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Introduction to Machine Learning

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Machine Learning – Today and the Past

History of AI
Turing Test
Driving Forces

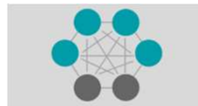
2

History of AI

The Dawn of AI
1950

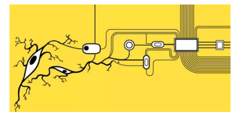
Perceptron
1958

1956
The Dartmouth Conference



The Boltzmann Machine
1983

1997
IBM's Deep Blue



Deep Learning
2006

2011
IBM's Watson

AlphaGo
2016

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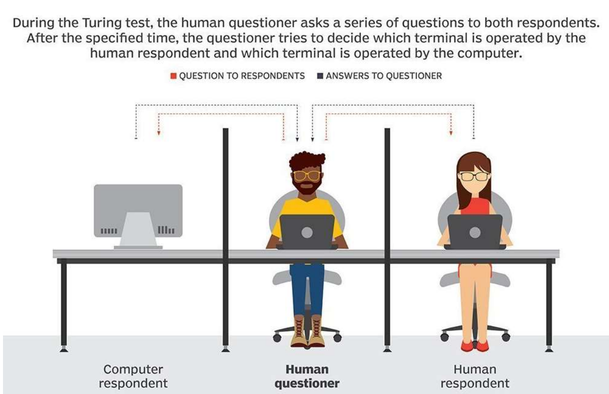
Turing Test



Eugene Goostman

- First **pass** on Jun 6, 2014
- 13-year old boy from Odessa, Ukraine

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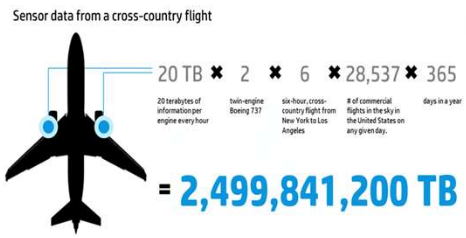
Driving Forces

Big Data

More data was created this year than in last **5,000** years
(but only 0.5% was analyzed)

For example:



= **2.5 ZB**

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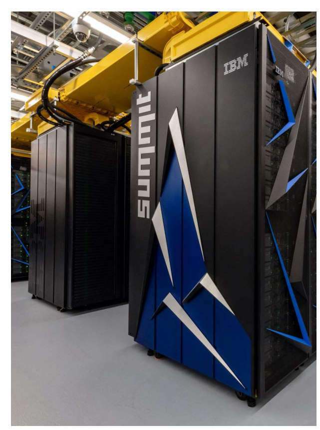
Driving Forces

Big Data

More data was created this year than in last **5,000** years
(but only 0.5% was analyzed)

Computing

If every person on Earth completes one calculation per second, it would take **305 days** to do what Summit can do in **1 second**



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Basic Concepts of machine learning

ML vs the Traditional Paradigm
Taxonomies of ML
Steps in ML Project

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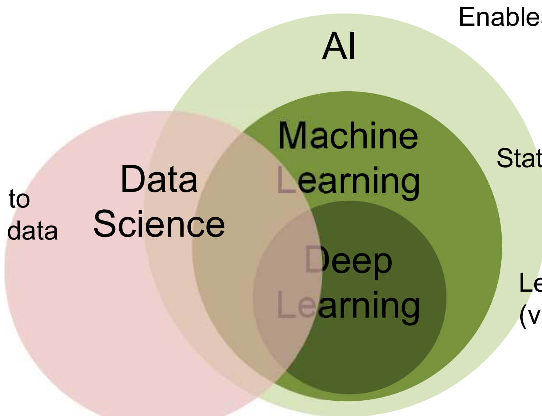
AI vs. ML vs…

Enables machine to "think"

Statistical tools to enable AI using data

Mathematical tools to manage & analyse data



Learning the way humans learn (via multi-neural network architecture)

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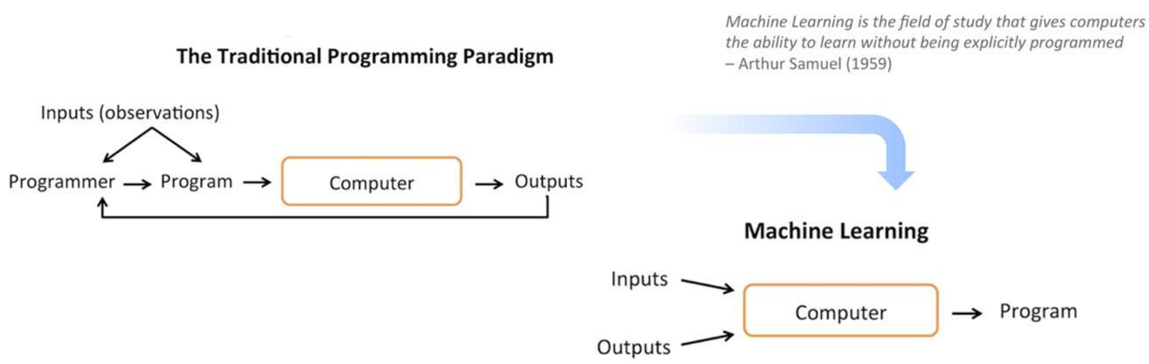
ML vs Traditional Programming



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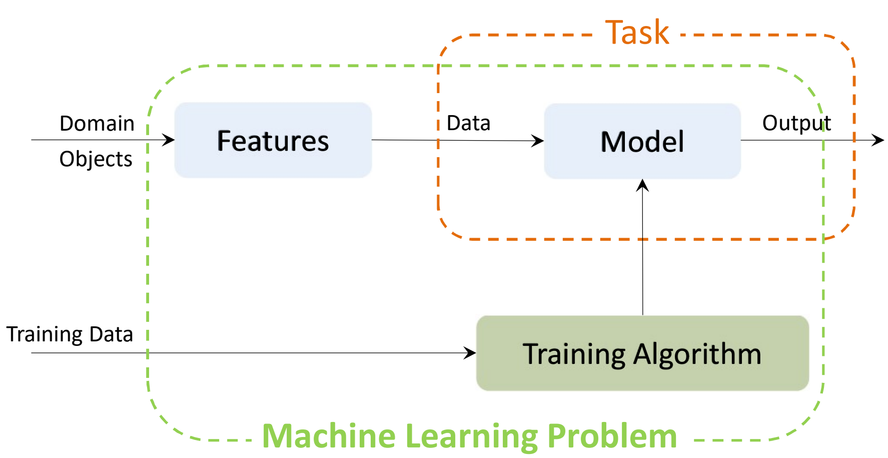
Task, Training, Model and Data



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Taxonomies of ML

Type of Data

- **Supervised ML**
  - Learning by problems and solutions
  - Using labeled examples to predict
- **Unsupervised ML**
  - Learning by problems
  - Explores data to learn hidden patterns
- **Reinforcement learning**
  - Learning by trying
  - Making strategic decisions

Type of Task

- **Regression**
  - Predict continuous value
- **Classification**
  - Predict discrete value
- **Decision making**
  - Predict the best alternative

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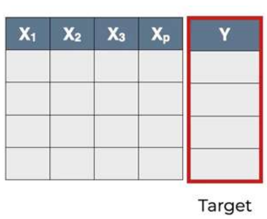
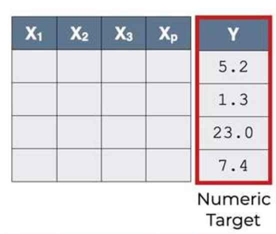
Data and Task

- Data
- Task

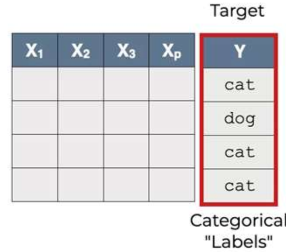


Supervised ML

Unsupervised ML



Regression Task



Classification Task

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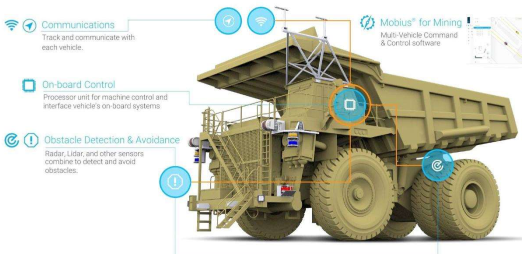
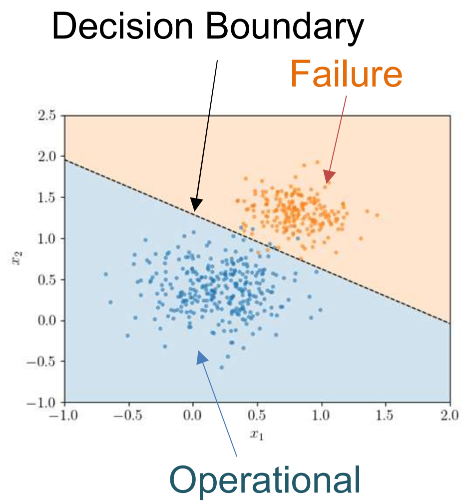
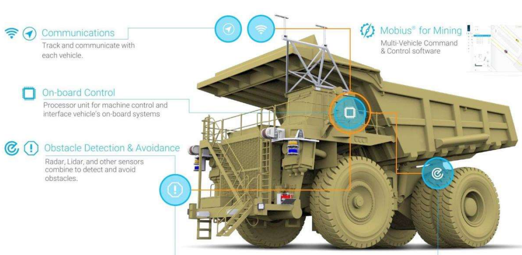
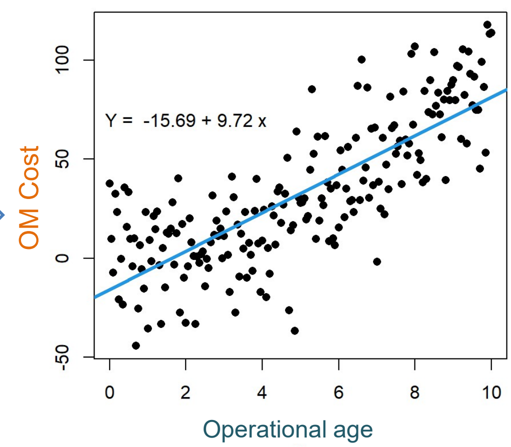
Classification Task





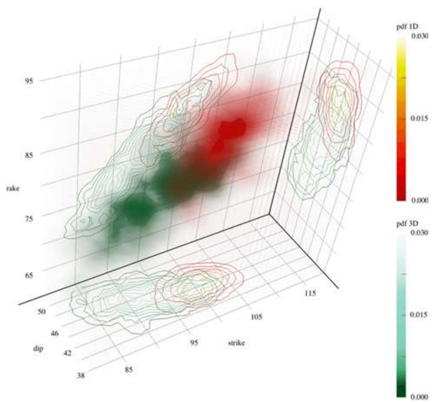
Regression Task





Task types

- Other tasks



dimension reduction

sequential mining

Steps in Machine Learning

1. Define the problem
2. Data Collection — The more, the better
3. Data Preparation — Duplicates, missing data, normalization, split
4. Choose a Model — Nature of tasks
5. Train the Model — Update learnable parameter to reduce loss
6. Evaluate the Model — Loss against unseen data
7. Tune Hyper-parameters of the Model — Learn unlearnables
8. Use the Model to Predict

Machine Learning in Practice

- Preparation of Data
  - One-hot Coding
  - Binning
  - Normalization
  - Standardization
  - Missing data & Imputation
  - Unbalanced data
- Three Sets
  - Training set
  - Validation set
  - Test set
- Selection of Learning Algorithm
  - Explainability
  - # of features and examples
  - Categorical vs. numerical features
  - Nonlinearity of the data
  - Training and Prediction speed
- Performance Evaluation
  - Confusion Matrix
  - Precision, Recall, Accuracy, AUC
- Overfitting and Underfitting

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Steps in ML Project

Data Preparation
Performance Evaluation

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Data collection

- Size
  - The more, the better
  - At least 10x more examples than number of trainable parameters
- Quality
  - Noise, even outliers
  - Missing values
  - Features
- Labeling
  - Direct vs. derived

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Data Preparation

- **1-Hot Coding: Categorical** to **numerical**

$$\text{Red} = [1,0,0] \qquad\qquad \text{Red} = 1$$
$$\text{Yellow} = [0,1,0] \quad \textbf{vs.} \quad \text{Yellow} = 2$$
$$\text{Green} = [0,0,1] \qquad\qquad \text{Green} = 3$$

- **Binning: Numerical** to **categorical**

$$\text{Age} \in [0,5) \quad \rightarrow \quad \text{Bucket} = 1$$
$$\text{Age} \in [6,12) \quad \rightarrow \quad \text{Bucket} = 2$$
$$\text{Age} \in [12,20) \quad \rightarrow \quad \text{Bucket} = 3$$

Data Preparation

- **Normalization**: **Range** to **[0,1]**

$$\bar{x} = \frac{x - \min\{x_1, \dots, x_n\}}{\max\{x_1, \dots, x_n\} - \min\{x_1, \dots, x_n\}}$$

  - Improves learning speed by preventing gradient of large range dominate the gradient descent

- **Standardization**: **Distribution** to **N(0, 1)**

$$\hat{x} = \frac{x - \mu\,\{x_1, \dots, x_n\}}{\sigma\{x_1, \dots, x_n\}}$$

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Data Preparation

- Normalization vs. Standardization

Normalization	Standardization
	Feature distribution is close to normal
No outliers	Some outliers
Usually recommended over standardization	

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Data Preparation

- Missing Features and Data Imputation
  - Replacing with an average of the feature

$$\tilde{x} = \frac{1}{M}\sum_{i}^{N} x_i$$

	col1	col2	col3	col4	col5
0	2	5.0	3.0	6	NaN
1	9	NaN	9.0	0	7.0
2	19	17.0	NaN	9	NaN

mean() →

	col1	col2	col3	col4	col5
0	2.0	5.0	3.0	6.0	7.0
1	9.0	11.0	9.0	0.0	7.0
2	19.0	17.0	6.0	9.0	7.0

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Data Preparation

- Other Data Imputation Methods
  - Most frequent value
  - 0 or any other constant
  - kNN
  - Regression
  - Extrapolation and interpolation

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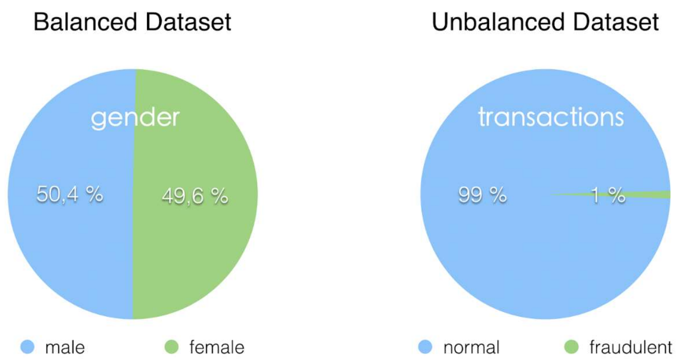
Data Preparation

- Unbalanced Datasets



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Data Preparation

- Unbalanced Datasets
  1. Carefully select performance metrics

     e.g., Accuracy vs Precision+Recall
  2. Resampling
     1. Under-sampling
     2. Over-sampling
     3. SMOTE (Synthetic Minority Over-sampling Technique)

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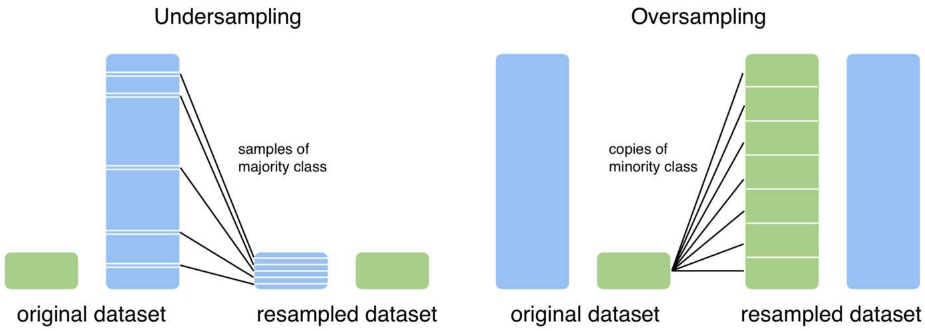
Data Preparation

- Unbalanced Datasets



Three Sets

- Training Set
  - To build the model
- Validation Set
  - To tune hyper-parameters
- Test Set
- Rule of Thumb
  - **70%:15%:15%** for **training** : **validation** : **test**

Selecting Learning Model

- Explainability
- # of features and examples
- Categorical vs. numerical features
- Nonlinearity
- Training speed
- Prediction speed

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ML Models

- Supervised ML
  - Linear Models
    - Linear Regression
    - Logistics Regression
    - Support Vector Machine
  - Non-linear Models
    - Naive Bayes Method
    - Decision Trees
    - Neural Networks
- Unsupervised ML
  - Principle Component Analysis
  - Clustering
  - Sequential Patterns

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Recommendations for Learning Algorithm

	Recommended	Not recommended
Explainability	kNN, **linear regression**, **decision tree**	NN, Kernel-methods
Large data set (feature/sample)	**NN**	SVM
Categorical	**NN**, **Logistic regression**, SVM, **Decision tree**	Linear regression
Non-linearity	**NN**, Kernel-methods	Linear regression, SVM
Training speed	**Regression**, **Decision tree**	NN
Prediction speed	**Regression**, **NN**	kNN, RNN

Back to Steps in Machine Learning

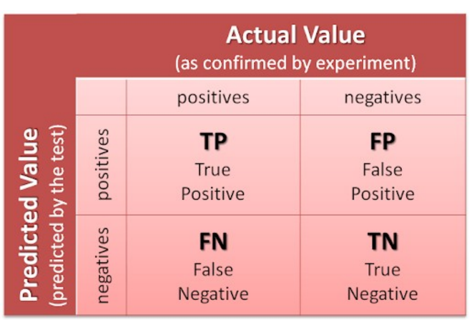
1. Define the problem
2. Data Collection
3. Data Preparation
4. Choose a Model
5. Train the Model
6. Evaluate the Model
7. Tune Hyper-parameters of the Model
8. Use the Model to Predict

Performance Evaluation

- Classification Tasks
  - Confusion matrix
  - Accuracy
  - Precision
  - Recall (sensitivity)
  - F1-score
  - AUC (Area Under ROC Curve)
- Regression Tasks
  - MAE
  - MSE
  - R^2

Classification Tasks

- Confusion Matrix



Predicted	Dove	Woodpecker	Robin	Crow	Starling	Sparrow	Finch	Goldfinch
Dove	11	0	1	0	0	1	0	0
Woodpe	0	9	0	1	1	0	0	0
Robin	0	2	13	0	0	1	0	0
Crow	1	0	0	9	0	0	0	0
Starling	0	0	1	0	12	1	1	0
Sparrow	0	1	2	0	0	13	1	0
Finch	1	0	0	0	0	0	6	1
Goldfinc	0	0	0	0	0	0	2	8

Evaluation of Binary Classification

– Accuracy

$$A = \frac{\#\ of\ correct\ predictions}{\#\ of\ all\ predictions}$$

$$= \frac{TP+TN}{TP+TN+FP+F}$$

– Recall (Sensitivity)

$$R = \frac{\#\ of\ correctly\ predicted\ positives}{\#\ of\ actual\ positives}$$

$$= \frac{TP}{TP+FN}$$

– Precision

$$P = \frac{\#\ of\ correctly\ predicted\ positives}{\#\ of\ all\ predicted\ positives}$$

$$= \frac{TP}{TP+}$$

– F1 score

$$F1 = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}}$$

$$= 2\frac{Precision \cdot Recall}{Precision + Recal}$$

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Evaluation of Binary Classification

	Actual Positive	Actual Negative	
Predicted Positive	**TP**=100	**FP**=10	$\hat{\mathbf{P}}$=110
Predicted Negative	**FN**=5	**TN**=50	$\hat{\mathbf{N}}$=55
	P=105	**N**=60	n=165

Recall

Precision

F1 score

Accuracy

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Evaluation of Multi-Type Classification

Predicted		Dove	Woodpecker	Robin	Crow	Starling	Sparrow	Finch	Goldfinch	TP	FP	FN	Precision	Recall	F1 score
	Dove	11	0	1	0	0	1	0	0						
	Woodpe	0	9	0	1	1	0	0	0						
	Robin	0	2	13	0	0	1	0	0						
	Crow	1	0	0	9	0	0	0	0						
	Starling	0	0	1	0	12	1	1	0						
	Sparrow	0	1	2	0	0	13	1	0						
	Finch	1	0	0	0	0	0	6	1						
	Goldfinc	0	0	0	0	0	0	2	8						

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Evaluation of Multi-Type Classification

Predicted		Dove	Woodpecker	Robin	Crow	Starling	Sparrow	Finch	Goldfinch	TP	FP	FN	Precision	Recall	F1 score
	Dove	11	0	1	0	0	1	0	0	11	2	2	0.846	0.846	0.846
	Woodpe	0	9	0	1	1	0	0	0	9	2	3	0.818	0.750	0.783
	Robin	0	2	13	0	0	1	0	0	13	3	4	0.813	0.765	0.788
	Crow	1	0	0	9	0	0	0	0	9	1	1	0.900	0.900	0.900
	Starling	0	0	1	0	12	1	1	0	12	3	1	0.800	0.923	0.857
	Sparrow	0	1	2	0	0	13	1	0	13	4	2	0.765	0.867	0.813
	Finch	1	0	0	0	0	0	6	1	6	2	4	0.750	0.600	0.667
	Goldfinc	0	0	0	0	0	0	2	8	8	2	1	0.800	0.889	0.842

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Regression Task

- MAE (Mean Absolute Error)

$$MAE = \frac{1}{n}\sum |y_i - \hat{y}|$$

- MSE (Mean Squared Error)

$$MSE = \frac{1}{n}\sum (y_i - \hat{y})^2$$

- R^2 (Coefficient of Determination)

$$R^2 = 1 - \frac{\text{Unexplainable Variation}}{\text{Total Variation}} = 1 - \frac{\sum (y_i - \hat{y})^2}{\sum (y_i - \bar{y})^2}$$

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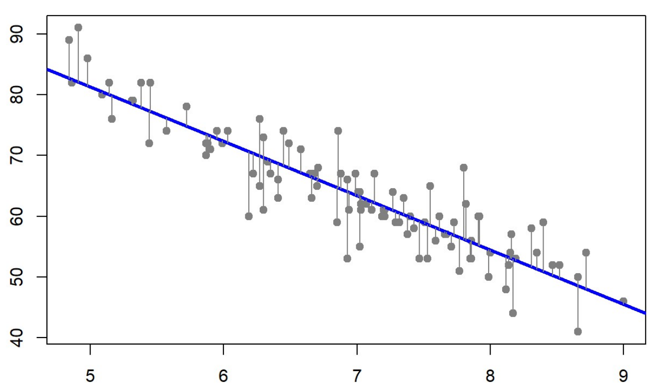
Regression Task

- MAE (Mean Absolute Error) and MSE (Mean Squared Error)



$$MAE = \frac{1}{n}\sum |y_i - \hat{y}|$$

$$MSE = \frac{1}{n}\sum (y_i - \hat{y})^2$$

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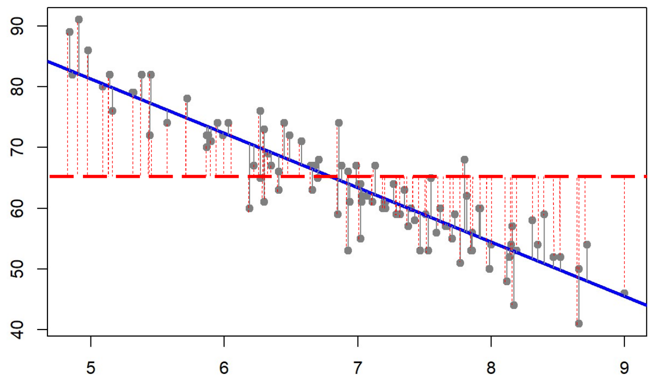
Regression Task

- R^2



Sum of the squared residuals:

$$SS_{res} = \sum (y_i - \hat{y})^2$$

Total variability/variation:

$$SS_{tot} = \sum (y_i - \bar{y})^2$$

$$R^2 = 1 - \frac{\sum (y_i - \hat{y})^2}{\sum (y_i - \bar{y})^2}$$

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Anomaly Detection on Track

- Subway power-rail may overheat and cause defects
  - 6.5 Km light metro line
  - In May 2017, a train was damaged during operation
  - Power rail anomaly can be caused by high temperature
- IR camera is used to identify anomalies, but the video must be viewed manually to detect the anomalies

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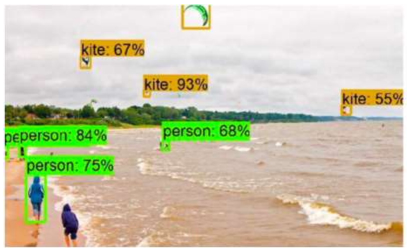
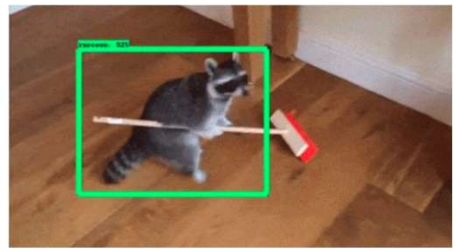
Anomaly Detection on Track

- Using TensorFlow Object Detection API & Microsoft Visual Object Tagging Tool to detect anomalies automatically





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Data and Preparation

- 2 sets of videos
  - Line 3
  - 1 set has 4 videos with 16,000 frames recorded in December 2017
    - Only 3 videos capture the power rail
    - Partially labelled by TTC with a total 45 anomalies
  - Another set has 8 videos with 10,000 frames recorded in May 2018
    - Only 2 videos capture the power rail
    - Not labelled
  - Winter images were chosen
    - Recorded using a thermal camera in resolution 640X512
    - Further labelling was done by the team to get a total of 668 anomalies

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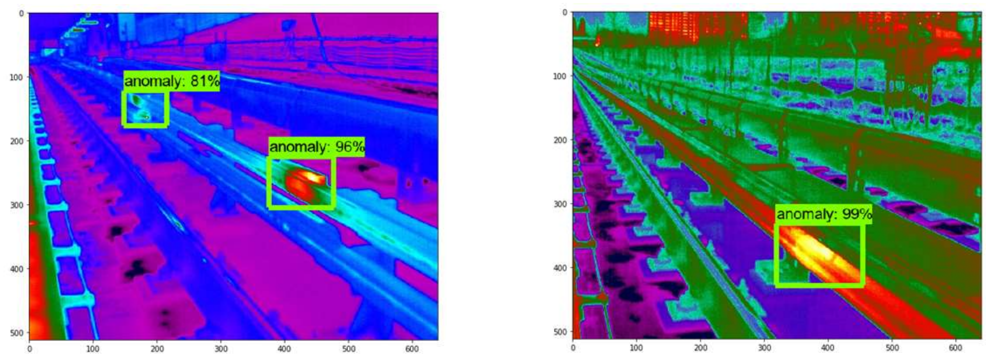
Anomaly Detection on Track

- ANN using Tensorflow Object Detection API



True Positives

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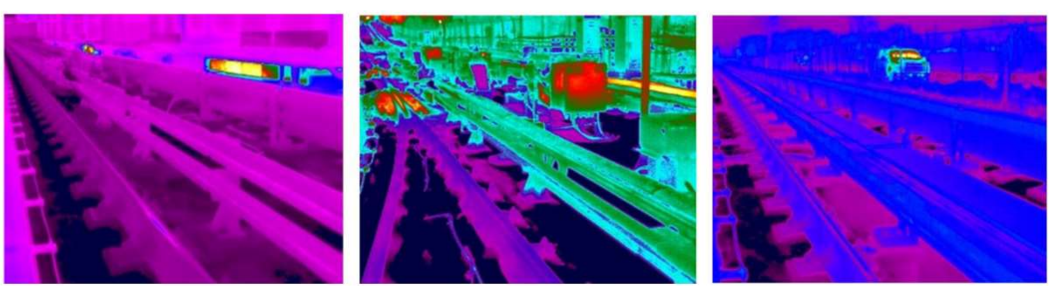
Anomaly Detection on Track

- Tricky cases



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Performance

- Balanced Tune-up

Method	Precision	Recall
Shallow AutoEncoder	47%	76%
Robust AutoEncoder	51%	88%
Isolation Forest	64%	94%
SVM	61%	93%

- Recall Maximization

Method	Precision	Recall
Isolation Forest	52%	**100%**
SVM	53%	**100%**

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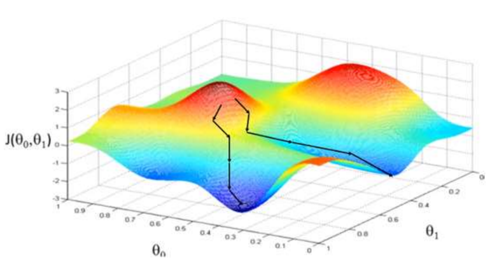
Gradient Descent for ML

- The most used learning algorithm




```
Repeat until convergence {
```

$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} \mathrm{MSE}(\theta)$$

```
}
```

$$MSE = \frac{2}{n} \sum (y_i - \hat{y})^2$$

$$\frac{\partial}{\partial \theta_j} \mathrm{MSE}(\theta) = \frac{2}{n} \sum_{i=1}^{n} (\theta^T \cdot x_i - y_i)[x_i]_j$$

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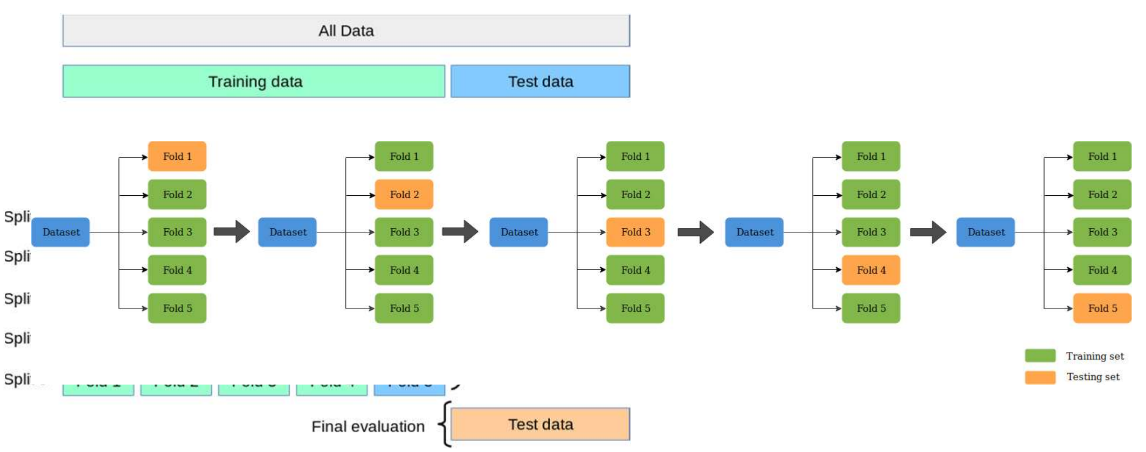
Cross Validation

- Cross validation (CV) usually means k-fold cross validation
  - Useful when data set is too small
  - In k-fold, every sample is used for training as well as for testing
  - Recommended in hyper-parameter tune up

- In k-fold CV
  - Data set is split into k subsets of equal size
  - The holdout method is repeated k times
  - Each time, (k-1) sets are used for training and 1 set for testing

k-Fold Cross Validation



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Model Training and Performance Improvement

A Case Study
Over-fitting and Under-fitting
Hyper-parameter tune up
Combining learners

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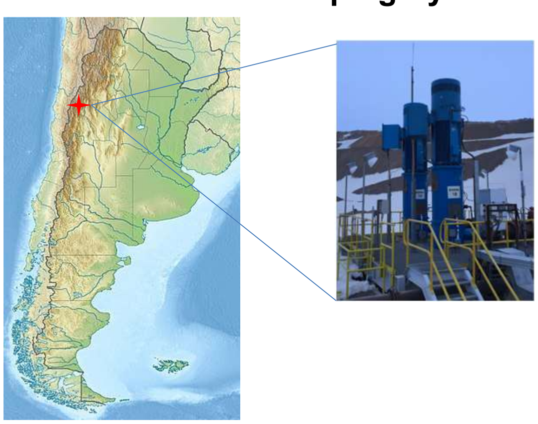
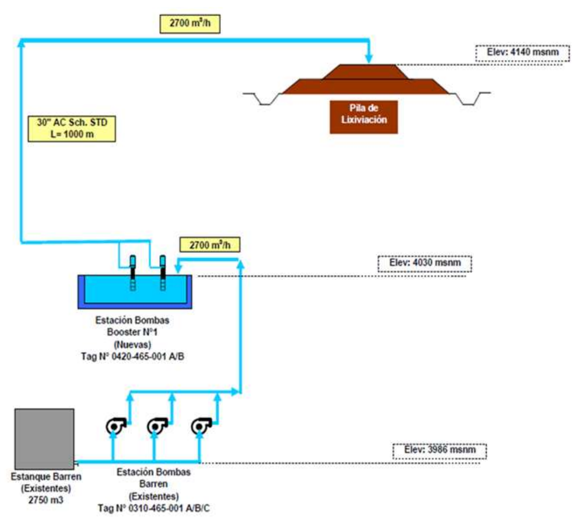
Case 1: Linear regression

Veladero Barren Pumping System





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Case 1: Linear regression

Situation

- Two pumps running full time with sensor data available
- Over the course of project, additional data including pressure, and any significant down time were added.
- For better understanding of the data, we sought to determine the relationships between different variables.

Objective

- Anomaly detection before the accident happens

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Case 1: Linear regression

Steps

Preprocessing → Data Transforming → Exploratory Data Analysis → Model Construction

Preprocessing:
- Missing values
- Outliers

Data Transforming:
- Format transforming
- Data splitting
- Seasonality

Exploratory Data Analysis:
- Correlation matrix
- Bivariate analysis
- Multivariate analysis

Model Construction:
- Regression models

The variables can be divided into three categories
- Performance variables: Discharge pressure and flow
- Control variables: Speed
- Monitoring variables: Vibration and temperature

We seek to predict the **performance variables** based on the control and monitoring variables.

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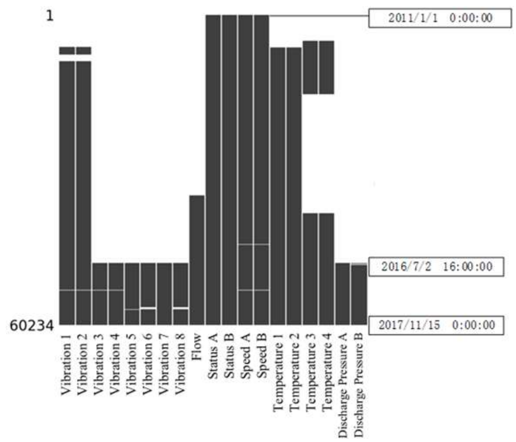
Case 1: Linear regression

Missing data

- The records available from 2011/1/1 to 2017/11/15
- Measurements were gradually introduced
- Records only from 2016/07/02 to 2017/11/15 have all the variables



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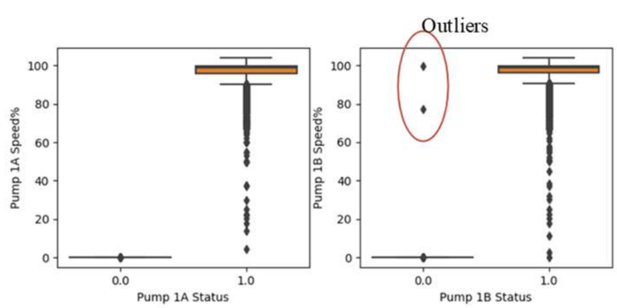
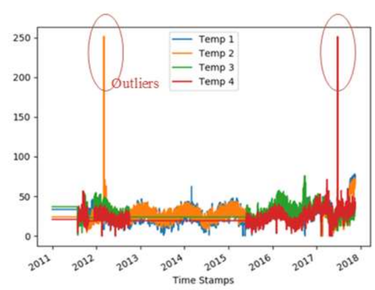
Case 1: Linear regression

Outliers

- Some obvious outliers can be excluded by univariate visualization.
- Also, some extremely high temperatures are clearly unreasonable.



The speeds of different status.



The temperatures

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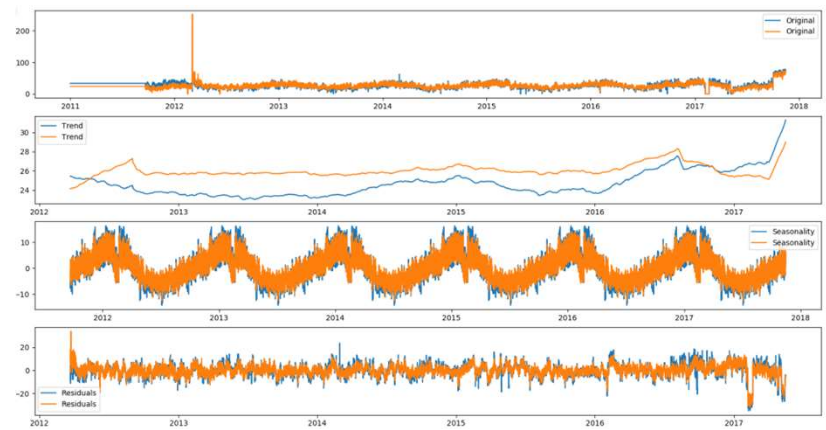
Case 1: Linear regression

Seasonality

- The residuals of the temperature are better options in the analysis.



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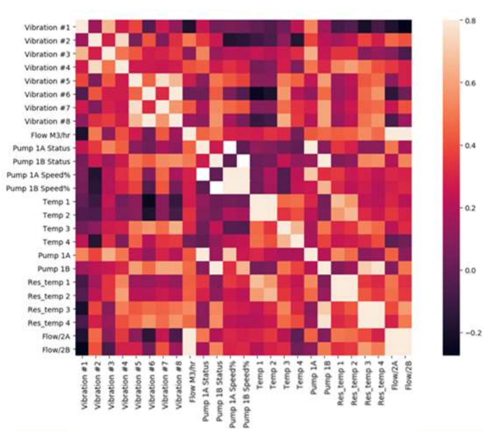
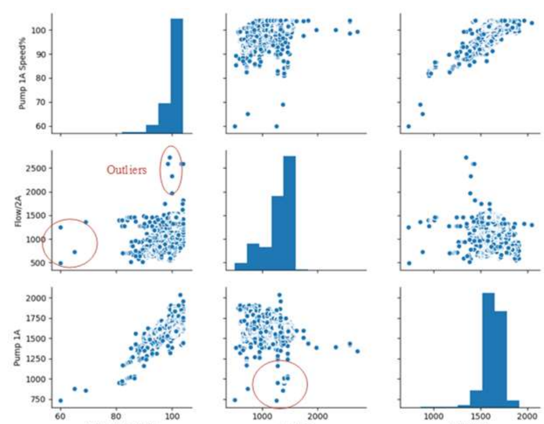
Case 1: Linear regression

Correlation & Scatter Plot





- Strong connection between **speed** & **pressure**

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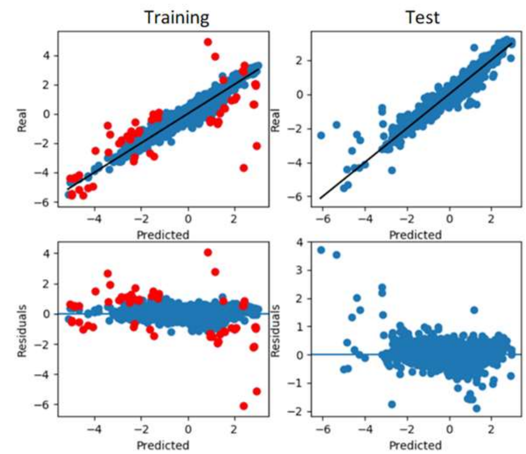
Case 1: Linear regression

Linear Regression

- **Speed ➔ Pressure**
- The R^2 values
  - 0.957 for Pump A
  - 0.952 for Pump B.



Early warning symptom

Symptoms = max(Threshold — Residuals, 0)

where Residuals =| Pressure(Real) – Pressure(Predicted) |

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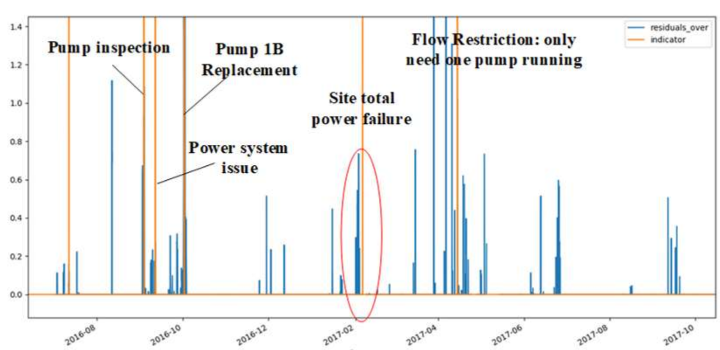
Case 1: Linear regression

Anomaly detection

- Threshold is set as 0.45.
- Continuous deviation of the residuals may be treated as an early warning signal.



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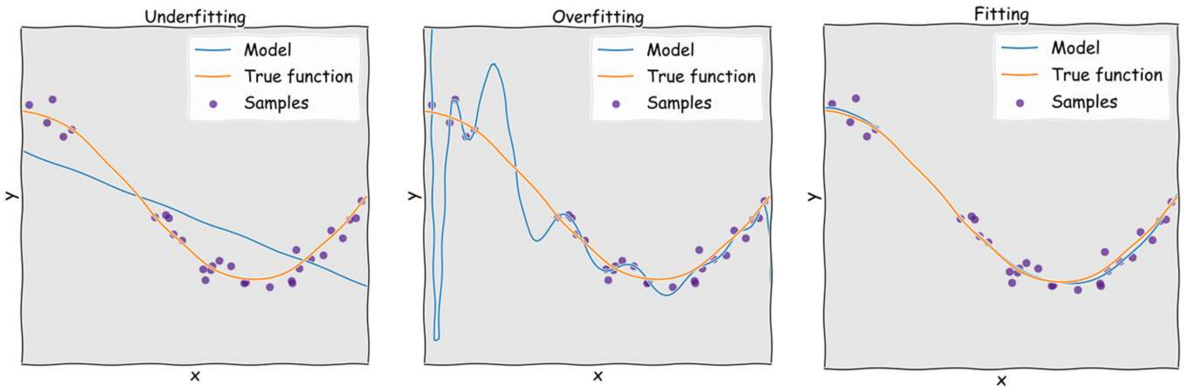
Model Complexity

- Under-fitting and Over-fitting



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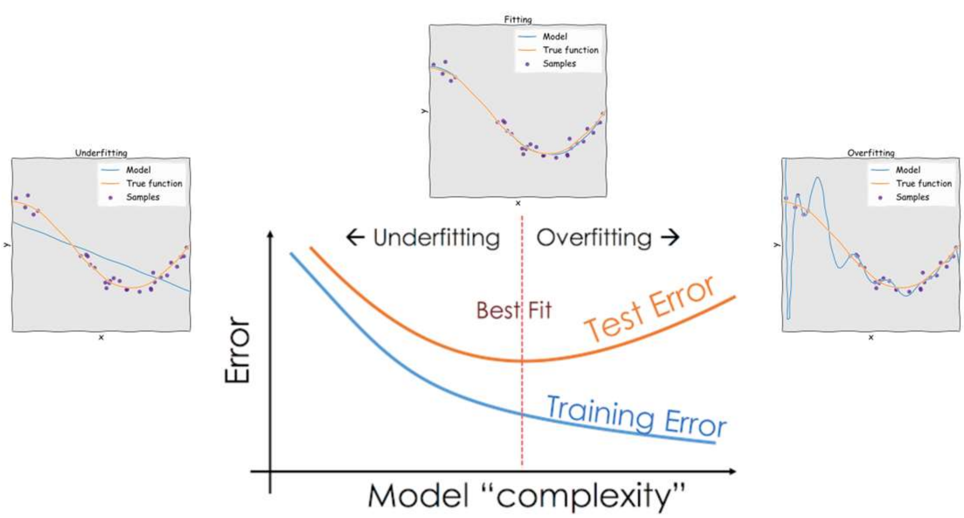
Overfitting and Underfitting



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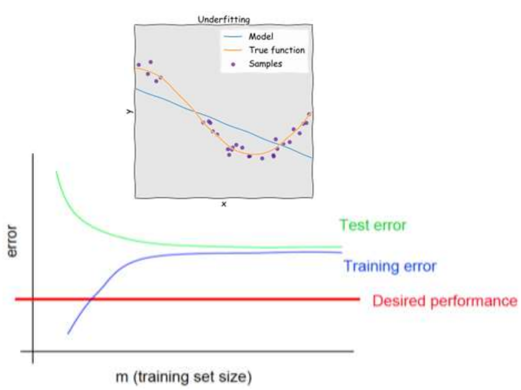
Overfitting and Underfitting

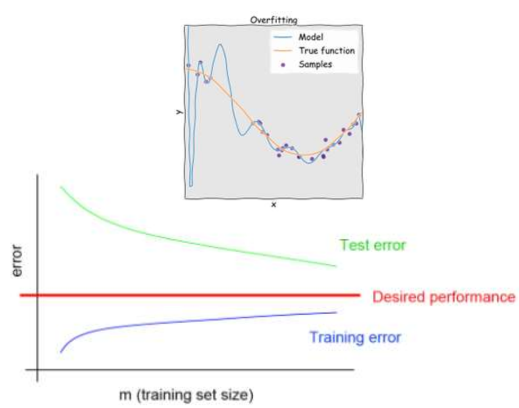
	Overfitting	Underfitting
Model Complexity	Higher	Lower
Degree of Training	More	Less
Size of Data	Smaller	Larger

Overfitting and Underfitting

- How to detect?



Underfitting



Overfitting

Hyper-Parameter Tuning

- Hyper-parameter
  - Not trainable unlike model parameters
  - Quite impactful on the model performance
  - Usually done with cross validation for more reliable performance evaluation
- Manual tuning using experience
- Grid search
  - Commonly used but time consuming
- Random search
- Bayesian optimization
  - Assuming Gaussian process as the objective to be optimized
  - Posterior of GP given samples
  - Relatively easy-to-compute acquisition function

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Combining Learners

- No single learner performs consistently better than others
- Performance can be improved by combining base learners
- Diversity vs accuracy of base learners
- Two questions:
  - How to generate diverse learners?
  - How to combine the predictions for best results?

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Generating Diverse Learners

- Different models
- Different hyperprameters
  - # of neurons in DL
  - k in k-nearest neighbor
  - error threshold in decision trees
  - kernel function in support vector machine
- Different input representation
  - Multiple sensors
  - Random subspace (of features)
- Different training sets
  - subsets of training set (bagging or boosting)
  - Partitioning of the training set

Combining Predictions

- Two major approaches
  - Parallel
    - Global: all base learners predict (e.g., voting)
    - Local: some learners are selected, requiring a gating model
  - Serial
    - Subsequent learners are trained where previous ones did not perform

Combining Prediction

- Voting
  - Simplest method to combine classifiers
  - Linear combination of predictions

$$y_i = \sum_j w_j d_{ji} \text{ where } w_j \geq 0, \sum_j w_j = 1$$

  - Classifier combination rules

	C_1	C_2	C_3
d_1	0.2	0.5	0.3
d_2	0.0	0.6	0.4
d_3	0.4	0.4	0.2
Sum	0.2	**0.5**	0.3
Median	0.2	**0.5**	0.4
Minimum	0.0	**0.4**	0.2
Maximum	0.4	**0.6**	0.4
Product	0.0	**0.12**	0.032

Combining Prediction

- Bagging
  - Short for "boostrap aggregating"
  - Base learners are trained with different subsets of training data
  - Base learners should be unstable so that their predictions on test sets are diverse

Steps:

- Given training set X of size N, n instances randomly drawn from X with replacement to make a subset $X_j, j = 1, \dots, L$.
- Base learners d_j are trained with X_j

Combining Prediction

- Boosting
  - In bagging, generating complementary base learners is by chance
  - In boosting, complementary base learners are actively generated by training the next learner on samples previous ones struggled.
  - In the original boosting algorithm (Schapire 1990)
    - Consists of 3 base learners and 3 subsets of samples
    - Train the 3 learner sequentially
    - Not expandible

The original boosting algorithm (Schapire 1990)

- During **training**
  1. Training set is divided into three: X_1, X_2, X_3
  2. Learner d_1 is trained on X_1 and tested on X_2
  3. Make a sample set X_2' with instances in X_2 misclassified by d_1 and the same number of instances in X_2 correctly classified by d_1
  4. Train d_2 on X_2'
  5. Test d_1 and d_2 on X_3 and make a sample set X_3' with instances in X_3 on which d_1 and d_2 disagree
  6. Train d_3 on X_3'
- During **testing**
  1. Given an instance, let d_1 and d_2 predict
  2. If they agree, the prediction is final; if they disagree, the prediction by d_3 is final.

AdaBoost Algorithm (Freund and Schapire 1996)

- Short for "adaptive boosting"
- Use the same training set over and over
- Arbitrary number of base learners
- Basic idea

  Sample instances that were misclassified with a higher probability

Training:
  For all $\{x^t, r^t\}_{t=1}^N \in \mathcal{X}$, initialize $p_1^t = 1/N$
  For all base-learners $j = 1, \ldots, L$
    Randomly draw $\mathcal{X}_j$ from $\mathcal{X}$ with probabilities p_j^t
    Train d_j using $\mathcal{X}_j$
    For each (x^t, r^t), calculate $y_j^t \leftarrow d_j(x^t)$
    Calculate error rate: $\epsilon_j \leftarrow \sum_t p_j^t \cdot 1(y_j^t \neq r^t)$
    If $\epsilon_j > 1/2$, then $L \leftarrow j - 1$; stop
    $\beta_j \leftarrow \epsilon_j / (1 - \epsilon_j)$
    For each (x^t, r^t), decrease probabilities if correct:
      If $y_j^t = r^t$, then $p_{j+1}^t \leftarrow \beta_j p_j^t$ Else $p_{j+1}^t \leftarrow p_j^t$
    Normalize probabilities:
      $Z_j \leftarrow \sum_t p_{j+1}^t; \quad p_{j+1}^t \leftarrow p_{j+1}^t / Z_j$
Testing:
  Given x, calculate $d_j(x), j = 1, \ldots, L$
  Calculate class outputs, $i = 1, \ldots, K$:
    $y_i = \sum_{j=1}^L \left(\log \frac{1}{\beta_j}\right) d_{ji}(x)$

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Thank you!

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