Elements of statistical learning: Chapter 2

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Introduction

Supervised learning

Goal is to use inputs to predict outputs.

- inputs are also referred to as *predictors*, *features* or *independent* variable
- outputs are also referred to as response or dependent variables

The outputs may be

- quantitative (takes values in \mathbb{R})
- qualitative (also known as categorical or discrete)
 - Ordered (e.g. small, medium or large)
 - Unordered (e.g. pass or fail, on or off)

Regression vs classification

We use *regression* to predict quantitative outputs and *classification* to predict qualitative outputs.

Notations

For different predictors $\{X_k\}_{k=1}^p$ across different observations $i=1,\cdots,n$ denote

 $X_{i,k}$ for random variable and $x_{i,k}$ for an observation

 X_i for a $p \times 1$ vector of variables $-i.e.X_i = [X_{i,1}, \cdots, X_{i,p}]^T$

X for a $N \times p$ matrix of variables across different obvs

In other words

$$\mathbf{X} = \begin{bmatrix} X_{11} & \cdots & X1p \\ X_{21} & \cdots & X2p \\ \vdots & \ddots & \vdots \\ X_{n1} & \cdots & X_{np} \end{bmatrix} = \begin{bmatrix} X_1' \\ X_2' \\ \vdots \\ X_n' \end{bmatrix}$$

Therefore, denotes (X_i, Y_i) as the random variables and (x_i, y_i) as the observed values at i.

Linear models and least squares

To predict Y (which would be denoted by \hat{Y}), we use the linear regression model, which may be expressed as

$$Y_i = \beta_0 + \beta_1 X_{i,1} + \dots + \beta_p X_{i,p} + \epsilon_i, \quad i = 1, \dots, n$$
 (1)

or as

$$Y_i = \beta_0 + \sum_{k=1}^{P} \beta_k X_{i,k} + \epsilon_i, \quad i = 1, \dots, n$$
 (2)

or as

$$Y_i = X_i'\beta + \epsilon_i, \quad , i = 1, \cdots, n$$
 (3)

where $X_i = [1, X_{i,1}, \dots, X_{i,p}]'$ and $\beta = [\beta_0, \beta_1, \dots, \beta_p]'$ are $(p+1) \times 1$ vectors.



In matrix notation, the above can be expressed as

$$\mathbf{Y} = \mathbf{X}\beta + \boldsymbol{\epsilon} \tag{4}$$

which if expanded is expressed as follows

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{1,1} & X_{1,2} & \cdots & X_{1,p} \\ 1 & X_{2,1} & X_{2,2} & \cdots & X_{2,p} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & X_{n,1} & X_{n,2} & \cdots & X_{n,n} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_n \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$
(5)

Least squares estimation

The least squares estimation in one approach to fit the model. In essence, we find the coefficiens β that minimize the sum of squared residuals. Thus, we wish to minimize $RSS(\beta)$

$$rg \min_{eta} RSS(eta) ext{ or } (oldsymbol{y} - oldsymbol{X}eta)'(oldsymbol{y} - oldsymbol{X}eta)$$

The above can be rearranged and expanded to (which is not necessary, as chain rule can be used)

$$(y - X\beta)'(y - X\beta) = (y' - \beta'X')(y - X\beta)$$
$$= y'y - y'X\beta - \beta'X'y + \beta'X'X\beta$$

Differentiating with respect to β yields

$$\frac{\partial RSS(\beta)}{\partial \beta} = 0 - X'y - X'y + 2\beta X'X$$
$$= -2X'y + 2\beta X'X$$

and as this is a minimization problem

$$\frac{\partial RSS(\beta)}{\partial \beta} = 0$$

$$-2X'y + 2\beta X'X = 0$$

$$\beta X'X = X'y$$

and thus so long as X'X is non-singular, the LS estimator of $\hat{\beta}$ is

$$\hat{\beta} = (\mathbf{X'X})^{-1}\mathbf{X'y} \tag{6}$$



Logit models

Now let us consider the case , where the dependent variable Y_i can assume only two categories (say win or lose), and hence two discrete values (i.e. $Y_i=0$ or $Y_i=1$), where as the vector of independent variables are continuous, say $X_i\in\mathbb{R}^p$.

In order to restrict Y_i to 0 and 1. In this case it would make sense to make the probability of $Y_i = 1$ and not the value of Y_i itself. This leads to a probability model, which specifies the probability of the outcome as a function of the predictor:

$$P[Y_i = 1] = P[X_i, \beta] \tag{7}$$

$$P[Y_i = 0] = 1 - P[X_i, \beta]$$
 (8)

Since P is a probability, it is bounded between 0 and 1. The regression equation may be revived by briefly denoting

$$P(X_i,\beta)=X_i'\beta$$



As we wish the pobability to vary monotically with X, we may use a *sigmoid* function:

$$P(X_i, \beta) = \frac{\exp(\beta' X_i)}{1 + \exp(\beta' X_i)}$$
(9)

Let us denote $Z_i = \beta' X_i$, then

$$\lim_{z \to \infty} \frac{\exp(z)}{1 + \exp(z)} = 1$$

and

$$\lim_{z \to -\infty} \frac{\exp(z)}{1 + \exp(z)} = 0$$

Therefore,

$$P[Y_i = 1] = \frac{\exp(\beta'X)}{1 + \exp(\beta'X)}$$

and

$$P[Y_i = 0] = \frac{1}{1 + \exp(\beta' X)}$$

Alternatively, one could look at the odd $P[Y_i = 1]/P[Y_i = 0]$, which may be expressed as

$$\frac{P[Y_i = 1]}{P[Y_i = 0]} = \frac{\exp(\beta' X)}{1 + \exp(\beta' X)} [1 + \exp(\beta' X)].$$
$$= \exp(\beta' X).$$

now taking the logarithm from both sides will yield

$$\log(odds) = \beta' X \tag{10}$$

where now log(odds) is no longer bounded by 0 and 1.

Nearet-neighbour algorithm

- A non-parametric approach used for both classification and regression
- ullet Input consists of the k closest training examples in the feature space.
- Output depends on whether K-NN is used or classification or regression.
- For classification, the output is a class membership
- \bullet For regression, this value is the average of the k nearest neighbbours
- Specifically it can be defined as

$$\hat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i, \tag{11}$$

where $N_k(x)$ is the neighbourhood of x defined by the k closest points x_i in the training sample.

• In other words, find the k nearest neighbours with x_i closest to x, and average their responses y_i .

L2 loss function

- Let random variables $X \in \mathbb{R}^p$ and $Y \in \mathbb{R}$ with joint distribution function F(x, y).
- A function g(X) is sought after for predicting Y, given values of the input X.
- This theory requires a loss function L(Y, g(X)) for penalizing errors in prediction.
- The most common and convenient is squared error loss

$$L(Y, g(X)) = (Y - g(X))^{2}$$
(12)

which gives us the following criterion

$$EPE = \mathbb{E}[(Y - g(X))^2] \tag{13}$$



EXTRA: Some probability recap

The expectation operator $\mathbb E$ is defined for discrete and continuous variables as follows

Discrete variables:

$$\mathbb{E}(X) = \sum_{i \in k} p_i x_i$$

where k are the number of categories. E.g. A coin has two possible states of head (quantified as 1) and tail (quantified as 0) with equal probability. Therefore, the expectated value of the outcome of a coin toss is

$$\mathbb{E}(X) = 0.5 \times 0 + 0.5 \times 1 = 0.5$$

Continuous variables:

$$\mathbb{E}[X] = \int_{\mathbb{R}} x f(x) dx$$

if density f(x) exists. Otherwise,

$$\mathbb{E}[X] = \int_{\mathbb{R}} x dF(x)$$

(noting that dF(X)/dx = f(x))

Multivatiate continuous variable

$$\mathbb{E}[g(X_1,\cdots,X_n)]=\int_{x_1}\cdots\int_{x_n}g(x_1,\cdots,x_n)dF(x_1,\cdots,x_n)$$

and where the density $f(x_1, \dots, x_n)$ exists

$$\mathbb{E}[g(X_1,\cdots,X_n)]=\int_{X_1}\cdots\int_{X_n}g(x_1,\cdots,x_n)f(x_1,\cdots,x_n)dx_1\cdots dx_n$$

Finally, note that

$$F(x,y) = F(x \mid y)F(y)$$

$$F(x,y) = F(y \mid x)F(x)$$

Therefore, returning to (13)

$$\mathbb{E}[(Y - g(X))^{2}] = \int_{x} \int_{y} (y - g(x))^{2} dF(y, x)$$

$$= \int_{x} \int_{y} (y - g(x))^{2} f(y, x) dy dx$$

$$= \int_{x} \int_{y} (y - g(x))^{2} f(y \mid x) f(x) dy dx$$

$$= \int_{x} \mathbb{E}_{y \mid x} [(Y - g(X))^{2} \mid X] f(x) dx$$

$$= \mathbb{E}_{x} \mathbb{E}_{y \mid x} [(Y - g(X))^{2} \mid X]$$

- As the above expression is conditioned on X, there is no longer any dependency between X and the function g.
- furthermore, $[Y g]^2$ is a convex function and we may minimize to solve for g

$$\begin{split} g(x) &=& \arg\min_{g} \mathbb{E}_{y|x}[(Y-g(X))^2 \mid X=x] \\ &\to & \frac{\partial}{\partial g} \int [y-g]^2 f(y\mid x) dy = 0 \\ &\to & \int \frac{\partial}{\partial g} [y-g]^2 f(y\mid x) dy = 0 \\ &\to & -2 \int [y-g] f(y\mid x) dy = 0 \\ &\to & 2g \int f(y\mid x) dy = 2 \int y f(y\mid x) dy \\ &\to & 2g \int f(y\mid x) dy = 2 \mathbb{E}_{Y|X}[Y\mid X=x] \end{split}$$

Note that

$$\int_{\mathbb{R}} f(y \mid x) dy = 1$$

Thus

$$\mathbb{E}[Y \mid X = x] = g(x)$$

This conditional function is also known as the regression function.
 Thus, the best predictor of Y at any point X = x is the conditional mean.

L1 loss function

 The L2 loss function is analytically more desirable, but an L1 criteria of the sort

$$\mathbb{E}[|Y - g(X)|]$$

is more robust to outliers. We may express (13) in the following manner using the L1 criteria:

$$\mathbb{E}[|Y - g(X)|] = \int \int |Y - g(X)|f(x, y)dydx$$

where as before it may be expressed as

$$\mathbb{E}_X \mathbb{E}_{Y|X}[|Y - g(X)||X]$$

and minimized by differentiating with respect to g - i.e.

$$\frac{\partial}{\partial g} \int |y - g(x)| f(y \mid x) dy = 0$$



The latter can be approxmiated by

$$\frac{\partial}{\partial g} \int |y - g| f(y \mid x) dy = \frac{\partial}{\partial g} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} |y_i - g|$$

$$\approx \frac{\partial}{\partial g} \frac{1}{n} \sum_{i=1}^{n} |y_i - g|$$
(14)

Note that the absolute function is piecewise

$$|y_i - g| =$$

$$\begin{cases} y_i - g, & y_i - g > 0 \\ g - y_i, & y_i - g < 0 \\ 0, & y_i = g \end{cases}$$

So that taking the derivative is not continuous at zero

$$\frac{\partial}{\partial g}|y_i - g| = \begin{cases} -1, & y_i - g > 0\\ 1, & y_i - g < 0\\ 0, & y_i = g \end{cases}$$

which is very similar to a sign function - i.e.

$$sgn(z) = \begin{cases} -1, & z < 0 \\ 1, & z > 0 \\ 0, & z = 0 \end{cases}$$

which implies that we may express (14) as

$$\frac{\partial}{\partial g} \int |y - g| f(y \mid x) dy = 0$$

$$\frac{1}{n} \sum_{i=1}^{n} -sgn(y_i - g) = 0$$

$$\sum_{i=1}^{n} sgn(y_i - g) = 0$$

The mean squared error at a nominated test point x_0 for a *deterministic* model of the form

$$Y = f(X) = \exp(-8||X||^2)$$

without any measurement errors, can be obtained by

$$MSE(x_0) = \mathbb{E}_T[(f(x_0) - \hat{y}_0)^2]$$

$$= \mathbb{E}_T[(f(x_0) - \mathbb{E}_T(\hat{y}_0) + \mathbb{E}_T(\hat{y}_0) - \hat{y}_0)^2]$$
add and deduct

Noting that by noting $\underbrace{f(x_0) - \mathbb{E}_T(\hat{y}_0)}_a$ and $\underbrace{\mathbb{E}_T(\hat{y}_0) - \hat{y}_0}_a$, the above is equivalent to $\mathbb{E}_T[(a+b)^2]$, and such can be expanded as follows

$$MSE(x_0) = \mathbb{E}_{\mathcal{T}}[(f(x_0) - \mathbb{E}_{\mathcal{T}}(\hat{y}_0))^2 + (\mathbb{E}_{\mathcal{T}}(\hat{y}_0) - \hat{y}_0)^2 + 2[(f(x_0) - \mathbb{E}_{\mathcal{T}}(\hat{y}_0))(\mathbb{E}_{\mathcal{T}}(\hat{y}_0) - \hat{y}_0)]$$

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which may further get expanded as

$$MSE(x_{0}) = \mathbb{E}_{T}[(f(x_{0}) - \mathbb{E}_{T}(\hat{y}_{0}))^{2} + (\mathbb{E}_{T}(\hat{y}_{0}) - \hat{y}_{0})^{2}$$

$$+ 2f(x_{0})\mathbb{E}_{T}(\hat{y}_{0}) - 2f(x_{0})\hat{y}_{0} - 2\mathbb{E}_{T}(\hat{y}_{0})\mathbb{E}_{T}(\hat{y}_{0}) + 2\mathbb{E}_{T}(\hat{y}_{0})\hat{y}_{0}]$$

$$= \mathbb{E}_{T}[(f(x_{0}) - \mathbb{E}_{T}(\hat{y}_{0}))^{2}] + \mathbb{E}_{T}[(\mathbb{E}_{T}(\hat{y}_{0}) - \hat{y}_{0})^{2}]$$

$$+ 2f(x_{0})^{2} - 2f(x_{0})\hat{y}_{0} - 2f(x_{0})^{2} + 2f(x_{0})\hat{y}_{0}$$

$$= \mathbb{E}_{T}[(f(x_{0}) - \mathbb{E}_{T}(\hat{y}_{0}))^{2}] + \mathbb{E}_{T}[(\mathbb{E}_{T}(\hat{y}_{0}) - \hat{y}_{0})^{2}]$$

Note that by definition

- Variance: $\mathbb{E}_T[(f(x_0) \mathbb{E}_T(\hat{y}_0))^2]$; and
- Bias: $\mathbb{E}_T[(\mathbb{E}_T(\hat{y}_0) \hat{y}_0)]$

Thus,

$$MSE(x_0) = \sigma_T^2(\hat{y}_0) + Bias^2(\hat{y}_0)$$
 (15)



Proofs of eq 2.26 and 2.27

Assume we know that the relationship between X and Y linear and follows the relationship

$$Y_i = X_i'\beta + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2)$$
 (16)

and the model is fitted using the LS estimator, which is

$$\hat{\beta} = (X'X)^{-1}X'Y$$

which may alternatively be expressed as

$$\hat{\beta} = (X'X)^{-1}X'(X\beta + \epsilon) = (X'X)^{-1}(X'X)\beta + (X'X)^{-1}X'\epsilon$$
$$= \beta + (X'X)^{-1}X'\epsilon$$

Thus, the linear model (16) can be expressed as

$$Y_i = X_i'[\beta + (X'X)^{-1}X'\epsilon] = X_i'\beta + X_i'(X'X)^{-1}X'\epsilon$$
$$= X_i'\beta + X(X'X)^{-1}X_i\epsilon$$

Thus, at a nominated test point x_0 , we have

$$\hat{y}_{0} = x'_{0}\beta + X(X'X)^{-1}x_{0}\epsilon
\hat{y}_{0} = x'_{0}\beta + \sum_{i=1}^{N} l_{i}(x_{0})\epsilon_{i}$$

where $l_i(x_0)$ is the i-th element of the N vector $X(X'X)^{-1}x_0$.

Proof of equation 2.27

Here, since our target is no longer deterministic (pay attention to the error term in (16), the expected prediction error can be written as

$$EPE(x_0) = \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} (y_0 - \hat{y}_0)^2$$
 (17)

which as before may get expanded to

$$\begin{split} EPE(x_0) &= \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}} [(y_0 - g(x_0)) + (g(x_0) - \hat{y}_0)]^2 \\ &= \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}} [(y_0 - g(x_0))^2] \\ &+ 2\mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}} [(y_0 - g(x_0))(g(x_0) - \hat{y}_0)] \\ &+ \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}} [(g(x_0) - \hat{y}_0)^2] \end{split}$$

The first term $\mathbb{E}_{y_0|x_0}\mathbb{E}_{\mathcal{T}}[(y_0-g(x_0))^2]$ is independent of the training set and as such can be expressed as

$$\mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau}[(y_0 - g(x_0))^2] = \mathbb{E}_{y_0|x_0}[(y_0 - g(x_0))^2]$$
$$= \int (y_0 - g(x_0))^2 f(y \mid x) dy$$

and as $\mathbb{E}(y_0) = g(x_0)$ the first term is nothing but the conditional variance σ^2 .

The second term can be factorized as before to get

$$\begin{split} \mathbb{E}_{y_{0}|x_{0}} \mathbb{E}_{\tau} [(y_{0} - g(x_{0}))(g(x_{0}) - \hat{y}_{0})] &= \mathbb{E}_{y_{0}|x_{0}} \mathbb{E}_{\tau} [y_{0}g(x_{0})] - \mathbb{E}_{y_{0}|x_{0}} \mathbb{E}_{\tau} [y_{0}\hat{y}_{0}] \\ &- \mathbb{E}_{y_{0}|x_{0}} \mathbb{E}_{\tau} [g(x_{0})^{2}] \\ &+ \mathbb{E}_{y_{0}|x_{0}} \mathbb{E}_{\tau} [g(x_{0})\hat{y}_{0}] \end{split}$$

 \hat{y}_0 is dependent on \mathcal{T} and $g(x_0) = \mathbb{E}[y_0]$, so it is a constant term that we can reduce above to

$$= g(x_0)\mathbb{E}_{y_0|x_0}[y_0] - \mathbb{E}_{y_0|x_0}[y_0\mathbb{E}_{\tau}[\hat{y}_0]] - g(x_0)^2 + g(x_0)\mathbb{E}_{y_0|x_0}\mathbb{E}_{\tau}[\hat{y}_0]$$

noting that

$$\mathbb{E}_{y|x_0}[y_0] = \int y_0 f(y_0 \mid x_0) dy = g(x_0)$$

and for the 2nd term in relationship

$$\mathbb{E}_{y_0|x_0}[y_0\mathbb{E}_{\tau}[\hat{y}_0]] = \mathbb{E}_{\tau}[\hat{y}_0]\mathbb{E}_{y_0|x_0}[y_0] = \mathbb{E}_{\tau}[\hat{y}_0]g(x_0)$$

and the last term we get

$$g(x_0)\mathbb{E}_{y_0|x_0}\mathbb{E}_{\tau}[\hat{y}_0] = g(x_0)\mathbb{E}[\hat{y}_0]$$



Therefore, since $\mathbb{E}_{y_0|x_0}[y_0] = g(x_0)$

$$\begin{split} \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [(y_0 - g(x_0)) (g(x_0) - \hat{y}_0)] &= g(x_0) \mathbb{E}_{y_0|x_0} [y_0] - \mathbb{E}_{y_0|x_0} [y_0 \mathbb{E}_{\tau} [\hat{y}_0]] \\ &- g(x_0)^2 + g(x_0) \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [\hat{y}_0] \\ &= g(x_0)^2 - g(x_0) \mathbb{E}_{\tau} [\hat{y}_0] \\ &- g(x_0)^2 + g(x_0) \mathbb{E}_{\tau} [\hat{y}_0] = 0 \end{split}$$

Thus,

$$\begin{split} EPE(x_0) &= \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [(y_0 - g(x_0))^2] + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [(g(x_0) - \hat{y}_0)^2] \\ &= \sigma^2 + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [(g(x_0) - \hat{y}_0)^2] \\ &= \sigma^2 + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [g(x_0)^2] - 2\mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [g(x_0)\hat{y}_0] + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau} [\hat{y}_0^2] \end{split}$$

Noting that

$$\mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau}[(g(x_0) - \mathbb{E}_{\tau}[\hat{y}_0])^2] = \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau}[g(x_0)^2] - 2\mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau}[g(x_0)\hat{y}_0] + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\tau}[\hat{y}_0]^2$$

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The expression in the brackets can be substituted with

$$\mathbb{E}_{y_0|x_0}\mathbb{E}_{\tau}[(g(x_0)-\mathbb{E}_{\tau}[\hat{y}_0])^2]-\mathbb{E}_{y_0|x_0}\mathbb{E}_{\tau}[\hat{y}_0]^2$$

which implies

$$\begin{split} EPE(x_0) &= \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}}[(y_0 - g(x_0))^2] + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}}[(g(x_0) - \hat{y}_0)^2] \\ &= \sigma^2 + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}}[(g(x_0) - \mathbb{E}_{\mathcal{T}}[\hat{y}_0])^2] \\ &- \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}}[\hat{y}_0]^2 + \mathbb{E}_{y_0|x_0} \mathbb{E}_{\mathcal{T}}[\hat{y}_0^2] \end{split}$$

noting that

$$\sigma_T^2(\hat{y}_0) = \mathbb{E}_T[\hat{y}_0^2] - \mathbb{E}_T[\hat{y}_0]^2$$

Hence

$$EPE(x_0) = \sigma^2(y_0 \mid x_0) + \mathbb{E}_{y_0 \mid x_0} \mathbb{E}_T[(g(x_0) - \mathbb{E}_T[\hat{y}_0])^2] + \sigma_T^2(\hat{y}_0)$$

= $\sigma^2(y_0 \mid x_0) + Bias^2(\hat{y}_0) + \sigma_T^2(\hat{y}_0)$