Big Data Computing

Master's Degree in Computer Science

2022-2023

Gabriele Tolomei

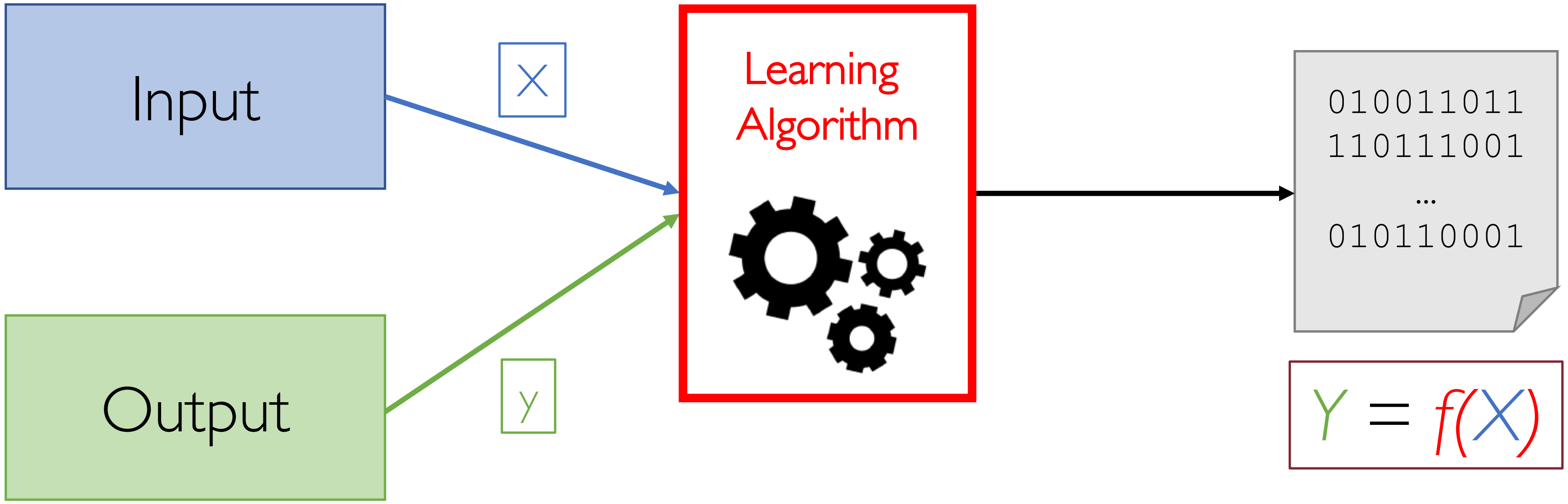
Department of Computer Science

Sapienza Università di Roma

tolomei@di.uniroma1.it

SAPIENZA UNIVERSITÀ DI ROMA

"Training" a Computer



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

A Bit of Notation

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

A Bit of Notation

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

A Bit of Notation

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

$\mathcal{Y}$ output space

$\mathcal{Y} \subseteq \mathbb{R}$ real-value label (regression)

$\mathcal{Y} = \{1, \ldots, k\}$ discrete-value label (k-ary classification)

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	input feature space
$\mathcal{Y}$	output space
$\mathcal{Y} \subseteq \mathbb{R}$	real-value label (regression)
$\mathcal{Y} = \{1, \ldots, k\}$	discrete-value label (k-ary classification)
$(\mathbf{x}_i, y_i)$	*i*-th labeled instance

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	input feature space
$\mathcal{Y}$	output space
$\quad \mathcal{Y} \subseteq \mathbb{R}$	real-value label (regression)
$\quad \mathcal{Y} = \{1, \ldots, k\}$	discrete-value label (k-ary classification)
$(\mathbf{x}_i, y_i)$	*i*-th labeled instance
$\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,n}) \in \mathcal{X}$	*n*-dimensional feature vector of the *i*-th instance

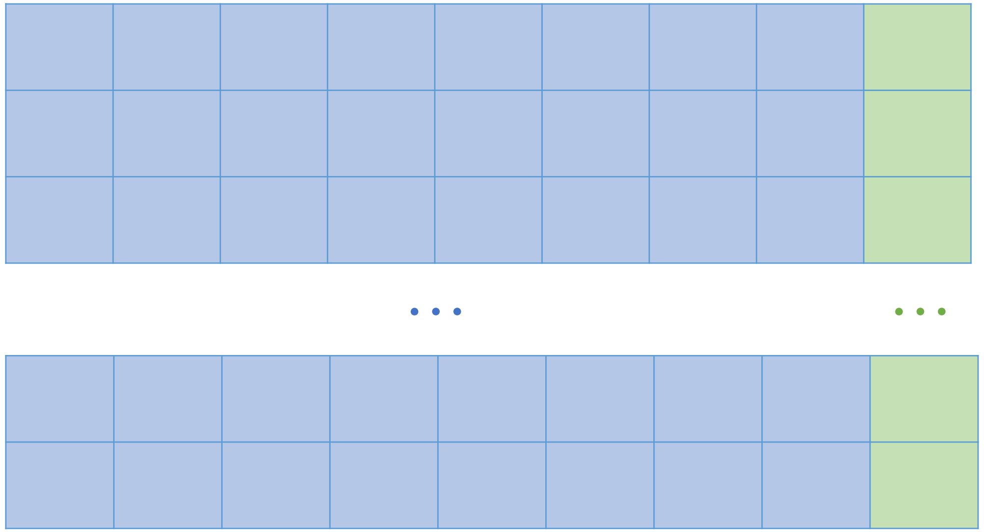
A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	input feature space
$\mathcal{Y}$	output space
$\mathcal{Y} \subseteq \mathbb{R}$	real-value label (regression)
$\mathcal{Y} = \{1, \ldots, k\}$	discrete-value label (k-ary classification)
$(\mathbf{x}_i, y_i)$	*i*-th labeled instance
$\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,n}) \in \mathcal{X}$	*n*-dimensional feature vector of the *i*-th instance
$y_i \in \mathcal{Y}$	label of the *i*-th instance

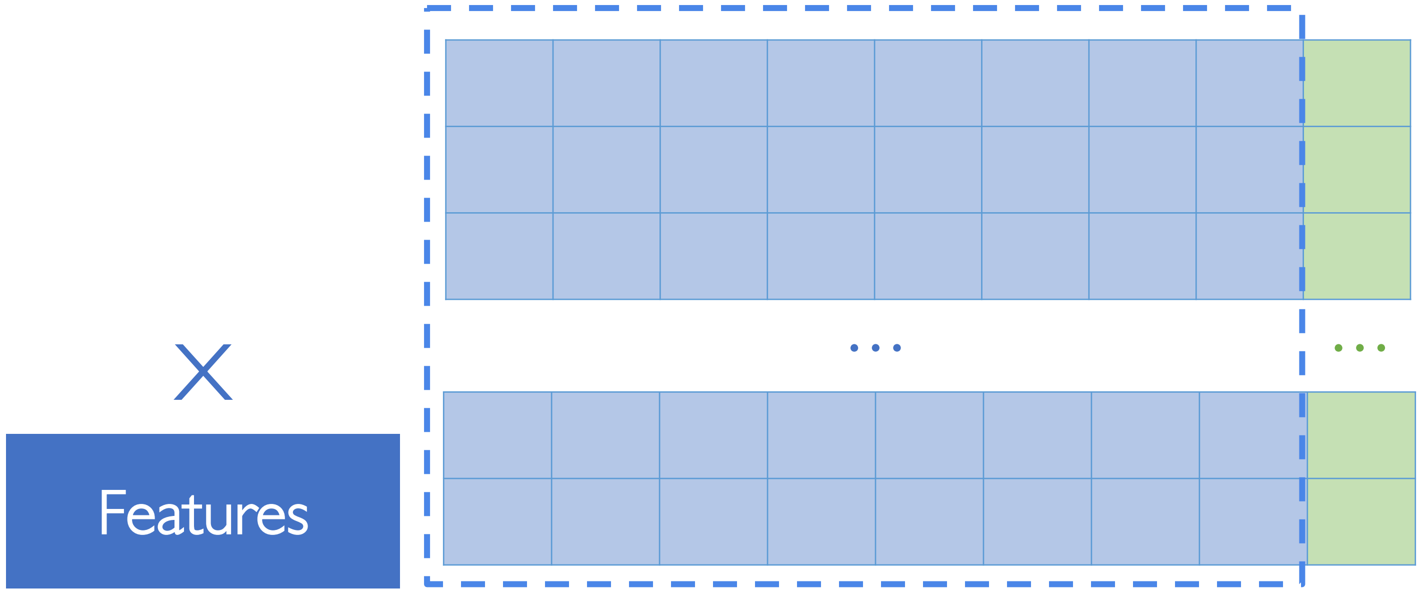
A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	input feature space
$\mathcal{Y}$	output space
$\quad \mathcal{Y} \subseteq \mathbb{R}$	real-value label (regression)
$\quad \mathcal{Y} = \{1, \ldots, k\}$	discrete-value label (k-ary classification)
$(\mathbf{x}_i, y_i)$	*i*-th labeled instance
$\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,n}) \in \mathcal{X}$	*n*-dimensional feature vector of the *i*-th instance
$y_i \in \mathcal{Y}$	label of the *i*-th instance
$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$	dataset of *m* i.i.d. labeled instances

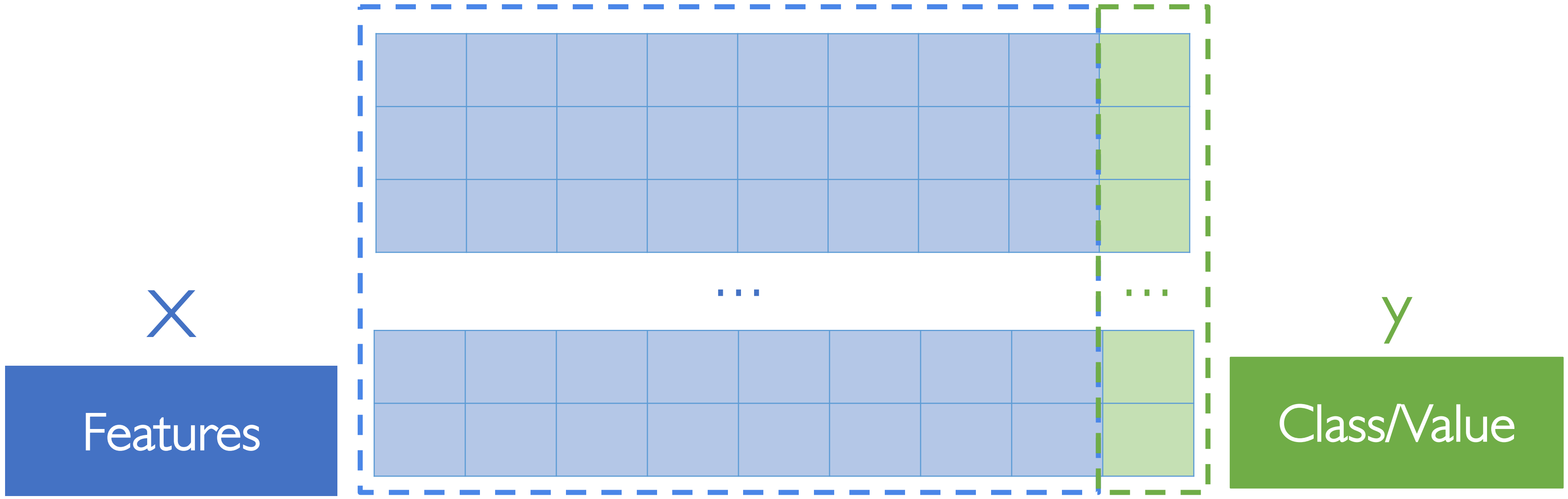
Model Training: Labeled Dataset



Model Training: Labeled Dataset

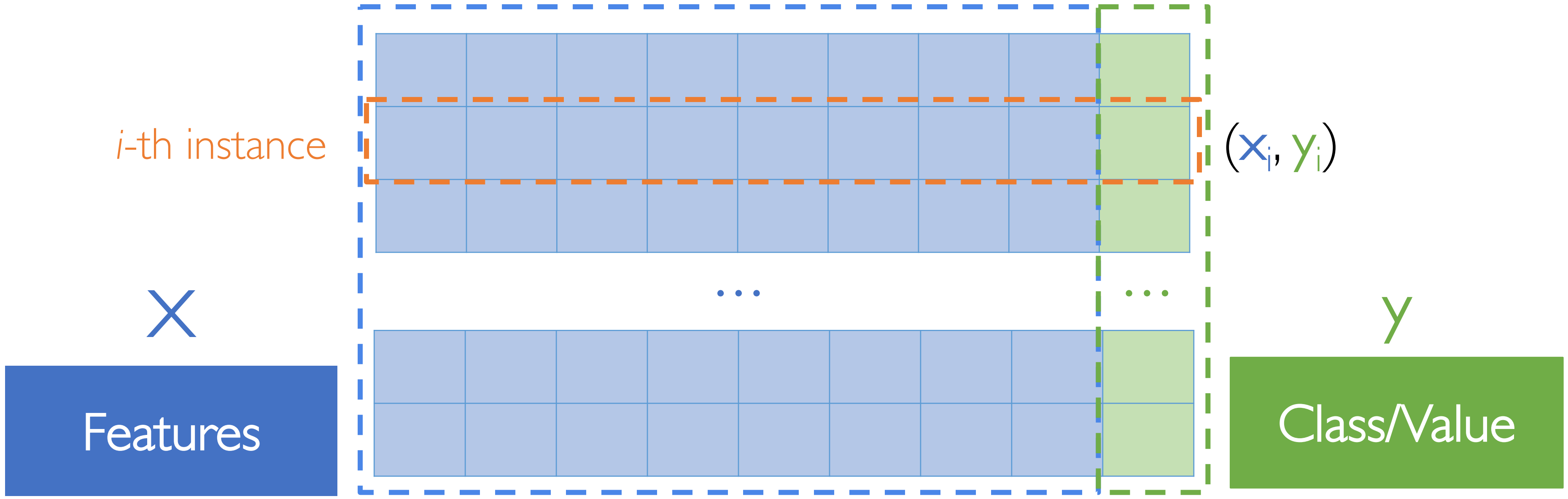


Model Training: Labeled Dataset



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

Model Training: Intuition

Idea

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

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

Model Training: Intuition

Idea

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

⇩

$$f = X \rightarrow Y$$

⇩

Problem

We cannot write down an algorithm which just implements f

Model Training: Learning f from Labeled Data

- Learning f means "finding" another function h^* which best approximates f using the data we observed

Model Training: Learning f from Labeled Data

- Learning f means "finding" another function h^* which best approximates f using the data we observed
- h^* is chosen among a family of functions H called hypothesis space by specifying two components:

Model Training: Learning f from Labeled Data

- Learning f means "finding" another function h^* which best approximates f using the data we observed
- h^* is chosen among a family of functions H called **hypothesis space** by specifying two components:
  - **loss function:** measures the error of using h^* instead of the true f

Model Training: Learning f from Labeled Data

- Learning f means "finding" another function h^* which best approximates f using the data we observed
- h^* is chosen among a family of functions H called hypothesis space by specifying two components:
  - 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

- The set of functions the learning algorithm will search through to pick the hypothesis h^* which best approximates the true target f

The Hypothesis Space H

- The set of functions the learning algorithm will search through to pick the hypothesis h^* which best approximates the true target f
- The larger the hypothesis space:
  - the larger will be the set of functions that can be represented 

The Hypothesis Space H

- The set of functions the learning algorithm will search through to pick the hypothesis h^* which best approximates the true target f
- The larger the hypothesis space:
  - the larger will be the set of functions that can be represented 
  - the harder will be for the learning algorithm to pick h^* 

The Hypothesis Space H

- The set of functions the learning algorithm will search through to pick the hypothesis h^* which best approximates the true target f
- The larger the hypothesis space:
  - the larger will be the set of functions that can be represented 
  - the harder will be for the learning algorithm to pick h^* 

Trade-off

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

The Loss Function

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

The Loss Function

- Measures the error we would make if a hypothesis *h* is used instead of the true (yet unknown) mapping *f*
- It can be computed only on the data we observed, therefore depends on the hypothesis and the dataset

$$L : \mathcal{H} \times \mathcal{D} \mapsto \mathbb{R}$$

The Loss Function

- Measures the error we would make if a hypothesis h is used instead of the true (yet unknown) mapping f
- It can be computed only on the data we observed, therefore depends on the hypothesis and the dataset

$$L : \mathcal{H} \times \mathcal{D} \mapsto \mathbb{R}$$

- 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)

The Learning Algorithm

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

The Learning Algorithm

- Defines the strategy we use to search the hypothesis space H for picking our **best** hypothesis h^*
- Here, "**best**" means the hypothesis that **minimizes** the loss function on the observed data (**Empirical Risk Minimization**)

The Learning Algorithm

- Defines the strategy we use to search the hypothesis space H for picking our best hypothesis h^*
- Here, "best" means the hypothesis that minimizes the loss function on the observed data (Empirical Risk Minimization)
- In other words, among all the hypotheses specified by H the learning algorithm will pick the one that minimizes L

The Learning Algorithm

- Defines the strategy we use to search the hypothesis space *H* for picking our **best** hypothesis h^*
- Here, "**best**" means the hypothesis that **minimizes** the loss function on the observed data (**Empirical Risk Minimization**)
- In other words, among all the hypotheses specified by *H* the learning algorithm will pick the one that minimizes *L*

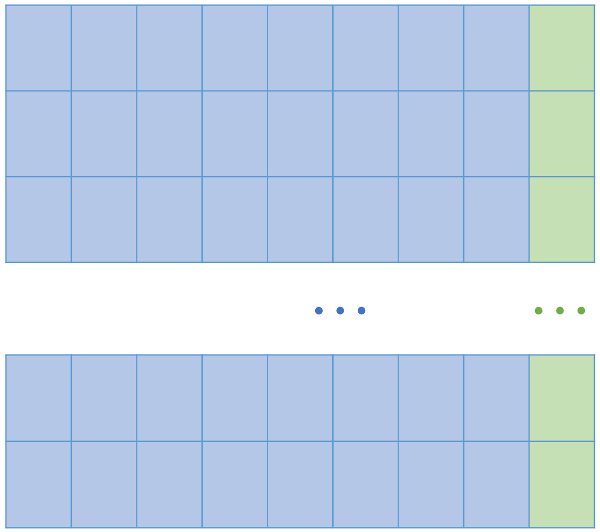
$$\boxed{h^* = \text{argmin}_{h \in \mathcal{H}} L(h, \mathcal{D})}$$

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

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

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

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

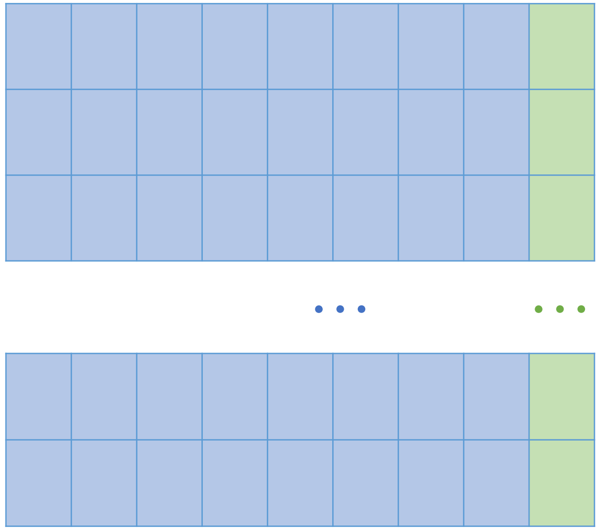


$(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$

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

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

$f = X \rightarrow Y$



$(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$

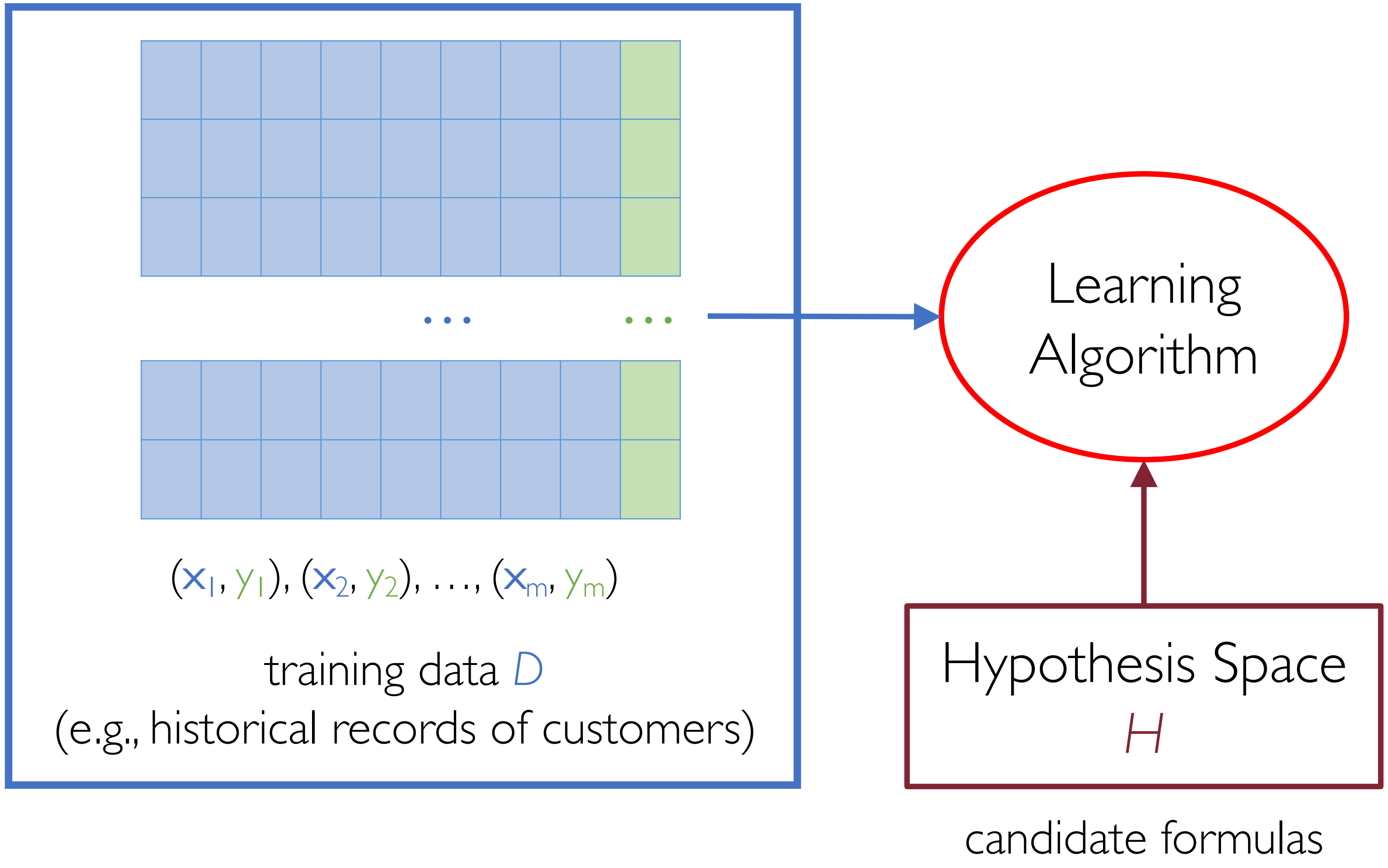
training data D
(e.g., historical records of customers)

Hypothesis Space
H

candidate formulas

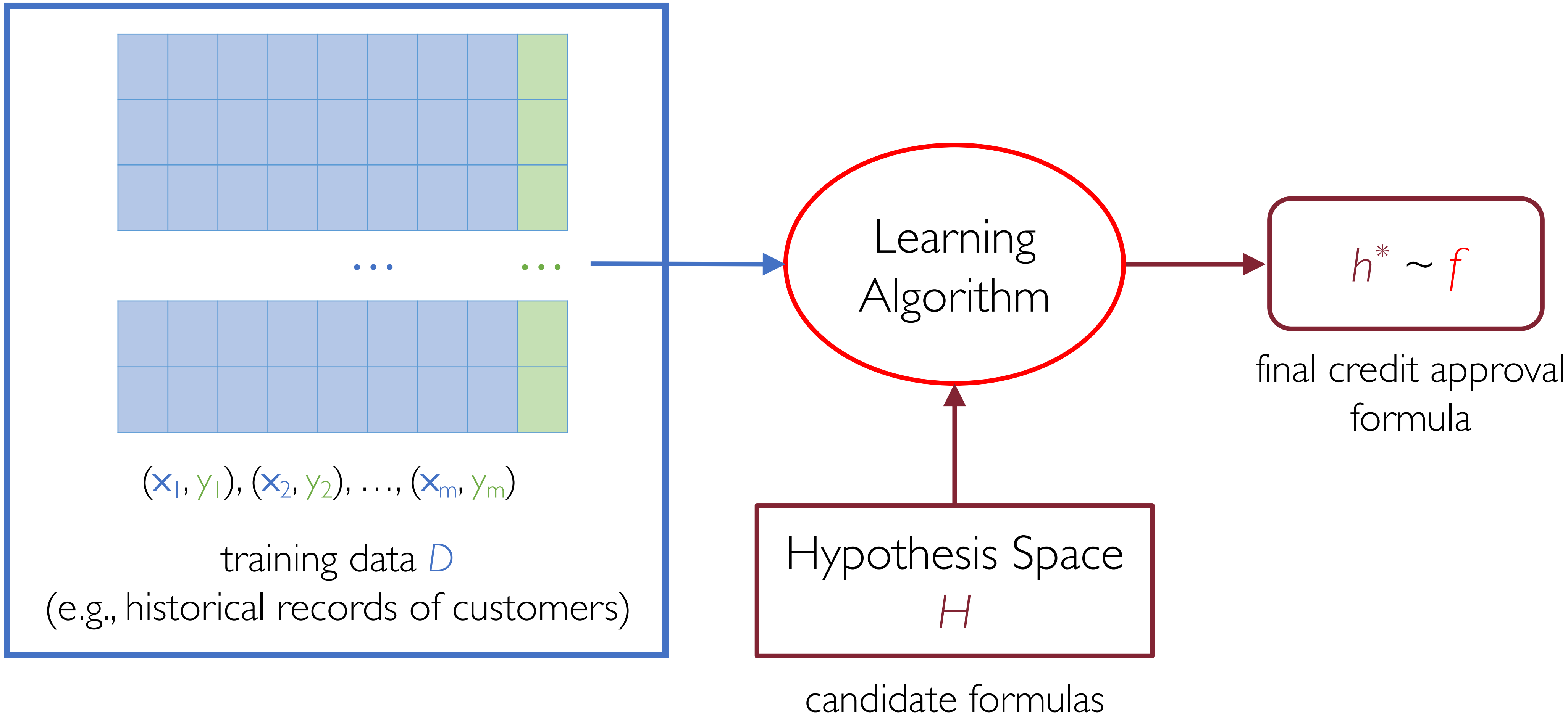
unknown target
(e.g., ideal credit approval function)

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



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

$$f = X \rightarrow Y$$



Learning f as an Optimization Problem

- We define the supervised learning problem as an optimization one

Learning f as an Optimization Problem

- We define the supervised learning problem as an optimization one
- By plugging in different loss functions combined with various hypothesis spaces we must solve a specific optimization problem

Learning f as an Optimization Problem

- We define the supervised learning problem as an optimization one
- 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

Learning *f* as an Optimization Problem

- We define the supervised learning problem as an optimization one
- 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

In-Sample vs. Out-of-Sample Error

- Minimizing the loss function on the observed data D just limits the in-sample error

In-Sample vs. Out-of-Sample Error

- Minimizing the loss function on the observed data D just limits the in-sample error
- Our ultimate hypothesis is to pick h^* which is able to generalize to unseen instances (i.e., minimize the out-of-sample error)

In-Sample vs. Out-of-Sample Error

- Minimizing the loss function on the observed data D just limits the in-sample error
- Our ultimate hypothesis is to pick h^* which is able to generalize to unseen instances (i.e., minimize the out-of-sample error)
- If we pick a hypothesis which just memorizes all the training instances, we will obtain a 0 in-sample error but <u>this is not learning</u>!

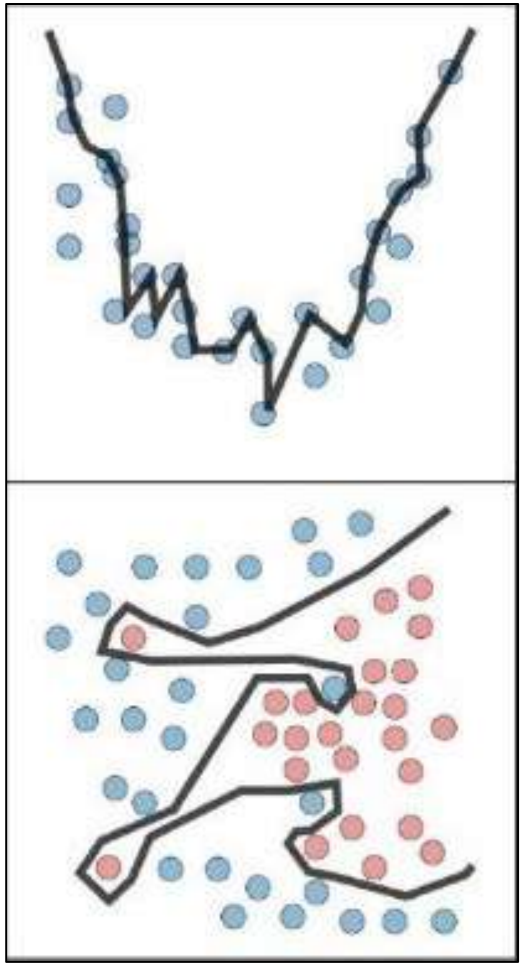
In-Sample vs. Out-of-Sample Error

- Minimizing the loss function on the observed data D just limits the in-sample error
- Our ultimate hypothesis is to pick h^* which is able to generalize to unseen instances (i.e., minimize the out-of-sample error)
- If we pick a hypothesis which just memorizes all the training instances, we will obtain a 0 in-sample error but this is not learning!
- At the same time we do not want h^* to perform poorly on D

Overfitting (High Variance)

Regression

Classification

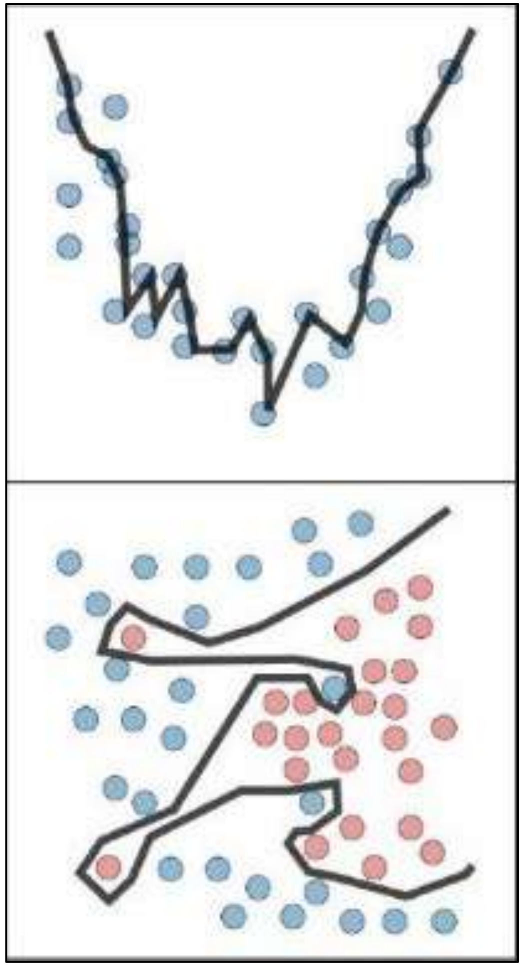


The hypothesis h^* is not learning the true f but it mimics its noise

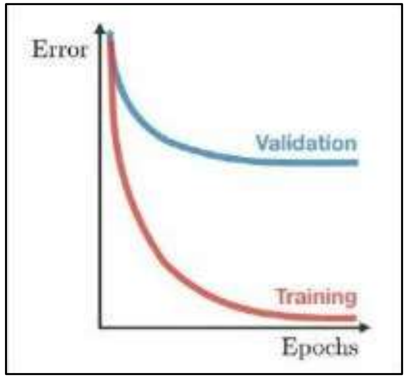
Overfitting (High Variance)

Regression

Classification



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

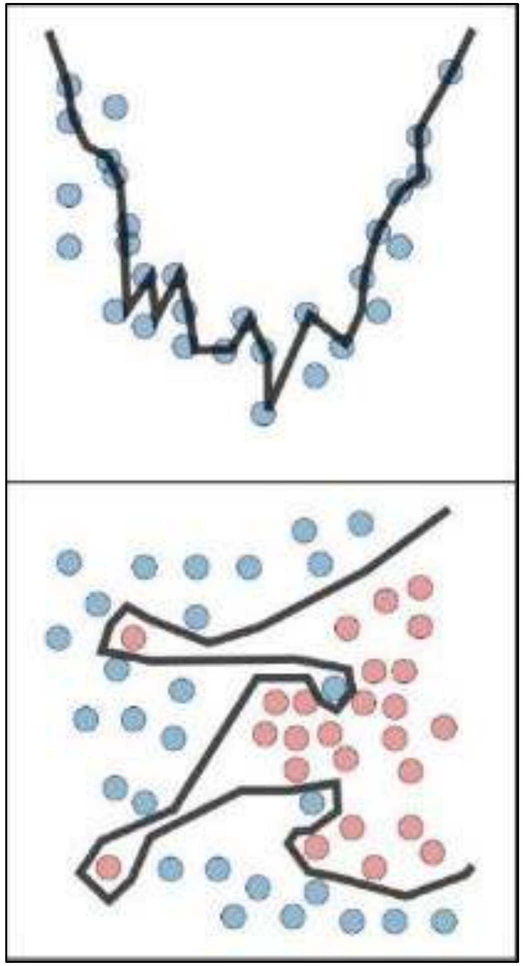


low in-sample error high out-of-sample error

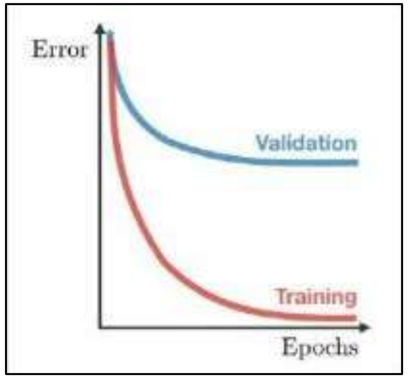
Overfitting (High Variance)

Regression

Classification



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



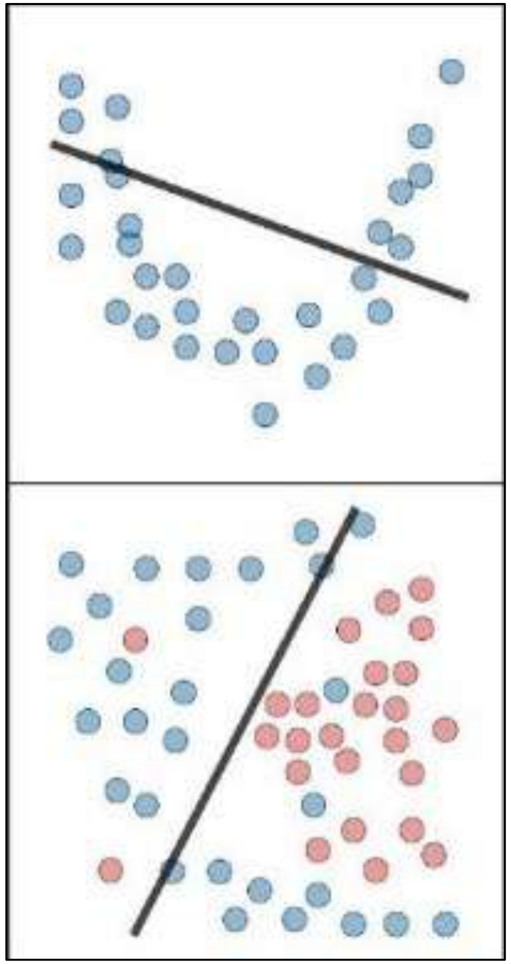
low in-sample error high out-of-sample error

- Regularization
- Get more data

Underfitting (High Bias)

Regression

Classification

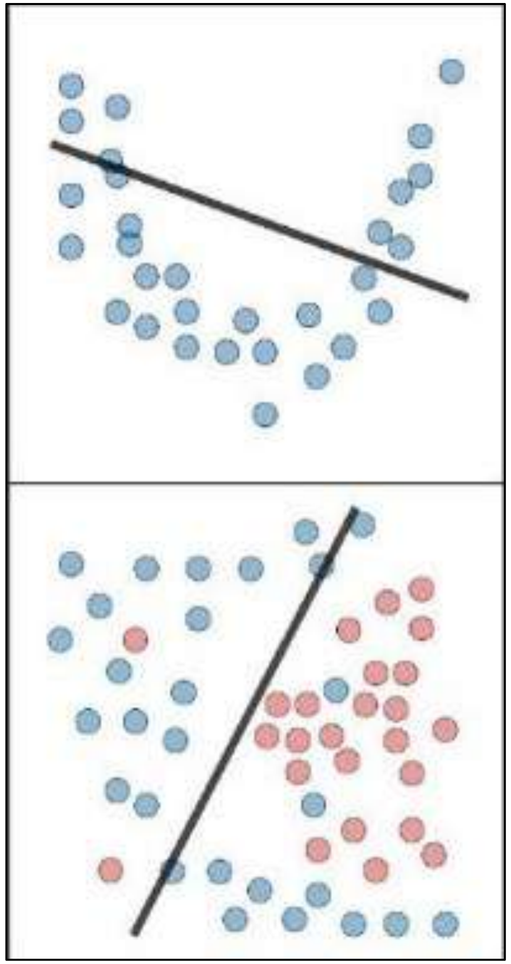


The hypothesis h^* is too "simple" for approximating the true f

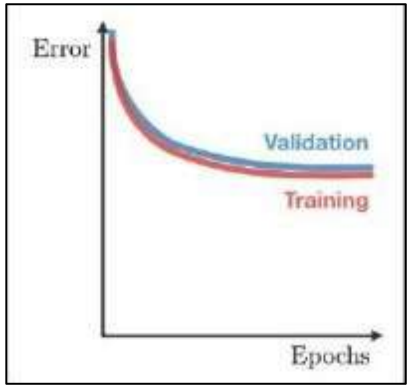
Underfitting (High Bias)

Regression

Classification



The hypothesis h^* is too "simple" for approximating the true f

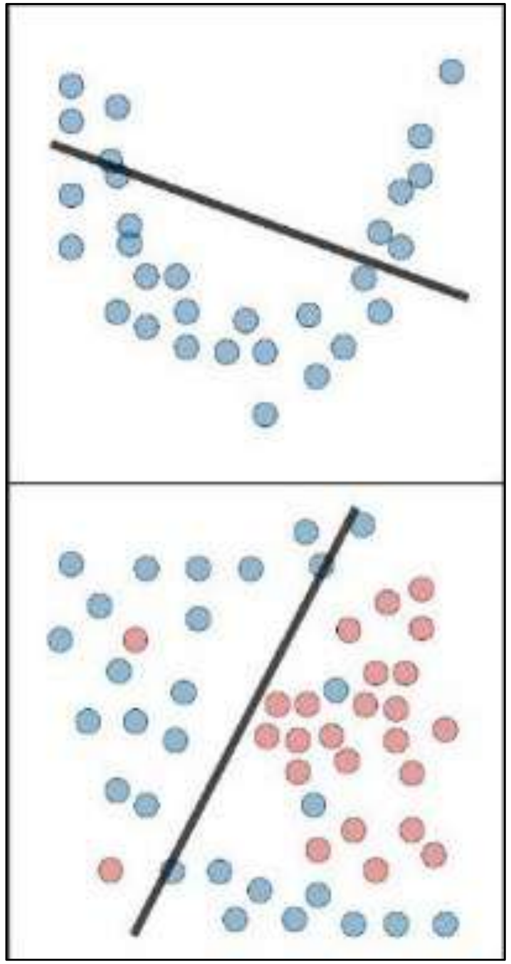


high in-sample error high out-of-sample error

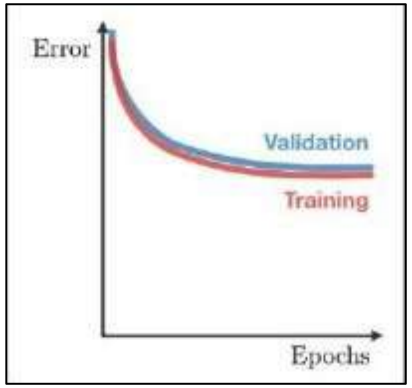
Underfitting (High Bias)

Regression

Classification



The hypothesis h^* is too "simple" for approximating the true f



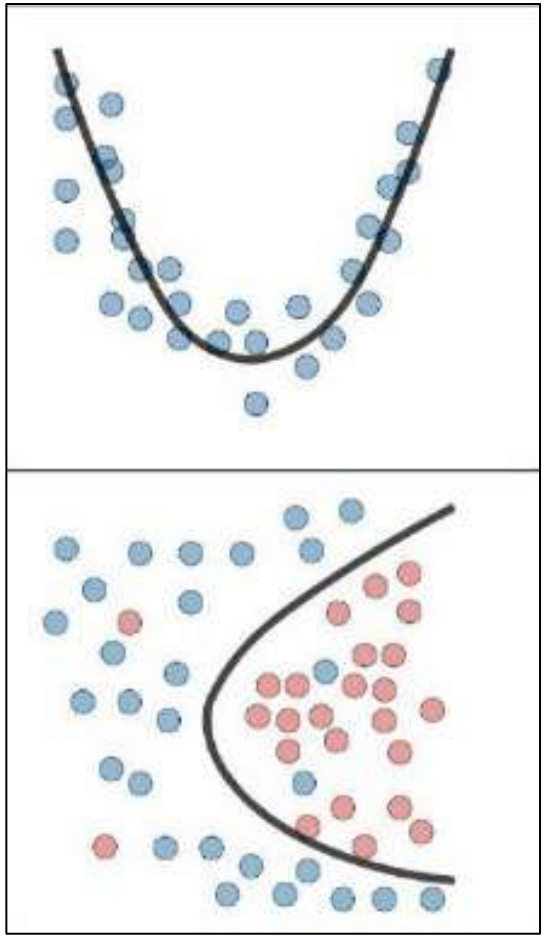
high in-sample error high out-of-sample error

- Increase model complexity
- Add more features

Bias-Variance Tradeoff

Regression

Classification



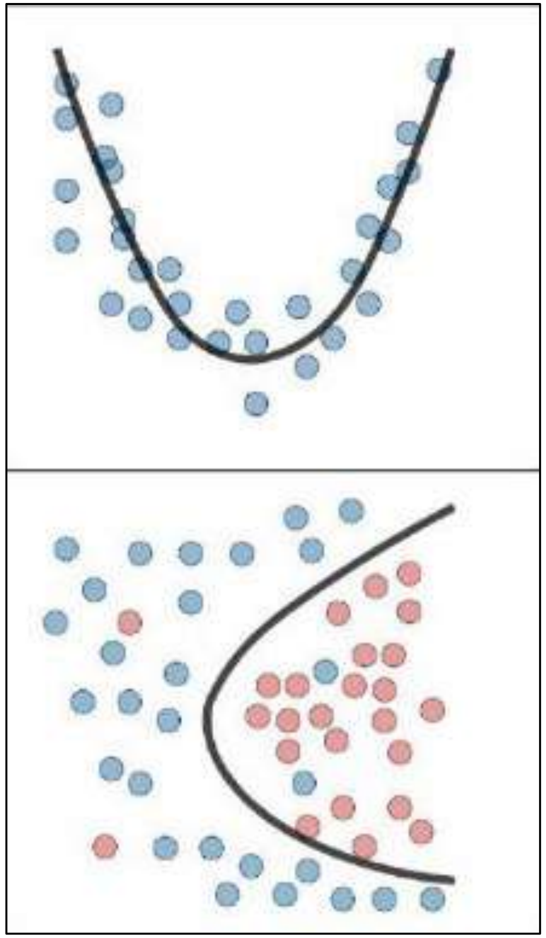
The hypothesis h^* is just right:
the simplest one explaining the data

Occam's razor

Bias-Variance Tradeoff

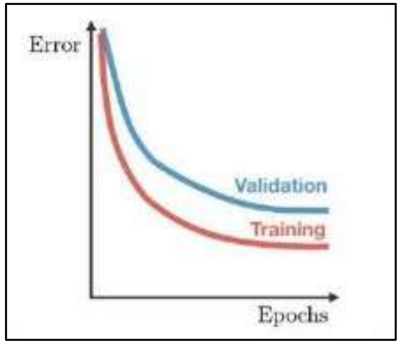
Regression

Classification



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

Occam's razor



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

Estimating Generalization Performance

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

Estimating Generalization Performance

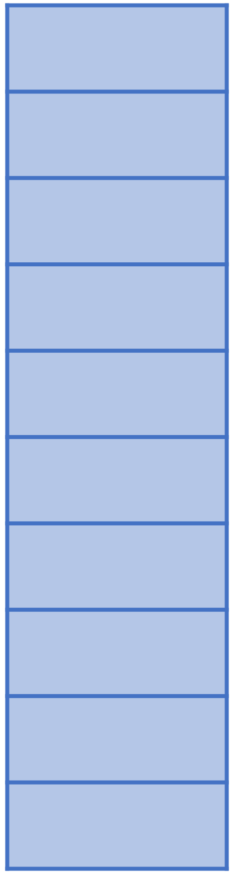
- Measuring the generalization (i.e., out-of-sample) performance online may be too risky
- Example: Don't want to deploy your new spam classifier in production knowing only its training (i.e., in-sample) performance

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 (i.i.d. assumption)

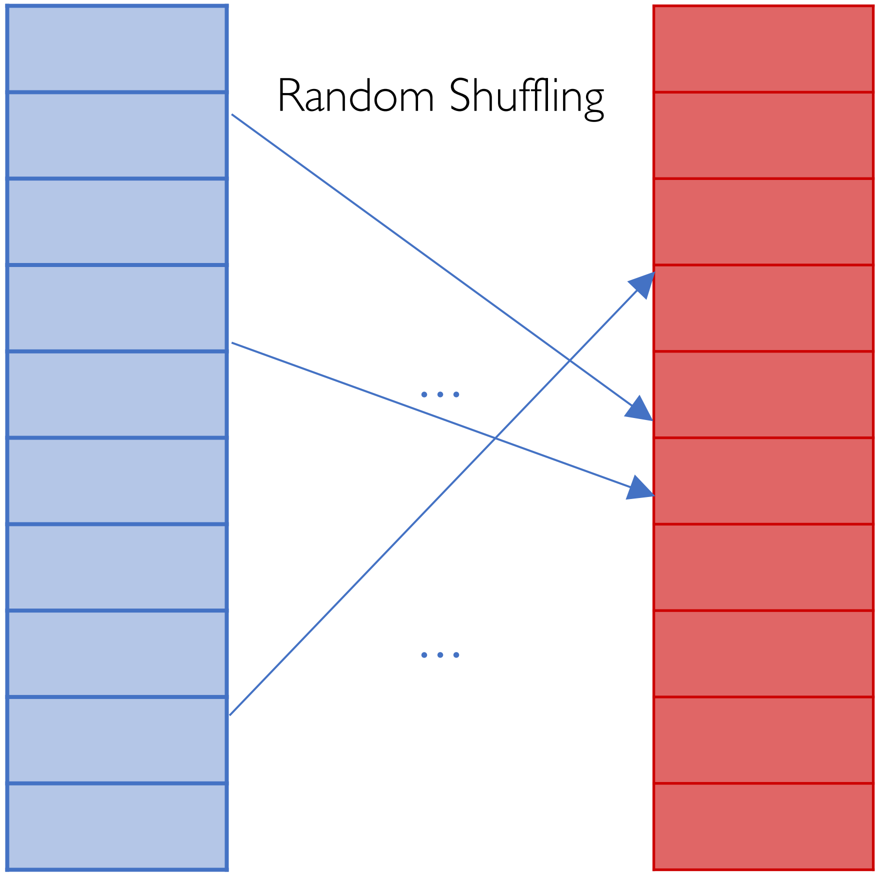
Dataset Splitting

Dataset
D

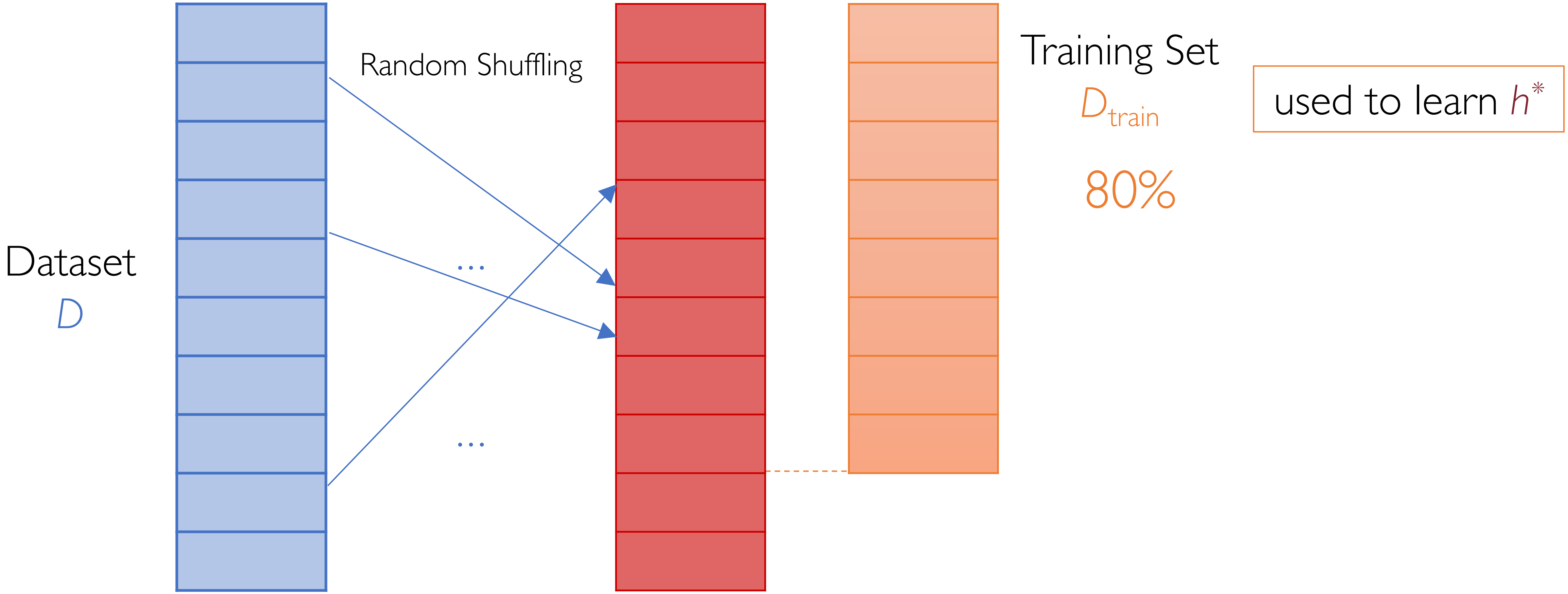


Dataset Splitting

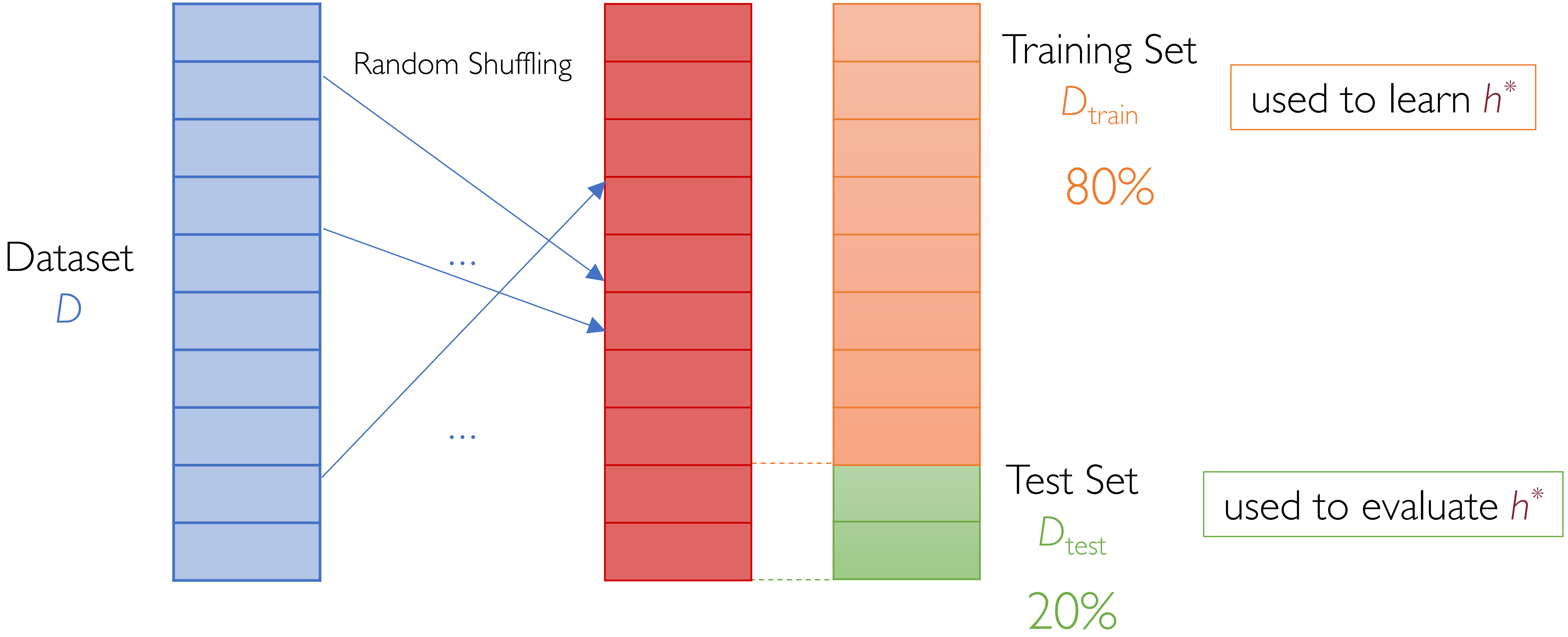
Dataset
D



Dataset Splitting

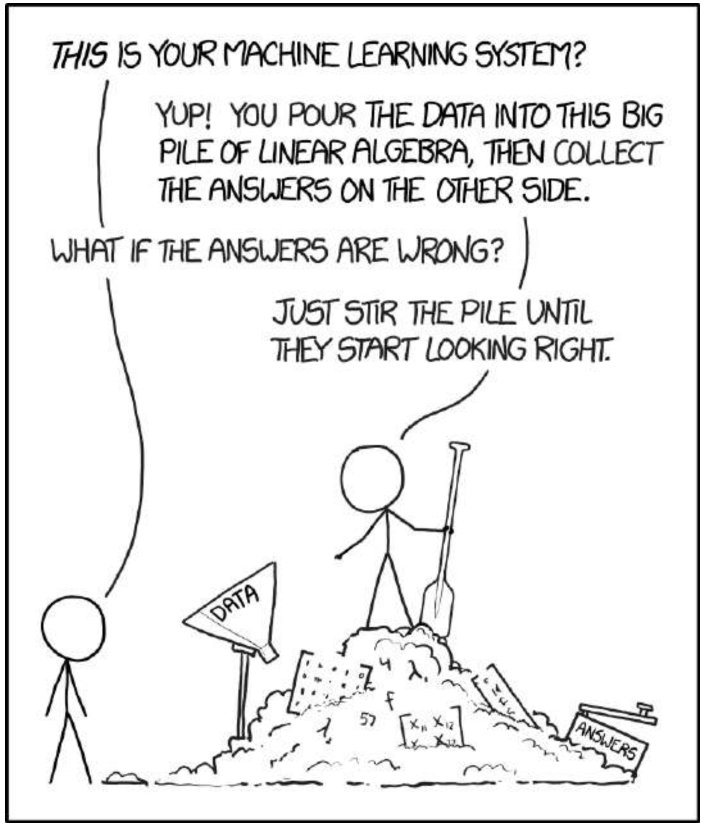


Dataset Splitting



How Much Data Do We Need?

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



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

K-Fold Cross Validation

- A generalization of the training/test splitting seen before

K-Fold Cross Validation

- A generalization of the training/test splitting seen before
- Pick a value for K (e.g., K=5 or 10)

K-Fold Cross Validation

- A generalization of the training/test splitting seen before
- Pick a value for K (e.g., K=5 or 10)
- Divide your dataset D into K distinct folds

K-Fold Cross Validation

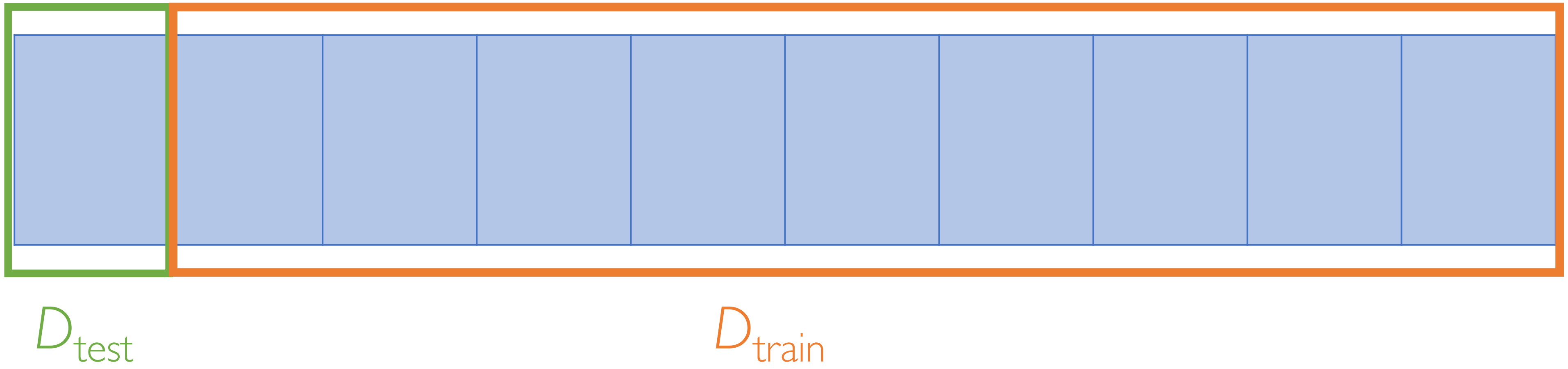
- A generalization of the training/test splitting seen before
- Pick a value for K (e.g., K=5 or 10)
- Divide your dataset D into K distinct folds
- Perform K rounds where h^* is:
  - leaned from K-1 training folds
  - evaluated on 1 remaining test fold

K-Fold Cross Validation

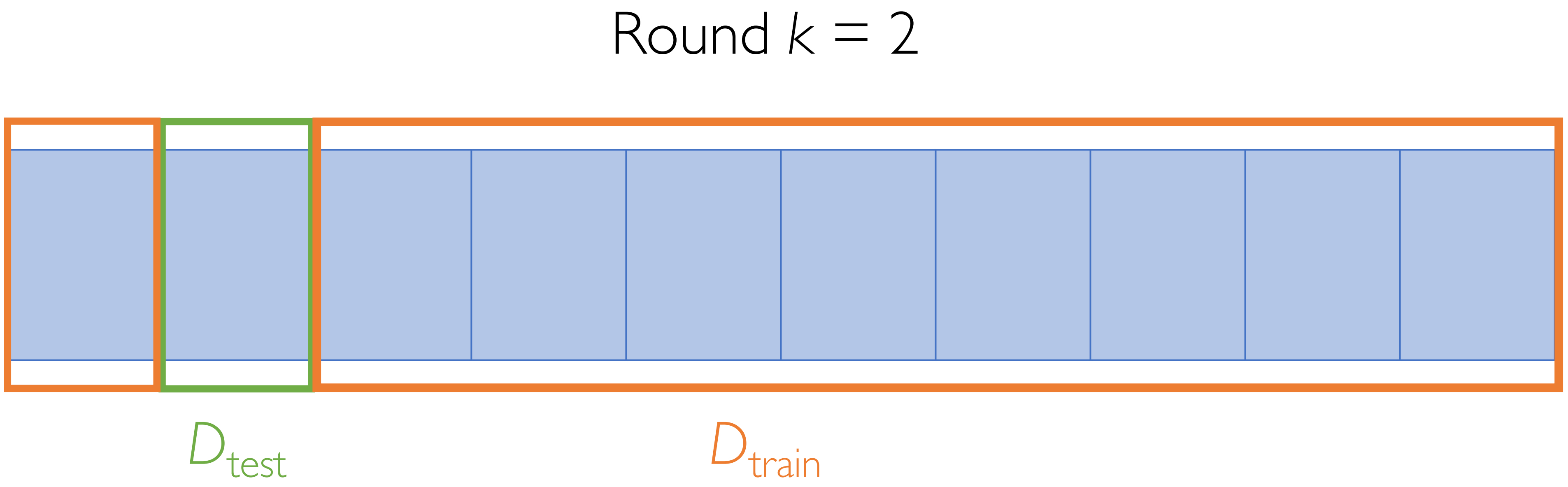
- A generalization of the training/test splitting seen before
- Pick a value for K (e.g., K=5 or 10)
- Divide your dataset D into K distinct folds
- Perform K rounds where h^* is:
  - leaned from K-1 training folds
  - evaluated on 1 remaining test fold
- The estimate of generalization error is the average across the K test folds of all the K rounds

K-Fold Cross Validation

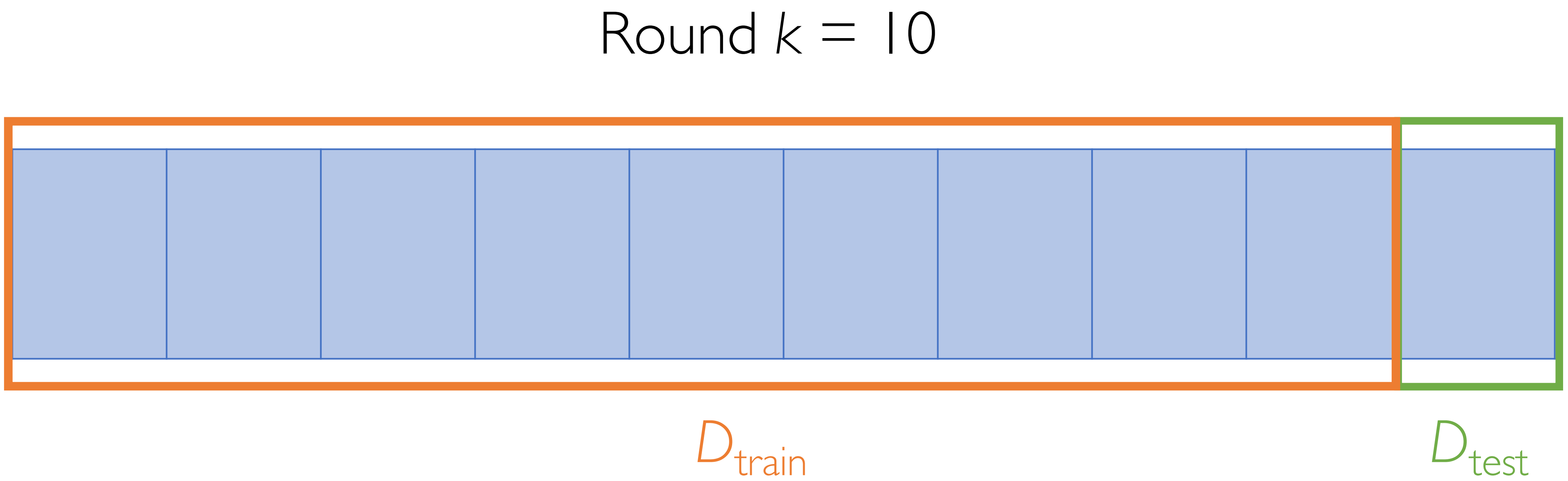
Round $k = 1$



K-Fold Cross Validation



K-Fold Cross Validation



Model Selection/Evaluation

Several different learning models to achieve the same task

Decision Trees

Random Forests

Logistic Regression

kNN

SVM

MLP

Model Selection/Evaluation

Several different learning models to achieve the same task

Decision Trees

Random Forests

Logistic Regression

kNN

SVM

MLP

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

Model Selection/Evaluation

Several different learning models to achieve the same task

Decision Trees

Random Forests

Logistic Regression

kNN

MLP

SVM

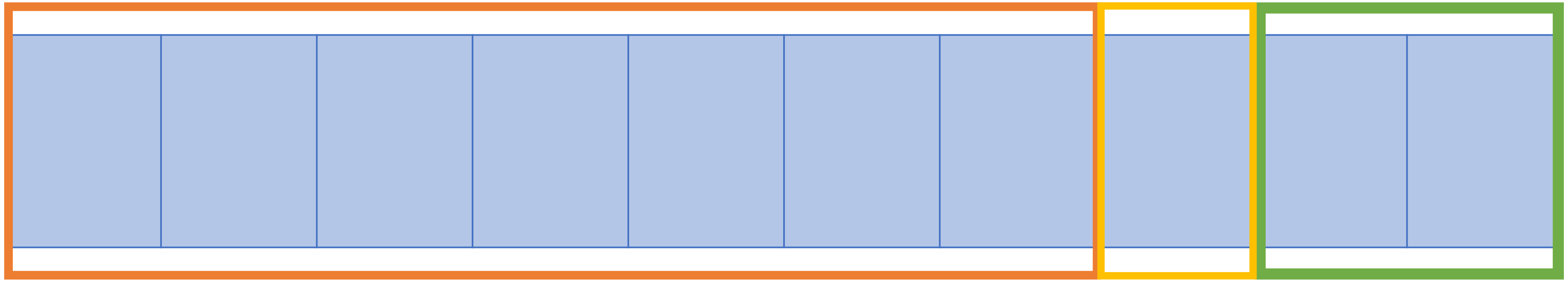
Each learning model has its own set of hyperparameters
(e.g., the number k of neighbors in kNN)

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



D_{train} D_{valid} D_{test}

Model Selection/Evaluation: Example

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

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%)

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%)

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., $k = 5$)

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

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%)

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

- Supervised Learning as an optimization problem
  - Hypothesis space (assumption)
  - Loss Function (objective)
  - Learning Algorithm (optimizer)

Take-Home Message of Today

- Supervised Learning as an optimization problem
  - Hypothesis space (assumption)
  - Loss Function (objective)
  - Learning Algorithm (optimizer)
- Regression vs. Classification

Take-Home Message of Today

- Supervised Learning as an optimization problem
  - Hypothesis space (assumption)
  - Loss Function (objective)
  - Learning Algorithm (optimizer)
- Regression vs. Classification
- Bias-Variance Tradeoff

Take-Home Message of Today

- Supervised Learning as an optimization problem
  - Hypothesis space (assumption)
  - Loss Function (objective)
  - Learning Algorithm (optimizer)
- Regression vs. Classification
- Bias-Variance Tradeoff
- Model selection vs. Model evaluation

Take-Home Message of Today

- Supervised Learning as an optimization problem
  - Hypothesis space (assumption)
  - Loss Function (objective)
  - Learning Algorithm (optimizer)
- Regression vs. Classification
- Bias-Variance Tradeoff
- Model selection vs. Model evaluation

Suggested reading: https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf