Machine Learning

Module 3.1 - Models: Linear and Logistic regressions

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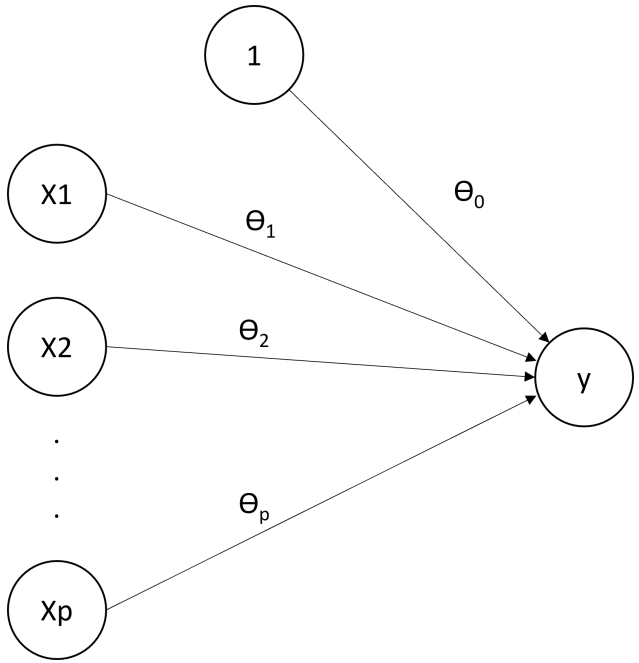
Linear regression

The prediction formula is

$$f(x;\theta) = \theta_0 + \theta_1 x_1 + \ldots + \theta_p x_p$$



The MSE and the OLS

The loss function is the **mean squared error**, MSE,

$$\bar{\mathcal{L}}(\theta) = \frac{1}{n}\sum_{i=1}^{n}\{y_i - f(x_i;\theta)\}^2.$$

The optimal parameter under this loss is called the **Ordinary Least Squares**, OLS,

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n}\sum_{i=1}^{n}\{y_i - f(x_i;\theta)\}^2.$$

The OLS

To find the OLS, the algorithm is exact and the final solution can be explicitly computed with the matrix-operation

$$\hat{\theta} = (X^T X)^{-1} X^T y,$$

where

- X is the so-called **design matrix** of size $n \times (p+1)$ and whose i-th row contains
$$[1, x_{i1}, \ldots, x_{ip}],$$
- y is the vector of length n whose i-th element is y_i.

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Logistic regression

The logistic regression is a model for **binary classification**. Prediction formula is in several steps:

- Compute the **linear predictor**

$$z(x;\theta) = \theta_0 + \theta_1 x_1 + \cdots + \theta_p x_p,$$

- Compute the **probability prediction** (sigmoid function):

$$p(x;\theta) = P(Y = 1|X = x) = \frac{\exp\{z(x;\theta)\}}{1 + \exp\{z(x;\theta)\}}.$$

- Compute the **prediction of the class**:

$$f(x;\theta) = \begin{cases} 1, & \text{if } p \geq 0.5, \\ 0, & \text{if } p < 0.5. \end{cases}$$

The sigmoid and the logit function

The **logit function** is the inverse of the **sigmoid function** and thus transforms $p(x;\theta)$ to $z(x;\theta)$.

$$z(x;\theta) = \log \frac{p(x;\theta)}{1 - p(x;\theta)}$$

Estimation

The loss function uses the probabilities $p(x;\theta)$ and not the final predictions. The loss is the **cross-entropy** also called **negative log-likelihood**:

$$\mathcal{L}(y,p) = -y\log p - (1-y)\log(1-p).$$

Interpretation,

- If $y = 1$, we want p to be large (close to 1). The contribution to the loss is

  $$\mathcal{L}(1,p) = -\log p$$

  It will be small indeed if p is large.
- If $y = 0$, we want p to be small (close to 0). The contribution to the loss is

  $$\mathcal{L}(0,p) = -\log(1-p)$$

  It will be small indeed if p is small.

Estimation

The overall loss is

$$\bar{\mathcal{L}}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} y_i \log p(x_i;\theta) + (1-y_i)\log\{1-p(x_i;\theta)\}.$$

The log in this formula can be in any base. Often,

- Machine learners use $\log_2$ for binary classification,
- Statisticians use ln.

This has no consequence on the final result. But it can bring confusion from time to time.

Optimal parameters

To obtain the optimal parameters, the best algorithm is the **Newton-Raphson** algorithm. It requires

- To compute the first and second derivatives of $\bar{\mathcal{L}}(\theta)$,
- To build a sequence of $\hat{\theta}_k$ that converges to the optimal one using these derivatives.

This algorithm is very fast and efficient. However, there is no explicit formula for $\hat{\theta}$, unlike the OLS.

The optimal $\hat{\theta}$ is called the **maximum likelihood estimator**, **MLE**.

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Interpretation

Linear and logistic regressions are highly interpretable in that

- the coefficients quantify the link between the features x and the outcome y.
- the certainty of the prediction can be quantify.

Interpretation of the coefficients

For the **linear regression**, coefficients are interpreted as *slopes*.

- When the feature x_1 increases by 1 unit, the outcome y increases in average by θ_1 units (same for all features $1, \dots, p$).
- A positive coefficient θ_j means a positive linear association between the feature x_j and the outcome y.
- The larger the coefficients, the larger the association, in absolute value. (note: pay attention to the scale!)
- For the categorical features, the coefficients estimate the average change in the outcome y when the feature switches from the reference level to any other level. It is thus a **contrast** with the reference level.

Note: one should not say that an increase in x_j *causes* an increase of the response. It is an association. The causality implies a direction and is more complex to establish.

Interpretation of the coefficients

For the **logistic regression**, because of the sigmoid transform, the interpretation of the coefficients is not direct like with the linear regression:

- With a positive θ_j, an increase of x_j is associated with an increase of the probability that $y = 1$.
- The larger the coefficient, the larger the increase. However, it the increase is not linear and depends on the other features.
- A negative coefficient means a decrease in the probability of the positive class ($y = 1$).

Note: coefficients can be interpreted in terms of odds ratio. We will not pursue this here.

Certainty for linear regression

For **linear regression**, certainty can be measured by **prediction intervals**. In practice, the main interest relies in the prediction interval for **the future value**[1].

Let x be a set of new features, the **point** prediction for $y(x)$ uses the estimate $\hat{\theta}$:

$$f(x;\hat{\theta}) = \hat{\theta}_0 + \hat{\theta}_1 x_1 + \cdots + \hat{\theta}_p x_p.$$

Now, rather than a point estimate, we want to build an interval $[L, U]$ such that

$$P(L \leq y(x) \leq U) = 1 - \alpha,$$

where α is usually set to 5% for an interval at 95%. To build this interval, we rely on probabilistic assumptions of the model.

[1] As opposed to prediction interval for the mean.

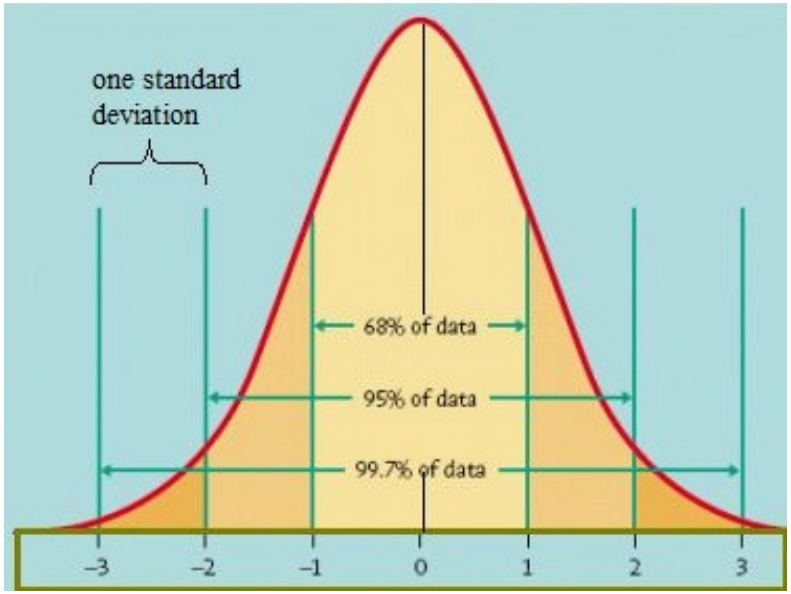
Certainty for linear regression

It is often assumed that the true response $y(x)$ for feature x satisfies

$$y(x) = \theta_0 + \theta_1 x_1 + \cdots + \theta_p x_p + \sigma e = f(x;\theta) + \sigma e,$$

where the residual e is standard normal, $e \sim N(0,1)$, and σ is the standard deviation.

In particular, we expect the residual distribution to be symmetric around 0 and (informally) respect the 68-95-99.7 rule:



source: http://www.statisticshowto.com/68-95-99-7-rule/

Certainty for linear regression

Therefore, to find $[L, U]$, we set

$$0.95 = P(L \leq y(x) \leq U) = P\left(\frac{L - f(x;\theta)}{\sigma} \leq e \leq \frac{U - f(x;\theta}{\sigma})\right).$$

Using the normal distribution, we find that

$$L - f(x;\theta) = -\sigma z_{1-\alpha/2}, \quad U - f(x;\theta) = \sigma z_{1-\alpha/2}.$$

This gives

$$L = f(x;\theta) - \sigma z_{1-\alpha/2}, \quad U = f(x;\theta) + \sigma z_{1-\alpha/2}.$$

For $\alpha = 5\%$, $z_{1-\alpha/2} = 1.96$, and

$$[L, U] = [f(x;\theta) \pm 1.96\sigma].$$

Certainty for linear regression

Using a plug-in estimate, this gives us a *rough* prediction interval (at 95%) of

$$\left[\hat{L}, \hat{U}\right] = \left[f(x;\hat{\theta}) \pm 1.96s\right],$$

where s is the unbiased estimate of the standard deviation

$$s^2 = \frac{1}{n-(p+1)} \sum_{i=1}^{n} \{y_i - f(x_i;\hat{\theta})\}^2.$$

This prediction interval is however hardly used/implemented because

- the estimate s carries uncertainty. If taken into account, the Student $t_{n-(p+1)}$ distribution should be used.
- the estimate $\hat{\theta}$ carries uncertainty. If taken into account, the estimate of s should be changed to $s\sqrt{1 + x^T(X^TX)^{-1}x}$.

Both adaptations widen the interval.

Certainty for logistic regression

The probability provides an interpretation of the certainty the model provides on a classification. Consider:

- $\hat{y} = 1$ with $\hat{p} = 0.99$: the prediction is **certain**.
- $\hat{y} = 1$ with $\hat{p} = 0.53$: the prediction is **uncertain**.

In both cases, the predicted class is the same but the probability provides a more precise view on it: if the instance is far in the class or on the edge between the two classes.

The prediction "Good" for a customer with a probability of 0.51 is uncertain. Alternatively, the prediction rule could set to a larger value than 0.5 to increase the certainty.

Also, a model with a lot of predictions close to 0.5 is considered as poor because of its uncertainty[2].

[2] A little thought on that will brings us back to the entropy.

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Occam's Razor

A parsimony principle:

> "All else being equal, the simplest explanation is the best one"

- In other words, among two models with approximately the same prediction quality, choose the simplest one.
- In practice, we remove from the model variables that do not impair too much the prediction quality.

Simplifying the model is a solution to **overfitting**. This will be studied later in the course.

Akaike Information Criterion

The **AIC** (Akaike Information Criterion) is

$$AIC = -2\hat{\ell} + 2k$$

where

- $\hat{\ell}$ is the maximum **log-likelihood** and measure the goodness-of-fit,
- k is the number of parameters and measure the model complexity.

Minimizing the AIC achieves a trade-off between the quality of prediction and the model complexity.

Akaike Information Criterion

For linear regressions,

- The number of parameters is $k = p + 2$ with $\theta_0, \theta_1, \ldots, \theta_p$ and σ,
- The log-likelihood part equals

$$-2\hat{\ell} = n \ln 2\pi + n \ln \hat{\sigma}^2 + \frac{1}{\hat{\sigma}^2} \sum_{i=1}^{n} \left\{ y_i - f(x; \hat{\theta}) \right\}^2,$$

where $\hat{\sigma}^2 = (n - p - 1)s^2/n$.

For logistic regressions,

- The number of parameters is $k = p + 1$ for $\theta_0, \theta_1, \ldots, \theta_p$,
- The log-likelihood part equals

$$-2\hat{\ell} = 2 \sum_{i=1}^{n} y_i \ln p(x_i; \hat{\theta}) + (1 - y_i) \ln\{1 - p(x_i; \hat{\theta})\}.$$

Variables selection with AIC

Automatic variable selection using stepwise minimization of the AIC can be performed. There are

- Backward: start from the most complete model and try to remove variable one at a time (if it decreases the AIC)
- Forward: start from the empty model and try to add one variable at a time (if it decreases the AIC).
- Both: start to add or remove at each step.

At each step, all the models in competition are fitted. The procedure is computationally intense.

Variable selection with penalization

A different approach consists of penalizing the loss function so that, during the training of the parameters, the variable selection applies directly.

The most common penalties are:

- L_1 penalty (LASSO)

$$\min_{\theta} \bar{\mathcal{L}}(\theta) + \lambda \sum_{j=1}^{p} |\theta_j|$$

- L_2 penalty (Ridge)

$$\min_{\theta} \bar{\mathcal{L}}(\theta) + \lambda \sum_{j=1}^{p} \theta_j^2$$

Usually, θ_0 is not penalized.

Variable selection with penalization

The penalty parameter $\lambda \geq 0$:

- If $\lambda = 0$, then there is no penalty.
- If $\lambda \longrightarrow \infty$, then $\theta \longrightarrow 0$.

For intermediate values, some components of θ will be small, pushed toward 0.

This is equivalent to variable selection: setting $\theta_j = 0$ is equivalent to not including x_j.

Selection of λ can be done with **cross-validation** (CV ; see later).

Variable selection with penalization

- L_1 shrink some of the θ_j, set some $\theta_j = 0$, select variables.
- L_2 shrink all the θ_j's, avoiding extremes θ_j, regularize θ.

Elastic net combines L_1 and L_2:

$$\min_{\theta} \bar{\mathcal{L}}(\theta) + \lambda \left\{ \alpha \sum_{j=1}^{p} |\theta_j| + \frac{1-\alpha}{2} \sum_{j=1}^{p} \theta_j^2 \right\}$$

with $0 \leq \alpha \leq 1$,

- If $\alpha = 0$, it is the ridge (L_2)
- If $\alpha = 1$, it is the LASSO (L_1)

Often, λ is selected by the data (CV), while α is set by the user.