Machine learning in systems biology I (unsupervised)

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INTRODUCTION

WHAT IS MACHINE LEARNING?

'A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E'
- Tom M. Mitchell [Mit97]

HISTORY OF MACHINE LEARNING

1943	First publication of neural network [MP43]
1956	Dartmouth Summer Research Project (Birthplace of modern Machine Learning)
1965	Nilson Machine Learning for pattern classification [Nil65]
1966	Following years: Many setbacks in Artificial Intelligence called 'AI-Winters'
1995	Support Vector Machines are first introduced
2002	Torch first release (open source library)
2006	Geoffrey Hinton coins 'Deep Learning' [HOT06]
>2006	Companies such as Netflix, Facebook, Microsoft, Google fund projects/prizes in and use machine learning/artificial intelligence

WORKFLOW

Machine learning techniques follow a similar workflow.

1. Define Problem (scope, feasability)
2. Gather Data (assumptions, constraints)
3. Pre-process Data (cleanup, drop)
4. Analyze Data (define features, find correlations)
5. Prepare Data (transform, normalize, drop)
6. Evaluate Models (train/test, classify/regress)
7. Tune Model (cross validation, fine tune parameters)
8. Apply model to problems, learn more

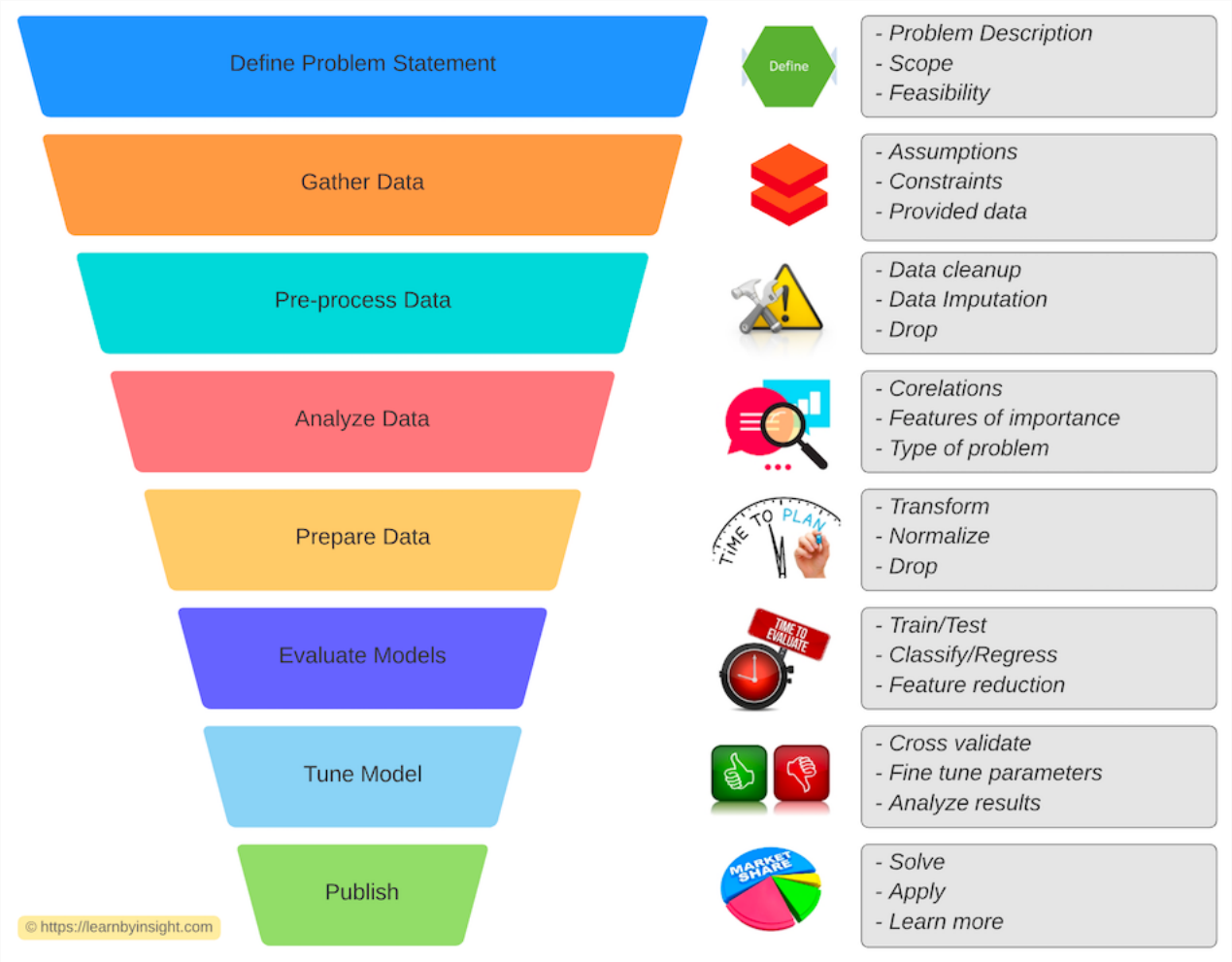

Figure 1: Machine Learning workflow [Mew20]

CONCEPTS

UNSUPERVISED AND SUPERVISED LEARNING

Supervised

- Fit model to labelled data (ie. with 'ground truth')
- Data is usually obtained experimentally or assigned by humans
- Previously labelled data can serve as testing set

Unsupvervised

- Data does not contain any labels (only inputs)
- Find structure in data (clustering, grouping)

Semi-supervised

- Combine partly labeled data with partly unlabeled data
- Can have huge performance benefits compared to unsupervised learning

TERMS

- Classification: Assign datapoints discrete categories (eg. cancerous, non-cancerous). Algorithms are called 'classifiers'.

  If discrete categories are mutually exclusive, we call them 'classes', otherwise 'labels'.
- Regression: Output continuous values (eg. predict free energy of protein system).
- Classification problems can also be solved with regression and thresholds/binning.
- Clustering: Predict groupings of similar datapoints.

TERMS

- Loss or Cost function:
  Measure deviation to ground truth in supervised learning.
  Implemented similarly in unsupervised situations.
- Parameters: Part of the model, will be adjusted by learning process of the model.
- Hyperparameters: Not part of the model but control learning process (eg. learning rate, number of iterations)
- Training: describes process of iterative learning and adjusting the parameters of the model to obtain better performance. Minimize the loss/cost-function.
- Validation: Use seperate dataset to test model.

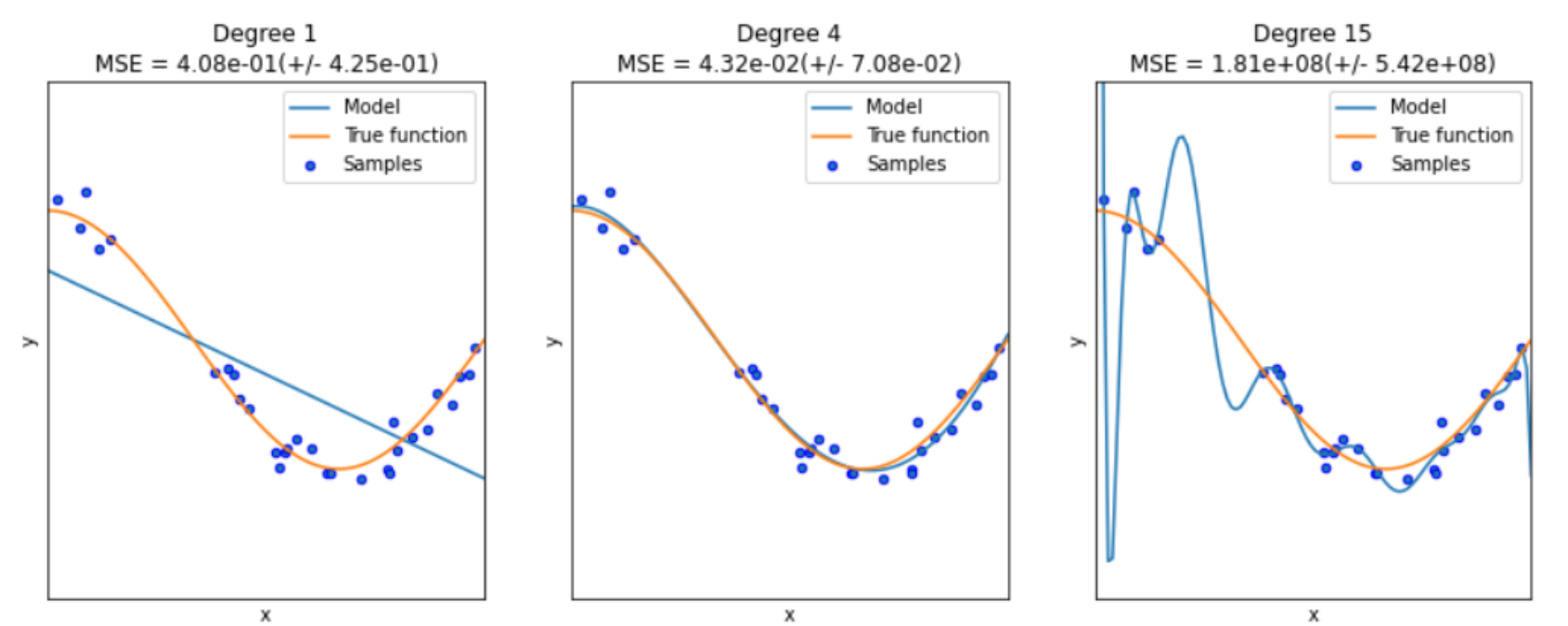

Figure 2: Underfitting, Optimal Fitting and Overfitting [Tri20]

INDUCTIVE BIAS AND VARIANCE

- Inductive Bias: Set of assumptions.
  Leads it to favour a particular type of solution over others.
  Often programmed in mathematical model.
  Example: Recurrent Neural Networks anticipate sequential dependencies
- Trade-off between bias and variance
  Different inductive biases typically lead to better performance, but higher constraints on the model.
  Lower bias makes fewer assumptions.
- Variance: How much does trained model change in response to training on different dataset.
- We want low bias and low variance.
- Low bias and low variance often conflict each other.
  $\Rightarrow$ Need to balance between them

MACHINE LEARNING TECHNIQUES

TRADITIONAL TECHNIQUES

BIOLOGY AGAIN

Questions?

LITERATURE

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