MATH 637: Mathematical Techniques in Data Science
Linear Regression: old and new (part 2)

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

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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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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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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

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

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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} \\
&+ \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 will later examine some useful alternatives to least squares.

Training error and test error

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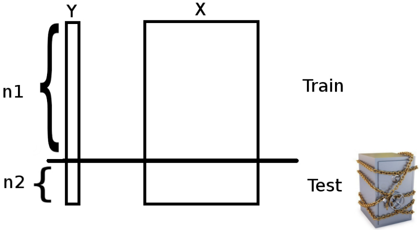
3. We use the fitted model to predict values of the test data and compute the **test error**.

Training error and test error (cont.)

Splitting data into training/test data:



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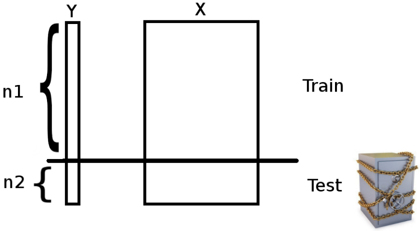

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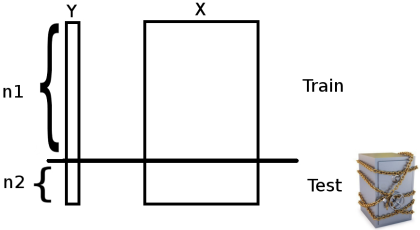

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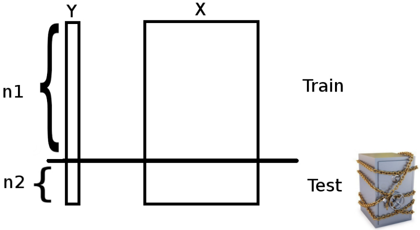

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$$\text{MSE}_{\text{test}} = \frac{1}{n_2} \sum_{i=1}^{n_2} (\widehat{Y}_{\text{test},i} - Y_{\text{test},i})^2.$$

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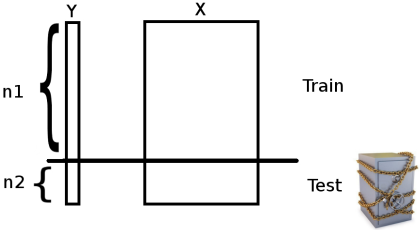

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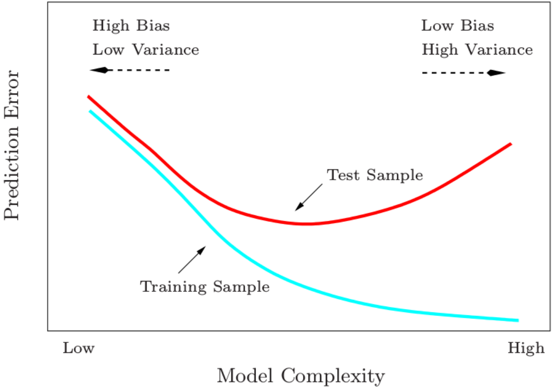
We choose a model that minimizes the test error.

Training error and test error (cont.)

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



ESL, Fig 2.11.

Training sets and test sets (Python)

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

- In some sense, the R^2 measures "how much better" is the prediction, compared to a constant prediction equal to the average of the $y_i s$.

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- The `score` method in `sklearn` returns the R^2.
- We want a model with a **test** R^2 as close to 1 as possible.

Lab - Part 1

- Load the Boston dataset. Read the description of the dataset.

```
from sklearn.datasets import load_boston
X, y = load_boston(return_X_y=True)
```

- Split the data into a training and a test set.

```
X_train, X_test, y_train, y_test =
train_test_split(X, y, test_size=0.25,
random_state=42)
```

- Fit the model on the training data.

```
lin_model = LinearRegression(fit_intercept=True)
lin_model.fit(X_train,y_train)
```

- Compute the mean squared error and the R^2 on the **test** data:

```
from sklearn.metrics import mean_squared_error
y_test_pred = lin_model.predict(X_test)
mean_squared_error(y_test, y_test_pred)
lin_model.score(X_test, y_test)
```

Lab - Part 2

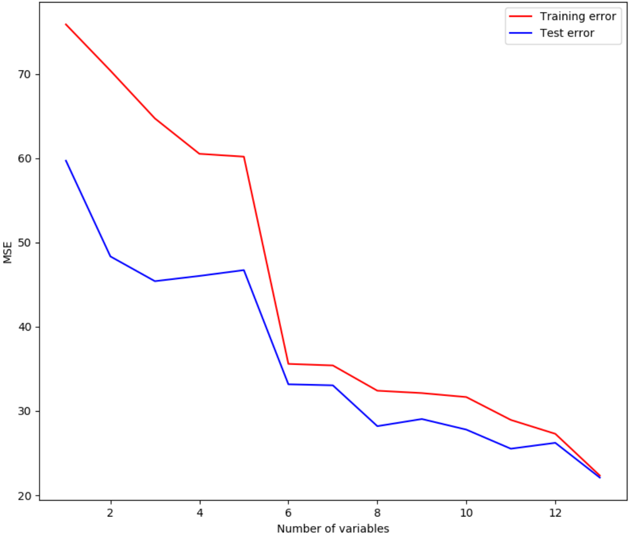
- Compute the training error and the test error obtained by using only the first i variables, for $i = 1, \ldots, 13$:

```
err_test = np.zeros(13)
err_train = np.zeros(13)

for i in range(13):
   X_train, X_test, y_train, y_test =
   train_test_split(X[:,0:i+1], y,
   test_size=0.25, random_state=42)
   lin_model = LinearRegression(fit_intercept=True)
   lin_model.fit(X_train,y_train)
etc...
```

- Plot the train and test error as a function of i.

Result



Training error
Test error
MSE
70
60
50
40
30
20
2
4
6
8
10
12
Number of variables