MATH 829: Introduction to Data Mining and Analysis
Linear Regression: old and new (part 2)

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1. $E(\epsilon_i) = 0$.
2. $\mathrm{Var}(\epsilon_i) = \sigma^2 < \infty$.
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Note:

- (3) means that the errors are *uncorrelated*. In particular, (3) holds if the errors are independent.
- The errors need not be normal, nor independent, nor identically distributed.

Gauss–Markov (cont.)

Remarks: In our model $\mathbf{Y} = \mathbf{X}\beta + \epsilon$,

- $\mathbf{X}$ is fixed.
- ϵ is random.
- $\mathbf{Y}$ is random.
- β is fixed, but unobservable.

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A *linear* estimator of β, is an estimator of the form $\hat{\beta} = C\mathbf{Y}$, where $C = (c_{ij}) \in \mathbb{R}^{p \times n}$ is a matrix, and

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An estimator is *unbiased* if $E(\hat{\beta}) = \beta$.

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Ultimately, we want to use $\hat{\beta}$ to predict Y, i.e., $\hat{Y}_i = X_{i1}\hat{\beta}_1 + X_{i2}\hat{\beta}_2 + \cdots + X_{ip}\hat{\beta}_p$.

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We define the mean squared error (MSE) of a linear combination of the coefficients of $\hat{\beta}$ by

$$\mathrm{MSE}(a^T\hat{\beta}) = E\left[\left(\sum_{i=1}^{n} a_i(\hat{\beta}_i - \beta_i)\right)^2\right] \qquad (a \in \mathbb{R}^p).$$

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Theorem (Gauss–Markov theorem)

Suppose $\mathbf{Y} = \mathbf{X}\beta + \epsilon$ where ϵ satisfies the previous assumptions. Let $\hat{\beta} = C\mathbf{Y}$ be a linear unbiased estimator of β. Then for all $a \in \mathbb{R}^p$,

$$MSE(a^T\hat{\beta}_{LS}) \leq MSE(a^T\hat{\beta}).$$

We say that $\hat{\beta}_{\mathrm{LS}}$ is the **best linear unbiased estimator** (BLUE) of β.

The bias-variance tradeoff

Let $Z = a^T\beta$ and $\hat{Z} = a^T\hat{\beta}$. (Note: Z is non-random). Then

$$\begin{aligned}
MSE(a^T\hat{\beta}) &= E\left[(a^T(\hat{\beta}-\beta))^2\right] = E\left[(\hat{Z}-Z)^2\right] \\
&= E(Z^2 - 2Z\hat{Z} + \hat{Z}^2) \\
&= E(Z^2) - 2E(Z\hat{Z}) + E(\hat{Z}^2) \\
&= Z^2 - 2ZE(\hat{Z}) + \mathrm{Var}(\hat{Z}) + E(\hat{Z})^2 \\
&= \underbrace{(Z - E(\hat{Z}))^2}_{\text{bias}^2} + \underbrace{\mathrm{Var}(\hat{Z})}_{\text{variance}}.
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Therefore, $\mathrm{MSE} = \text{Bias-squared} + \text{Variance}.$

As a result, if $\hat{\beta}$ is unbiased, then $\mathrm{MSE}(a^T\beta) = \mathrm{Var}(\hat{Z})$.

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Proof. Let $\hat{\beta} = C\mathbf{Y}$ where $C = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + D$ for some $D \in \mathbb{R}^{p\times n}$. We will compute $E(\hat{\beta})$ and $\mathrm{Var}(a^T\hat{\beta})$.

$$\begin{aligned} E(\hat{\beta}) &= E\left[((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + D)\mathbf{Y}\right] \\ &= E\left[((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + D)(\mathbf{X}\beta + \epsilon)\right] \\ &= (I + D\mathbf{X})\beta. \end{aligned}$$

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We now compute $\mathrm{Var}(a^T\hat{\beta})$.

Gauss–Markov (cont.)

Recall:

$$\mathrm{Var}(a^T \hat{\beta}) = a^T \Sigma a,$$

where $\Sigma = (\mathrm{Cov}(\hat{\beta}_i, \hat{\beta}_j)) = \mathrm{Var}(\hat{\beta})$.

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Using these formulas, we obtain

$$\begin{aligned}
\mathrm{Var}(\hat{\beta}) &= \mathrm{Var}(C\mathbf{Y}) \\
&= C\,\mathrm{Var}(\mathbf{Y})C^T = \sigma^2 CC^T \\
&= \sigma^2((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + D)((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T + D)^T \\
&= \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1} \\
&\quad + \sigma^2\left[(\mathbf{X}^T\mathbf{X})^{-1}\underbrace{\mathbf{X}^T D^T}_{=(DX)^T=0} + \underbrace{D\mathbf{X}}_{=0}(\mathbf{X}^T\mathbf{X})^{-1} + DD^T\right] \\
&= \sigma^2\left[(X^TX)^{-1} + DD^T\right].
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Therefore,

$$\begin{aligned}\mathrm{Var}(a^T \hat{\beta}) = a^T(\sigma^2 (X^T X)^{-1} + \sigma^2 D D^T) a &\geq a^T \sigma^2 (X^T X)^{-1} a \\ &= \mathrm{Var}(a^T \hat{\beta}_{\mathrm{LS}}).\end{aligned}$$

This concludes the proof. □

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Moreover, according to the Gauss–Markov theorem, for every **unbiased estimator** $\hat{\beta}$,

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We can often increase the prediction accuracy by sacrificing a little bit of bias to reduce the variance of the estimator.
We will later examine some useful alternatives to least squares.

Training error and test error

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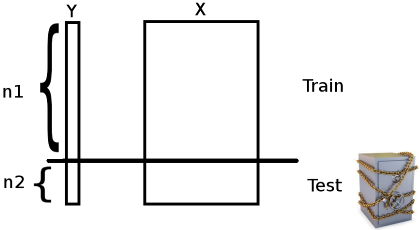
3. We use the fitted model to predict values of the test data and compute the **test error**.

Training error and test error (cont.)

Splitting data into training/test data:



In the case of least squares:

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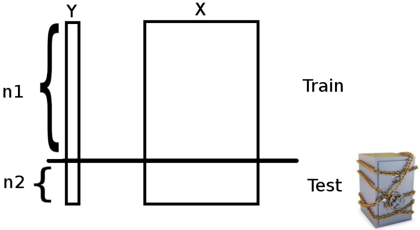

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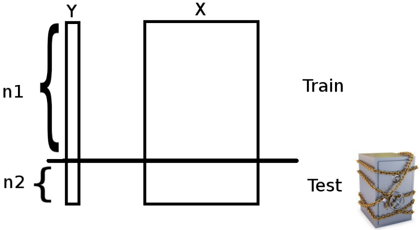

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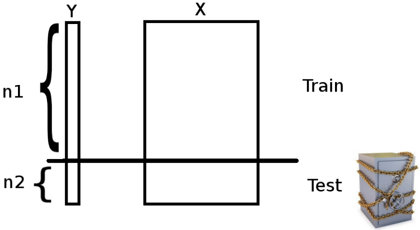

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3. Test error:

$$\text{MSE}_{\text{test}} = \frac{1}{n_2} \sum_{i=1}^{n_2} (\widehat{Y}_{\text{test},i} - Y_{\text{test},i})^2.$$

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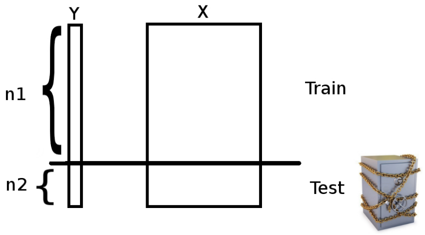

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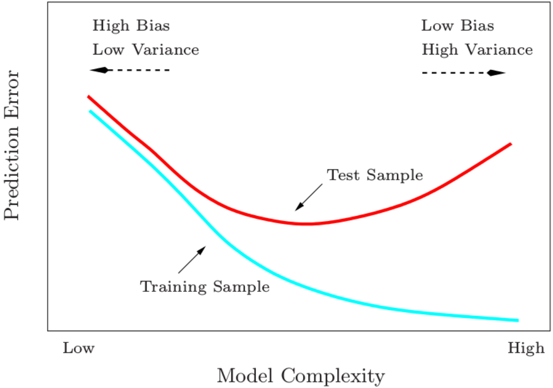
We choose a model that minimizes the test error.

Typical behavior of the test and training error, as model complexity is varied.



ESL, Fig 2.11.

Training sets and test sets (Python)

Scikit-learn provides a function to split the data automatically for us.

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```
from sklearn.cross_validation import train_test_split

# Split data into training and test sets
X_train, X_test, y_train, y_test =
  train_test_split(X, y, test_size=0.25,
  random_state=42)

# Fit model on training data
lin_model = LinearRegression(fit_intercept=True)
lin_model.fit(X_train,y_train)

# Returns the coefficient of determination R^2.
lin_model.score(X_test, y_test)
```

The coefficient of determination

- Regression models are often ranked using the *coefficient of determination* called "R squared" and denoted R^2.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \overline{y})^2}.$$

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- We want a model with a **test** R^2 as close to 1 as possible.