but we did it directly in matrix form.

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

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

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

Linear regression: Higher dimensions

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

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

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

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

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

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

Linear regression: Higher dimensions

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

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

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

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

The MSE reads:

$$\ell(\boldsymbol{\Theta}) = \|\mathbf{Y} - \mathbf{X}\boldsymbol{\Theta}\|_2^2 = \mathrm{tr}(\mathbf{Y}^\top\mathbf{Y}) - 2\mathrm{tr}(\mathbf{Y}^\top\mathbf{X}\boldsymbol{\Theta}) + \mathrm{tr}(\boldsymbol{\Theta}^\top\mathbf{X}^\top\mathbf{X}\boldsymbol{\Theta})$$

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

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

Wrap-up

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

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

This case can be solved in closed form.

Wrap-up

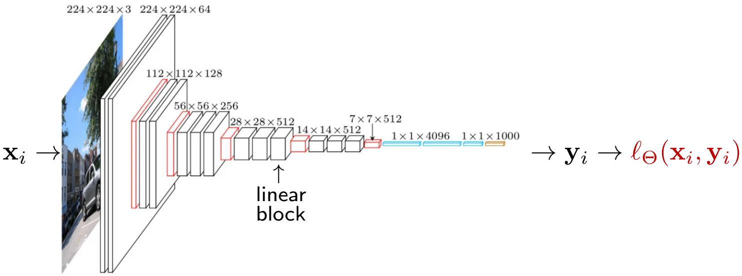
$$\mathbf{x}_i \rightarrow f_{\boldsymbol{\Theta}} \rightarrow \mathbf{y}_i \rightarrow \ell_{\Theta}(\mathbf{x}_i, \mathbf{y}_i)$$

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

This case can be solved in closed form.

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

Wrap-up



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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`