Big Data Computing

Master's Degree in Computer Science

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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 compute 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 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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Problem

Solution/Algorithm
explicitly designed by human

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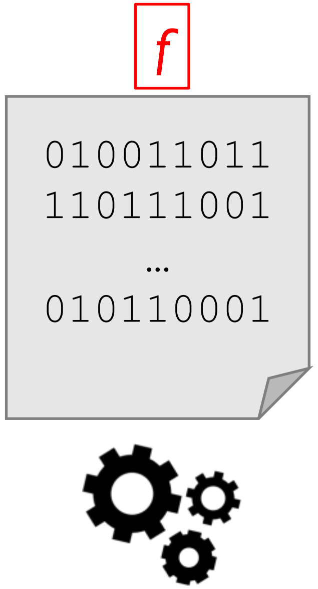
010011011
110111001
…
010110001

Encoding of
Computable Function f

Programming a Computer



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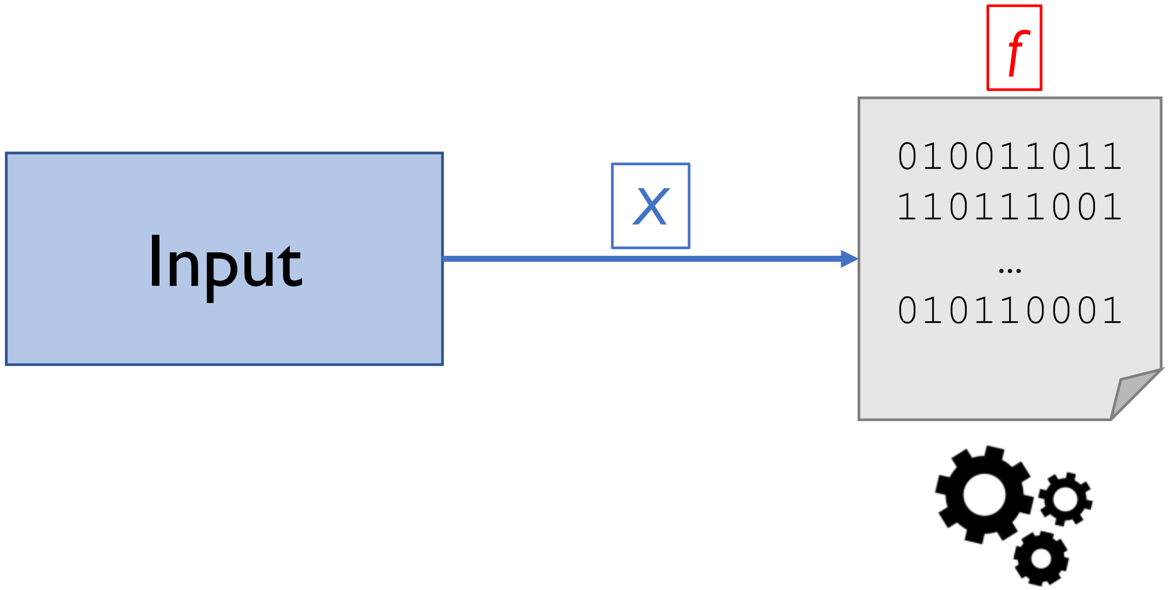

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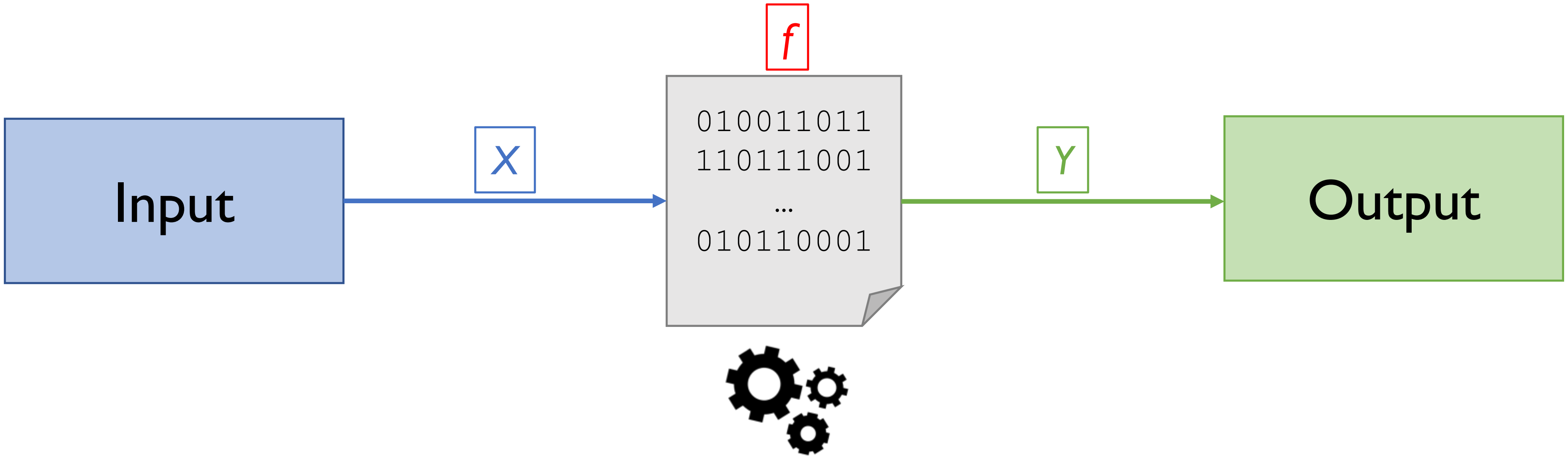

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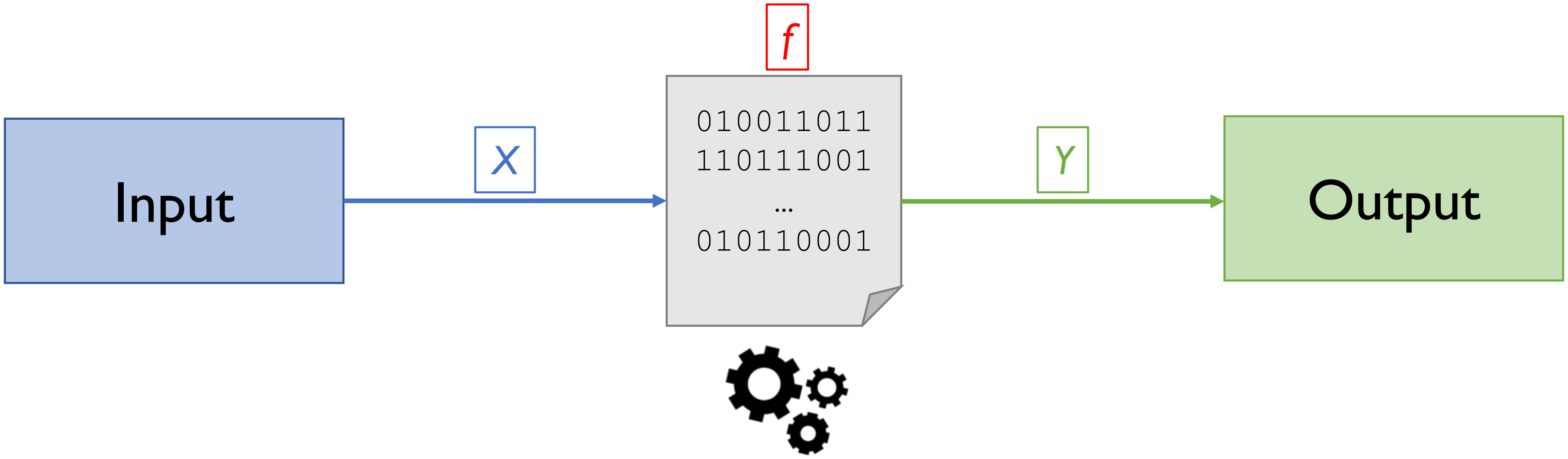

$$\boxed{Y = f(X)}$$

Can We Always Do That?

Chihuahua or Muffin?

[Copyright @teenybiscuit]

Chihuahua

Muffin

Programming vs. "Training" a Computer

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$\Downarrow$

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

"Training" a Computer

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Labeled Data

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

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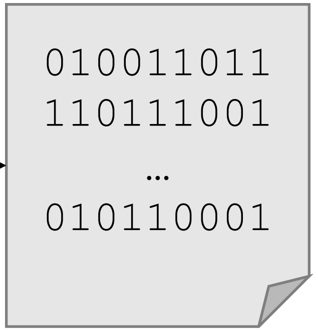

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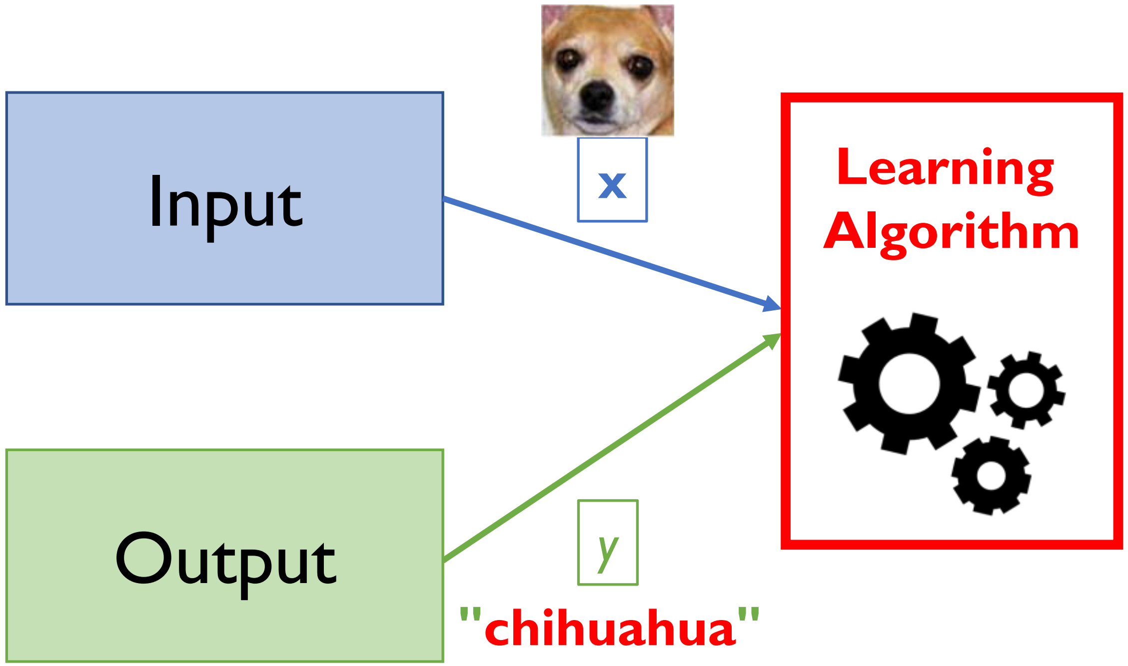

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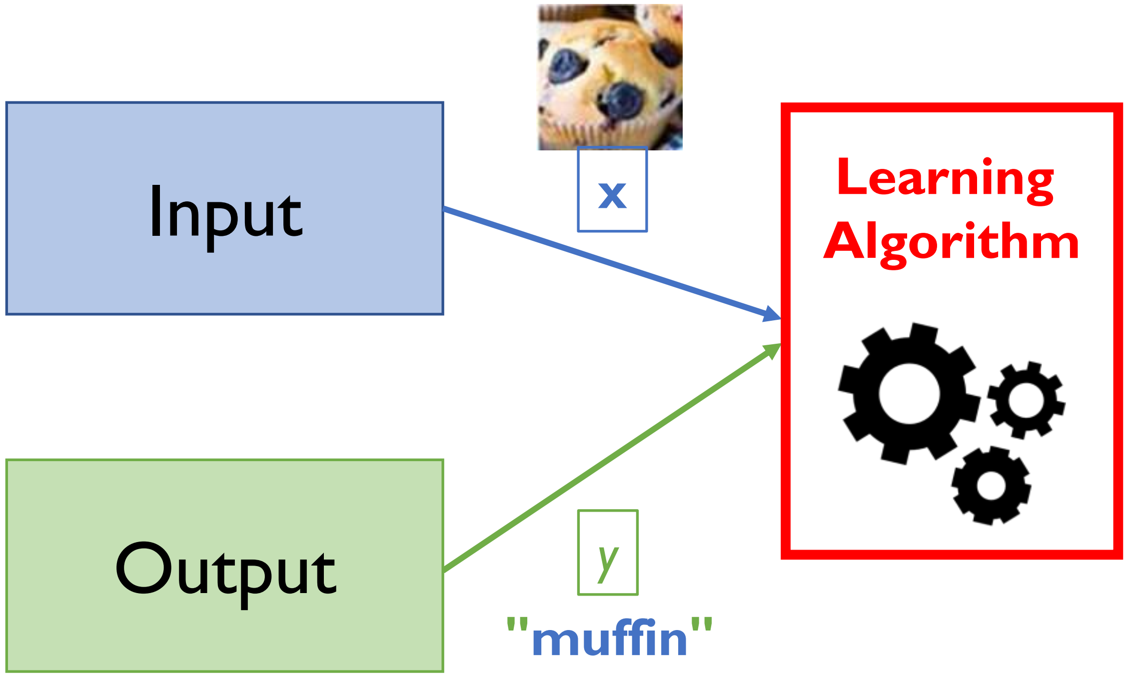

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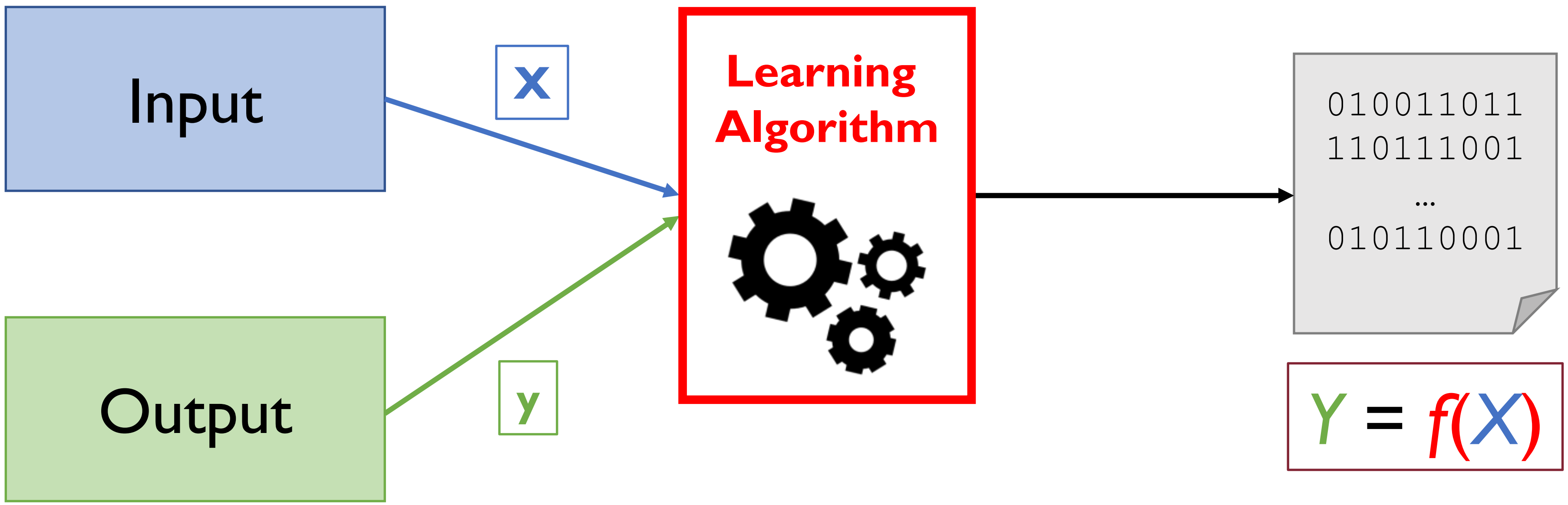

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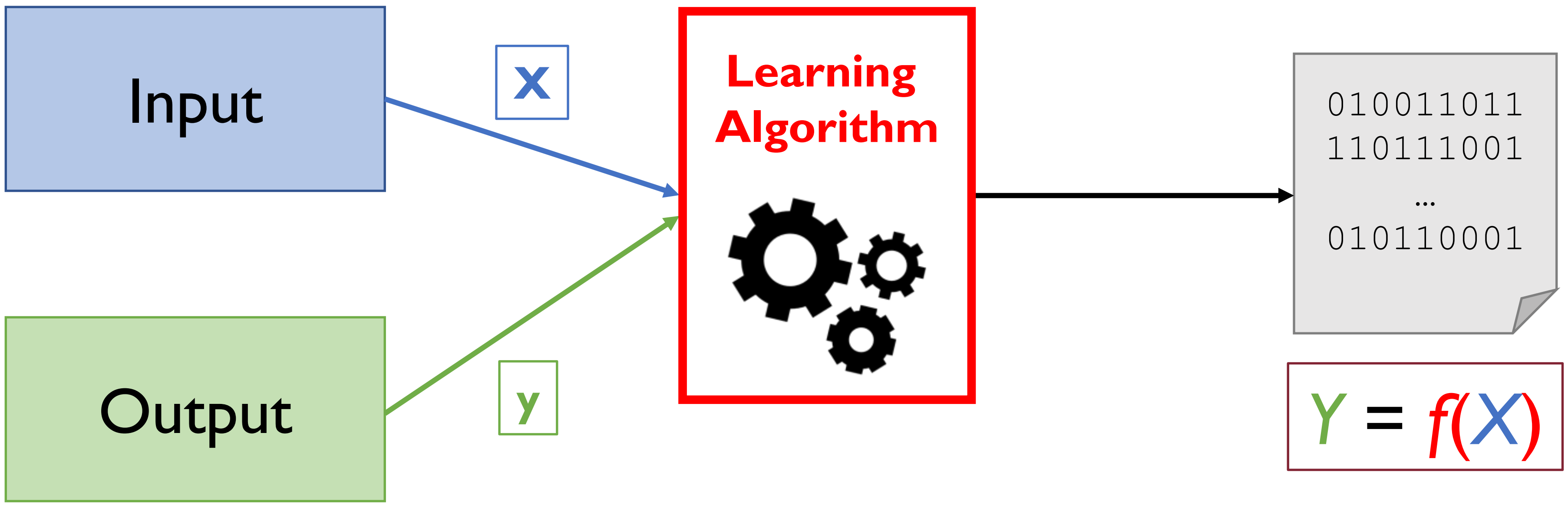

Eventually, the function *f* is **learned** by the learning algorithm from a (large) set of **labeled data**

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"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**

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

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- Any ML technique needs data to operate on!
- 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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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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- Traditionally done manually by human experts
- 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**)
  - Siamese 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)

Feature Engineering: Challenges and Solutions

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	

Feature Engineering: Challenges and Solutions

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Class imbalance	Instances labeled with the class of interest represents a tiny fraction of the total	Over-/Under-sampling, cost-sensitive learning

Feature Engineering: Challenges and Solutions

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Strong multicollinearity	Linear relationship between one or more features	

Feature Engineering: Challenges and Solutions

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

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$ input feature space

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$\mathcal{Y} \in \{1, \ldots, k\}$ — discrete-value label of the *i*-th instance (k-ary classification)

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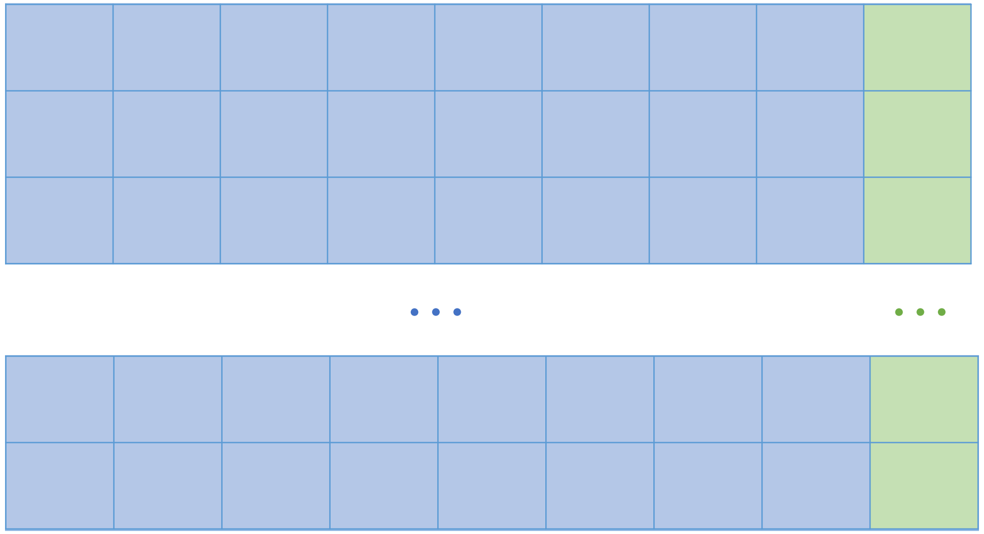
$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$	dataset of *m* i.i.d. labeled instances

Model Training: Labeled Dataset



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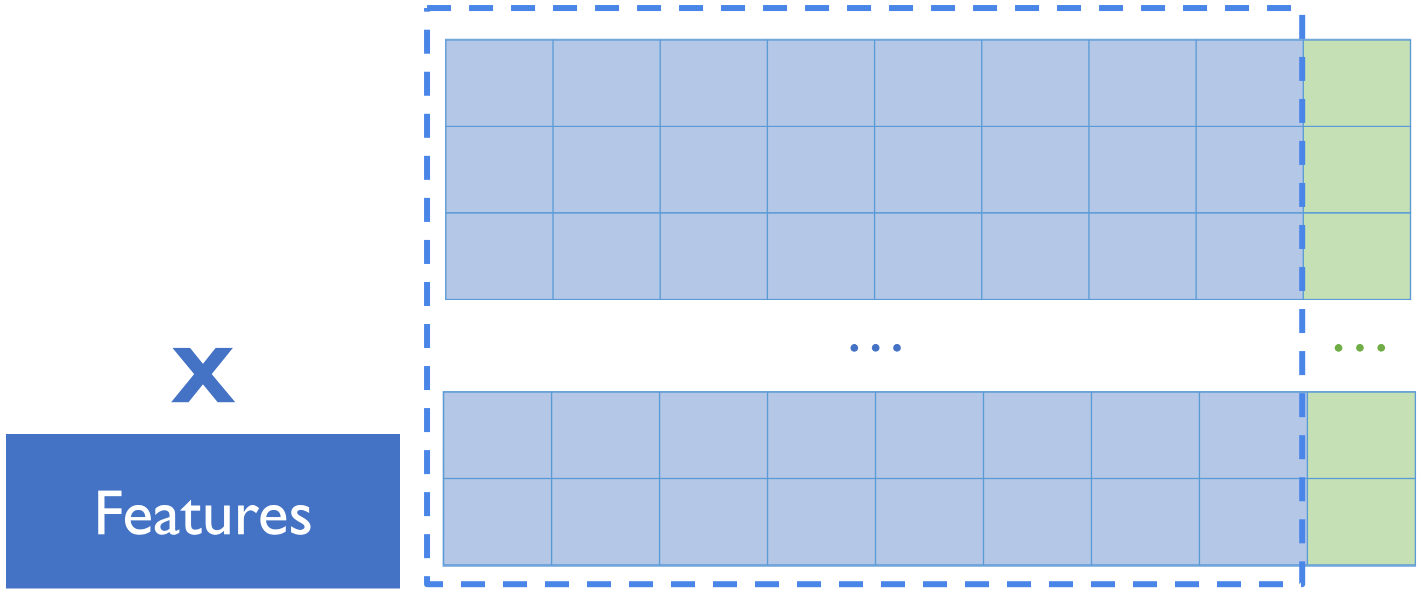

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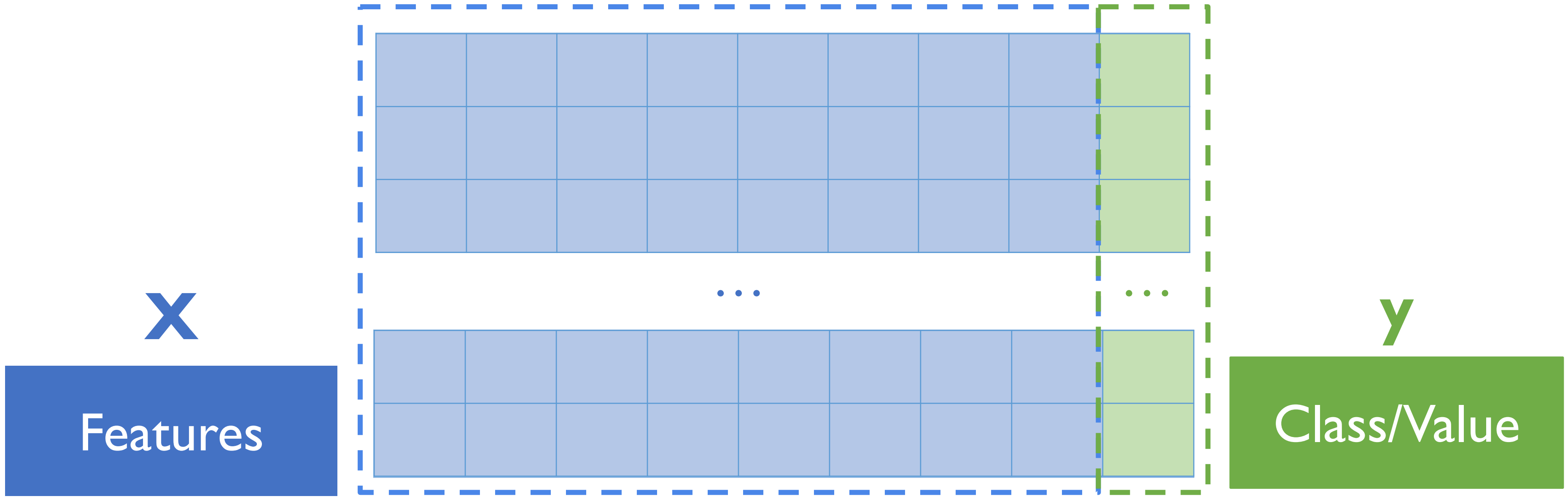
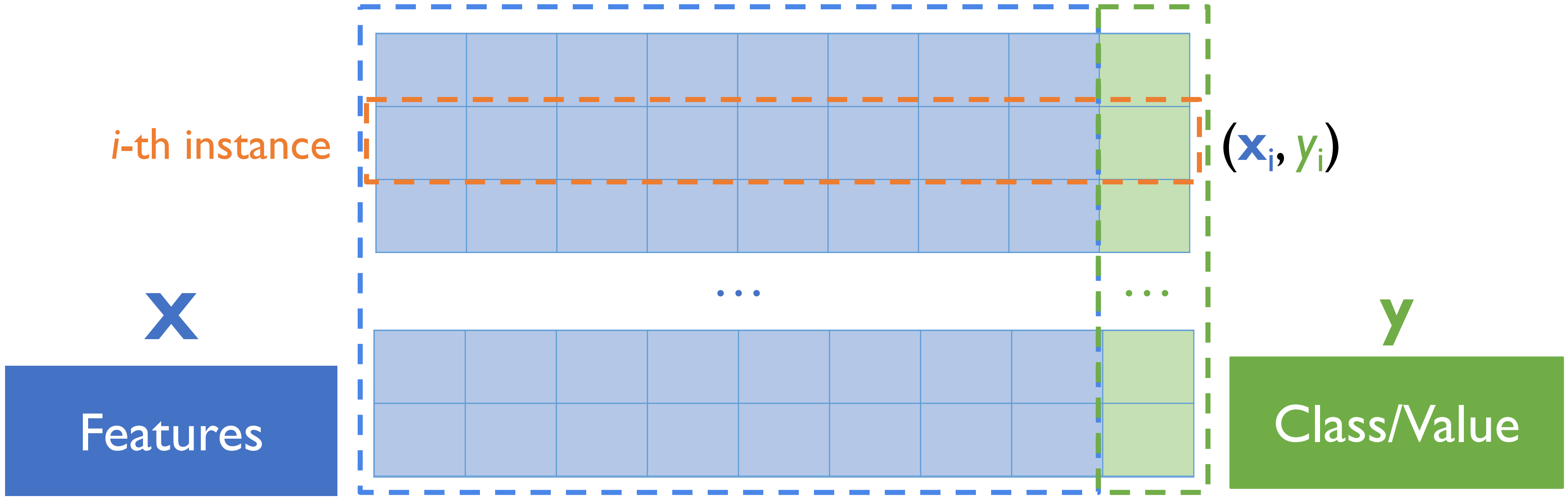


Model Training: Labeled Dataset

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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Problem

We cannot write down an algorithm which just implements f

Model Training: Learning f from Labeled Data

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  - **learning algorithm:** explores the hypothesis space to pick the function which minimizes the loss on the observed data

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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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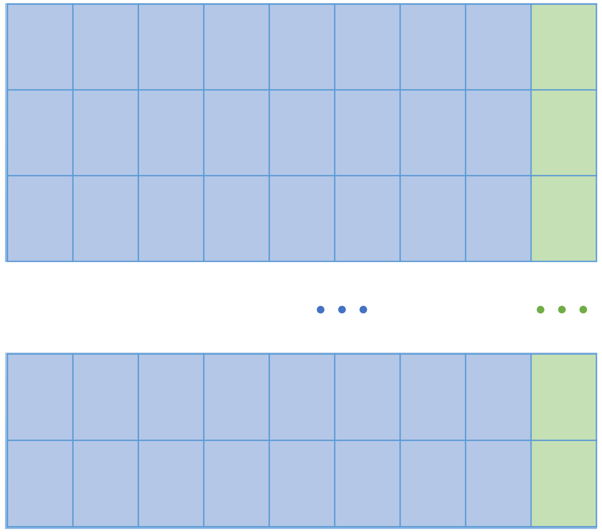

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training data D
(e.g., historical records of customers)

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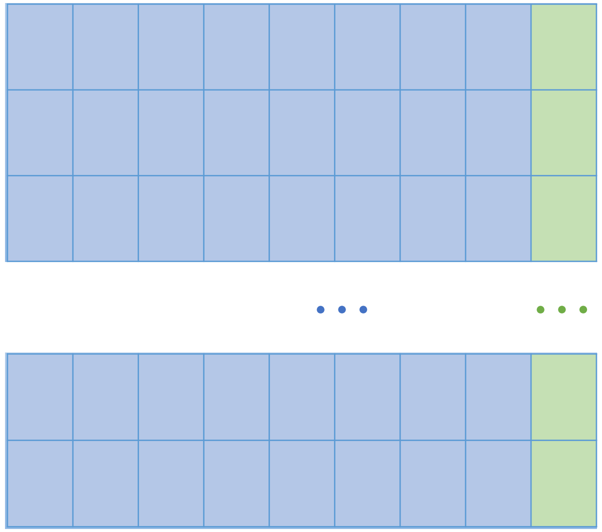

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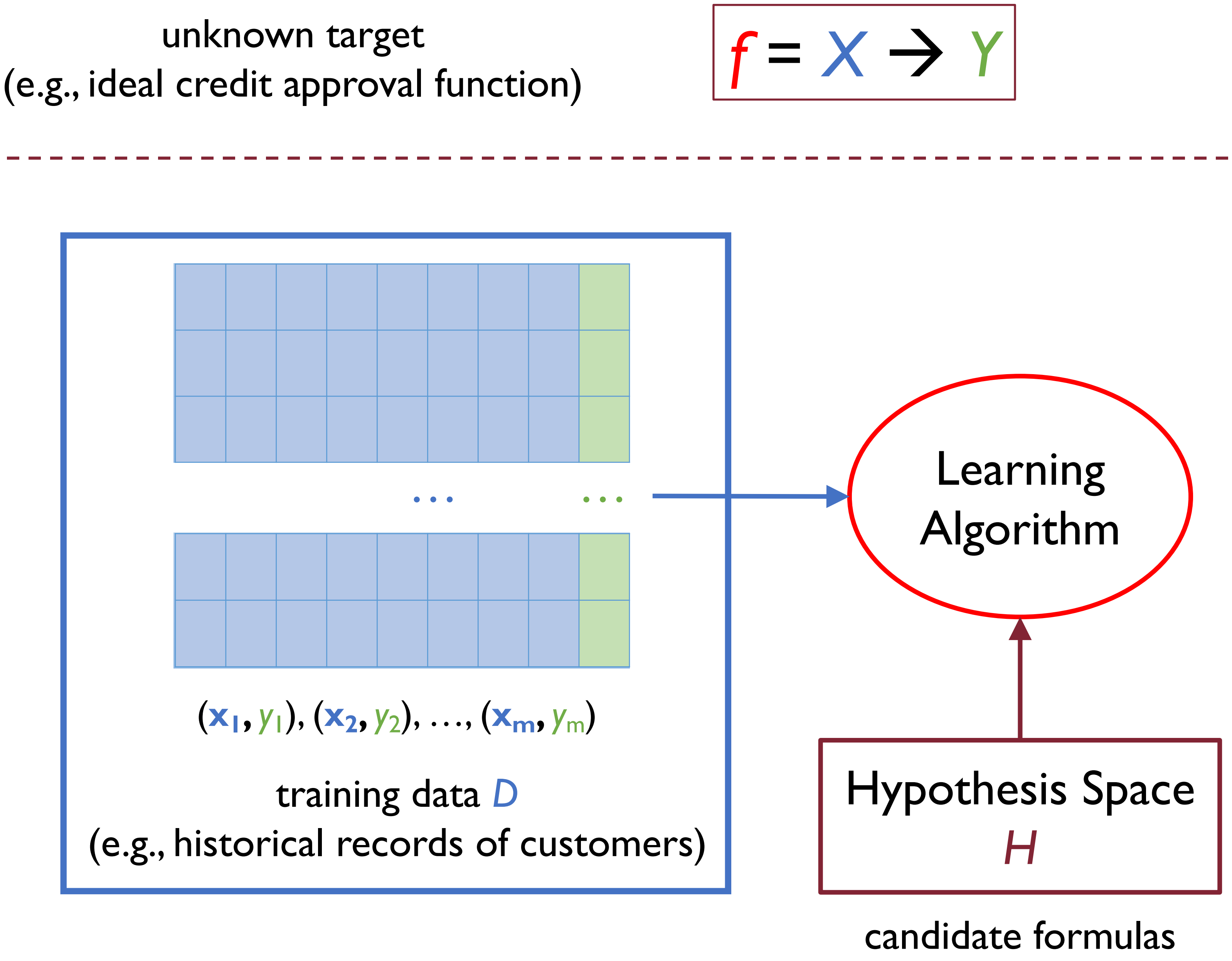
Hypothesis Space
H

candidate formulas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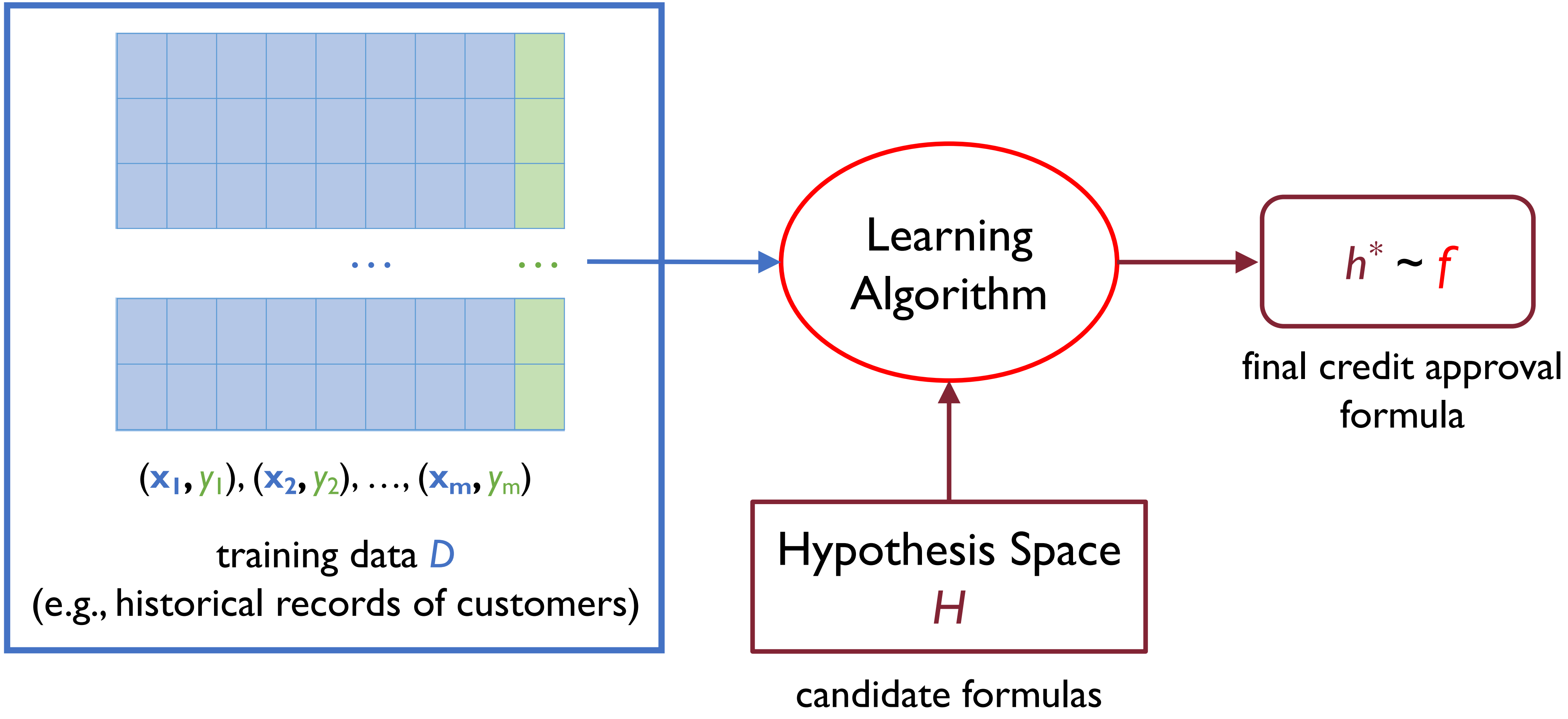

Learning *f* as an Optimization Problem

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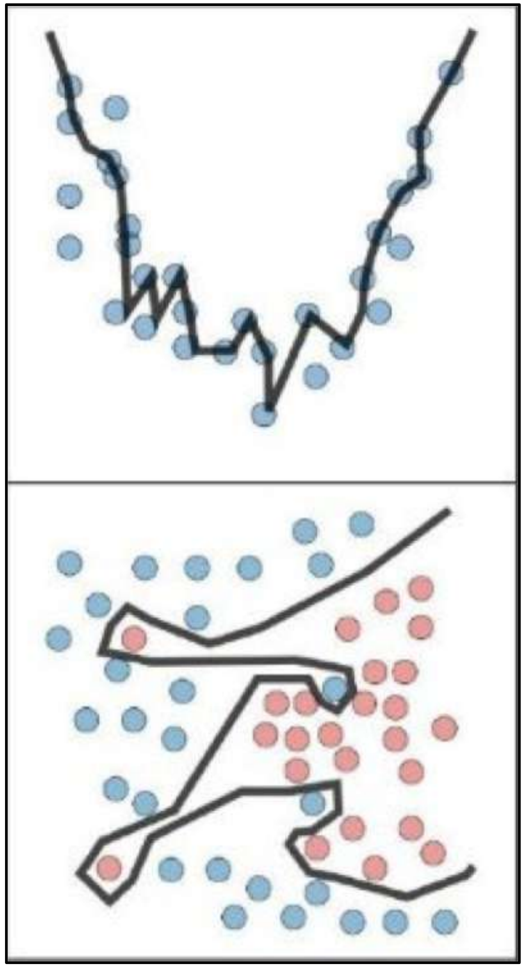
- At the same time we do not want h^* to perform poorly on D

Overfitting (High Variance)

Regression

Classification



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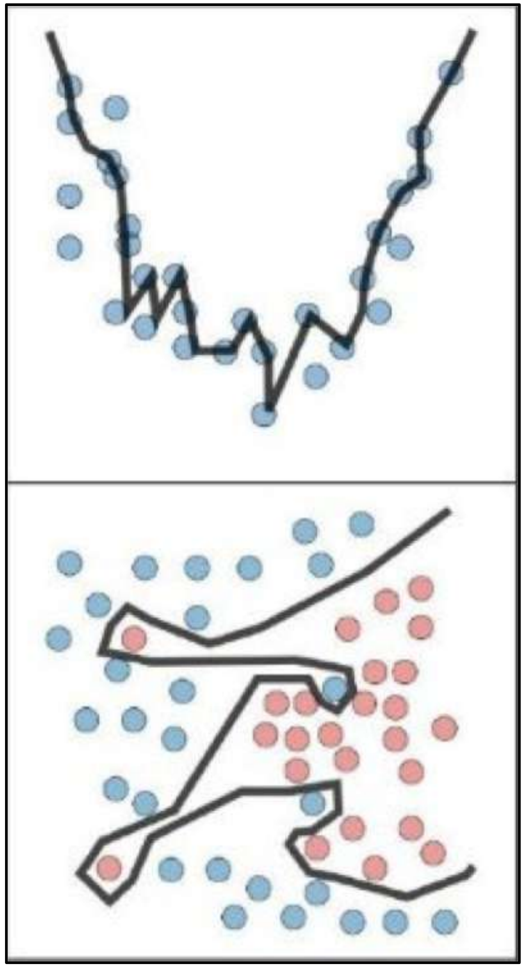

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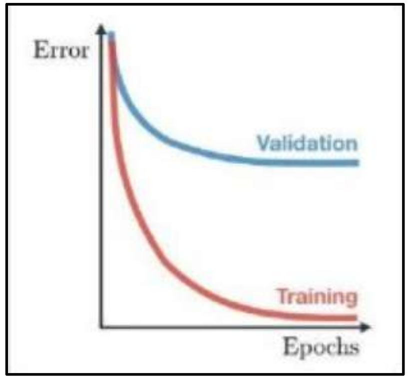

low in-sample error high out-of-sample error

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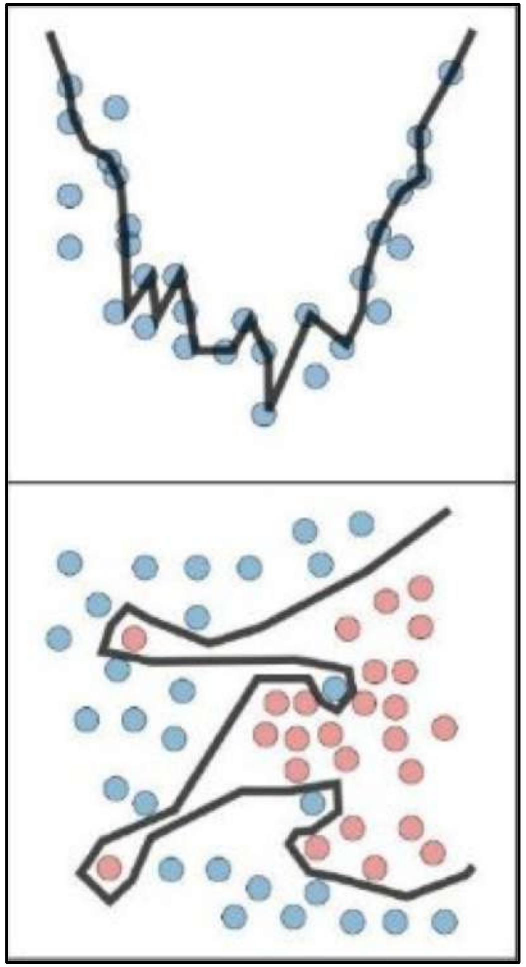

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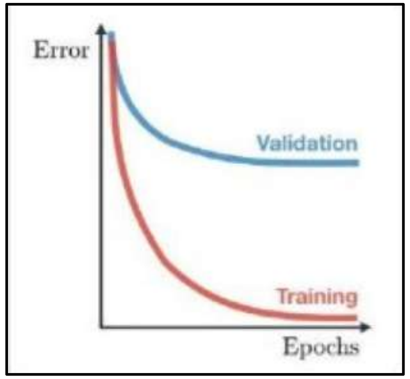

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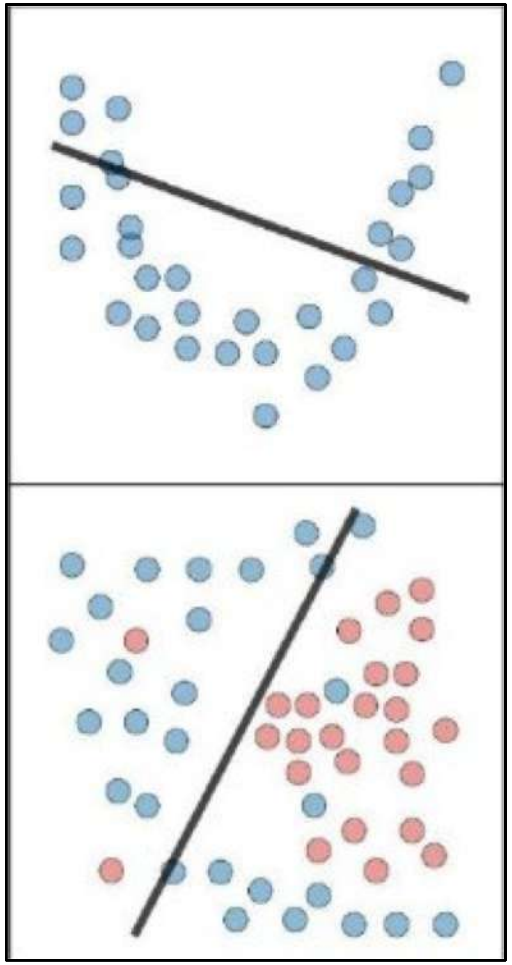
- Regularization
- Get more data

Underfitting (High Bias)

Regression

Classification



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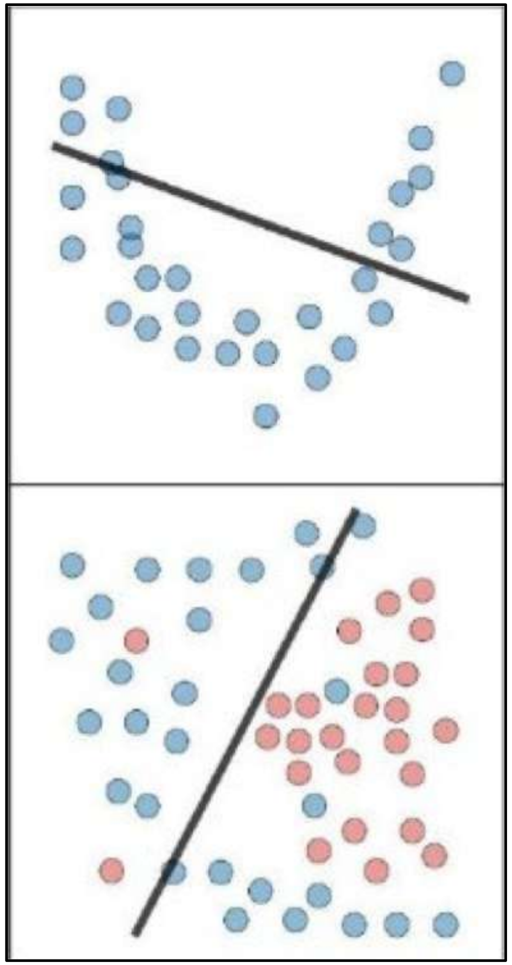

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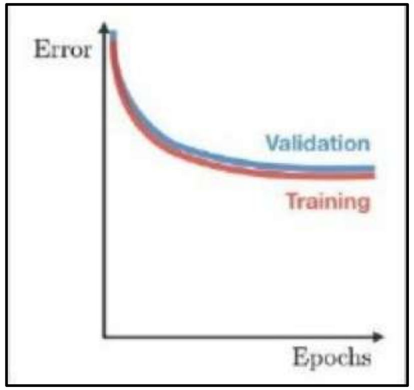

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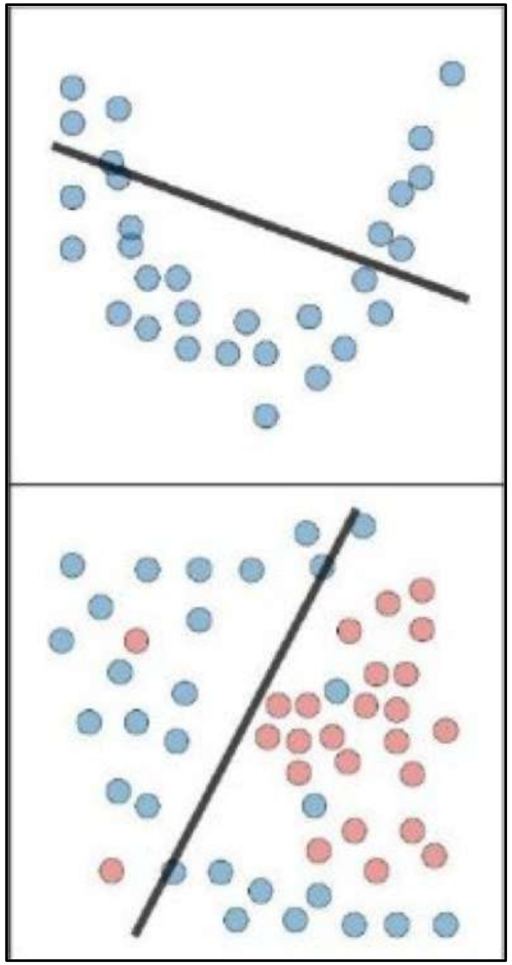

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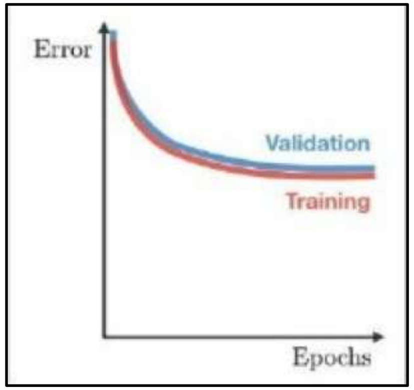


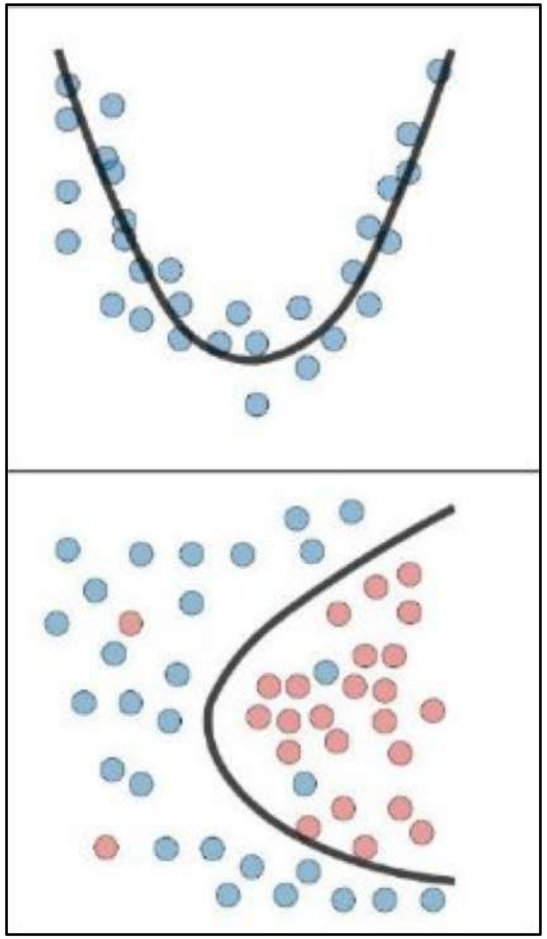
high in-sample error high out-of-sample error

- 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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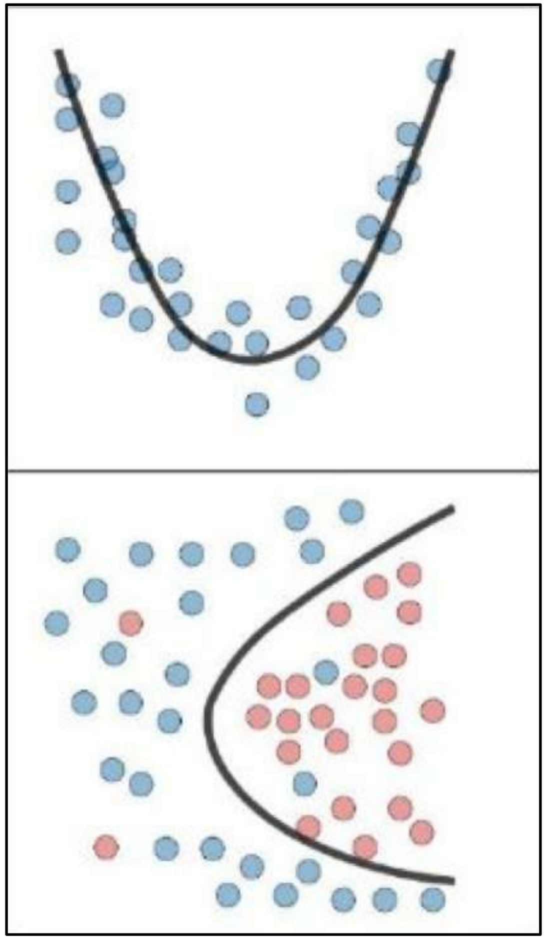

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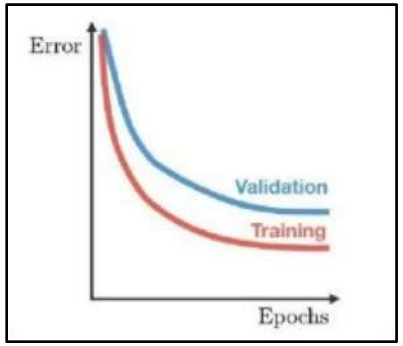

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Estimating Generalization Performance

- Measuring the generalization (i.e., out-of-sample) performance online may be too risky
  - e.g., don't want to deploy your new spam classifier in production knowing only its training (i.e., in-sample) performance

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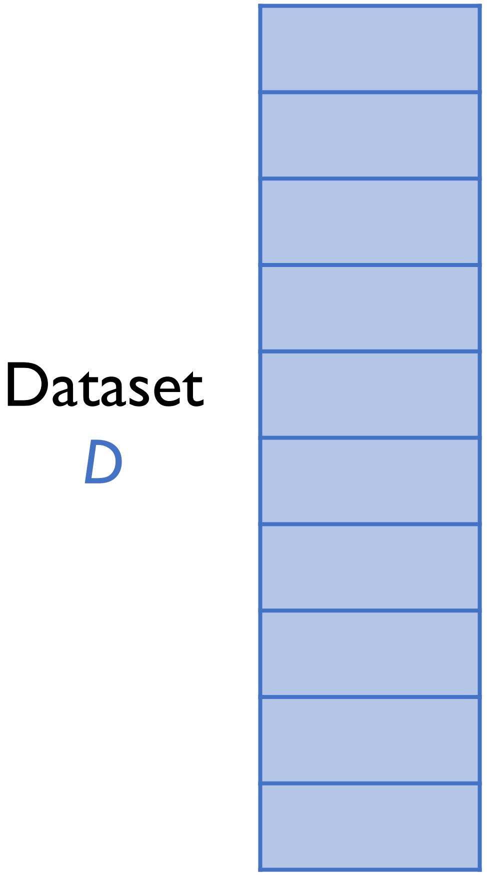
- Measuring the generalization (i.e., out-of-sample) performance online may be too risky
  - e.g., don't want to deploy your new spam classifier in production knowing only its training (i.e., in-sample) performance
- **Solution:** Estimate the generalization performance using training set
  - As long as it holds true the assumption that training and test instances are both drawn from the same probability distribution

Dataset Splitting



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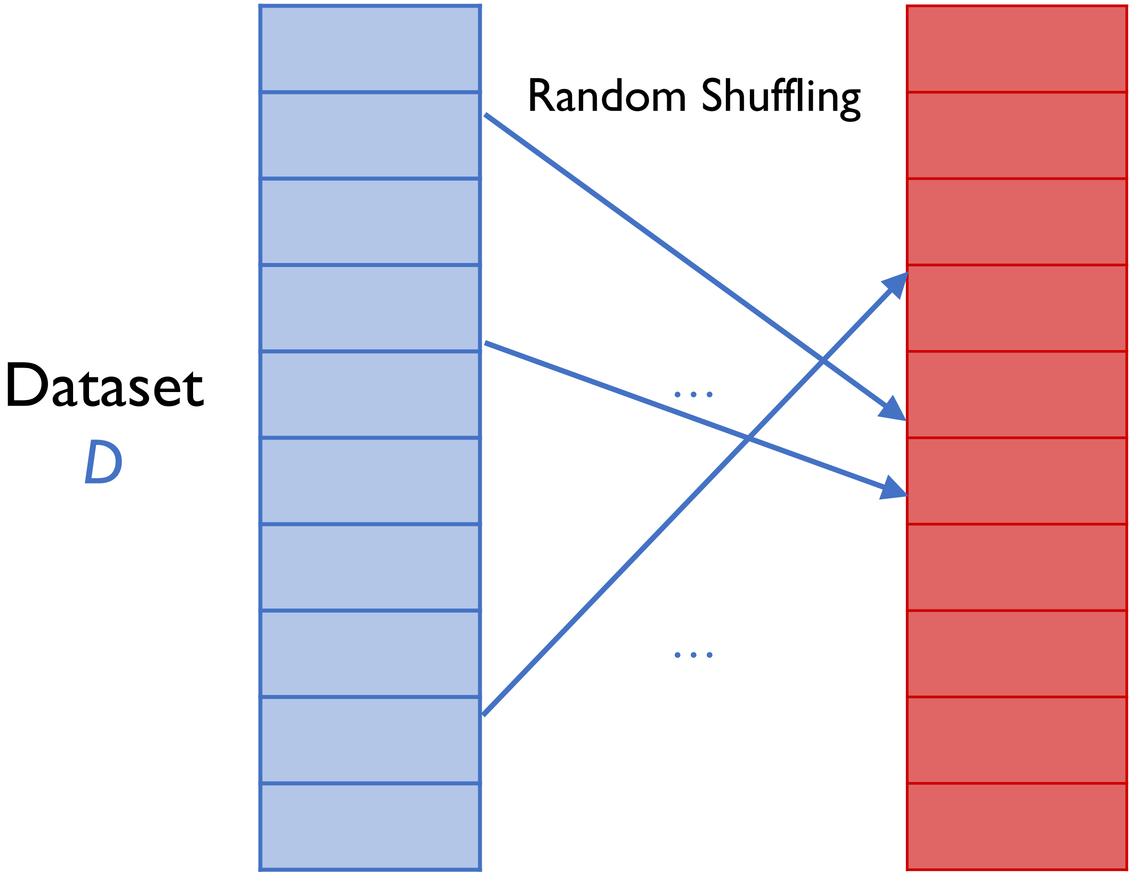

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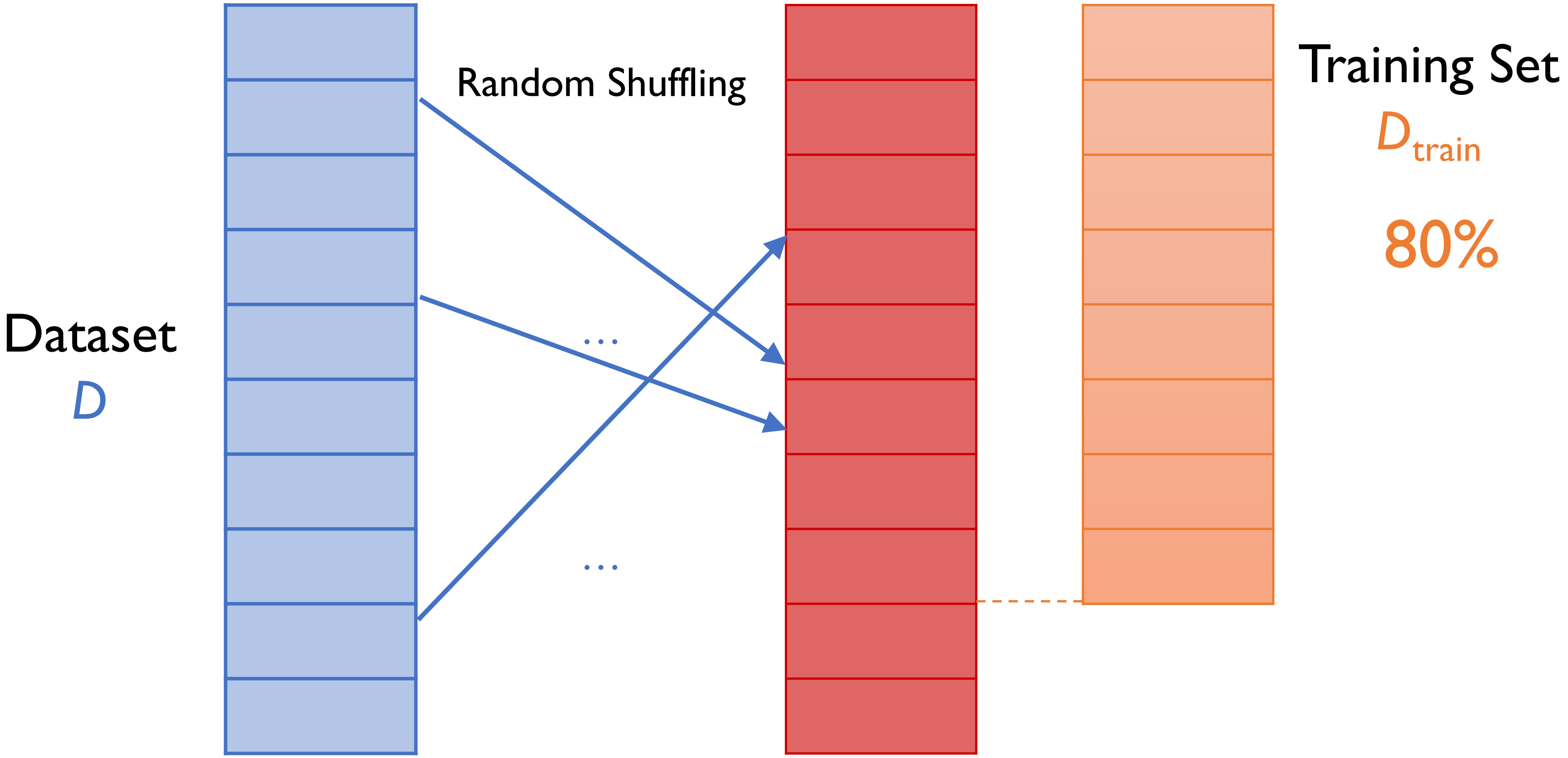
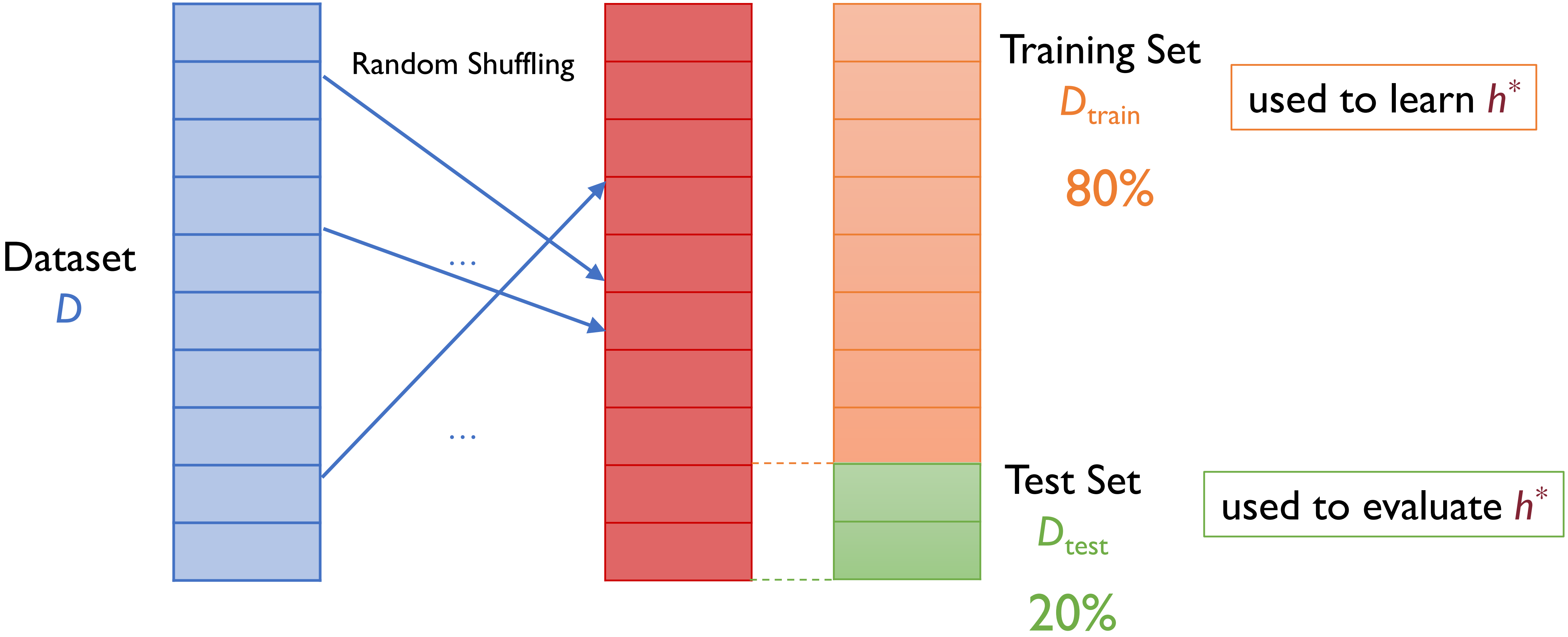


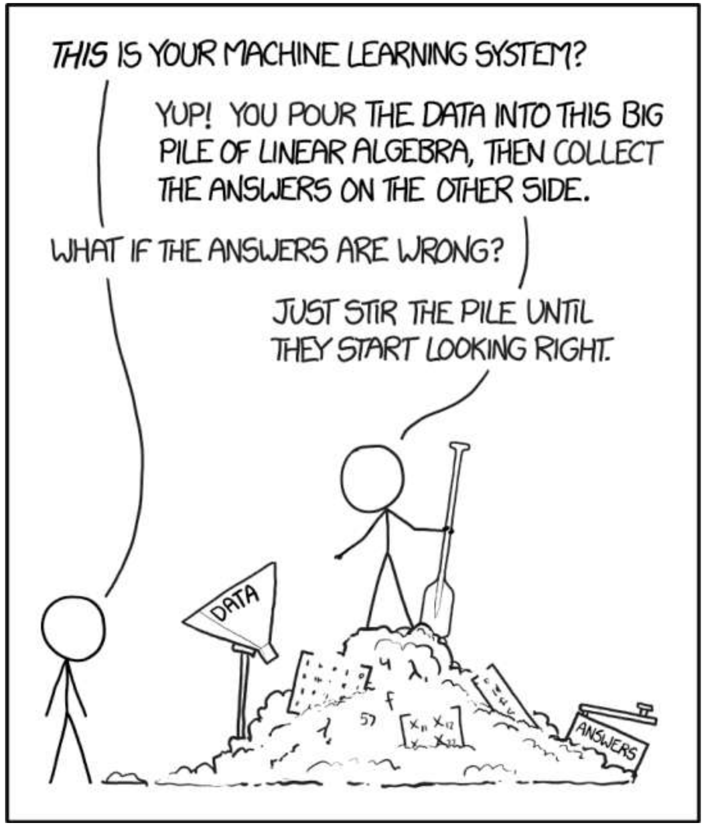
used to learn h^*

Dataset Splitting



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

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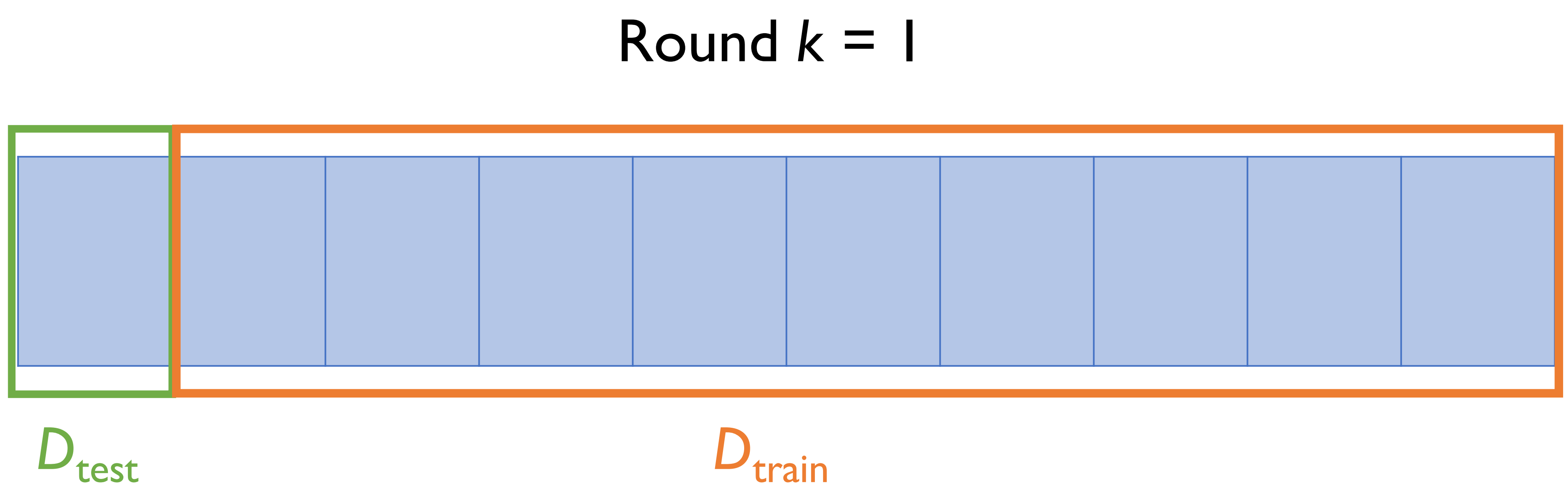

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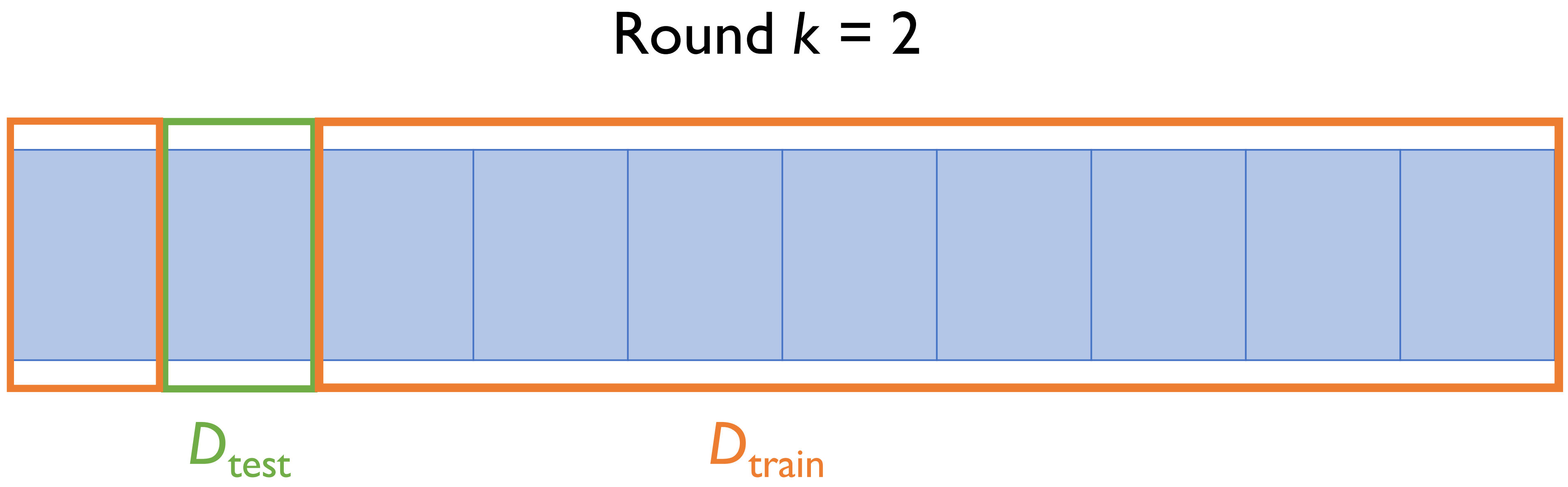
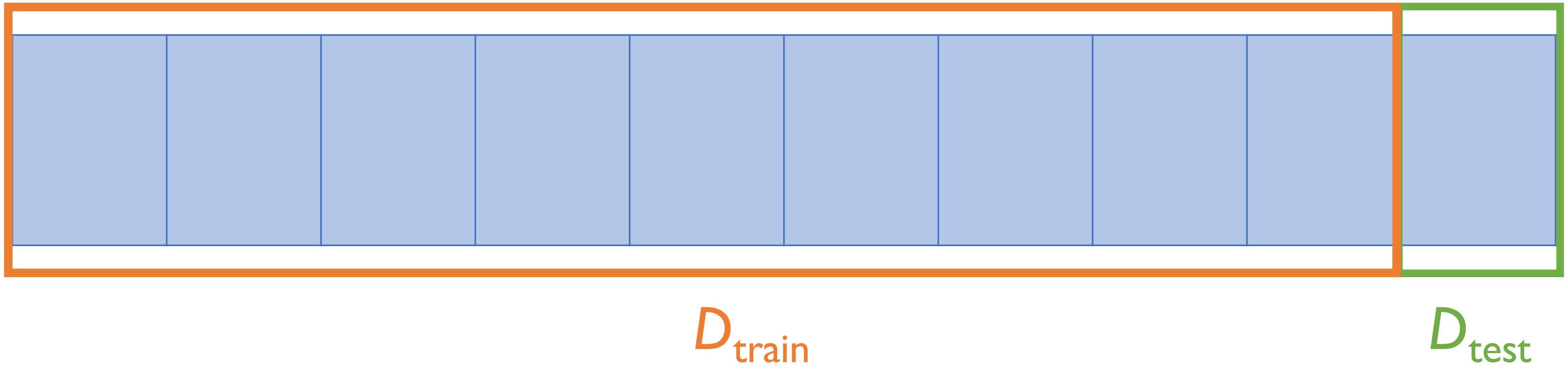


K-Fold Cross Validation

Round k = 10



Model Selection/Evaluation

Several different learning models to achieve the same task

Decision Trees

Random Forests

Logistic Regression

*k*NN

SVM

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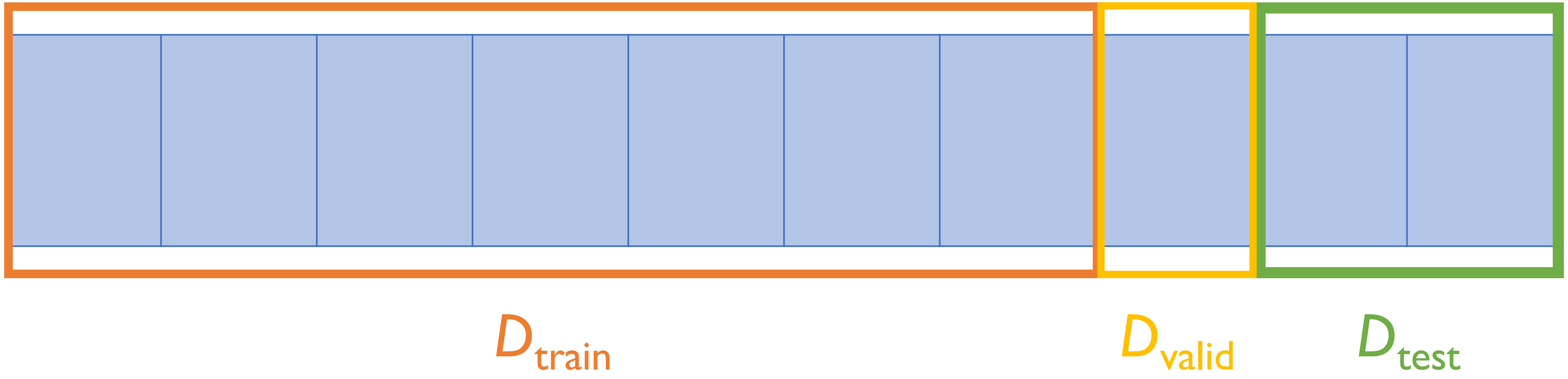
How do we select the best model?

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

Take-Home Message of Today

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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