Part I: The Elements of Machine Learning

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December 2, 2019

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Over Fitting Problems

Model Evaluation and Selection

Philosophy



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Philosophy			

- Examples.
- Two kinds of information

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Philosophy

- Examples.
- Two kinds of information
 - x information: accessible, cheap.



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- Prediction: automated, accurate, safe and objective solution.
- Ability of prediction V.S. interpretation.



Over Fitting Problems

Model Evaluation and Selection



Over Fitting Problems

Model Evaluation and Selection

Observations from my lovely son \heartsuit

• At beginning, he repeatedly asked me: "What is this, papa?"



Over Fitting Problems

Model Evaluation and Selection

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- After a while, his question style was switched from special to general.
 "Papa, is this an apple?"



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Over Fitting Problems

Model Evaluation and Selection

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- It's so magical! I did not summarize any rule for him!



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• Data: Target variable y, feature variables X.



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Logit function

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- Perceptron classfier: Sign(w'x)
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Non-linear Extension

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Help!			



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Model Evaluation and Selection

Help!



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Model Evaluation and Selection

Polynomial Regression



Model Evaluation and Selection

Polynomial Regression

• In simple linear regression, we fit the data as a linear function of x



Model Evaluation and Selection

Polynomial Regression

- In simple linear regression, we fit the data as a linear function of x
- Here, it seems that we need to fit our data as a curve.



Model Evaluation and Selection

Polynomial Regression

- In simple linear regression, we fit the data as a linear function of x
- Here, it seems that we need to fit our data as a curve.
- Polynomial regression

 $y_i = w_0 + w_1 x_i + w_2 x_i^2 + \dots + w_k x_i^k + \epsilon_i$


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Non linear Separable



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Non linear Separable

• Non linear separable. Hyper plain decision boundary seems does not work here...



Model Evaluation and Selection

Non linear Separable

- Non linear separable. Hyper plain decision boundary seems does not work here...
- It seems that the decision boundary is an ellipse.

$$\frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} = 1$$

$$(\chi_1, \chi_2) \longrightarrow (\chi_1^2, \sqrt{2}\chi_1, \chi_2, \chi_2^2)$$



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• In the first problem, we did a transformation $\phi: \mathbb{R} \to \mathbb{R}^k$

$$x \rightarrow (x, x^2, ..., x^k)$$

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Non-Linear Extension

Model Evaluation and Selection

 $\gamma = \beta_0 + \beta_1 \times_0 + \beta_1 \times_2^2 + \beta_2 \times_3^2 + \beta_2 \times_4^2$



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Non-Linear Extension

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Non-Linear Extension

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Overfitting			

• The final aim of building a model is generalization.

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Overfitting			

- The final aim of building a model is generalization.
- Training set V.S. validation set.

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Overfitting			

- The final aim of building a model is generalization.
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- Not only take into account the errors within the training set, E_T , but also the prediction error from validation set, E_V

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Overfitting

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- Not only take into account the errors within the training set, E_T , but also the prediction error from validation set, E_V
- E_T is the measure of the goodness of fit; E_V is a measure of the overfitting.

	Orange	Red
$E_T(m)$	Perfect	Good enough
$E_V(m)$	Poor	Good
Complexity	Complicate	Simple

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K Nearest Neighbors, follwing the local majority

• Predict the label as the majority of the *K* surroundings.

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- Annotated observations $\{\mathbf{x}_i, y_i\}_{i=1}^N$



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- For a new observation **x**_{new}, find the *K* nearest neighbors given a metric.



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- It also can be applied for regression problem.
- Memory based method and lazy learner.



• Model parameters:

• Hyper parameters:

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 - (Logistic) regression, the regression coefficients.

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Hyper-parameters and Model selection

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 - KNN, the number of neighbors K.
- How to choose (tuning) the hyper-parameters?

Hyper-parameters and Model selection

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 - (Logistic) regression, the regression coefficients.
 - LDA, the parameters of each Gaussian model.
 - Perceptron, the weight parameters.
- Hyper parameters:
 - Polynomial regression, the order of polynomial.
 - Principal component regression, the number of components.
 - KNN, the number of neighbors K.
- How to choose (tuning) the hyper-parameters?
- Choose the "best" model.

Model Evaluation and Selection

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Evaluation

- Regression:
 - Mean Square Error (MSE): $\frac{1}{N} \sum_{i=1}^{N} (\hat{y}_i y_i)^2$
 - Mean Absolute Error (MSA): $\frac{1}{N} \sum_{i=1}^{N} |\hat{y}_i y_i|$
 - R square and F-statistic
- Classification:
 - Accuracy

$$\frac{1}{N}\sum_{i=1}^{N}\mathbf{1}\{\widehat{y}_i\neq y_i\}$$

- Confusion matrix
- Kappa statistics

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Leave One Out Cross Validation

- Suppose the sample size of the training data is N
- For each observation *i*
 - Leave the *i*th case out, and train the model with the rest.
 - Predict the *i*th case using the trained model.
- Calculate the average accuracy or other metrics.

For K=1....K



• Computational cost is high.

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k-Fold Cross Validation

- Randomly divide the training data set into k even parts.
- For each group *i*,
 - Excluding the *i*th group, train the model with the rest.
 - Predict the *i*th group using the trained model.
- Calculate the average performance.



• Provide a way to estimate the standard deviation of the estimation of performance.

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Procedure

- Spliting the data into three parts: training set, validation set and testing set.
- Fit and validate different models with training/validatoin set and the corresponding validation method.
- Select the model with the "best" performance.
- Train the "best" model by using train set + validation set.
- Estimate the performance of the model by using the testing set.