W1. Introduction and Machine Learning Pipeline

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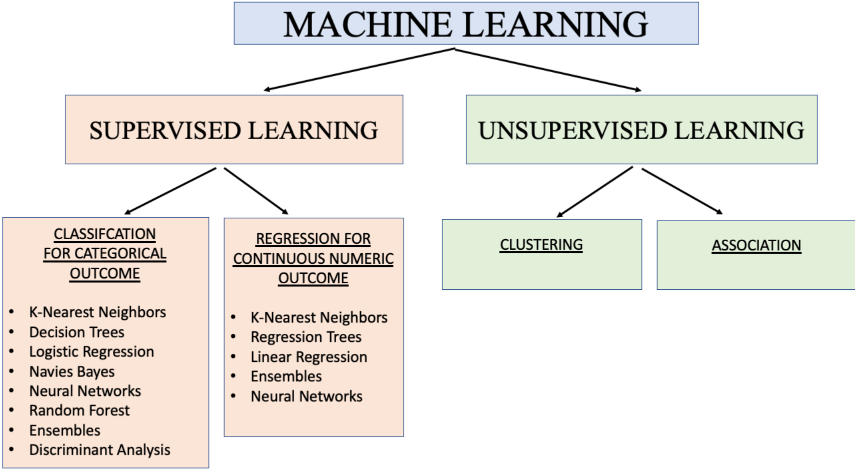
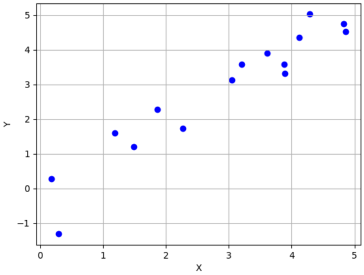
Week 1

ML Quadrants



Machine Learning and Statistical Models

- A simple example: Suppose we observe a dataset:



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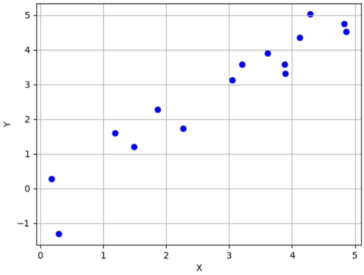

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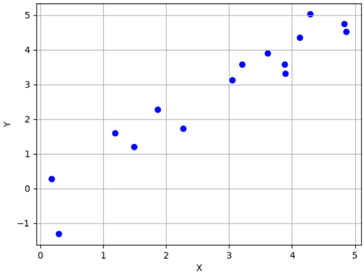

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- What is a statistical model?

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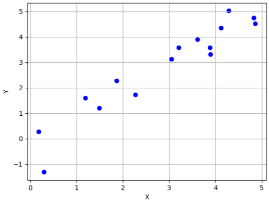

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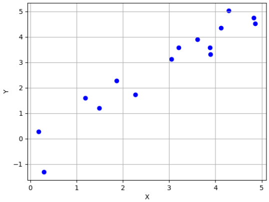

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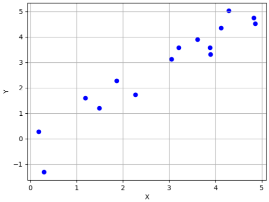
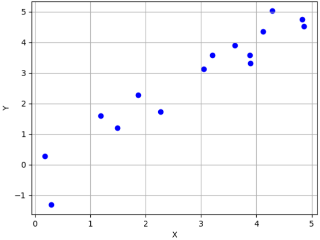


- **What is machine learning**?
  - Machine Learning is the study of computational algorithms that often applies to (unstructured) big data, e.g., image and text, with a particular focus on prediction.

Statistical Model

Statistical model: is a mathematical model (built up a set of statistical assumptions) and is mostly concerned about estimation and inference, e.g., hypothesis testing. It is mostly useful for small data and applies to scenarios that demands interpretability.



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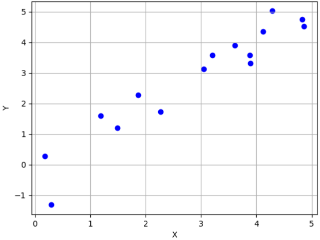

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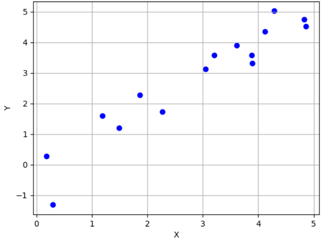

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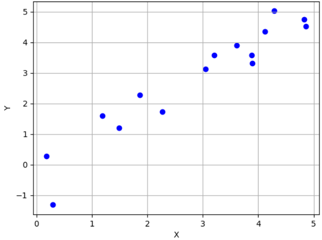
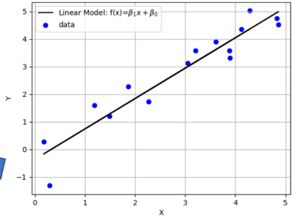


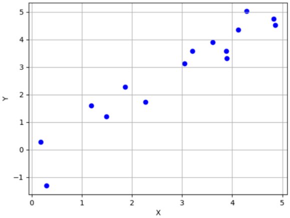
Assumptions:

- $Y = f(X) + \epsilon$, where f is a true model
- X and ϵ are independent
- $\mathbb{E}(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$

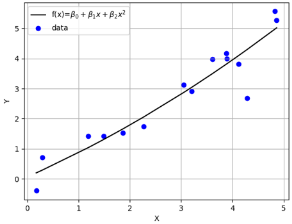
An example: how to determine the form of f



Assumption: the relationship between X and Y is Linear!



Assumption: the relationship between X and Y is Quadratic!



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- Parametric models vs non-parametric models
- Training data vs testing data
- Bias and variance tradeoff
- Model validation

Parametric models v.s. Non-parametric models

- **Parametric models**: Situations like linear regression, in which we can describe the functional form of $f(x)$ using *a fixed number of parameters* are called parametric models. Like

$$f(x) = \beta_0 + \beta^T x$$

Parametric models v.s. Non-parametric models

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- Once we know assume the parametric form of f, the estimation of f reduces to estimating the parameters β_0 and β.

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- For example, the value of k in the K-nearest neighbor classifier that grows as you see more and more data. Other examples include the depth in decision tree, and the number of layers and the width in deep neural networks.
- In this course, a non-parametric models is one that does not make explicit assumptions about the form of f.

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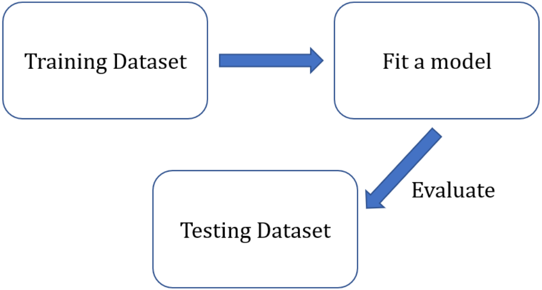

Let us take regression as an example

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- **Response/label**: Y is a quantitative random variable. Generally, Y is something we want to predict, say this image is a cat or dog or your starting salary after graduation.
- **The relationship between $\boldsymbol{X}$ and Y**:

$$Y = f^*(\boldsymbol{X}) + \epsilon, \tag{1}$$

where $\mathbb{E}(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$.

Statistical machine learning for regression

- **Goal**: Find a function $f(\boldsymbol{X})$ for predicting Y (or approximate f^* well)
- **Loss function**: square loss

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- The averaged loss (expected error, also called as "risk") of f:

$$R(f) = \mathbb{E}_{\boldsymbol{X},Y}\big[L(f(\boldsymbol{X}), Y)\big] = \mathbb{E}\big[(Y - f(\boldsymbol{X}))^2\big]$$

Deeper look at the risk function R

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- From the above decomp, we can tell $R(f)$ attains its minimum at

$$f^*(\boldsymbol{X}) = \mathbb{E}(Y|\boldsymbol{X}).$$

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  - Minimize the averaged squared loss on a training dataset $\{\boldsymbol{x}_i, y_i\}_{i=1}^{n}$

$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (f(\boldsymbol{x}_i) - y_i)^2$$

How to evaluate $\widehat{f}$: bias and variance tradeoff

- Based on the training dataset $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, we obtain an estimator $\widehat{f}$

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- Assess the quality of $\widehat{f}$ at $\boldsymbol{X} = \boldsymbol{x}_0$ (note that $Y = f^*(x_0) + \epsilon$):

$$\begin{aligned}
&\mathbb{E}_\epsilon\left[(\widehat{f}(\boldsymbol{X}) - Y)^2 | \boldsymbol{X} = \boldsymbol{x}_0\right] \\
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- Here, $(\boldsymbol{x}_0, Y)$ is the testing dataset.

Bias and Variance tradeoff

- Reducible part can be decomposed into two components

$$\mathbb{E}_D\left[\widehat{f}(\boldsymbol{x}_0) - \mathbb{E}(Y|\boldsymbol{X} = \boldsymbol{x}_0)\right]^2$$
$$= \underbrace{\mathbb{E}_D\left[\widehat{f}(\boldsymbol{x}_0) - \mathbb{E}(\widehat{f}(\boldsymbol{X})\right]^2}_{Variance} + \underbrace{\left[\mathbb{E}_D(\widehat{f}(\boldsymbol{x}_0)) - \mathbb{E}(Y|\boldsymbol{X} = \boldsymbol{x}_0)\right]^2}_{Bias^2},$$

where the expectation is taken with respect to the training dataset D (that takes care of the randomness in $\widehat{f}$.)

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  where the expectation is taken with respect to the training dataset D (that takes care of the randomness in $\widehat{f}$.)
  - **Variance**: represents the variability of the predicted value. The randomness comes from the training dataset.

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where the expectation is taken with respect to the training dataset D (that takes care of the randomness in $\widehat{f}$.)

- **Variance**: represents the variability of the predicted value. The randomness comes from the training dataset.
- **Squared Bias**: The second term is the squared bias. If $\mathcal{F}$ is chosen well, so that the mean across all training data sets is the true function, then bias is 0.

Training MSE v.s. Testing MSE

- Let $D_r = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ and $D_e = \{(\boldsymbol{x}_i', y_i')\}_{i=1}^m$ be training and testing datasets, respectively. Train an estimator from D_r

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- Evaluate $\widehat{f}$ by the mean squared error (MSE):

$$\text{Training MSE} : \frac{1}{n} \sum_{i=1}^{n} (\widehat{f}(\boldsymbol{x}_i) - y_i)^2$$

$$\text{Testing MSE} : \frac{1}{m} \sum_{i=1}^{m} (\widehat{f}(\boldsymbol{x}_i') - y_i')^2$$

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- **Question**: Which one can be used for assessing the quality of $\widehat{f}$?

An example.

- We generate $\{(x_i, y_i)\}_{i=1}^n$ in the following way

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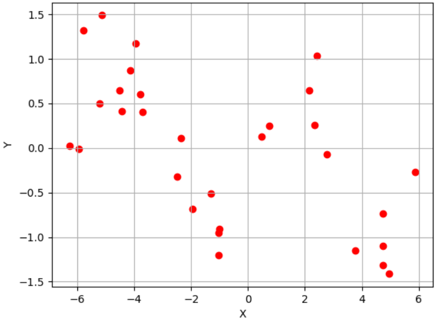

An example: linear regression model

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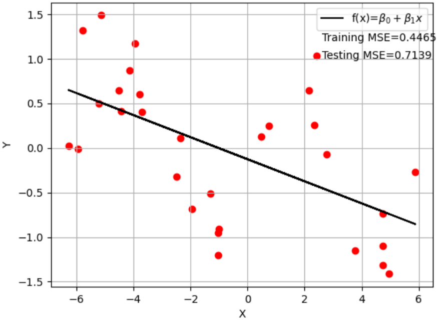

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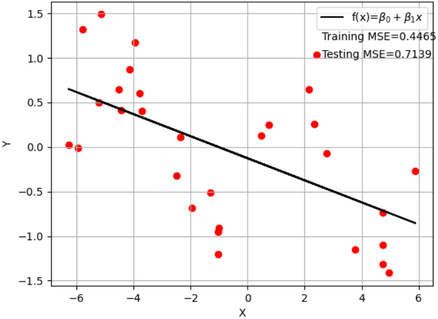

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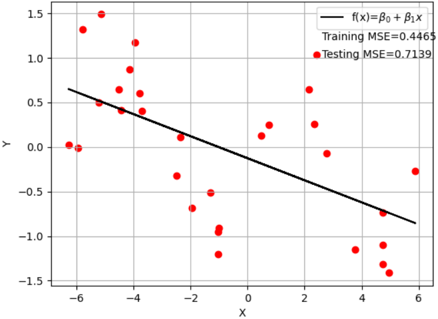
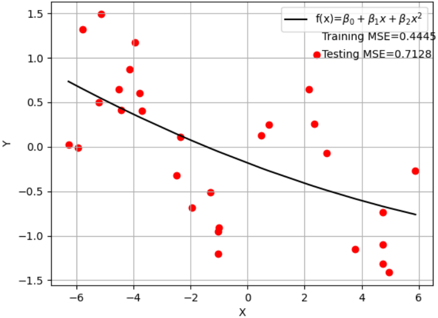


- Training MSE is 0.4465
- Testing MSE is 0.7139

An example: quadratic regression

- We fit a quadratic model $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2$



- Training MSE is 0.4445 (improve 0.0020)
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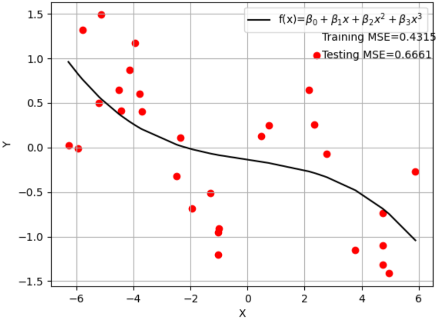

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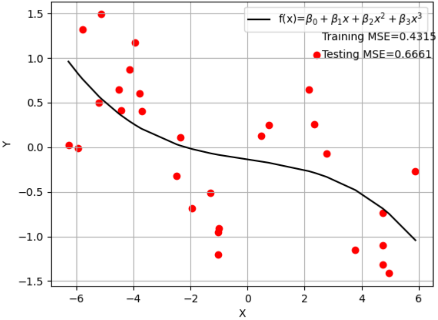

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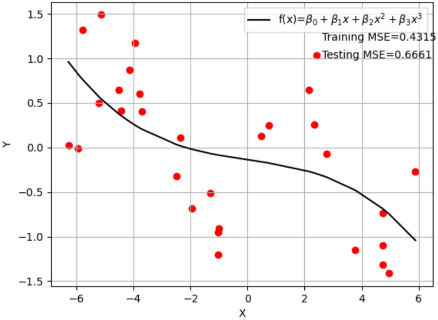
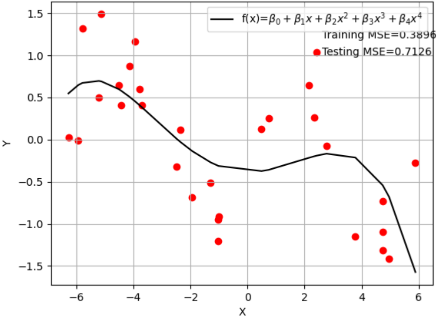


- Training MSE is 0.4315 (improve 0.0130)
- Testing MSE is 0.6661(improve by 0.0467)

An example: higher order polynomial

- We fit a polynomial model (with order 4)$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4$



- Training MSE is 0.3896 (improve 0.0419)
- Testing MSE is 0.7126 (increase by 0.0464): start fitting noise ratehr than signal....

An example: conclusion

Metrics	Model 1	Model 2	Model 3	Model 4
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- General questions: how to select the best fitting model from a bunch of candidate models?
- Use model validation!

Model validation

- **Training Set**: The training set is a subset of the dataset used to train the machine learning model. The model learns patterns, relationships, and features from this set.

Model validation

- **Validation Set**: The validation set is a separate subset of data that is not used for training the model. It is used during the training phase to assess the model's performance on data it has not seen before.

Model validation

- **Test Set**: The test set (or holdout set) is another independent subset of data that is not used during training or validation. It is reserved for the final evaluation of the model's performance after training is complete.
- In other words, we have three datasets: training, validation and testing.

Validation dataset

- **Validation dataset** is a sample of data held back from training your model that is used to give an *estimate of model performance* given the current model's hyperparameters, e.g., order of polynomial in f.

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  - D_r: training dataset (Fit your model using this dataset)
  - D_v: validation dataset (Evaluate your model using this dataset)

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- The true test error (testing MSE) is 0.2350 evaluated using the 268 testing samples

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- For each repetition, we further split the training dataset into "training" (350 samples) and validation (150 samples)
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- Compute the **validation error** (i.e., testing error computed based on the validation set) and compare it with the true testing error

Simulation

If we try training-validation split multiple times.

```
0.3133333 0.2350746
0.3000000 0.2350746
0.2600000 0.2350746
0.2933333 0.2350746
0.2800000 0.2350746
0.2666667 0.2350746
0.3466667 0.2350746
0.2933333 0.2350746
0.3200000 0.2350746
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```

- **Left**: Validation error and **Right**: True Testing error

Conclusion:

- Disadvantages of this approach:
  (1) the **validation error** (that supposed to approximate the test error) is **highly variable**, depending on how you split the dataset.

  (2) In the validation approach, only a subset of training set are used to fit the model (350 out of 500). Since statistical methods tend to perform worse when trained on fewer observations, this suggests that the validation error tends to **overestimate** the test error since the training set and testing set are often larger.

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- **Objective**: Estimate the test error associated with a given statistical learning method in order to
  - evaluate its performance with less variability (model assessment)
  - select the appropriate level of flexibility (select the best model or parameters)
- **Mechanism**: holding out a subset of the training observations from the fitting process and then applying the fitted model to those held out observations.

K-Fold Cross-Validation

- **K-Fold Cross-Validation**: The dataset is divided into K subsets (or folds). The model is trained on K-1 folds and validated on the remaining fold. This process is repeated K times, with each fold serving as the validation set exactly once.

Stratified K-Fold Cross-Validation

- **Stratified K-Fold Cross-Validation**: Similar to K-Fold, but the data is divided into K folds while ensuring that each fold maintains the same class distribution as the original dataset. This is particularly useful for imbalanced datasets (to be covered in week 5).

Leave-One-Out Cross-Validation

- **Leave-One-Out Cross-Validation (LOOCV)**: In LOOCV, only one data point is used for validation, and the model is trained on the remaining data. This process is repeated for each data point in the dataset. So, if there are 100 datapoints, we will repeat this procedure 100 times.

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- Computationally expensive (or even infeasible) when the number of observations in the training data is large. Except if you are using linear regression (where an explicit formula is available).
- The validation MSE from LOOCV is based on averaging n individual fold-based error estimates. Each of these individual estimates is based on almost the same data. Therefore, these estimates are highly correlated with each other.

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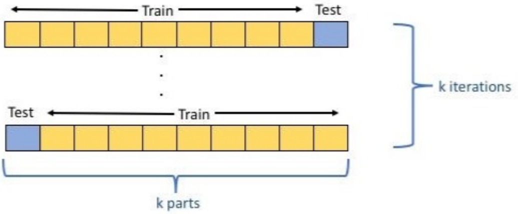
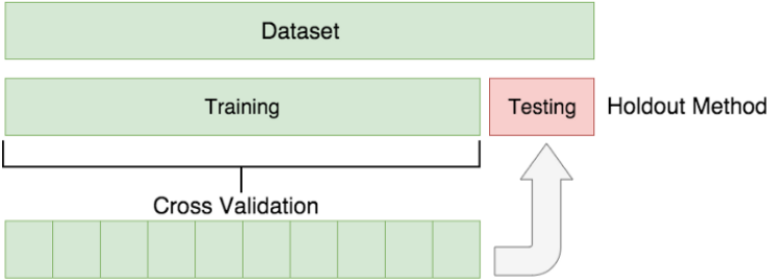


The complete picture on training, validation and testing



An example: 6-fold Cross-Validation

1 Suppose a dataset $D = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{6n}$ is given. We split it into 6 parts

$$D_1 = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}, D_2 = \{(\boldsymbol{x}_i, y_i)\}_{i=n+1}^{2n}, D_2 = \{(\boldsymbol{x}_i, y_i)\}_{i=2n+1}^{3n}$$
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2. We repeat the following step from $j = 1, 2, 3, 4, 5, 6$: (1) Construct a dataset $D_{-j} = \cup_{i \neq j} D_i$; (2) Train a function via

$$\widehat{f}_{-j} = \arg\min_{f \in \mathcal{F}} \frac{1}{5n} \sum_{i \in D_{-j}} (f(\boldsymbol{x}_i) - y_i)^2$$

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3. Compute the validation error of $\widehat{f}_{-j}, j = 1, \ldots, 6$

$$VE_j(\widehat{f}_{-j}) = \frac{1}{n} \sum_{i=(j-1)n+1}^{jn} (\widehat{f}_{-j}(\boldsymbol{x}_i) - y_i)^2$$

6-fold Cross-Validation: Procedure

4 Use the averaged validation errors as an estimate of testing error

$$\text{Testing Error Estimate} : \frac{1}{6}\sum_{j=1}^{6} VE_j(\widehat{f}_{-j})$$