# Learning Phases

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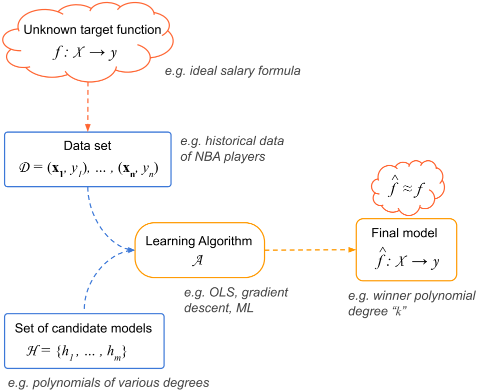
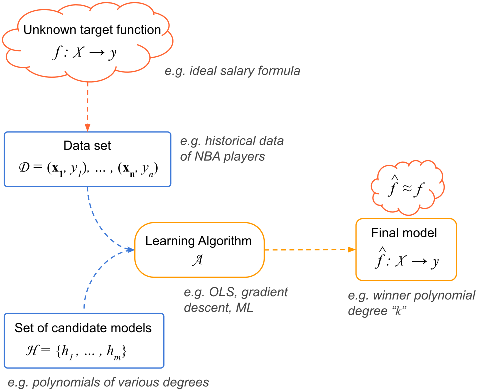
# Review: Theoretical Framework for Supervised Learning


Unknown target function
$f: \mathcal{X} \to y$
e.g. ideal salary formula
Data set
$\mathcal{D} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
e.g. historical data of NBA players
$\hat{f} \approx f$
Learning Algorithm
$\mathcal{A}$
Final model
$\hat{f}: \mathcal{X} \to y$
e.g. OLS, gradient descent, ML
e.g. winner polynomial degree "$k$"
Set of candidate models
$\mathcal{H} = \{h_1, \ldots, h_m\}$
e.g. polynomials of various degrees

- The target function $f$ is unknown, and we can never really "discover" $f$. We can only find a good enough approximation to $f$ by estimating $\hat{f}$.
- The idea of a good approximation $\hat{f} \approx f$ is also theoretical because we don't know $f$.

# Review: Theoretical Framework for Supervised Learning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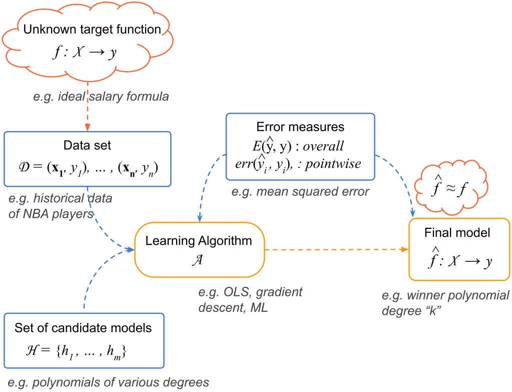
e.g. polynomials of various degrees

- The dataset $\mathcal{D}$ is influenced by the unknown target function.
- The hypothesis set $\mathcal{H}$ is the type of ML models that we want to try out (e.g., linear models, polynomial models, non-parametric models, etc.)

# Review: Theoretical Framework for Supervised Learning



Unknown target function

$f : \mathcal{X} \rightarrow y$

*e.g. ideal salary formula*

Data set

$\mathcal{D} = (\mathbf{x_1}, y_1), \dots, (\mathbf{x_n}, y_n)$

*e.g. historical data of NBA players*

Error measures

$E(\hat{y}, y)$ : *overall*

$err(\hat{y}_i, y_i)$, : *pointwise*

*e.g. mean squared error*

$\hat{f} \approx f$

Learning Algorithm

$\mathcal{A}$

*e.g. OLS, gradient descent, ML*

Final model

$\hat{f} : \mathcal{X} \rightarrow y$

*e.g. winner polynomial degree "k"*

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*e.g. polynomials of various degrees*

- The learning algorithm $\mathcal{A}$ is the set of instructions to be carried out when learning from data with the individual error function $err()$.
- The overall measure of error $E()$ is used to determine which model $h()$ is the best approximation $\hat{f}()$ to the target model $f()$.

# Review: Theoretical Framework for Supervised Learning

- In ML, the individual error function is known as the **loss function**:
  - Squared error: $err(\hat{f}, f) = (\hat{y}_i - y_i)^2$
  - Absolute error: $err(\hat{f}, f) = |\hat{y}_i - y_i|$
  - Misclassification error: $err(\hat{f}, f) = \mathbf{1}[\hat{y}_i \neq y_i]$
  - $\dots$
- The overall measure of error is the **cost function** or **risk**:
  1. **In-sample Error** $E_{in}$: the average of individual errors from data points of the in-sample data $\mathcal{D}_{in}$:

     $$E_{in}(\hat{f}, f) = \frac{1}{n} \sum_i err(\hat{f}(\mathbf{x}_i), f(\mathbf{x}_i))$$

  2. **Out-of-sample Error** $E_{out}$: the theoretical mean, or expected value, of the individual errors over the entire input space:

     $$E_{out}(\hat{f}, f) = \mathbb{E}_{\mathbf{x} \sim \mathcal{X}} \left[ err(\hat{f}(\mathbf{x}), f(\mathbf{x})) \right]$$

     The point $\mathbf{x}$ denotes a general data point in the input space $\mathcal{X}$.

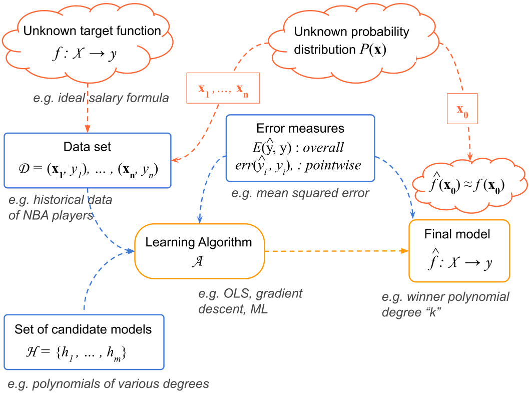
# Review: Theoretical Framework for Supervised Learning

- A good approximation $\hat{f} \approx f$ means that $E_{out}(\hat{f}, f) \approx 0$.
- However, we never have access to $E_{out}$ because out-of-sample data is theoretical: taking expectation over the entire input space $\mathcal{X}$.
- We solve this problem via:

$$E_{out}(\hat{f}) \approx 0 \Rightarrow \begin{cases} E_{in}(\hat{f}) \approx 0 & \text{practical result} \\ E_{out}(\hat{f}) \approx E_{in}(\hat{f}) & \text{theoretical result} \end{cases}$$

- The first goal is achievable because we have access to our training data $D_{in}$.
- To achieve the second goal, we need to assume a probability distribution $P$ over the input space $\mathcal{X}$: $\mathbf{x}_0 \sim P$. We need $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ are independent identically distributed (i.i.d.) samples from this distribution $P$.

# Review: Theoretical Framework for Supervised Learning



Unknown target function $f : \mathcal{X} \to \mathcal{Y}$

e.g. ideal salary formula

Unknown probability distribution $P(\mathbf{x})$

$\mathbf{x}_1, \dots, \mathbf{x}_n$

$\mathbf{x}_0$

Data set $\mathcal{D} = (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$

e.g. historical data of NBA players

Error measures

$E(\hat{y}, y)$ : *overall*

$err(\hat{y}_i, y_i)$, : *pointwise*

e.g. mean squared error

$\hat{f}(\mathbf{x}_0) \approx f(\mathbf{x}_0)$

Learning Algorithm $\mathcal{A}$

e.g. OLS, gradient descent, ML

Final model $\hat{f} : \mathcal{X} \to \mathcal{Y}$

e.g. winner polynomial degree "k"

Set of candidate models $\mathcal{H} = \{h_1, \dots, h_m\}$

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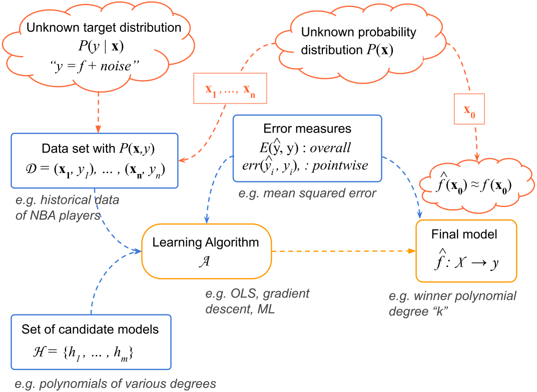

Unknown target distribution
$P(y \mid \mathbf{x})$
"$y = f + noise$"
Unknown probability distribution $P(\mathbf{x})$
$\mathbf{x}_1, \ldots, \mathbf{x}_n$
$\mathbf{x}_0$
Data set with $P(\mathbf{x}, y)$
$\mathcal{D} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
e.g. historical data of NBA players
Error measures
$E(\hat{y}, y)$ : overall
$err(\hat{y}_i, y_i)$, : pointwise
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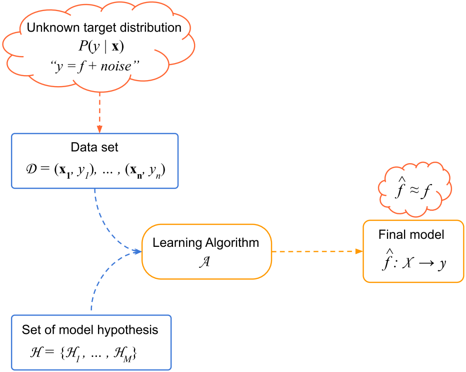
- In practice, there will be some noise: $y = f(\mathbf{x}) + \varepsilon$. We want to learn a **target conditional distribution** $P(y|\mathbf{x})$.
- Our data follow a joint probability distribution:

$$P(\mathbf{x}, y) = P(\mathbf{x})P(y|\mathbf{x})$$

# Learning Phases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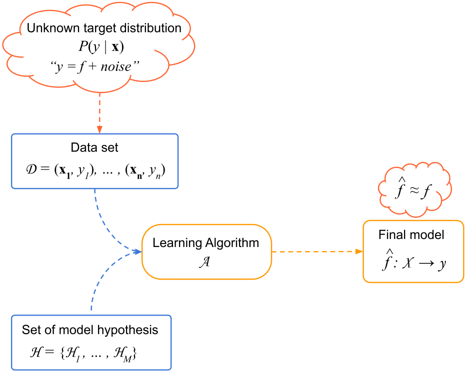
Final model
$\hat{f} : \mathcal{X} \to y$
Set of model hypothesis
$\mathcal{H} = \{\mathcal{H}_1, \dots, \mathcal{H}_M\}$

- We need to fit different models: i.e., working with different classes of hypothesis. For example: principal component regression $\mathcal{H}_1$, ridge regression $\mathcal{H}_2$, LASSO $\mathcal{H}_3$.
- Each type of models has tuning parameters that need to be determined through trial-error steps.

# Learning Phases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Learning Algorithm
$\mathcal{A}$
Final model
$\hat{f} : \mathcal{X} \to y$
Set of model hypothesis
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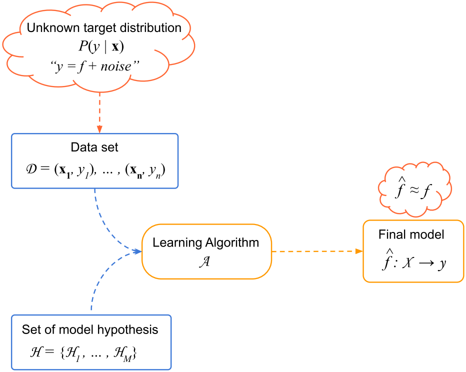
- For each hypothesis class, we need to find the optimal tuning parameter, which involves choosing a finalist model: the best principal component regression, the best polynomial regression model, etc.
- Among these finalist models, we need to select the best model $\hat{f}$.

# Learning Phases



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Data set
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Learning Algorithm
$\mathcal{A}$

$\hat{f} \approx f$

Final model
$\hat{f} : \mathcal{X} \to y$

Set of model hypothesis
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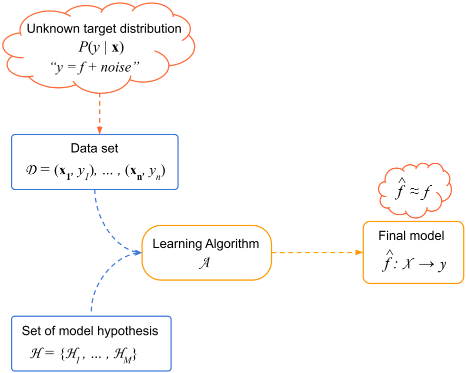
- Finally, we need to measure the predicting performance of the final model $\hat{f}$: measuring how the model behaves with out-of-sample data points.

# Learning Phases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Learning Algorithm
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$\hat{f} \approx f$
Final model
$\hat{f} : \mathcal{X} \rightarrow y$
Set of model hypothesis
$\mathcal{H} = \{\mathcal{H}_1, \ldots, \mathcal{H}_M\}$

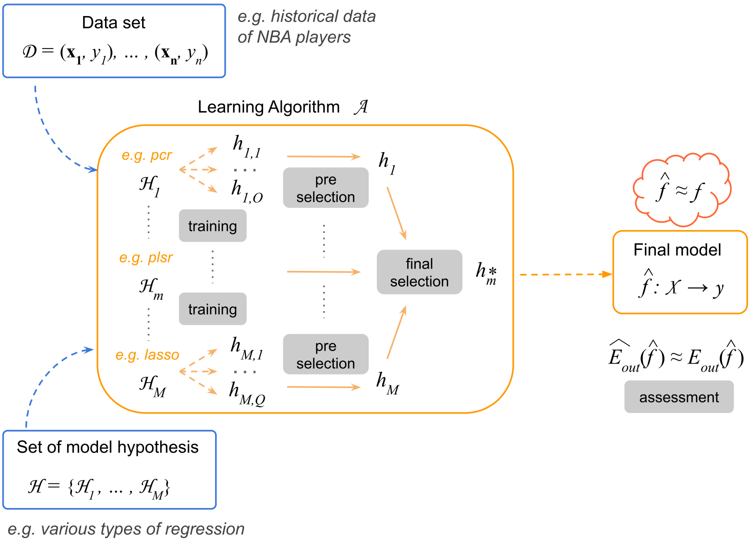
Three phases in supervised learning:

1. Model training
2. Model selection
3. Model assessment

# Learning Phases

1. Training: We need to consider different classes of hypothesis $\mathcal{H}_1, \ldots, \mathcal{H}_m, \ldots, \mathcal{H}_M$. Given some data, for each hypothesis class $\mathcal{H}_m$, we fit a model $h_m$.
2. Selection: We choose a model from a set of candidate models.
   - Pre-Selection: Choose a finalist model from a set of models belonging to a certain class of hypothesis.
   - Final-Selection: Choose a final model among a set of finalist models.
3. Assessment: Given a final model $\hat{f}$, how can we estimate the out-of-sample error $E_{out}(\hat{f})$?

# Learning Phases


Data set
$\mathcal{D} = (\mathbf{x_1}, y_1), \ldots, (\mathbf{x_n}, y_n)$
e.g. historical data of NBA players
Learning Algorithm $\mathcal{A}$
e.g. pcr
$\mathcal{H}_1$
$h_{1,1}$
$h_{1,O}$
training
pre selection
$h_1$
e.g. plsr
$\mathcal{H}_m$
training
final selection
$h_m^*$
e.g. lasso
$\mathcal{H}_M$
$h_{M,1}$
$h_{M,Q}$
pre selection
$h_M$
$\hat{f} \approx f$
Final model
$\hat{f} : \mathcal{X} \rightarrow y$
$\widehat{E}_{out}(\hat{f}) \approx E_{out}(\hat{f})$
assessment
Set of model hypothesis
$\mathcal{H} = \{\mathcal{H}_1, \ldots, \mathcal{H}_M\}$
e.g. various types of regression

What data should we use to perform each task?

# Model Assessment

- Given a final model $h$, how to measure its prediction quality?
- In-sample error $E_{in}$ measures **the resubstitution power** of the model $h$ (i.e., how well the model fits the learning data).

$$E_{in}(h) = \frac{1}{|\mathcal{D}_{in}|} \sum_{\mathbf{x}_i \in \mathcal{D}_{in}} err(h(\mathbf{x}_i) = \hat{y}_i, y_i)$$

- Out-of-sample error $E_{out}$ measures **the generalization power** of the model $h$:

$$E_{out}(h) = \mathbb{E}[err(h(\mathbf{x}_0) = \hat{y}_0, y_0)]$$

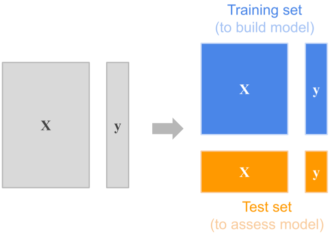
- Because we don't have access to out-of-sample dataset $\mathcal{D}_{out}$, we need to find a proxy set $\mathcal{D}_{proxy} \subset \mathcal{D}_{out}$ to compute $E_{proxy}$ and use it to approximate $E_{out}$:

$$\underbrace{\hat{E}_{out}(h)}_{\mathcal{D}_{proxy}} \approx \underbrace{E_{out}(h)}_{\mathcal{D}_{out}}$$

# Model Assessment - Holdout Test Set

- How can we estimate $E_{out}$?
- Our dataset $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$. If we use all $n$ data points to train/fit a model, then we have a good measure for $E_{in}$, but we don't have any out-of-sample data points to get an **honest** approximation $\hat{E}_{out}$ of $E_{out}$.
- Why not use $E_{in}$ as an estimate $\hat{E}_{out}$ of $E_{out}$?
- We may have a model that produces very small in-sample error $E_{in} \approx 0$ but does not perform well on out-of-sample data points.
- Given that the only available dataset is $\mathcal{D}$, the Holdout Method splits $\mathcal{D}$ into two subsets:
    1. **The training set** $\mathcal{D}_{train}$ for training/fitting the model.
    2. **The test set** $\mathcal{D}_{test}$ to be used a proxy for $\mathcal{D}_{out}$ for the assessment purpose.

# Model Assessment - Holdout Test Set

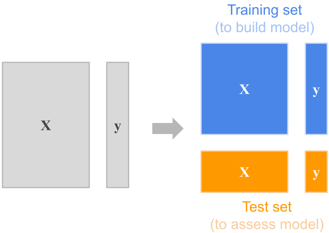


Taking random sample of size $a$ without replacement from $\mathcal{D}$:

$$\mathcal{D} \to \begin{cases} \mathcal{D}_{train} & \text{size } n - a \\ \mathcal{D}_{test} & \text{size } a \end{cases}$$

We fit a model using $\mathcal{D}_{train}$ to obtain a model $h^{-}(\mathbf{x})$

# Model Assessment - Holdout Test Set



Taking random sample of size $a$ without replacement from $\mathcal{D}$:

$$\mathcal{D} \rightarrow \begin{cases} \mathcal{D}_{train} & \text{size } n - a \\ \mathcal{D}_{test} & \text{size } a \end{cases}$$

With the remainder points in $\mathcal{D}_{test}$, we can measure the performance of $h^{-}(\mathbf{x})$ as:

$$E_{test}(h^{-}) = \frac{1}{a} \sum_{l=1}^{a} err(h^{-}(\mathbf{x}_l), y_l); \quad (\mathbf{x}_l, y_l) \in \mathcal{D}_{test}$$

# Model Assessment - Holdout Test Set

- If $\mathcal{D}_{test}$ is a representative sample of $\mathcal{D}_{out}$, $E_{test}$ gives an unbiased estimate of $E_{out}$. Why?
- Consider an out-of-sample point $(\mathbf{x}_0, y_0) \in \mathcal{D}_{test}$, given an error function, we can measure:

$$err(h(\mathbf{x}_0), y_0)$$

- Let's determine its expectation over the input space $\mathcal{X}$:

$$\mathbb{E}_{\mathcal{X}}[err(h(\mathbf{x}_0), y_0)]$$

- This is the definition of out-of-sample error $E_{out}$. Therefore $err(h(\mathbf{x}_0), y_0)$ is an **unbiased estimate** of the out-of-sample error.

# Model Assessment - Holdout Test Set - Expectation

- Let's consider a set $\mathcal{D}_{test} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_a, y_a)\}$ containing $a > 1$ points. We can get $E_{test}$ by

$$E_{test}(h) = \frac{1}{a} \sum_{l=1}^{a} err(h(\mathbf{x}_l), y_l)$$

- Is $E_{test}(h)$ an unbiased estimate of $E_{out}(h)$?

$$\begin{aligned} \mathbb{E}_{\mathcal{X}}[E_{test}(h)] &= \mathbb{E}_{\mathcal{X}}\left[\frac{1}{a} \sum_{l=1}^{a} err(h(\mathbf{x}_l), y_l)\right] \\ &= \frac{1}{a} \sum_{l=1}^{a} \mathbb{E}_{\mathcal{X}}[err(h(\mathbf{x}_l), y_l)] \\ &= \frac{1}{a} \sum_{l=1}^{a} E_{out}(h) = E_{out}(h) \end{aligned}$$

- $E_{test}(h)$ is an **unbiased estimate** of $E_{out}(h)$. What about its **variance**?

# Model Assessment - Holdout Test Set - Variance

- The variance[1] of $E_{test}(h)$ is given by:

$$\begin{aligned} Var[E_{test}(h)] &= Var\left[\frac{1}{a}\sum_{l=1}^{a} err(h(\mathbf{x}_l), y_l)\right] \\ &= \frac{1}{a^2}\sum_{l=1}^{a} Var[err(h(\mathbf{x}_l), y_l)] = \frac{s^2}{a} \end{aligned}$$

  Assume that the variance $Var[err(h(\mathbf{x}_0), y_0)] = s^2$ is constant.

- As we increase the number $a$ of test data points, the variance of the estimator $E_{test}(h)$ decreases. The more test points we use, the more reliably $E_{test}(h)$ estimates $E_{out}(h)$.
- But the larger $a$ is, the smaller the training dataset will be.

[1] `https://eli.thegreenplace.net/2009/01/07/variance-of-the-sum-of-independent-variables`

# Model Assessment - Holdout Algorithm

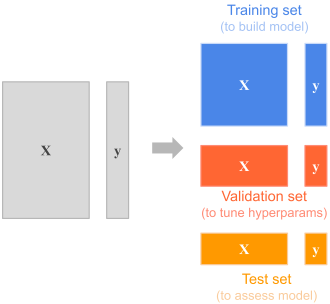
1. Compile the available data into $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$.
2. Choose $a \in \mathbb{N}$ points from $\mathcal{D}$ to get a test set $\mathcal{D}_{test}$, and place the remaining $n - a$ points into the training set $\mathcal{D}_{train}$.
3. Use $\mathcal{D}_{train}$ to fit a particular model $h^{-}(\mathbf{x})$.
4. Measure the performance of $h^{-}$ using $\mathcal{D}_{test}$:

$$E_{test}(h^{-}) = \frac{1}{a} \sum_{l=1}^{a} err(h^{-}(\mathbf{x}_l), y_l)$$

   where $(\mathbf{x}_l, y_l) \in \mathcal{D}_{test}$.

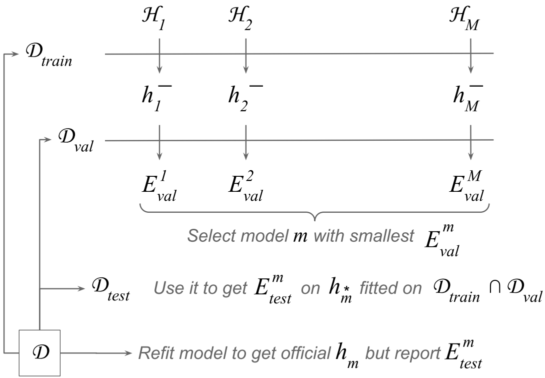
5. Generate the final model $\hat{h}$ by refitting $h^{-}$ to the entire dataset $\mathcal{D}$.

# Model Selection - Three-Way Holdout Method



- The test set $\mathcal{D}_{test}$ can only be used at the end of the learning process to quantify the generalization error of the final model. We don't use this set to make any **learning decisions**.
- Thus, we create a validation set $\mathcal{D}_{val}$ for selecting the final model from a set of finalist models.

# Model Selection



$\mathcal{H}_1$ $\mathcal{H}_2$ $\mathcal{H}_M$

$\mathcal{D}_{train}$

$h_1^-$ $h_2^-$ $h_M^-$

$\mathcal{D}_{val}$

$E_{val}^1$ $E_{val}^2$ $E_{val}^M$

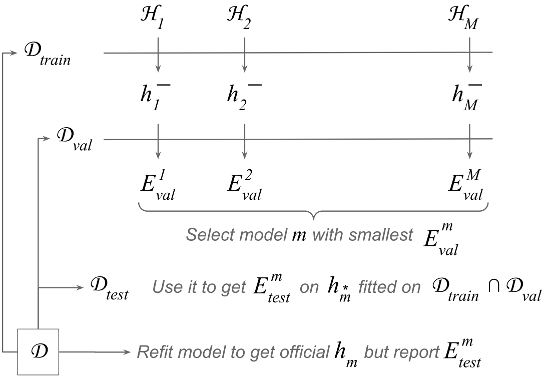
Select model $m$ with smallest $E_{val}^m$

$\mathcal{D}_{test}$ Use it to get $E_{test}^m$ on $h_m^*$ fitted on $\mathcal{D}_{train} \cap \mathcal{D}_{val}$

$\mathcal{D}$ Refit model to get official $h_m$ but report $E_{test}^m$

- $\mathcal{H}_m$ represents the $m$-th hypothesis class. $h_m^-$ is the finalist model from class $\mathcal{H}_m$.
- After a finalist model $h_m^-$ has been pre-selected for each hypothesis class, we use $\mathcal{D}_{val}$ to compute validation error $E_{val}^m$.

# Model Selection



$\mathcal{H}_1$
$\mathcal{H}_2$
$\mathcal{H}_M$
$\mathcal{D}_{train}$
$h_1^-$
$h_2^-$
$h_M^-$
$\mathcal{D}_{val}$
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Select model $m$ with smallest $E_{val}^m$
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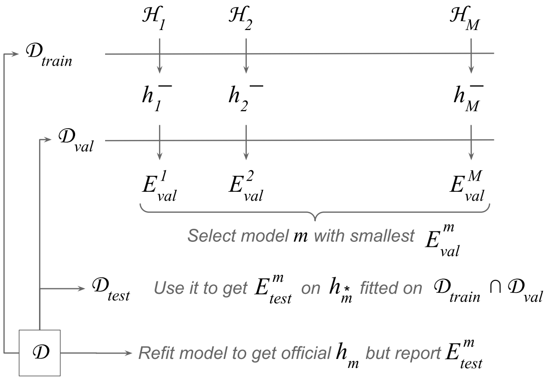
Use it to get $E_{test}^m$ on $h_m^*$ fitted on $\mathcal{D}_{train} \cap \mathcal{D}_{val}$
$\mathcal{D}$
Refit model to get official $h_m$ but report $E_{test}^m$

- After selecting the best model $h_m^-$ with the smallest $E_{val}^m$, a model $h_m^*$ is fitted using $\mathcal{D}_{train} \cap \mathcal{D}_{val}$

# Model Selection



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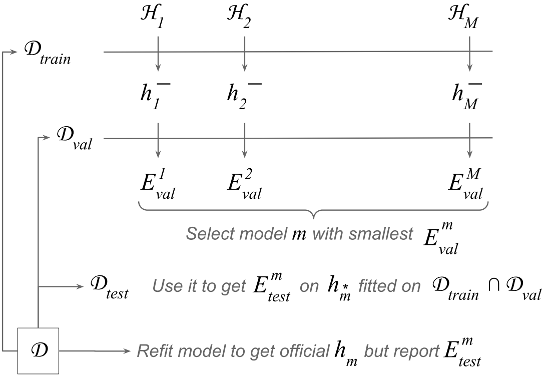
$\mathcal{D}$
Refit model to get official $h_m$ but report $E_{test}^m$

- The performance of $h_m^*$ is assessed by using $\mathcal{D}_{test}$ to obtain $E_{test}^m = E_{test}(h_m^*)$.
- Finally, the “official” model is the model fitted on the entire dataset $\mathcal{D}$.

# Model Selection



$\mathcal{H}_1$ $\mathcal{H}_2$ $\mathcal{H}_M$

$\mathcal{D}_{train}$

$h_1^-$ $h_2^-$ $h_M^-$

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Select model $m$ with smallest $E_{val}^m$

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$\mathcal{D}$ Refit model to get official $h_m$ but report $E_{test}^m$

- Choosing the best model (smallest $E_{val}^m$) is a **learning decision**.
- Thus, $E_{val}^m$ is a **biased estimate** of $E_{out}$.
- The larger the test and validation sets are, the more reliable the estimates of the out-of-sample performance. But the smaller the training set will be.

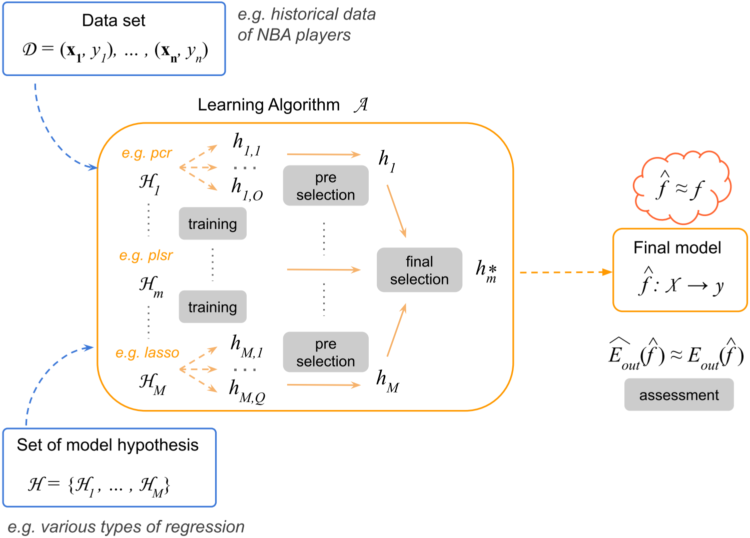
# Model Training

- For each hypothesis class, we need to train all candidate models and pre-select the finalist models using the training set $\mathcal{D}_{train}$.
- For example, $\mathcal{H}_m$ is principal component regression (PCR), we need to train several models

  $$h_{1,m}, h_{2,m}, \ldots, h_{q,m}$$

  with $1, 2, \ldots, q$ are the number of principal components (i.e., **the tuning parameter** - hyperparameter).
- Using $\mathcal{D}_{train}$ to fit all possible PCR models, and also to choose the one with the smallest error $E_{train}$ can cause overfitting.
- We could use $\mathcal{D}_{val}$ to pre-select the finalist model for $\mathcal{H}_m$, but then we don't have **fresh** data points for the final-selection phase.
- $\longrightarrow$ Resampling methods.

# Learning Phases



Data set

$\mathcal{D} = (\mathbf{x_1}, y_1), \ldots, (\mathbf{x_n}, y_n)$

*e.g. historical data of NBA players*

Learning Algorithm $\mathcal{A}$

*e.g. pcr*

$\mathcal{H}_1$

$h_{1,1}$ ... $h_{1,O}$

$h_1$

pre selection

training

*e.g. plsr*

$\mathcal{H}_m$

training

final selection

$h_m^*$

*e.g. lasso*

$\mathcal{H}_M$

$h_{M,1}$ ... $h_{M,Q}$

pre selection

$h_M$

$\hat{f} \approx f$

Final model

$\hat{f} : \mathcal{X} \rightarrow y$

$\widehat{E}_{out}(\hat{f}) \approx E_{out}(\hat{f})$

assessment

Set of model hypothesis

$\mathcal{H} = \{\mathcal{H}_1, \ldots, \mathcal{H}_M\}$

*e.g. various types of regression*

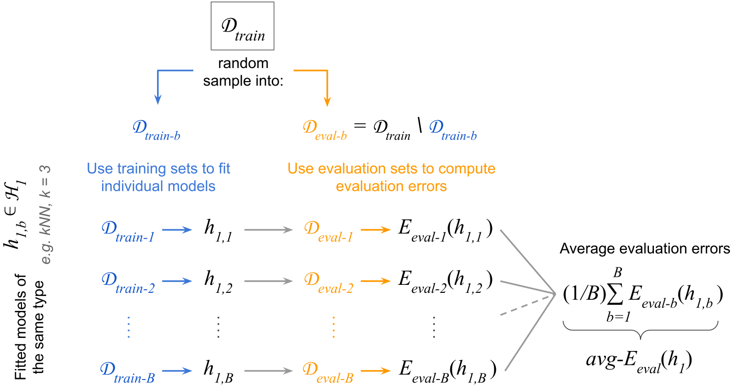
# Resampling Approaches - General Sampling Blueprint

- We have a limited dataset.
- We want to generate multiple training sets, multiple evaluation sets to be used for both training phase and the pre-selection phase.
- The training set is the one we usually apply resampling.
- For example, we want to fit a $k$-Nearest Neighbor ($k$NN) model with $k = 3$ neighbors.
- We randomly split the training set into two subsets:
  1. $\mathcal{D}_{train-b}$ to train a model $h_{1,b}$.
  2. $\mathcal{D}_{eval-b} = \mathcal{D}_{train} \setminus \mathcal{D}_{train-b}$ to evaluate $h_{1,b}$.
- The procedure is repeated $B$ times. We average all the evaluation errors to get a single measure indicating the performance of the particular type of trained models:

$$E_{eval} = \frac{1}{B} \sum_{b=1}^{B} E_{eval-b}$$

- The average measure $E_{eval}$ would be the typical performance of 3-NN models.

# Resampling Approaches



$\mathcal{D}_{train}$

random sample into:

$\mathcal{D}_{train\text{-}b}$

$\mathcal{D}_{eval\text{-}b} = \mathcal{D}_{train} \setminus \mathcal{D}_{train\text{-}b}$

Use training sets to fit individual models

Use evaluation sets to compute evaluation errors

Fitted models of the same type

$h_{1,b} \in \mathcal{H}_1$

e.g. kNN, $k = 3$

$\mathcal{D}_{train\text{-}1} \rightarrow h_{1,1} \rightarrow \mathcal{D}_{eval\text{-}1} \rightarrow E_{eval\text{-}1}(h_{1,1})$

$\mathcal{D}_{train\text{-}2} \rightarrow h_{1,2} \rightarrow \mathcal{D}_{eval\text{-}2} \rightarrow E_{eval\text{-}2}(h_{1,2})$

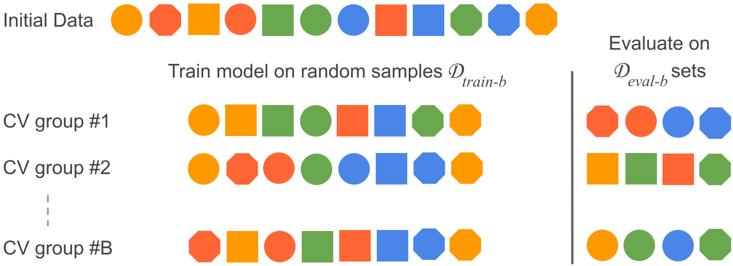
$\vdots$

$\mathcal{D}_{train\text{-}B} \rightarrow h_{1,B} \rightarrow \mathcal{D}_{eval\text{-}B} \rightarrow E_{eval\text{-}B}(h_{1,B})$

Average evaluation errors

$$\underbrace{(1/B)\sum_{b=1}^{B} E_{eval\text{-}b}(h_{1,b})}_{avg\text{-}E_{eval}(h_1)}$$

# Monte Carlo Cross Validation



Initial Data

Train model on random samples $\mathcal{D}_{train\text{-}b}$

Evaluate on $\mathcal{D}_{eval\text{-}b}$ sets

CV group #1

CV group #2

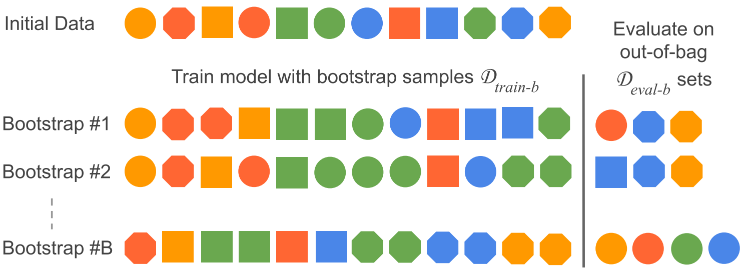
CV group #B

# Monte Carlo Cross Validation - Repeated Holdout

1. Compile training dataset $\mathcal{D}_{train} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
2. Repeat the Holdout method $B$ times ($B$ is very large, e.g., 500).
   - Generate $\mathcal{D}_{train-b}$ by sampling $n - r$ elements without replacement from $\mathcal{D}_{train}$.
   - Generate $h_b^-$ by fitting a model to $\mathcal{D}_{train-b}$.
   - Compute $E_{eval-b} = \frac{1}{r} \sum_i err(h_b^-(\mathbf{x}_i), y_i)$; where $(\mathbf{x}_i, y_i) \in \mathcal{D}_{eval-b}$.
3. Obtain an overall value for $E_{eval}$ by averaging the $E_{eval-b}$ values:

$$E_{eval} = \frac{1}{B} \sum_{b=1}^{B} E_{eval-b}$$

# Bootstrap Method


Initial Data
Train model with bootstrap samples $\mathcal{D}_{train\text{-}b}$
Evaluate on out-of-bag $\mathcal{D}_{eval\text{-}b}$ sets
Bootstrap #1
Bootstrap #2
Bootstrap #B

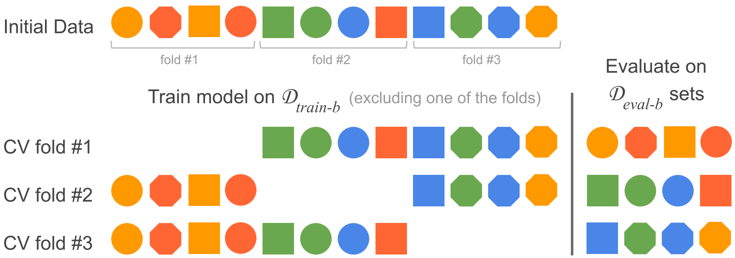
- A bootstrap sample is a random sample of the data taken **with replacement**.
- The bootstrap sample has the same size as $\mathcal{D}_{train}$.
- Some individuals are reprensented multiple times in the bootstrap while others are not selected at all. The unselected individuals are out-of-bag elements.

# Bootstrap Algorithm

1. Compile training dataset $\mathcal{D}_{train} = (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$
2. Repeat the following steps for $b = 1, 2, \dots, B$ where $B$ is very large (e.g., 500):
   - Generate $\mathcal{D}_{train-b}$ by sampling $n$ times **with replacement** from $\mathcal{D}_{train}$.
   - Generate $\mathcal{D}_{eval-b}$ by compiling out-of-bag elements ($\mathcal{D}_{eval-b}$ should not contain repeated elements).
   - Compute $E_{eval-b} = \frac{1}{r_b} \sum_i err(h_b^-(\mathbf{x}_i), y_i)$; where $(\mathbf{x}_i, y_i) \in \mathcal{D}_{eval-b}$ and $r_b$ is the size of $\mathcal{D}_{eval-b}$.
3. Obtain an overall value for bootstrap $E_{eval}$ by averaging the $E_{eval-b}$ values:

$$E_{eval}^{bootstrap} = \frac{1}{B} \sum_{b=1}^{B} E_{eval-b}$$

# $K$-Fold Cross Validation


Initial Data
fold #1
fold #2
fold #3
Train model on $\mathcal{D}_{train\text{-}b}$ (excluding one of the folds)
Evaluate on $\mathcal{D}_{eval\text{-}b}$ sets
CV fold #1
CV fold #2
CV fold #3

- Split $\mathcal{D}_{train}$ into $K$ sets of equal size. Each subset is called a **fold**.
- At each iteration $b$, a fold is held out for the evaluation purpose $\mathcal{D}_{eval-b}$, and the remaining folds are merged into $\mathcal{D}_{train-b}$ for the training purpose.
- At the end $b = K$, the cross-validation error $E_{cv}$ is defined as the average $E_{eval}$, which is computed from all evaluation errors $E_{eval-b}$.

# Leave-One-Out Cross Validation (LOOCV)

A special case of $K$-Fold cross validation is when each fold contains one single data point, i.e., $K = n$.

1. Compile training dataset $\mathcal{D}_{train} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
2. For $i = 1, 2, \ldots, n$:
   - Generate the $i$-th training dataset by removing the $i$-th element from $\mathcal{D}_{train}$: $\mathcal{D}_{train-i} = \mathcal{D}_{train} \setminus \{(\mathbf{x}_i, y_i)\}$
   - Fit the model to $\mathcal{D}_{train-i}$ to obtain $h_i^-$.
   - Use the point $(\mathbf{x}_i, y_i)$ to compute $E_{eval-i} = err(h_i^-(\mathbf{x}_i), y_i)$
3. Obtain cross-validation error $E_{cv}$ by averaging the individual errors:

$$E_{cv} = \frac{1}{n} \sum_{i}^{n} E_{eval-i}$$

# Example - Tuning the parameter $\lambda$ of Ridge Regression

The ridge regression coefficients:

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

$\lambda$ is a tuning parameter (i.e., a hyperparameter). How to find the finalist model of the hypothesis class of ridge regression models?

# Example - Tuning the parameter $\lambda$ of Ridge Regression

1. Split $\mathcal{D}_{train} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$ into $K$ folds:

$$\mathcal{D}_{train} = \mathcal{D}_{fold-1} \cup \mathcal{D}_{fold-2} \cup \dots \cup \mathcal{D}_{fold-K}$$

2. Create $K$ training sets:

$$\begin{aligned}
\mathcal{D}_{train-1} &= \mathcal{D}_{train} \setminus \mathcal{D}_{fold-1}; \mathcal{D}_{eval-1} = \mathcal{D}_{fold-1} \\
\mathcal{D}_{train-2} &= \mathcal{D}_{train} \setminus \mathcal{D}_{fold-2}; \mathcal{D}_{eval-2} = \mathcal{D}_{fold-2} \\
&\dots\dots \\
\mathcal{D}_{train-K} &= \mathcal{D}_{train} \setminus \mathcal{D}_{fold-K}; \mathcal{D}_{eval-K} = \mathcal{D}_{fold-K}
\end{aligned}$$

3. For $\lambda_l = 0.001, 0.002, \dots, \lambda_L$:
   1. For $b = 1, 2, \dots, K$:
      - Fit ridge regression model $h_{l,b}$ with $\lambda_l$ on $\mathcal{D}_{train-b}$
      - Compute $E_{eval-b}(h_{l,b})$ on $\mathcal{D}_{eval-b}$
   2. Compute cross-validation error $E_{cv-l} = \frac{1}{K} \sum_{b=1}^{K} E_{eval_b}(h_{l,b})$
4. Compare all $L$ cross-validation errors $E_{cv-1}, E_{cv-2}, \dots, E_{cv-L}$ and choose the $\lambda^*$ that yields the smallest $E^*_{cv}$.
5. Use $\lambda^*$ to fit the finalist model $\mathbf{w} = (\mathbf{X}^\top \mathbf{X} + \lambda^* \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$.