

Lecture II: Linear regression and classification. Loss functions

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Linear predictors generalities

Loss functions

Least squares linear regression

Linear regression as minimizing L_{LS}

Linear regression as maximizing likelihood

Linear Classifiers

Linear Discriminant Analysis (LDA)

OPTIONAL – QDA (Quadratic Discriminant Analysis)

Logistic Regression

OPTIONAL – The PERCEPTRON algorithm

Reading HTF Ch.: 2.1–5, 2.9, 7.1–4 bias-variance tradeoff, Murphy Ch.: 1., 8.6¹, Bach Ch.:

¹Neither textbook is close to these notes except in a few places; take them as alternative perspectives or related reading

Linear predictors

- ▶ Linear predictors for regression

$$f(x) = \beta^T x \quad (1)$$

where $Y \in \mathbb{R}$, $X \in \mathbb{R}^d$ and $\beta \in \mathbb{R}^d$ is a **vector of parameters**.

Hence, the **model class** is $\mathcal{F} = \{\beta \in \mathbb{R}^d\}$ the set of all linear functions over \mathbb{R}^d .

- ▶ Linear predictors for classification

$$\hat{y}(x) = \text{sgn}(\beta^T x) \quad (2)$$

i.e. **the decision boundary is linear**

Transforming categorical inputs into real values

- ▶ if X_j takes two values (e.g. “yes”, “no”), map it to $\{\pm 1\}$ or $\{0, 1\} \subset \mathbb{R}$.
- ▶ **discrete multivariate inputs**
 - ▶ Let X_j take values in $\Omega_j = \{0, \dots, r-1\}$.
 - ▶ One defines the $r-1$ binary variables $\tilde{X}_{jk} = \mathbf{1}_{\lfloor X_j = k \rfloor}$, $k = 1 : r-1$. The variable X_j is replaced with \tilde{X}_{jk} , $k = 1 : r-1$
 - ▶ the parameter β_j with $r-1$ parameters $\beta_{j1} \dots \beta_{jr-1}$, $r-1$ representing the coefficients of $\tilde{X}_{j1}, \dots, \tilde{X}_{jr-1}$.

This substitution is widely used to parametrize any function of a discrete variable as a linear function

Example: The demographic variable Race takes values in $\{\text{African, Asian, Caucasian, } \dots\}$; the corresponding parameters in the model will be $\hat{\beta}_{\text{Asian}}, \hat{\beta}_{\text{Caucasian}}, \dots$

The intercept as a slope

- Sometimes we like f to have an **intercept** $f(x) = \beta^T x + \beta_0$, with $x, \beta \in \mathbb{R}^d$. Such a function is **affine**, not linear, and not **homogeneous**. Here is a trick to get the best of both worlds.
- Add a dummy input $x_0 \equiv 1$ to x . Then its coefficient β_0 is the intercept.

$$\tilde{x} \leftarrow \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_d \end{bmatrix} \in \mathbb{R}^{d+1} \quad \tilde{\beta} \leftarrow \begin{bmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_d \end{bmatrix} \in \mathbb{R}^{d+1} \quad f(x) = \tilde{\beta}^T \tilde{x} \quad (3)$$

- in classification, β_0 is called **threshold** or **bias term**

The linear predictor as classifier

The linear predictor can be used for [binary] classification with the sign trick from Lecture I.

$$f(x) = \text{sgn} \beta^T x \quad (4)$$

Later in the course we will see a natural way to use real-valued predictors for multi-way classification.

What is the meaning of the β parameter for (4)?

In the following lectures we will see three possible “interpretations” for β , which correspond three different ways to construct a linear classifier for a problem.

How good is a regressor? Measuring the "Error"

- ▶ Prediction error for y^i : $e^i = y^i - f(x^i)$
- ▶ "Error" of f on \mathcal{D}
 - ▶ "Err" = $\frac{1}{n} \sum_{i=1}^n e^i$ **X**
 - ▶ "Err" = $\frac{1}{n} \sum_{i=1}^n |e^i|$?
 - ▶ ... norms!
- ▶ Let $\mathbf{e} = [e^1 \ e^2 \ \dots \ e^n]$.
- ▶ \mathbf{e} is a vector in \mathbb{R}^n . $\frac{1}{n} \sum_{i=1}^n |e^i| = \frac{1}{n} \|\mathbf{e}\|_1$
- ▶ But we can use other norms, e.g. $\frac{1}{n} \|\mathbf{e}\|_2$, $\frac{1}{n} \|\mathbf{e}\|_\infty$.

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- ▶ But we can use other norms, e.g. $\frac{1}{n} \|\mathbf{e}\|_2$, $\frac{1}{n} \|\mathbf{e}\|_\infty$.
- ▶ Formally, "Err" as above is called **loss** function.

Loss functions

The **loss function** represents the cost of error in a prediction problem. We denote it by L , where

$L(y, \hat{y})$ = the cost of predicting \hat{y} when the actual outcome is y

As usually $\hat{y} = f(x)$ or $\text{sgn}f(x)$, we will typically abuse notation and write $L(y, f(x))$.

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► For **Regression**

► **Least-Squares** L_2 Loss $L_{LS}(y, f(x)) = \frac{1}{n} \|e\|_2^2$

► L_1 Loss $L_{LS}(y, f(x)) = \frac{1}{n} \|e\|_1$

► **Statistical losses...**

► For **Classification**

► **Misclassification Error (0-1 Loss)** $L_{01} = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{[y^i \neq \hat{y}^i]}$

► **Statistical losses...**

Loss functions for classification

For classification, a natural loss function is the **misclassification error** (also called **0-1 loss**)

$$L_{01}(y, f(x)) = \mathbf{1}_{[y \neq f(x)]} = \begin{cases} 1 & \text{if } y \neq f(x) \\ 0 & \text{if } y = f(x) \end{cases} \quad (5)$$

Sometimes different errors have different costs. For instance, classifying a HIV+ patient as negative (a **false negative** error) incurs a much higher cost than classifying a normal patient as HIV+ (**false positive** error). This is expressed by **asymmetric misclassification costs**. For instance, assume that a false positive has cost one and a false negative has cost 100. We can express this in the matrix

$f(x) :$	+	-
true : +	0	100
-	1	0

In general, when there are p classes, the matrix $L = [L_{kl}]$ defines the loss, with L_{kl} being the cost of misclassifying as l an example whose true class is k .

Training set loss and expected loss

- ▶ **Training set loss**
- ▶ **Objective of prediction** = to minimize loss on future data,

$$\text{minimize } L(f) = E_{P(X,Y)}[L(Y, f(X))] \text{ over } f \in \mathcal{F} \quad (6)$$

We call $L(f)$ above **expected loss**.

Example (Misclassification error $L_{01}(f)$)

$L_{01}(f)$ = probability of making an error on future data.

$$L_{01}(f) = P[Yf(X) < 0] = E_{P_{XY}}[\mathbf{1}_{[Yf(X) < 0]}] \quad (7)$$

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We call $L(f)$ above **expected loss**.

- ▶ $L(f)$ cannot be minimized or even computed directly, because we don't know the data distribution P_{XY} .
- ▶ Therefore, in **training** we use the **traing set** loss.
- ▶ ... we approximate data distribution P_{XY} by the sample \mathcal{D} .
- ▶ The **empirical loss** (or **empirical error** or **training error**) is the average loss on \mathcal{D}

$$\hat{L}(f) = \frac{1}{n} \sum_{i=1}^n 1_{[y^i f(x^i) < 0]} \quad (7)$$

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$$\hat{L}(f) = \frac{1}{n} \sum_{i=1}^n 1_{[y^i f(x^i) < 0]} \quad (7)$$

- ▶ And we approximate $L(f)$ the expected loss by a **different** data set $\mathcal{D}^{\text{test}}$ from the same P_{XY} .
- ▶ The size of $\mathcal{D}^{\text{test}}$ is n' , not necessarily equal to n .

- ▶ Problem: how to learn a linear predictor from data?
- ▶ Now: examples of what one can do
- ▶ Later lectures: larger view of the estimation problem for predictors

(Linear) least squares regression

- define **data matrix** or (transpose) **design matrix**

$$\mathbf{X} = \begin{bmatrix} (x^1)^T \\ (x^2)^T \\ \vdots \\ (x^i)^T \\ \vdots \\ (x^n)^T \end{bmatrix} \in \mathbb{R}^{N \times n} \quad \text{and} \quad \mathbf{Y} = \begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^n \end{bmatrix}, \quad \mathbf{E} = \begin{bmatrix} \varepsilon^1 \\ \varepsilon^2 \\ \vdots \\ \varepsilon^d \end{bmatrix} \in \mathbb{R}^d$$

- Then we can write

$$\mathbf{Y} = \mathbf{X}\beta + \mathbf{E}$$

- The solution $\hat{\beta}$ is chosen to minimize the sum of the squared errors $\sum_{i=1}^d (\varepsilon^i)^2 = \sum_{i=1}^d (y^i - \beta^T x^i)^2 = \|\mathbf{E}\|^2$

$$\hat{\beta} = \underset{\beta \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^d (y^i - \beta^T x_i)^2$$

- This **optimization** problem is called a **least squares** problem. Its solution is

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \tag{8}$$

- Underlying statistical model $y = \beta^T x + \varepsilon$, $\varepsilon \sim N(0, \sigma^2)$ (and i.i.d. sampling of $(x^{1:N}, y^{1:N})$ of course).

Then $\hat{\beta}$ from (8) is the **Maximum Likelihood** (ML) estimator of the parameter β .

The statistical view of Machine Learning: Likelihood

The statistical view of Machine Learning: Likelihood

- What is random? **the noise** $\epsilon^{1:n}$
- Express noise as function of $(x^{1:n}, y^{1:n})$

$$\epsilon^i = y^i - \beta_0 - \beta^T x^i \sim N(0, \sigma^2) \quad (9)$$

- Likelihood

- Let $p_{0, \sigma^2}(\epsilon) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{\epsilon^2}{2\sigma^2}} = N(\epsilon; 0, \sigma^2)$

- Then

$$L(\beta_0, \beta_{1:d}, \sigma^2) = \prod_{i=1}^n p_{0, \sigma^2}(\epsilon^i) \quad (10)$$

$$= \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\epsilon^i)^2}{2\sigma^2}} \quad (11)$$

$$= \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(y^i - \beta_0 - \beta^T x^i)^2}{2\sigma^2}} \quad (12)$$

- **log-likelihood**

$$l(\beta_0, \beta_{1:d}, \sigma^2) = \quad (13)$$

$$= \sum_{i=1}^n \left\{ -\frac{1}{2} \ln \sigma^2 - \frac{1}{2} \ln(2\pi) - \frac{1}{2} (y^i - \beta_0 - \beta^T x^i)^2 \frac{1}{2\sigma^2} \right\} \quad (14)$$

$$= -\frac{n}{2} \ln \sigma^2 - \frac{1}{2} \ln(2\pi) - \text{constant} - \frac{1}{2} \sum_{i=1}^n (y^i - \beta_0 - \beta^T x^i)^2 \quad (15)$$

Maximizing the log-likelihood w.r.t β

- For simplicity, let $\beta_0 = 0$; hence $y^i = \beta^T x^i + \epsilon^i$
- log-likelihood

$$l(\beta_{1:d}, \sigma^2) = -\frac{n}{2} \ln \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (y^i - \beta_0 - \beta^T x^i)^2 + \text{constant} \quad (16)$$

- For any σ^2 ,

$$\operatorname{argmax}_{\beta} l(\sigma^2, \beta) = \operatorname{argmin}_{\beta} \sum_{i=1}^n (y^i - \beta_0 - \beta^T x^i)^2 \quad (17)$$

a **Least Squares Problem**

- In matrix form $\min_{\beta} \|y - \mathbf{X}\beta\|^2$
- Solution

$$\beta^{\text{ML}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T y \quad (18)$$

with $(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \equiv \mathbf{X}^\dagger$ the **pseudoinverse** of \mathbf{X}

- β^{ML} is **linear** in y !

Linear Discriminant Analysis (LDA)

Fitting a linear predictor for classification, first approach. (We are in the binary classification case)

- Assume each class is generated by a Normal distribution

$$P_{X|Y}(x|+) = \mathcal{N}(x; \mu_+, \Sigma_+), \quad P_{X|Y}(x|-) = \mathcal{N}(x; \mu_-, \Sigma_-) \quad \text{and} \quad P_Y(1) = p$$

- Given x , what is the probability it came from class $+$?

$$P_{Y|X}(+|x) = \frac{P_Y(1)P_{X|Y}(x|+)}{P_Y(1)P_{X|Y}(x|+) + P_Y(-)P_{X|Y}(x|+ -)} \quad \text{and} \quad P_{Y|X}(-|x) = 1 - P_{Y|X}(+|x) \quad (19)$$

This formula is true whether the distributions $P_{X|Y}$ are normal or not.

- We assign x to the class with maximum posterior probability.

$$\hat{y}(x) = \operatorname{argmax}_{y \in \{\pm 1\}} P_{Y|X}(y|x) \quad (20)$$

This too, holds true whether the distributions $P_{X|Y}$ are normal or not.

LDA – continued

Now we specialize to the case of normal class distribution. We assume in addition that $\Sigma_+ = \Sigma_- = K^{-1}$.

- ▶ **Decision rule:** $\hat{y} = 1$ iff $P_{Y|X}(+|x) > P_{Y|X}(-|x)$
- ▶ or equivalently iff

$$0 \leq f(x) = \ln \frac{P_{Y|X}(+|x)}{P_{Y|X}(-|x)} \quad (21)$$

$$= \ln \frac{p}{1-p} - \frac{1}{2} \left[x^T K x - 2\mu_+^T K x + \mu_+^T K \mu_+ \right] - \frac{1}{2} \left[x^T K x - 2\mu_-^T K x + \mu_-^T K \mu_- \right] \quad (22)$$

$$= [K(\mu_+ - \mu_-)]^T x + \ln \frac{p}{1-p} + \frac{\mu_-^T K \mu_- - \mu_+^T K \mu_+}{2} \quad (23)$$

$$= \beta^T x + \beta_0 \quad (24)$$

- ▶ The above is a **linear** expression in x , hence this classifier is called **(Fisher's) Linear Discriminant**
- ▶ Note that if we change the variables to $x \leftarrow \sqrt{K}x$, $\mu_{\pm} \leftarrow \sqrt{K}\mu_{\pm}$, and if we shift the origin to $\frac{\mu_+ + \mu_-}{2}$ (24) becomes

$$2\mu_+^T x + \ln \frac{p}{1-p} \quad (25)$$

This has a geometric interpretation

LDA Algorithm

LDA Algorithm

Train

1. Estimate μ_+ from data $\{(x^i, y^i), y^i = +1\}$
2. Estimate μ_- from data $\{(x^i, y^i), y^i = -1\}$
3. Estimate Σ jointly for both classes, calculate $K = \Sigma^{-1}$. **Exercise** Derive the formula for this estimate, in the Max Likelihood setting
4. Estimate $p = |\{(x^i, y^i), y^i = +1\}|/n$.

predict Now apply (24) to classify new data x

OPTIONAL – QDA (Quadratic Discriminant Analysis)

- If we do not assume $\Sigma_+ = \Sigma_-$ then (21) is a quadratic function of x **Exercise** Plot the curve $f(x) = 0$ in (21) for various data sets in two dimensions. What kind of curves do you observe? Can the decision region be bounded?

$$f(x) = \ln \frac{p}{1-p} - \frac{1}{2} \ln |\Sigma_+| + \frac{1}{2} \ln |\Sigma_-| \quad (26)$$

$$- \frac{1}{2} \left[x^T \Sigma_+^{-1} x - 2\mu_+^T \Sigma_+^{-1} x + \mu_+^T \Sigma_+^{-1} \mu_+ \right] \quad (27)$$

$$+ \frac{1}{2} \left[x^T \Sigma_-^{-1} x - 2\mu_-^T \Sigma_-^{-1} x + \mu_-^T \Sigma_-^{-1} \mu_- \right] \quad (28)$$

$$= \left[\ln \frac{p}{1-p} - \frac{1}{2} \ln |\Sigma_+| + \frac{1}{2} \ln |\Sigma_-| - \frac{1}{2} \mu_+^T \Sigma_+^{-1} \mu_+ + \frac{1}{2} \mu_-^T \Sigma_-^{-1} \mu_- \right] \quad (29)$$

$$+ \underbrace{\left[\mu_+^T \Sigma_+^{-1} - \mu_-^T \Sigma_-^{-1} \right] x}_{\text{linear}} - \underbrace{\frac{1}{2} x^T \left[\Sigma_+^{-1} - \Sigma_-^{-1} \right] x}_{\text{quadratic}} \quad (30)$$

Logistic Regression

Fitting a linear predictor for classification, another approach.

Let $f(x) = \beta^T x$ model the **log odds** of class 1

$$f(X) = \frac{P(Y = 1|X)}{P(Y = -1|X)} \quad (31)$$

Then

- ▶ $\hat{y} = 1$ iff $P(Y = 1|X) > P(Y = -1|X)$
 - ▶ just like in the previous case! so what's the difference?

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- ▶ $\hat{y} = 1$ iff $P(Y = 1|X) > P(Y = -1|X)$
 - ▶ just like in the previous case! so what's the difference?
 - ▶ Answer: We don't assume each class is Gaussian, so we are in a more general situation than LDA
- ▶ What is $p(x) = P(Y = 1|X = x)$ under our linear model?

$$\ln \frac{p}{1-p} = f, \quad \frac{p}{1-p} = e^f, \quad p = \frac{e^f}{1+e^f} \quad 1-p = \frac{1}{1+e^f} \quad (32)$$

- ▶ Note that we can put the last two formulas together as

$$P[y | x] = \frac{1}{1 + e^{-yf(x)}} = \phi(yf(x)) \quad (33)$$

- ▶ where $\phi(z) = \frac{1}{1+e^{-z}}$ is the **logistic** function

Estimating the parameters by Max Likelihood

- ▶ The likelihood of a data point is $P(y|x) = \phi(yf(x))$
- ▶ The log-likelihood for a single pair (x, y) is $l(\beta; (x, y)) = -\ln(1 + e^{-yf(x)})$
- ▶ Log-likelihood of the data set \mathcal{D}

$$l(\beta; \mathcal{D}) = \frac{1}{n} \sum_{i=1}^n l(\beta; (x^i, y^i)) = \frac{1}{n} \sum_{i=1}^n \ln(1 + e^{-y^i f(x^i)}) \quad (34)$$

- ▶ The optimal β maximizes $l(\beta; \mathcal{D})$. It is the value of β that sets the gradient $\nabla l(\beta; \mathcal{D}) = 0$.
- ▶ Unfortunately, this maximization problem does not have a closed form solution! We maximize the (log)likelihood by iterative methods (e.g. gradient ascent) to obtain the β of the classifier.

The gradient of $l(\beta; \mathcal{D})$

- ▶ For a single data point $l(\beta; (x, y)) = -\ln(1 + e^{-yf(x)}) = \phi(yf(x))$
- ▶ First calculate

$$\frac{\partial f}{\partial \beta} = \frac{\partial}{\partial \beta}(\beta^T x) = x \quad (35)$$

- ▶ Then, note $\phi' = \phi(1 - \phi)$,
- ▶ Putting them together

$$\frac{\partial l}{\partial f} = \frac{\partial \ln \phi(yf)}{\partial f} = \frac{y\phi(yf)(1 - \phi(yf))}{\phi(yf)} = y(1 - \phi(yf)) \quad (36)$$

- ▶ Finally

$$\frac{\partial l}{\partial \beta} = \frac{\partial l}{\partial f} \frac{\partial f}{\partial \beta} = (1 - \phi(yf))yx \quad (37)$$

- ▶ The gradient of the log-likelihood of the dataset \mathcal{D} is now

$$\frac{\partial l(\beta; \mathcal{D})}{\partial \beta} = \frac{1}{n} \sum_{i=1}^n \left(1 - \underbrace{\phi(e^{y^i f(x^i)})}_{P(y_i | x^i, \beta)} \right) y_i x^i \quad (38)$$

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- ▶ Interpretation: The infinitesimal change of β to increase log-likelihood for a single data point is along the direction of x , with the sign of y

OPTIONAL – The PERCEPTRON algorithm

Fitting a linear predictor for classification, third approach.

Define $f(x) = \beta^T x$ and find β that classifies all the data correctly (when possible).

PERCEPTRON **Algorithm**

Input labeled training set \mathcal{D}

Initialize $\beta = 0$, for all i , $x^i \rightarrow \frac{x^i}{||x^i||}$ (normalize the inputs)

Repeat until no more mistakes

for $i = 1 : N$

1. if $\text{sgn}(\beta^T x^i) \neq y^i$ (a mistake)
 $\beta \leftarrow \beta + y^i x^i$

(Other variants exist)

The perceptron algorithm and linearly separable data

- \mathcal{D} is **linearly separable** iff there is a β_* so that $\text{sgn} \beta_*^T x^i = y^i$ for all $i = 1, \dots, N$.
If one such β_* exists, then there are an infinity of them

Theorem

Let \mathcal{D} be a linearly separable data set, and define

$$\gamma = \min_i \frac{|\beta_*^T x^i|}{\|\beta_*\| \|x^i\|}. \quad (39)$$

Then, the number of mistakes made by the PERCEPTRON algorithm is at most $1/\gamma^2$.

- Note that if we scale the examples to have norm 1, then γ is the minimum distance to the hyperplane $\beta_*^T x = 0$ in the data set.
Exercise Show that if \mathcal{D} is linearly separable, the scaling $x^i \rightarrow \frac{x^i}{\|x^i\|}$ leaves it linearly separable.
- If \mathcal{D} is not linearly separable, the algorithm oscillates indefinitely.