

Generalization. Out of Sample Performance.

Big Data y Machine Learning para Economía Aplicada

Ignacio Sarmiento-Barbieri

Universidad de los Andes

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Predicting Well

$$y = f(X) + u \quad (1)$$

- Interest on predicting y

Linear Regression

$$y = f(X) + u \quad (2)$$

$$= \beta_0 + \beta_1 X_1 + \cdots + \beta_k X_k + u \quad (3)$$

- ▶ If $f(X) = X\beta$, obtaining $f(\cdot)$ boils down to obtaining β
- ▶ We learn these β s by minimizing a loss function on the sample.

Linear Regression

- Quadratic loss \rightarrow OLS

$$\mathcal{L}(\beta) = \frac{1}{n} \sum_{i=1}^n (y_i - f_{\beta}(X_i))^2 \quad (4)$$

$$= \sum_{i=1}^n \left(y_i - \hat{\beta}_0 - \sum_{j=1}^k \hat{\beta}_j x_{ji} \right)^2 \quad (5)$$

- Compute β s using sample data
 - QR
 - SVD
 - Gradient Descent

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Generalization Overview

- ▶ In ML we care in out-of-sample prediction
- ▶ Generalization refers to a model's performance on unseen data.
- ▶ The ultimate goal is **not** minimizing the in-sample loss, but achieving low error out-of-sample on unseen data.

Training and Test Loss

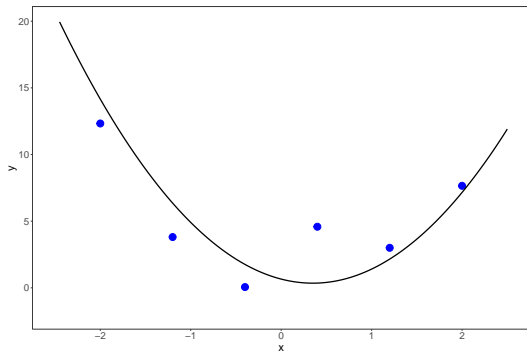
- ▶ Unseen data is typically referred as **test data**,
- ▶ While the sample data is called the **training data**.
- ▶ The expected loss over the test distribution is called the test loss.
- ▶ Test risk is defined as:

$$\mathbb{E}_{(X,y) \sim F}[(y - f_{\beta}(X))^2]$$

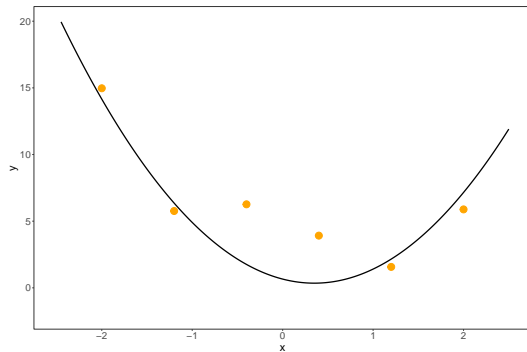
Overfitting and Underfitting

- ▶ Successfully minimizing training error does not always result in a small test error.
- ▶ A model is said to overfit if it predicts accurately on training data but poorly on test (unseen) data.
- ▶ A model underfits if its training error is relatively large, which usually means test error is also large.
- ▶ Understanding overfitting and underfitting helps in choosing appropriate model parameterizations.

Overfitting and Underfitting. Bias-Variance Tradeoff



(a) Training Data



(b) Testing Data

Overfitting and Underfitting. Bias-Variance Tradeoff

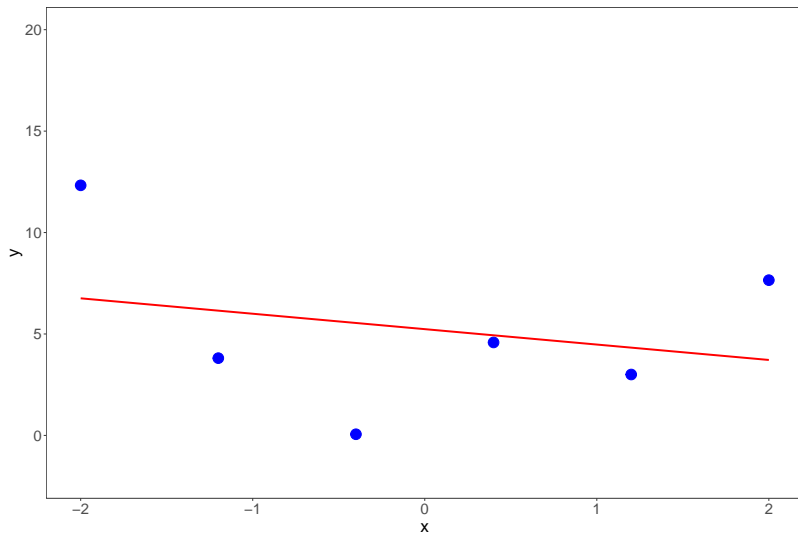
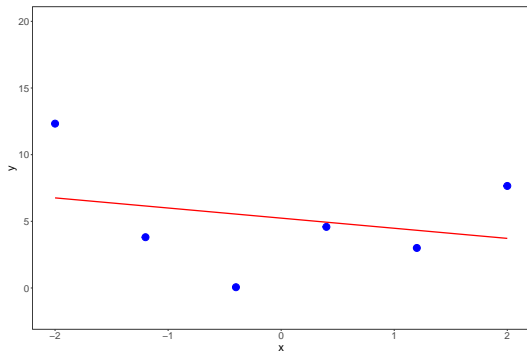


Figure 2: Training Data

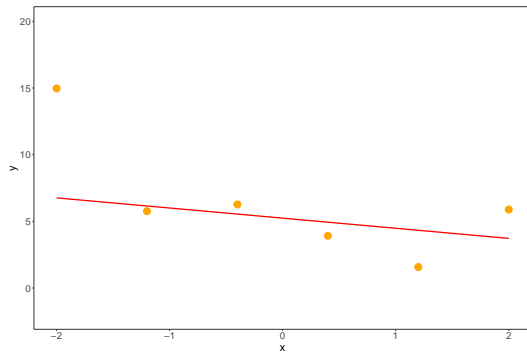
Generalization. Out of Sample Performance.

Overfitting and Underfitting. Bias-Variance Tradeoff

Out-of-Sample Performance



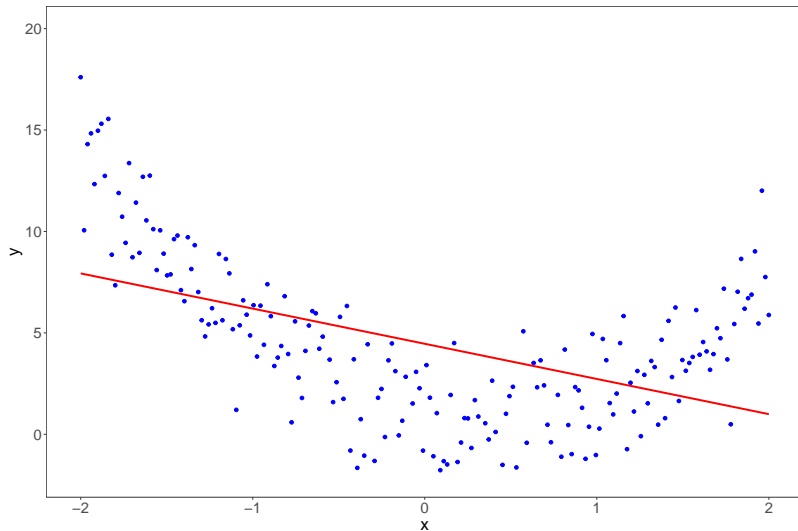
(a) Training Data



(b) Testing Data

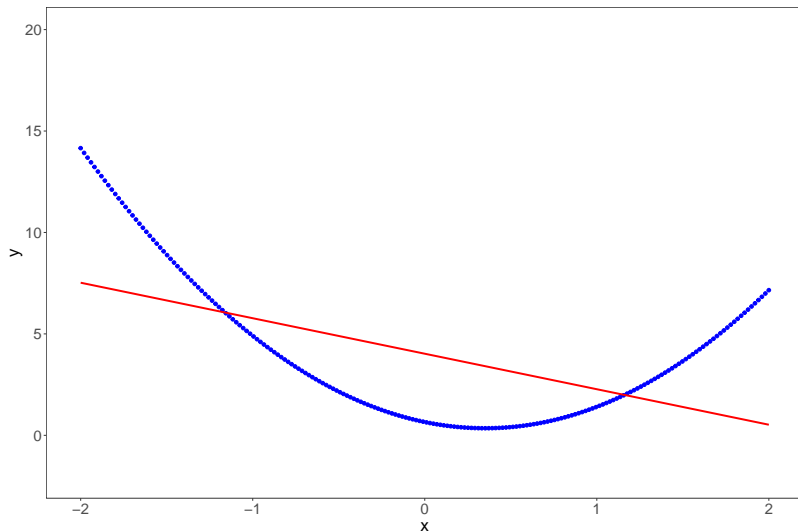
Overfitting and Underfitting. Bias-Variance Tradeoff

More data?



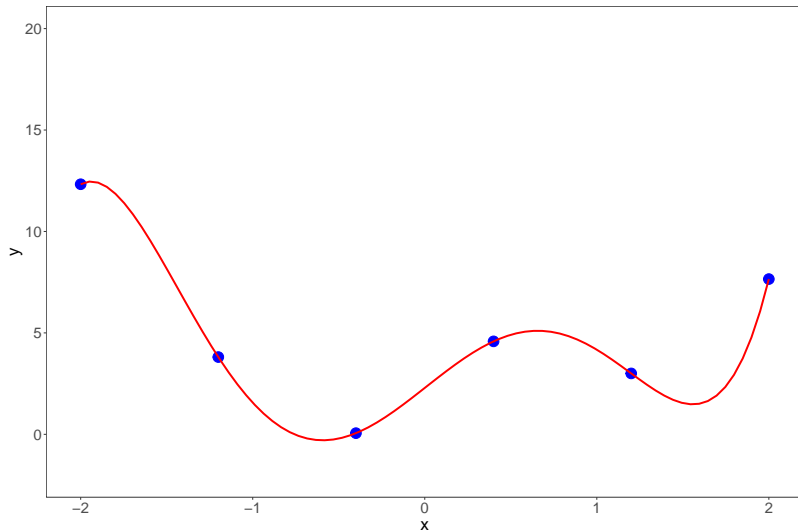
Overfitting and Underfitting. Bias-Variance Tradeoff

Noiseless data?



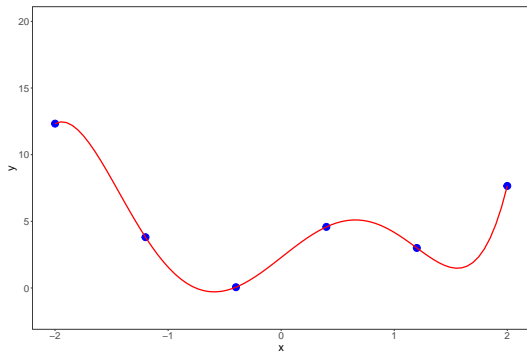
Overfitting and Underfitting. Bias-Variance Tradeoff

More Complex Model

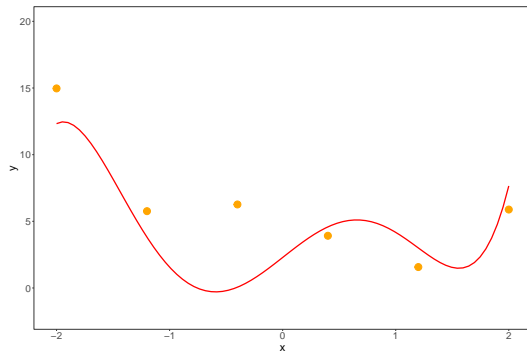


Overfitting and Underfitting. Bias-Variance Tradeoff

Out-of-Sample Performance



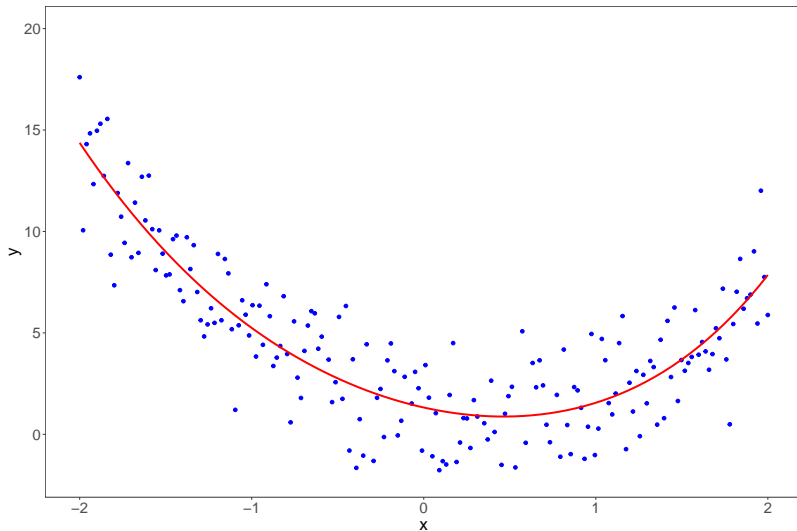
(a) Training Data



(b) Testing Data

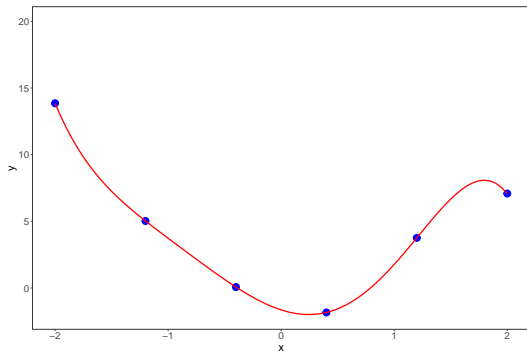
Overfitting and Underfitting. Bias-Variance Tradeoff

More Data

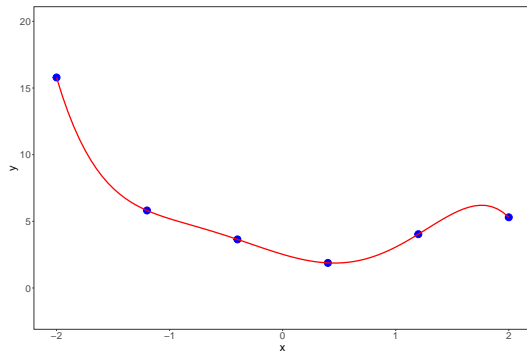


Overfitting and Underfitting. Bias-Variance Tradeoff

Variance



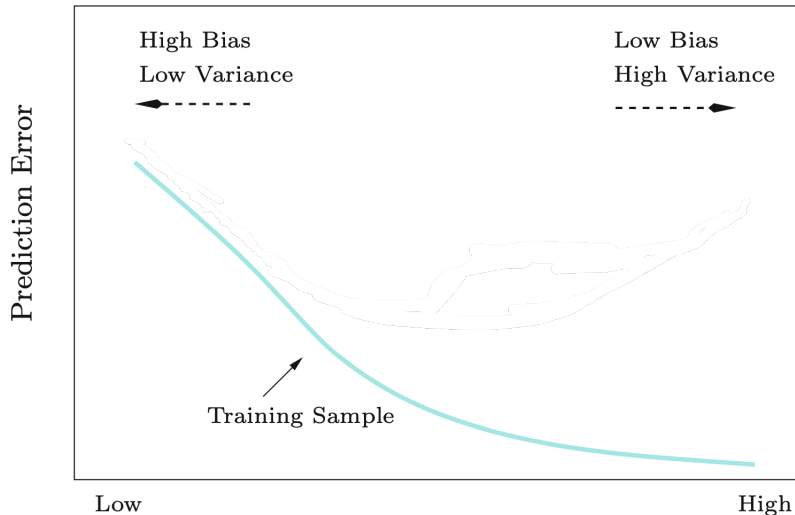
(a) Training Data 2



(b) Training Data 3

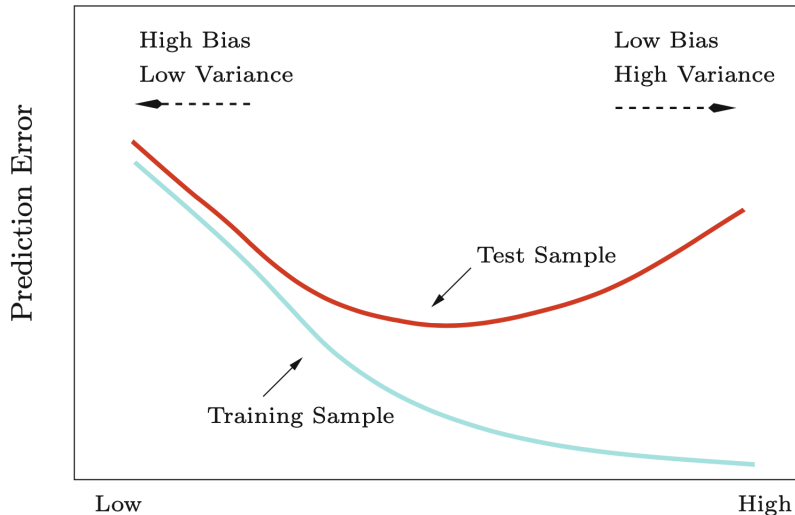
Overfitting and Underfitting. Bias-Variance Tradeoff

In-Sample Prediction and Overfit



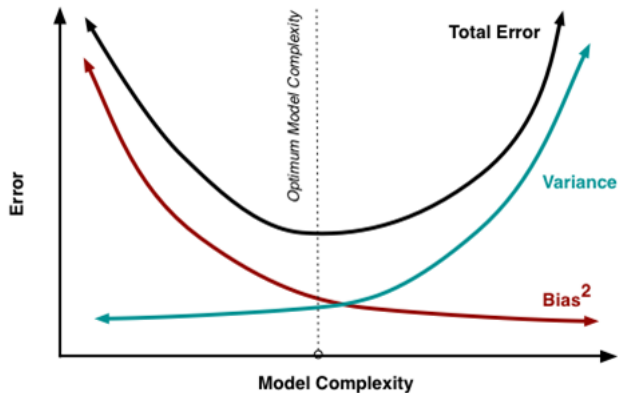
Overfitting and Underfitting. Bias-Variance Tradeoff

Out-of-Sample Prediction and Overfit



Mathematical Decomposition for Regression

Bias-Variance Tradeoff



Source: <https://tinyurl.com/y4lvjxpc>

- ML best kept secret: By tolerating some bias we can have significant gains in variance

Example polynomial revisited

- ▶ Suppose that the true model is $y = f(X) + u$
 - ▶ f is a polynomial of degree p^*
 - ▶ p^* is finite but unknown
 - ▶ $E(u) = 0$ and $V(u) = \sigma^2$
- ▶ We fit polynomials with increasing degrees $p = 1, 2, \dots$
- ▶ What happens when we increase the degree of the polynomial?

Example polynomial revisited

- The expected prediction error of a regression fit $\hat{f}(X)$ at a point $X = x_0$, is

$$\begin{aligned}MSE(x_0) &= MSE(y - \hat{f}(x_0) | X = x_0) \\ &= Bias^2(f, \hat{f}(x_0)) + V(\hat{f}(x_0)) + Irreducible\ Error\end{aligned}\tag{6}$$

Example polynomial revisited

► Bias ?

Example polynomial revisited

- ▶ Bias ?
- ▶ Variance?

Example polynomial revisited

- ▶ Bias ?
- ▶ Variance?
- ▶ Trace.
 - ▶ If $A_{m \times m}$ with typical element a_{ij} . The **trace** of A, $tr(A)$ is the sum of the elements of its diagonal: $tr(A) \equiv \sum_{s=1}^m a_{ss}$
 - ▶ Properties
 - ▶ For any square matrices A, B, and C: $tr(A + B) = tr(A) + tr(B)$
 - ▶ Cyclic property: $tr(ABC) = tr(BCA) = tr(CAB)$
 - ▶ If $m = 1$ $tr(A)=A$

Key Insights on Bias-Variance Tradeoff

- ▶ The bias term reflects the error introduced by the model's inability to approximate the true function f^* .
- ▶ The variance term reflects the sensitivity of the model to the specific training set.
- ▶ As dataset size increases, variance generally decreases.
- ▶ The noise term σ^2 is unavoidable and cannot be predicted.
- ▶ The decomposition for classification problems is less clear than for regression problems, but still present.

Agenda

- ① Review
- ② Generalization. Out-of-sample Performance
- ③ Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- ④ Review

Train and Test Sets. In-Sample and Out-of-Sample Prediction.

- ▶ Como seleccionamos la parametrización que minimize el error de predicción fuera de muestra?
- ▶ Problema: solo contamos con una muestra

Test Error

- ▶ Para seleccionar la mejor parametrización con respecto al Test Error (error de prueba), es necesario estimarlo.
- ▶ Hay dos enfoques comunes:
 - ▶ Podemos estimar indirectamente el error de la prueba haciendo un ajuste al error de entrenamiento para tener en cuenta el sesgo debido al sobreajuste \Rightarrow Penalización ex post: AIC, BIC, etc.

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Test Error

AIC

- ▶ Akaike (1969) fue el primero en ofrecer un enfoque unificado al problema de la selección de modelos.
- ▶ Elegir el modelo j tal que se minimice:

$$AIC(j) = \log \left(\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y})^2 \right) - p_j \quad (7)$$

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Test Error

SIC/BIC

- ▶ Schwarz (1978) mostró que el AIC es inconsistente, (cuando $n \rightarrow \infty$, tiende a elegir un modelo demasiado grande con probabilidad positiva)
- ▶ Schwarz (1978) propuso:

$$SIC(j) = \log \left(\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y})^2 \right) - \frac{1}{2} p_j \log(n) \quad (8)$$

Test Error

AIC vs BIC

$$AIC(j) = \log \left(\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y})^2 \right) - p_j \quad (9)$$

$$SIC(j) = \log \left(\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y})^2 \right) - p_j \frac{1}{2} \log(n) \quad (10)$$

Test Error

- ▶ Para seleccionar la mejor parametrización con respecto al Test Error (error de prueba), es necesario estimarlo.
- ▶ Hay dos enfoques comunes:
 - ▶ Podemos estimar indirectamente el error de la prueba haciendo un ajuste al error de entrenamiento para tener en cuenta el sesgo debido al sobreajuste \Rightarrow Penalización ex post: AIC, BIC, etc.
 - ▶ Levantarnos de nuestros bootstraps (resampling methods) y estimar directamente el Test Error (error de prueba)

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Test Error

Cross-Validation



photo from <https://www.dailydot.com/parsec/batman-1966-labels-tumblr-twitter-vine/>

Agenda

- 1 Review
- 2 Generalization. Out-of-sample Performance
- 3 Out-of-Sample Error Estimation
 - AIC: Akaike Information Criterion
 - SIC/BIC: Schwarz/Bayesian Information Criterion
 - Cross-Validation
- 4 Review

Review

Hoy

- ▶ Bias-Variance Tradeoff (Dilema Sesgo/Varianza)
- ▶ Sobreajuste y Selección de modelos
 - ▶ AIC y BIC
 - ▶ Enfoque de Validación
 - ▶ LOOCV
 - ▶ K-fold Cross-Validation (Validación Cruzada)