5. Generalization and regularization

Outline

Generalization

Model selection

- two models, A and B, are learned on the same training dataset.
- model A has an error of 0.1 on the training set and model B has an error of 1.0.
- which model is better?

Model selection

- two models, A and B, are learned on the same training dataset.
- model A has an error of 0.1 on the training set and model B has an error of 1.0.
- which model is better?
- answer: unknown.
- training error is not a good metric for comparing and selecting models

Test error

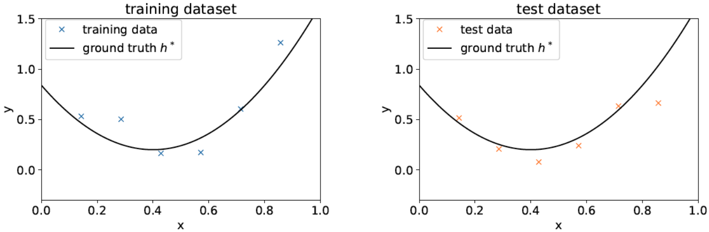
- to compare models, we need to evaluate them on a test set
- the error on the test set is called the **test error**
- measures whether the model generalizes to well to unseen data
- the ultimate goal of machine learning is to minimize the test error, not the training error.
- minimizing the training error is merely an approach towards the goal.
- reducing the training error does not necessarily always reduce the test error
- can be decomposed into three components: bias, variance, and irreducible error

Underfits and overfits

- underfits
  - when both the training and test errors are high
  - cannot make accurate predictions on the training set
  - model being too simple to capture the underlying structure of the data
- overfits
  - when the training error is much lower than the test error
  - make accurate predictions on the training set but not on the test set
  - model being too flexible and captures noise in the training data
- both are related to the bias-variance decomposition of the test error

Bias-variance tradeoff

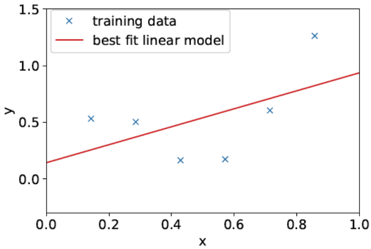
- an example of regression from `https://cs229.stanford.edu/main_notes.pdf`
- the ground true: $y^{(i)} = h^*(x^{(i)}) + \xi^{(i)}$
- h^* is a quadratic function and $\xi^{(i)} \sim N(0, \sigma^2)$ is the noise.

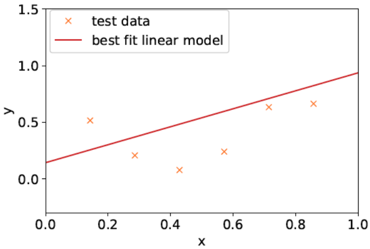


- goal: learn a model $h(x)$ to approximate h^* using training data

Underfits

- fit a linear model with limited noisy data

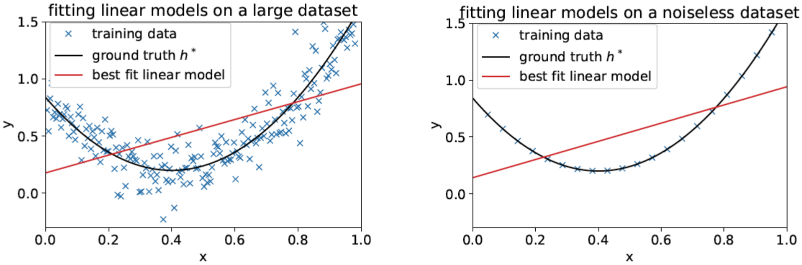




- both training and test errors are large

Underfits

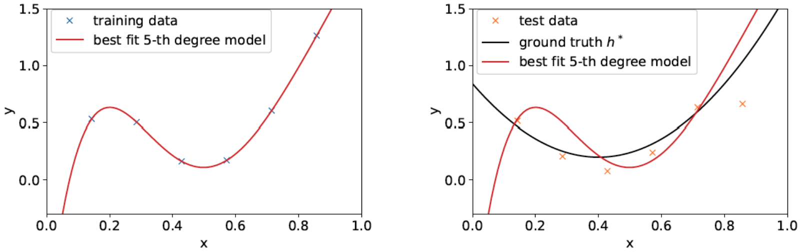
- fit a linear model with more or noiseless data



- using more training data does not help reduce either error
- the **bias** of a model is the test error when the model is trained on a very (infinitely) large training set
- models that underfit the data have high bias

Overfits

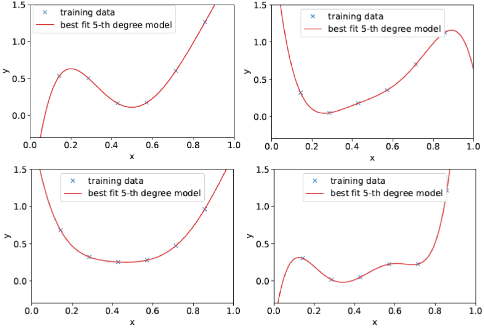
- fit a 5-th degree polynomial with noisy data



- very small (zero) training error but large test error
- the model is so flexible that it even fits the patterns in training data that is due to noise

Overfits

- fit a 5-th degree polynomial on different training sets

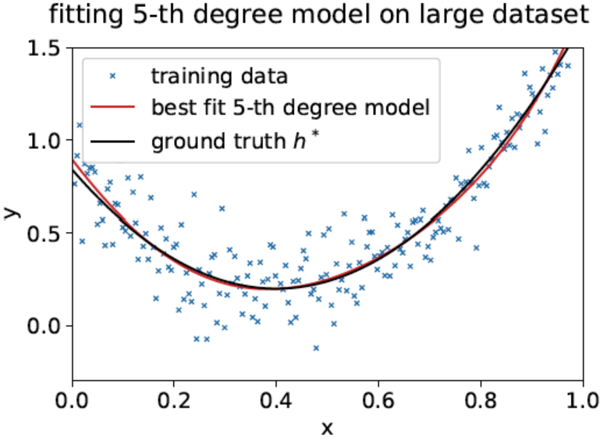


- the model fits the noise in the training set, but the noise could be different in different training sets

- the **variance** of a model is the amount of variations across models trained on different training sets

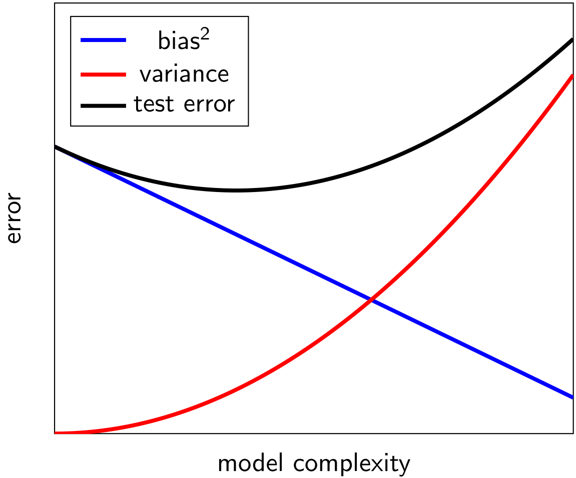
Overfits

- fit a 5-th degree polynomial with more data



- large training set helps reduce the variance of the model

Bias-variance tradeoff



The bias-variance decomposition for regression

- Draw a training dataset $S = \{(x^{(i)}, y^{(i)})\}_{i=1}^{n}$ such that $y^{(i)} = h^{\star}(x^{(i)}) + \xi^{(i)}$ where $\xi^{(i)} \in N(0, \sigma^2)$
- Train a model on the dataset S, denoted by $\hat{h}_S$.
- Take a test example (x, y) such that $y = h^{\star}(x) + \xi$ where $\xi \sim N(0, \sigma^2)$,
- the expected test error (averaged over the random draw of the training set S and the randomness of ξ):

$$\mathsf{MSE}(x) = \mathbb{E}_{S,\xi}\left[(y - h_S(x))^2\right]$$

The bias-variance decomposition

- conceptually useful for understanding what contributes to the test error

$$
\begin{aligned}
\mathsf{MSE}(x) &= \mathbb{E}\left[(y - h_S(x))^2\right] \\
&= \mathbb{E}\left[\left(\xi + (h^\star(x) - h_S(x))\right)^2\right] \\
&= \mathbb{E}\left[\xi^2\right] + \mathbb{E}\left[\left(h^\star(x) - h_S(x)\right)^2\right] \\
&= \sigma^2 + \mathbb{E}\left[\left(h^\star(x) - h_S(x)\right)^2\right] \\
&= \sigma^2 + \left(h^\star(x) - h_{\mathsf{avg}}(x)\right)^2 + \mathbb{E}\left[\left(h_{\mathsf{avg}}(x) - h_S(x)\right)^2\right] \\
&= \underbrace{\sigma^2}_{\text{unavoidable}} + \underbrace{\left(h^\star(x) - h_{\mathsf{avg}}(x)\right)^2}_{\triangleq \text{bias}^2} + \underbrace{\mathrm{var}(h_S(x))}_{\triangleq \text{variance}}
\end{aligned}
$$

- in practice, the bias and variance are not directly computable

Model selection in practice

- in practice, we do not have access to the true underlying function $h^\star$
- when training data is limited, we cannot estimate $h_{\mathsf{avg}}(x)$ or var$(h_S(x))$ accurately
- the bias-variance decomposition is a conceptual tool for understanding the test error
- there are more practical ways to estimate the test error and select models

Model selection in practice

- the most common approach is to split the dataset into training, validation, and test sets

- the training set is used to train models
- the validation set is used to estimate the test error and select models
- the test set is used to evaluate the final model; should be kept in a "vault" and be brought out only at the end of evaluating the model
- if the test set is used repeatedly to select models with smallest test error, the test error of the final chosen model will underestimate the true test error