Teoria degli Algoritmi

Corso di Laurea Magistrale in Matematica Applicata

a.a. 2020-21

SAPIENZA
UNIVERSITÀ DI ROMA

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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

Human vs. Computer

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  - 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
...
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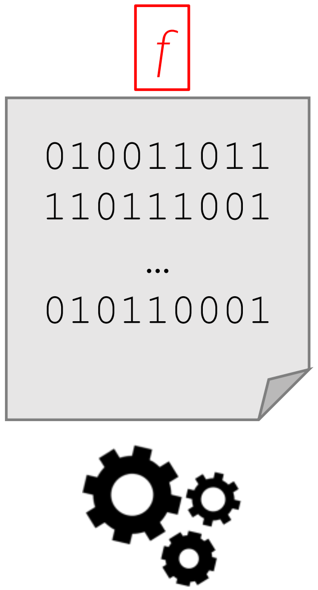
```

Encoding of
Computable Function f

Programming a Computer



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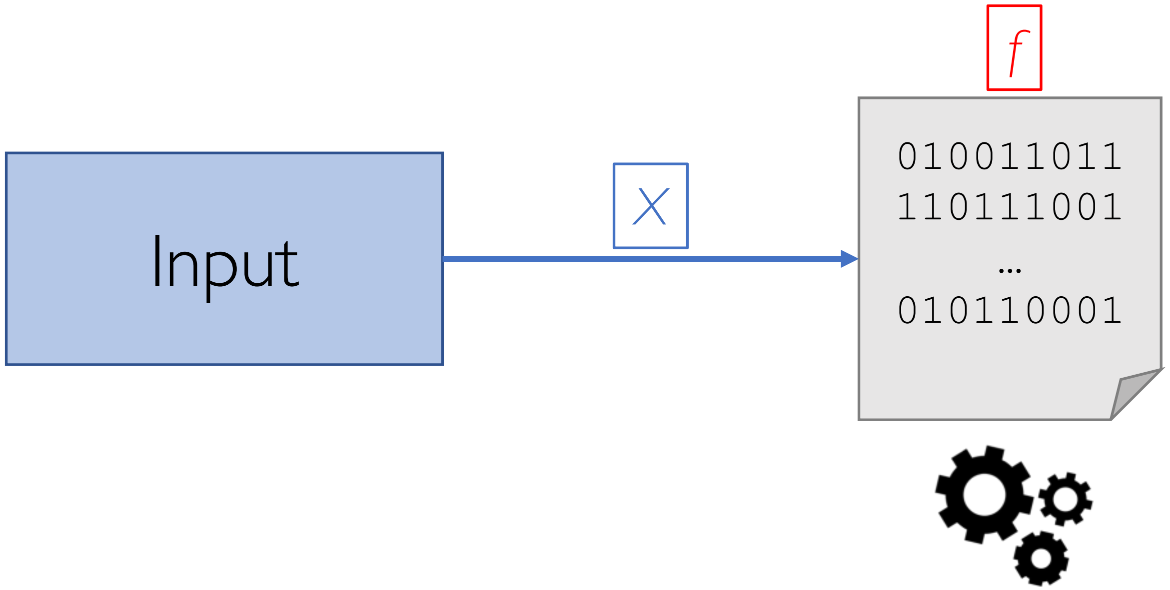

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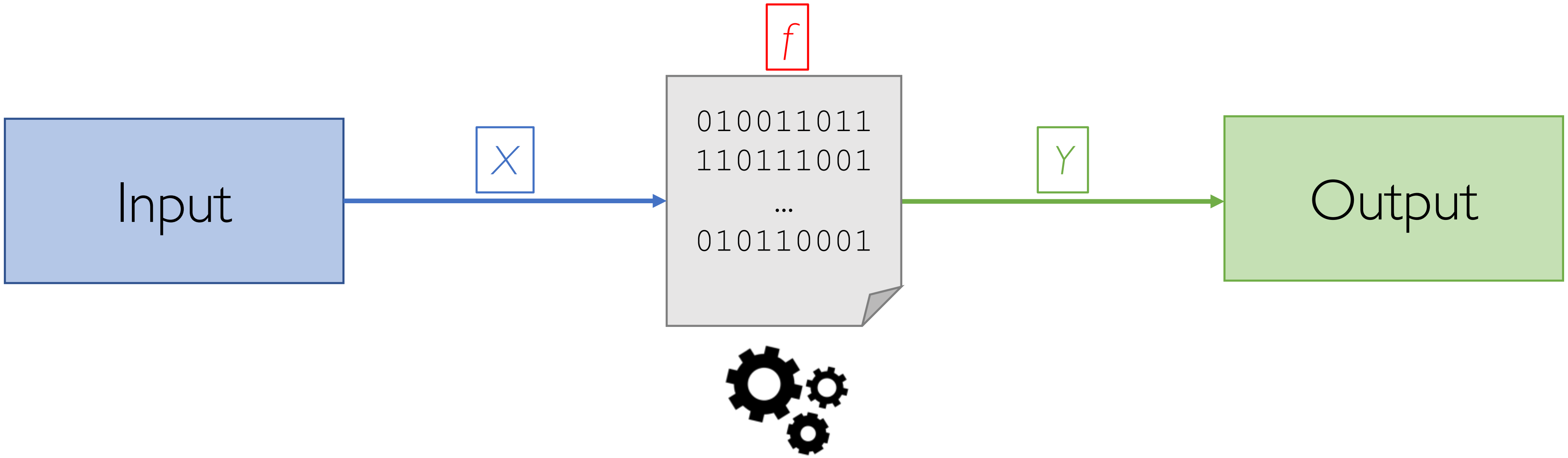

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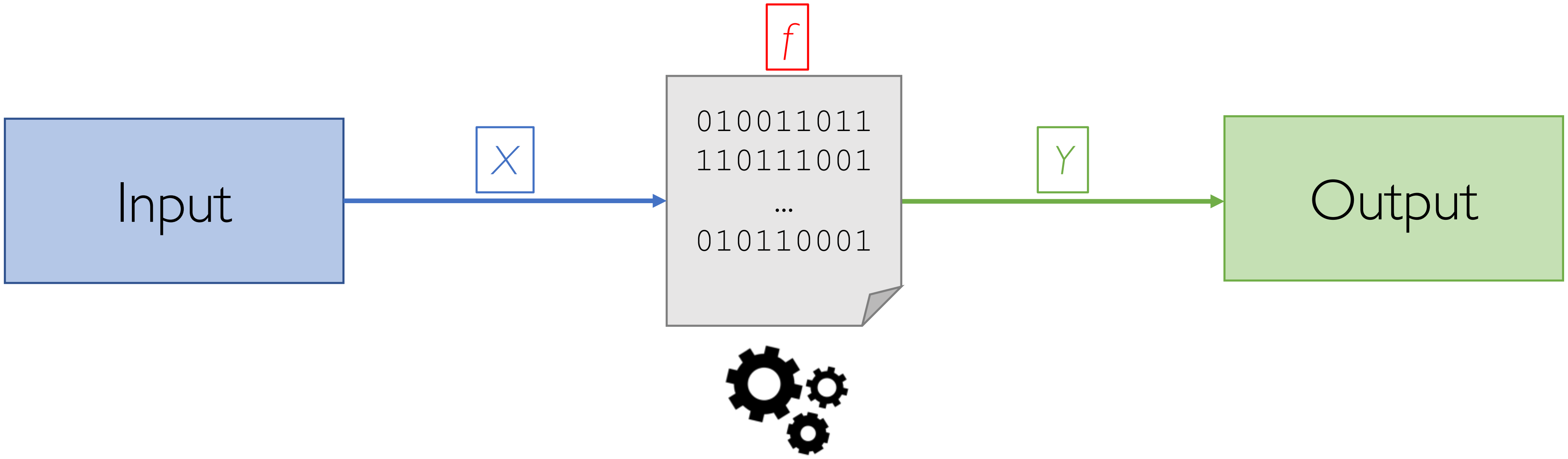

$$\boxed{Y = f(X)}$$

Can We Always Do That?

Chihuahua or Muffin?

[Copyright @teenybiscuit]

Chihuahua

Muffin

Programming vs. "Training" a Computer

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

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⇩

Programming vs. "Training" a Computer

"Training" a Computer

Problem

Labeled Data

"Training" a Computer

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

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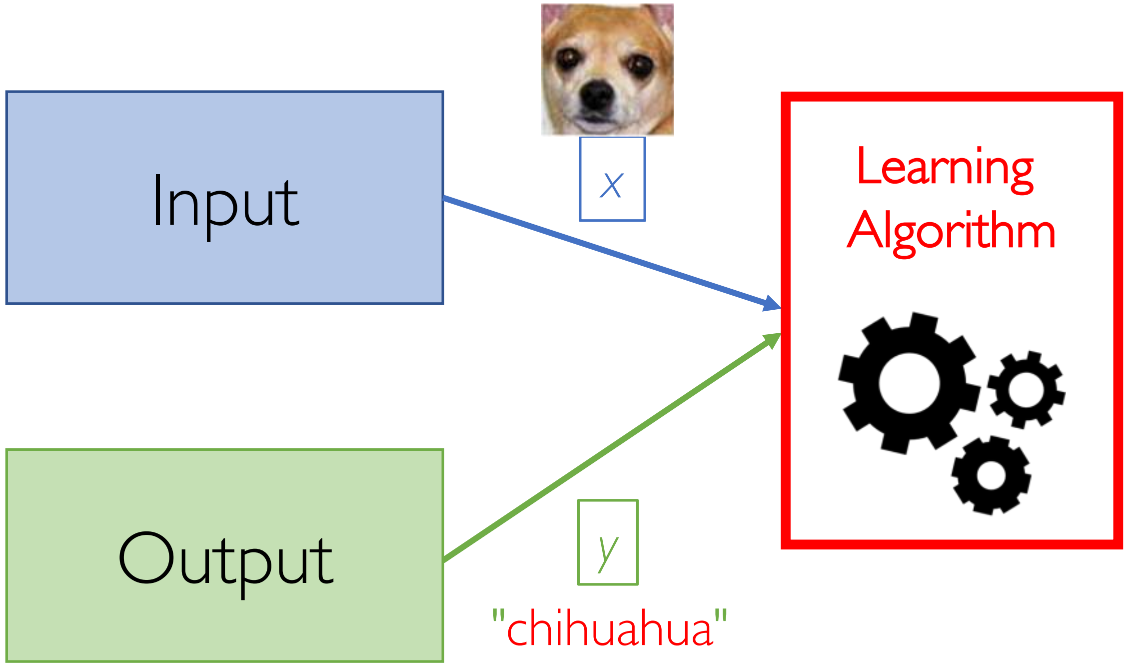

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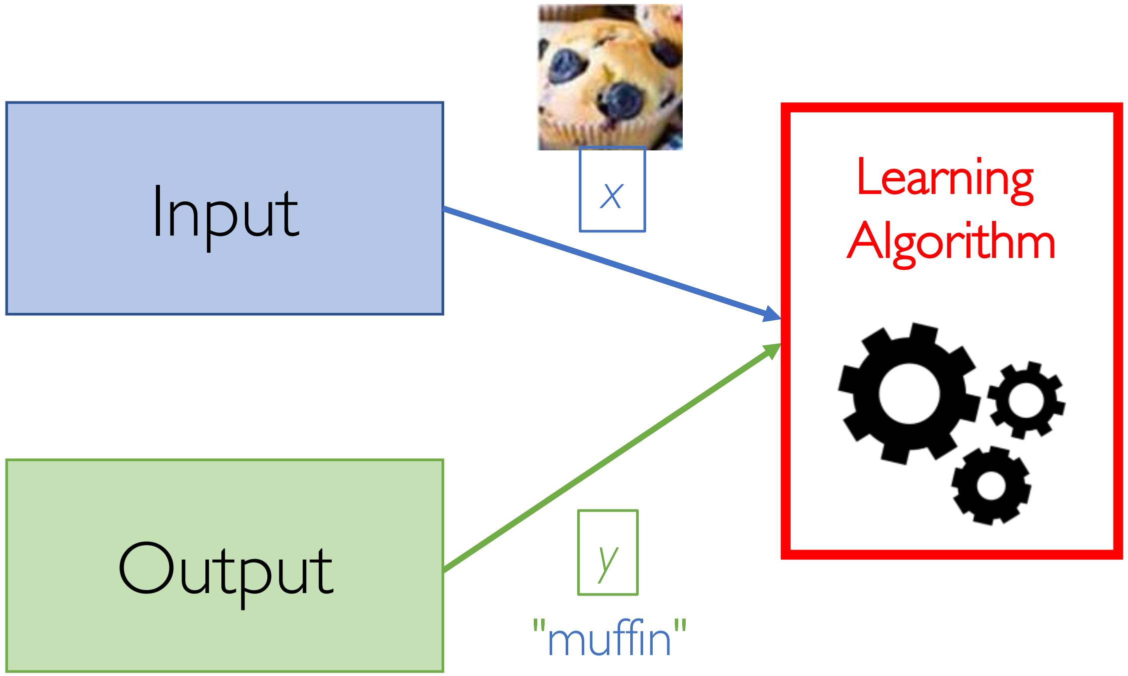

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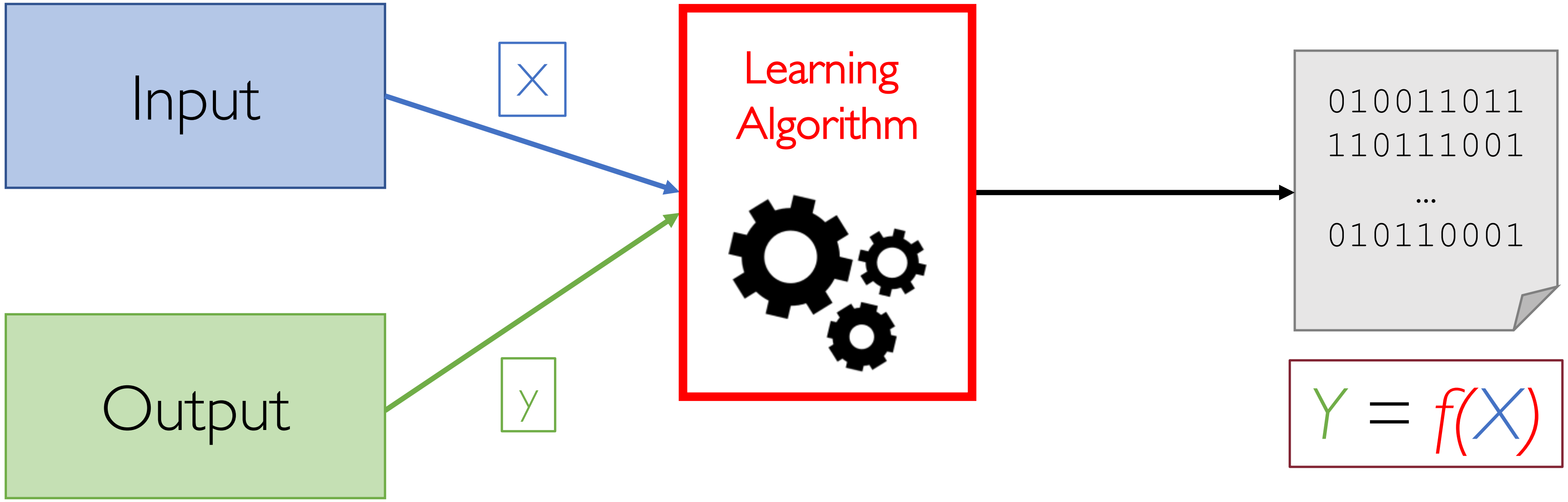

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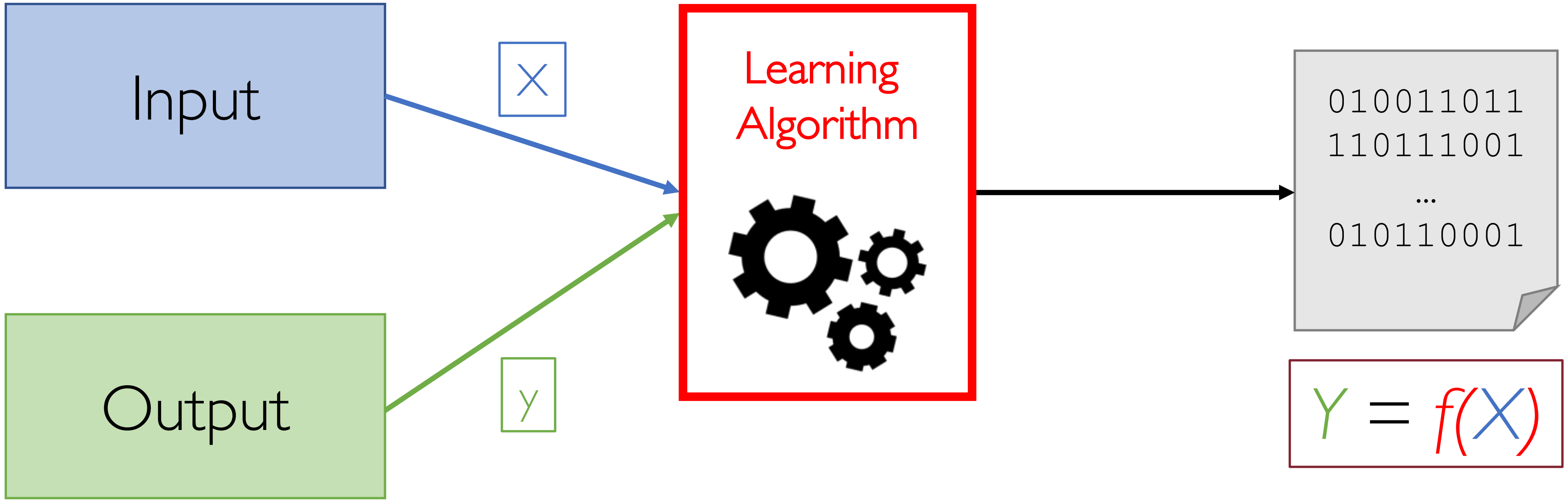

Eventually, the function f is **learned** by the learning algorithm from a (large) set of **labeled data**

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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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e.g., y = price of a house

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Regression

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Classification

The target y we want to predict is a discrete value

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

A Bit of Notation

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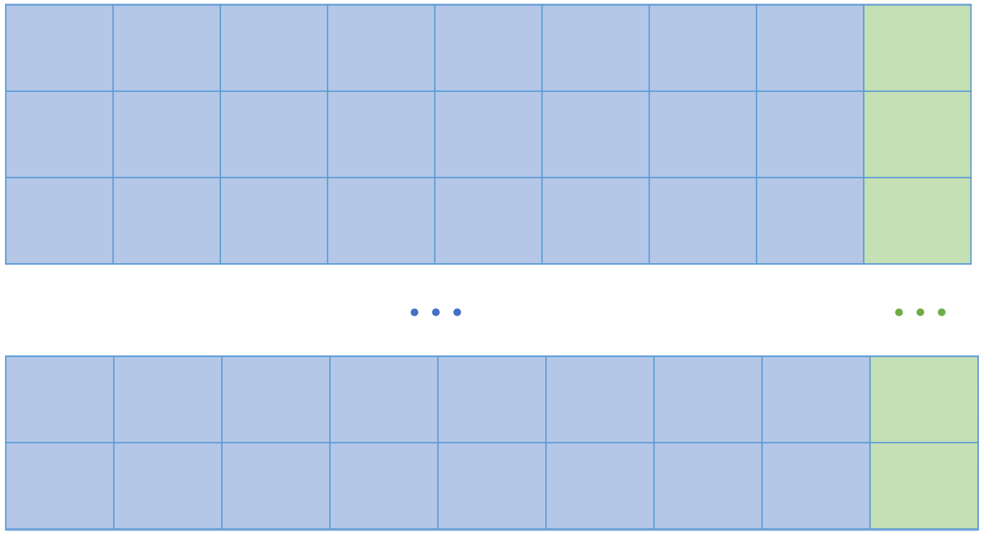
$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$	dataset of *m* i.i.d. labeled instances

Model Training: Labeled Dataset



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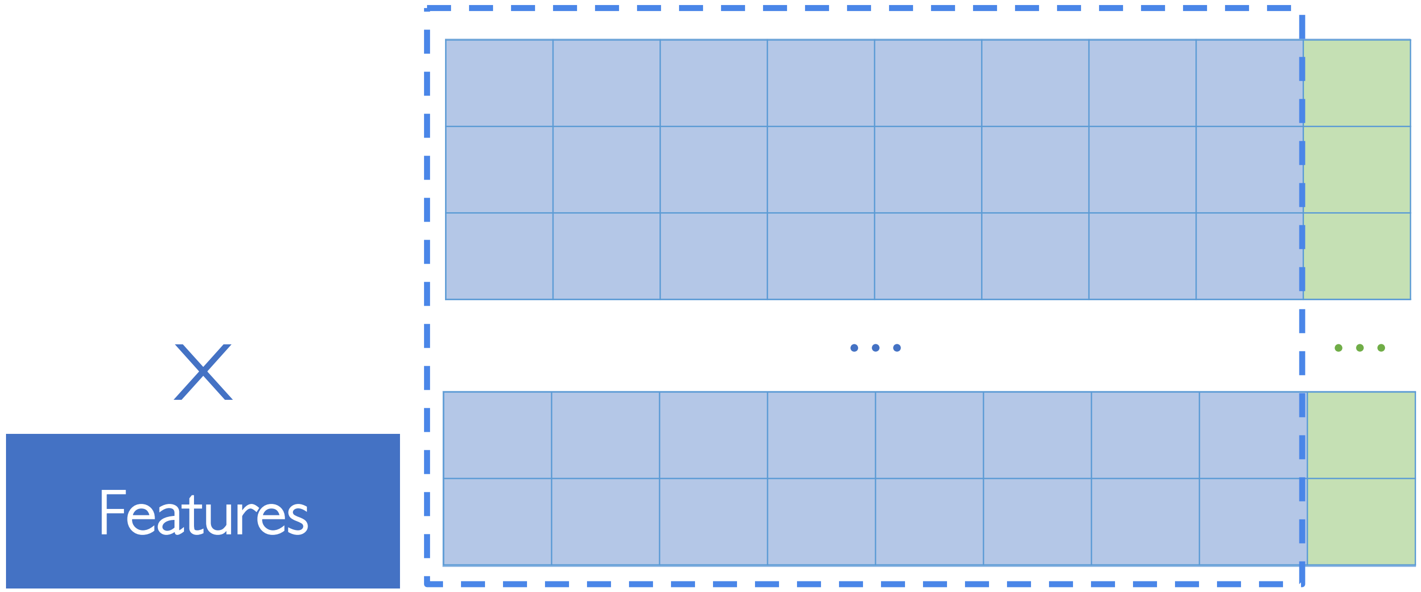

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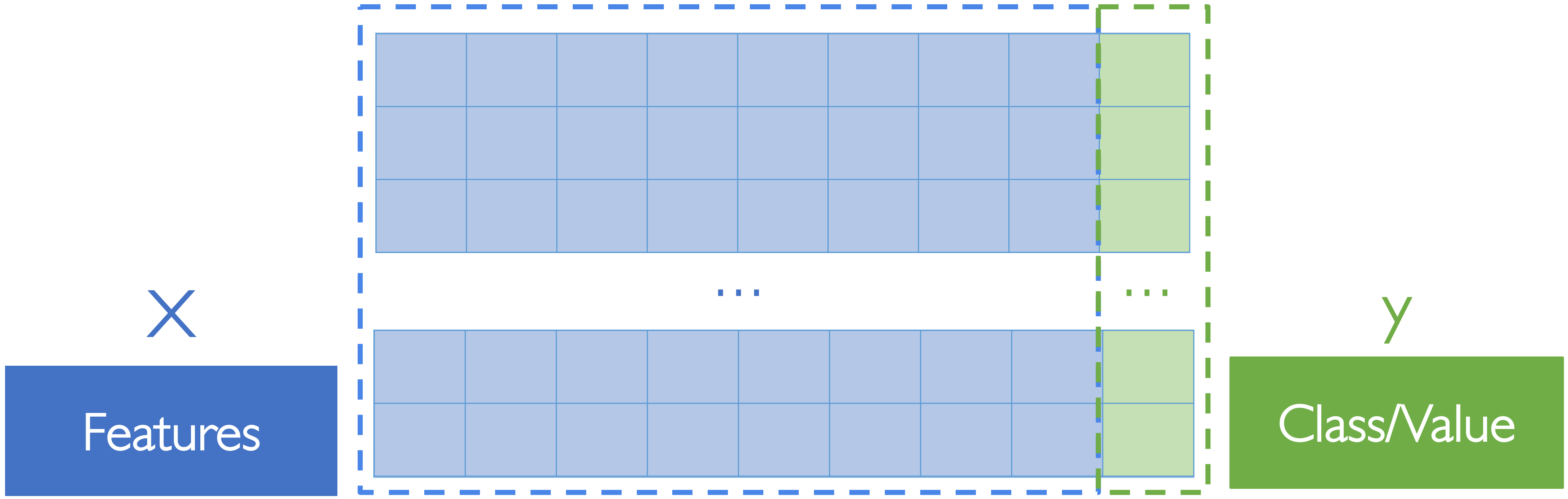
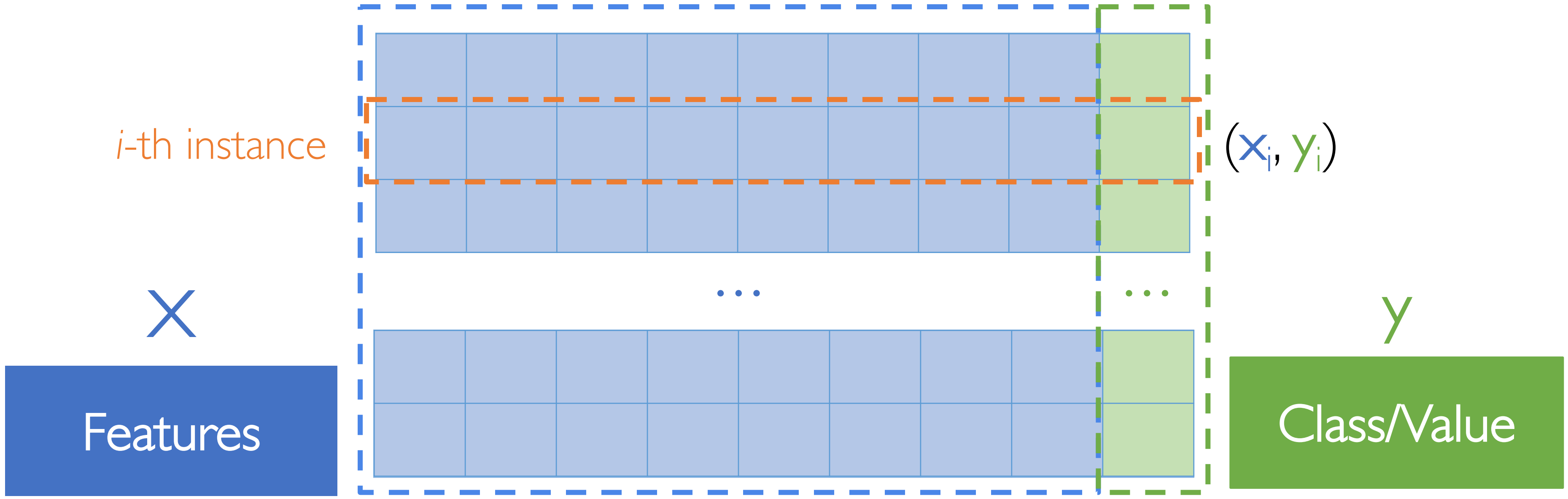


Model Training: Labeled Dataset

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



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

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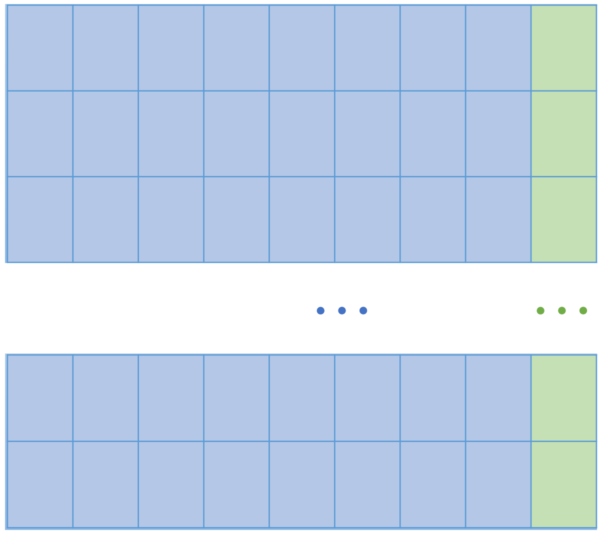

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(e.g., historical records of customers)

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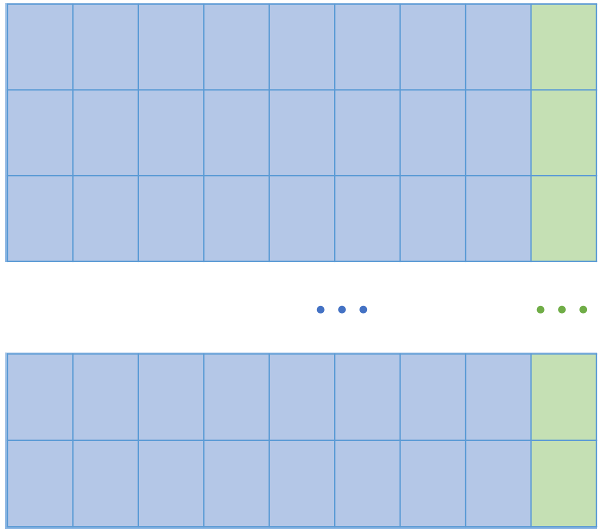

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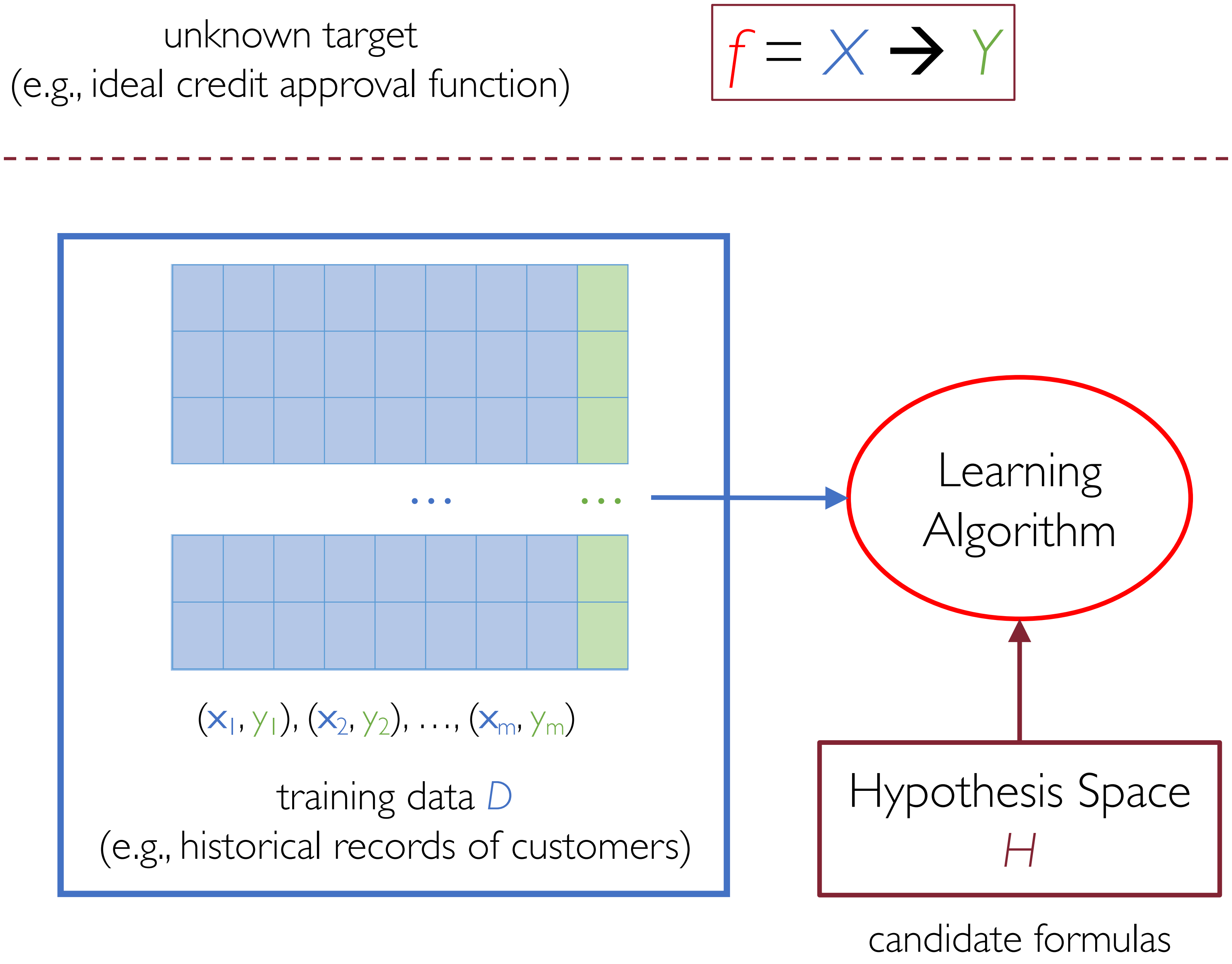
Hypothesis Space
H

candidate formulas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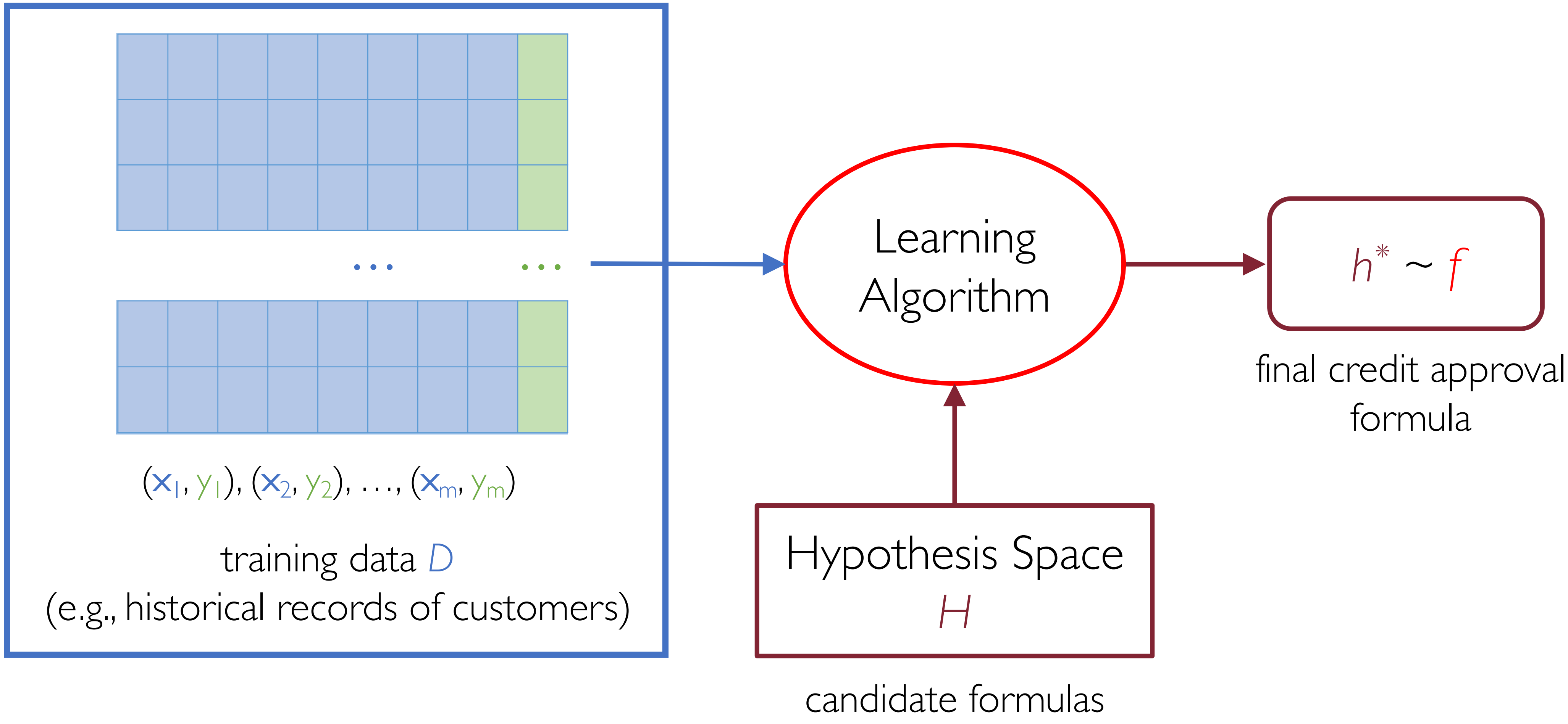

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- By plugging in different loss functions combined with various hypothesis spaces we must solve a specific optimization problem
- Those choices are usually "mathematically convenient": e.g., convex objective functions are guaranteed to have a unique 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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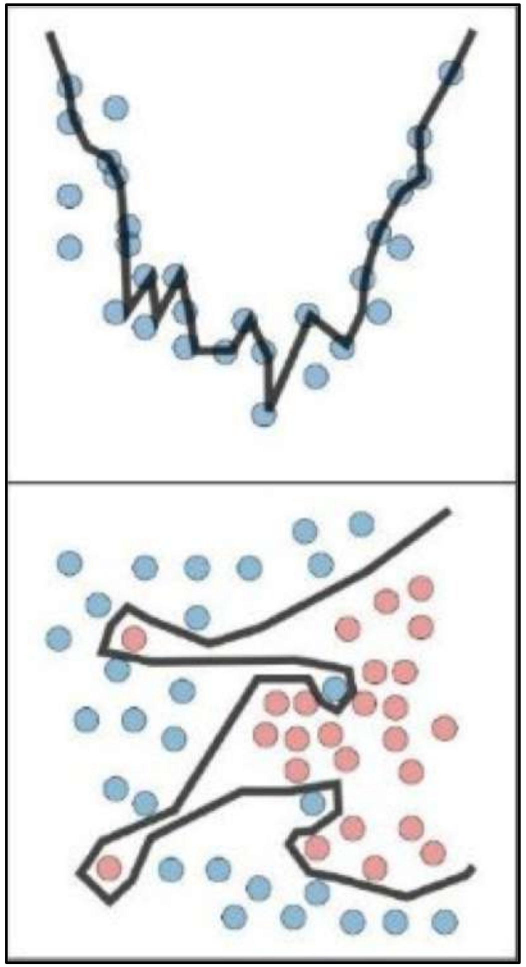
- At the same time we do not want h^* to perform poorly on D

Overfitting (High Variance)

Regression

Classification



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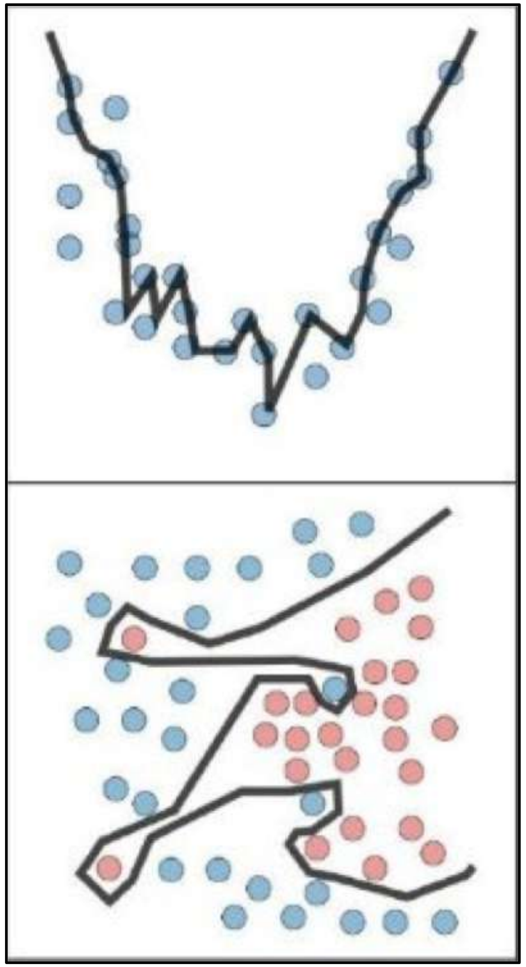

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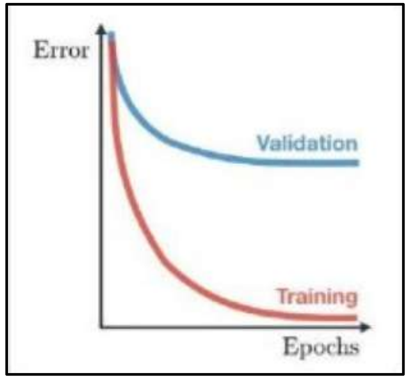

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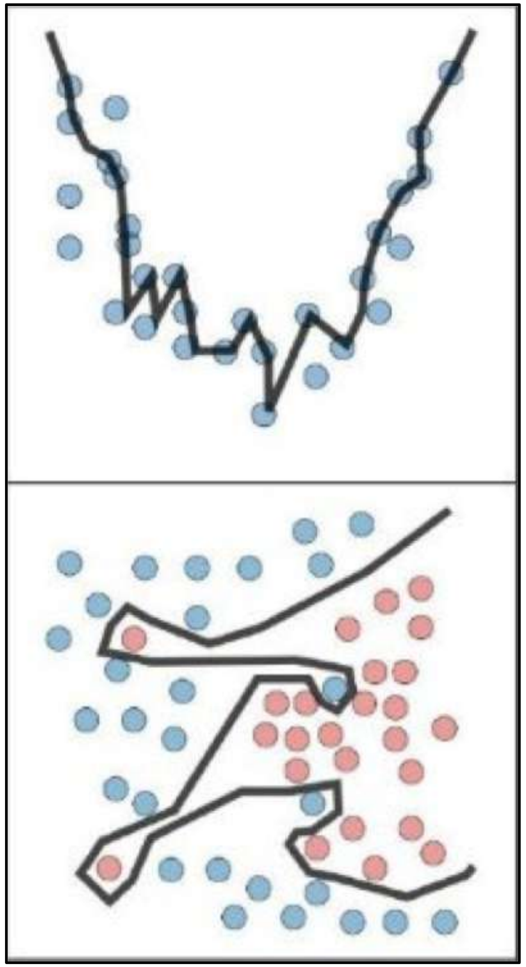

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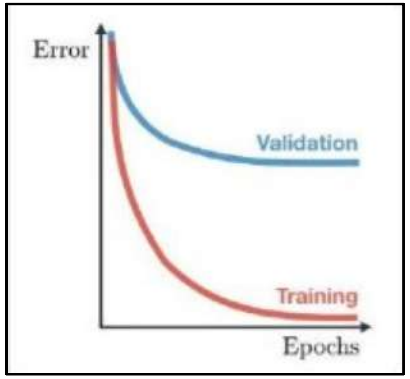

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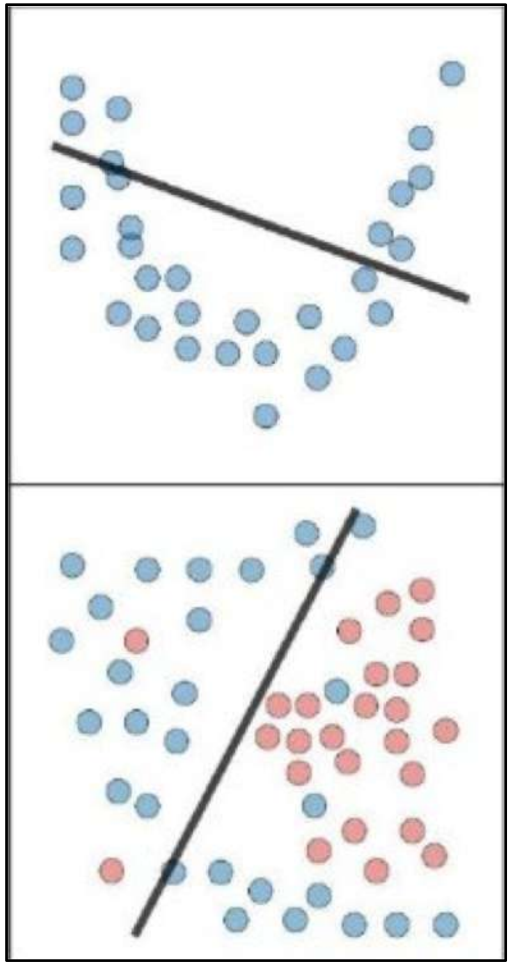
- Regularization
- Get more data

Underfitting (High Bias)

Regression

Classification



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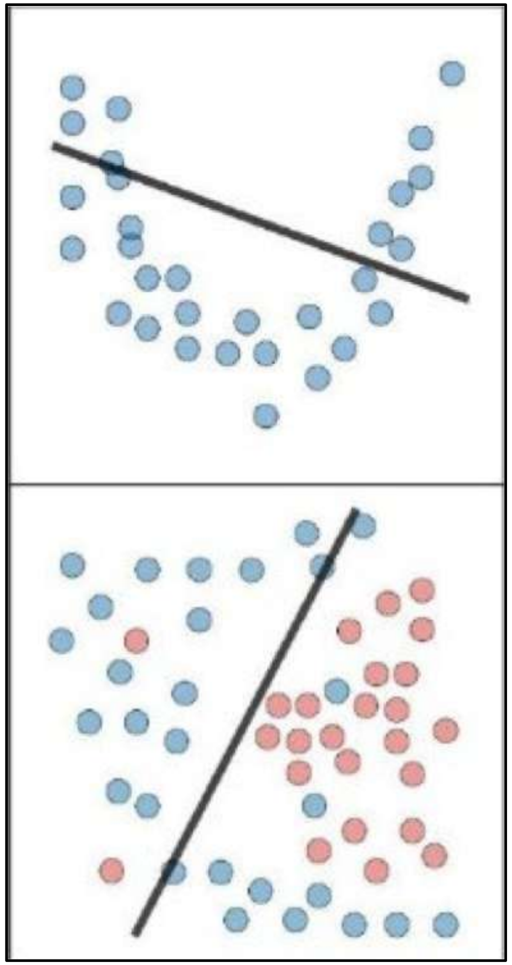

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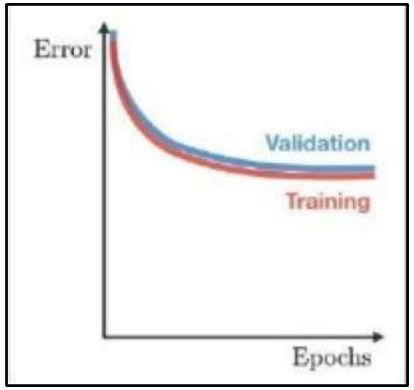

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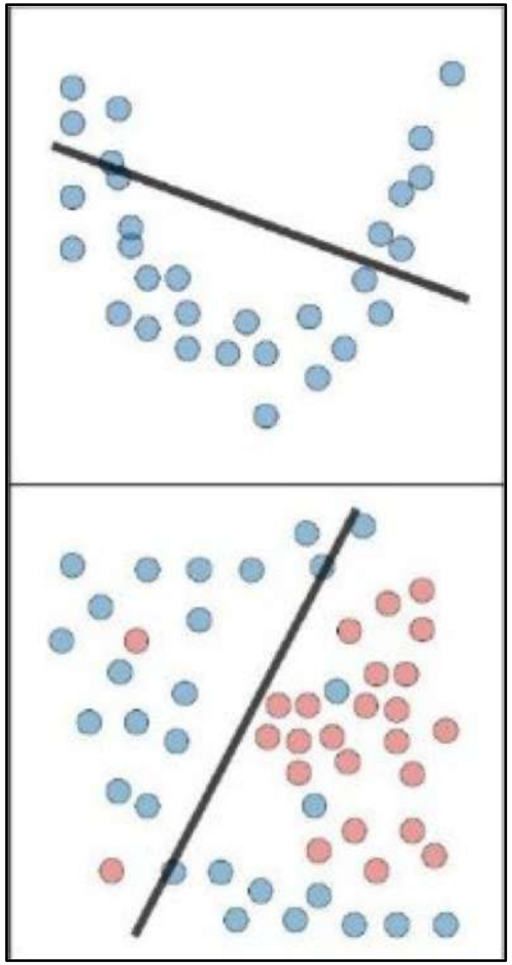

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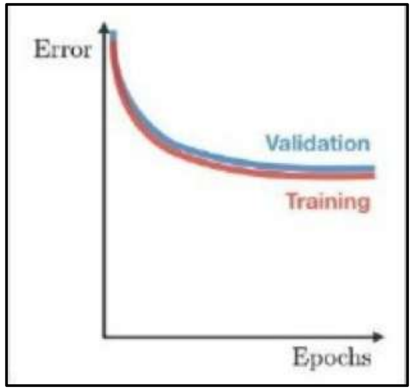

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- Increase model complexity
- Add more features

Bias-Variance Tradeoff

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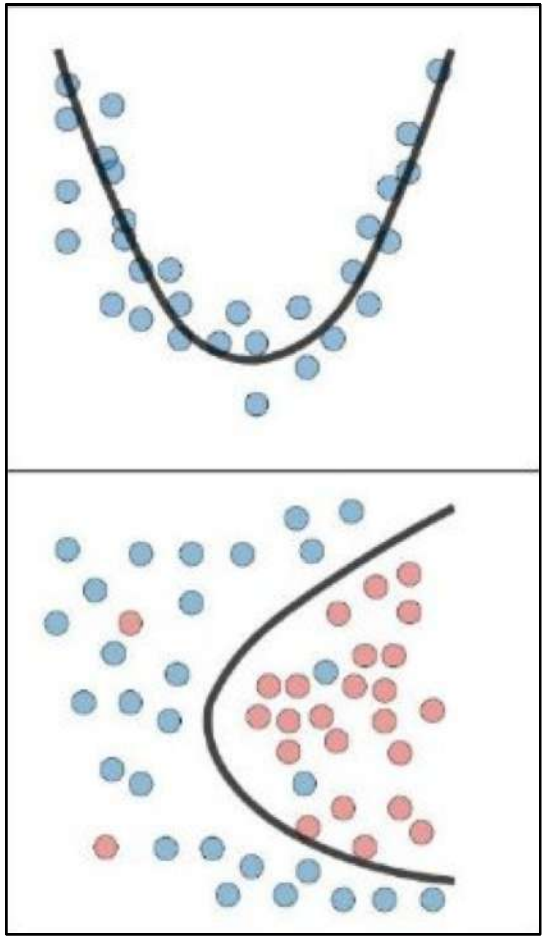

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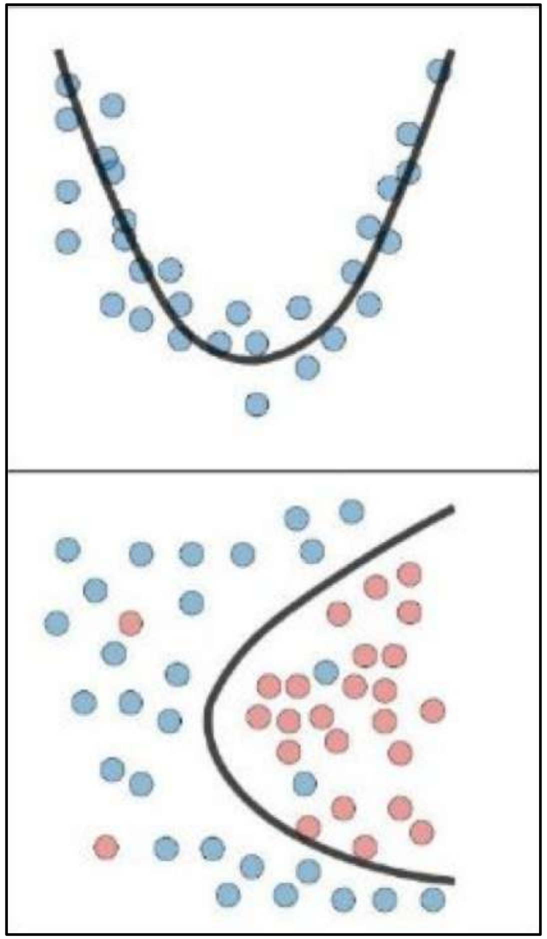

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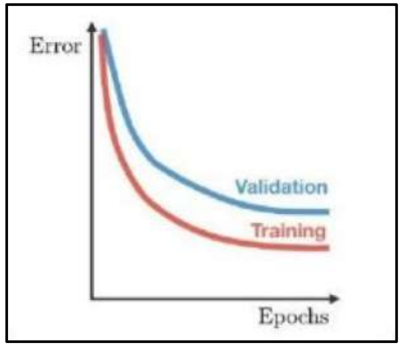

low in-sample error low out-of-sample error

Estimating Generalization Performance

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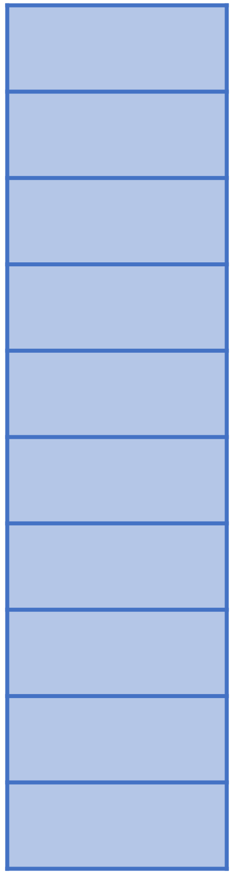
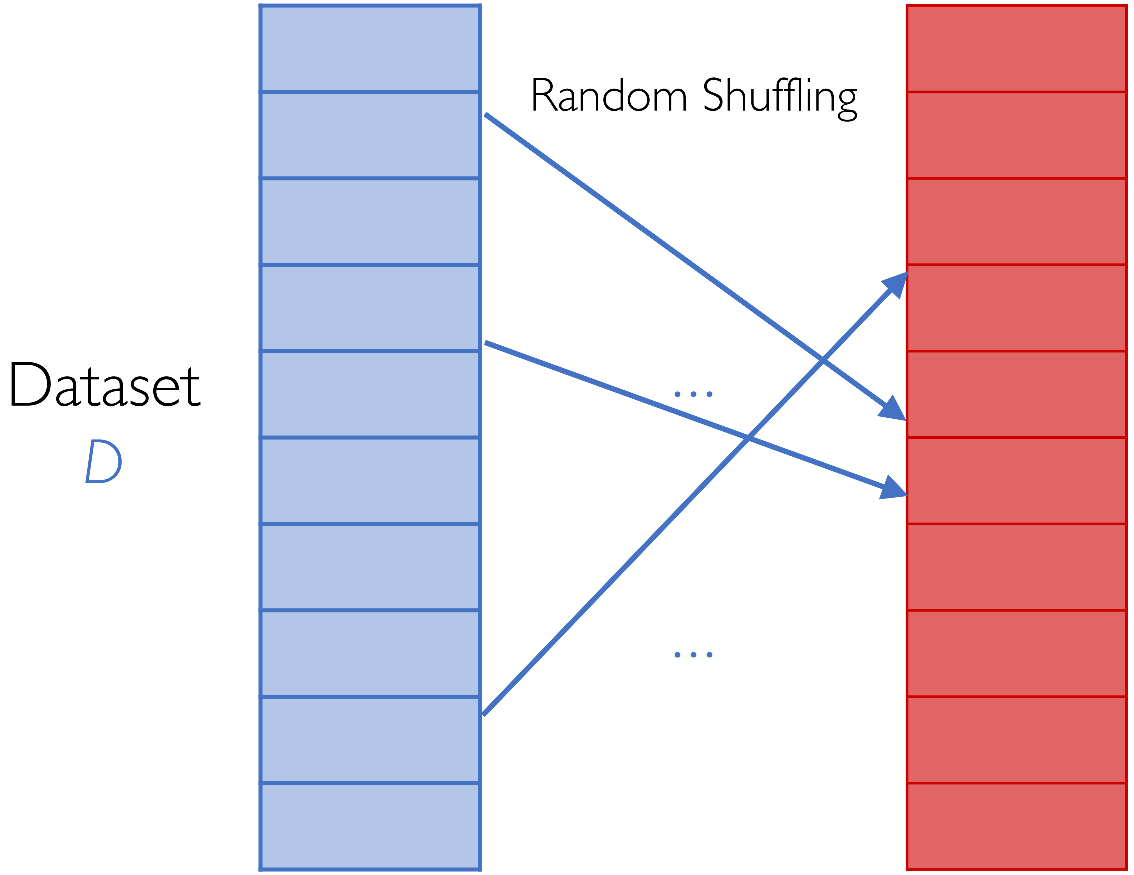
- Solution: Estimate the generalization performance using training set
  - As long as it holds true the assumption that training and test instances are both drawn from the same probability distribution (i.i.d. assumption)

Dataset Splitting

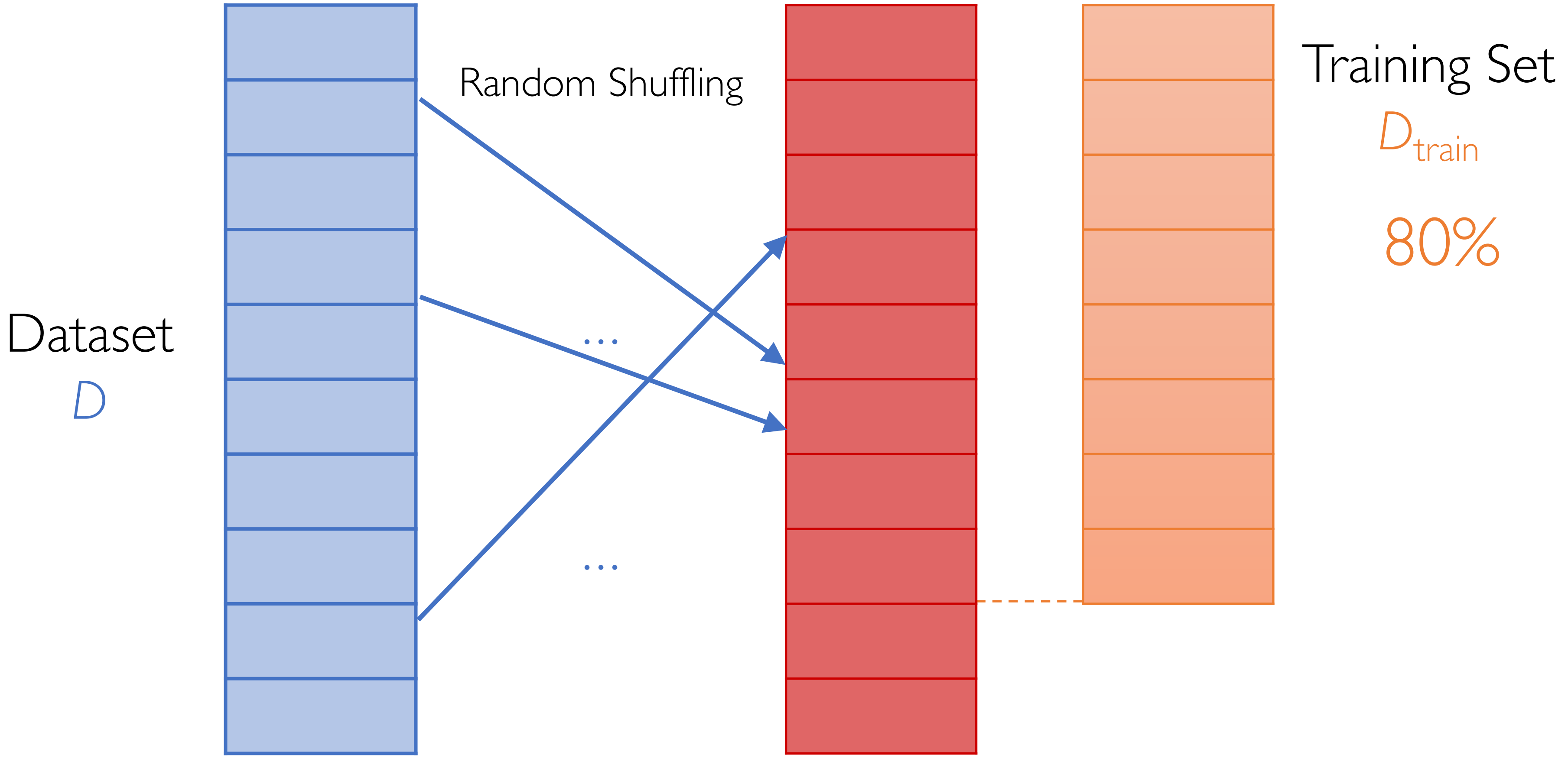
Dataset
D



Dataset Splitting

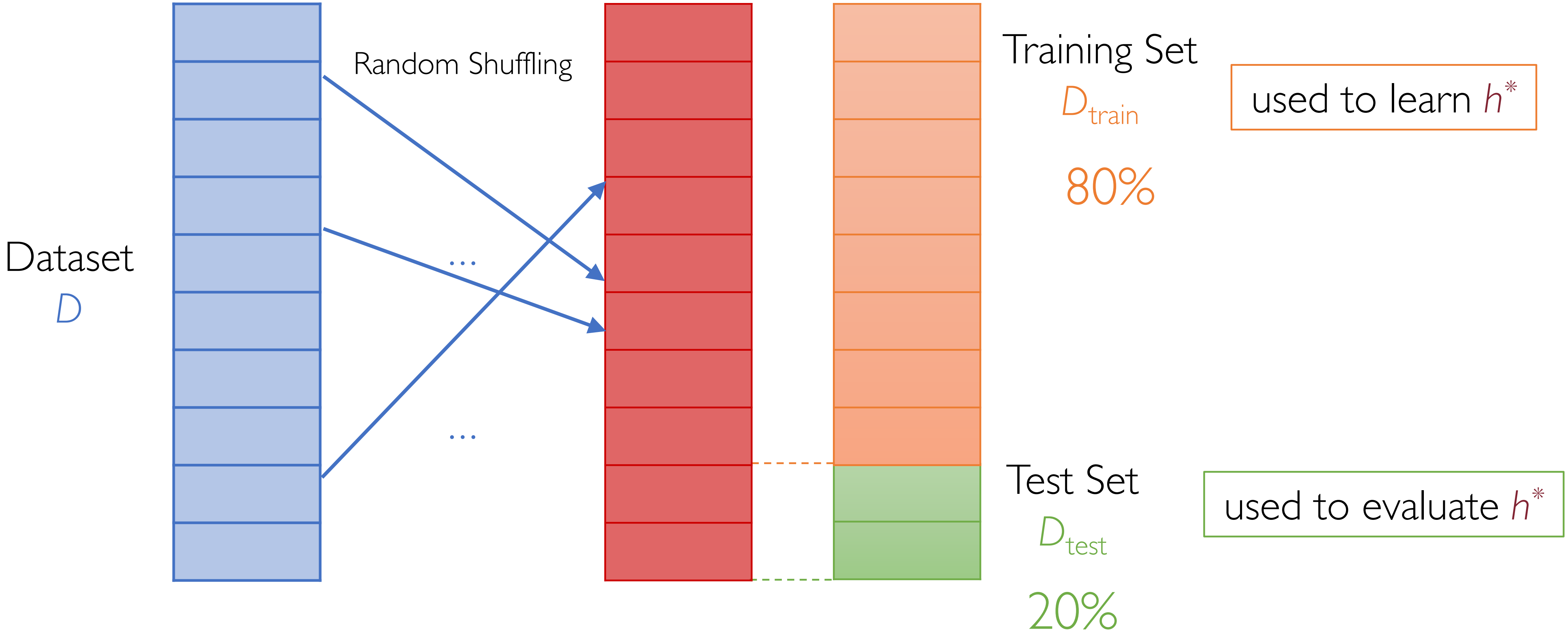


Dataset Splitting



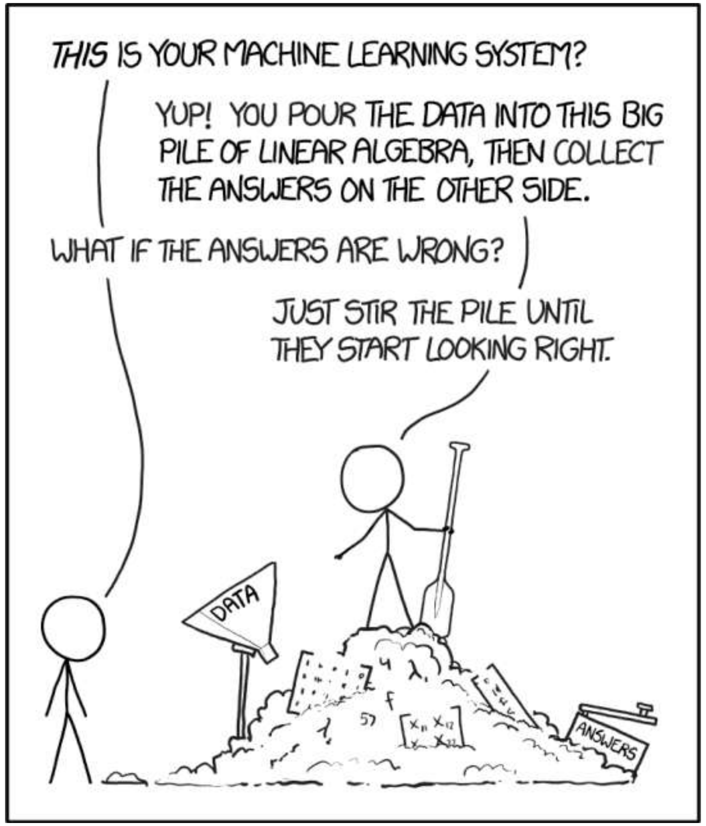
used to learn h^*

Dataset Splitting



How Much Data Do We Need?

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



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