KAZAKH-BRITISH TECHNICAL UNIVERSITY

Introduction to Machine Learning
Week 3

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Definition

The goal of the supervised learning approach is to learn a **mapping** from inputs $\mathbf{x}$ to outputs y, given a *labeled set* of input-output pairs:

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n},$$

where:

- $\mathcal{D}$ is the **training set**.
- n is the number of training examples.
- $\mathbf{x}_i$: Each training example is a vector of numbers called *features*, *attributes*, *covariates*, or *explanatory variables*:
  - They are usually stored on an $n \times p$ **design matrix**.
  - Their structure may be more complex, such as an image, a text, a sequence, a graph, ...
- y_i is the **response variable**:
  - It can be a *categorical* or *nominal* variable from a finite set.
  - Or a *real-valued scalar*.

As we know the real value of y_i, it is possible to compare the prediction with the observable and therefore compute **error metrics**.

Classification

When the response variable y_i is categorical, the problem is known as **classification** (or pattern recognition).

- detecting if an e-mail is ham or spam
- recognizing parts of speech (verbs, subject, pronouns, etc.)
- face detection on an image
- market segmentation

Regression

When the response variable y_i is a real-valued scalar, the problem is known as **regression**.

- predict the wage of an individual
- predict the value of a financial asset
- predict the temperature at any location in a building

Supervised learning

With supervised learning problems, we assume that there exists a relationship between the input variables x and the output variable y:

$$y = f(x) + \epsilon,$$

where f is a fixed but unknown function of the predictors, and ϵ is a random error term.

Mispecification Bias

- Let's consider a quite general model: $y = f(X) + \varepsilon$.
- Assume that X is fixed.
- The expected (squared) prediction error, or EPE, is equal to :

$$\begin{aligned} E(y-\hat{y})^2 &= E[f(X)+\varepsilon-\hat{f}(X)]^2 \\ &= \underbrace{E[f(X)-\hat{f}(X)]^2}_{\text{Reducible}} + \underbrace{Var(\varepsilon)}_{\text{Irreducible}} \end{aligned}$$

- The focus of Machine Learning is to estimate f with the aim of minimizing the reducible error.

- Reducible error = $[\text{Bias}(\hat{f}(X))]^2 + \text{Var}(\hat{f}(X))$.

Mispecification Bias

Assuming that the data are generated by a specific model, or that the model is correctly specified (i.e. $f(x) = \hat{f}(x)$),

remains to assume that the (misspecification) bias is zero:

$$Bias(\hat{f}) = 0$$
$$E[f(X) - \hat{f}(X)]^2 = 0$$

Estimating f

We are interested in estimating the function f, for two main reasons:

- to **predict** the value of y for some inputs that may nor be available.
- to estimate the **impact** of X on y i.e., for *inference* purposes.

Estimating f for prediction

If we are interested in estimating f for prediction purposes:

- we want to get $\hat{y} = \hat{f}(x)$ where $\hat{f}$ is the estimation of f
- we may not be interested that much in the exact form of $\hat{f}$ and may view it as a black box... as long as it gets accurate predictions

Estimating f for inference

When we are interested in estimating the mapping from x to y for inference purposes, we want to know **how variations in the inputs** x **affect the output** y.

In that case, we may want to know what are the important predictors among x that can explain the variations of the response.

Besides, we may want to know more about the relationship between predictors and the response:

- what is the magnitude?
- what is the sign of the relationship?
- is it linear? non-linear?

Accuracy Vs. Interpretability Trade-off

There is therefore a trade-off between prediction accuracy and model interpretability.

Depending on the goal of the estimation, one might prefer giving-up some accuracy and turn to more restrictive model to get more interpretable results.

Definition

A **Cost function**[1] measures the performance of a machine learning model for given data.

It quantifies the error between predicted and expected values and present that error in the form of a single real number.

It is often denoted as :

$$\mathcal{L}(\mathcal{D}),$$

$$\text{where : } \mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$$

[1] Also called **Loss function**

Regression Loss functions

$$\text{Mean Squared Error (MSE)} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \tag{1}$$

$$\text{Mean Absolute Error (MAE)} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{2}$$

Binary Classification Loss functions

Misclassification Rate :

$$\mathcal{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(y_i \neq \hat{y}_i) \tag{3}$$

Binary Cross Entropy Loss :

$$\mathcal{L}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} [y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)] \tag{4}$$

Multiclass Classification Loss functions

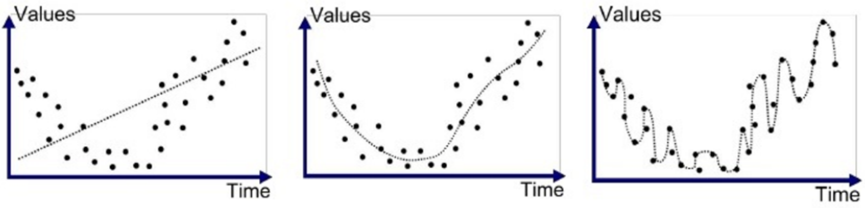
Cross entropy Loss :

$$\mathcal{L}(\theta) = -\sum_{i=1}^{N} y_i \log(\hat{y}_i) \tag{5}$$

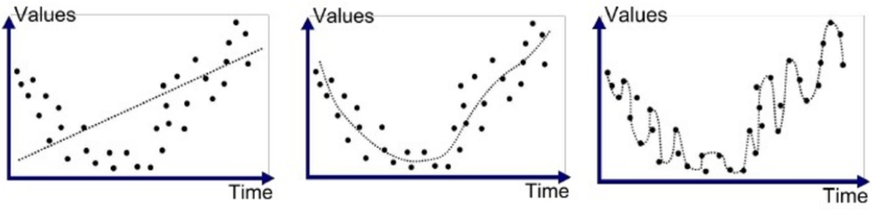
Cross Entropy Loss :

$$\mathcal{L}(\theta) = -\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K} y_{ik} \log(\hat{y}_{ik}). \tag{6}$$

Model Selection



Model Selection

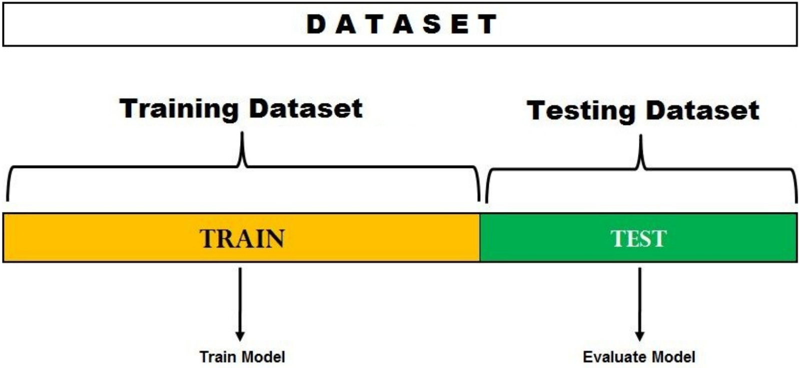


Underfitted

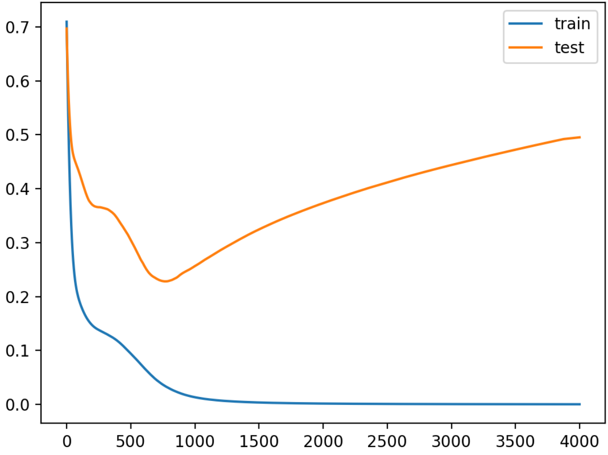
Good Fit/Robust

Overfitted

Data split


DATASET
Training Dataset
Testing Dataset
TRAIN
TEST
Train Model
Evaluate Model

Train and test Loss



Thank you for your attention !