Lecture Notes: Basics of ML

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Contents

1	Intr	oduction	2
2	Supervised learning framework		2
	2.1	Regression setting	2
	2.2	Classification setting	2
A	Useful Formulas and Good Practices		
	A.1	Definitions and notations	3
	A.2	Gradients	3
	A.3	Linear Algebra	4
	A.4	Convexity	4
	A.5	Good practices and sanity checks	4

1 Introduction

Slides of the general introduction can be found here.

2 Supervised learning framework

- 2.1 Regression setting
- 2.2 Classification setting

A Useful Formulas and Good Practices

A.1 Definitions and notations

Keep in mind that these are the notations I like to use, but these are obviously personal and others will use different ones!!

- the notation x will always be used for input data. E.g. $x_1, \ldots, x_n \in \mathbb{R}^d$ could be some dataset. n is then the number of training samples, and d the dimension of each data point. Similarly, y will used for output data, e.g. $y_1, \ldots, y_n \in \mathbb{R}$ (or $\in \{0, 1\}$) are output data (or labels).
- $X = \begin{pmatrix} & x_1 & \\ & \vdots & \\ & x_n & \end{pmatrix} \in \mathbb{R}^{n \times d}$ corresponds to data / feature / design /observation matrix. It has $n = "number \ of \ samples"$ rows and $d = "dimension \ of \ datapoints"$ columns.
- $y = (y_1, \ldots, y_n) \in \mathbb{R}^n$ corresponds to the output vector.
- for a vector $u \in \mathbb{R}^d$, we let $||u||_2 := \sqrt{\sum_{i=1}^d u_i^2}$ denote the Euclidean norm of u (also called ℓ_2 -norm).
- for vectors $u, v \in \mathbb{R}^d$, we denote $\langle u, v \rangle := \sum_{i=1}^d u_i, v_i$ to be the inner product of u and v. Notice that $||u||^2 = \langle u, u \rangle$. Two vectors are said to be orthogonal if their inner product is null.
- for vectors x_1, \ldots, x_n , their span corresponds to the linear space which they generate: $\operatorname{span}(x_1, \ldots, x_n) \coloneqq \{\lambda_1 x_1 + \ldots, \lambda_n x_n, \text{ where } \lambda_1, \ldots, \lambda_n \in \mathbb{R}\}.$
- the rank of a matrix corresponds to the dimension of the span of its columns, which is equal to the dimension of the span of its rows. Therefore for $X \in \mathbb{R}^{n \times d}$, it holds that $\operatorname{rank}(X) \leq \min(n, d)$. A matrix is said to be full rank if $\operatorname{rank}(X) = \min(n, d)$.
- a matrix $A \in \mathbb{R}^{d \times d}$ is said to be symmetric if $A^{\top} = A$. It is said to be positive semi-definite (we write this as $A \succeq 0$) if for all vector $u \in \mathbb{R}^d$, $u^{\top}Au \geq 0$. This is equivalent to saying that all the eigenvalues of A are positive.
- the null space (sometimes called kernel) of a matrix $A \in \mathbb{R}^{n \times d}$ is defined as $Ker(A) = \{w \in \mathbb{R}^d, Aw = 0\}$.

A.2 Gradients

If $f: \mathbb{R}^d \to \mathbb{R}$ is twice differentiable, then its gradient $\nabla f: \mathbb{R}^d \to \mathbb{R}^d$ and hessian $\nabla^2 f: \mathbb{R}^d \to \mathbb{R}^{d \times d}$ are defined as:

$$\nabla f(w) = \left(\frac{\partial f}{\partial w_i}(w)\right)_{1 \le i \le d} \quad \nabla^2 f(w) = \left(\frac{\partial^2 f}{\partial w_i \partial w_i}(w)\right)_{1 \le i, j \le d}$$

- For a vector $b \in \mathbb{R}^d$, the gradient of the linear function $f : \mathbb{R}^d \to \mathbb{R}$, $f(w) = \langle a, w \rangle$ is equal to $\nabla f(w) = b$.
- For a (not necessarily symmetric) matrix $A \in \mathbb{R}^{d \times d}$, $f(w) = \frac{1}{2} w^{\top} A w$ is a quadratic function. Its gradient is $\nabla f(w) = \frac{1}{2} (A + A^{\top}) w$, which is equal to A w if and only if A is a symmetric matrix. The hessian of f is equal to $\nabla^2 f(w) = \frac{1}{2} (A + A^{\top})$.

A.3 Linear Algebra

- For a matrix $A \in \mathbb{R}^{d \times d}$, it holds that $w^{\top} A w = \sum_{i,j=1}^{d} w_i w_j A_{i,j}$.
- It holds that $X^{\top}X = \sum_{i=1}^{n} x_i x_i^{\top} \in \mathbb{R}^{d \times d}$ and $XX^{\top} = (\langle x_i, x_j \rangle)_{1 \leq i, j \leq n} \in \mathbb{R}^{n \times n}$.
- Let $L(w) = \frac{1}{2} \sum_{i=1}^{n} (y_i \langle w, x_i \rangle)^2$, then $L(w) = \frac{1}{2} ||y Xw||^2$ and $\nabla L(w) = X^{\top}(Xw y)$.
- if n < d ("underparametrised setting), then the matrix $X^{\top}X$ cannot be invertible, because $\operatorname{span}(x_1, \ldots, x_n)$ cannot be equal to \mathbb{R}^d . However, if $n \geq d$ and $\operatorname{span}(x_1, \ldots, x_n) = \mathbb{R}^d$, then $X^{\top}X$ is invertible.
- Rank-nullity theorem: for $A \in \mathbb{R}^{d \times n}$, it holds that $\operatorname{rank}(A) + \dim \operatorname{Ker}(A) = d$.

A.4 Convexity

A function $f: \mathbb{R}^d \to \mathbb{R}$ is said to be convex if for all $w_1, w_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$, $f(\lambda w_1 + (1 - \lambda)w_2) \le \lambda f(w_1) + (1 - \lambda)f(w_2)$ (DO A DRAWING TO VISUALISE THIS!).

- if f is convex and differentiable, then for all $w_1, w_2 \in \mathbb{R}^d$, it holds that $f(w_2) \ge f(w_1) + \langle \nabla f(w_1), w_2 w_1 \rangle$ (DO A DRAWING TO VISUALISE THIS!).
- if f is convex, then all local minima are global. Therefore, if $\nabla f(w^*) = 0$, then w^* is a global minimum. However, keep in mind that there exist convex functions which do not have any minima! (the exponential function for example)

A.5 Good practices and sanity checks

Math sanity checks Always check that the math makes sense!

- If $f: \mathbb{R}^d \to \mathbb{R}$, then for a vector $w \in \mathbb{R}^d$, $\nabla f(w)$ must belong to \mathbb{R}^d ! So for example if $f(w) = \frac{1}{2} ||x||^2$, then writing that " $\nabla f(w) = ||x||$ " doesn't make sense.
- Check that the matrix operations are allowed: if $L(w) = ||y Xw||^2$, writing that $||\nabla L(w)|| = X(Xw y)||$ doesn't make sense because the operations XX and Xy don't make sense for $n \neq d$ (and also because of the remark right above).

Dimensional sanity check. Even if an expression is mathematically well-formed, it might be meaningless from the point of view of "units" or "dimensions." A quick check is to make sure your formulas are *homogeneous*: every term you add or compare should have the same "type."

Example. Suppose our data are temperature observations y_i measured in degrees Celsius. A feature vector $x \in \mathbb{R}^d$ could represent input quantities such as:

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x = ([altitude in meters], [pressure in pascals], [wind speed in meters per second]).
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A parameter vector $w \in \mathbb{R}^d$ scales each feature so that the inner product $\langle w, x \rangle$ has the same unit as y (degrees Celsius). In our small example the units of w are

$$([^{\circ}C] \cdot [meters]^{-1}, [^{\circ}C] \cdot [pascals]^{-1}, [^{\circ}C] \cdot [meters]^{-1} \cdot [seconds])$$

Now notice that:

- $\langle w, x \rangle$ makes sense: each coordinate of w carries the reciprocal unit of the corresponding coordinate of x, so the sum yields something in degrees Celsius.
- w + x does not make sense: w and x do not have the same units (adding "degrees per meter" to "meters" is meaningless).