Model Evaluation through a Monte Carlo Experiment
Machine Learning Concepts
CEU, Winter 2024

1. The goal of this problem is to conduct Monte Carlo simulations about the mean squared error of various regression models.

   a) Let X_1, X_2 and X_3 be independent uniform[0,2] variables and let $\epsilon \sim N(0,1)$, independent of $X = (X_1, X_2, X_3)$. Generate $n = 500$ observations on these variables and compute the corresponding outcomes from the model

   $$Y_i = X_{1i}^3 - 3.5X_{1i}^2 + 3X_{1i} + \epsilon_i, \qquad i = 1, \ldots, n.$$

   Note that $f(X) = f(X_1) = X_1^3 - 3.5X_1^2 + 3X_1$, i.e., the predictors X_2 and X_3 are useless (irrelevant).

   b) Estimate three different regression models using the data generated under part a) as the training sample:

   - Model 1: The OLS regression of Y on a constant and X_1
   - Model 2: The OLS regression of Y on a constant, X_1, X_1^2 and X_1^3
   - Model 3: The OLS regression of Y on a constant, X_1, X_2, X_3, and all powers and cross-products of order 2 and 3. (This means all terms of the form $X_1^a X_2^b X_3^c$ where $a, b, c \in \{0, 1, 2\}$ and $a + b + c = 2$ or $a + b + c = 3$.)

   c) Compute the estimate $\hat{f}_m(x)$ from each model $m = 1, 2, 3$ for $x = (0.1, 0, 0)$ and $x = (1.1, 0, 0)$. Compute the true value $f(x)$.

   d) Repeat steps a) through c) many times, say, $R = 5000$. Then you'll have R possible estimates $\hat{f}_m(x)$ from each model for the two value of x. Compute $bias[\hat{f}_m(x)]$, $Var[\hat{f}_m(x)]$ and $MSE[\hat{f}_m(x)] = bias^2[\hat{f}_m(x)] + Var[\hat{f}_m(x)]$ for all models and x. Organize your results into a table.

   e) Pick 10 of your training samples and produce three separate figures where you plot the 10 estimates $x_1 \mapsto \hat{f}_m(x_1, 0, 0)$ over a fine grid of x_1 values (go from 0 to

2 in small steps) for $m = 1, 2, 3$. Add the plot of $f(x_1, 0, 0)$ to each figure. This will help you visualize and understand the results under part d).

f) Interpret the results you have obtained under part d) and e). Discuss bias-variance tradeoff, underfit, overfit, etc.