JPL-Caltech Virtual Summer School

Big Data Analytics

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Supervised Learning

Jet Propulsion Laboratory

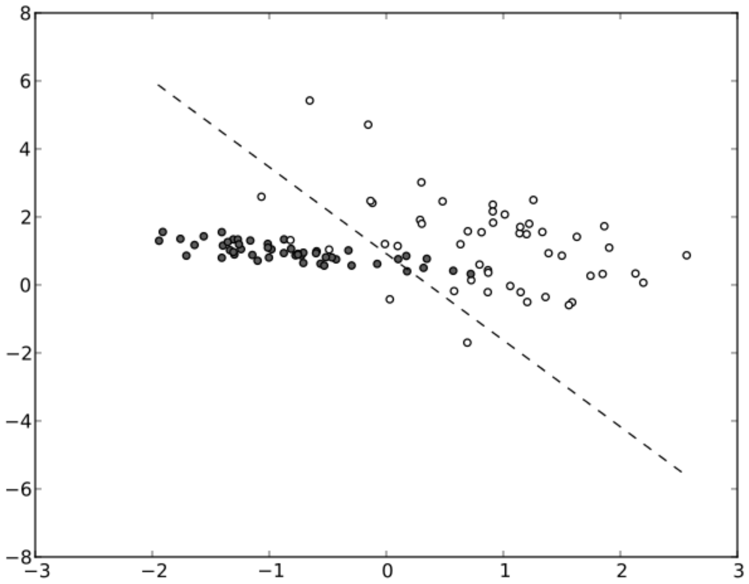
Keck Institute for Space Studies

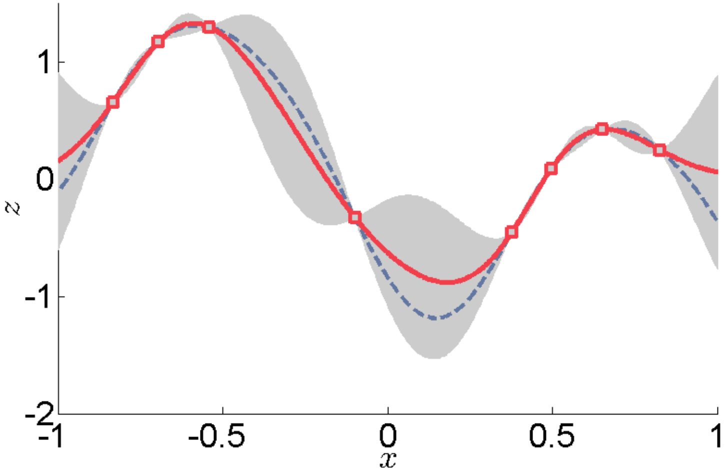
Sponsored by the Jet Propulsion Laboratory and by the Keck Institute for Space Studies, California Institute of Technology

Caltech

Outline

- Supervised Learning
- How to create a training set
- Steps
- Cross-Validation
- Overfitting

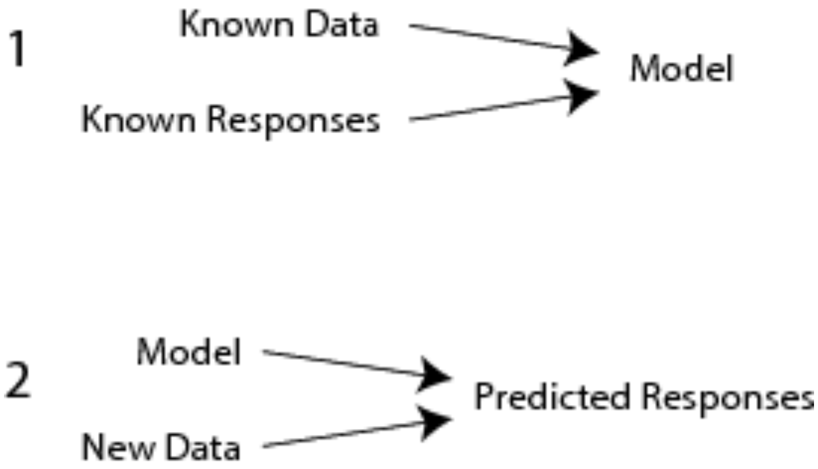




Pictures credit: Wikipedia.org

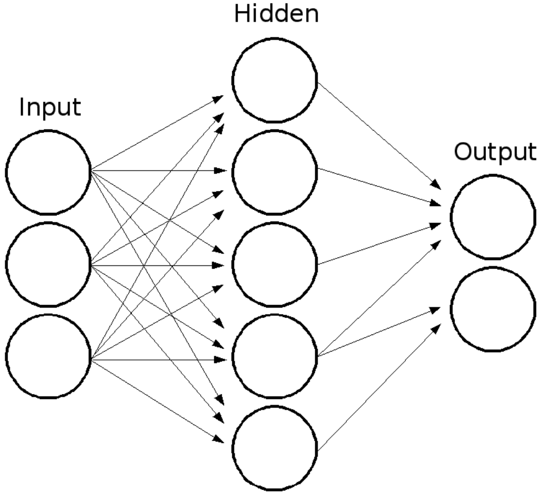
Supervised Learning

- For some examples the correct results (targets) are known and are given in input to the model during the learning process.
- Generalization: ability of a learning machine to perform accurately on new, unseen examples.



1 Known Data → Model
Known Responses → Model

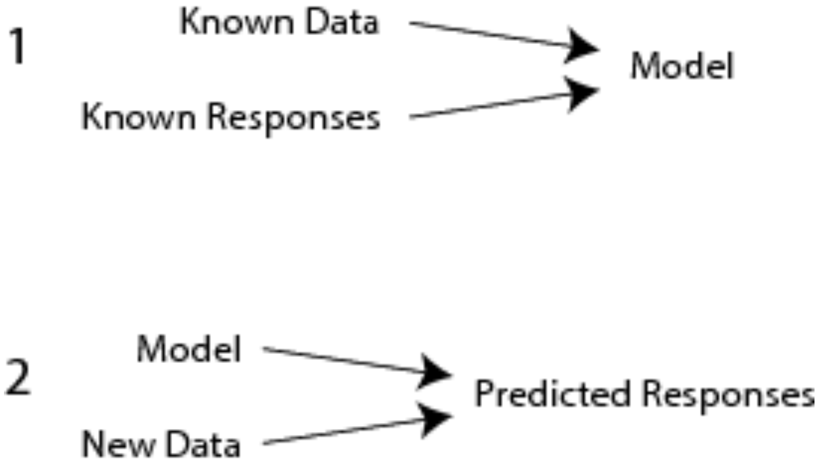
2 Model → Predicted Responses
New Data → Predicted Responses



Images credits: Mathworks

Supervised Learning

- Common tasks:
  - classification: categorical output, data can be separated in specific classes;
  - regression: for continuous outputs.



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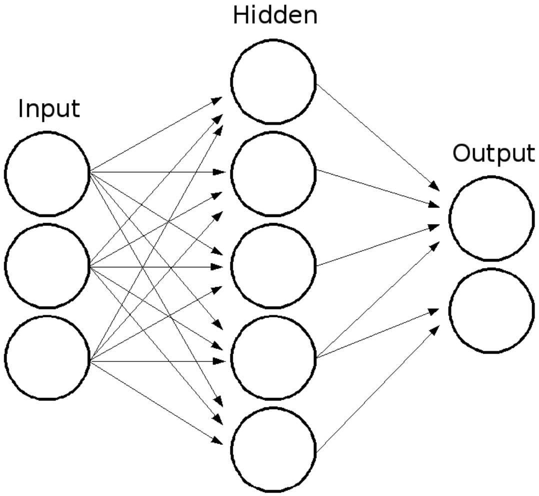


Images credits: Mathworks

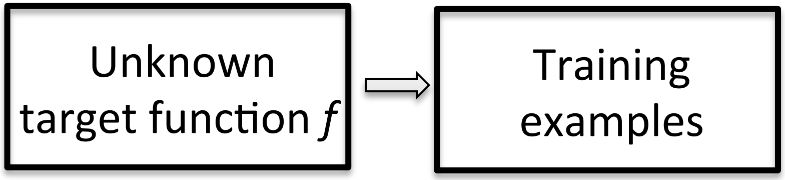
Supervised Learning

- Training data consists of a set of training examples $D = (\mathbf{x_1}, y_1),(\mathbf{x_2}, y_2),\ldots,(\mathbf{x_n}, y_n)$ where:
  - $\mathbf{x}_1, \ldots, \mathbf{x}_n$: input parameters (feature vector)
  - y : output value (target vector)
  - Example: credit approval
    - $\mathbf{x}$ = [age, gender, annual salary, current debt]
    - y = {accept, deny} = {+1, -1}

Training examples

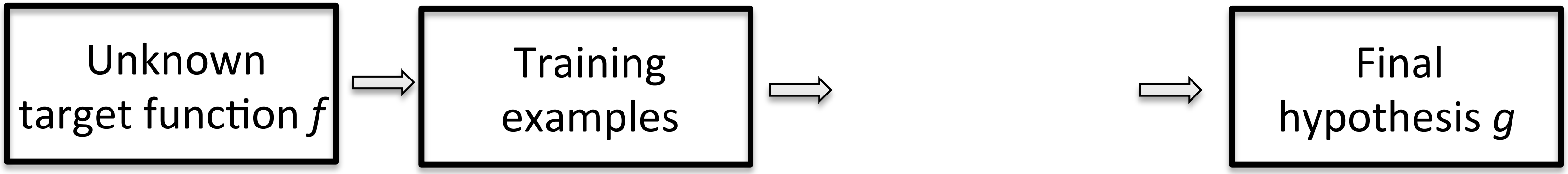
Supervised Learning

- Training data consists of a set of training examples.
- Target function: $f(\mathbf{x}_\mathrm{i}) = y_i$ (function to learn, unknown)
  - – example: ideal credit approval formula



Supervised Learning

- Training data consists of a set of training examples
- Ideal target function *f*
- Hypothesis: $g(\mathbf{x}_i) \approx y_i$ (approximate *f*, known)
  - – example: reliable credit score



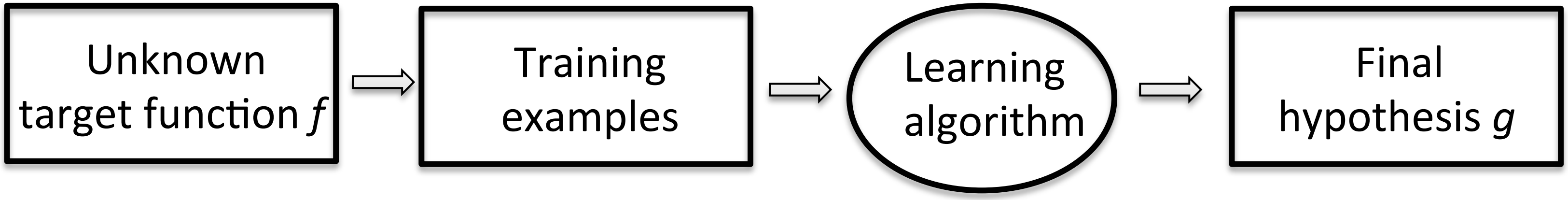
Unknown target function *f*

Training examples

Final hypothesis *g*

Supervised Learning

- Training data consists of a set of training examples
- Ideal target function *f*
- Hypothesis *g* that best approximate *f*
- Learning algorithm
  - – connect target function and hypothesis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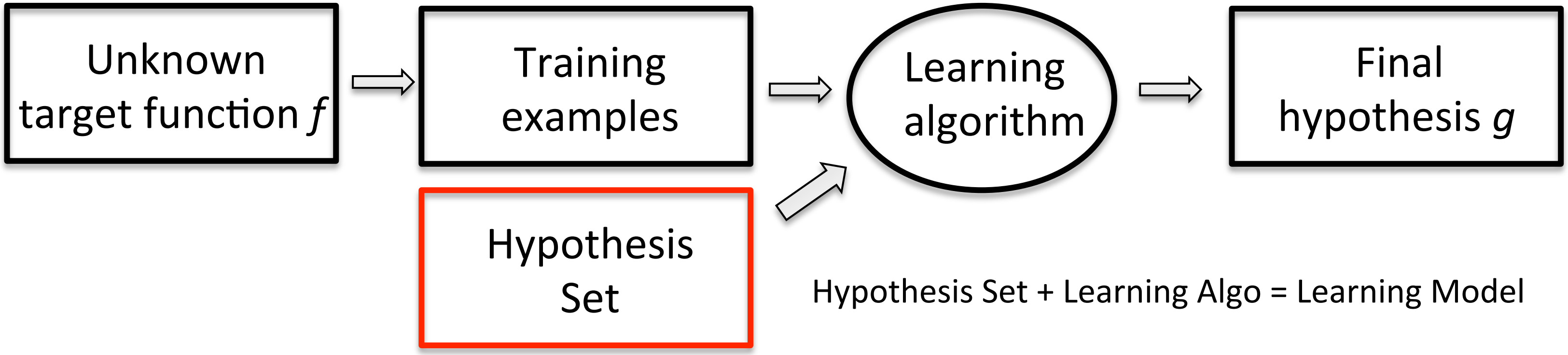
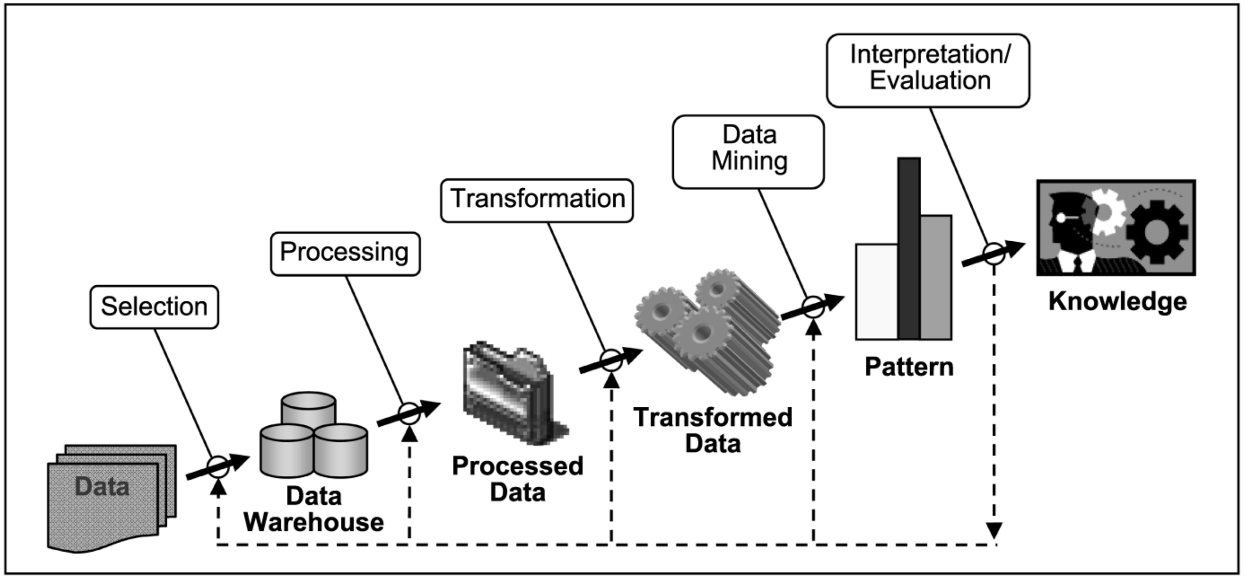
Supervised Learning

- Training data consists of a set of training examples
- Ideal target function *f*
- Hypothesis *g* that best approximate *f*
- Learning algorithm
  - – connect target function and hypothesis
- Hypothesis Set
- Predict new inputs: $y_{new}=g(\mathbf{x}_{new})$



Hypothesis Set + Learning Algo = Learning Model

Supervised Learning in a nutshell



Supervised Learning in a nutshell

① Define the data to be used as a learning set

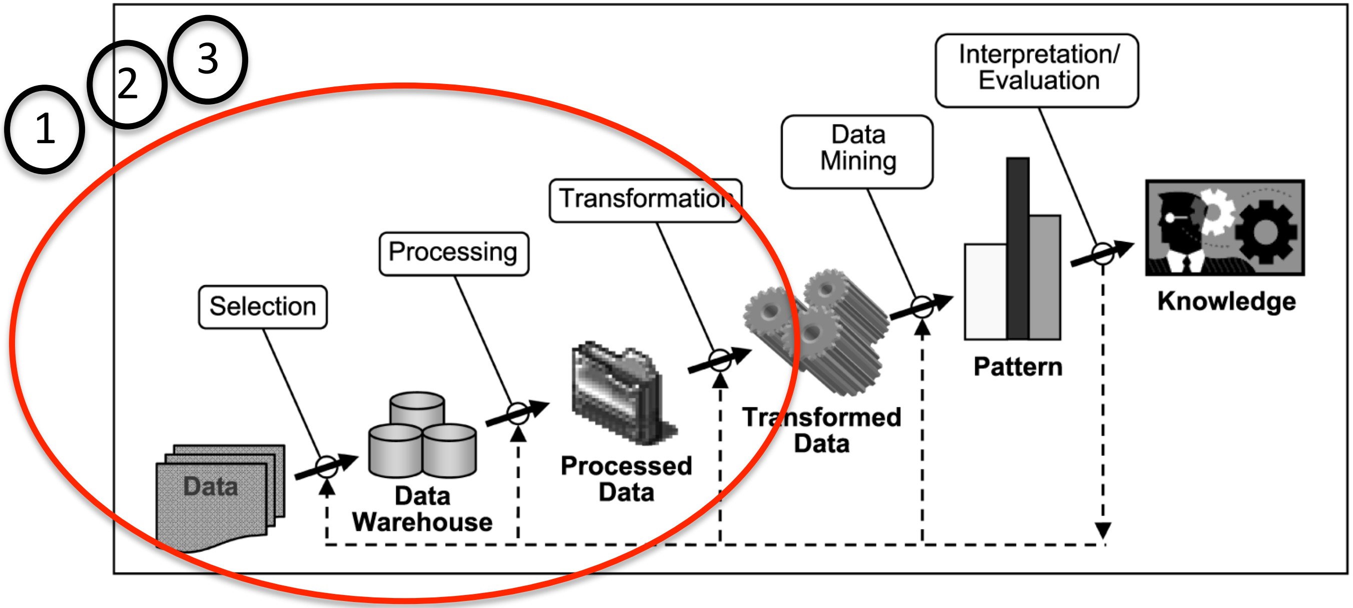
- eg, handwriting analysis: single character or entire words?

② Prepare the training set

- eg, create training, validation and test sets

③ Transform the input data in feature vectors (X,Y)

- eg, extract/select features to avoid the curse of dimensionality



Supervised Learning in a nutshell

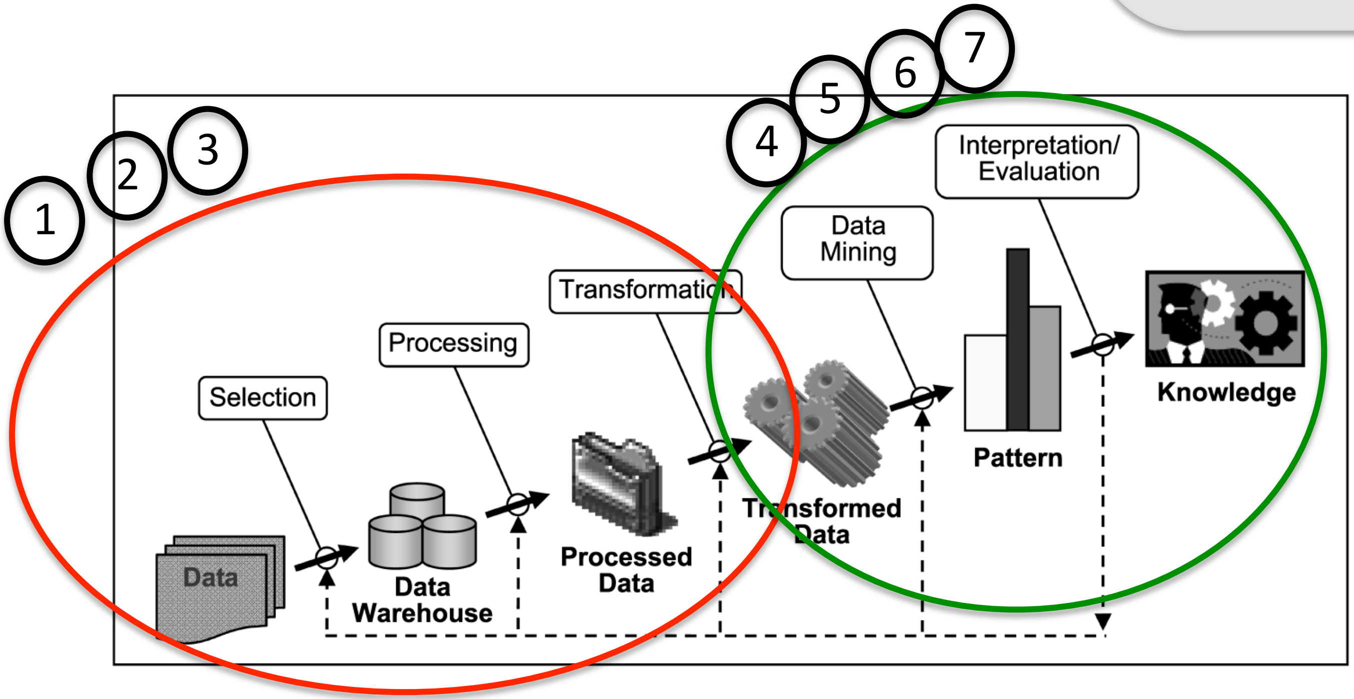
④ Choose the learning model
- eg, Neural Network and Back propagation

⑤ Choose a validation model
- eg, cross validation, random splits, etc

⑥ Run the algorithm, compute the accuracy and update until satisfied
- eg, minimize the loss, minimize the MSE, etc

⑦ Use final model to make predictions

Supervised Algorithms
Neural Networks (MLP)
Boltzmann Machines
RBM
Decision Trees
Nearest Neighbor
Naive Bayes Classifiers
Bayesian Networks
GPR
...

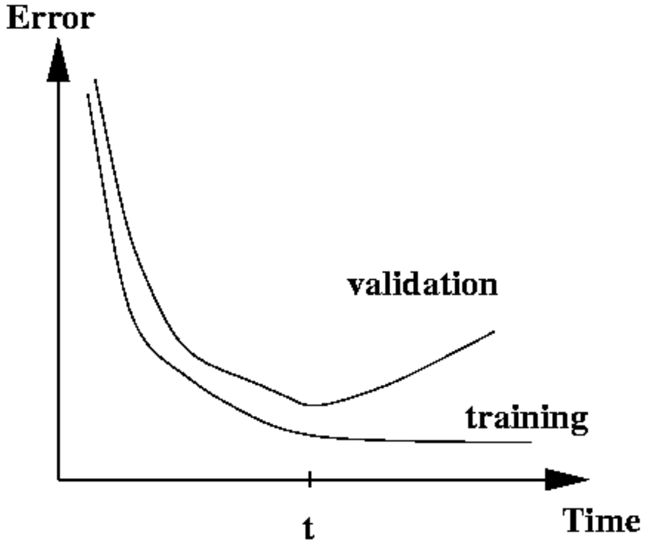


Learning set

- All eventualities must be covered: the learning dataset must be representative of the underlying model.
- Split the data in three independent data sets:
  - training set;
  - validation set;
  - test set.

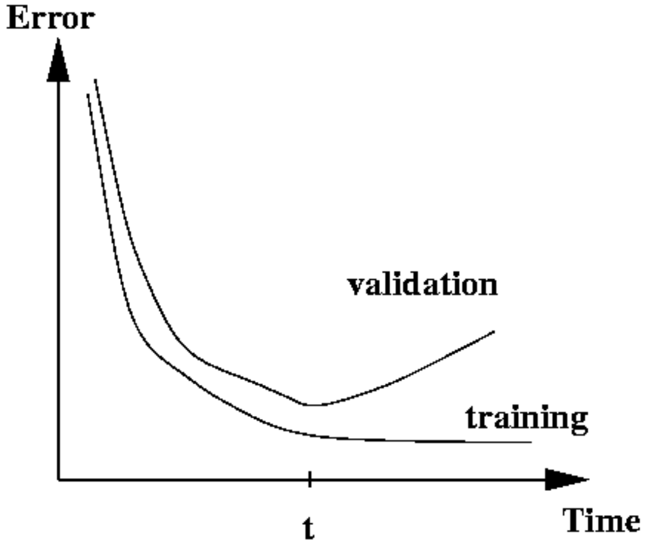
Training Set

- **Training set**: a set of examples used for learning, where the target value is known.
- The goal of the learning algorithm is to build a model which makes accurate predictions on the training set.
- Training set accuracy does not give a good indication about the generalization power of the model.
- Add a Validation set.



Validation Set

- Set of examples used to tune the architecture of a classifier and estimate the error.
- Used for model selection.
- The validation data has to be representative of the range of inputs the classifier is likely to encounter.
- How to create it?
  - – gather new data;
  - – random split:
    - 80-20
    - cross-validation

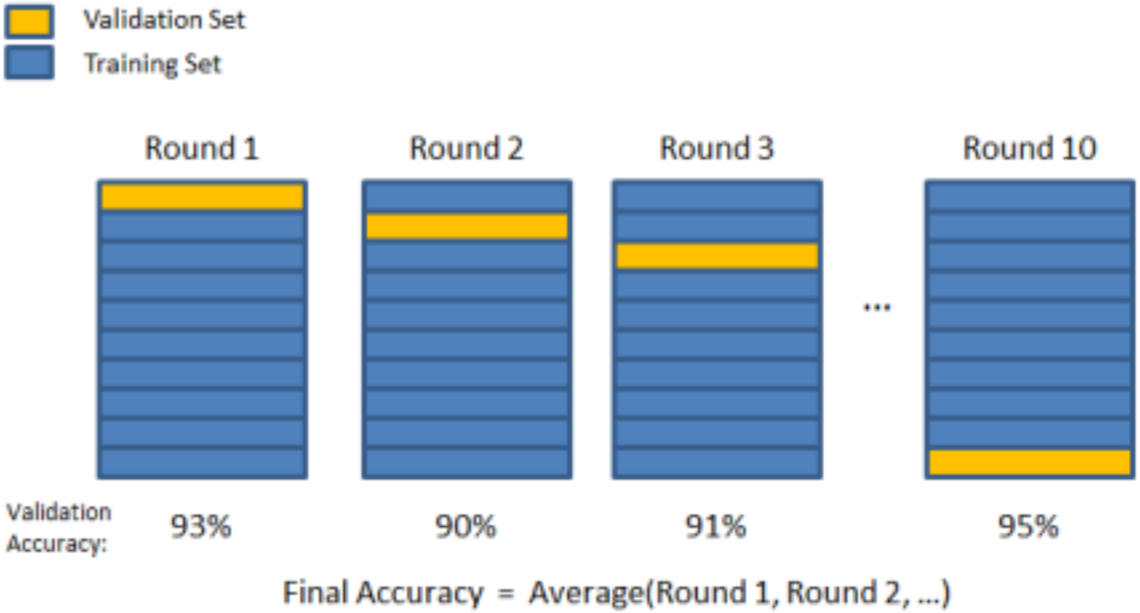


Cross-Validation

- C-V techniques are used for assessing how the results of a statistical analysis will generalize to an independent data set.
- Exhaustive Cross-Validation
  - leave one out cross validation (LOOCV)
  - leave p-out cross validation
- Non-exhaustive Cross-Validation
  - *k*-fold cross validation
  - repeated random sub-sampling validation
- Choose also according to your model/task.

K-fold cross-validation

- How it works:
  - randomly partition the original into *k* subsamples;
  - of the *k* subsamples, one is retained as the validation data for testing the model, and the remaining *k* − 1 are used as training data;
  - the process is then repeated *k times*, with each of the *k* subsamples used exactly once as the validation data;
  - the *k* results can be averaged (or otherwise combined) to produce a single estimation.



Picture credit: chrisjmccormick

Repeated random sub-sampling

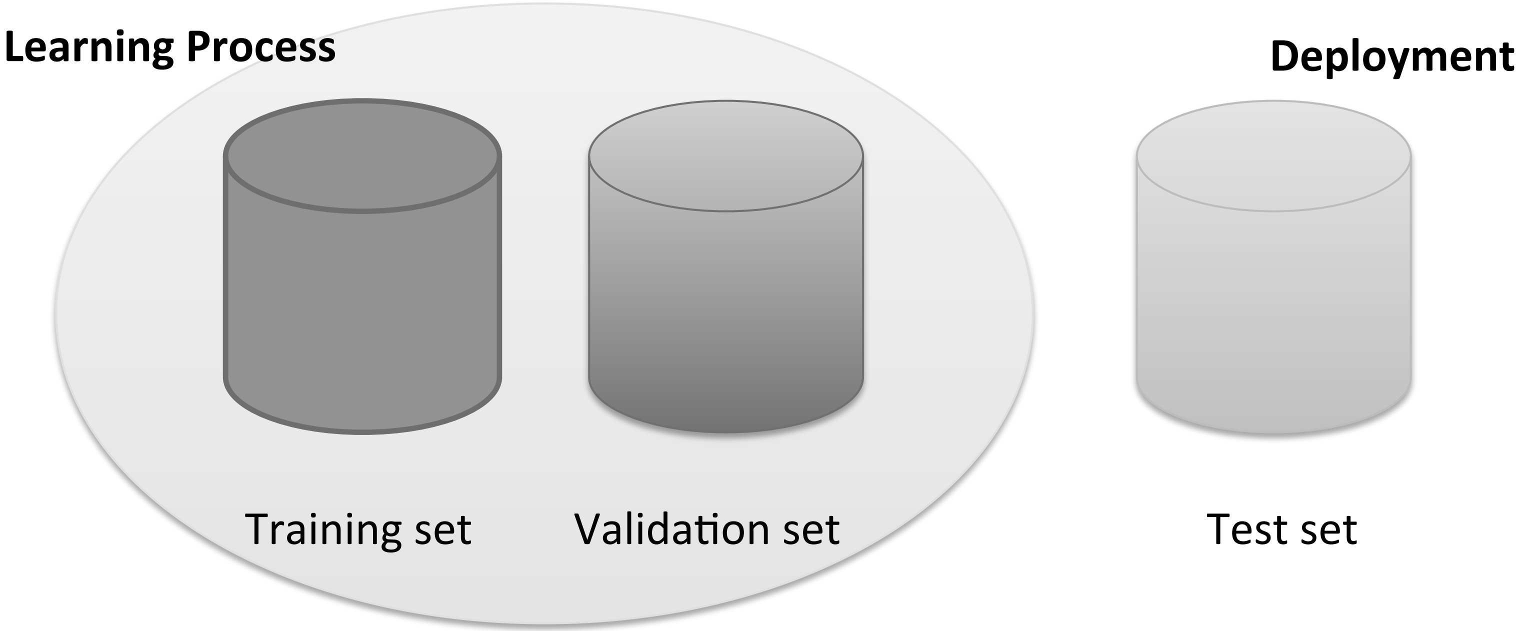
- Repeated Random Sub-Sampling
  - at each step: randomly split the dataset into two subsets: training and validation;
  - compute the validation errors.
  - average the results over the splits.
- Advantage: proportion of the sets not dependent on the number of folds.
- Disadvantage: some samples may never be selected for validation, some may be selected more than once.

LOOCV

- Leave One Out Cross Validation
  - use a single **observation** from the original sample as the validation data, and the remaining observations as the training data;
  - repeat n-times such that each observation in the sample is used once as the validation data;
  - computationally expensive.

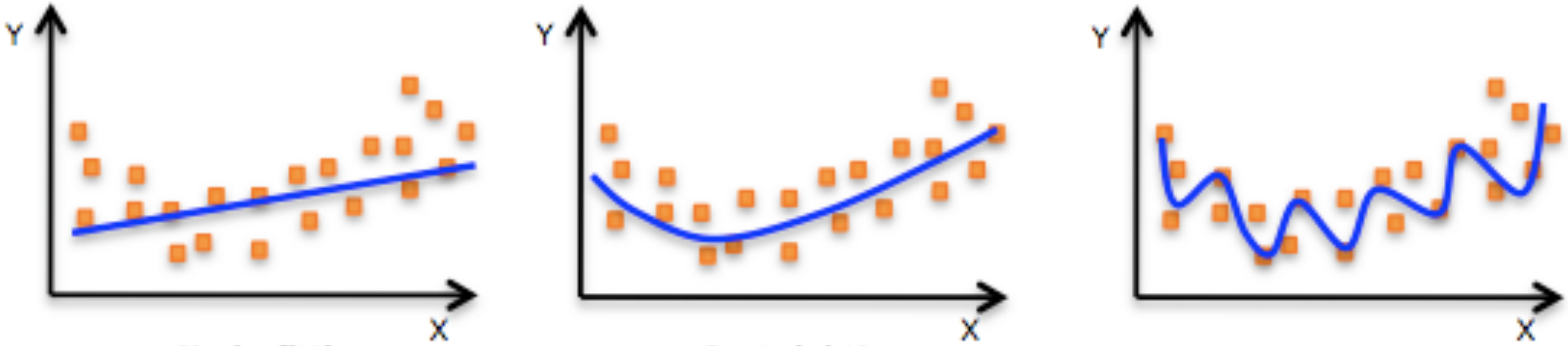
Test Set

- **Test set**: used only to assess the performances of a fully trained classifier.
- It is **never used** during the training process so that the error on the test set provides an unbiased estimate of the generalization error.



A common problem: OVERFITTING

- Model is not be able to generalize.
- Learn the “data” and not the underlying function.
- Performs well on the data used during the training and poorly with new data.
- How to avoid: cross-validation, early stopping, regularization, Bayesian priors, model comparison.



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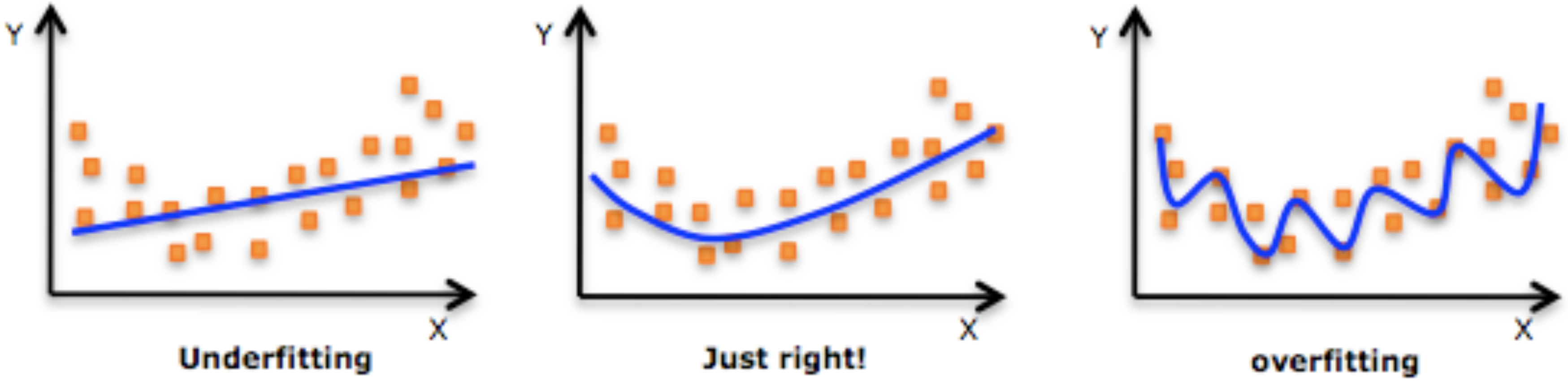

Underfitting

Just right!

overfitting

Overfitting in supervised learning

- Example: overfitting in supervised learning.
- Blu is the training error, red the validation error, over time.
- If the validation error increase while the training error decrease it is a warning sign for overfitting.

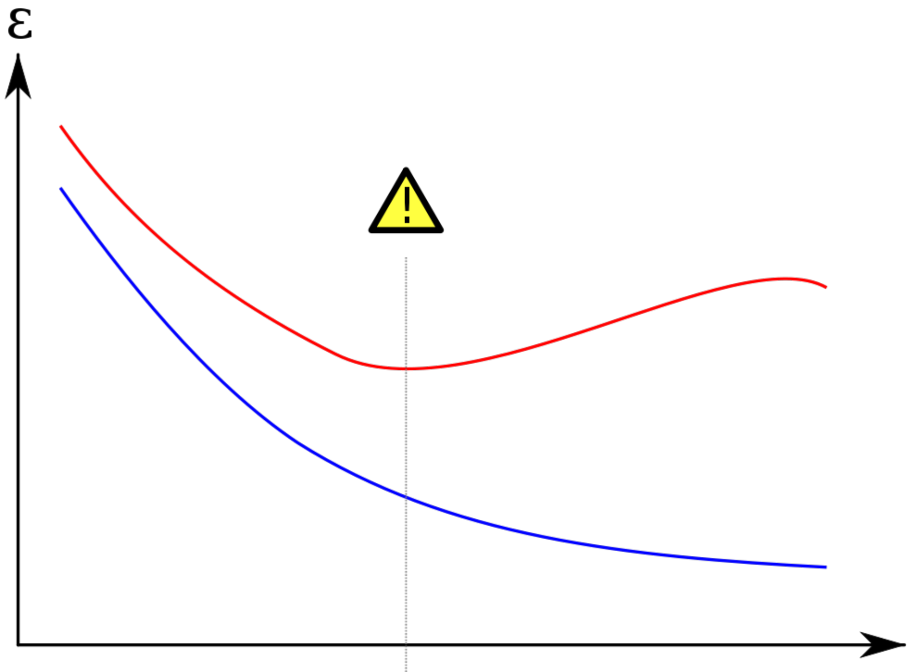

Image credit: Wikipedia.

Summary

- Supervised Learning: general concepts
- Target function and hypothesis
- Training, Validation and Test Set
- Different types of cross-validation
- Overfitting

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