DATASCI 347 Machine Learning

Lecture 2: Bias-variance decomposition

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Suggested reading: ISL Chapter 2

Lecture plan

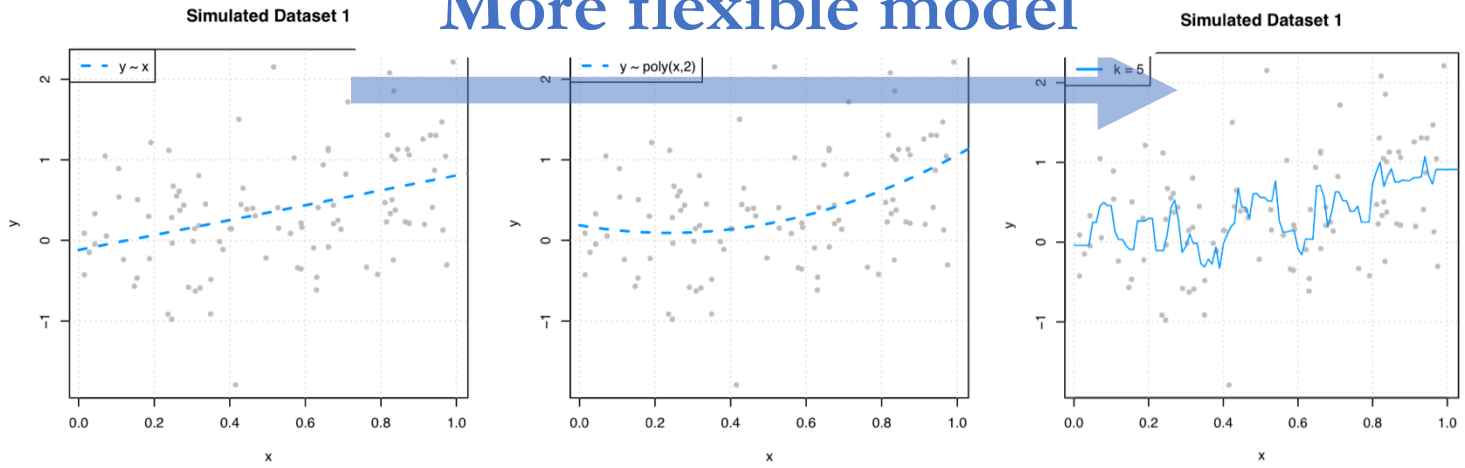
- Bias-variance decomposition for regression problems (MSE)

Training vs. test data and MSE

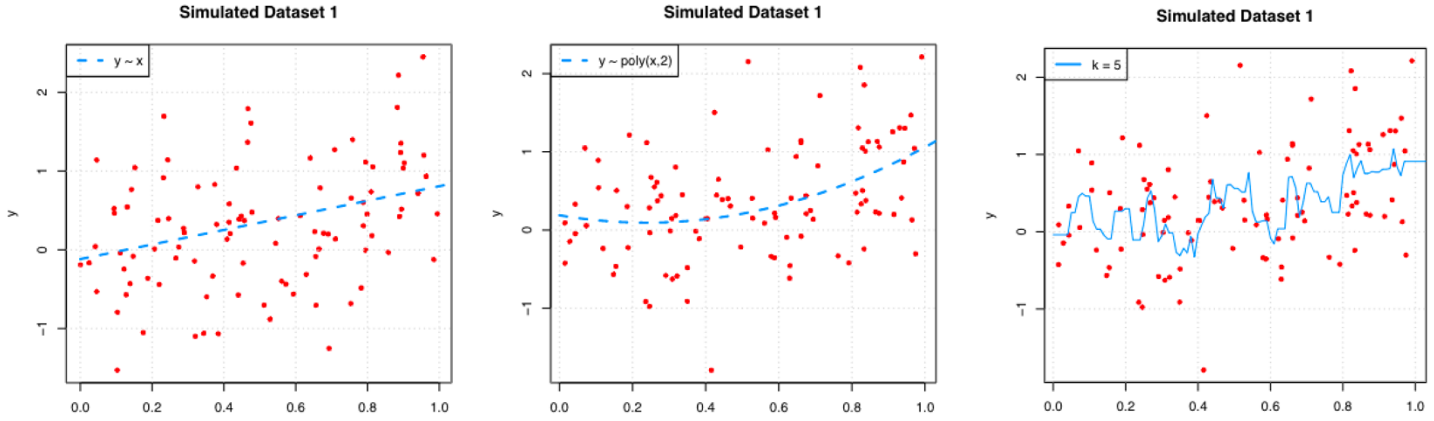
- **Training data**: data $(X_1, Y_1), (X_2, Y_2), \cdots, (X_n, Y_n)$ used to fit f
- **Training MSE**: $\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{f}(X_i))^2$
- **Test data**: data, $(X_1', Y_1'), (X_2', Y_2'), \ldots, (X_m', Y_m')$ previous unseen and *not used* to fit f
- **Test MSE**: $\text{MSE} = \frac{1}{m}\sum_{i=1}^{m}(Y_i' - \hat{f}(X_i'))^2$
- We care **more about test MSE** than training MSE
  - It measures **how well the model generalizes**
- *A low training MSE does not imply a low test MSE*

MSE varies with model flexibility

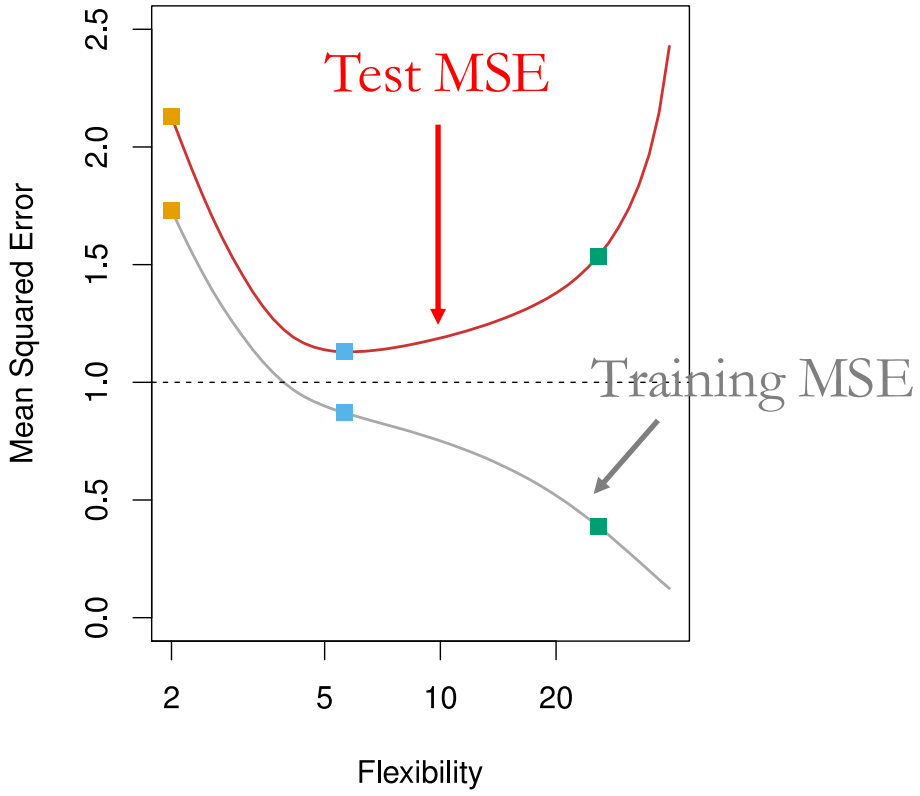
More flexible model



Training MSE = 0.439 | Training MSE = 0.425 | Training MSE = 0.354



Test MSE = 0.533 | Test MSE = 0.518 | Test MSE = 0.564



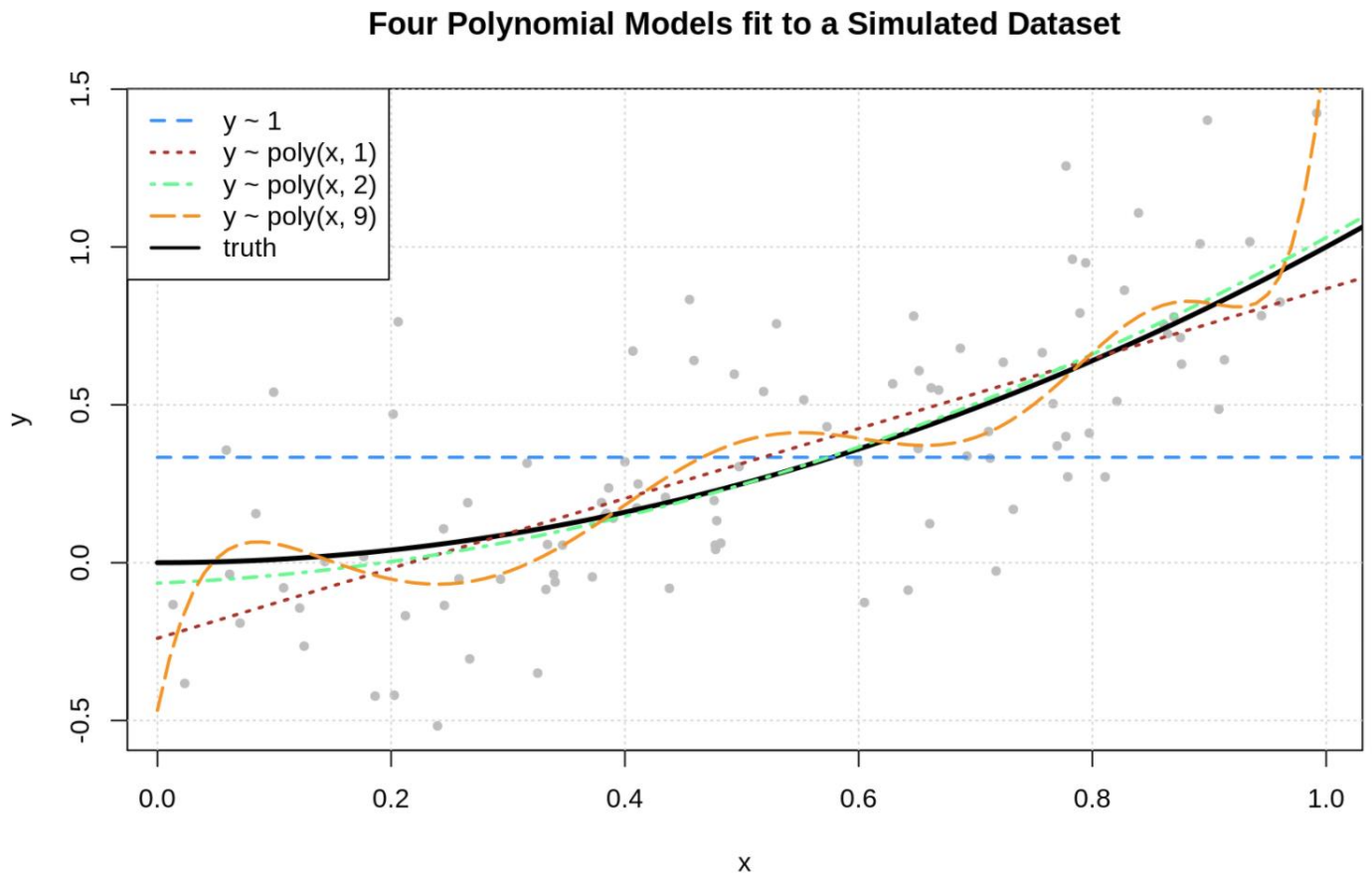
Why does MSE vary with model flexibility?

- Suppose the *true regression function* is $f(x) = x^2$ (x is a scalar)

- We fit *models of increasing flexibility* to approximate this function
  - Constant model: $\hat{f}_0(x) = \hat{\beta}_0$
  - Linear model: $\hat{f}_1(x) = \hat{\beta}_0 + x \cdot \hat{\beta}_1$
  - Quadratic model: $\hat{f}_2(x) = \hat{\beta}_0 + x \cdot \hat{\beta}_1 + x^2 \cdot \hat{\beta}_2$
  - Ninth degree polynomial model: $\hat{f}_9(x) = \hat{\beta}_0 + x \cdot \hat{\beta}_1 + \cdots + x^9 \cdot \hat{\beta}_9$

  - The model is *more flexible* if the *polynomial degree is larger*

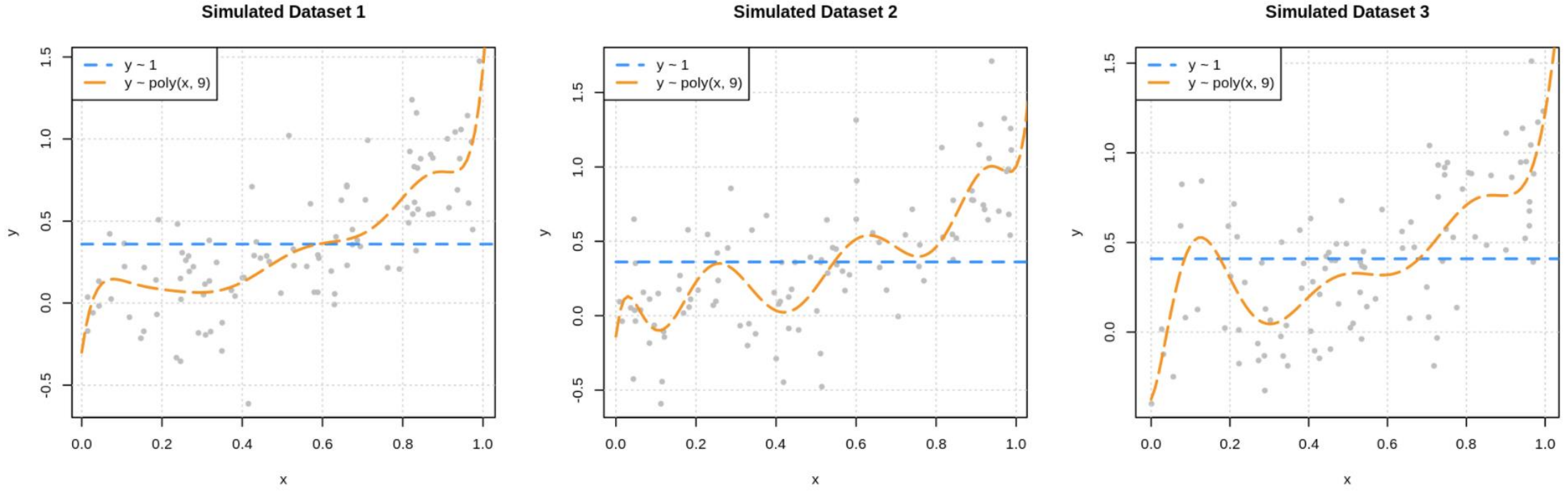
Four fitted models



- Zero predictor model fits poorly
- Linear model is reasonable
- Quadratic model fits much better
- Ninth degree model seems rather wild

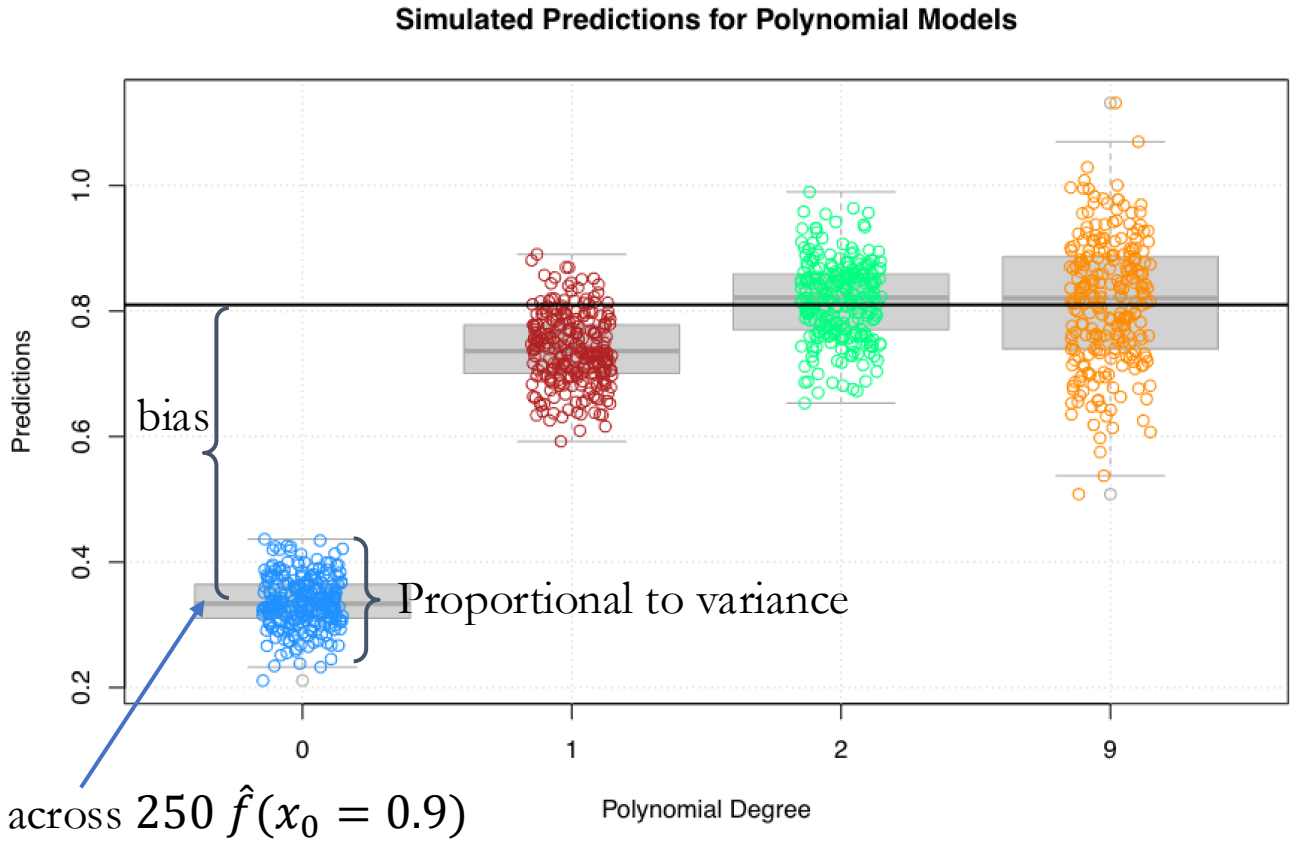
Model fits change across training datasets

- In general, the fitted model depends on the training data
- When we refit the same model on different datasets:
  - The **constant model** $\hat{f}_0(x)$ changes only slightly
  - The **9th-degree polynomial** $\hat{f}_9(x)$ can change dramatically
- This variability across training sets is called the **variance of the model**
  - The variance of $\hat{f}_0(x)$ is smaller than the variance of $\hat{f}_9(x)$



Predicting $f(x_0)$ at a specific point x_0

- We study prediction at a single test input
- Test point: $x_0 = 0.9$
- True value: $f(x_0 = 0.9) = x_0^2 = 0.81$
- We generate **250 independent training datasets**
- For each dataset, we fit polynomial models of degree 0,1,2, and 9, and record the prediction $\hat{f}(x_0 = 0.9)$



Average prediction across 250 $\hat{f}(x_0 = 0.9)$

Each dot = one prediction $\hat{f}(x_0)$ from a different dataset
The **horizontal line** = true value $f(x_0) = 0.81$
The **center of the cloud** = average prediction
The **spread of the cloud** $\propto$ variance of the model

Bias and variance of prediction at x_0

- The squared bias

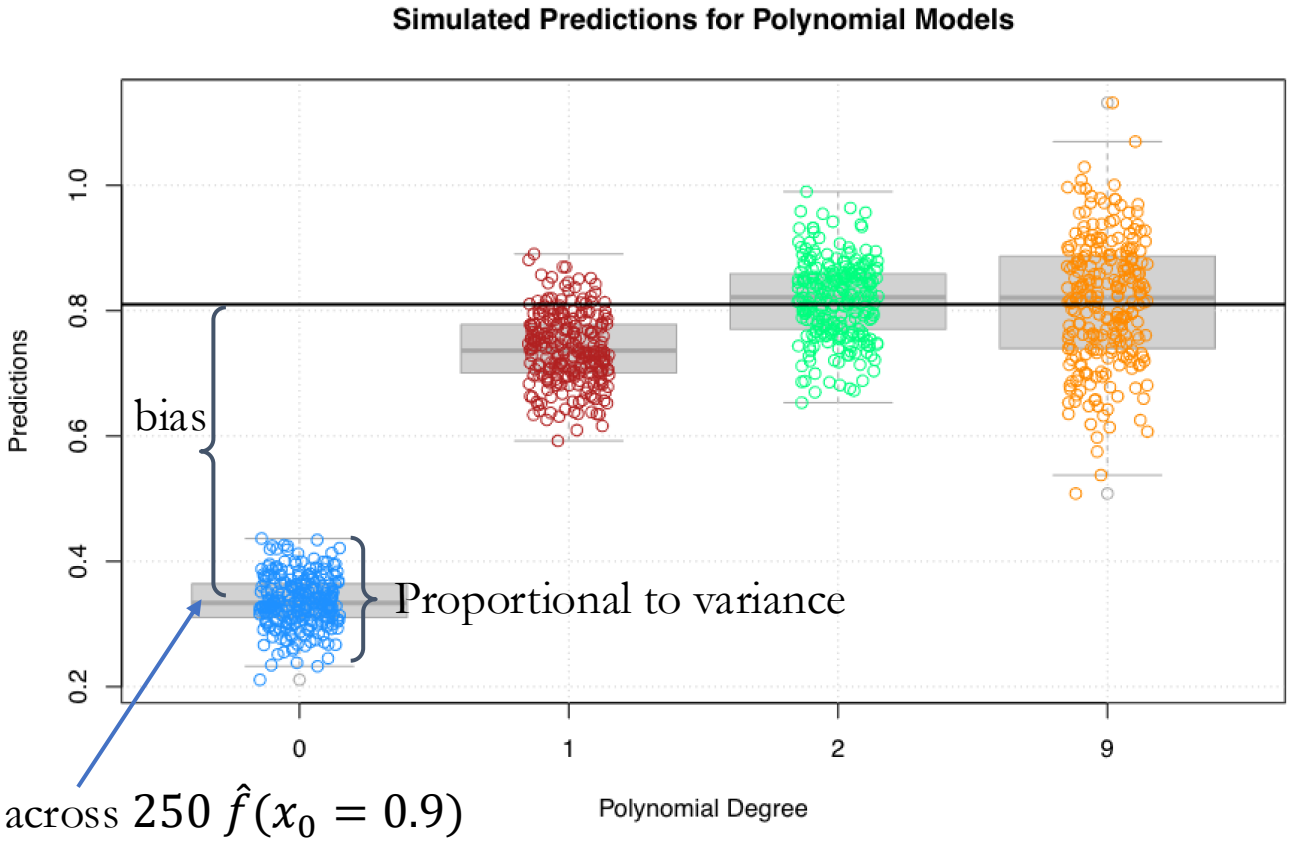
  $\hat{f}_2(x) \approx \hat{f}_9(x) < \hat{f}_1(x) < \hat{f}_0(x)$

  - Increasing degree from **2 to 9 does not meaningfully reduce bias**

- Variance

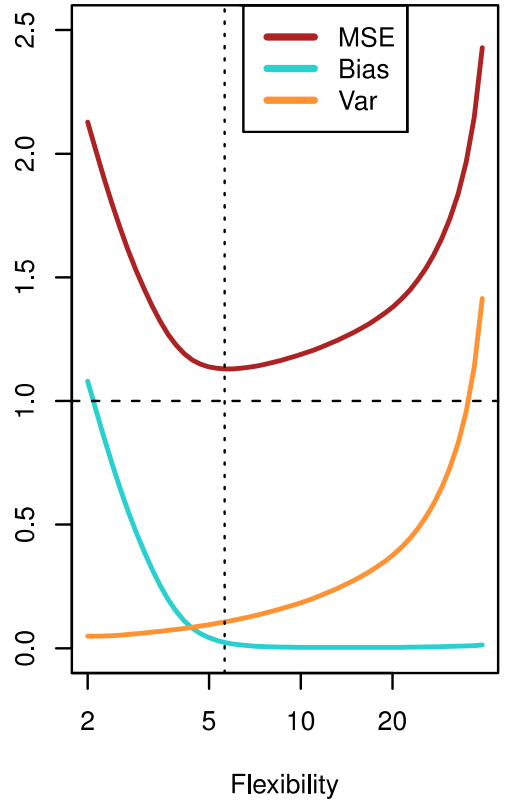
  $\hat{f}_0(x) < \hat{f}_1(x) < \hat{f}_2(x) < \hat{f}_9(x)$

  ➢Increasing degree increases variance



Combining bias and variance

- The **test mean squared error (MSE)** depends on both **bias** and **variance**



- As model flexibility increases:
  - Bias decreases
  - Variance increases

- Their combined effect produces the **U-shaped test MSE curve**

Analyzing test MSE

- Suppose the true regression function is f
- The response satisfies $Y = f(X) + \varepsilon$, with $\mathrm{E}[\varepsilon \mid X] = 0$
- Let the training dataset be $\mathcal{D} = \{(X_1, Y_1), (X_2, Y_2), \cdots, (X_n, Y_n)\}$
- The fitted model $\hat{f}$ *depends on training data* $\mathcal{D}$
  - If we change the training data $\mathcal{D}$, we get a different estimate $\hat{f}$
- Prediction at a fixed test point x_0
  - The MSE at x_0 can be decomposed as

$$\mathrm{MSE}(x_0) = \underbrace{E_{Y|X,\mathcal{D}}}\left[\left(Y - \hat{f}(X)\right)^2 \mid X = x_0\right] = \underbrace{E_{\mathcal{D}}\left[\left(f(x_0) - \hat{f}(x_0)\right)^2\right]} + \underbrace{V_{Y|X}[Y \mid X = x_0]}$$

Expected value over $\mathcal{D}$ and $Y|X$ | Reducible error | Irreducible error

Decomposition of MSE

- The MSE at x_0 can be decomposed as

$$\text{MSE}(x_0) = \underbrace{E_{Y|X,\mathcal{D}}}\left[\left(Y - \hat{f}(X)\right)^2 \mid X = x_0\right] = \underbrace{E_{\mathcal{D}}\left[\left(f(x_0) - \hat{f}(x_0)\right)^2\right]}_{\text{Reducible error}} + \underbrace{V_{Y|X}[Y \mid X = x_0]}_{\text{Irreducible error}}$$

Expected value over $Y|X$ and $\mathcal{D}$

- The MSE at x_0 is the **expected prediction error** for
  - a **new response** Y_0
  - at a **fixed input** $X_0 = x_0$
  - using a **model** $\hat{f}$ trained on random data $\mathcal{D}$

- Two sources of *randomness*
  - Noise in the outcome: Y_0 is random because $Y = f(X) + \varepsilon$ and ε is random
  - Randomness in fitted model $\hat{f}$: $\hat{f}$ is random because it depends on randomly sampled $\mathcal{D}$

Irreducible error

- The MSE at x_0 can be decomposed as

$$\text{MSE}(x_0) = \underbrace{E_{Y|X,\mathcal{D}}}\left[\left(Y - \hat{f}(X)\right)^2 \mid X = x_0\right] = \underbrace{E_{\mathcal{D}}\left[\left(f(x_0) - \hat{f}(x_0)\right)^2\right]}_{\text{Reducible error}} + \underbrace{V_{Y|X}[Y \mid X = x_0]}_{\text{Irreducible error}}$$

Expected value over $Y|X$ and $\mathcal{D}$

  - Irreducible error: the variance of Y given that $X = x_0$
    - If $Y = f(X) + \varepsilon$ with $\text{E}[\varepsilon] = 0$ and $\text{V}[\varepsilon] = \sigma_\varepsilon^2$, then $V_{Y|X}[Y \mid X = x_0] = \sigma_\varepsilon^2$
    - Irreducible error can not be reduced for any $\hat{f}$

Reducible error

- The MSE at x_0 can be decomposed as

$$\text{MSE}(x_0) = \underbrace{E_{Y|X,\mathcal{D}}}\left[\left(Y - \hat{f}(X)\right)^2 \mid X = x_0\right] = \underbrace{E_{\mathcal{D}}\left[\left(f(x_0) - \hat{f}(x_0)\right)^2\right]}_{\text{Reducible error}} + \underbrace{V_{Y|X}[Y \mid X = x_0]}_{\text{Irreducible error}}$$

Expected value over $Y|X$ and $\mathcal{D}$

  - Reducible error: the expected squared error by using $\hat{f}(x_0)$ to estimate $f(x_0)$
    - The randomness comes from training data $\mathcal{D}$ used to obtain $\hat{f}$ (both f and x_0 are fixed)
    - Reducible error can be reduced by using a better $\hat{f}$

Bias-variance decomposition of reducible error

- *Reducible error* can be decomposed as the *squared bias* and *variance*

$$E_{\mathcal{D}}\left[\left(f(x_0)-\hat{f}(x_0)\right)^2\right]=\underbrace{\left(f(x_0)-E_{\mathcal{D}}[\hat{f}(x_0)]\right)^2}_{\text{bias}^2(\hat{f}(x_0))}+\underbrace{E_{\mathcal{D}}\left[\left(\hat{f}(x_0)-E_{\mathcal{D}}[\hat{f}(x_0)]\right)^2\right]}_{\text{var}(\hat{f}(x_0))}$$

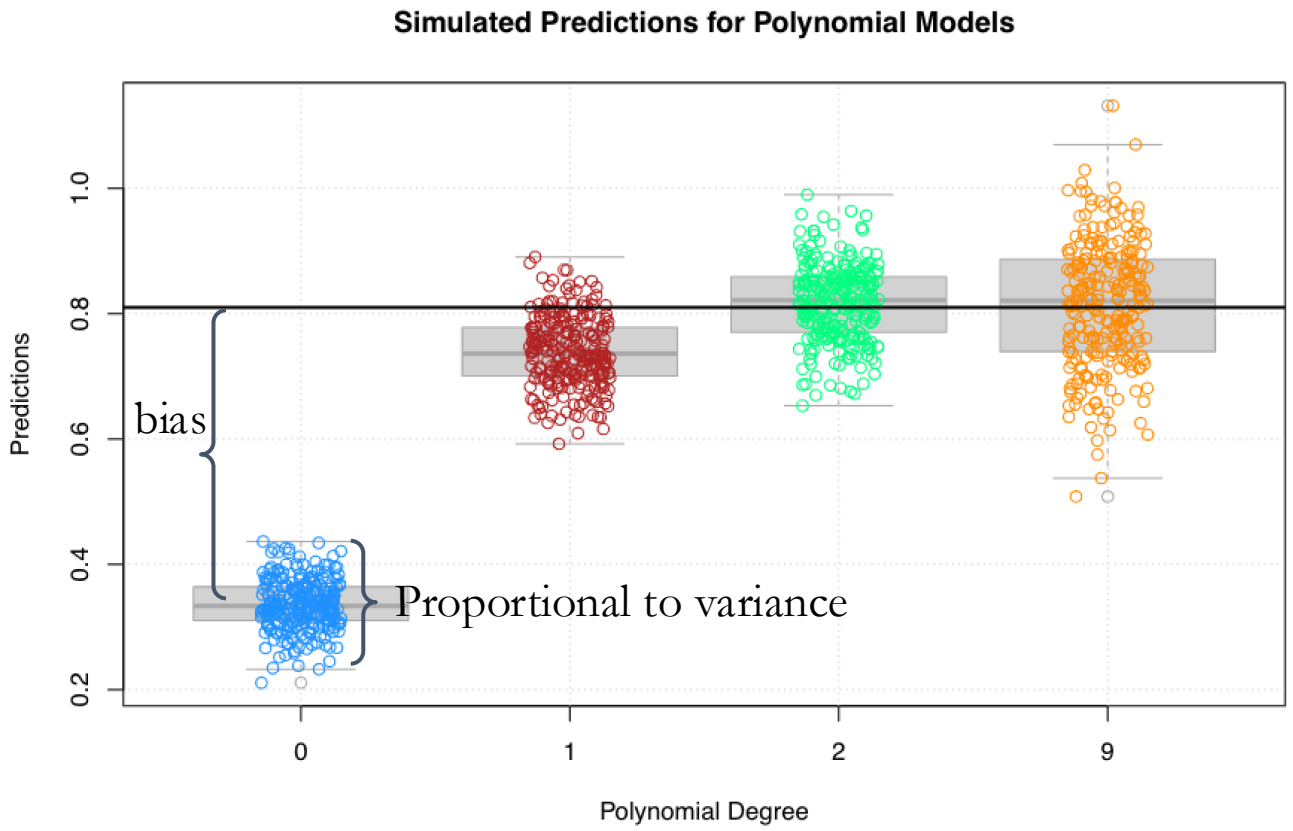
- *Take home exercise: Prove this decomposition*
- Hint: Use the property

$$E_{\mathcal{D}}\left[\left(f(x_0)-\hat{f}(x_0)\right)^2\right]=E_{\mathcal{D}}\left[\left(\underbrace{f(x_0)-E_{\mathcal{D}}[\hat{f}(x_0)]}_{A}+\underbrace{E_{\mathcal{D}}[\hat{f}(x_0)]-\hat{f}(x_0)}_{B}\right)^2\right]$$

$$E_{\mathcal{D}}[(A+B)^2]=A^2+2A\underbrace{E_{\mathcal{D}}[B]}_{=0}+E_{\mathcal{D}}[B^2]=A^2+E_{\mathcal{D}}[B^2]$$

(A is nonrandom and $E_{\mathcal{D}}[A^2]=A^2$)

Recall our toy example



Summing up the decomposition

- The MSE at x_0 can be decomposed as

$$\text{MSE}(x_0) = \underbrace{\text{bias}^2\left(\hat{f}(x_0)\right) + \text{var}\left(\hat{f}(x_0)\right)}_{\text{Reducible error}} + \underbrace{\sigma_\varepsilon^2}_{\text{Irreducible error}}$$

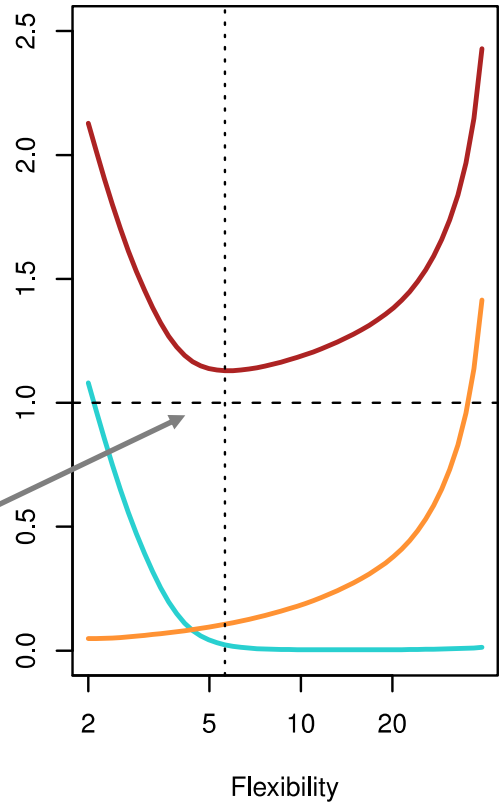
Visualizing the bias-variance tradeoff

$Y = f(X) + \varepsilon$
$\mathrm{Var}(\varepsilon) = 1$

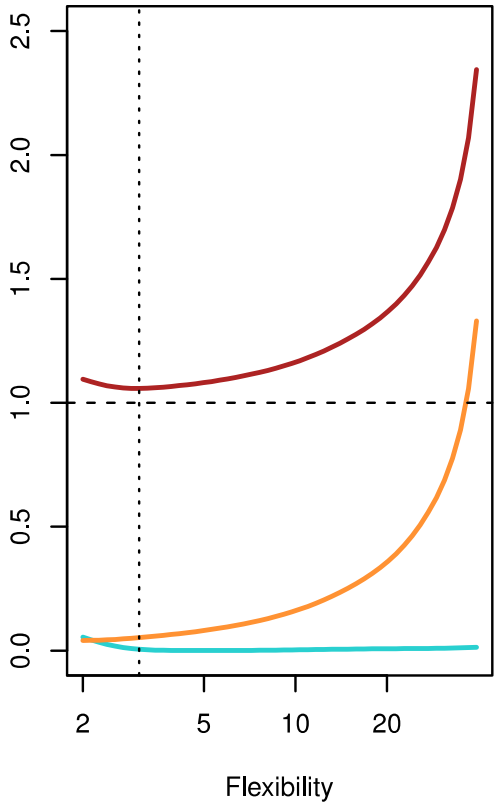
SNR: Signal-to-noise ratio
Signal measured by $f(X)$
Noise measured by ε

Irreducible error

f is complicated, low SNR



f is simple, low SNR



f is complicated, high SNR