

Linear Regression Models

Segment 4 – Model Diagnostics

Topic 1 – In-Sample Estimation of Prediction Error

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Topics



- 1. Prediction error
- 2. Train-Test-Validation Split
- 3. Validation
- 4. Testing
- 5. Linear Regression Example











true population relationship $Y = f(X) + \varepsilon$,





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• Prediction error:

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• The fitted model \hat{f} should minimize the *expected* prediction error on new unseen data.

Prediction error



• Recall the prediction problem and the associated error:

true population relationship
$$Y=f(X)+\varepsilon,$$
 using data build approximation $Y\approx \hat{f}(X).$

squared error
$$\left(Y-\hat{f}(X)\right)^2$$
 , absolute deviation $\left|Y-\hat{f}(X)\right|$.

- The fitted model \hat{f} should minimize the *expected* prediction error on new unseen data.
- How do we calculate the expected prediction error?





• Split data into three groups:



• Split data into three groups: (1) train









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data
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$$\underbrace{\left[\frac{\left(\mathbf{x}^{(1)},y^{(1)}\right),\ldots,\left(\mathbf{x}^{(k)},y^{(k)}\right)}{\mathsf{train}}}\right]}_{\mathsf{data}}$$





$$\underbrace{\left[\frac{\left(\mathbf{x}^{(1)},y^{(1)}\right),\ldots,\left(\mathbf{x}^{(k)},y^{(k)}\right)}{\mathsf{train}}}_{\mathsf{train}} \underbrace{\left(\mathbf{x}^{(k+1)},y^{(k+1)}\right),\ldots,\left(\mathbf{x}^{(l)},y^{(l)}\right)}_{\mathsf{validation}}$$

data





$$\underbrace{\left[\frac{\left(\mathbf{x}^{(1)},y^{(1)}\right),\ldots,\left(\mathbf{x}^{(k)},y^{(k)}\right)}{\mathsf{train}}}_{\mathsf{train}} \quad \underbrace{\left(\mathbf{x}^{(k+1)},y^{(k+1)}\right),\ldots,\left(\mathbf{x}^{(l)},y^{(l)}\right)}_{\mathsf{validation}} \quad \underbrace{\left(\mathbf{x}^{(l+1)},y^{(l+1)}\right),\ldots,\left(\mathbf{x}^{(n)},y^{(n)}\right)}_{\mathsf{test}}\right]}_{\mathsf{test}}$$

data



• Split data into three groups: (1) train (2) validation (3) test:

$$\underbrace{\begin{bmatrix} \mathbf{x}^{(1)}, y^{(1)} \end{pmatrix}, \dots, \mathbf{x}^{(k)}, y^{(k)} \end{pmatrix}}_{\text{train}} \quad \underbrace{\begin{pmatrix} \mathbf{x}^{(k+1)}, y^{(k+1)} \end{pmatrix}, \dots, \mathbf{x}^{(k)}, y^{(l)} \end{pmatrix}}_{\text{validation}} \quad \underbrace{\begin{pmatrix} \mathbf{x}^{(l+1)}, y^{(l+1)} \end{pmatrix}, \dots, \mathbf{x}^{(k)}, y^{(n)} \end{pmatrix}}_{\text{test}} \\ \mathbf{data}$$

• Build different models (\hat{f}) using training data.





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- Build different models (\hat{f}) using training data.
- Estimate prediction error for different models and pick the best one using validation data.



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- Build different models (\hat{f}) using training data.
- Estimate prediction error for different models and pick the best one using validation data.
- Finally, assess the best model's performance using test data.







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- Choose the model \hat{f}_{best} with the smallest estimated generalization error.
- Once we have the best model \hat{f}_{best} , what is the need for the test data?





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$$\frac{1}{n-l} \sum_{j=l+1}^{n} \left[y^{(j)} - \hat{f}_{\mathsf{best}} \left(\mathbf{x}^{(j)} \right) \right]^{2}.$$

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- The test data is used to obtain an unbiased estimate of the generalization error of the best model and assess its performance.







• We will simulate a dataset with 1000 samples:



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• We will simulate a dataset with 1000 samples: 750 train, 150 validation.



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Y~X_1	10.9	10.6	11.0



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$Y \sim X_1 + X_2 + I(X_1^2) + I(X_2^2)$	5.2	4.8	5.3

Summary



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 Describe how model performance can be studied using prediction error.

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- Describe how model performance can be studied using prediction error.
- Differentiate between train, test, and validation parts of the data for assessing model performance