Machine Learning

Supervised Machine Learning – Regression

Part 2: Model Flexibility, Overfitting, Bias-Variance Trade-Off

Parametric Modeling – Part 2

Parametric Modeling

Consider that *f* can take the parametric form

$$f(x) \approx m(x; a) \ \forall x \in I, a \in H$$

Training:

- 1. Identify parametric model m
- 2. Identify model parameters *a*

Training the Parameters (recap)

Assume the simplified case that true m is known.

Then, to train \hat{f} is to train the parameters of the model, a, which can take values in set H.

Given training data $S = \{(y_n, x_n)\}_{n=1}^N$ and loss function L, we train

$$\hat{f}(\mathbf{x}) = m(\mathbf{x}; \widehat{\mathbf{a}})$$

where

$$\hat{a} = \operatorname{argmin}_{b \in H} L(b; S)$$

We call this "fitting the model parameters to the training data."

For MSE training,
$$L(\boldsymbol{b}, S) = \frac{1}{N} \sum_{n=1}^{N} (y_n - m(\boldsymbol{x}_n; \boldsymbol{b}))^2$$

Other loss functions?

Better parameter training:

- Fewer parameters
- More training data N
- Lower noise variance, σ_{ϵ}^2

Identifying Model

- True knowledge of m in f is rarely the case. Needs domain expertise and simple f.
- Need to select hypothetical model \widehat{m} (call it <u>hypothesis</u>) to approximate the true m in f

Model Flexibility

• Affine model:

$$m(x, a) = a_0 + a_1 x_1 + a_2 x_2$$

• Quadratic model:

$$m'(\mathbf{x}, \mathbf{a}) = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_1 x_2 + a_4 x_1^2 + a_5 x_2^2$$

• It holds that:

$$m(\mathbf{x}, [a_0, a_1, a_2]^T) = m'(\mathbf{x}, [a_0, a_1, a_2, a_3 = 0, a_4 = 0, a_5 = 0]^T)$$

- m' is more "flexible" than m
 - m' has more parameters than m
 - m' can become m for certain parameter configuration

Select Hypothesis and Train Parameters – Considerations

We want $\hat{f}(x) = \widehat{m}(x; \widehat{a}) \approx f(x) = m(x; a)$.

What if *m* is more flexible than \widehat{m} ?

What if \widehat{m} is more flexible than m?

What is more important, to select \widehat{m} correctly or to train \widehat{a} well?

Place in order of preference:

- \square $\widehat{m} = m$, poor parameter training
- \square \widehat{m} more flexible than m, excellent parameter training
- \square \widehat{m} less flexible than m, poor parameter training
- \square $\widehat{m} = m$, excellent parameter training
- \square \widehat{m} less flexible than m, excellent parameter training

Select Hypothesis and Train Parameters – Considerations

We want $\hat{f}(x) = \widehat{m}(x; \widehat{a}) \approx f(x) = m(x; a)$.

Given ample low-noise training data...

- \square Overestimate flexibility of m?
- \square Underestimate flexibility of m?

Given limited and or highly-noisy training data...

- \square Overestimate flexibility of m?
- \Box Underestimate flexibility of m?

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma^2_\epsilon$

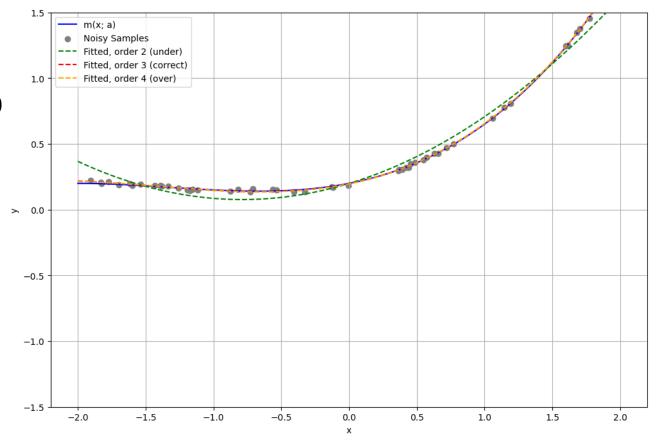
Model Estimation:

 \widehat{m} estimated as:

- 2nd deg. poly. (3 param.)
- 3rd deg. poly. (4 param.)
- 4th deg. poly. (5 param.)

Mod. Est. Quality:

2nd deg. too low 3rd deg. is correct 4th deg. can be



Param. Training:

 \widehat{m} fitted with:

- N=50 samples
- $\sigma_{e} = 0.01$

Param. Tr. Quality:

Enough low-noise data. All models train well.

Correct and highflexibility trained models perform best.

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma^2_\epsilon$

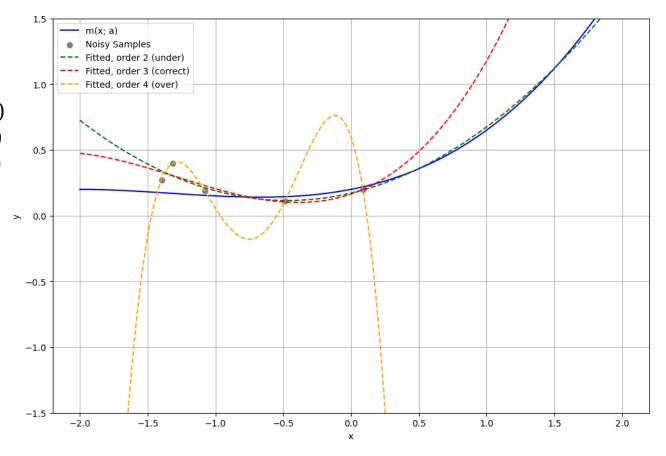
Model Estimation:

\widehat{m} estimated as:

- 2nd deg. poly. (3 param.)
- 3rd deg. poly. (4 param.)
- 4th deg. poly. (5 param.)

Mod. Est. Quality:

2nd deg. too low 3rd deg. is correct 4th deg. can be



Param. Training:

\widehat{m} fitted with:

- N=5 samples
- $\sigma_{\epsilon} = 0.1$

Param. Tr. Quality:

Limited noisy data. Flexible models do not train well.

Moderately-trained low-flexibility model performs better (!) than poorly-trained correct-flexibility and high-flexibility models.

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma^2_\epsilon$

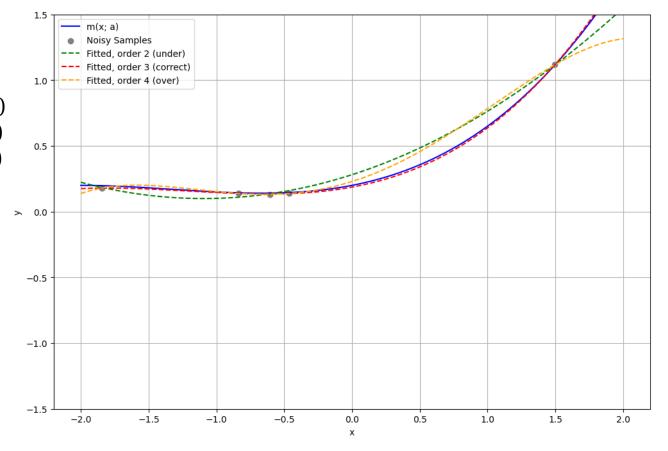
Model Estimation:

 \widehat{m} estimated as:

- 2nd deg. poly. (3 param.)
- 3rd deg. poly. (4 param.)
- 4th deg. poly. (5 param.)

Mod. Est. Quality:

2nd deg. too low 3rd deg. is correct 4th deg. can be



Param. Training:

 \widehat{m} fitted with:

- N=5 samples
- $\sigma_{\epsilon} = 0.01$

Param. Tr. Quality:

Limited low-noise data. Still, high-flexibility model does not train very well.

Correct-flexibility trained model performs best.

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma^2_\epsilon$

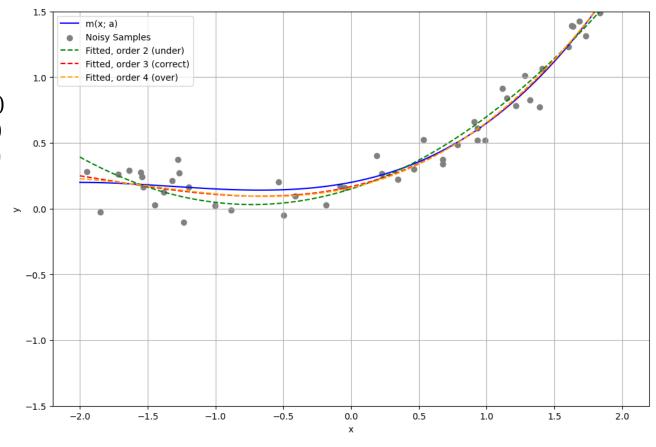
Model Estimation:

\widehat{m} estimated as:

- 2nd deg. poly. (3 param.)
- 3rd deg. poly. (4 param.)
- 4th deg. poly. (5 param.)

Mod. Est. Quality:

2nd deg. too low 3rd deg. is correct 4th deg. can be



Param. Training:

\widehat{m} fitted with:

- N=50 samples
- $\sigma_{e} = 0.1$

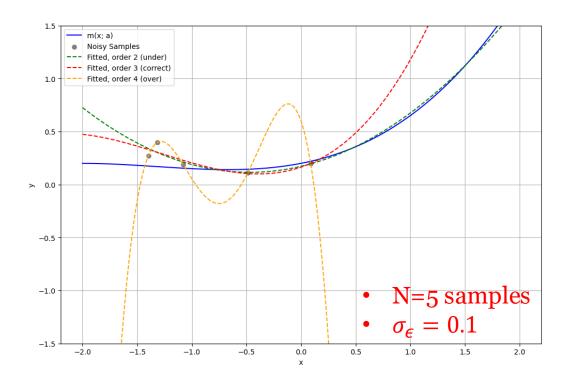
Param. Tr. Quality:

Enough noisy data. High-flexibility model does not train very well.

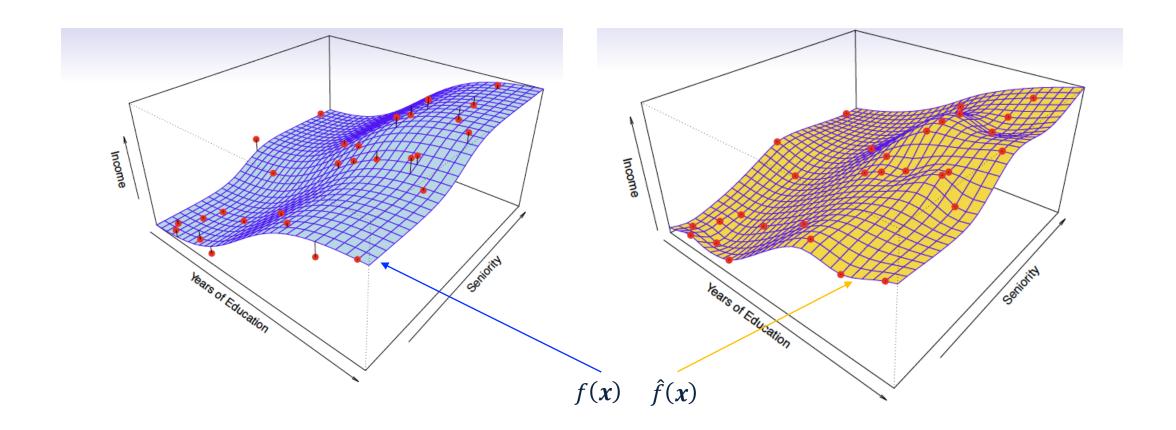
Correct-flexibility trained model performs best.

Overfitting

- For any \widehat{m} , \widehat{a} is optimized so that $\widehat{f}(x) = \widehat{m}(x; \widehat{a})$ fits the training data as closely as allowed by the \widehat{m} .
- If \widehat{m} is flexible, $\widehat{f}(x)$ will fit well the training data.
- This is positive, for many and/or low-noise data.
- This is negative, for limited and/or noisy data.
- Overfitting: The trained model \hat{f} overfits data and captures the noise within it. For high noise intensity, overfitted model fails to represent m and express other "unseen" data ("generalize").



Overfitting (cont'd)



Measuring Model Accuracy

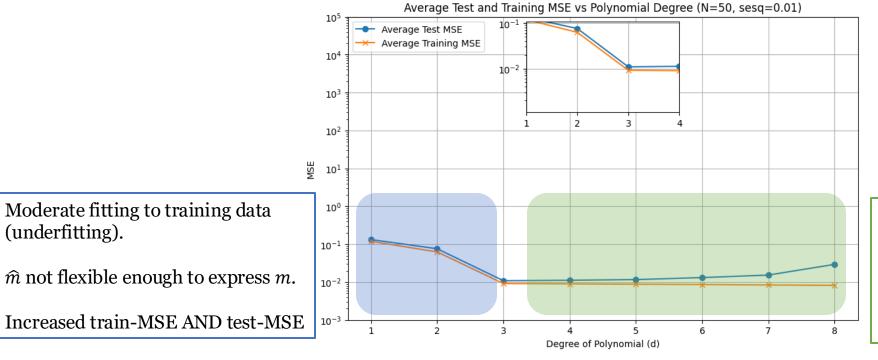
- \square Consider $\hat{f}(\mathbf{x}) = \widehat{m}(\mathbf{x}; \mathbf{a})$ trained on data $S_{tr} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$.
- \square We could examine MSE on S_{tr} .

$$MSE_{tr} = \frac{1}{|S_{tr}|} \sum_{(y,x) \in S_{tr}} |y - \hat{f}(x)|^2$$

- ☐ This will be low. This is exactly what parameter training/fitting optimized.
- \square Instead, we should examine MSE on fresh (unseen) <u>test data</u> $S_{te} = \{(x_i, y_i)\}_{i=1}^M$:

$$MSE_{te} = \frac{1}{|S_{te}|} \sum_{(y,x) \in S_{te}} |y - \hat{f}(x)|^2$$

 $d=1; m(x; \boldsymbol{a})$ is 3rd degree polynomial (4 parameters); $f(x)=m(x; \boldsymbol{a})+\epsilon; E\{\epsilon^2\}=\sigma_\epsilon^2$



- Fitting well the training data.
- Slightly overfitting as *d* increases because of enough training data and low noise intensity. Limited effect on test-MSE.

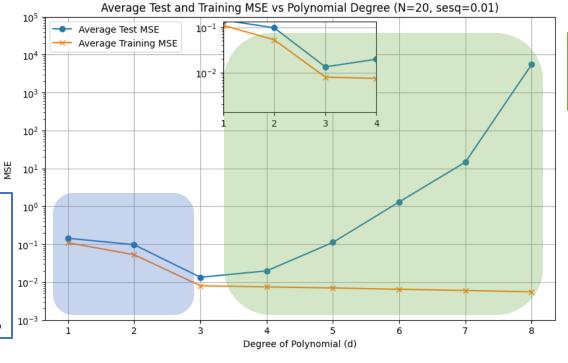
Param. Training: N=50 samples; $\sigma_{\epsilon}^2 = 0.01$

Moderate fitting to training data

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(underfitting).

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma_\epsilon^2$



Pronounced overfitting as *d* increases due to limited data. test-MSE increases fast.

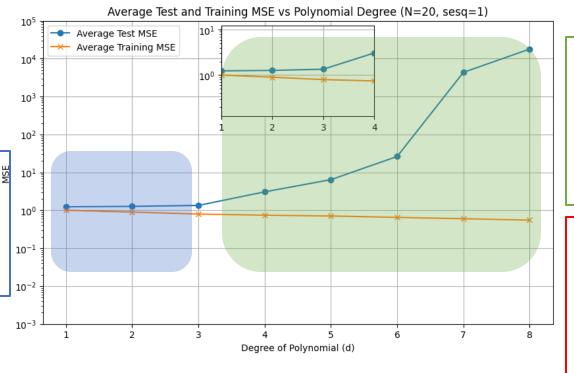
- Moderate fitting to training data (underfitting).
- \widehat{m} not flexible enough to express m.
- Increased train-MSE AND test-MSE

Param. Training: N=20 samples; $\sigma_{\epsilon}^2 = 0.01$

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma^2_\epsilon$



- \widehat{m} not flexible enough to express m.
- Increased train-MSE AND test-MSE



Param. Training: N=20 samples; $\sigma_{\epsilon}^2 = 1$

- Moderate fitting to data (higher train-MSE floor), even for high d, due to high σ_{ϵ}^2 .
- Yet, higher test-MSE than before due to capturing part of the highintensity noise.

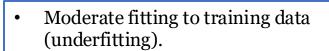
• <u>Previous figure:</u>

Overfitting (low train-MSE) at high d, capturing most of the low-intensity noise. High test-MSE.

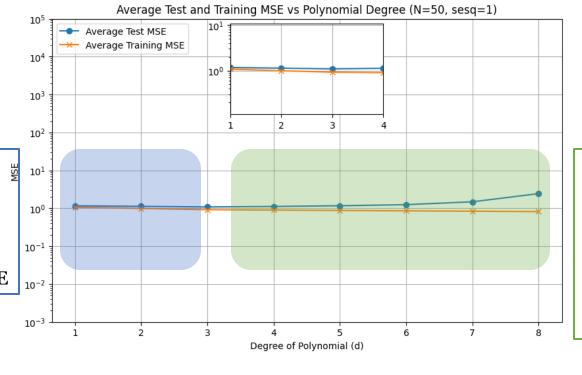
• This figure:

Moderate fitting (higher train-MSE) at high *d*, capturing part of the high-intensity noise. Higher test-MSE.

 $d=1;\ m(x;\boldsymbol{a})\ \text{is 3}^{\text{rd}}\ \text{degree polynomial (4 parameters)};\ f(x)=m(x;\boldsymbol{a})+\epsilon;\ E\{\epsilon^2\}=\sigma_\epsilon^2$

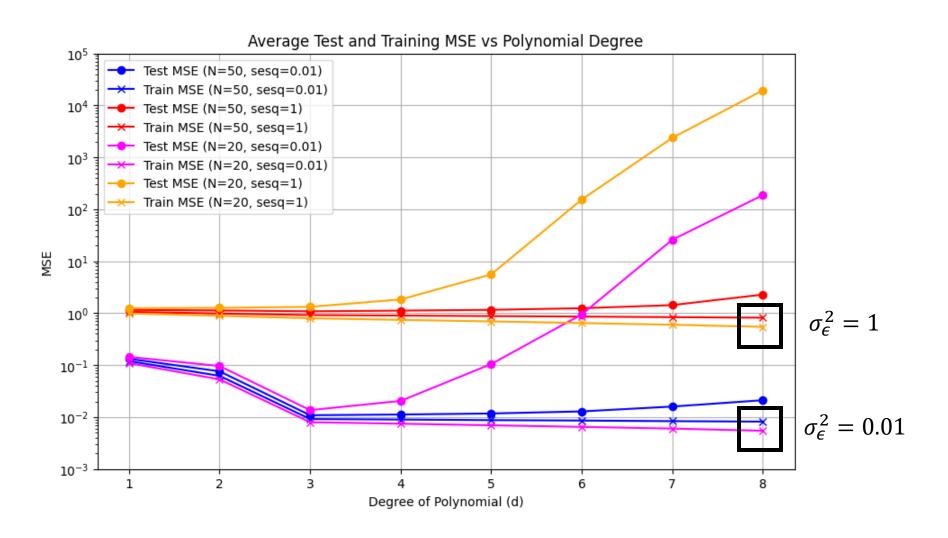


- \widehat{m} not flexible enough to express m.
- Increased train-MSE AND test-MSE

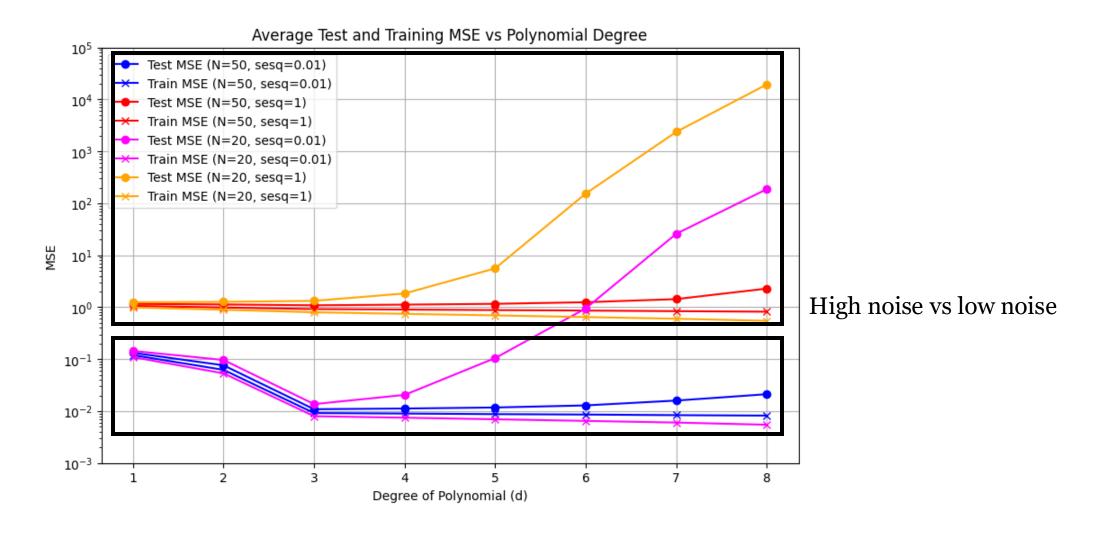


- Low fitting to data (flat train-MSE floor), even for high d, due to both low N and high σ_{ϵ}^{2} .
- Captures little of the high-intensity noise, which is averaged out due to high *N*. Low test-MSE.

Param. Training: N=50 samples; $\sigma_{\epsilon}^2 = 1$



Measuring Model Accuracy



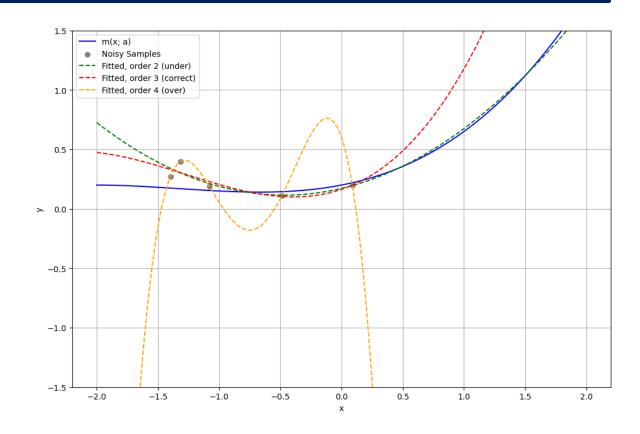
How to Combat Overfitting?

Buy better training data:

- More examples
- Less noise

Fixed training data:

- Lower hypothesis flexibility
- Suboptimal parameter fitting



Bias and Variance

- \square Assume that you have chosen \widehat{m} and you train the model over **random** dataset S to obtain \widehat{f} .
- \square For any unseen input x and corresponding output $y(x) = f(x) + \epsilon$, the model exhibits:
 - ☐ Bias:

☐ Variance:

☐ MSE:

Mean over S

$$\operatorname{Bias}_{S}\left(\hat{f}(\boldsymbol{x})\right) = f(\boldsymbol{x}) - E_{S}\left[\hat{f}(\boldsymbol{x})\right]$$

Bias: Error of $\hat{f}(x)$ to express f(x), in the mean over S.

$$Var_{S}(\hat{f}(x)) = E_{S}[\hat{f}(x) - E_{S}[\hat{f}(x)])^{2}$$

Variance of trained $\hat{f}(x)$, over S.

$$MSE_{S,\epsilon}\left(\hat{f}_S(x)\right) = E_{S,\epsilon}\left[\left(y(x) - \hat{f}(x)\right)^2\right]$$

SE attained by trained $\hat{f}(x)$ on unseen x, in the mean over S and error in y(x).

Bias and Variance (cont'd)

Simplify notation: $Bias(\hat{f}) = f - E[\hat{f}], Var(\hat{f}) = E[(\hat{f} - E[\hat{f}])^2], \text{ and } MSE(\hat{f}) = E[(y - \hat{f})^2]$

Then we find:

$$MSE_{S,\epsilon} = E\left[\left(y - \hat{f}\right)^{2}\right] = E\left[\left(f + \epsilon - \hat{f}\right)^{2}\right] = E\left[\left(f - \hat{f}\right)^{2} + \epsilon^{2} + 2\epsilon\left(f - \hat{f}\right)\right]$$
$$= E\left[\left(f - \hat{f}\right)^{2}\right] + E\left[\epsilon^{2}\right] + 2E\left[\left(f - \hat{f}\right)\epsilon\right] = E\left[\left(f - \hat{f}\right)^{2}\right] + \sigma_{\epsilon}^{2}$$

In turn we find:

$$E\left[\left(f-\hat{f}\right)^{2}\right] = E\left[f^{2} + \hat{f}^{2} - 2f\hat{f}\right] = f^{2} + E\left[\hat{f}^{2}\right] - 2fE\left[\hat{f}\right]$$

$$= f^{2} + E\left[\hat{f}^{2}\right] - 2fE\left[\hat{f}\right] + E\left[\hat{f}\right]^{2} - E\left[\hat{f}\right]^{2} - 2E\left[\hat{f}\right]^{2} + 2E\left[\hat{f}\right]^{2}$$

$$= f^{2} + E\left[\hat{f}^{2} + E\left[\hat{f}\right]^{2} - 2E\left[\hat{f}\right]^{2}\right] - 2fE\left[\hat{f}\right] + E\left[\hat{f}\right]^{2}$$

$$= (f - E\left[\hat{f}\right])^{2} + E\left[\hat{f}^{2} + E\left[\hat{f}\right]^{2} - 2E\left[\hat{f}\right]\hat{f}\right] = (f - E\left[\hat{f}\right])^{2} + E\left[(\hat{f} - E\left[\hat{f}\right])^{2}\right] = Bias^{2}(\hat{f}) + Var(\hat{f})$$

Bias and Variance (cont'd)

We proved that, for any given x, the MSE is:

$$MSE_{S,\epsilon}(\hat{f}(x)) = \left(Bias_S(\hat{f}(x))\right)^2 + Var_S(\hat{f}(x)) + \sigma_{\epsilon}^2$$

The mean MSE over all (random) unseen data is:

$$MSE = E_{x} \left[MSE_{S,\epsilon} \left(\hat{f}(x) \right) \right] = E_{x} \left[\left(Bias_{S} \left(\hat{f}(x) \right) \right)^{2} + Var_{S} \left(\hat{f}(x) \right) \right] + \sigma_{\epsilon}^{2}$$

Bias and Variance (cont'd)

☐ We proved that the MSE is:

$$MSE = E_{x} \left[\left(Bias_{S} \left(\hat{f}(x) \right) \right)^{2} + Var_{S} \left(\hat{f}(x) \right) \right] + \sigma_{\epsilon}^{2}$$

$$MSE = \underbrace{E_{x} \left[\left(f(x) - E_{S} \left[\hat{f}(x) \right] \right)^{2} \right]}_{B} + \underbrace{E_{x} \left[E_{S} \left[\left(\hat{f}(x) - E_{S} \left[\hat{f}(x) \right] \right)^{2} \right] \right]}_{V} + \sigma_{\epsilon}^{2}$$

- ☐ How to reduce MSE?
 - \Box Consider σ_{ϵ}^2 given.
 - ☐ Reduce Bias and/or Variance.
 - ☐ Two things to tune: hypothesis and number of training data.

High Bias

$$MSE = \underbrace{E_{x} \left[\left(f(x) - E_{S} \left[\hat{f}(x) \right] \right)^{2} \right]}_{B} + \underbrace{E_{x} \left[E_{S} \left[\left(\hat{f}(x) - E_{S} \left[\hat{f}(x) \right] \right)^{2} \right] \right]}_{V} + \sigma_{\epsilon}^{2}$$

High B:

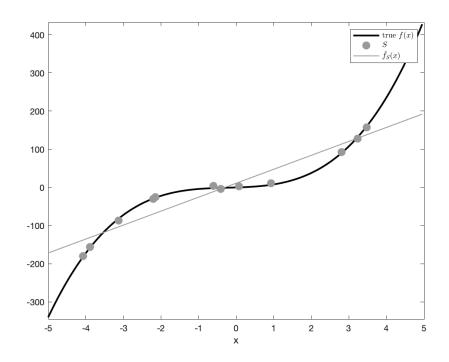
- Over the unseen points (in the mean), over the possible training datasets of size N (in the mean), your model is far from true f.
- \square This is because hypothesis \widehat{m} is too rigid (not flexible enough).
- \square Cannot fit true f and generalize to unseen data.

Remedy:

 \square For fixed *N*, increase the flexibility (e.g., #parameters) of \widehat{m} .

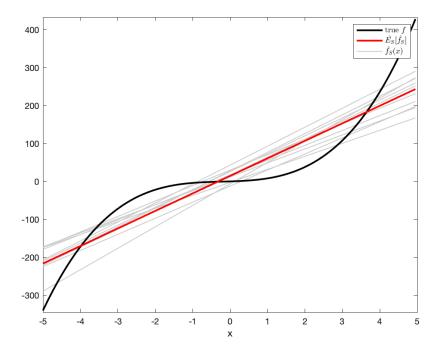
Example 4 – High Bias

True: $f(x) = 3x^3 + 2x^2 + 3x$. Hypothesis: line (simpler). N = 12, $\sigma_{\epsilon} = 5$.



Model cannot fit the training data (underfitting).

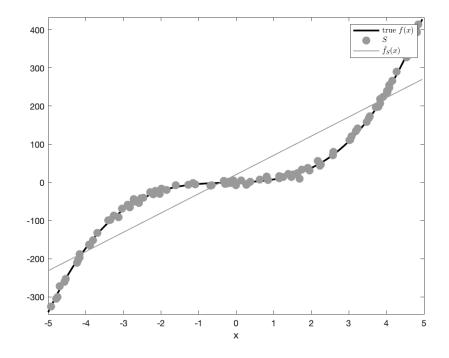
$$B = \frac{E_x}{\left[\left(f(x) - E_S \left[\hat{f}(x) \right] \right)^2 \right]}$$



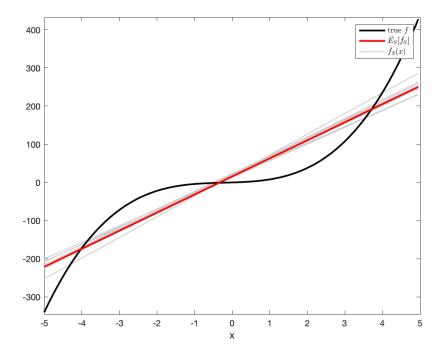
from the mean model (over all training datasets of size *N*). Both model instances and mean model are far from the true *f*.

Example 4 - Increase Data

Same simple hypothesis. Increase N = 64.



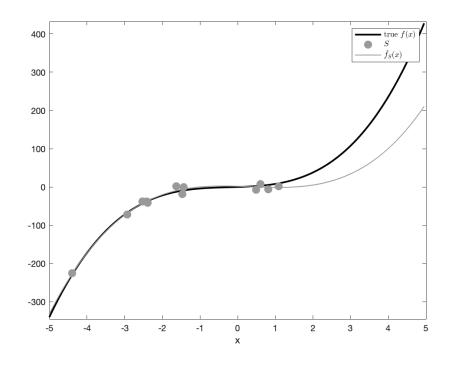
Still underfitting.



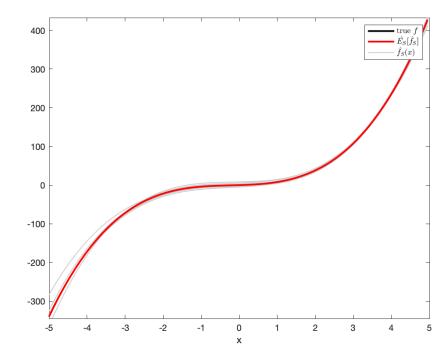
- Bias remains. Variance (and, thus, MSE) somewhat decreased.
- Increasing the amount of data typically drops variance.

Example 4 - Increase Flexibility

Keep N = 12 data. Increase flexibility to deg-3 polynomial.



- Fits data better, but not all of them and not perfectly.
- Since $\sigma > 0$ this is good; the model can generalize.



- Bias eliminated.
- Variance remains.

High Variance

$$MSE = \underbrace{E_{x} \left[\left(f(x) - E_{S} \left[\hat{f}(x) \right] \right)^{2} \right]}_{B} + \underbrace{E_{x} \left[E_{S} \left[\left(\hat{f}(x) - E_{S} \left[\hat{f}(x) \right] \right)^{2} \right] \right]}_{V} + \sigma_{\epsilon}^{2}$$

High *V*:

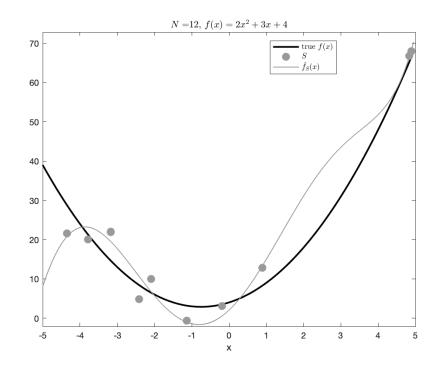
- Over the unseen points (in the mean), model instances across different training datasets of size N deviate a lot from the mean model (in the mean).
- ☐ This is because our hypothesis is too flexible and overfits to each specific training dataset.
- \square Each training dataset contains error and deviates from true f.
- \Box Thus, overfitted model is far from the true f and cannot express unseen data (generalize).

Remedy:

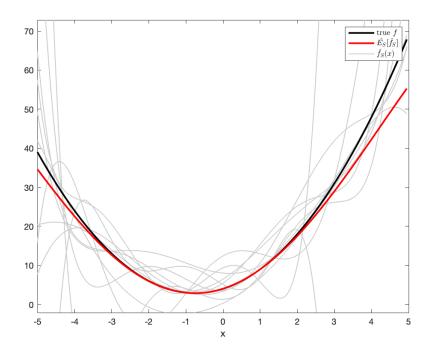
- ☐ For same number of data, reduce flexibility to reduce variance.
- ☐ For same hypothesis, increase the number of data to reduce variance.

Example 5 - High Variance

True: $f(x) = 2x^2 + 3x + 4$. Hypothesis: deg-6 polynomial (more complex). N = 12, $\sigma = 5$.



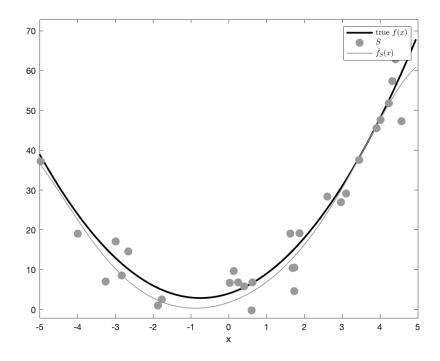
Model fits more to the training data than true *f*. **Overfitting.**



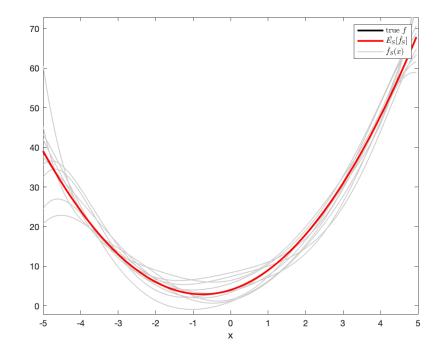
- The mean model (over all datasets of size *N*) matches the true *f*. Minimal Bias.
- But each **model instance** is far from the mean model and the true *f*. **High Variance**.

Example 5 - Increase Data

Same flexible hypothesis. **Increase** N = 32.



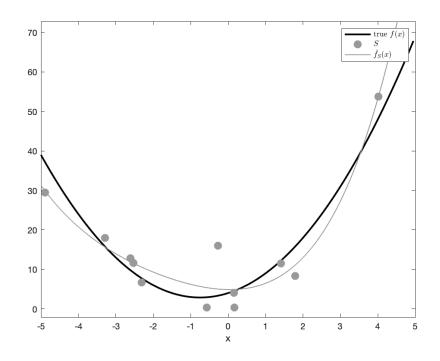
Model cannot fit to training data. Not complex enough for increased N. Model balances among training data, staying closer to the true f.



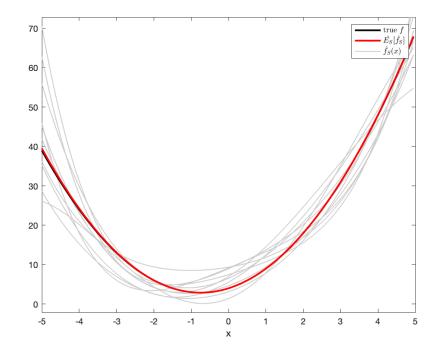
- The mean model matches the true f. No Bias.
- Now each model instance is closer to the mean model and the true f. Variance reduced.

Example 5 - Reduce Flexibility

Keep same N. Reduce flexibility to deg-4 polynomial.



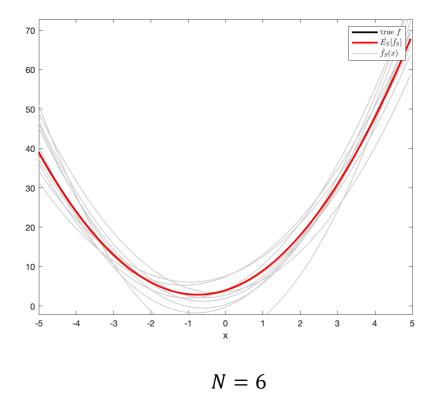
Model cannot fit to all training data. Not complex enough. Model balances among training data, staying closer to the true *f*.

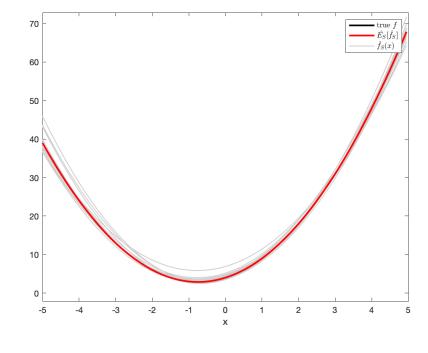


- The mean model almost the true f. Low bias.
- Each **model instance** is closer to the mean model and the true *f*. **Variance reduced.**

Example 5 - Correct Hypothesis

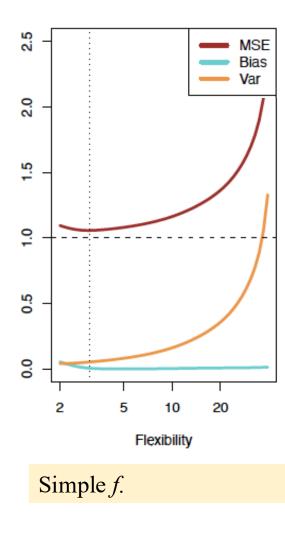
For correct hypothesis, even N = 6 suffices. More training data will be better of course.





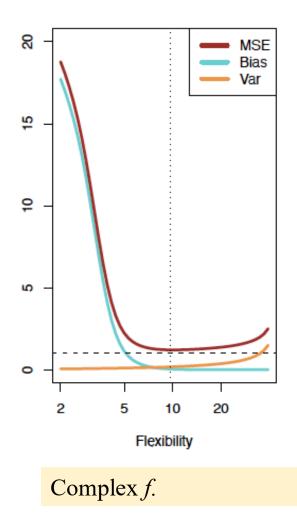
$$N = 32$$

Bias-Variance Trade-Off



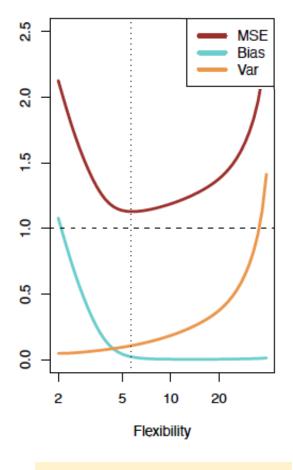
- ☐ For lower model flexibility,
 - □ Some very little bias exists. Simple model underfits.
 - ☐ Assuming enough data, variance is low.
 - ☐ Therefore, MSE is low.
- ☐ As flexibility increases to the best spot,
 - ☐ Bias further reduces.
 - ☐ Variance starts increasing but remains low.
 - ☐ MSE remains low.
- ☐ As flexibility increases excessively,
 - ☐ Variance increases. Flexible model overfits to training data.
 - ☐ Bias remains low.
 - ☐ Following the variance, MSE increases.

Bias-Variance Trade-Off (cont'd)



- ☐ For lower model flexibility,
 - ☐ Bias is very high. Sever underfitting.
 - ☐ Assuming enough data, variance is low.
 - ☐ Following the bias, MSE is very high.
- ☐ As flexibility increases toward the best spot,
 - ☐ Bias rapidly drops.
 - ☐ Variance remains low.
 - ☐ MSE rapidly drops, following the bias.
- ☐ As flexibility starts increasing excessively,
 - ☐ Bias remains low.
 - ☐ Variance starts increasing. As #parameters increase, while *N* remains fixed, mild overfitting starts appearing.
 - ☐ Following the variance, MSE starts increasing.

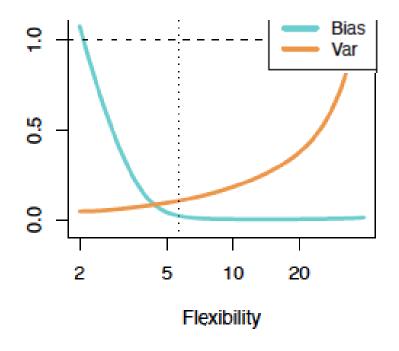
Bias-Variance Trade-Off (cont'd)



Moderately complex f.

- ☐ For low flexibility,
 - ☐ Bias is very high, leading to high MSE. Underfitting.
 - ☐ Assuming enough data, variance is low.
- \square As flexibility increases to the best spot (complexity of true f),
 - ☐ Bias drops drastically.
 - ☐ Variance starts increasing but remains relatively low.
 - ☐ Following the bias, MSE drops drastically.
- ☐ As flexibility increases excessively,
 - ☐ Given data are not enough any more to sustain low variance. Model too flexible for the given amount of data. Variance increases. Overfitting.
 - ☐ Bias remains low.
 - ☐ Following the variance, MSE increases.

Bias-Variance Trade-Off (cont'd)



- ☐ Figure expresses what is known as Bias-Variance Trade-Off.
- ☐ We want to be about where Bias and Variance meet.
- ☐ But we do not have the Bias/Variance curves when we design/train the model...
 - \square This is why we wish we have a good guess of what the true f complexity is.