Theory of Statistical Learning
Part II

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Outline

1. Linear predictors
   Linear classification
   Linear regression
   Ridge regression
   Polynomial regression
   Logistic regression

2. Tree-based classifiers
   Partition rules
   Random forests

3. Boosting

1. Linear predictors

1.1. Linear classification

Linear functions

- $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \mathbb{R}$
- thus $x_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,d})^\top$
- we consider no bias term (otherwise *affine*):

$$\left\{h : x \mapsto w^\top x, w \in \mathbb{R}^d\right\} .$$

- **Reminder:** given two vectors $u, v \in \mathbb{R}^d$,

$$\langle u, v \rangle = u^\top v = \sum_{j=1}^{d} u_i v_i .$$

- binary classification: 0-1 loss, $\mathcal{Y} = \{-1, +1\}$
- **Important:** compose h with $\phi : \mathbb{R} \to \mathcal{Y}$ (typically the sign)

The sign function

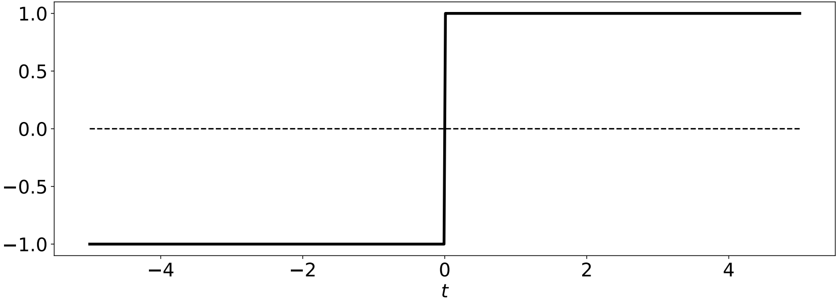


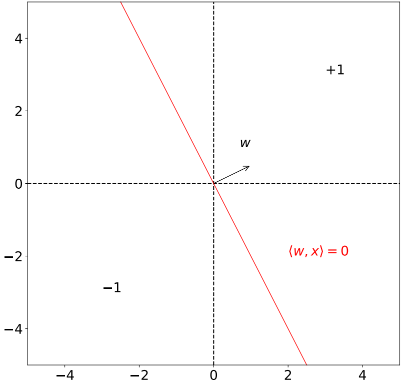
Figure: the sign function

Halfspaces

- thus our function class is

$$\mathcal{H} = \{x \mapsto \operatorname{sign}\left(w^\top x\right), w \in \mathbb{R}^d\}.$$

- gives label $+1$ to vector pointing in the same direction as w



VC dimension of halfspaces

Proposition: the VC dimension of halfspaces in dimension d is exactly $d + 1$.

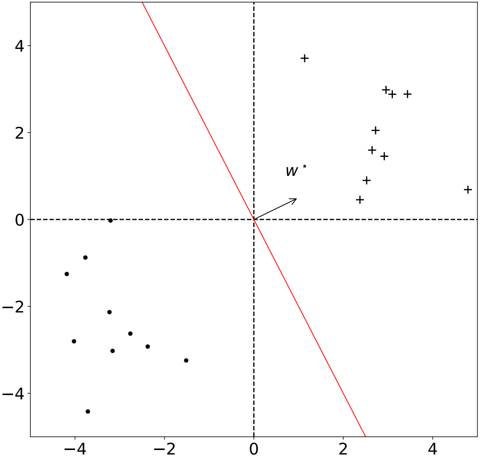
- **Consequence:** $\mathcal{H}$ is PAC learnable with sample complexity

$$\Omega\left(\frac{d + \log(1/\delta)}{\varepsilon}\right) .$$

Linearly separable data

- **Important assumption:** data is linearly separable
- that is, there is a $w^\star \in \mathbb{R}^d$ such that

$$y_i = \mathrm{sign}\left(\langle w^\star, x_i \rangle\right) \quad \forall 1 \leq i \leq n\,.$$



Linear programming

- **Empirical risk minimization:** recall that we are looking for w such that
$$\hat{\mathcal{R}}_S(w) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{y_i \neq \mathrm{sign}(w^\top x_i)}$$
is minimal
- **Question:** how to solve this?
- we want $y_i = \mathrm{sign}\left(w^\top x_i\right)$ for all $1 \leq i \leq n$
- equivalent formulation: $y_i \langle w, x_i \rangle > 0$
- we know that there is a vector that satisfies this condition $(w^\star)$
- let us set $\gamma = \min_i \{y_i \langle w^\star, x_i \rangle\}$ and $\overline{w} = w^\star / \gamma$
- we have shown that there is a vector such that $y_i \langle \overline{w}, x_i \rangle \geq 1$ for any $1 \leq i \leq n$ (and it is an ERM)

Linear programming, ctd.

- define the matrix $A \in \mathbb{R}^{n \times d}$ such that

$$A_{i,j} = y_i x_{i,j} \,.$$

- **Intuition:** observations $\times$ labels
- remember that we have the ± 1 label convention
- define $v = (1, \ldots, 1)^\top \in \mathbb{R}^n$
- then we can rewrite the above problem as

$$\text{maximize} \quad \langle u, w \rangle \text{ subject to } Aw \leq v \,,$$

  with $u = 0$ for instance
- we call this sort of problems **linear programs**[1]
- solvers readily available, e.g., `scipy.optimize.linprog` if you use Python

[1] Boyd, Vandenberghe, *Convex optimization*, Cambridge University Press, 2004

The perceptron

- another possibility: the *perceptron*[2]
- **Idea:** iterative algorithm that constructs $w^{(1)}, w^{(2)}, \dots, w^{(T)}$
- update rule: at each step, find i that is misclassified and set

$$w^{(t+1)} = w^{(t)} + y_i x_i \,.$$

- **Question:** why does it work?
- pushes w in the right direction:

$$y_i \langle w^{(t+1)}, x_i \rangle = y_i \langle w^{(t)} + y_i x_i, x_i \rangle = y_i \langle w^{(t)}, x_i \rangle + \|x_i\|^2$$

- remember, we want $y_i \langle w, x_i \rangle > 0$ for all i

[2] Rosenblatt, *The perceptron, a perceiving and recognizing automaton*, tech report, 1957

1.2. Linear regression

Least squares

- regression $\Rightarrow$ squared-loss function

$$\ell(y, y') = (y - y')^2 \,.$$

- still looking at linear functions:

$$\mathcal{H} = \{h : x \mapsto \langle w, x \rangle \text{ s.t. } w \in \mathbb{R}^d\} \,.$$

- empirical risk in this context:

$$\hat{\mathcal{R}}_S(h) = \frac{1}{n} \sum_{i=1}^{n} (w^\top x_i - y_i)^2 = F(w) \,.$$

- also called **mean squared error**
- empirical risk minimization: we want to minimize $w \mapsto F(w)$ with respect to $w \in \mathbb{R}^d$
- F is a convex, smooth function

Least squares, ctd.

- let us compute the gradient of F:

$$\begin{aligned}
\frac{\partial F}{\partial w_j}(w) &= \frac{1}{n}\sum_{i=1}^{n} \frac{\partial}{\partial w_j}(w^\top x_i - y_i)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n} 2\frac{\partial}{\partial w_j} w^\top x_i (w^\top x_i - y_i) \\
\frac{\partial F}{\partial w_j}(w) &= \frac{2}{n}\sum_{i=1}^{n}(w^\top x_i - y_i) x_{i,j}\,.
\end{aligned}$$

Least squares, ctd.

- we can rewrite it, define

$$A = X^\top X = \sum_{i=1}^{n} x_i x_i^\top \in \mathbb{R}^{d \times d} \text{ and } b = \sum_{i=1}^{n} y_i x_i \in \mathbb{R}\,,$$

then solving $\nabla F(w) = 0$ is equivalent to

$$Aw = b\,.$$

- if A is invertible, straightforward:

$$\boxed{\hat{w} = A^{-1} b}$$

- computational cost: $\mathcal{O}\left(d^3\right)$ (inversion is actually a bit less)
- what happens when A is not invertible?

Singular value decomposition

- since A is symmetric, it has an eigendecomposition

$$A = VDV^\top ,$$

  with $D \in \mathbb{R}^d$ diagonal and V orthonormal
- define D^+ such that

$$D^+_{i,i} = 0 \text{ if } D_{i,i} = 0 \text{ and } D^+_{i,i} = \frac{1}{D_{i,i}} \text{ otherwise.}$$

- define $A^+ = VD^+V^\top$
- then we set

$$\boxed{\hat{w} = A^+ b\,.}$$

Singular value decomposition, ctd.

- why did we do that?
- let v_i denote the ith column of V, then

$$
\begin{aligned}
A\hat{w} &= AA^{+}b && \text{(definition of } \hat{w}\text{)} \\
&= VDV^{\top}VD^{+}V^{\top}b && \text{(definition of } A^{+}\text{)} \\
&= VDD^{+}V^{\top}b && \text{(}V\text{ is orthonormal)} \\
A\hat{w} &= \sum_{i:D_{i,i}\neq 0} v_i v_i^{\top} b\,.
\end{aligned}
$$

- in definitive, $A\hat{w}$ is the projection of b onto the span of v_i such that $D_{i,i} \neq 0$
- since the span of these v_i is the span of the x_i and b is in the linear span of the x_i, we have $A\hat{w} = b$
- cost of SVD: $\mathcal{O}\left(dn^2\right)$ if $d > n$ (SVD of X)

Exercise

Exercise: Of course, one does not have to use the squared loss. Instead, we may prefer to use

$$\ell(y, y') = |y - y'| \ .$$

1. show that, for any $c \in \mathbb{R}$,

$$|c| = \min_{a \geq 0} a \quad \text{subject to} \quad a \geq c \text{ and } a \geq -c \, .$$

2. use the previous question to show that ERM with the absolute value loss function is equivalent to minimizing the linear function $\sum_{i=1}^{n} s_i$, where the s_i satisfy linear constraints
3. write it in matrix form, that is, find $A \in \mathbb{R}^{2n\times(n+d)}$, $v \in \mathbb{R}^{d+n}$, and $b \in \mathbb{R}^{2n}$ such that the LP can be written

$$\text{minimize } c^\top v \quad \text{subject to} \quad Av \leq b \, .$$

Correction of the exercise

1. The absolute value is the smallest positive number larger than both c and $-c$ for any real number c.
2. In that case, the empirical risk can be written

$$\hat{\mathcal{R}}_S(w) = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - w^\top x_i\right| \,.$$

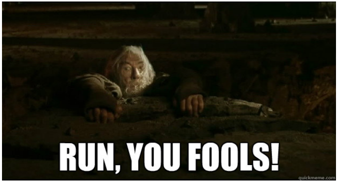
We deduce the result from question 1.
3. One possibility is to define $v = (w_1, \ldots, w_d, s_1, \ldots, s_n)^\top \in \mathbb{R}^{n+d}$, $c = (0, \ldots, 0, 1, \ldots, 1)^\top \in \mathbb{R}^{d+n}$, $b = (y_1, \ldots, y_n, -y_1, \ldots, -y_n)^\top \in \mathbb{R}^{2n}$, and

$$A = \begin{pmatrix} -X & -I_n \\ X & -I_n \end{pmatrix} \in \mathbb{R}^{2n\times(n+d)}\,,$$

with $X \in \mathbb{R}^{n\times d}$ the matrix whose lines are the x_is and I_n the identity matrix.

Recap

- **What happens when we invoke** `sklearn.linear_model.LinearRegression` with default parameters?
- `fit_intercept` is True $\rightarrow$ assumes that the data is not centered (our maths are not totally accurate)
- `normalize` is False $\rightarrow$ we are responsible for the normalization of our data
- behind the scenes, calls `scipy.linalg.lstsq` when fitting, which itself calls LAPACK (Linear Algebra PACKage)[3]
- LAPACK is coded in Fortran90



[3] `http://www.netlib.org/lapack/`

1.3. Ridge regression

Ridge regression

- same hypothesis class: linear functions

$$\mathcal{H} = \{h : x \mapsto w^\top x, w \in \mathbb{R}^d\}$$

- squared loss:

$$\ell(y, y') = (y - y')^2 \,.$$

- **Idea:** regularization:

$$\text{minimize} \left\{ \frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \lambda \left\| w \right\|^2 \right\},$$

with $\left\| u \right\|^2 = u_1^2 + \cdots + u_d^2$ and $\lambda > 0$ a *regularization parameter*

Exercise

Exercise: Let $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$ be n given training samples. For any $w \in \mathbb{R}^d$, set

$$F(w) = \frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \lambda \|w\|^2 .$$

Notice that F is a convex smooth function. Find its minimizer $\hat{w}$ in closed-form. Recall that we defined

$$A = \sum_{i=1}^{n} x_i x_i^\top \quad \text{and} \quad b = \sum_{i=1}^{n} y_i x_i .$$