FYS-STK4155 Week 36

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Exercise 1

Show that

$$\mathbb{E}[(\boldsymbol{y}-\tilde{\boldsymbol{y}})^2] = \mathrm{Bias}[\tilde{\boldsymbol{y}}] + \mathrm{Var}[\tilde{\boldsymbol{y}}] + \sigma^2$$

where $\boldsymbol{y}$ is defined by $\boldsymbol{y} = f(\boldsymbol{x}) + \boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon} \sim N(0, \sigma^2)$ is a normal distributed error and $f(\boldsymbol{x})$ is the approximated function given our model $\tilde{\boldsymbol{y}}$ obtained by minimizing $(\boldsymbol{y}-\tilde{\boldsymbol{y}})^2$ with $\tilde{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\beta}$. Explain what the terms mean and discuss their interpretations. Perform then a bias-variance analysis of a simple one-dimensional function by studying the MSE value as a function of the complexity of your model. Use OLS only. Discuss the bias and variance trade-off as function of your model complexity (the degree of the polynomial) and the number of data points. **Solution:**
For ease of notation we write $f(\boldsymbol{x}) = f$ and simply ignore vector notation since everything is a scalar in the end. Then we have

$$\begin{aligned}
\mathbb{E}[(\boldsymbol{y}-\tilde{\boldsymbol{y}})^2] = \mathbb{E}[(f+\boldsymbol{\varepsilon}-\tilde{\boldsymbol{y}})^2] &= \mathbb{E}[(f-\tilde{\boldsymbol{y}})^2] + 2\underbrace{\mathbb{E}[(f-\tilde{\boldsymbol{y}})\boldsymbol{\varepsilon}]}_{=0} + \underbrace{\mathbb{E}[\boldsymbol{\varepsilon}^2]}_{=\sigma^2} \\
&= \mathbb{E}[((f-\mathbb{E}[\tilde{\boldsymbol{y}}]) - (\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{\boldsymbol{y}}]))^2] + \sigma^2 \\
&= \mathbb{E}[(f-\mathbb{E}[\tilde{\boldsymbol{y}}]))^2] + \mathbb{E}[(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{\boldsymbol{y}}])^2] - 2\,\mathbb{E}[((f-\mathbb{E}[\tilde{\boldsymbol{y}}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{\boldsymbol{y}}]))] + \sigma^2 \\
&= \mathrm{Bias}[\tilde{\boldsymbol{y}}] + \mathrm{Var}[\tilde{\boldsymbol{y}}] + \sigma^2 - 2\,\mathbb{E}[(f-\mathbb{E}[\tilde{\boldsymbol{y}}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{\boldsymbol{y}}])]
\end{aligned}$$

where $\mathbb{E}[(f-\tilde{\boldsymbol{y}})\boldsymbol{\varepsilon}] = 0$ is justified by $\boldsymbol{\varepsilon}$ being independent and we note that the wrong definition of the Bias is given in the problem text (with that definition σ^2 gets put into the 'Bias'). All that remains is to show that the last term is 0. Since $\mathbb{E}[f] = f$ and $\mathbb{E}[f\,\mathbb{E}[\tilde{\boldsymbol{y}}]] = f\,\mathbb{E}[\mathbb{E}[\tilde{\boldsymbol{y}}]] = f\,\mathbb{E}[\tilde{\boldsymbol{y}}]$ then

$$\begin{aligned}
\mathbb{E}[(f-\mathbb{E}[\tilde{y}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])] &= \mathbb{E}[f\tilde{\boldsymbol{y}} - f\,\mathbb{E}[\tilde{\boldsymbol{y}}] - \tilde{\boldsymbol{y}}\,\mathbb{E}[\tilde{y}] + \mathbb{E}^2[\tilde{\boldsymbol{y}}]] \\
&= f\,\mathbb{E}[\tilde{\boldsymbol{y}}] - f\,\mathbb{E}[\tilde{\boldsymbol{y}}] - \mathbb{E}^2[\tilde{\boldsymbol{y}}] + \mathbb{E}^2[\tilde{\boldsymbol{y}}] = 0
\end{aligned}$$

Since I have already written it in down I just want to quickly show why (I believe at least) the definition given in the problem text is wrong:

$$\begin{aligned}
\mathbb{E}[(\boldsymbol{y}-\tilde{\boldsymbol{y}})^2] &= \mathbb{E}[((\boldsymbol{y}-\mathbb{E}[\tilde{y}]) - (\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}]))^2] \\
&= \mathbb{E}[(\boldsymbol{y}-\mathbb{E}[\tilde{y}])^2] + \mathbb{E}[(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])^2] - 2\,\mathbb{E}[(\boldsymbol{y}-\mathbb{E}[\tilde{y}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])] \\
&\underbrace{=}_{\text{wrong}} \mathrm{Bias}[\tilde{\boldsymbol{y}}] + \mathrm{Var}[\tilde{\boldsymbol{y}}] - 2\,\mathbb{E}[(\boldsymbol{y}-\mathbb{E}[\tilde{y}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])]
\end{aligned}$$

Then we have

$$\begin{aligned}\mathbb{E}[(\boldsymbol{y}-\mathbb{E}[\tilde{y}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])] &= \mathbb{E}[(f+\boldsymbol{\varepsilon}-\mathbb{E}[\tilde{y}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])] \\ &= \mathbb{E}[(f-\mathbb{E}[\tilde{y}])(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])]+\mathbb{E}[\boldsymbol{\varepsilon}(\tilde{\boldsymbol{y}}-\mathbb{E}[\tilde{y}])]\end{aligned}$$

I have already shown explicitly that the first term is 0 and the second term is 0 due to the same reasons as above. So with this definition we would get the wrong result that

$$\mathbb{E}[(\boldsymbol{y}-\tilde{\boldsymbol{y}})^2] = \mathrm{Bias}[\tilde{\boldsymbol{y}}] + \mathrm{Var}[\tilde{\boldsymbol{y}}]$$