Deep Learning & Applied AI

Linear regression, convexity, and gradients

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SAPIENZA
Università di Roma

2nd semester a.y. 2019/2020 · March 04, 2020

A glimpse into neural networks

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

A glimpse into neural networks

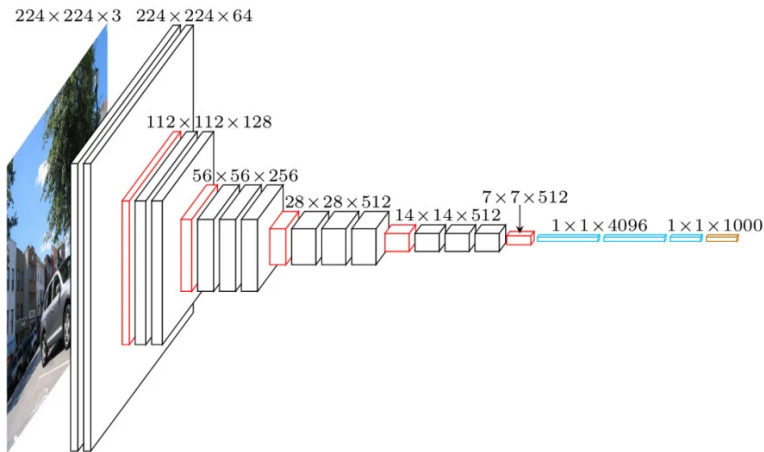In deep learning, we deal with highly parametrized models called deep neural networks:
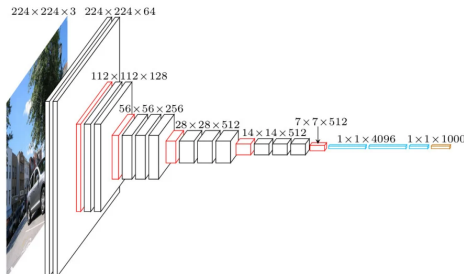

$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

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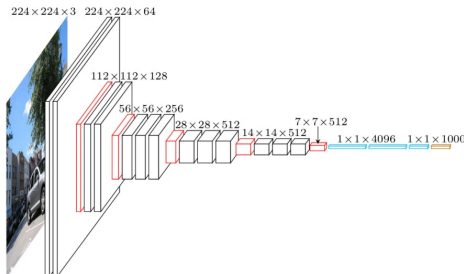
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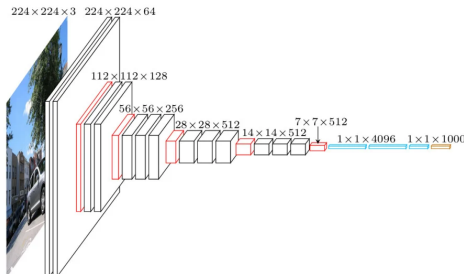
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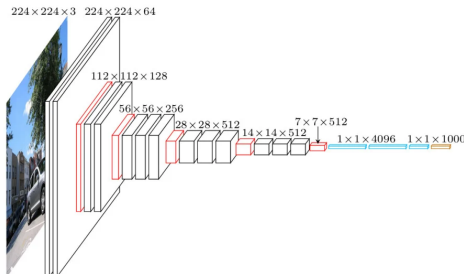- Finding the parameter values is called training...

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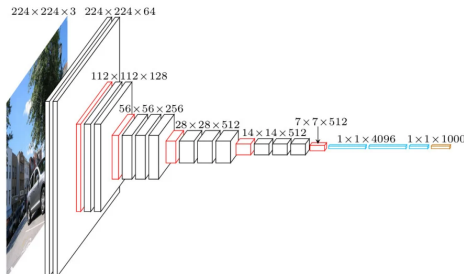- ...which is done by minimizing a function called loss

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- Finding the parameter values is called training...
- ...which is done by minimizing a function called loss
- Minimization requires computing gradients, called backpropagation
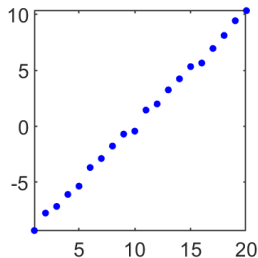
Parametrized models

The parameters describe the behavior of the network, and must be solved for.
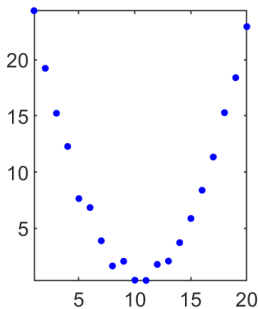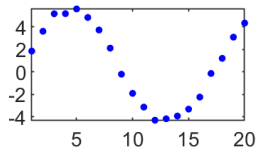
$$y = ax + b \qquad\qquad y = ax^2 + bx + c \qquad\qquad y = a\sin(x) + bx + c$$

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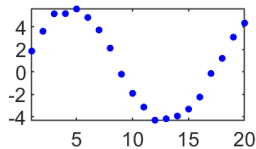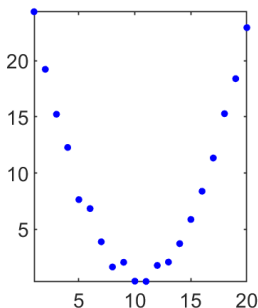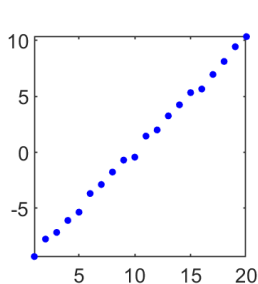
$$f_{a,b}(x) = ax + b$$

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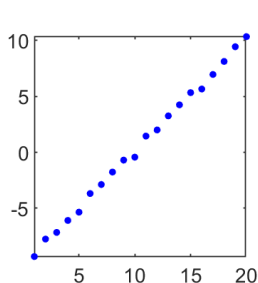
$$f_{\Theta_f}(x)$$
$$\Theta_f \equiv \{a, b\}$$
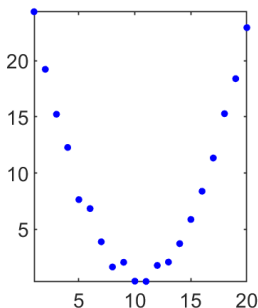
$$g_{\Theta_g}(x)$$
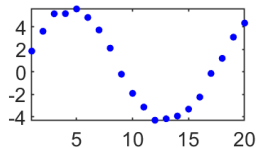
$$h_{\Theta_h}(x)$$

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:
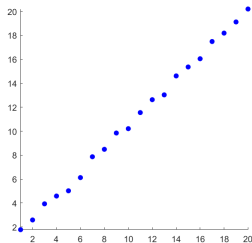
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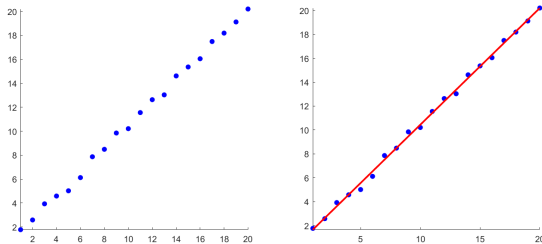
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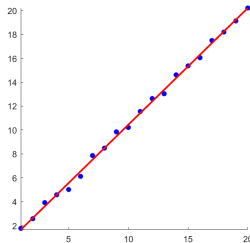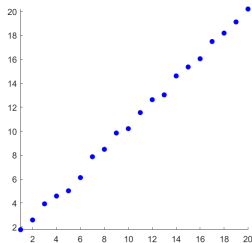
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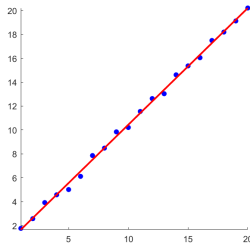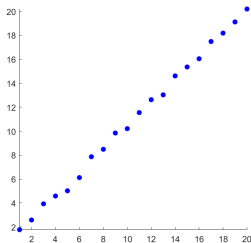
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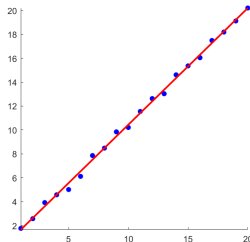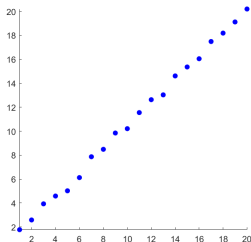
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Model: linear $+$ bias (we ignore the noise)

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

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

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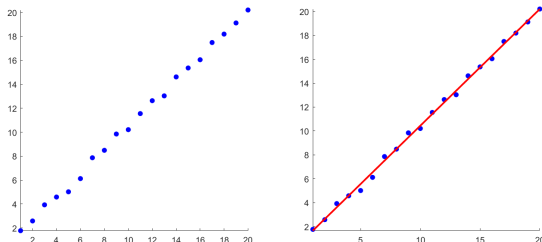
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Given a and b, we have a mapping that gives new output from new input.

Linear regression

The equations:

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

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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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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).

Linear regression

We are considering the following case:

$$\mathbf{x}_i \rightarrow \boxed{f_{\boldsymbol{\Theta}}} \rightarrow \mathbf{y}_i \rightarrow \ell_{\Theta}(\mathbf{x}_i, \mathbf{y}_i)$$
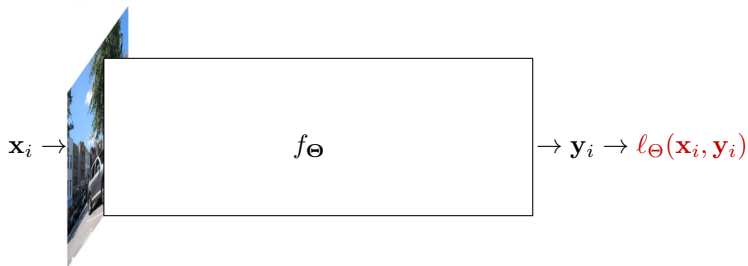
where $f_{\boldsymbol{\Theta}}$ is linear, and $\ell_{\boldsymbol{\Theta}}$ is quadratic.

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We need to solve the general minimization problem:

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

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

We will mostly deal with unconstrained problems.

Convex functions

Jensen's inequality:

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

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

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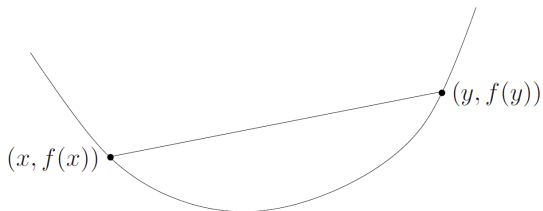
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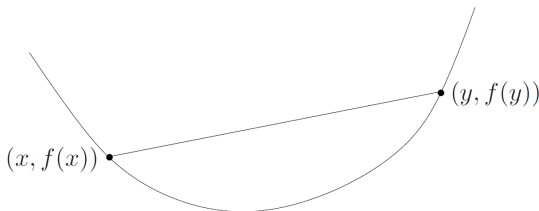
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Let us further assume that f is a differentiable function, so that we can compute its derivative $\frac{df}{dx}$ at all points x.

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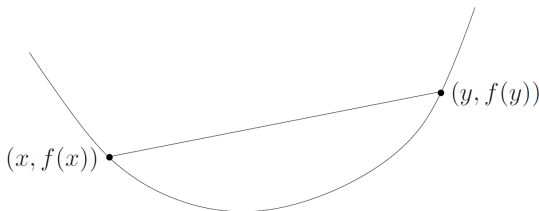
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Let us further assume that f is a differentiable function, so that we can compute its derivative $\frac{df}{dx}$ at all points x.

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

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

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

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

Convex functions: Global minima

$$\underbrace{\frac{df(x)}{dx}(y - x) + f(x)}_{\text{1st−order Taylor at } f(x)} \leq f(y)$$
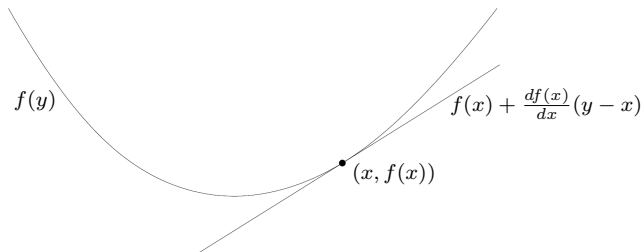
Thus, if $\frac{df(x)}{dx} = 0$:

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

and x is a global minimizer of f.

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

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

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Convexity is defined as before:

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

and we also have the global optimality condition:

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

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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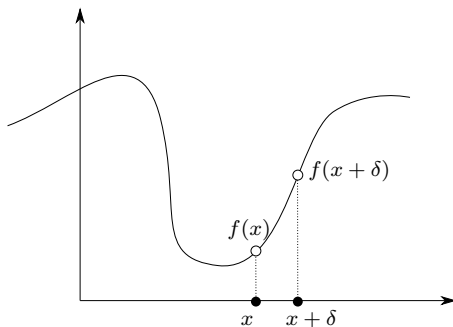
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$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$
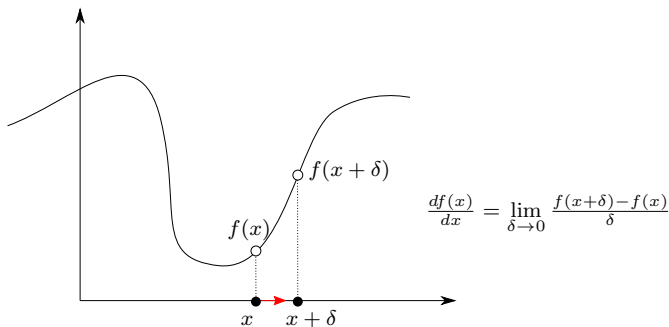
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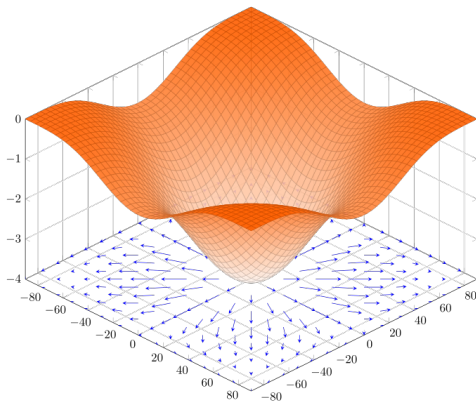
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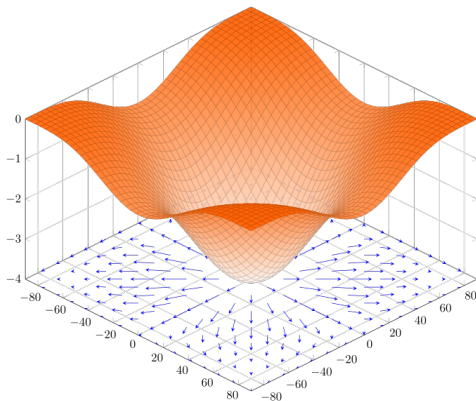
The length of the gradient vector encodes its strength.

Vector lengths

The Euclidean distance measures the length of a straight line connecting two points:
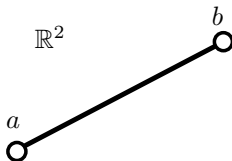
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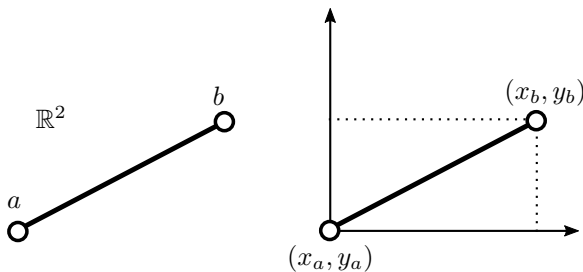
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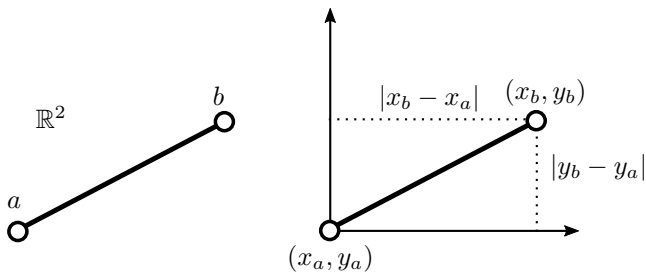
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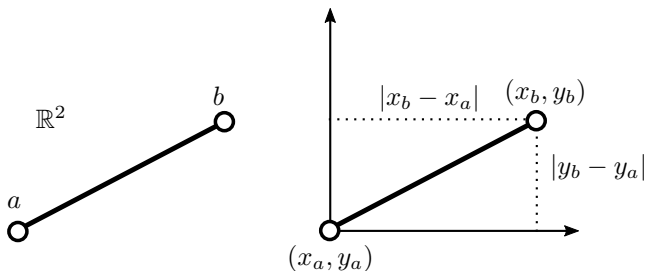
Apply Pythagoras' theorem: $d(a, b) = (|x_b - x_a|^2 + |y_b - y_a|^2)^{\frac{1}{2}}$

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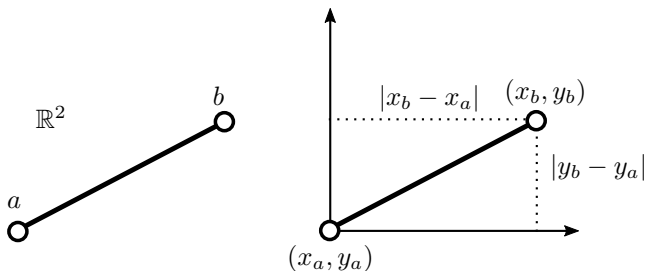
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In matrix notation:

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

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

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

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

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 $\mathbb{R}^k$:

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

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

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

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

L_p unit balls in $\mathbb{R}^2$
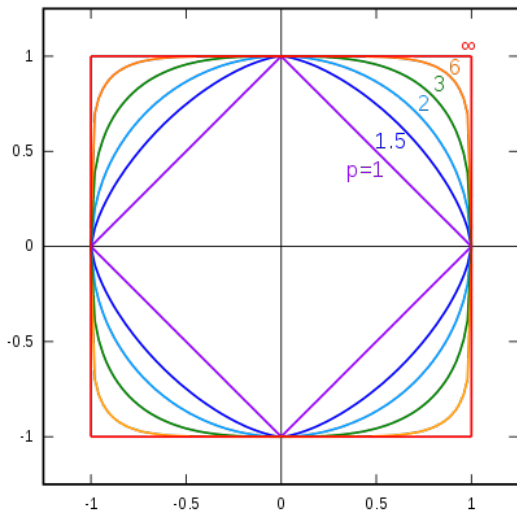
Convex functions: Examples

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

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Some convex functions appearing in deep learning (check convexity!):

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$$f(\alpha \mathbf{x} + (1-\alpha)\mathbf{y}) = \max_i \{\alpha x_i + (1-\alpha)y_i\}$$

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$$\begin{aligned} f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) &= \max_i\{\alpha x_i + (1-\alpha)y_i\} \\ &\leq \alpha \max_i\{x_i\} + (1-\alpha)\max_i\{y_i\} \end{aligned}$$

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&\leq \alpha \max_i \{x_i\} + (1-\alpha) \max_i \{y_i\} \\
&= \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y})
\end{aligned}$$

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:

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$$
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&= \sum_{i=1}^{n} \begin{pmatrix} 2ax_i^2 - 2x_i y_i + 2bx_i \\ 2b - 2y_i + 2ax_i \end{pmatrix}
\end{aligned}
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$$\nabla_\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, 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.

Familiarize with matrix calculus.

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

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:

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

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

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

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

We get a closed form solution to our problem.

A note on the gradient in matrix form

In the previous slide, for the differentiation step:

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

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

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

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

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

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

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

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

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

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

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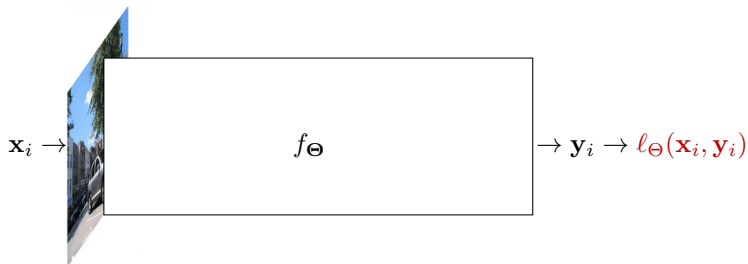
The MSE reads:

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

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

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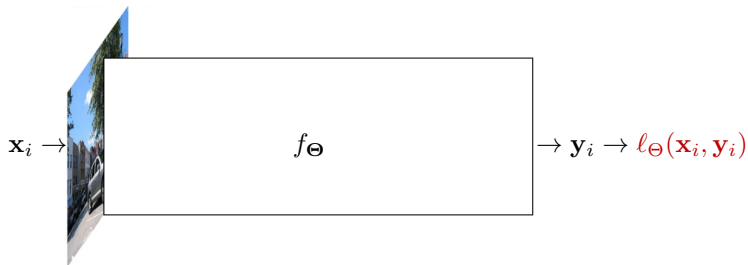
Wrap-up

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

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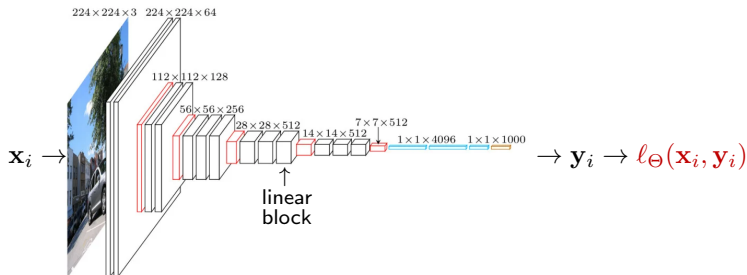
This case can be solved in closed form.

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.

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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.

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`