ISOM 3360

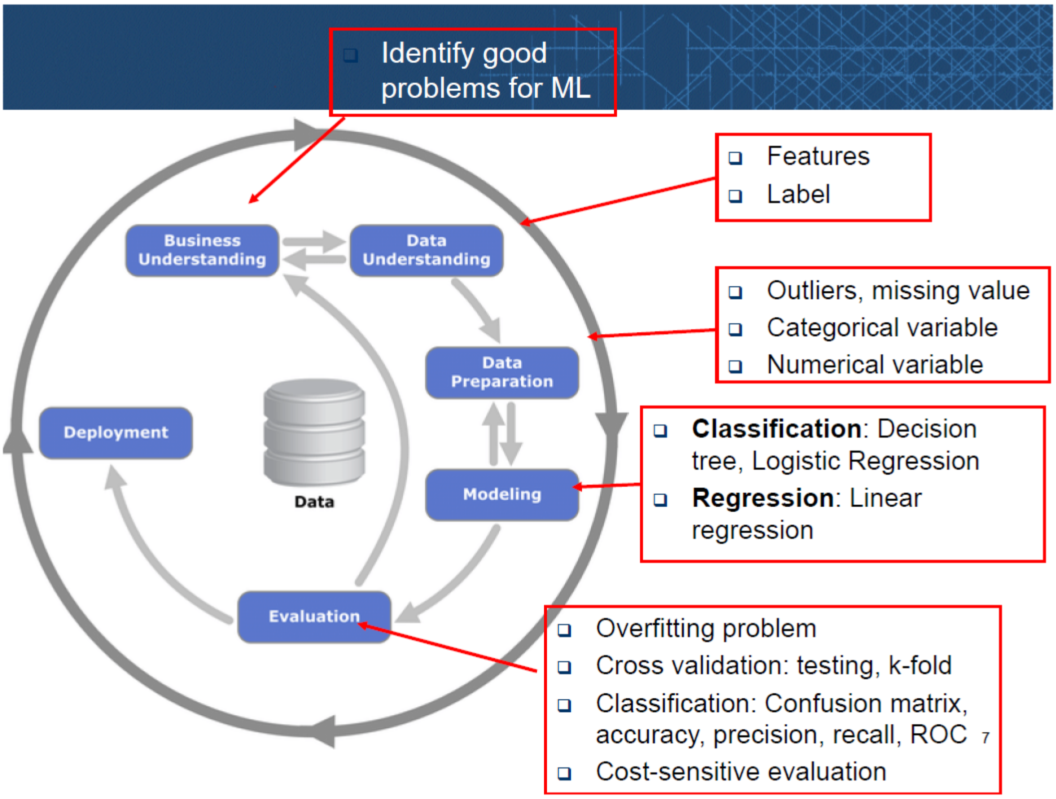
ISOM 3360 - Data Mining for Business Analytics

Spring 2020, HKUST

This repository contains code of labs and assignments.

For reference only, please DO NOT COPY.

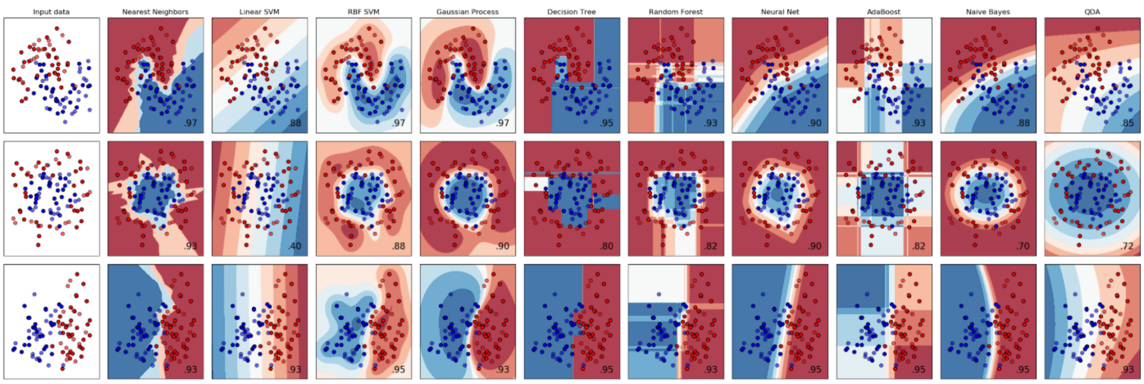
Overview of Data Mining



Supervised learning (prediction of labels)

Unsupervised learning (relationship mining)

Classification <u>decision boundaries</u>:



Strengths and weakness

ML tends to work well when

- Learning a simple concept
- Lots of (good quality) data available

ML tends to work poorly when

- Learning complex concepts from a small amount of data
- Performing on new types of data
  - e.g. photos taken in big hospitals and small hospitals are different types, because small hospitals may rotate.

Data preparation

- Size: > 10 × number of features

- Quality: label errors, noisy features, unreliable source

Outliers: > 3 σ away from the mean

Missing values handling

- Ignore instances/features
- Fill in:
  - Global constant (Null or 0)
  - **Feature mean**
  - Feature mean for samples in each class
  - Feature mode/medium/...

Feature transformation

- Categorical: **one-hot encoding**
- Numerical:
  - **normalization** (after visualization)
    - scaling to range: e.g. min-max: $(x - x_{min})/(x_{max} - x_{min})$
    - clipping: capped above/below a threshold ⇒ bell shape
    - log scaling: $\log(x)$ for long-tailed data
    - z-score scaling: $(x - \mu)/\sigma$ for normal data
  - **discretization**
    - binning

Balancing

Degree of Imbalance	**Proportion of the Minority Class**
Mild	20% - 40%
Moderate	1% - 20%
Extreme	< 1%

- Resample
- Generate synthetic data for the minority class

Modeling

Train-test split

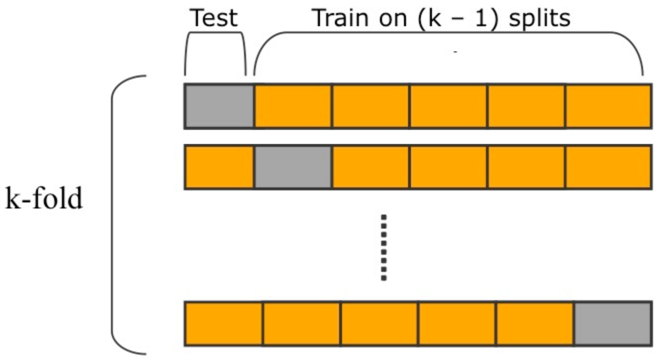
Avoid data leakage: never use testing data in data preparation (e.g. `fillna`) or modeling

Testing set:

- Large enough to yield statistically meaningful results
- Is representative of the data set as a whole

Cross validation

k-fold (k = 10)



Overfitting

Noise or random fluctuations in the training data is picked up and learned.

Decision threshold

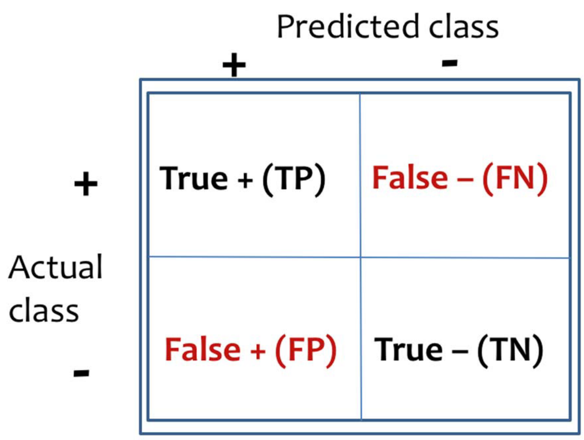
Probabilistic predictions: e.g. p >= 0.5 ⇒ y = 1

Determine the confusion matrix and ROC curve.

Model Evaluation

Benchmark: the naïve learner e.g. random guess, **majority class classifier**

Confusion Matrix



Accuracy = (TP + TN) / (TP + TN + FP + FN)

Error Rate = 1 - Accuracy

Precision = TP / (TP + FP)

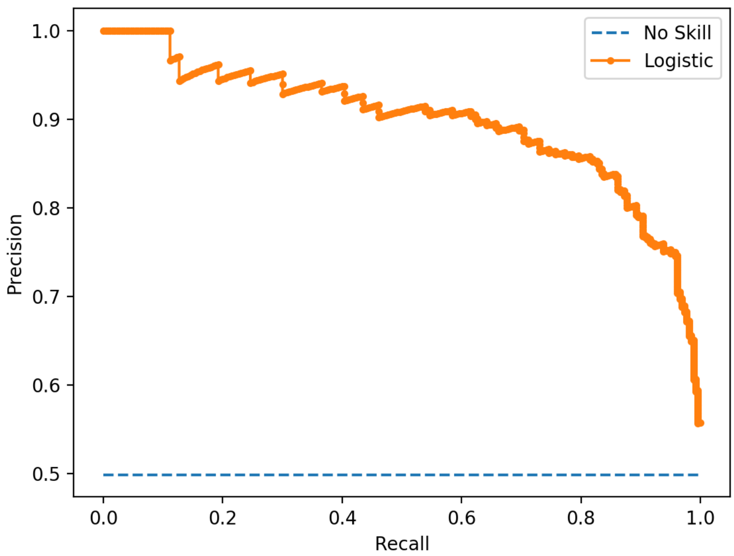
Recall (TPR) = TP / (TP + FN)

Fall-out (FPR) = FP / (FP + TN)

A confusion matrix is determined by its **decision threshold**.

Threshold ↑ , Precision ↑ , Recall ↓

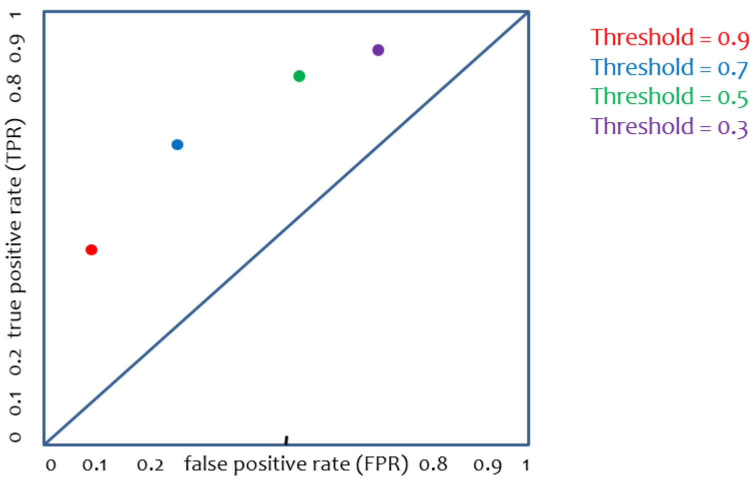
Precision-Recall Curve



high precision → few results

Useful for imbalanced datasets where the positive class is the minority (e.g. web search).

ROC Curve



- Diagonal: random guess, AUC = 0.5
  - (1, 1): y = 1
  - (0, 0): y = 0
- (0, 1): perfect model, AUC = 1
- (1, 0): perfect model = Not(y)

AUC

Area Under (the ROC) Curve: between 0.5 (random) and 1 (perfect).

- aggregate measure of performance across all possible thresholds
- probability that the model ranks a random positive example higher than a random negative example

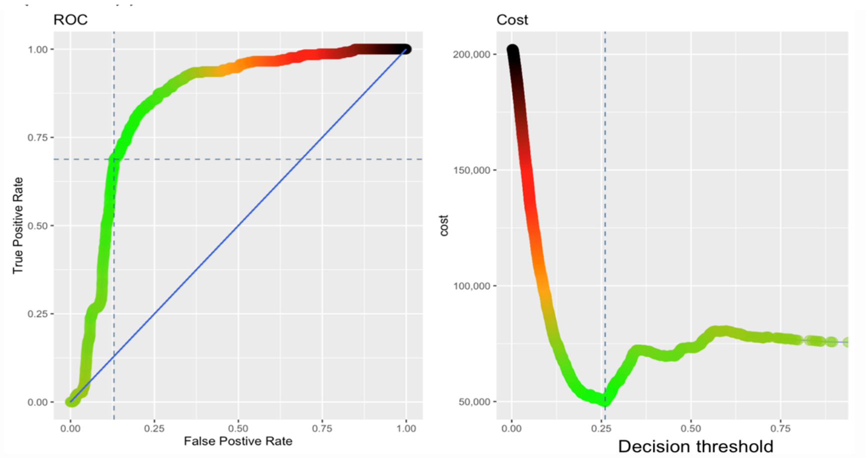
Cost-sensitive classification

Cost = FP × (cost of FP) + FN × (cost of FN)

When the costs of FP (Type I error) and FN (Type II error) are different,

Minimize the cost → Minimize the type of error with the higher cost.

Examples: credit card applications, spam filtering, medical diagnosis, customer churn



Prediction bias

Bias = average of predictions – average of actual labels

Significant non-zero bias ⇒ Error in model

Decision Tree

Find features with high predictability.

Structure:

- upside down if-else tree
- **root** node contains all training examples
- **leaf** node
- numerical features may be discretized

Metrics

Gini Impurity

Information Gain

Entropy: uncertainty/impurity in the dataset; always non-negative

$$H(S) = \sum_{x \in X} -p(x) \log_2 p(x)$$

where p(x) is the proportion of class x in the dataset S.

Information Gain: decrease in entropy after a split

$$IG(A, S) = H(S) - \sum_{t \in T} p(t) H(t)$$

where T are the subsets crated from splitting S by feature A.

ID3 Algorithm

Only for classification, only handles categorical features.

1. Calculate the entropy of every feature using the dataset S.
2. Split the set S into subsets using the feature for which the information gain is maximum.

3. Make a decision tree node containing that feature, divide the dataset by its branches, and calculate the entropy of each branch
4. - If a branch has entropy of 0, it's a leaf node.
   - If `depth = max_depth` or `size < min_samples_split` , it's a leaf node.
   - Else:
     - If additional splits obtain no information gain, it's a leaf node.
     - Else, go back to Step 2.

Decision boundaries

Parallel to the axes.

Pros and Cons

Pros

- easy to understand, implement, and use (good for non-DM-savvy stakeholders)
- computationally cheap
- require little data preparation (no need for one-hot encoding)

Cons

- can overfit, need pruning
- unstable structure (one minor change can make the tree completely different)
- decision boundaries are parallel to the axes
- accuracy is mediocre

Linear Regression

Basics

$$
\begin{aligned}
h_{\mathbf{w}}(\mathbf{x}) &= \mathbf{w}^T\mathbf{x} \\
&= w_0 + \sum_{i=1}^{n} w_i x_i \\
\mathbf{w} &= \underset{\mathbf{w}}{\operatorname{argmin}} \sum (h_{\mathbf{w}}(x) - y)^2 \\
&= (X^T X)^{-1} X^T y
\end{aligned}
$$

For univariate linear regression,

$$
\begin{aligned}
w_1 &= \frac{\sum (x-\bar{x})(y-\bar{y})}{\sum (x-\bar{x})^2} \\
w_0 &= \bar{y} - w_1\bar{x}
\end{aligned}
$$

Lasso Regression

$$
\mathbf{w} = \underset{\mathbf{w}}{\operatorname{argmin}} \sum (h_{\mathbf{w}}(x) - y)^2 + \lambda \sum |w|
$$

L1 Regularization: $\lambda \uparrow$, fitness $\uparrow$, model complexity $\uparrow$.

- Penalize models with too many features $\Rightarrow$ Generate **sparse models**
- Penalize features with large coefficients

Evaluation

Root Mean Squared Error (RMSE): penalize large prediction errors

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum(\hat{y}-y)^2}$$

Mean Absolute Error (MAE):

$$\mathrm{MAE} = \frac{1}{N}\sum|\hat{y}-y|$$

Both RMSE and MAE are sensitive to outliers.

Pros and Cons

Pros

- Simple and easy to interpret

Cons

- Oversimplifies problems by assuming linearity
- Sensitive to outliers

Logistic Regression

Basics

Softmax function

$$\sigma = \frac{\exp(x_k)}{\sum \exp(x)}$$

Conditional probabilities

$$\begin{aligned} P(y=k \mid \mathbf{x}) &= \sigma(\mathbf{w}_k^T \mathbf{x}) \\ &= \frac{\exp(\mathbf{w}_k^T \mathbf{x})}{\sum \exp(\mathbf{w}^T \mathbf{x})} \end{aligned}$$

For binary classification, we have

$$\begin{aligned} P(y=1 \mid \mathbf{x}) &= \sigma(\mathbf{w}_1^T \mathbf{x}) \\ &= \frac{\exp(\mathbf{w}_1^T \mathbf{x})}{\exp(\mathbf{w}_0^T \mathbf{x}) + \exp(\mathbf{w}_1^T \mathbf{x})} \\ &= \frac{1}{1+\exp[(\mathbf{w}_1 - \mathbf{w}_0)^T \mathbf{x}]} \\ &= \frac{1}{1+\exp(\mathbf{w}^T \mathbf{x})} \end{aligned}$$

where $\mathbf{w} = \mathbf{w}_1 - \mathbf{w}_0$.

So, we have the sigmoid function

$$s = \frac{1}{1+\exp(-x)}$$

And we can get the conditional probability from

$$P(y=1 \mid \mathbf{x}) = s(\mathbf{w}^T \mathbf{x})$$

Decision boundaries

- Univariate: parallel to y-axis
- Multivariate: linear but not parallel to y-axis