

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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Clustering

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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

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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

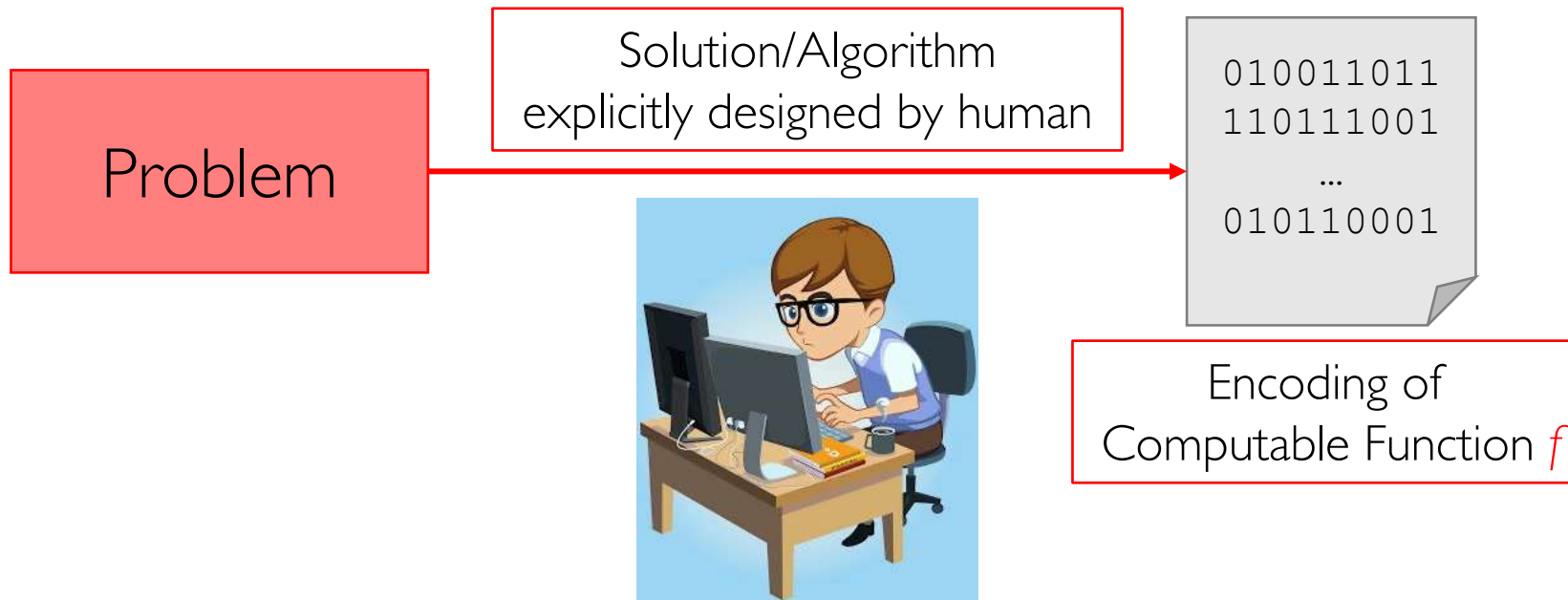
Programming a Computer

Problem

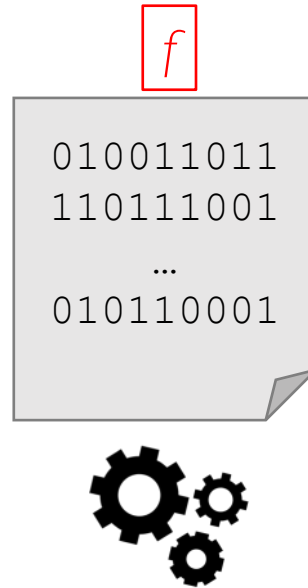
Solution/Algorithm
explicitly designed by human



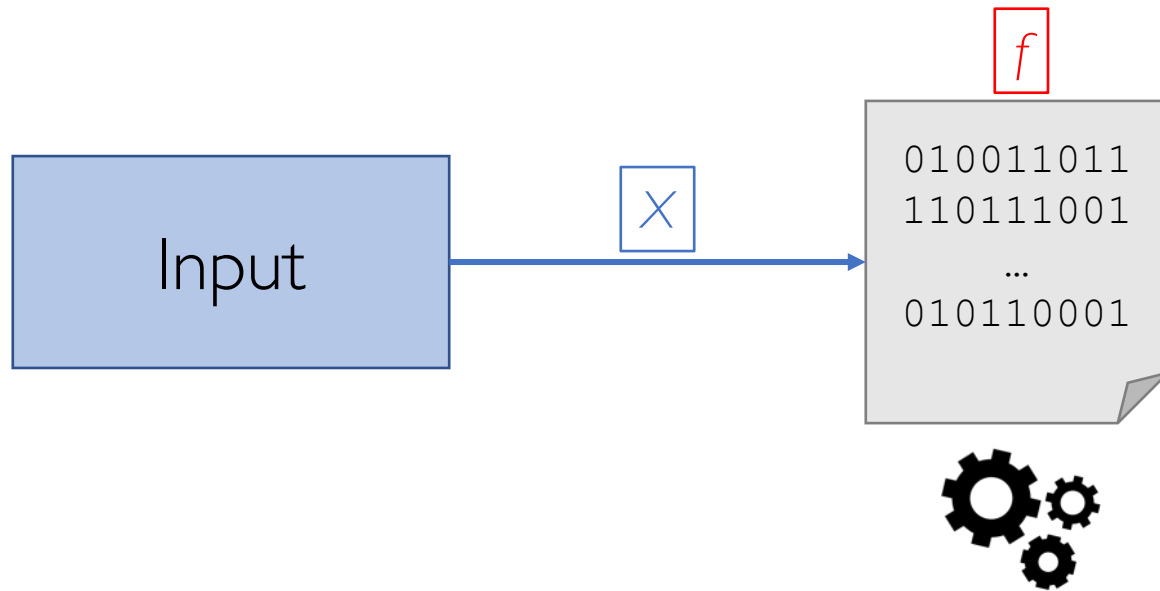
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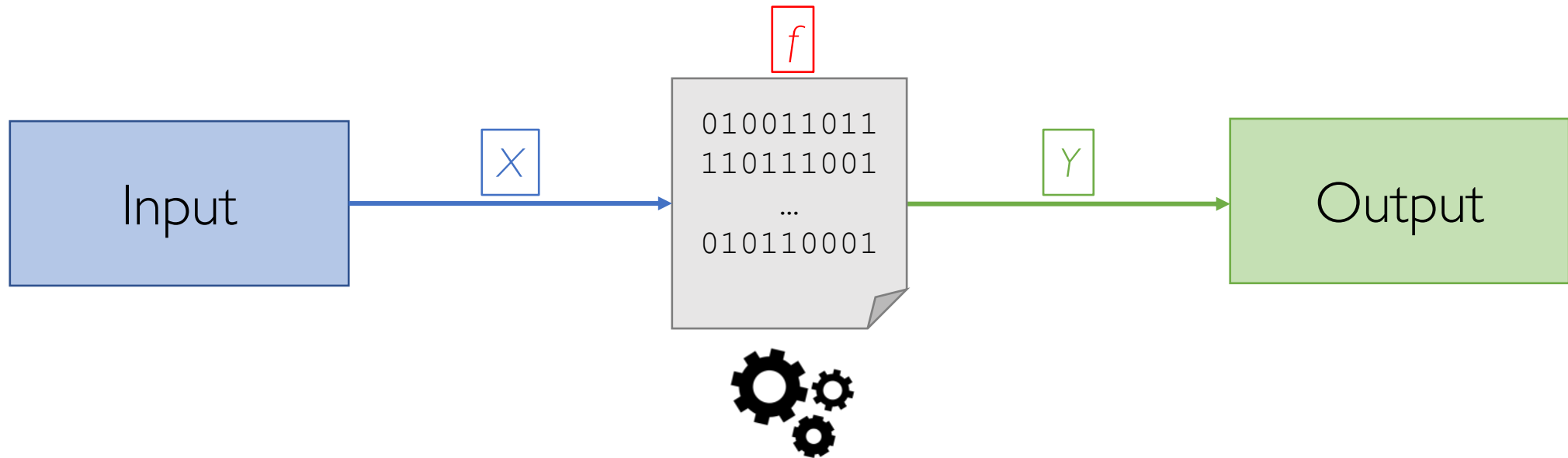
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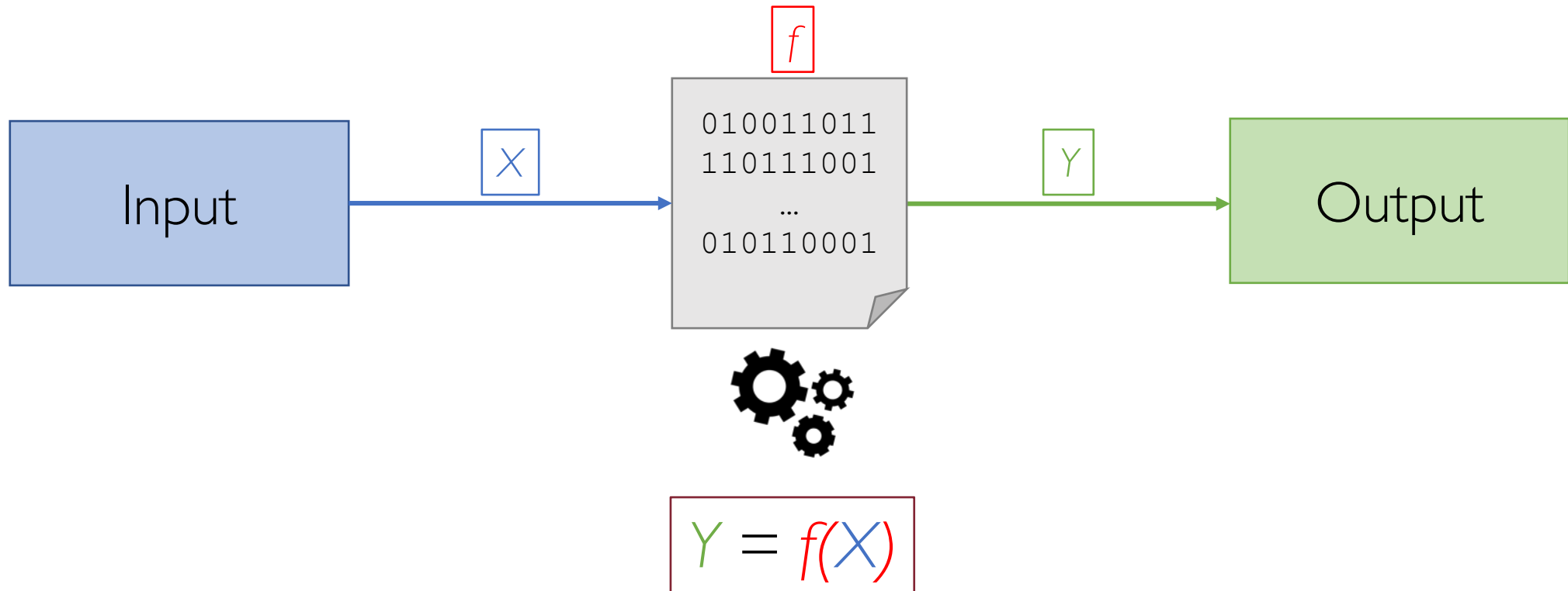
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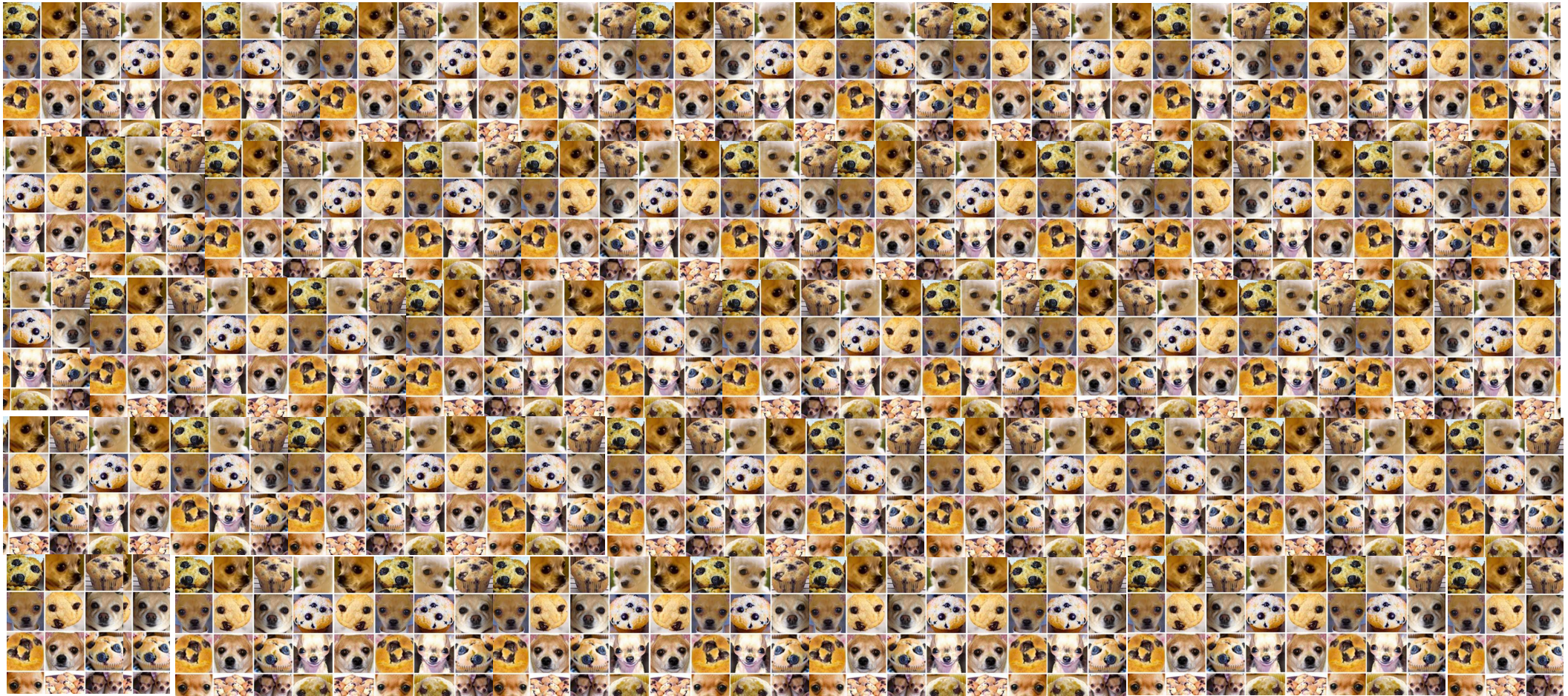


Programming a Computer



Can We Always Do That?

Chihuahua or Muffin?



[Copyright @teenybiscuit]

Chihuahua



Muffin



Programming vs. "Training" a Computer

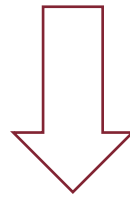
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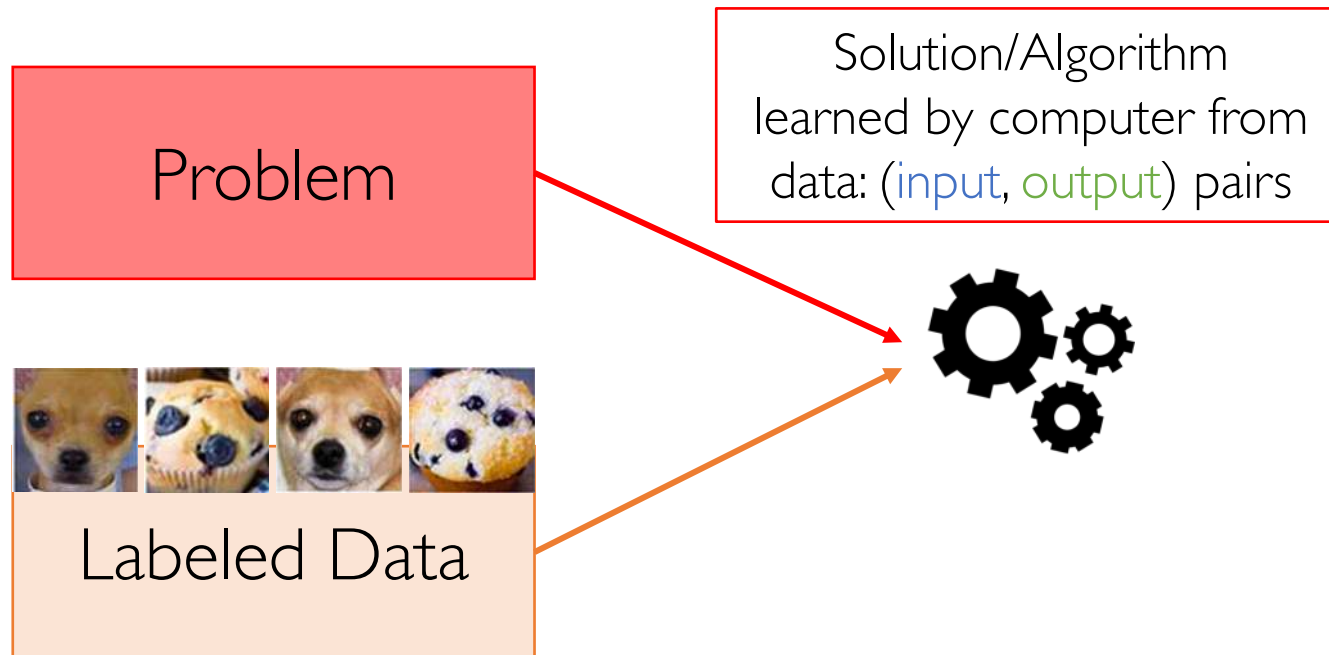
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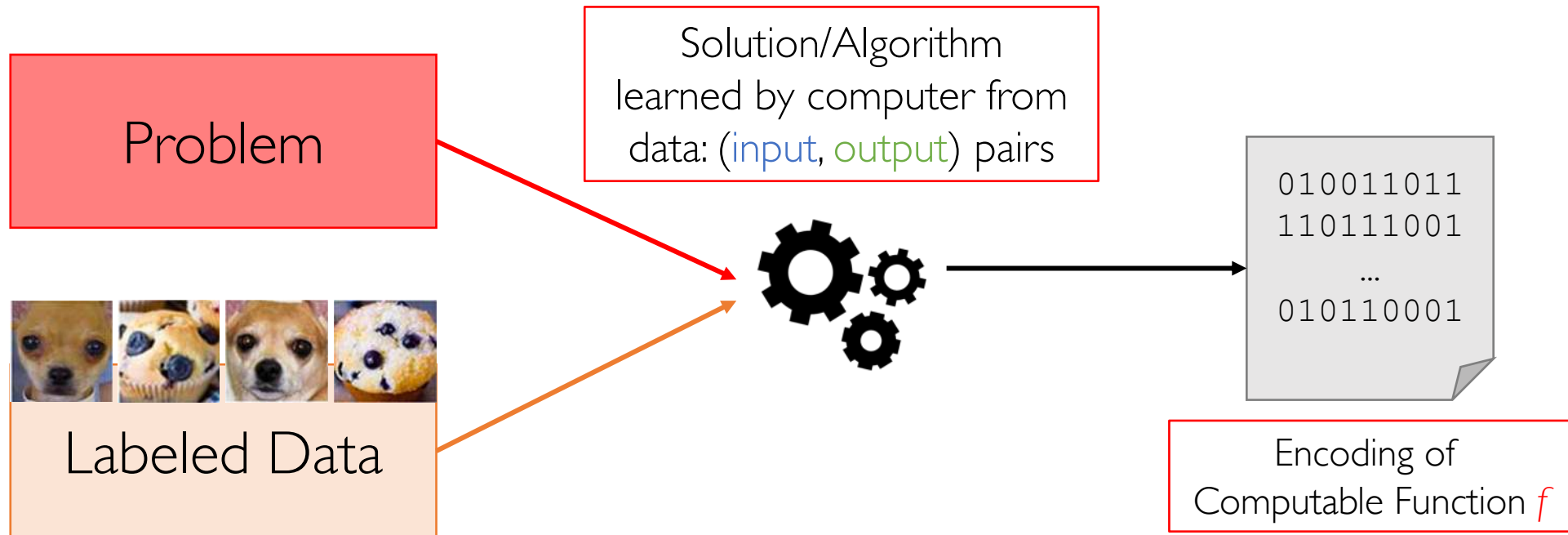


Labeled Data

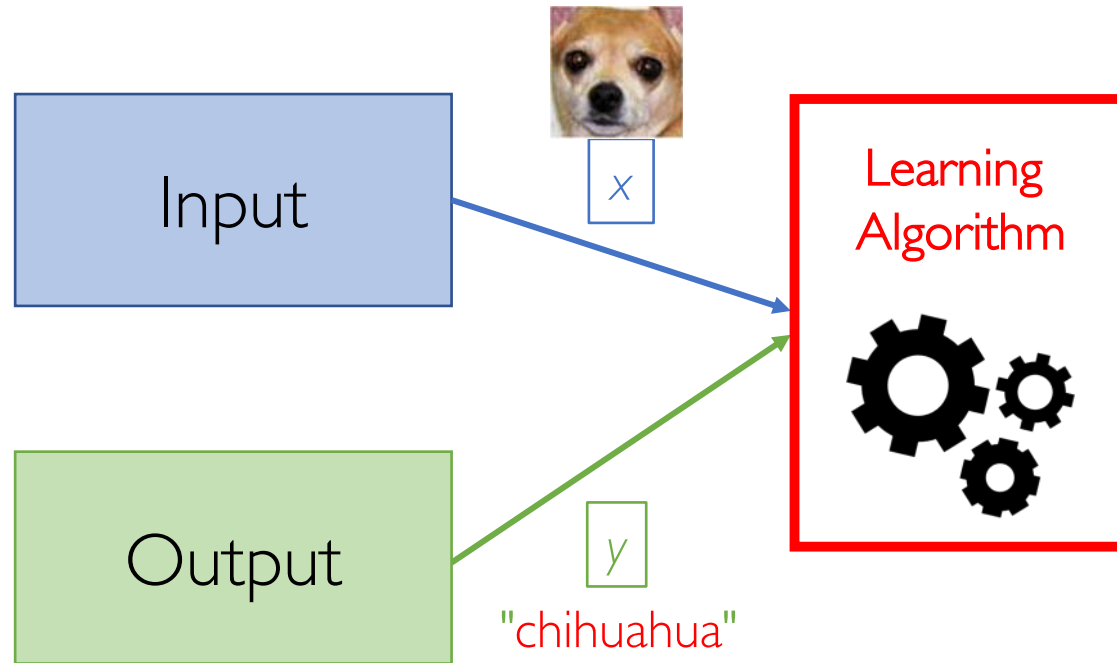
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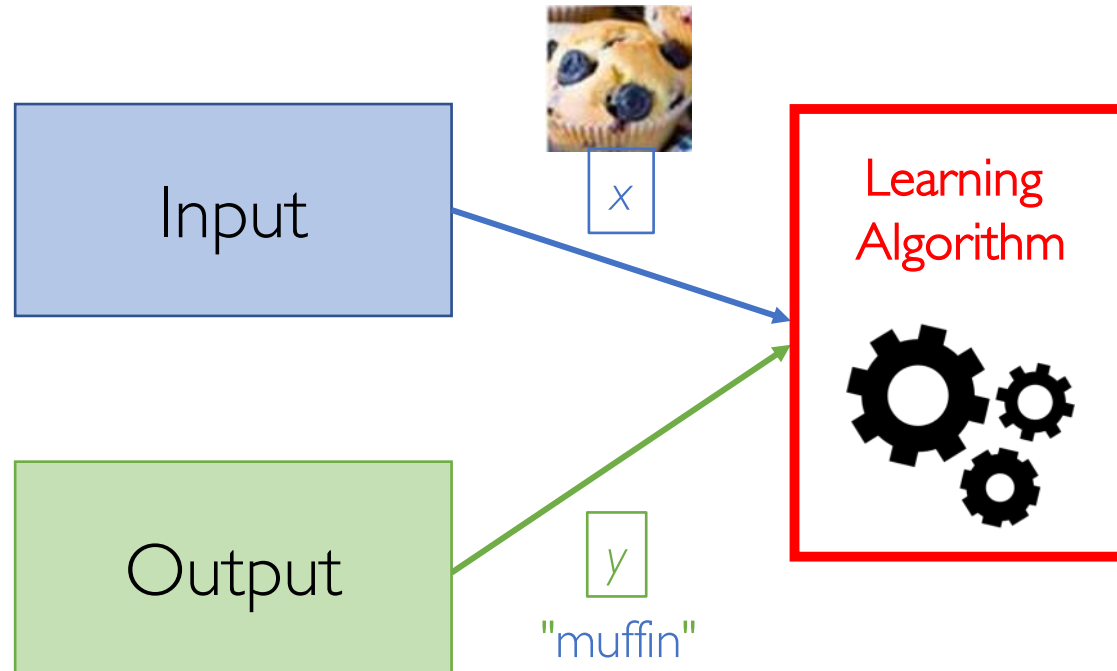
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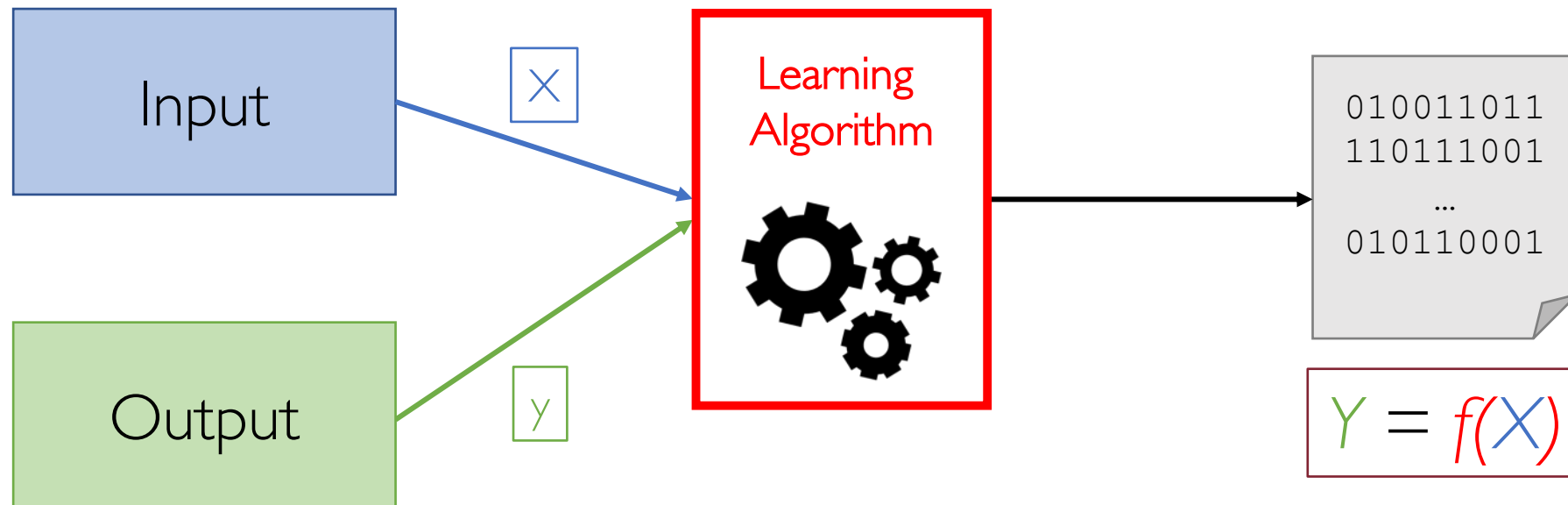
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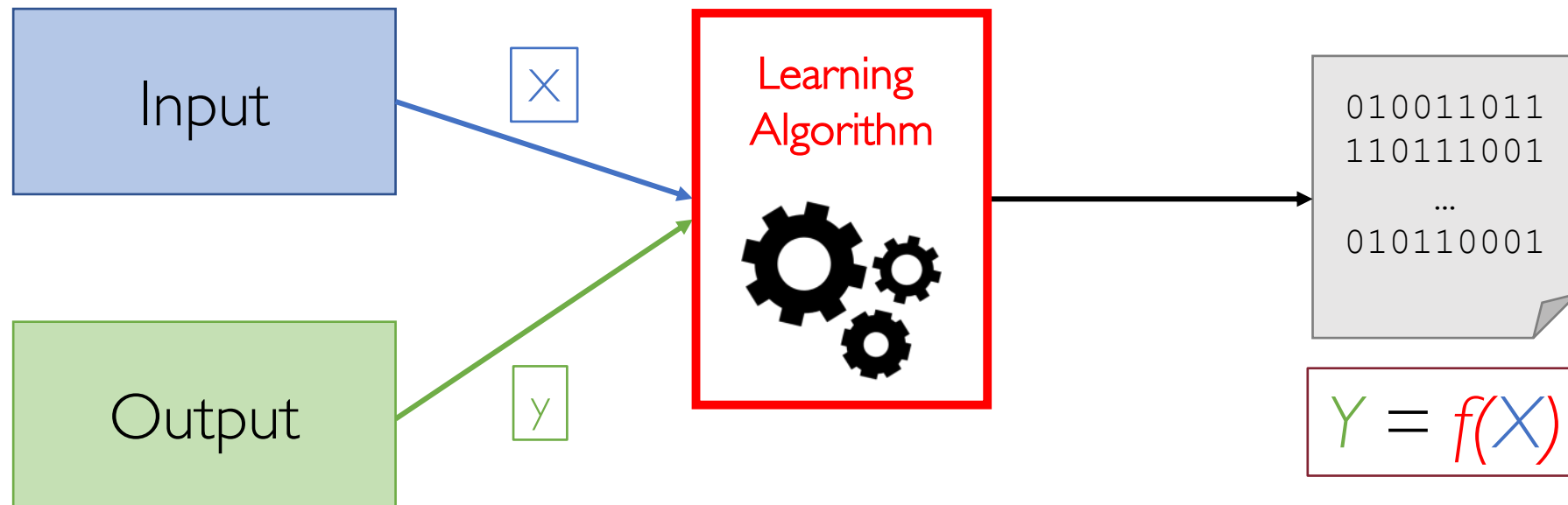
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Eventually, the function f is **learned** by the learning algorithm from a (large) set of **labeled data**

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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

Machine Learning

Machine Learning: Taxonomy

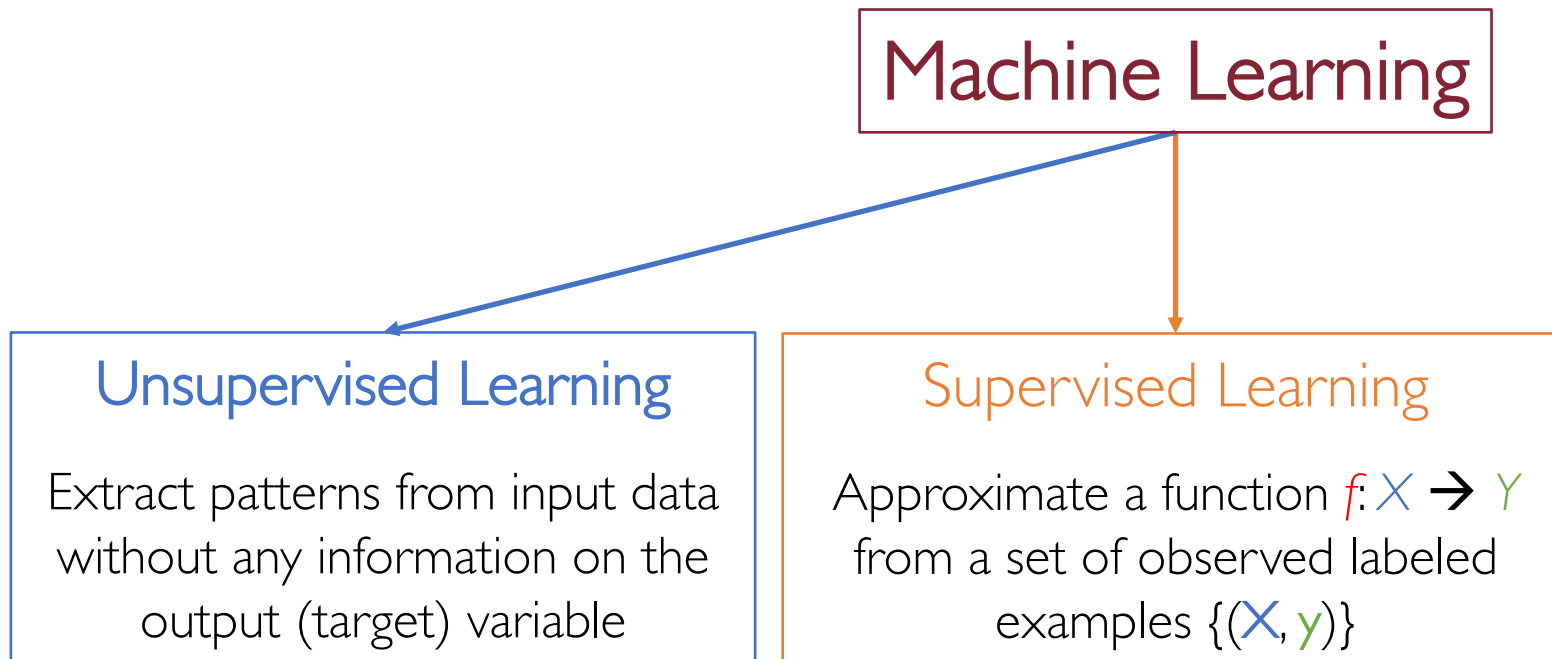
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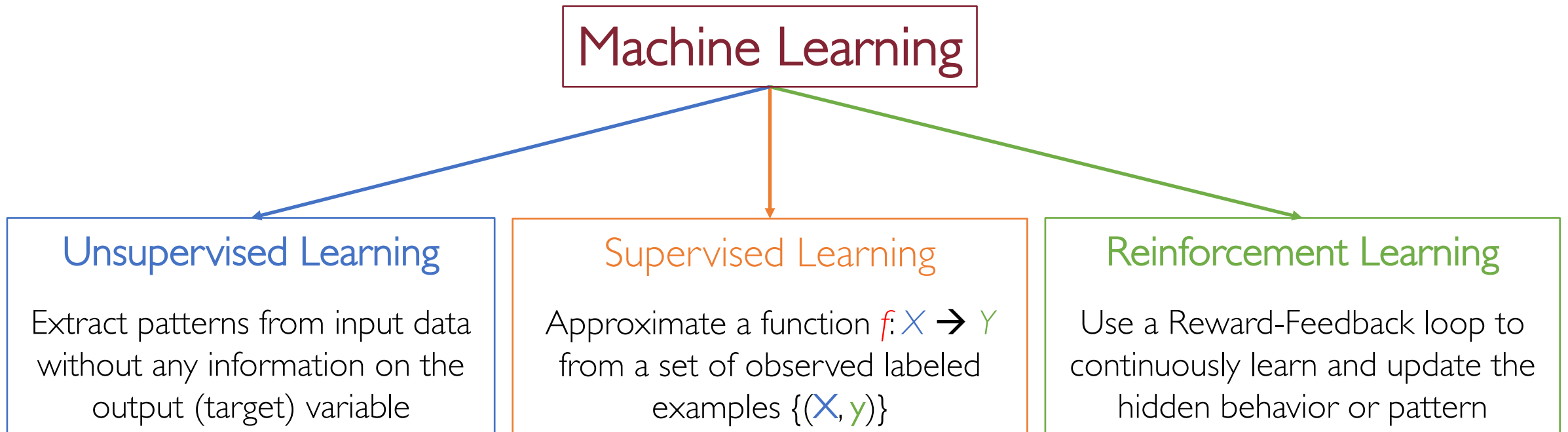
Unsupervised Learning

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

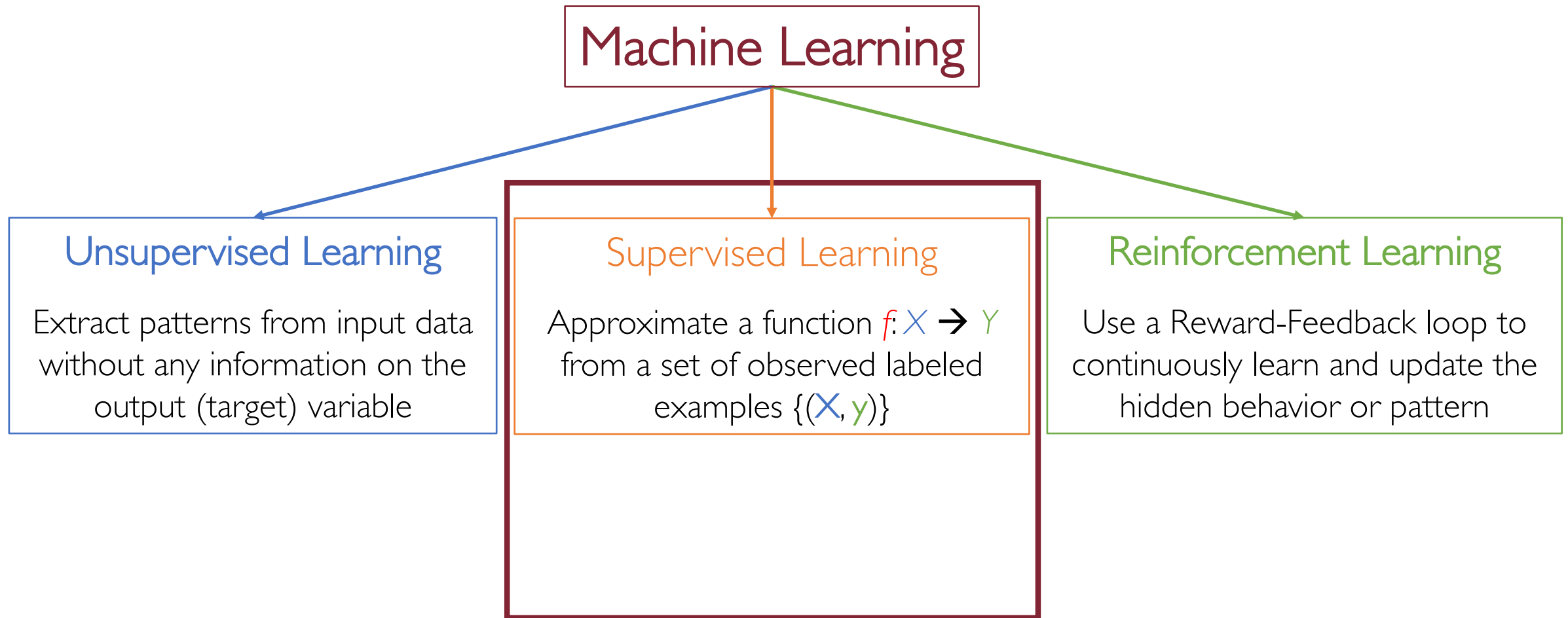
Machine Learning: Taxonomy



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Supervised Learning: What Do We Predict?

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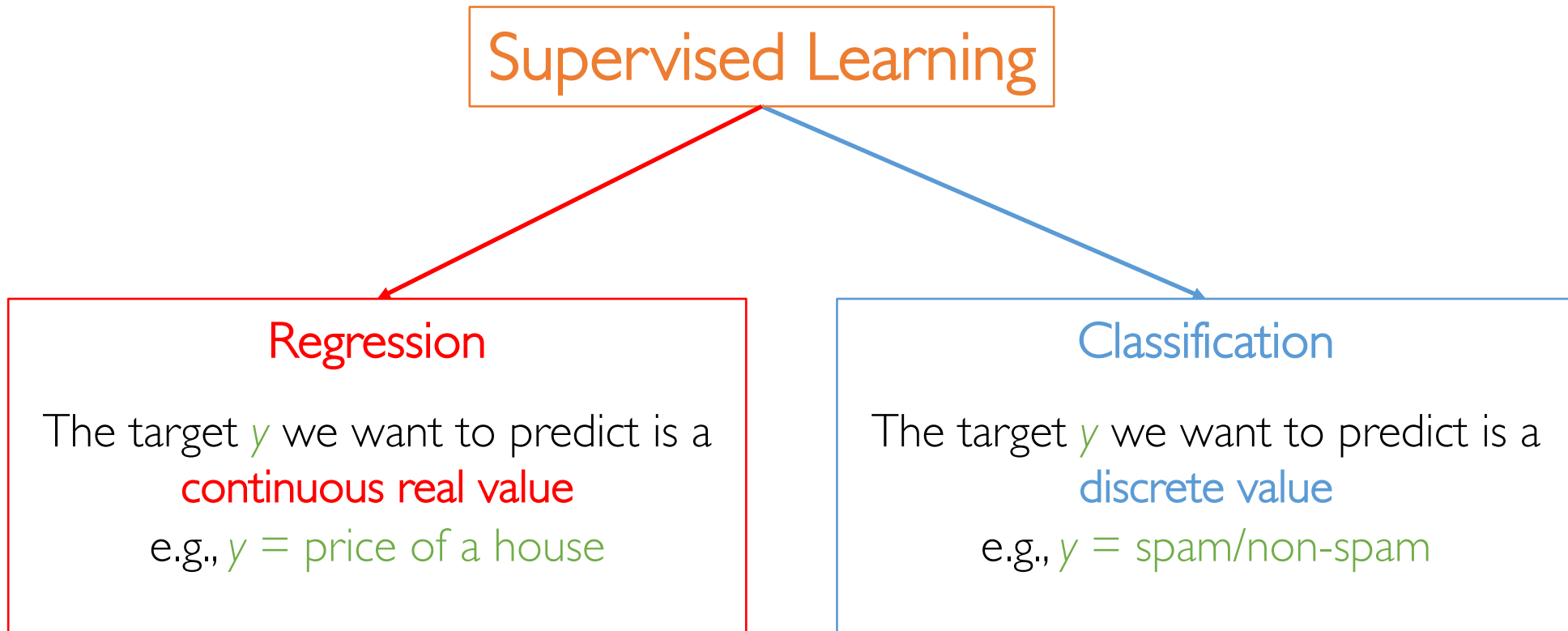
Supervised Learning



Regression

The target y we want to predict is a
continuous real value
e.g., $y = \text{price of a house}$

Supervised Learning: What Do We Predict?



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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- Supervised Learning requires **labeled data** which may be even harder to get
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- Might involve combining multiple and heterogeneous data sources

Feature Engineering



Domain Objects

Feature Engineering

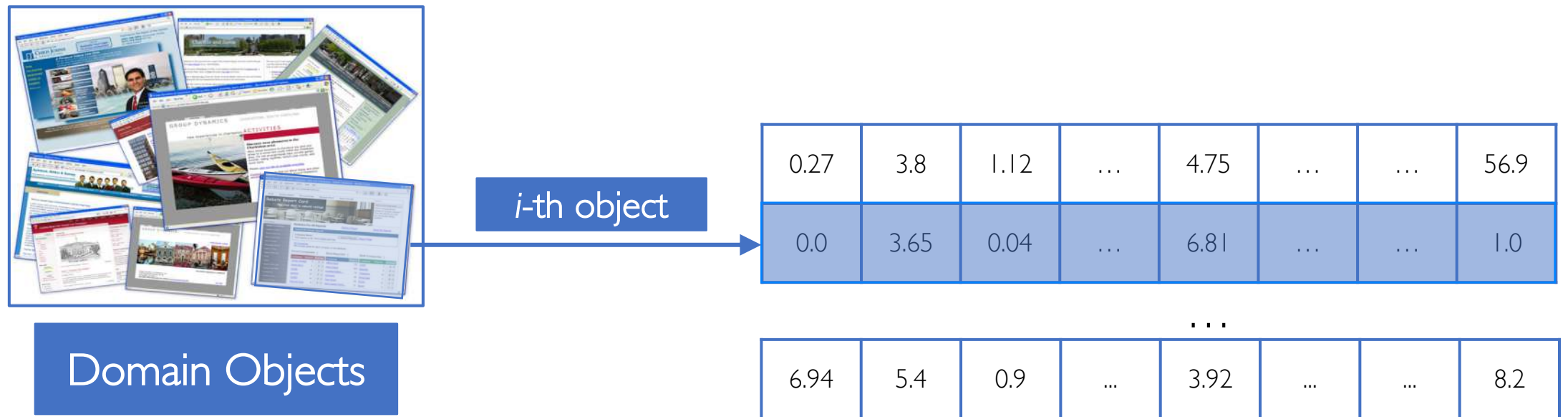
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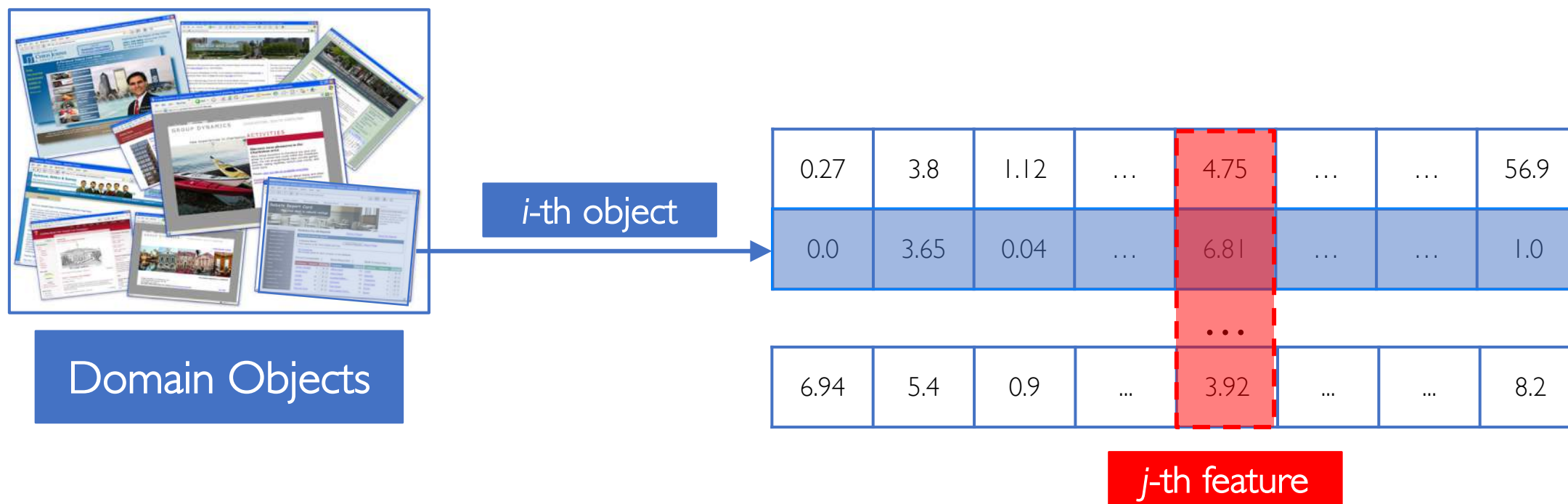
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- Each feature is a **property** of an instance of our domain
 - e.g., **number_of_bedrooms** in the case our domain objects are “houses”

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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!

Feature Engineering: Challenges and Solutions

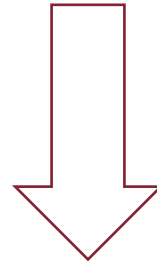
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Data Preprocessing

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 (<i>trimming</i> or <i>winsorising</i>)

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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 <i>one-hot encoding</i>

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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)

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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	

Feature Engineering: Challenges and Solutions

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

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$$\mathcal{X} \subseteq \mathbb{R}^n$$

input feature space

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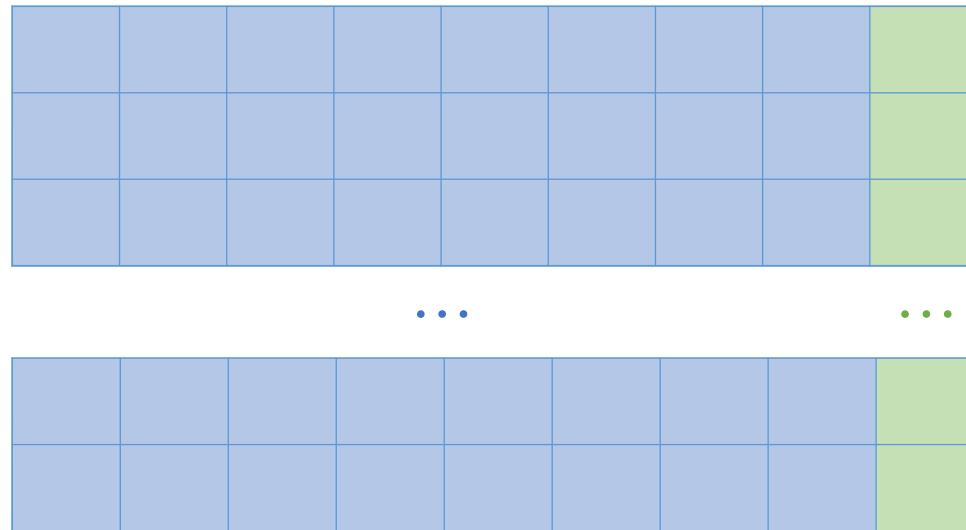
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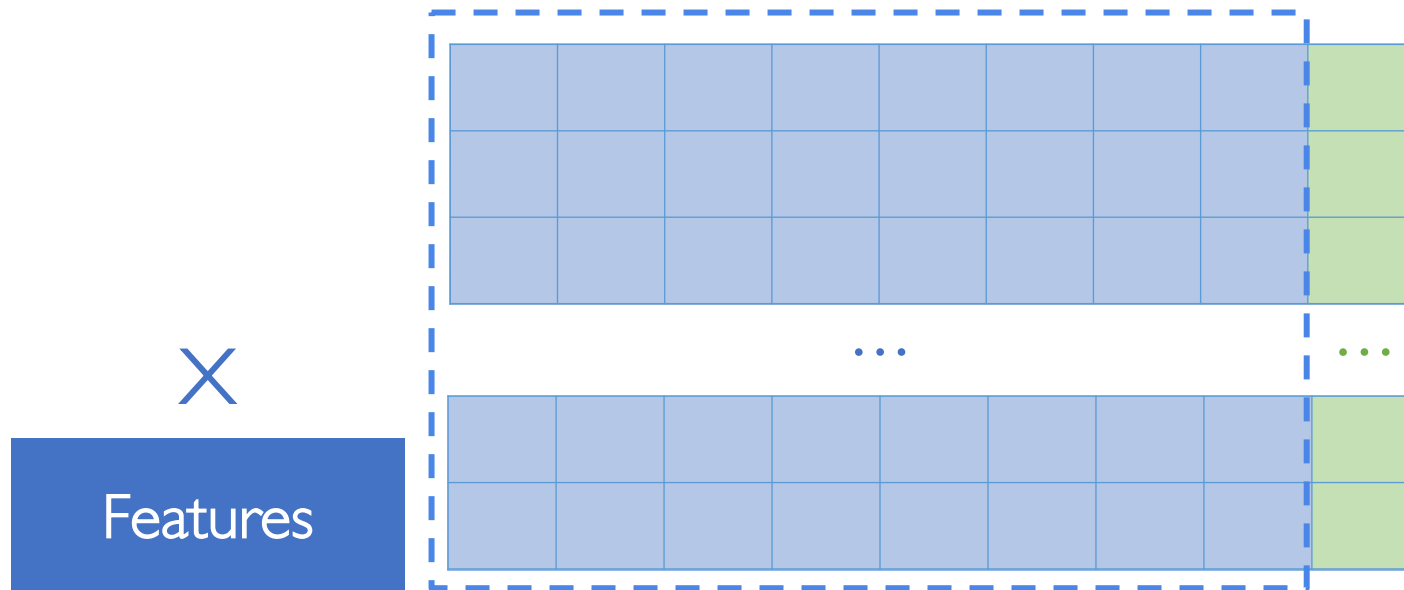
$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)\}$$

dataset of m i.i.d. labeled instances

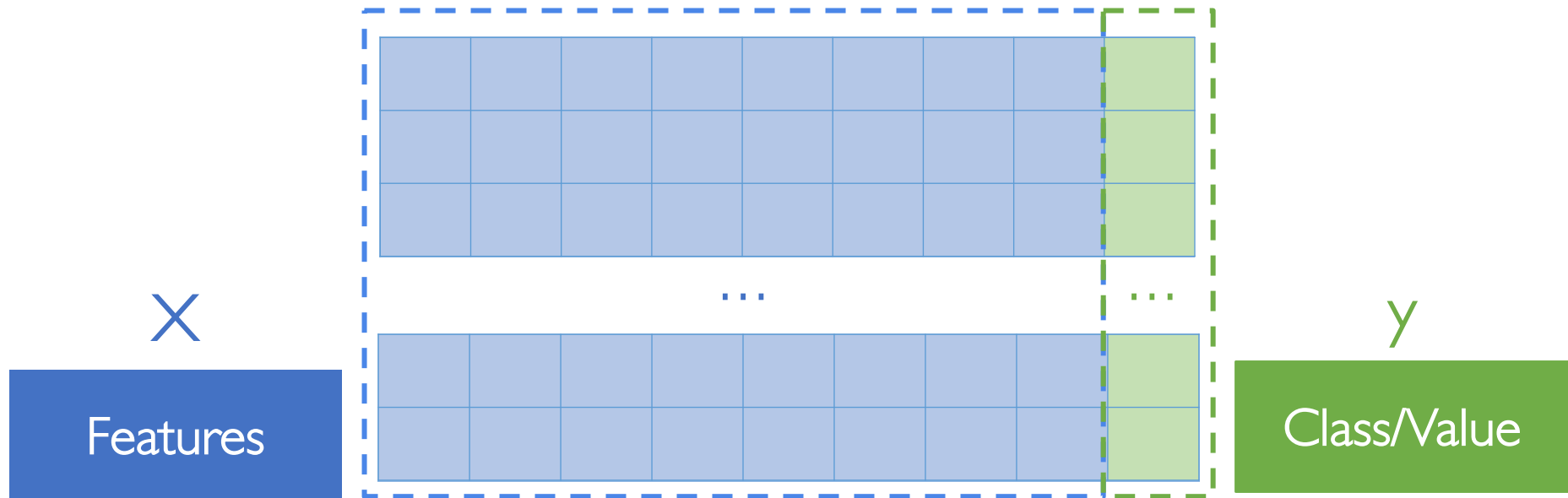
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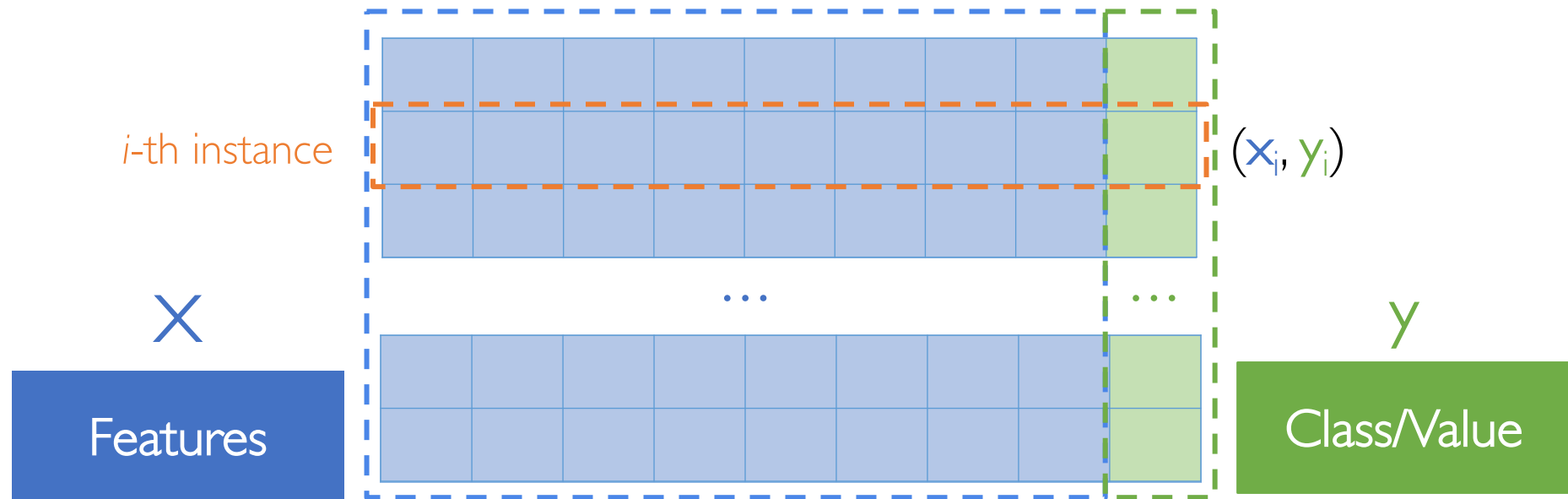


Model Training: Labeled Dataset



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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 - **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

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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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- Measures the error we would make if a hypothesis h is used instead of the true (yet unknown) mapping f

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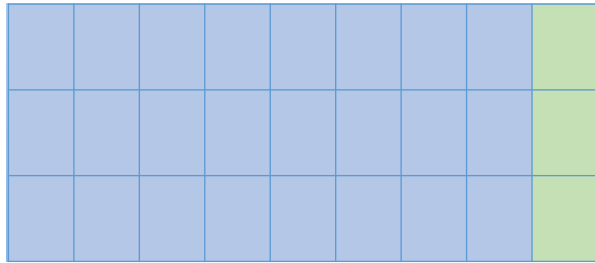
$$h^* = \operatorname{argmin}_{h \in \mathcal{H}} L(h, \mathcal{D})$$

unknown target
(e.g., ideal credit approval function)

$$f = X \rightarrow Y$$

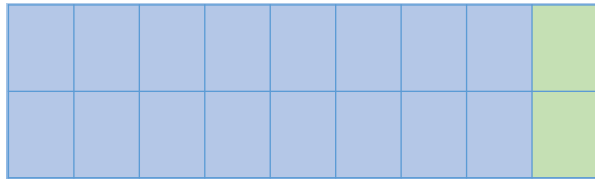
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A diagram showing a grid of training data. It consists of two rows of blue squares, each followed by a green square. The first row has 8 blue squares and 1 green square. The second row has 8 blue squares and 1 green square. Below the first row, there are three blue dots and three green dots, indicating continuation of the data.

...



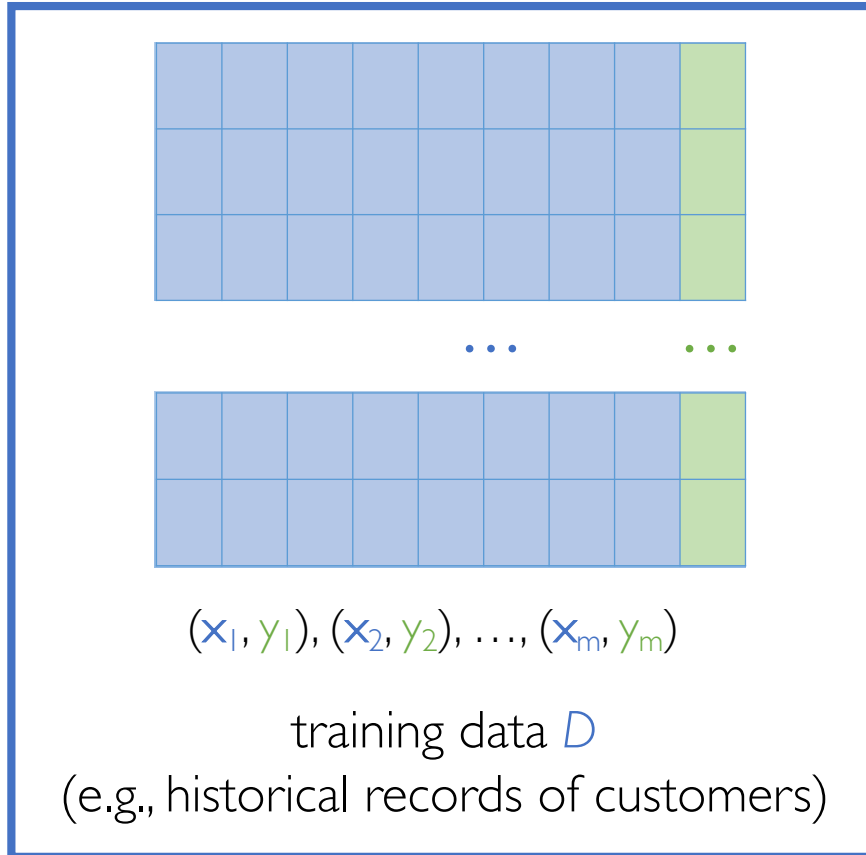
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training data D
(e.g., historical records of customers)

unknown target
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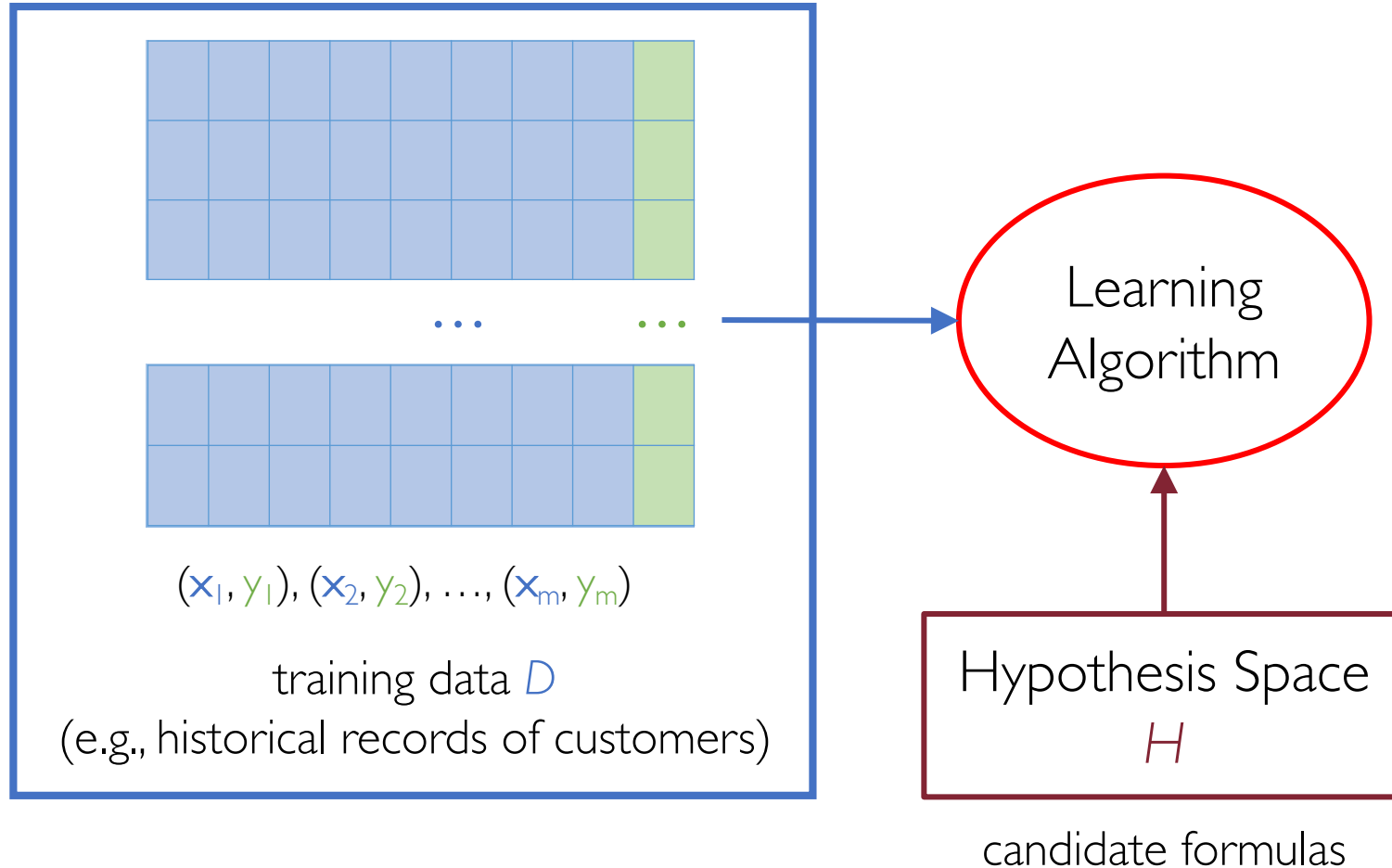
Hypothesis Space

H

candidate formulas

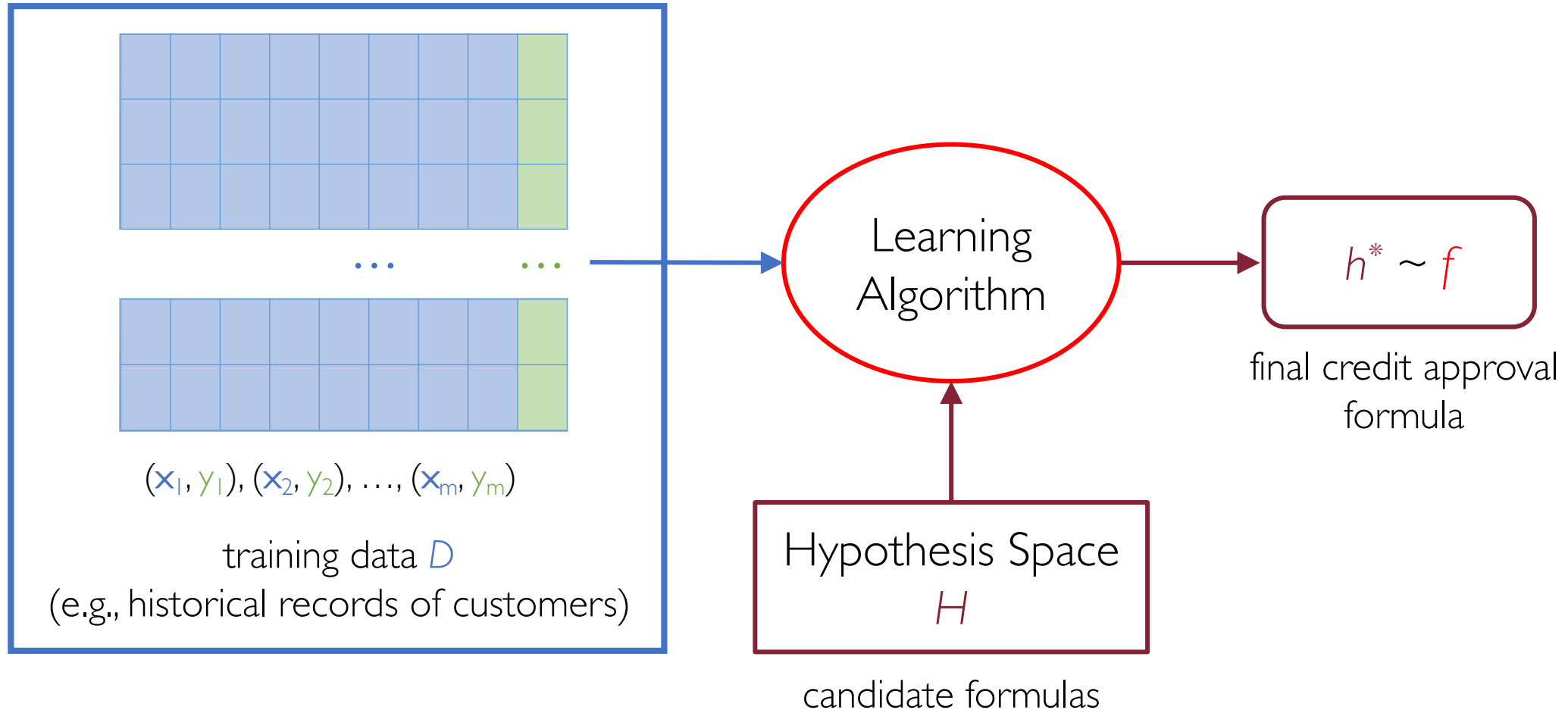
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Learning f as an Optimization Problem

- We define the supervised learning problem as an optimization one

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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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In-Sample vs. Out-of-Sample Error

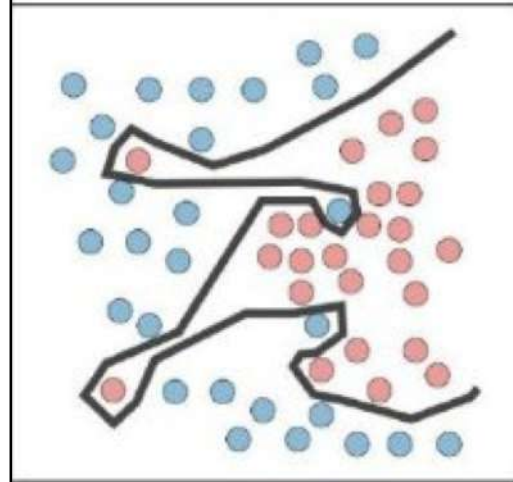
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- At the same time we do not want h^* to perform poorly on D

Overfitting (High Variance)

Regression



Classification



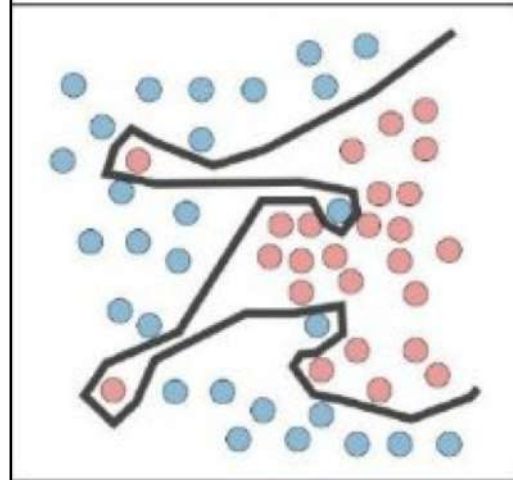
The hypothesis h^* is not learning the true f but it mimics its noise

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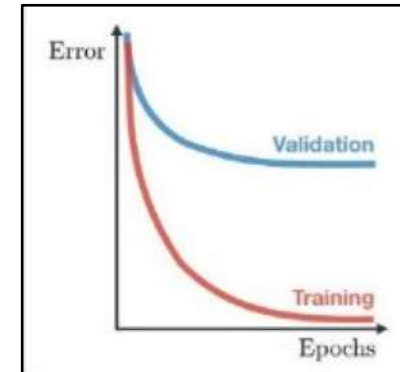
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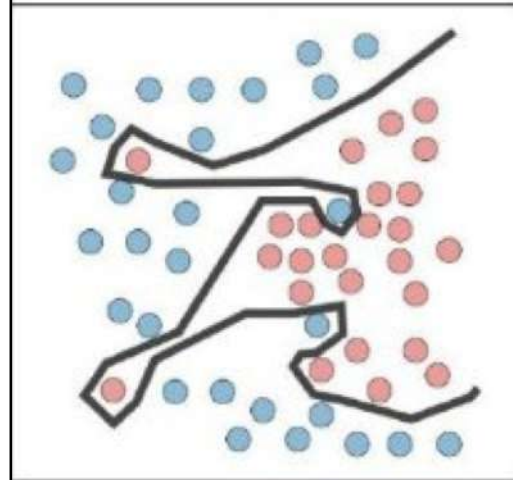
low in-sample error high out-of-sample error

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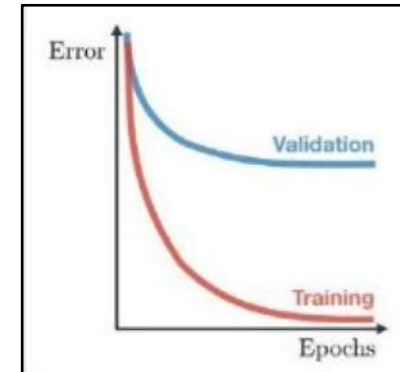
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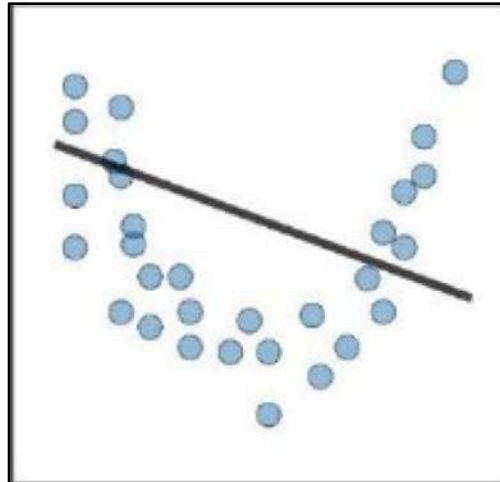


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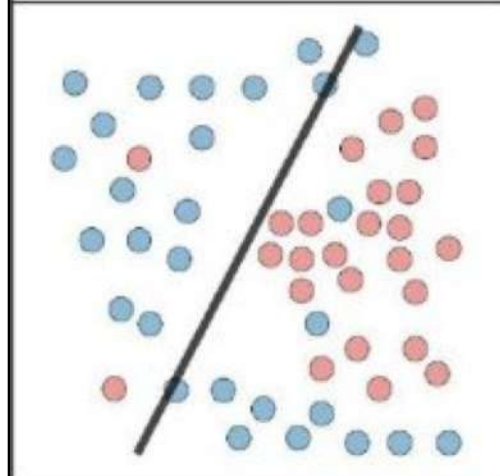
- Regularization
- Get more data

Underfitting (High Bias)

Regression



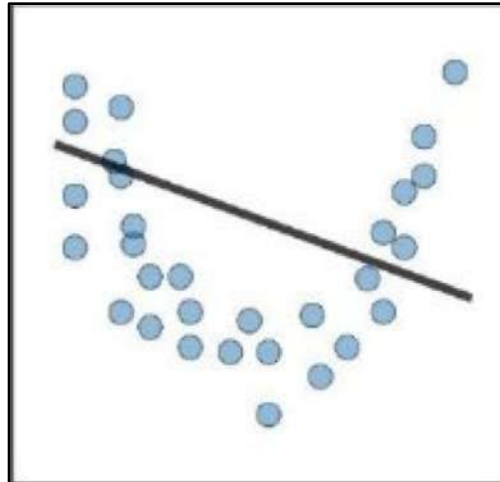
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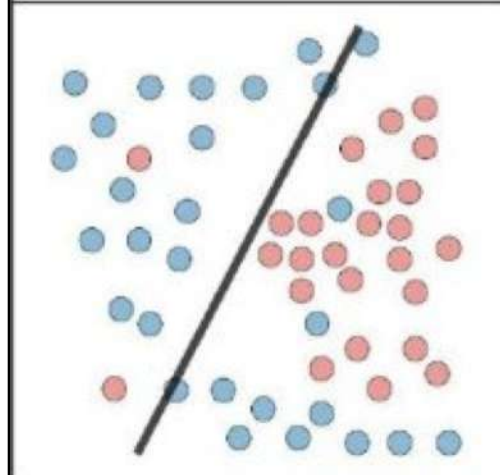
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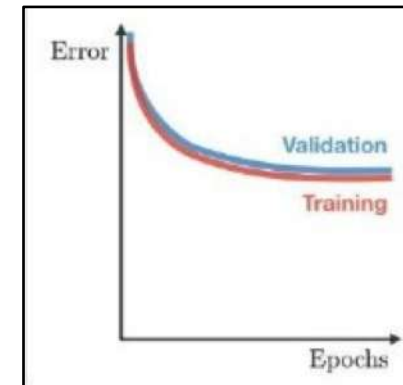
Regression



Classification



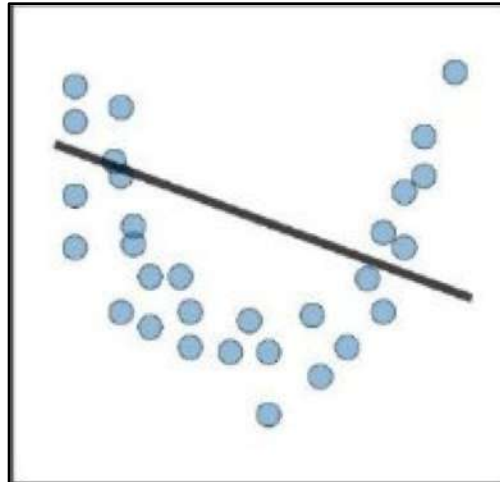
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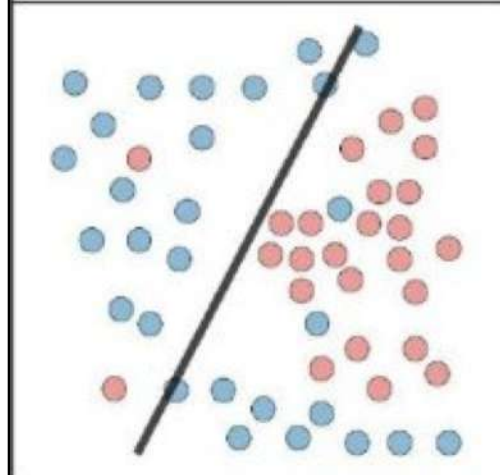
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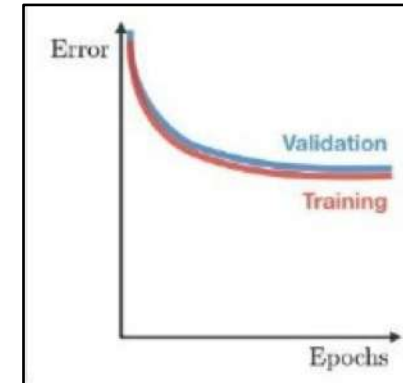
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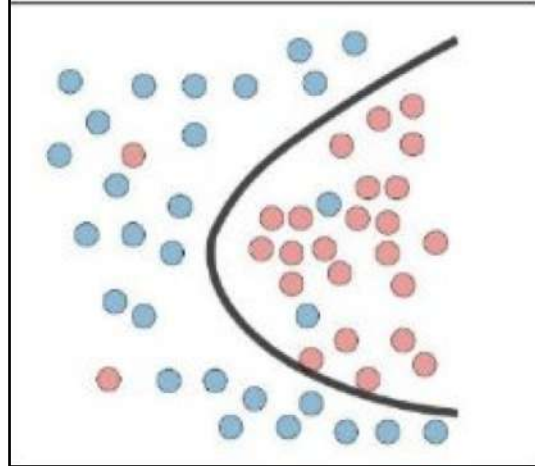
- Increase model complexity
- Add more features

Bias-Variance Tradeoff

Regression



Classification



The hypothesis h^* is just right:
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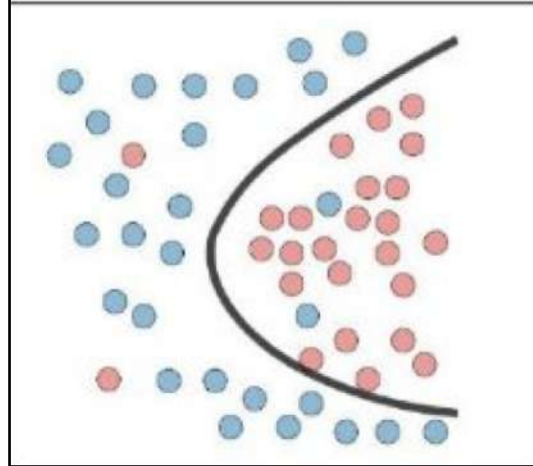
Occam's razor

Bias-Variance Tradeoff

Regression

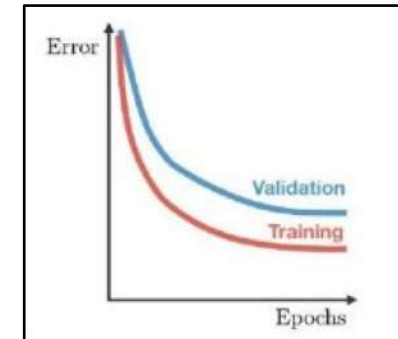


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Estimating Generalization Performance

- Measuring the generalization (i.e., out-of-sample) performance online may be too risky

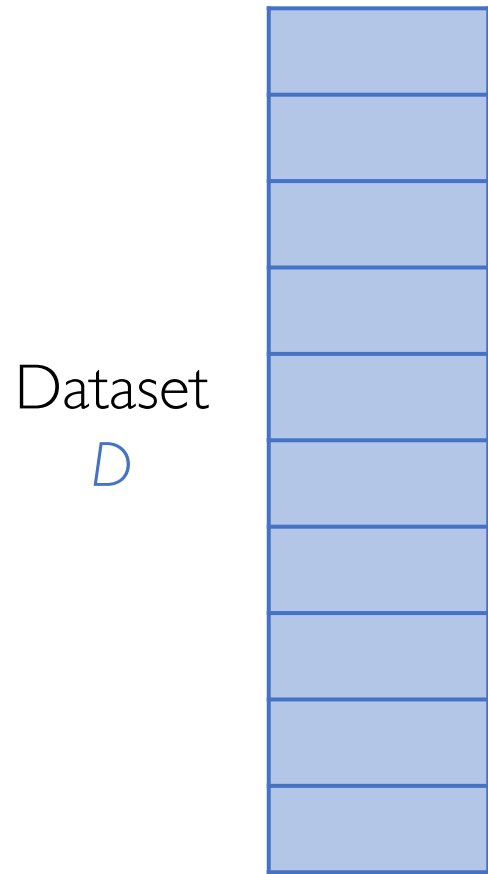
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- **Example:** Don't want to deploy your new spam classifier in production knowing only its training (i.e., in-sample) performance

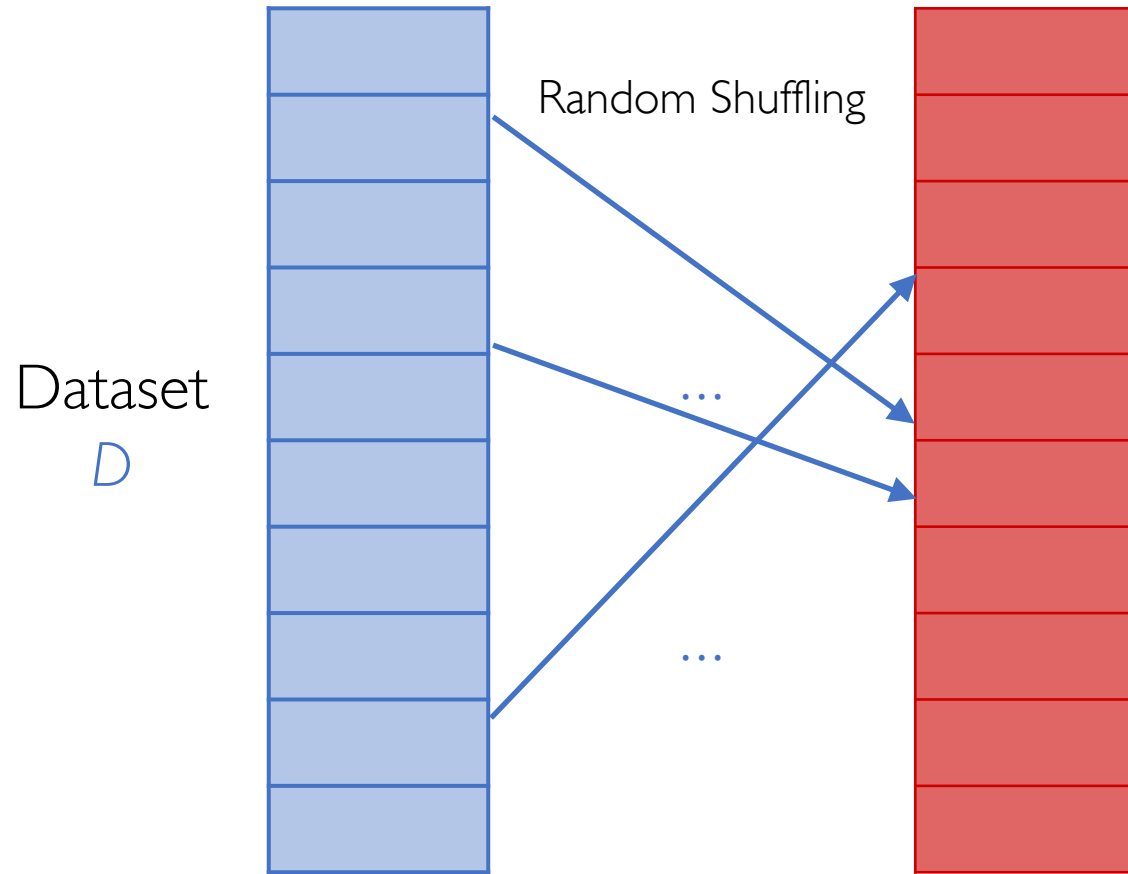
Estimating Generalization Performance

- Measuring the generalization (i.e., out-of-sample) performance online may be too risky
- **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

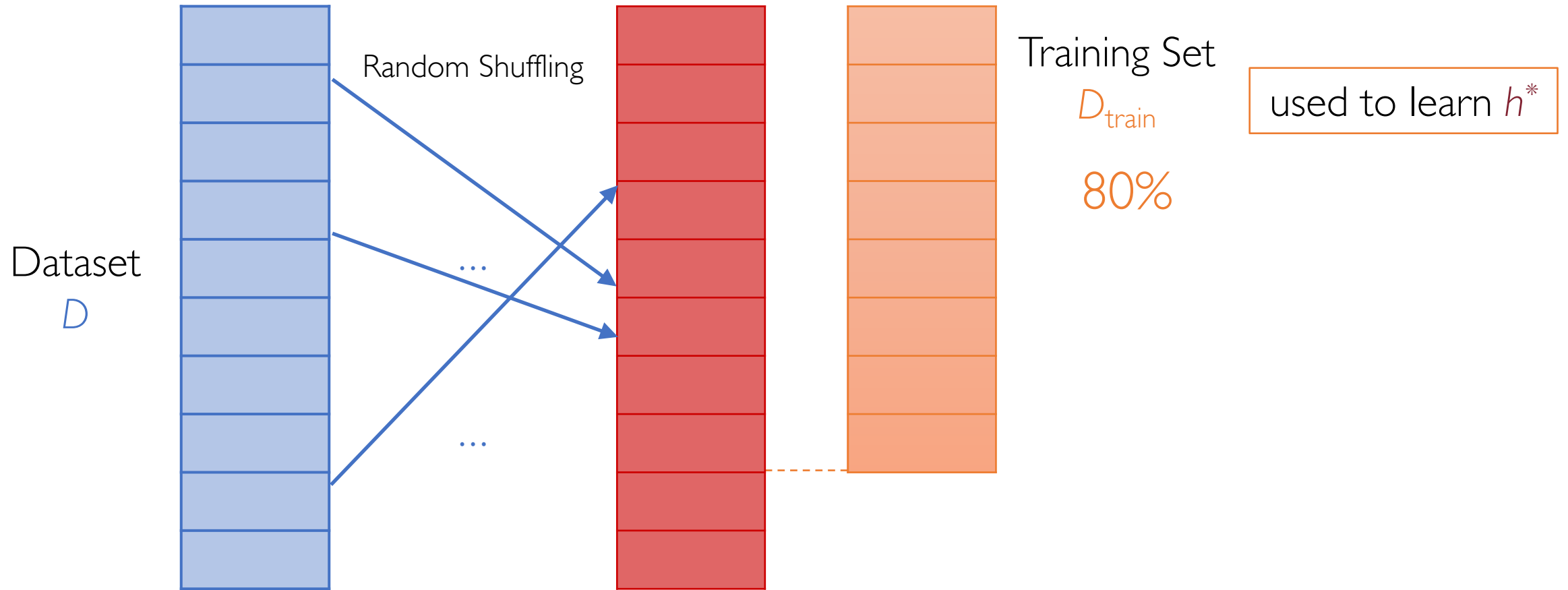
Dataset Splitting



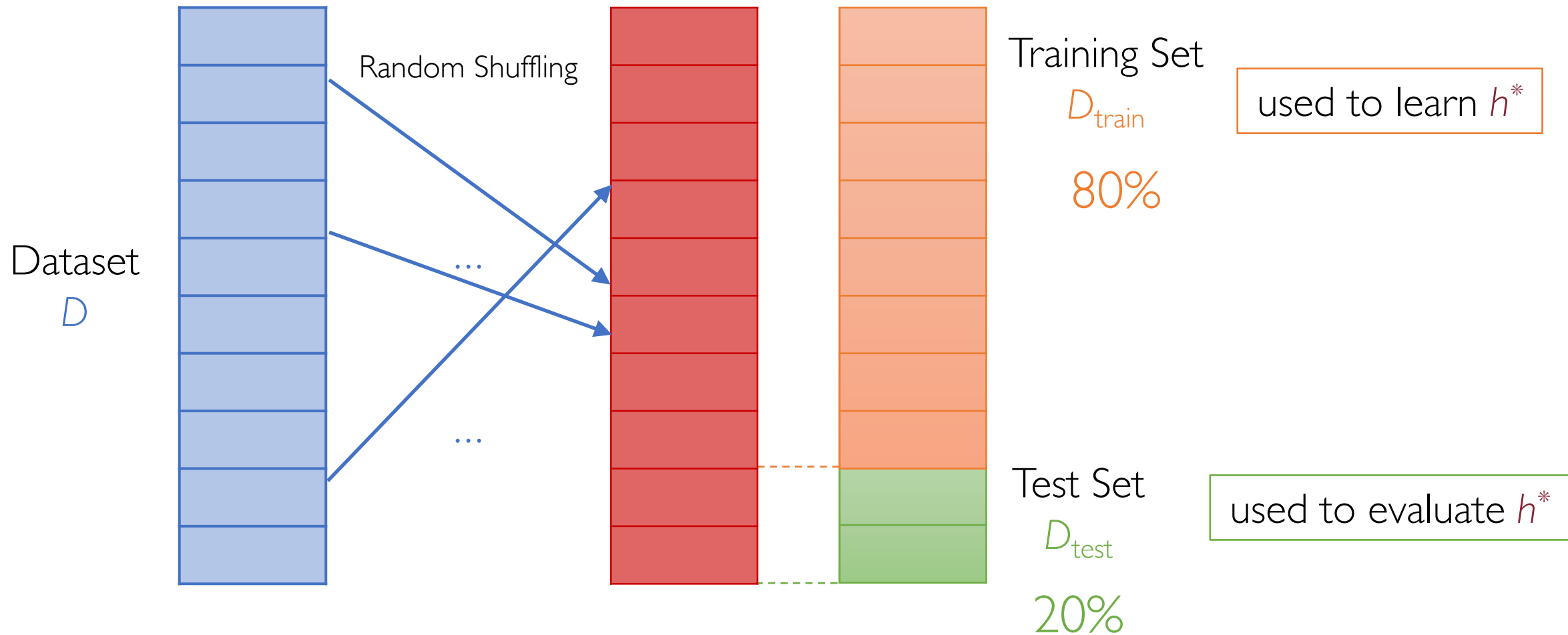
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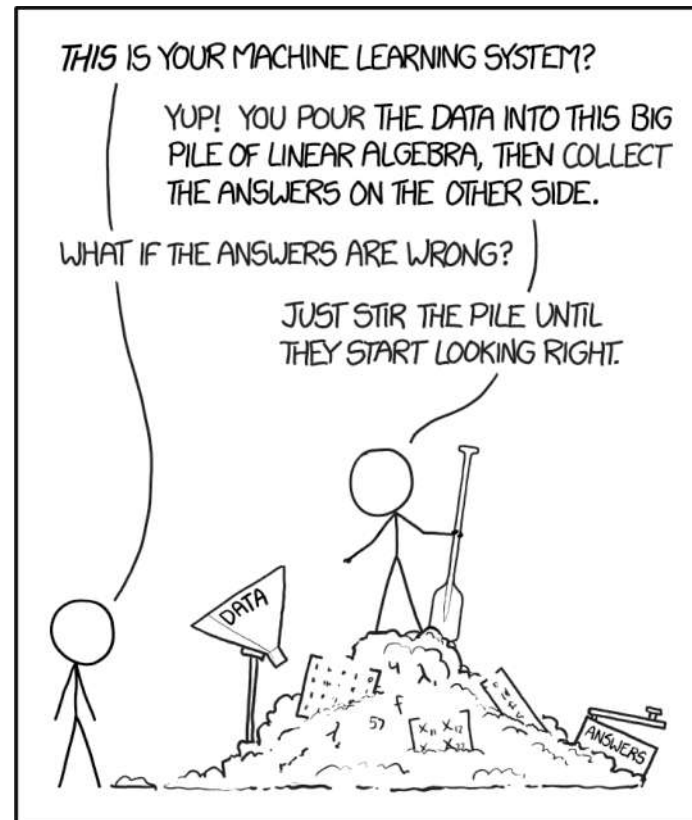


Dataset Splitting



How Much Data Do We Need?

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



K-Fold Cross Validation

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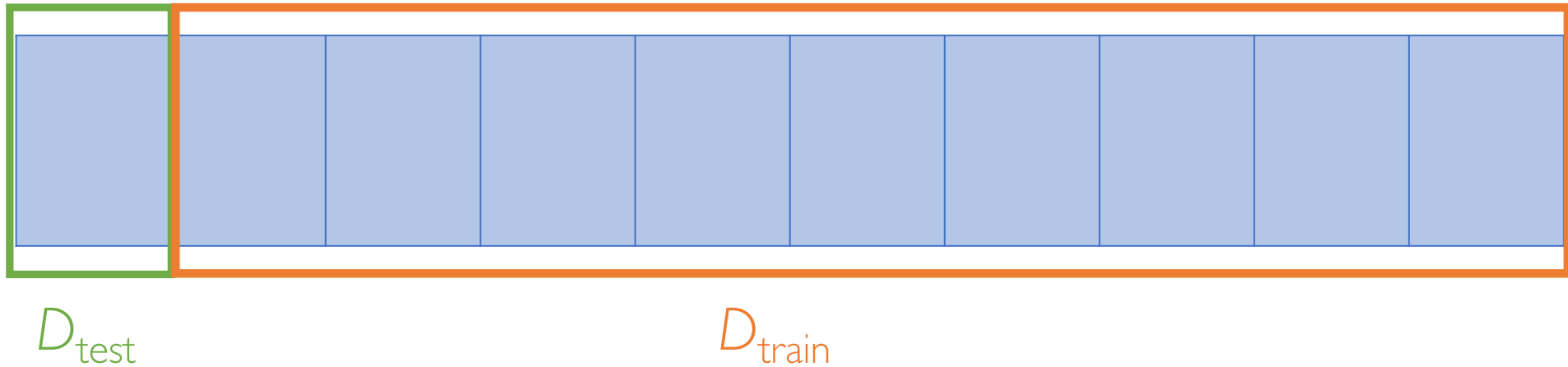
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- The estimate of generalization error is the average across the K test folds of all the K rounds

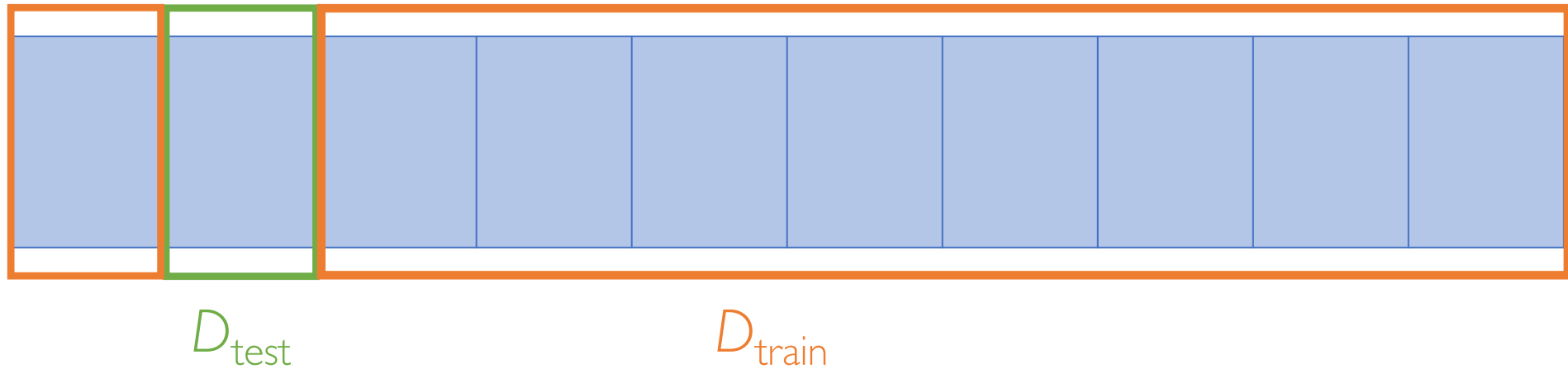
K-Fold Cross Validation

Round $k = 1$



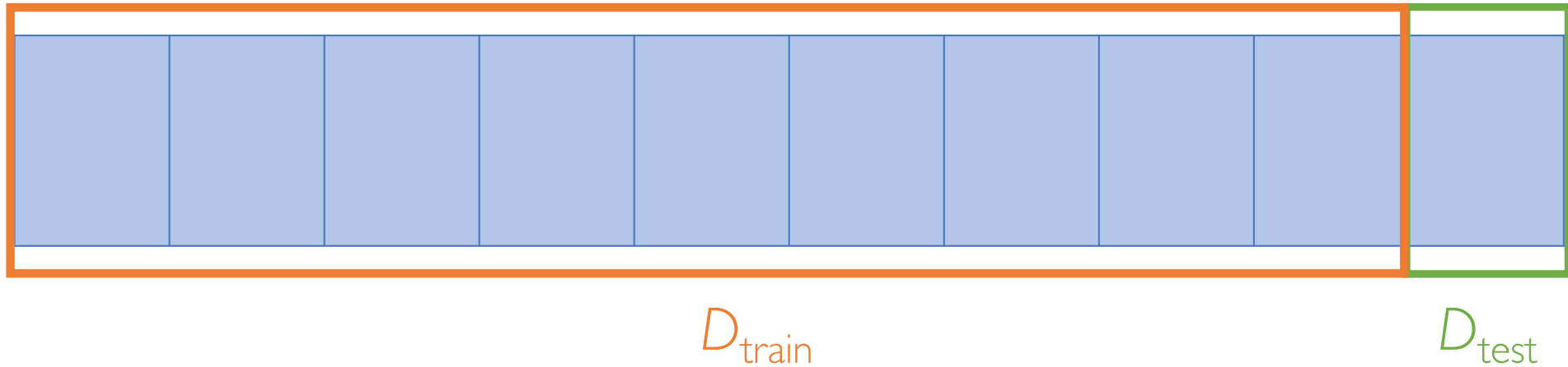
K-Fold Cross Validation

Round $k = 2$



K-Fold Cross Validation

Round $k = 10$



Model Selection/Evaluation

Several different learning models to achieve the same task



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Each learning model has its own set of **hyperparameters** (e.g., the number k of neighbours in kNN)

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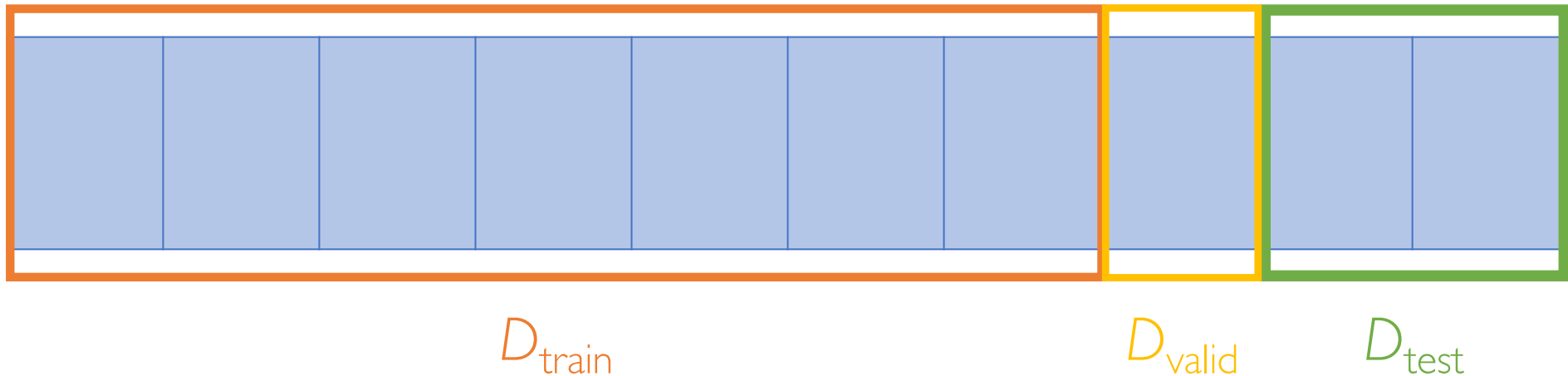
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How do we select the best model?

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 k NN 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)
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Suggested reading: <https://homes.cs.washington.edu/~pedrod/papers/cacml2.pdf>