Big Data Computing

Master's Degree in Computer Science

2020-2021

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SAPIENZA
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Recap from Last Lecture(s)

2 unsupervised learning techniques to extract "structural" patterns from raw data

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- Formalized as an NP-hard optimization problem
- K-means and its variants as effective heuristics that work in practice

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Principal Component Analysis (PCA)

- Reduce data dimensionality
- Automatically extract features from raw data
- Resort to computing the eigenvectors and eigenvalues of the covariance matrix

SUPERVISED LEARNING

Human vs. Computer

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- Example
  - Task/Problem: Find the maximum element of a list of 1 million unsorted numbers
  - Solution/Algorithm: Scan all the numbers in the set and keep track of the largest found "so far"
  - Code/Program: Encode the algorithm above into one specific programming language (e.g., C/C++, Java, Python)

Programming a Computer

Problem

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Solution/Algorithm
explicitly designed by human

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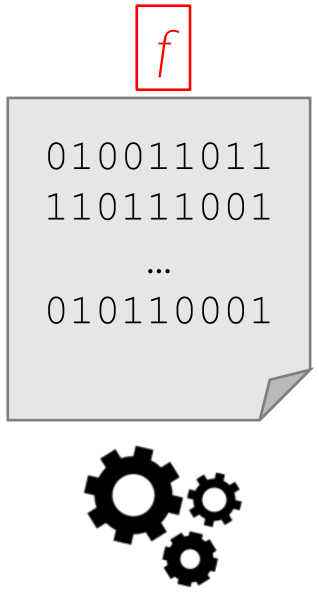
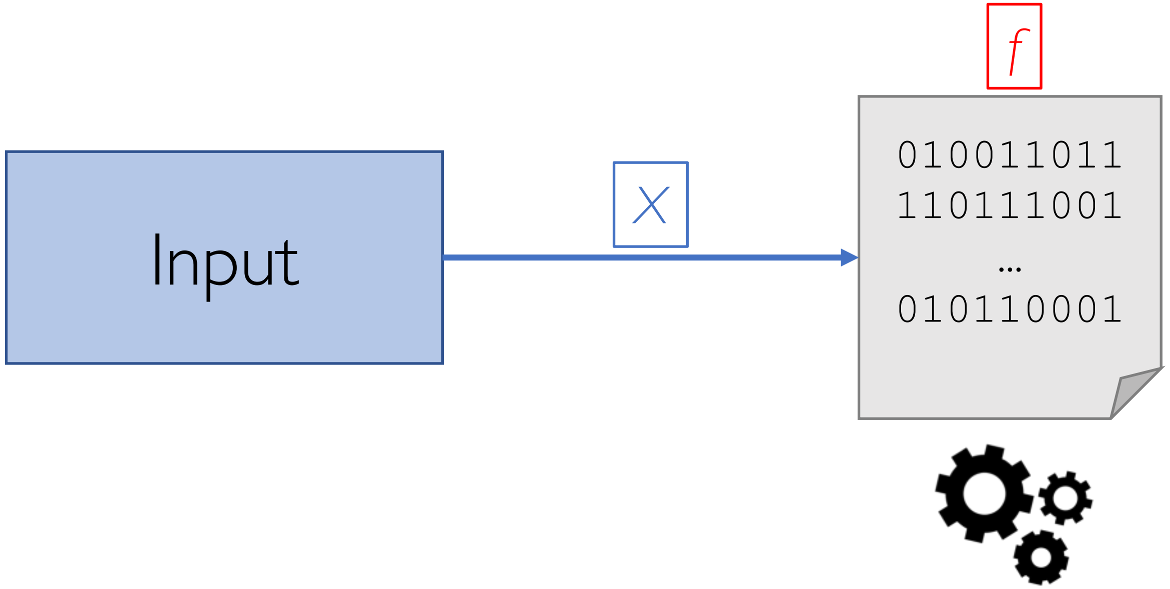
```
010011011
110111001
...
010110001
```

Encoding of
Computable Function f

Programming a Computer



Programming a Computer



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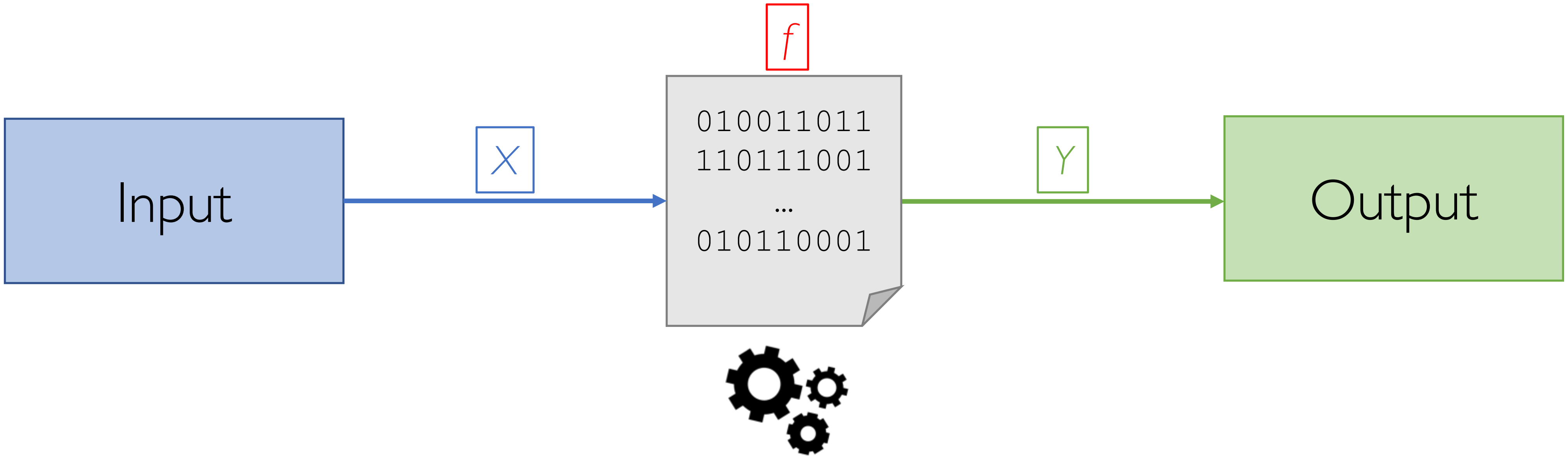

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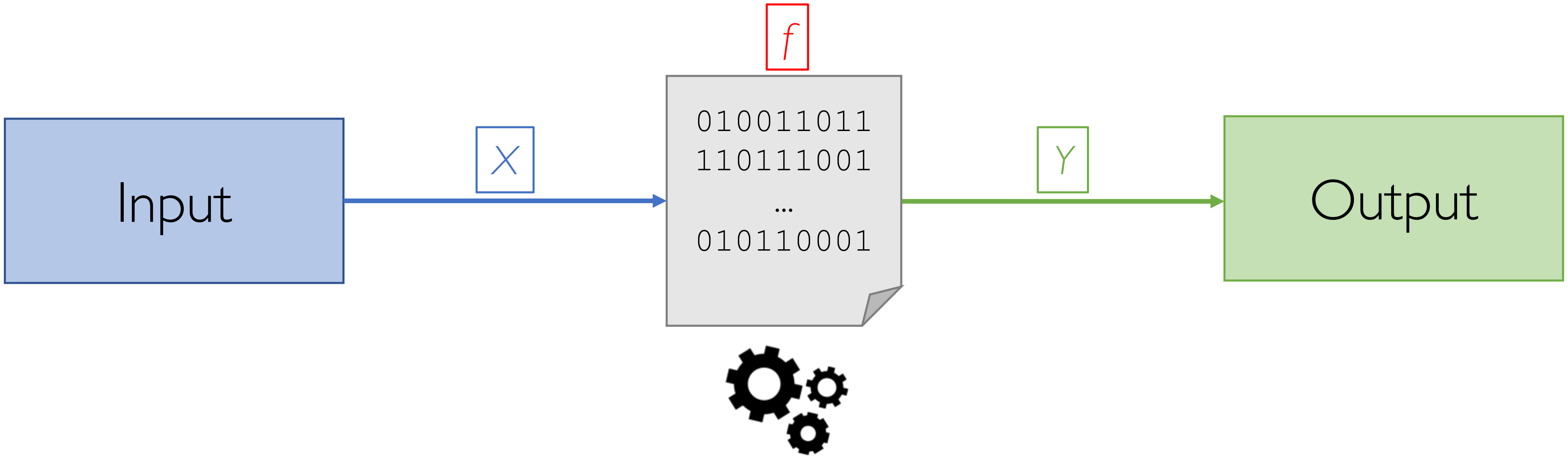

$$\boxed{Y = f(X)}$$

Can We Always Do That?

Chihuahua or Muffin?

[Copyright @teenybiscuit]

Chihuahua

Muffin

Programming vs. "Training" a Computer

- There exist some problems like the chihuahua vs. muffin above which are too hard to be solved directly

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$\Downarrow$

$\boxed{\text{Programming vs. "Training" a Computer}}$

"Training" a Computer

Problem

Labeled Data

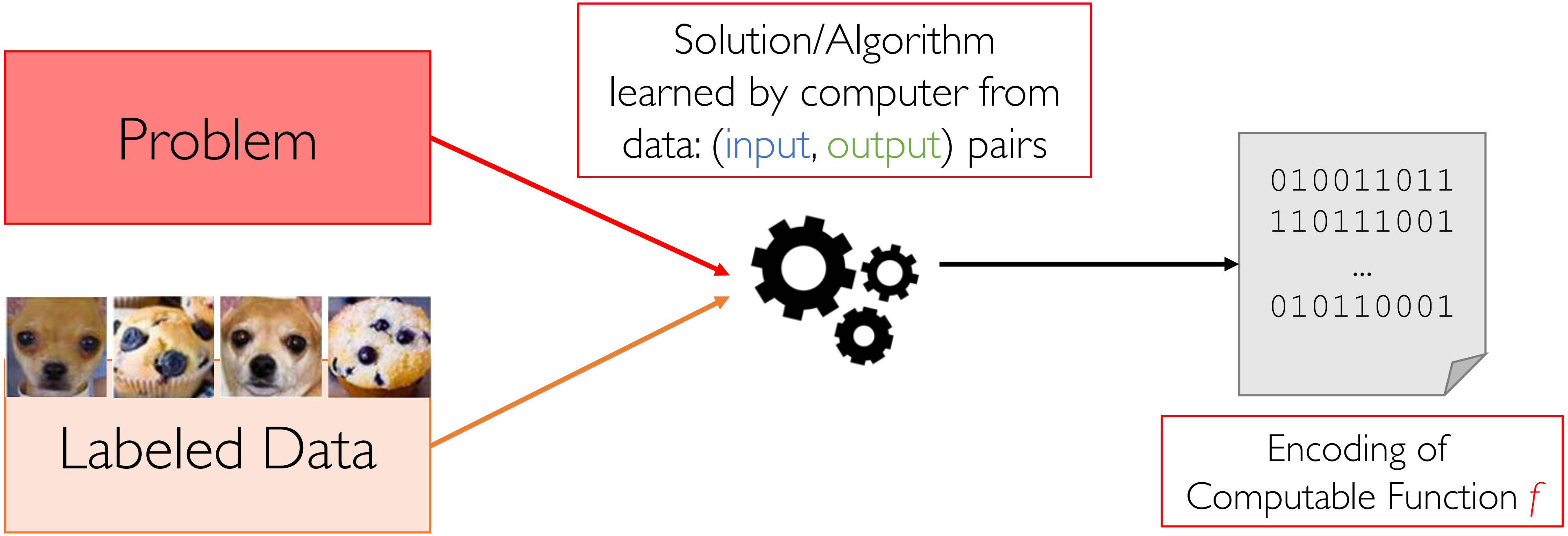
"Training" a Computer

Solution/Algorithm learned by computer from data: (input, output) pairs

Problem

Labeled Data

"Training" a Computer



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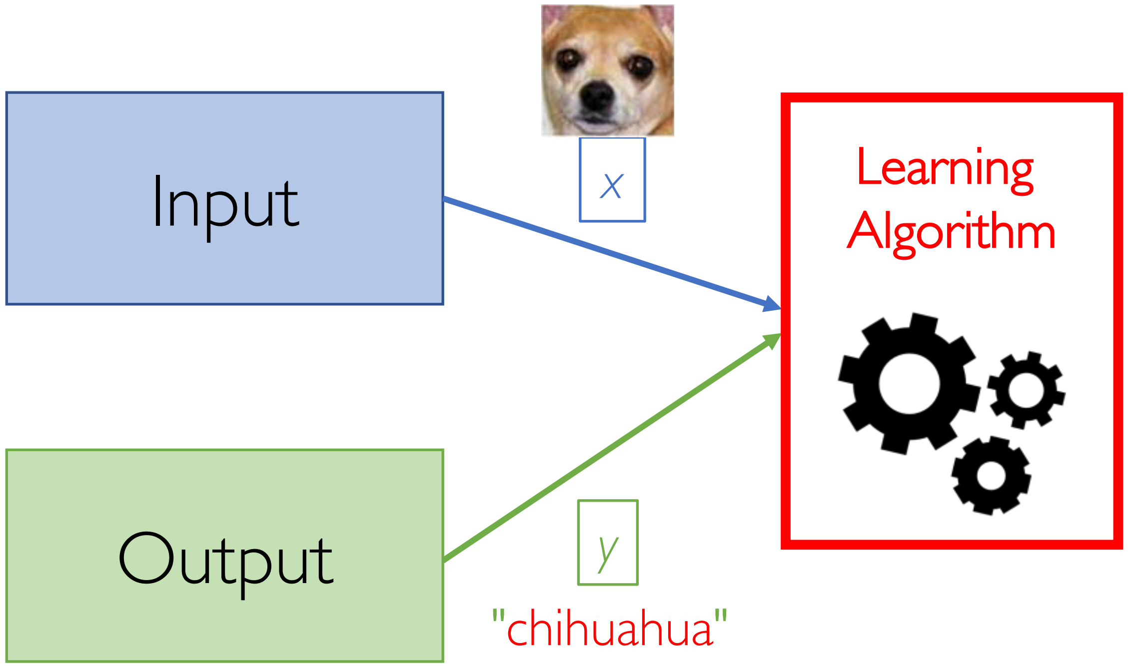

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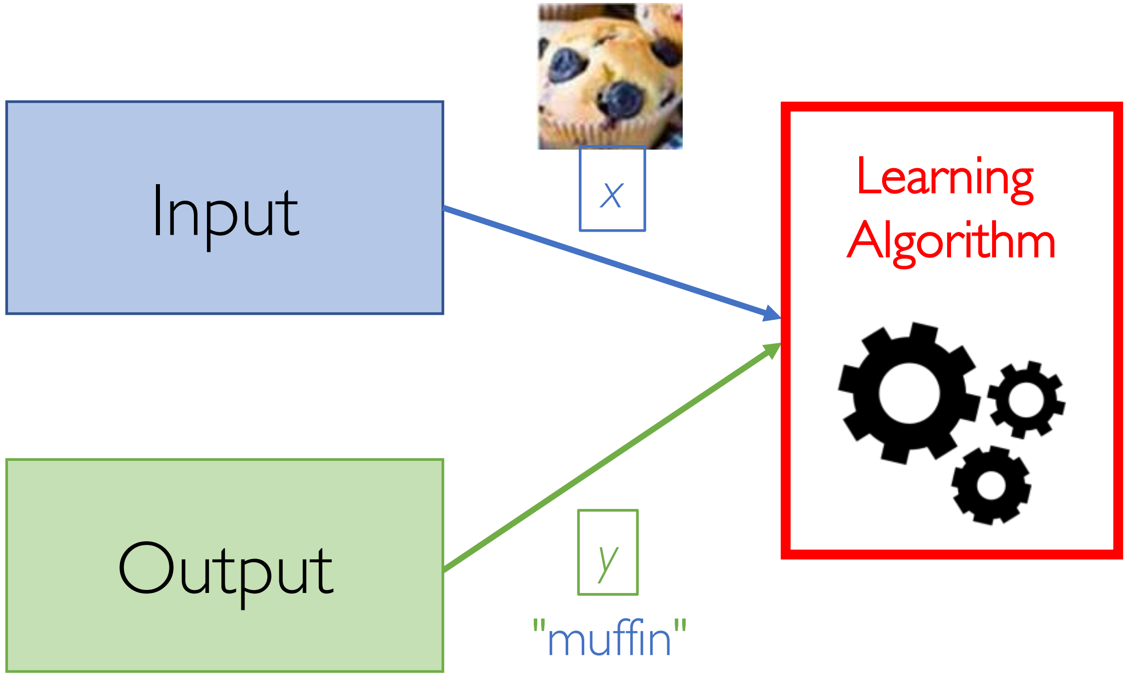

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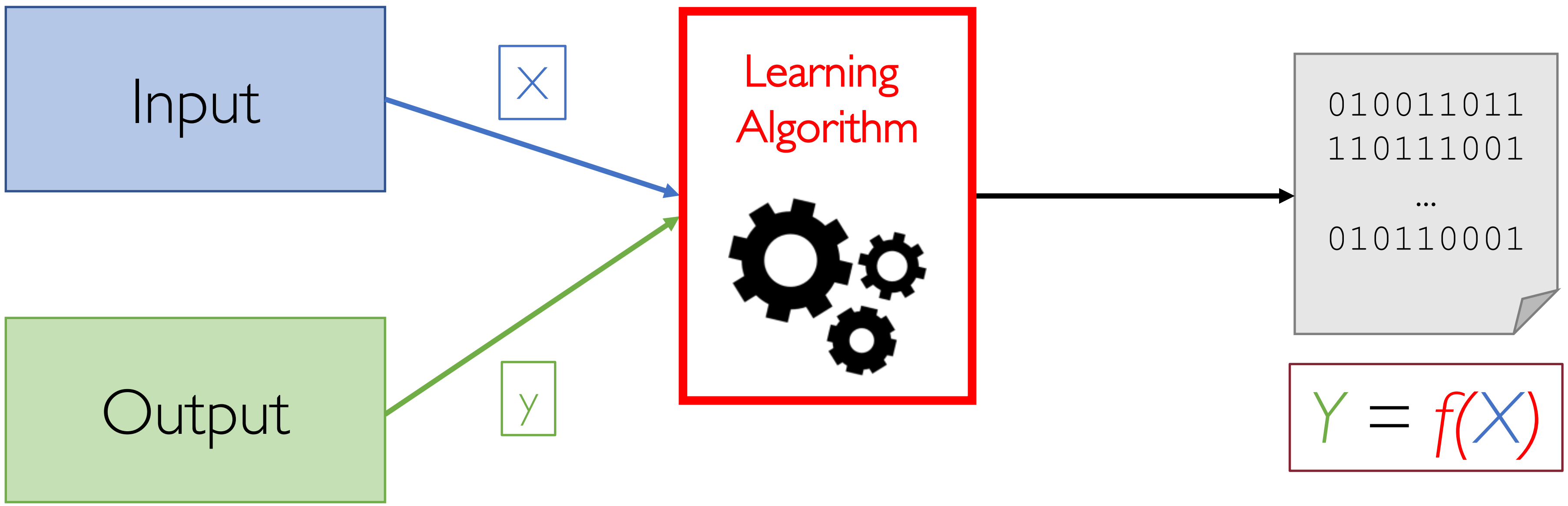

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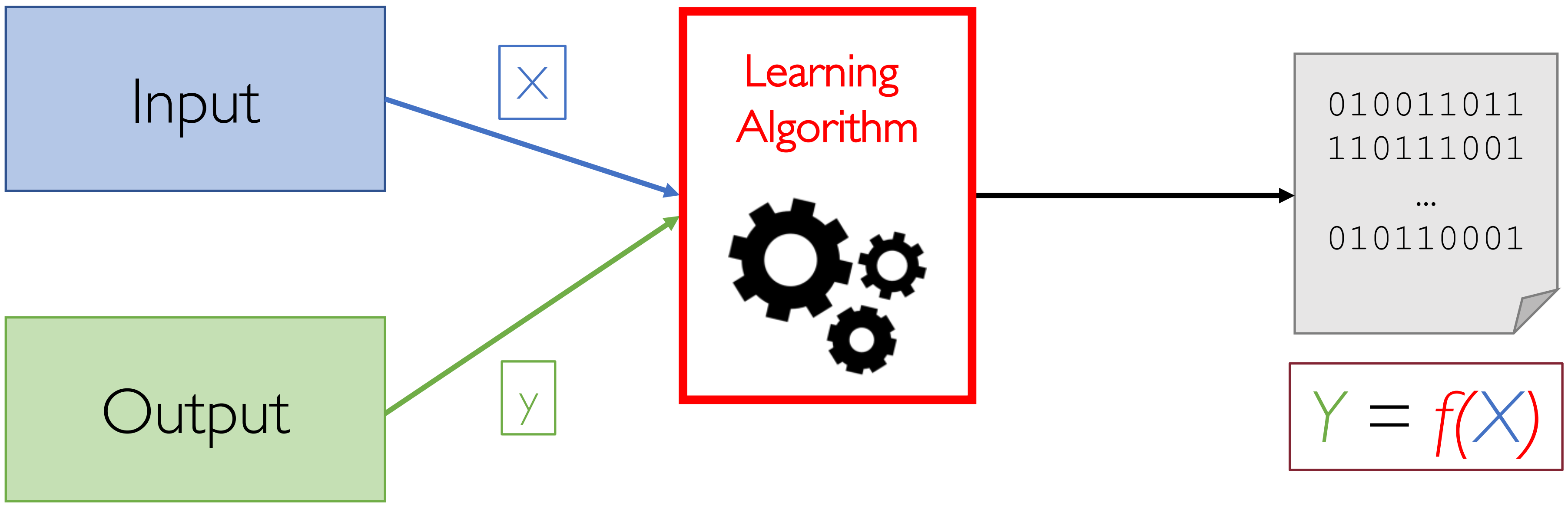

Eventually, the function f is learned by the learning algorithm from a (large) set of labeled data

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Arthur Samuel

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"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 Mitchell

Machine Learning: Taxonomy

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Unsupervised Learning

Extract patterns from input data without any information on the output (target) variable

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Regression

The target y we want to predict is a **continuous real value**

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Regression

The target y we want to predict is a continuous real value

e.g., y = price of a house

Classification

The target y we want to predict is a discrete value

e.g., y = spam/non-spam

The Supervised Learning Pipeline

The Stages of Supervised Learning

0. Be sure your problem needs <u>actually</u> to be tackled using Machine Learning techniques

(i.e. there is no point in adopting any fancy ML solution if it can be solved "directly"!)

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3. **Model training:** "build" one (or more) learning models

4. **Model selection/evaluation:** pick the best-performing model according to some quality metrics

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- Supervised Learning requires labeled data which may be even harder to get
  - e.g., emails + spam/non-spam tags
- Might involve combining multiple and heterogeneous data sources

Feature Engineering

Domain Objects

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Collected data need to be encoded with a machine-readable format

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Domain Objects

i-th object

0.27	3.8	1.12	…	4.75	…	…	56.9
0.0	3.65	0.04	…	6.81	…	…	1.0

…

6.94	5.4	0.9	…	3.92	…	…	8.2

Each domain object is translated into a *n*-dimensional vector of features

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i-th object

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j-th feature

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- Each feature is a property of an instance of our domain
  - e.g., **`number_of_bedrooms`** in the case our domain objects are "houses"

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  - e.g., **`number_of_bedrooms`** in the case our domain objects are "houses"
- Each feature can be either derived locally from an instance
  - e.g., **`annual_income`** of a person
- Or it can be the result of more complex computation involving the whole data collection
  - e.g., **`tf-idf`** of a word of a document w.r.t. a corpus

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- Require in-depth knowledge of the specific domain of application
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- Tedious and time-consuming process
- Techniques to **automatically** learn data representation (i.e., features):
  - K-means clustering, PCA, autoencoders (**unsupervised**)
  - Neural Networks (**supervised**)

Feature Engineering: Challenges and Solutions

Collected (raw) data is far from being perfect!

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↓

Data Preprocessing

Feature Engineering: Challenges and Solutions

Challenge	Description	
Missing values	A feature value may not be available for one or more instances	

Feature Engineering: Challenges and Solutions

Challenge	Description	Solution
Missing values	A feature value may not be available for one or more instances	Replace missing values with the **median** (continuous) or the **mode** (categorical) of the existing values

Feature Engineering: Challenges and Solutions

Challenge	Description	
Sparsity	Most of the instances contain just a small subset of the features	

Feature Engineering: Challenges and Solutions

Challenge	Description	Solution
Sparsity	Most of the instances contain just a small subset of the features	Use "sparse-friendly" data structures (e.g., DOK)

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Challenge	Description	
Outliers	One or more instances have out-of-range values for one or more features	

Feature Engineering: Challenges and Solutions

Challenge	Description	Solution
Outliers	One or more instances have out-of-range values for one or more features	Retention vs. Exclusion (*trimming* or *winsorising*)

Feature Engineering: Challenges and Solutions

Challenge	Description	
Mix of continuous and discrete values	Feature set contains both numerical and categorical values	

Feature Engineering: Challenges and Solutions

Challenge	Description	Solution
Mix of continuous and discrete values	Feature set contains both numerical and categorical values	Transform categorical features using *one-hot encoding*

Feature Engineering: Challenges and Solutions

Challenge	Description	
Multiple feature magnitudes	Feature set contains very wide range of values	

Feature Engineering: Challenges and Solutions

Challenge	Description	Solution
Multiple feature magnitudes	Feature set contains very wide range of values	Standardization (min-max, z-scores)

Feature Engineering: Challenges and Solutions

Challenge	Description	
Class imbalance	Instances labeled with the class of interest represents a tiny fraction of the total	

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Strong multicollinearity	Linear relationship between one or more features	

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Strong multicollinearity	Linear relationship between one or more features	Dimensionality reduction (PCA)

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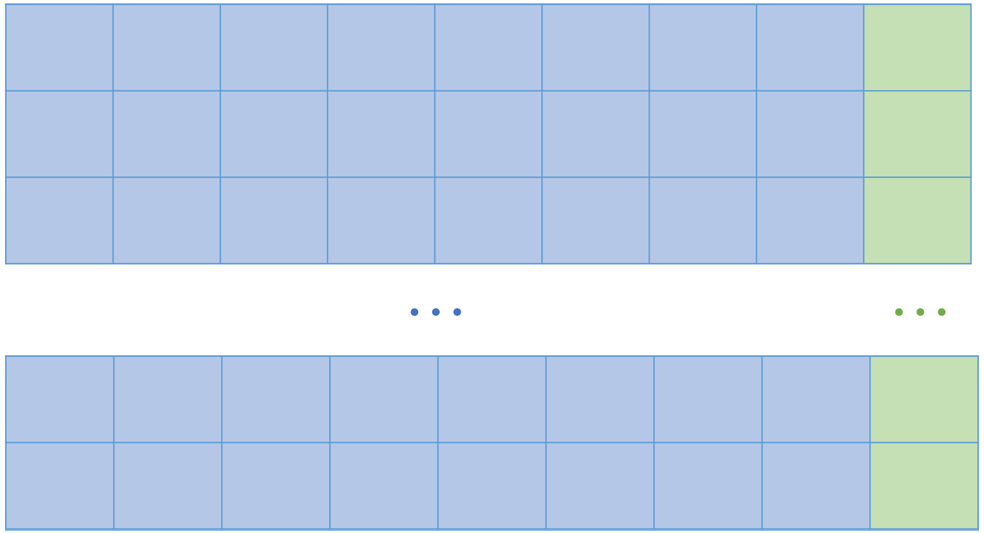
$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$	dataset of *m* i.i.d. labeled instances

Model Training: Labeled Dataset



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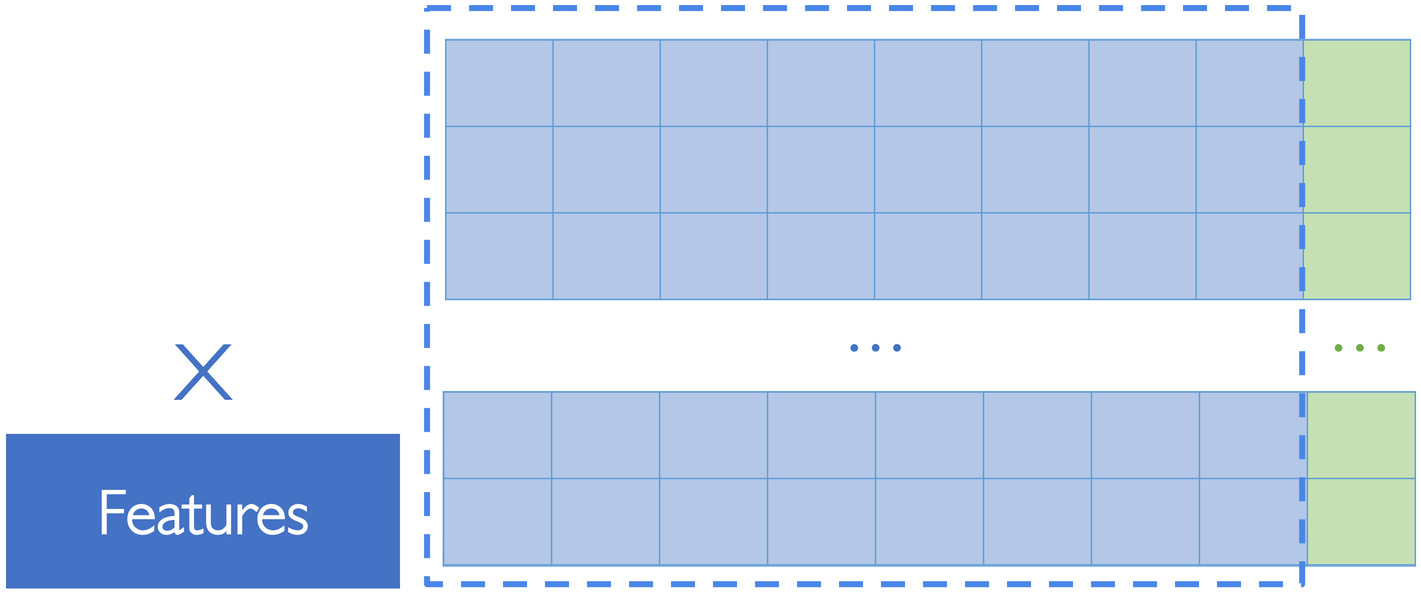

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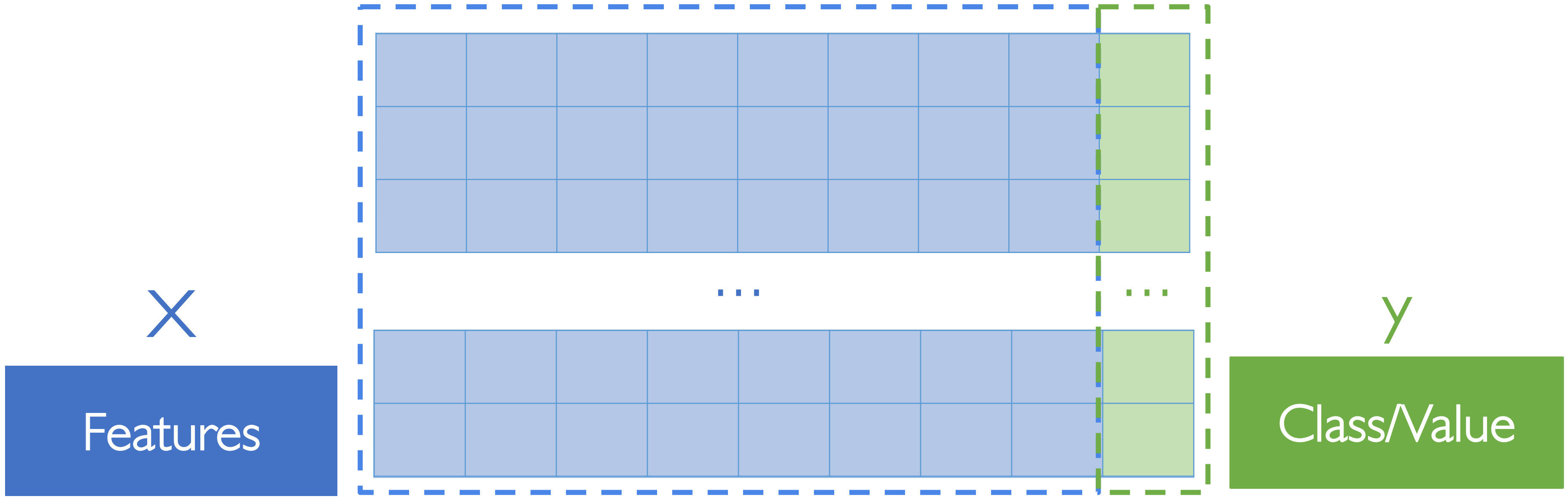
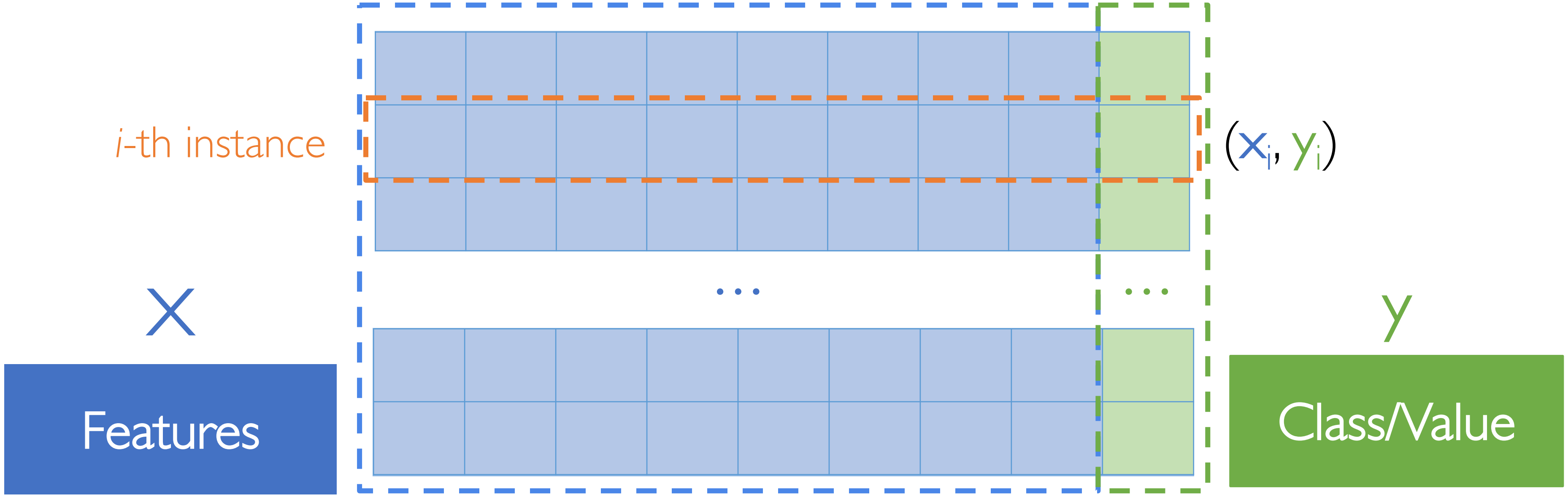


Model Training: Labeled Dataset

Each instance comes with the class label (classification) or the value (regression) we want to predict



Model Training: Intuition

Idea

There is an unknown target function f which puts in a relationship elements of X with elements of Y

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$$\downarrow$$

$$\boxed{f = X \rightarrow Y}$$

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Problem

We cannot write down an algorithm which just implements f

Model Training: Learning f from Labeled Data

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  - loss function: measures the error of using h^* instead of the true f
  - learning algorithm: explores the hypothesis space to pick the function which minimizes the loss on the observed data

The Hypothesis Space H

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Trade-off

Put some constraints on H, e.g., limit the search space only to linear functions

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- This in-sample error (a.k.a. empirical loss) is an estimate of the out-of-sample error (a.k.a. expected loss or risk)

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- Defines the strategy we use to search the hypothesis space H for picking our **best** hypothesis h^*

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$$\boxed{h^* = \text{argmin}_{h \in \mathcal{H}} L(h, \mathcal{D})}$$

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(e.g., ideal credit approval function)

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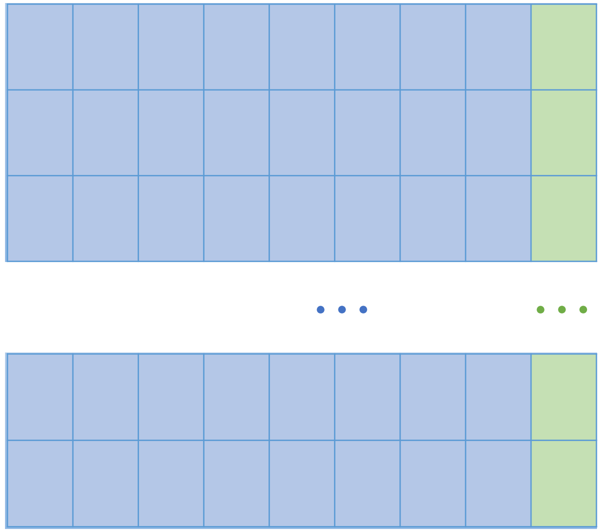

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training data D
(e.g., historical records of customers)

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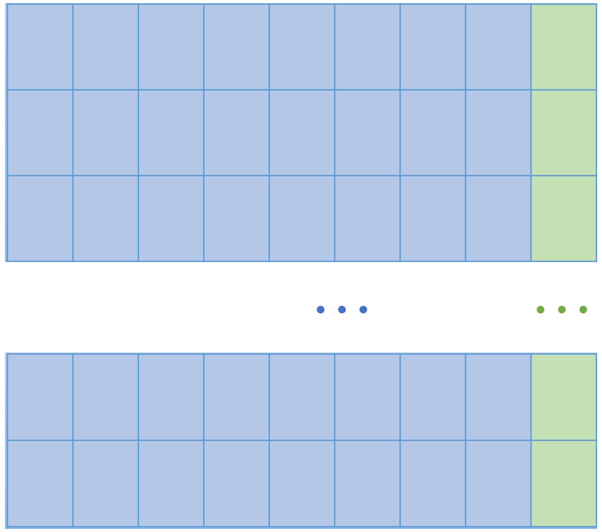

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Hypothesis Space
H

candidate formulas

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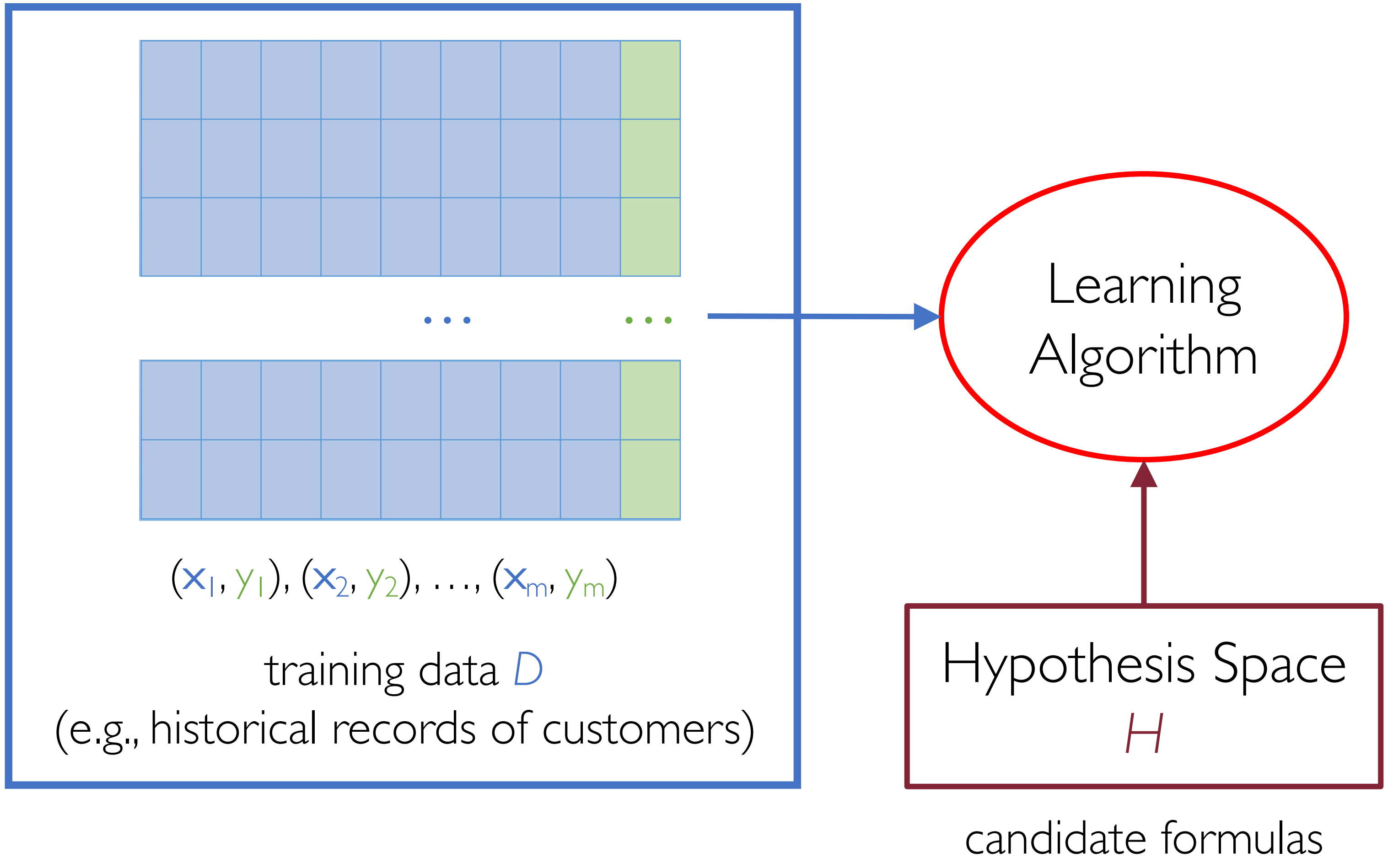

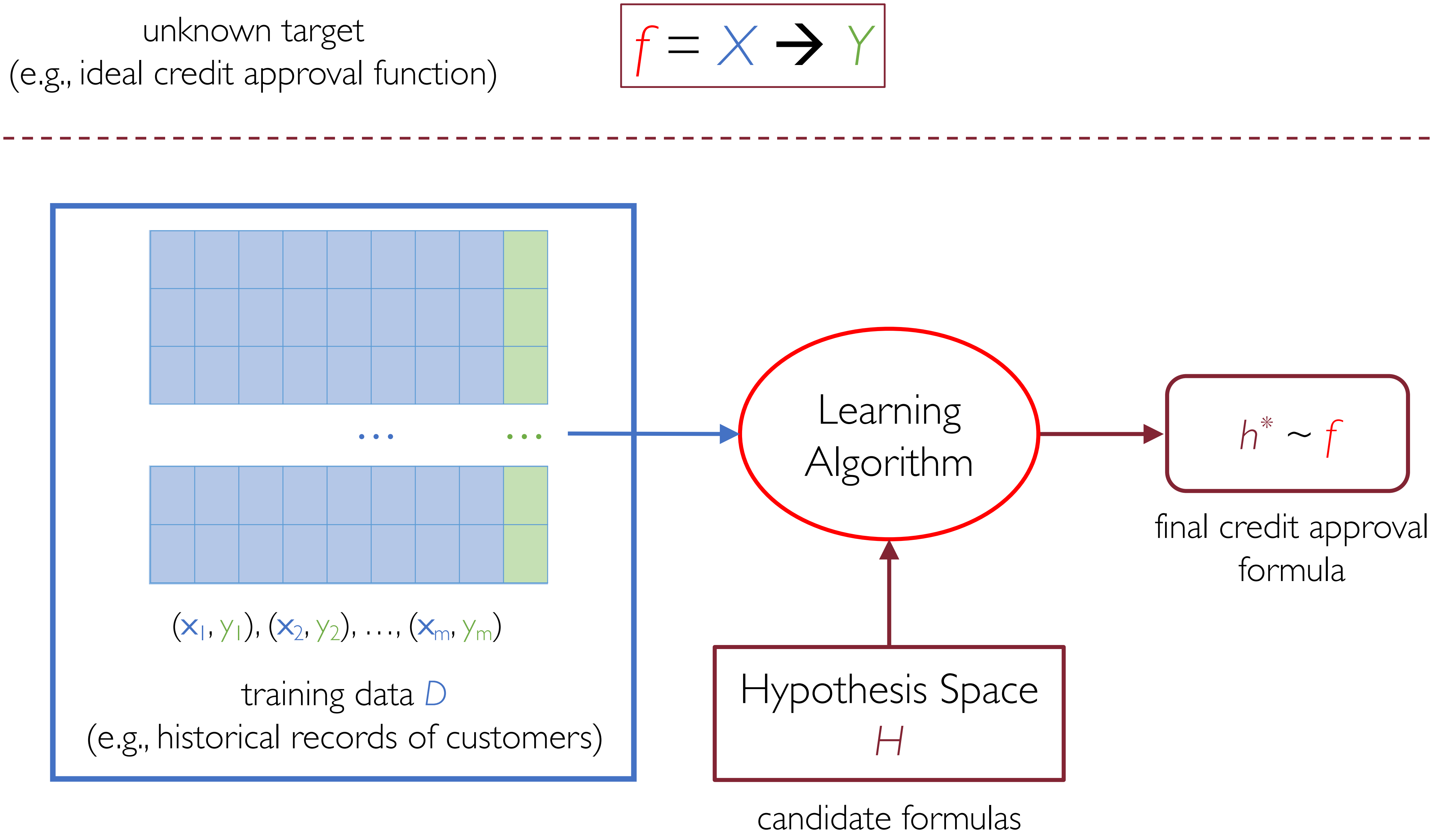
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Learning Algorithm
$h^* \sim f$
final credit approval formula
Hypothesis Space H
candidate formulas

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- By plugging in different loss functions combined with various hypothesis spaces we must solve a specific optimization problem
- Those choices are usually "mathematically convenient": e.g., convex objective functions are guaranteed to have a unique global minimum
- Even though closed-form solutions to the optimization problem rarely exist, there are numerical methods which work: e.g., gradient descent

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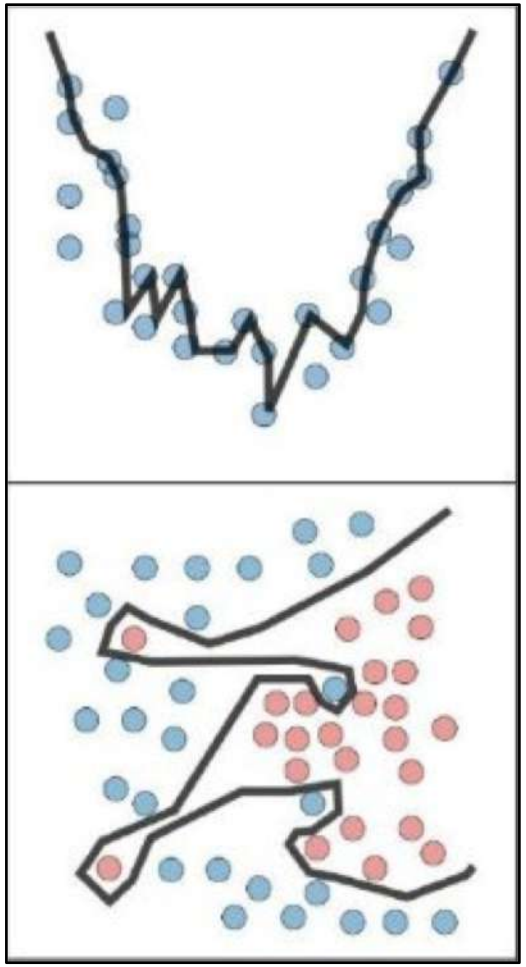
- At the same time we do not want h^* to perform poorly on D

Overfitting (High Variance)

Regression

Classification



The hypothesis h^* is not learning the true f but it mimics its noise

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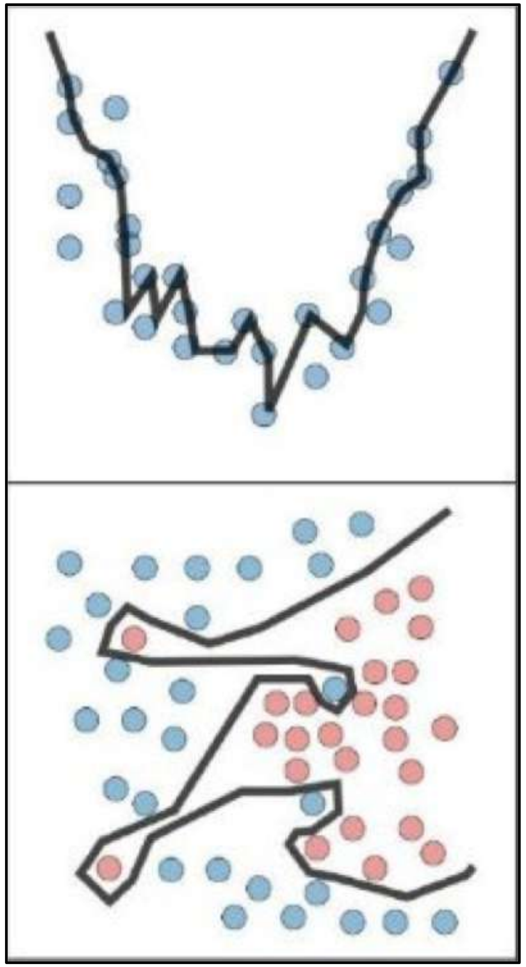

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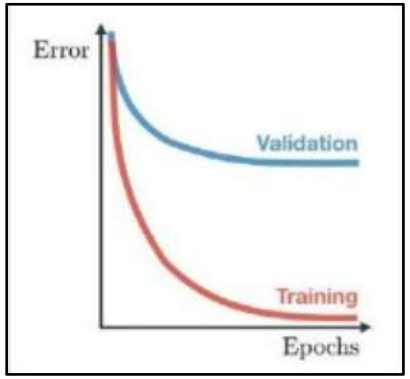

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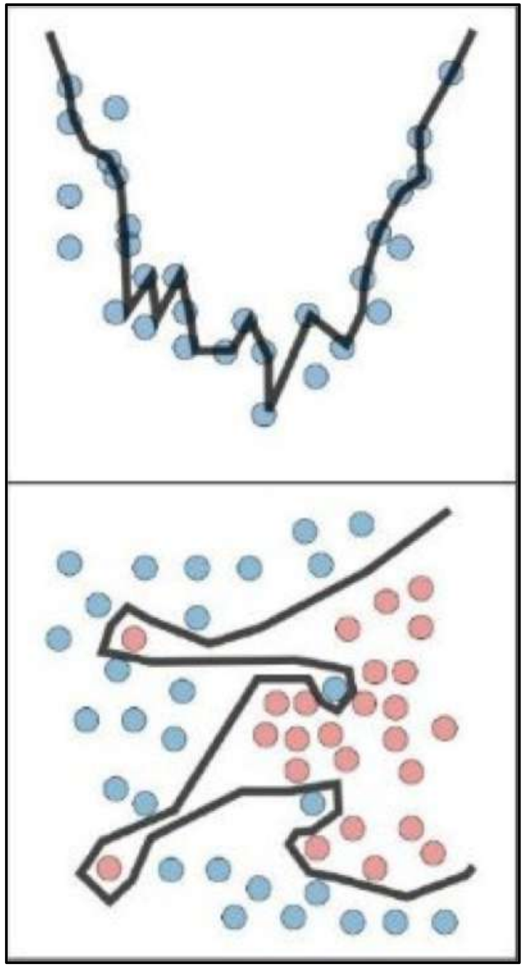

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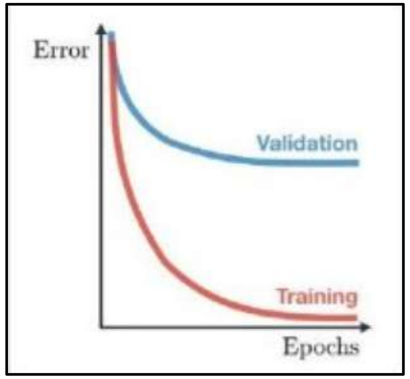

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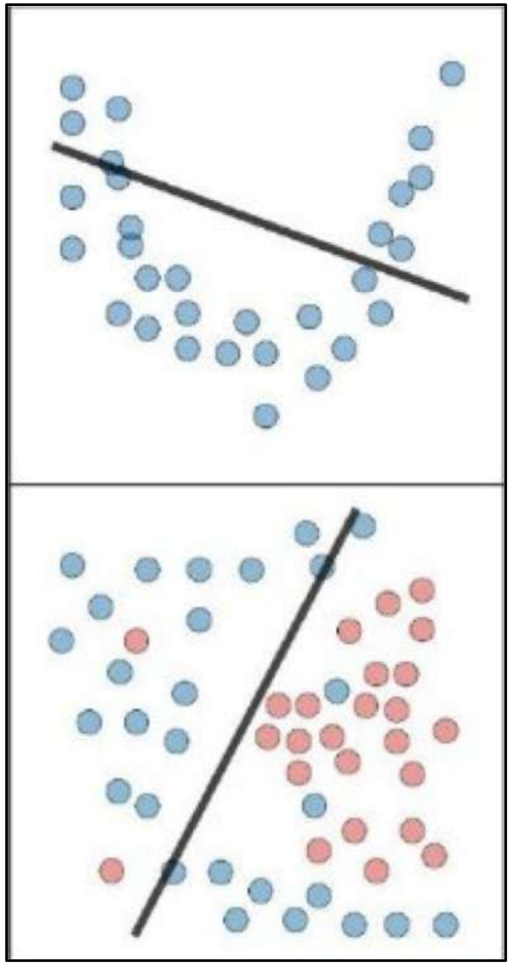
- Regularization
- Get more data

Underfitting (High Bias)

Regression

Classification



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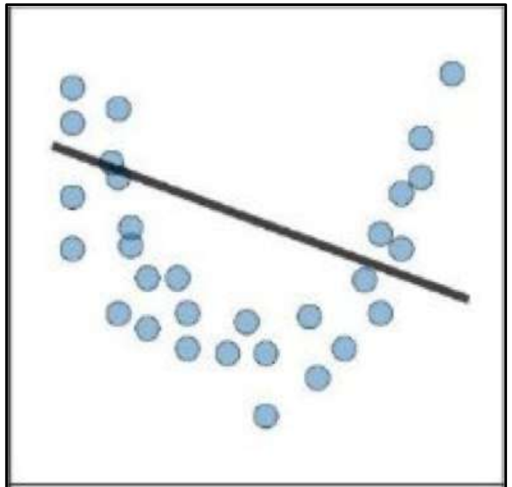

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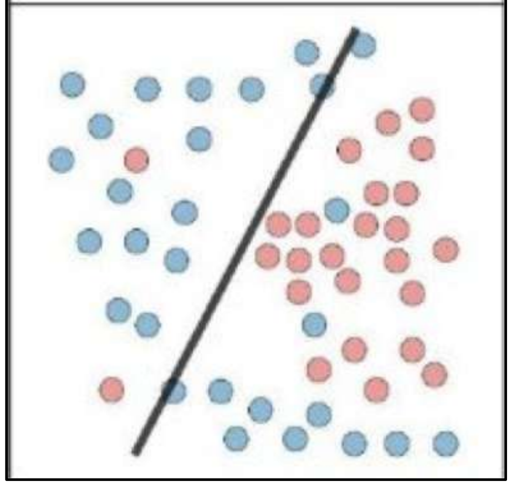

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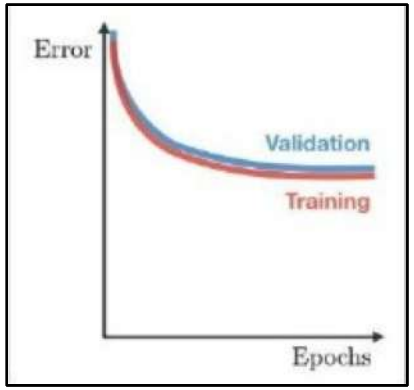

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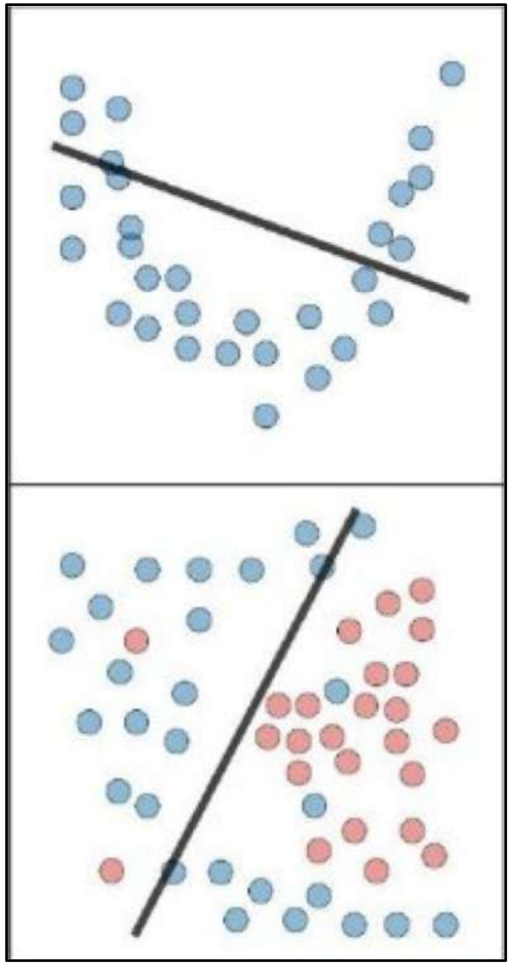

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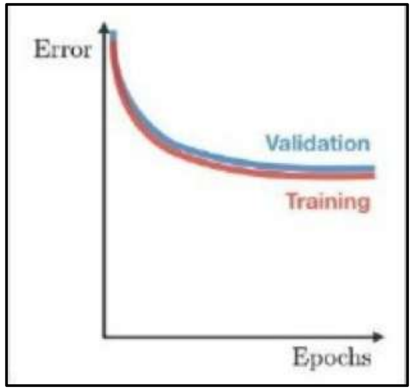


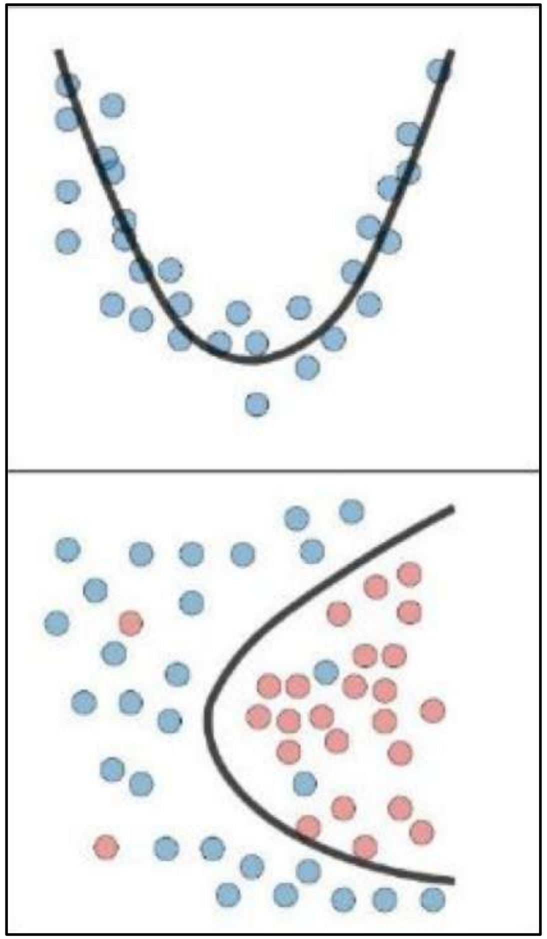
high in-sample error high out-of-sample error

- Increase model complexity
- Add more features

Bias-Variance Tradeoff

Regression

Classification



The hypothesis h^* is just right:
the simplest one explaining the data

Occam's razor

Bias-Variance Tradeoff

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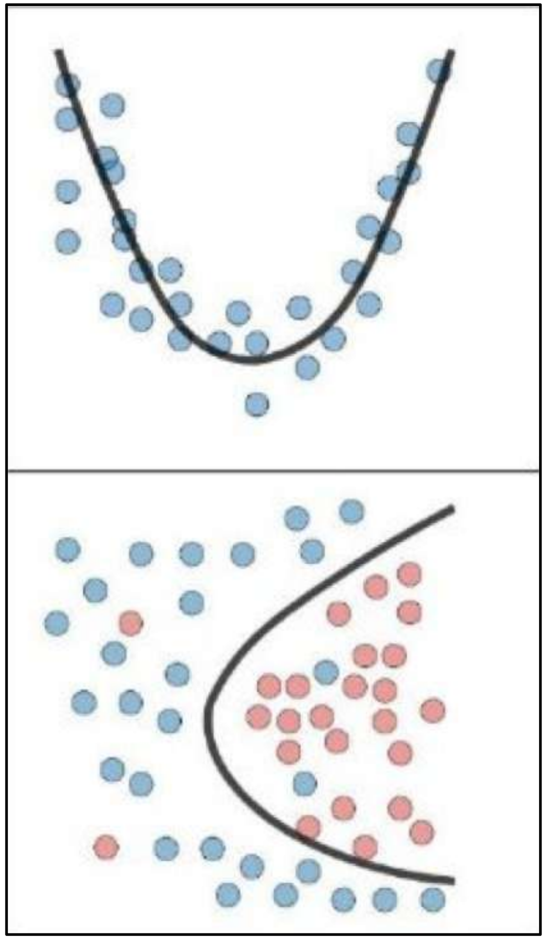

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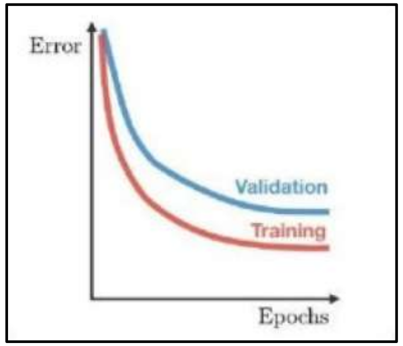

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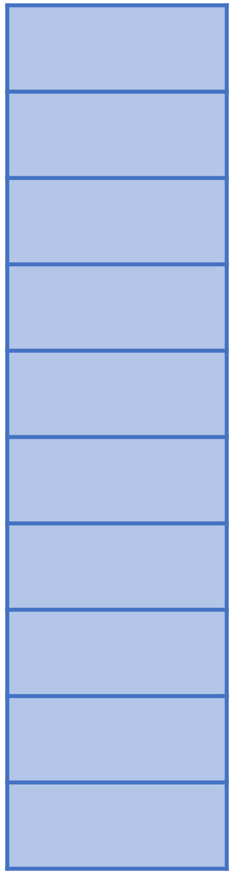
- Example: Don't want to deploy your new spam classifier in production knowing only its training (i.e., in-sample) performance
- Solution: Estimate the generalization performance using training set
  - As long as it holds true the assumption that training and test instances are both drawn from the same probability distribution (i.i.d. assumption)

Dataset Splitting

Dataset
D



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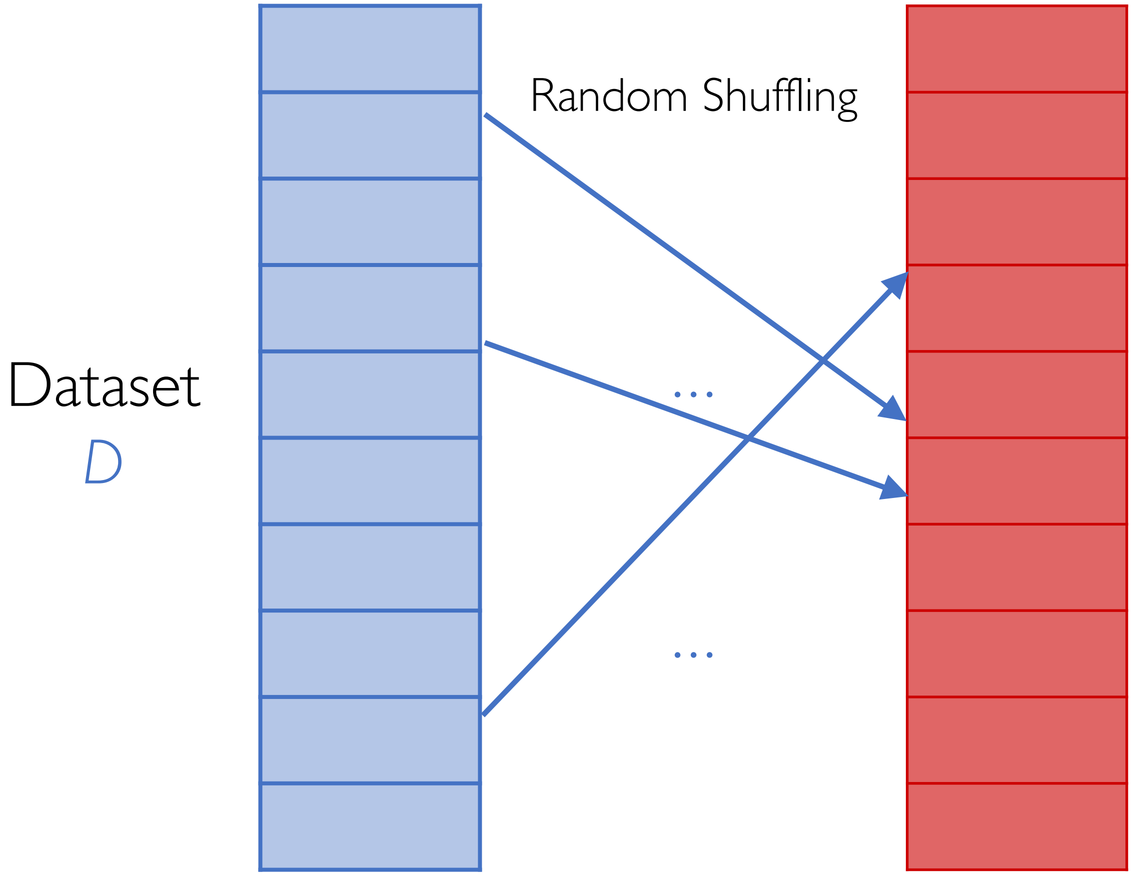

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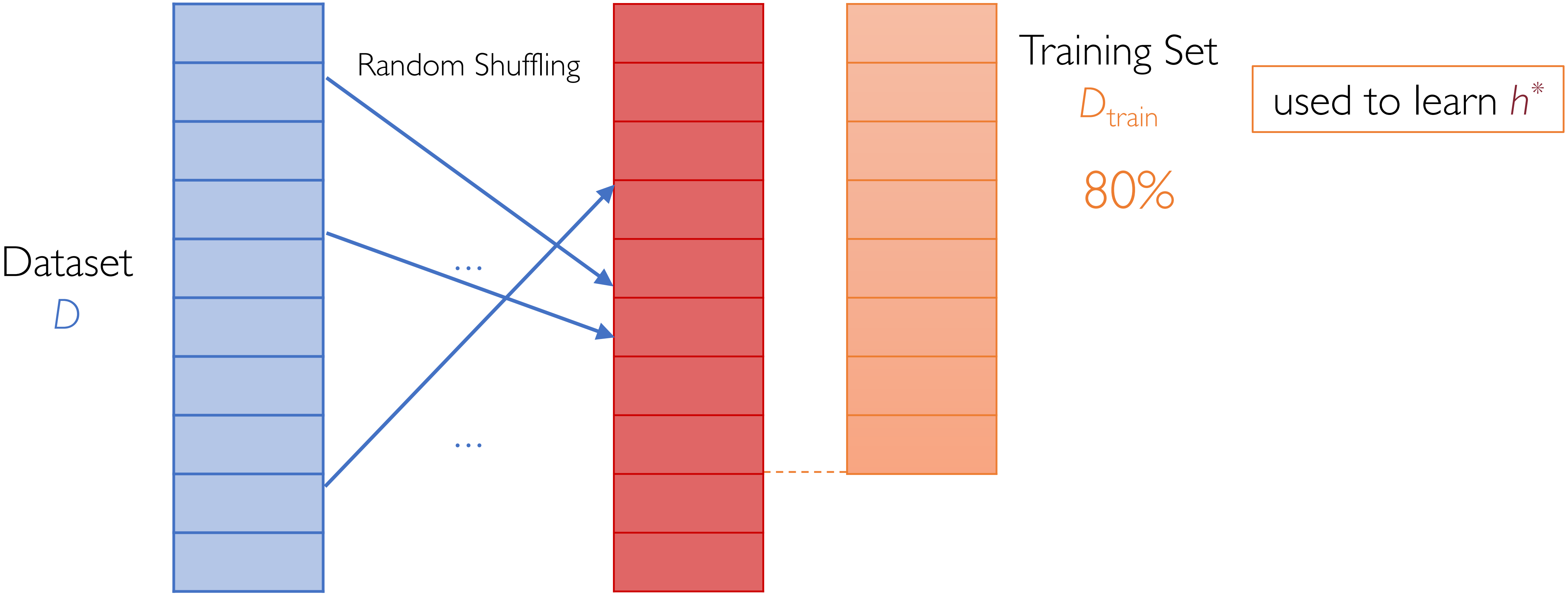

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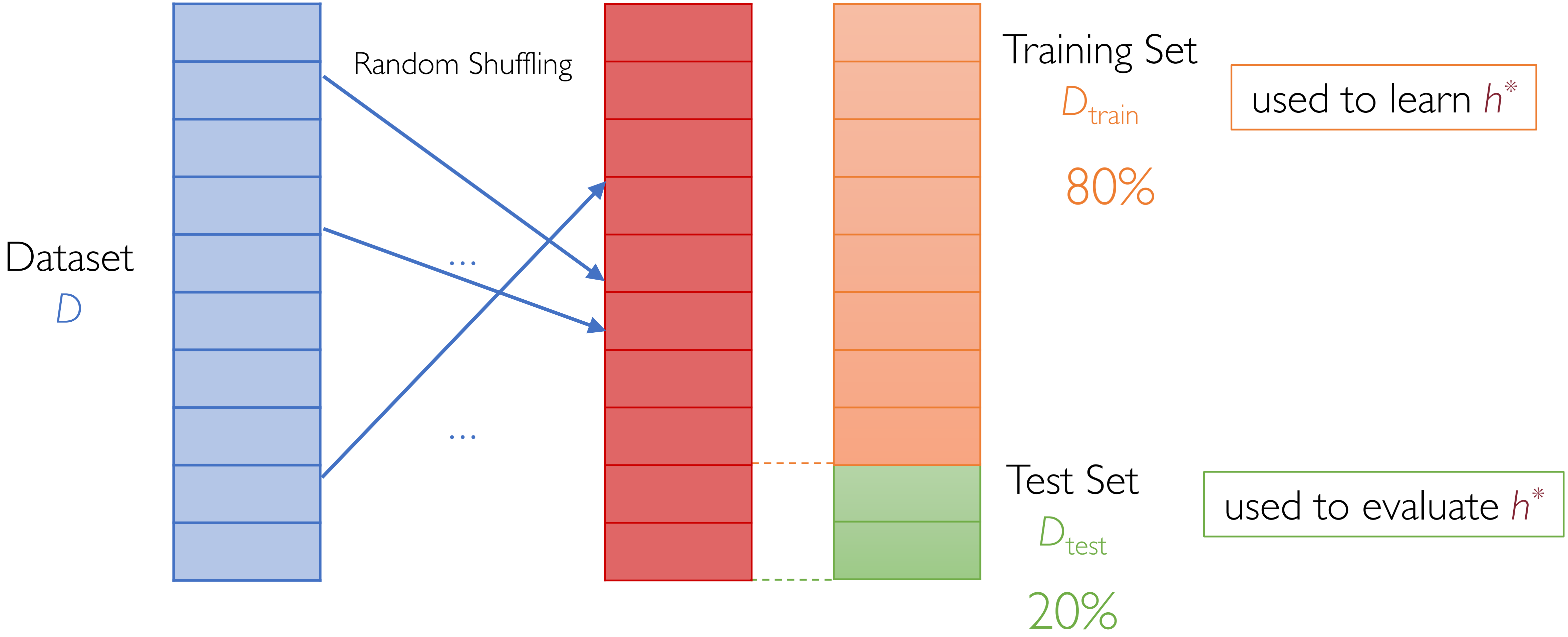
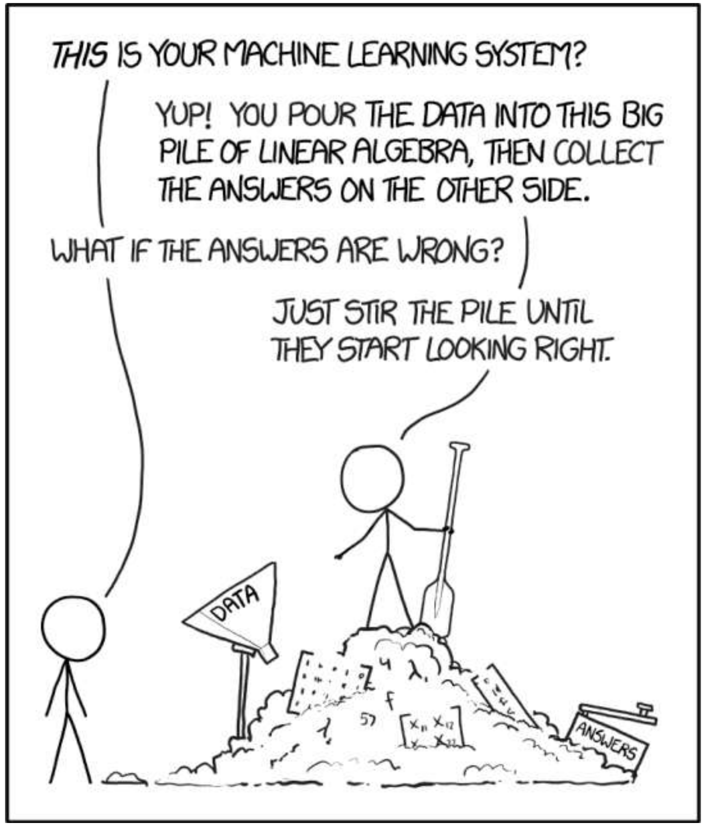


How Much Data Do We Need?

In general, the more data we have the better we learn



source: https://xkcd.com/1838/

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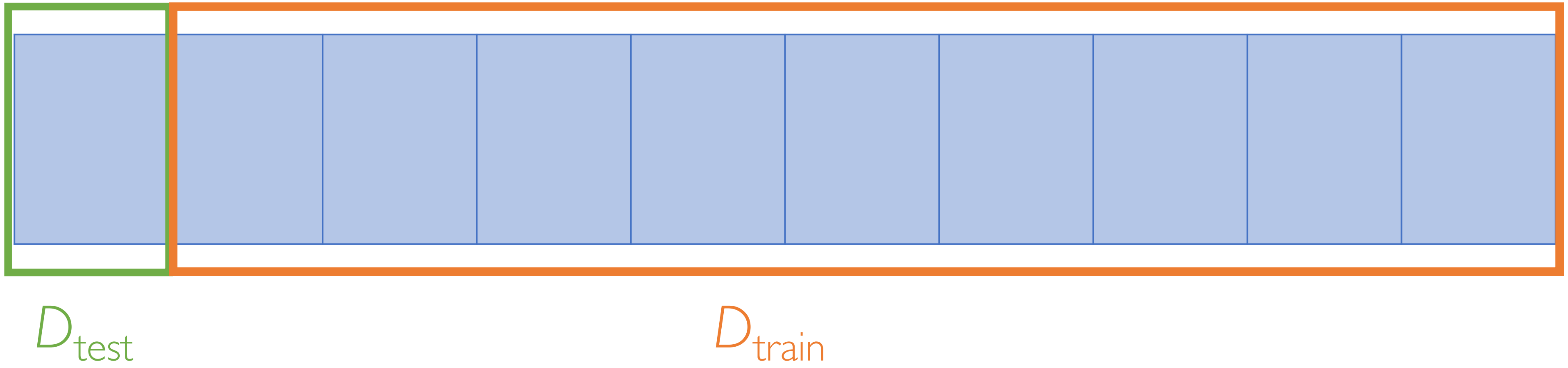
- The estimate of generalization error is the average across the K test folds of all the K rounds

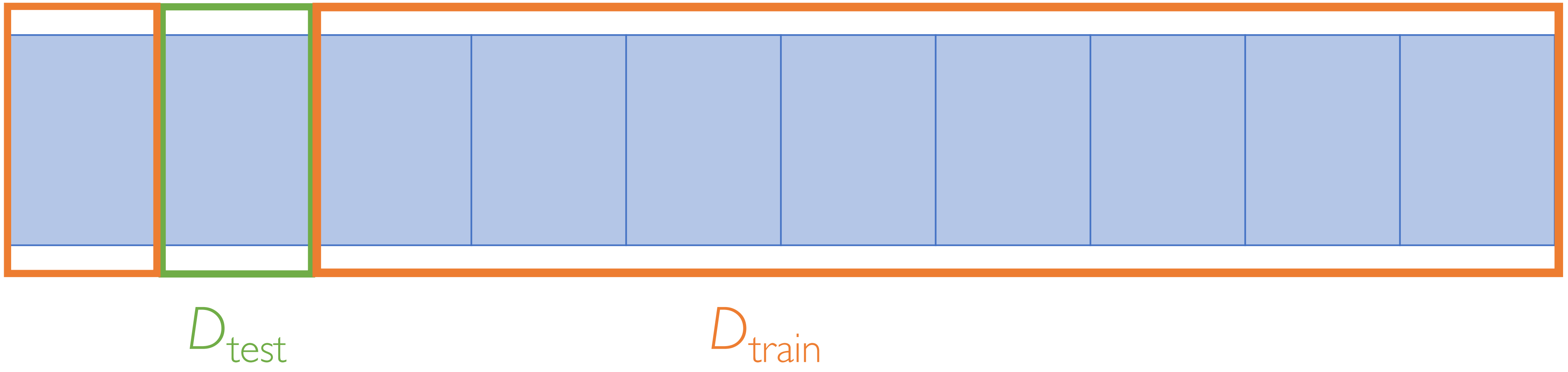
K-Fold Cross Validation

Round $k = 1$



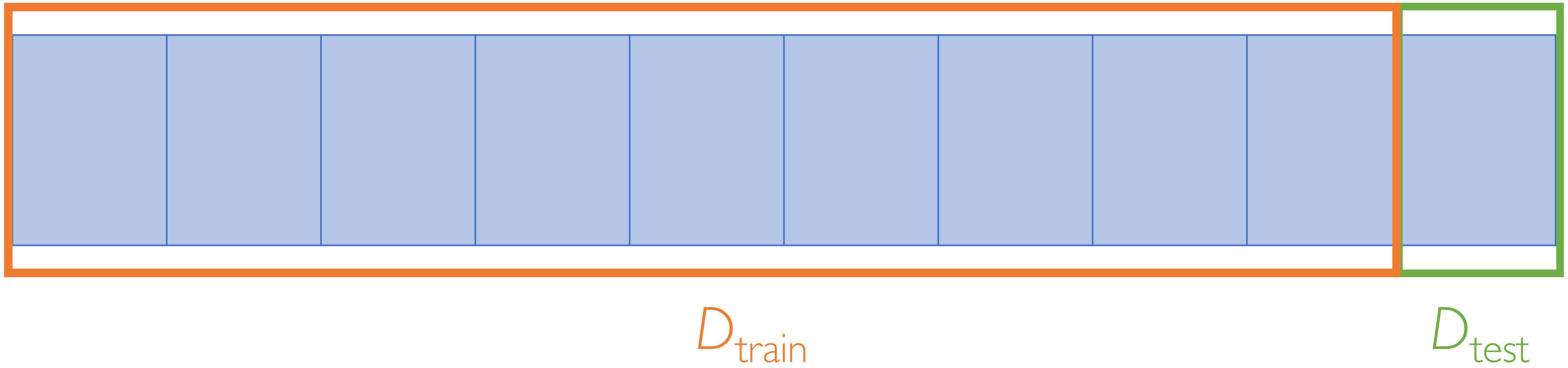
K-Fold Cross Validation

Round $k = 2$



K-Fold Cross Validation

Round $k = 10$



Model Selection/Evaluation

Several different learning models to achieve the same task

Decision Trees

Random Forests

Logistic Regression

kNN

SVM

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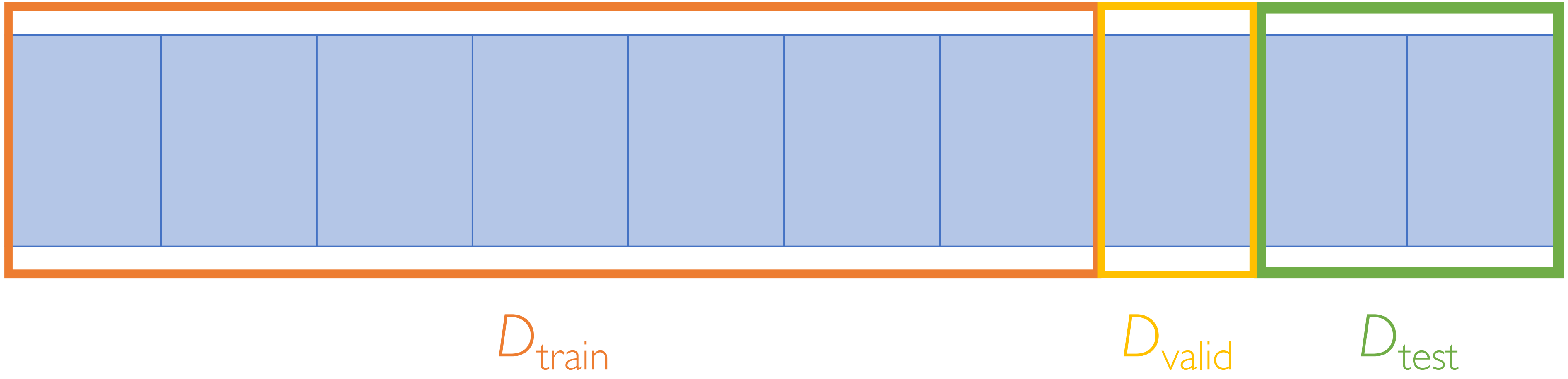
How do we select the best model?

Model Selection/Evaluation: Validation Set

Separate hyperparameter selection from model evaluation

D_{valid} is used to validate hyperparameters



Model Selection/Evaluation: Example

Select which value of $k = \{2, 5, 10\}$ of a kNN gives the best performance

1) Train a separate model for each value of k on the training set (e.g., 70%)
2) Measure the error of each model on the validation set (e.g., 10%)
3) Select the model whose value of k gives the best performance on the validation set (e.g., $k = 5$)
4) Re-train only this model on the training + validation set
5) Measure the performance on the test set (e.g., 20%)

Note:

The strategy above can also be extended to K-fold Cross Validation

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  - Hypothesis space (assumption)
  - Loss Function (objective)
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Suggested reading: https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf