Bias-Variance Tradeoff

CS229: Machine Learning

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Stanford University

Slides include content developed by and co-developed with Emily Fox

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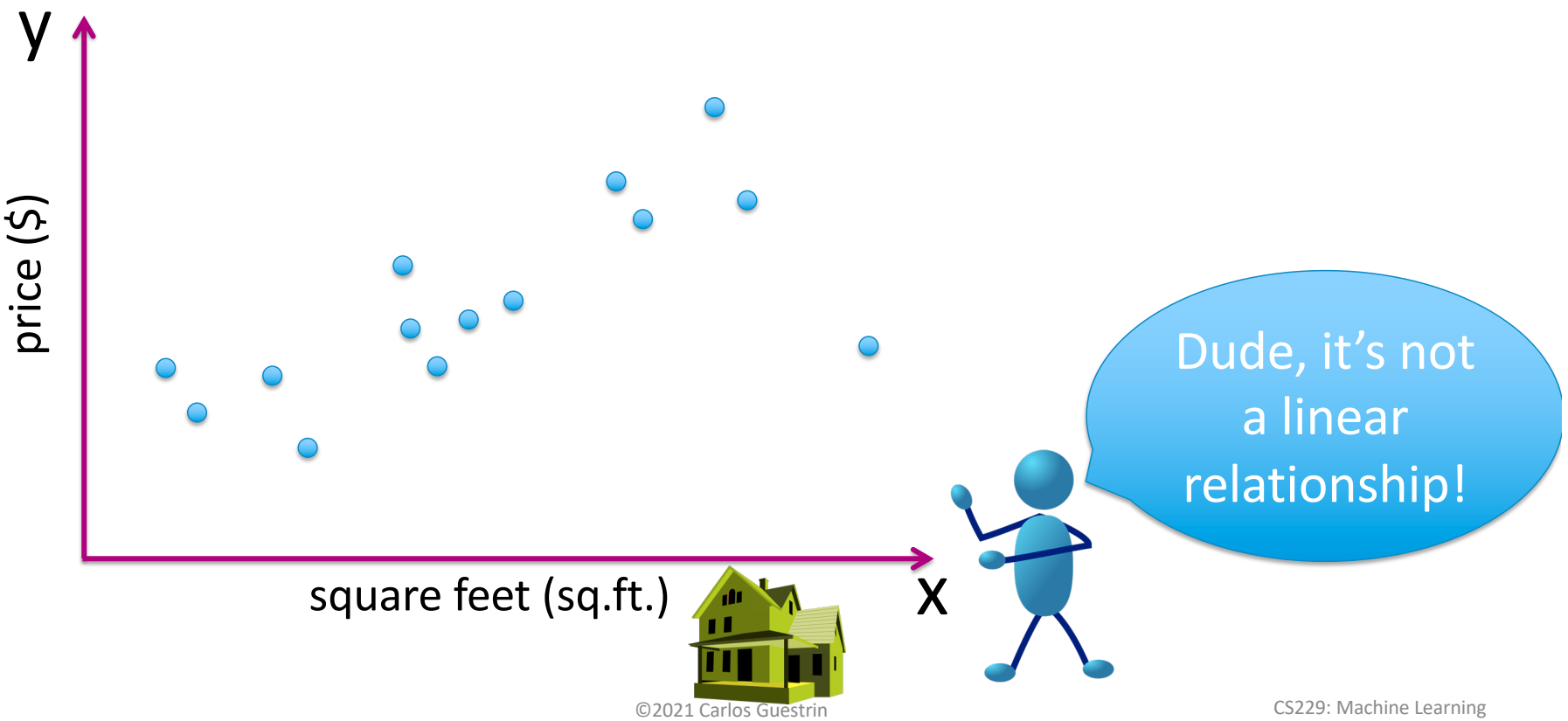
Fit data with a line or … ?



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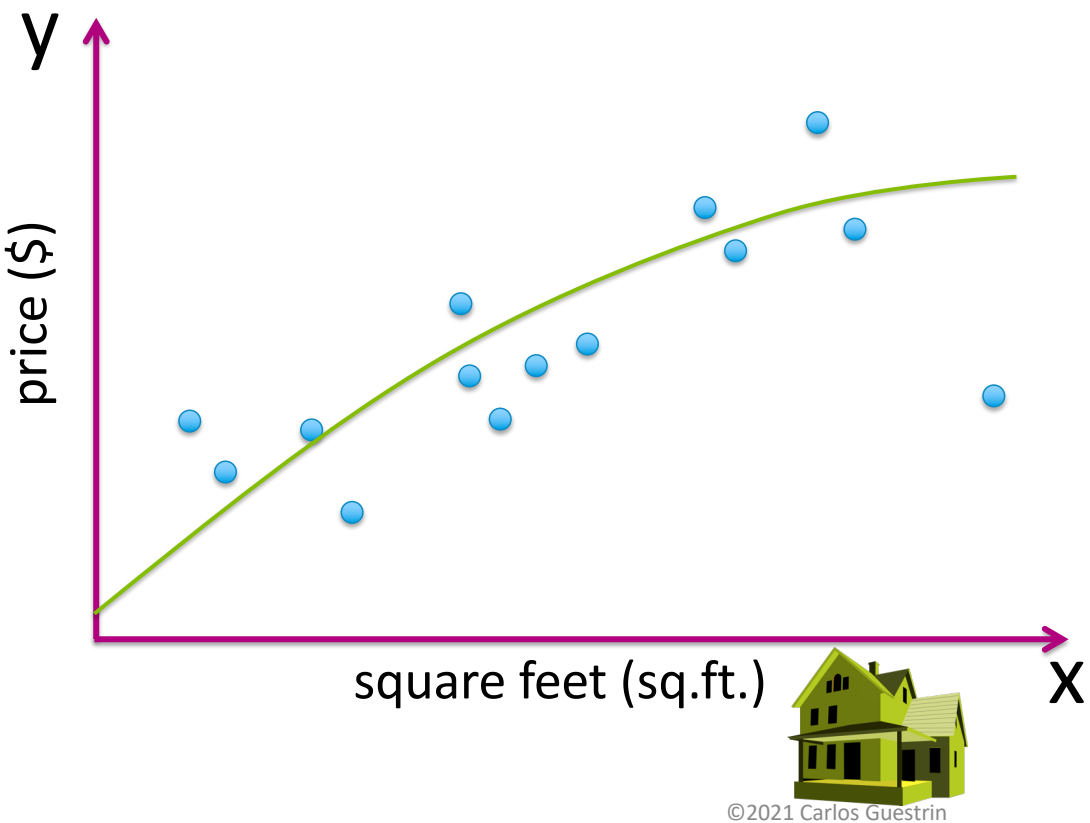
What about a quadratic function?



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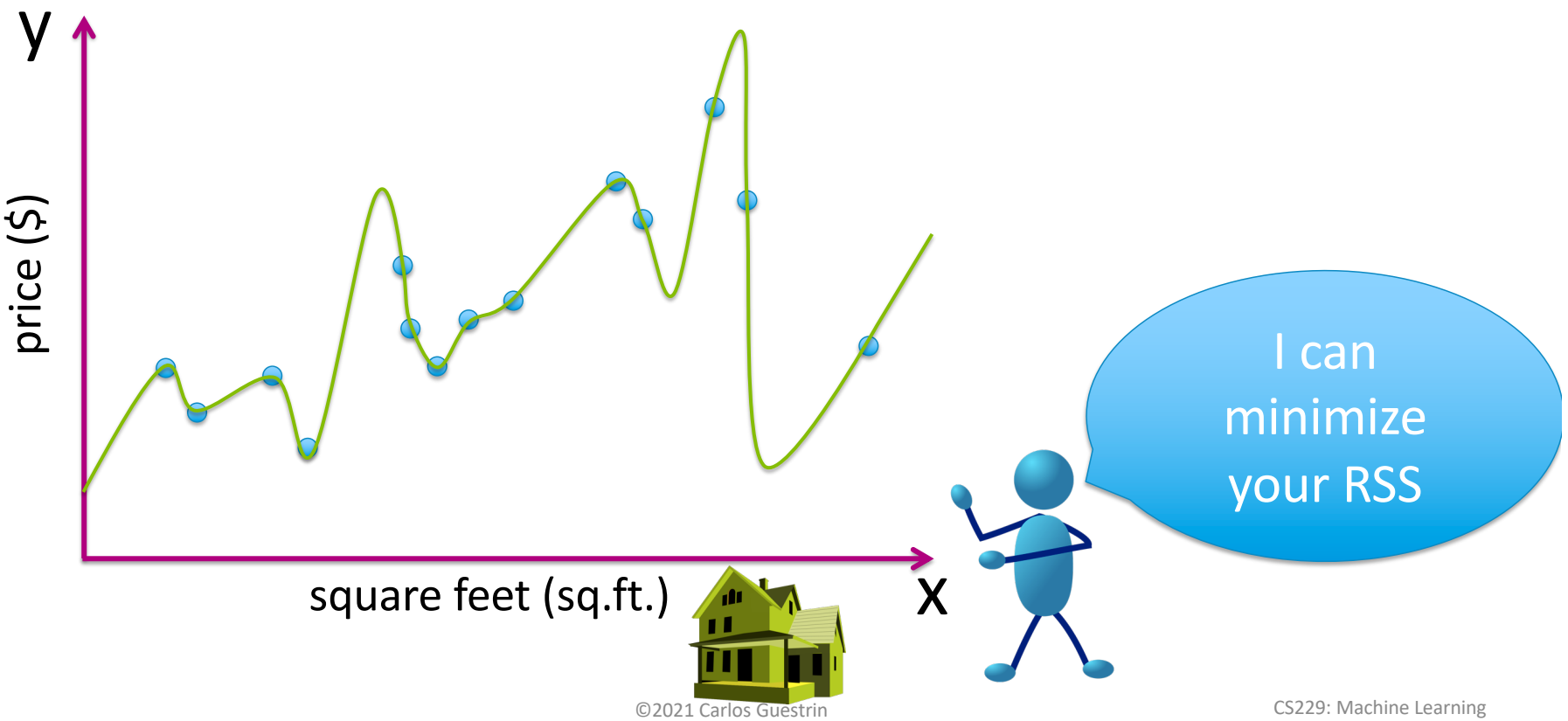
Even higher order polynomial



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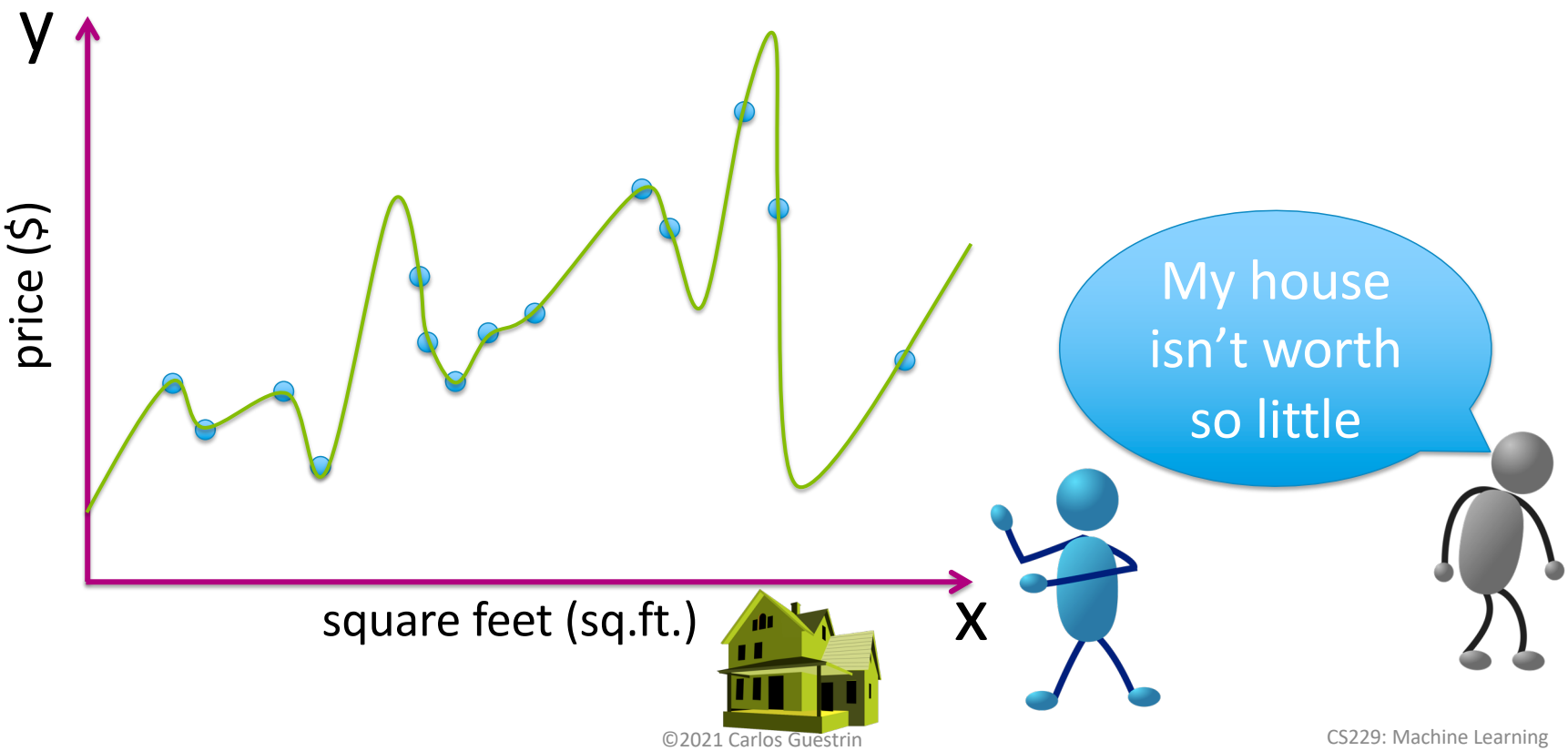
Do you believe this fit?



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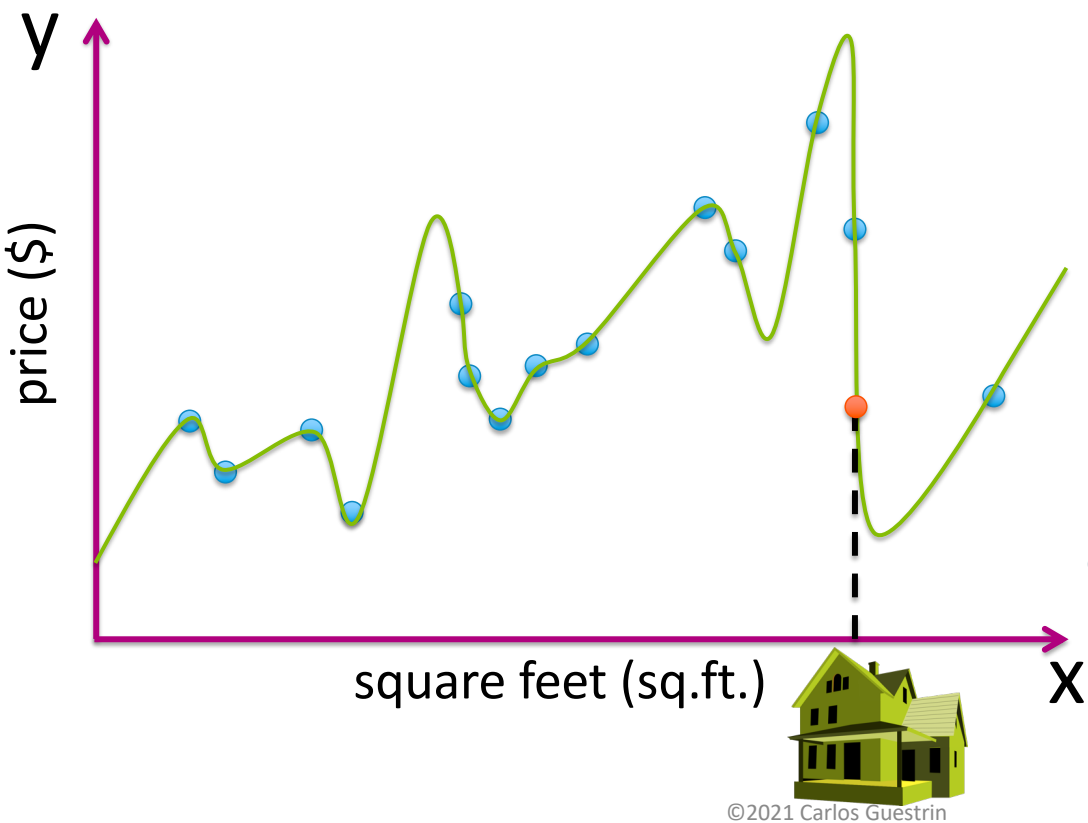
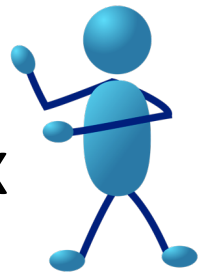
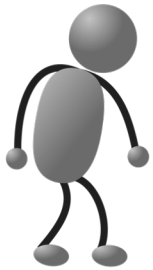
Do you believe this fit?



Minimizes RSS,
but bad predictions





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"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful." George Box, 1987.

Assessing the loss

Assessing the loss
Part 1: Training error

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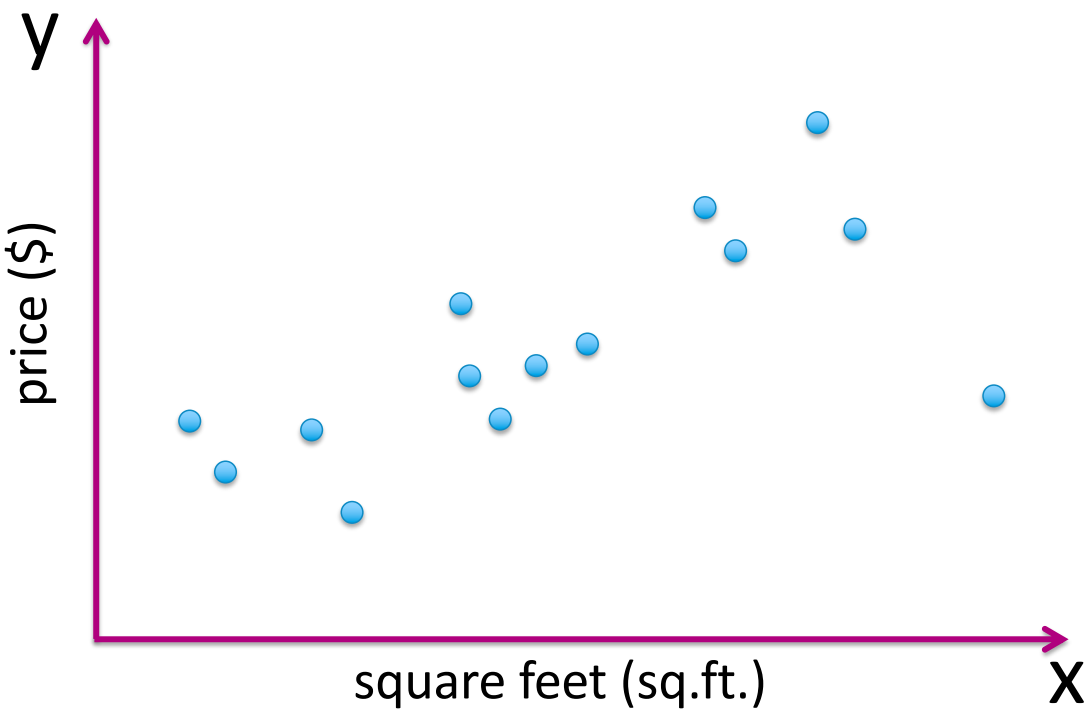
Define training data



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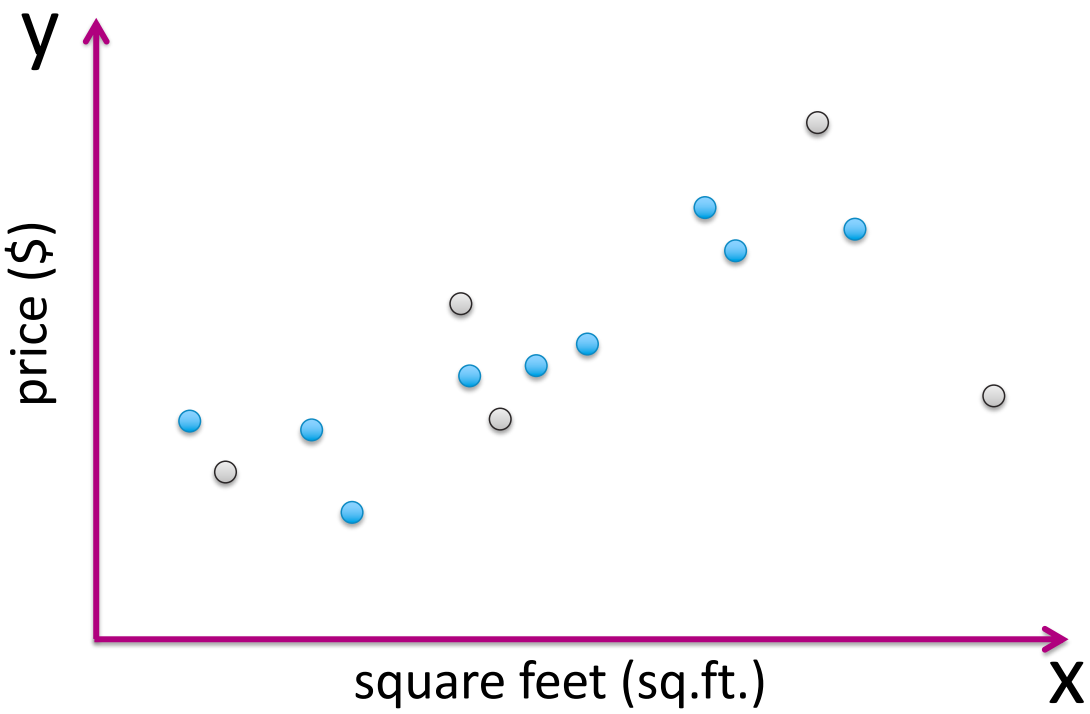
Define training data



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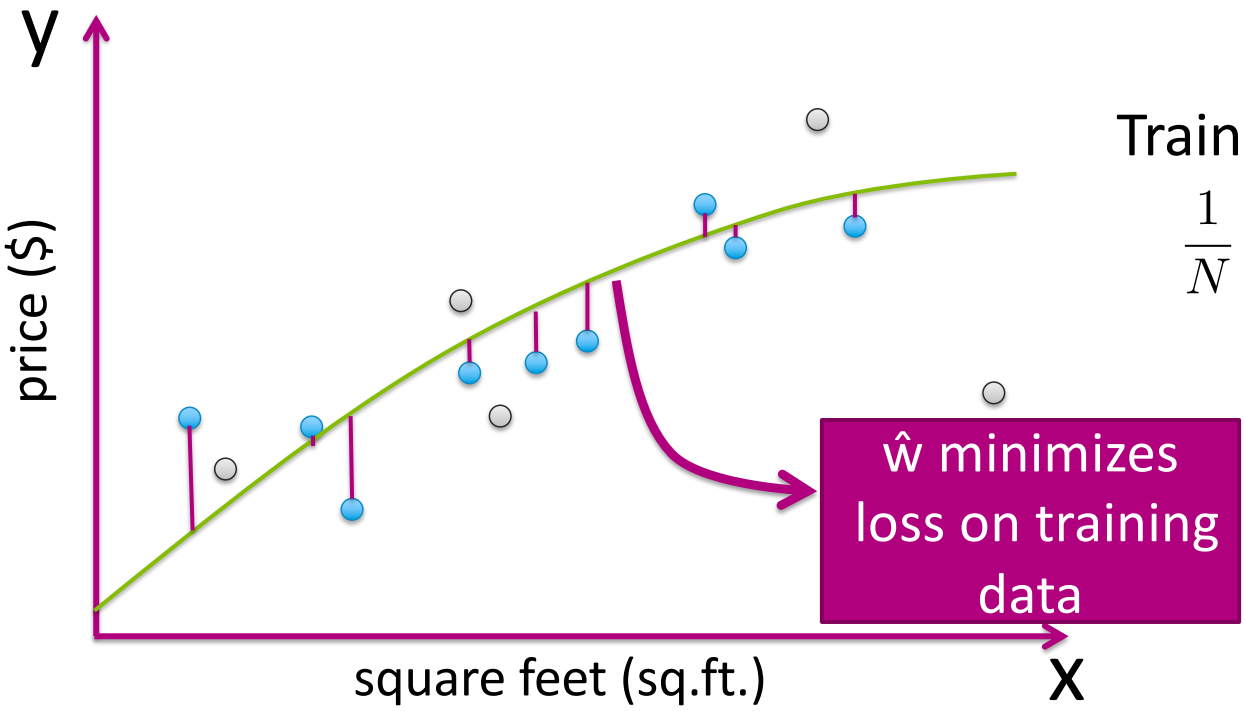
Example:
Fit quadratic to minimize RSS



Training error ($\hat{w}$) =

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\hat{w}}(x_i))^2$$

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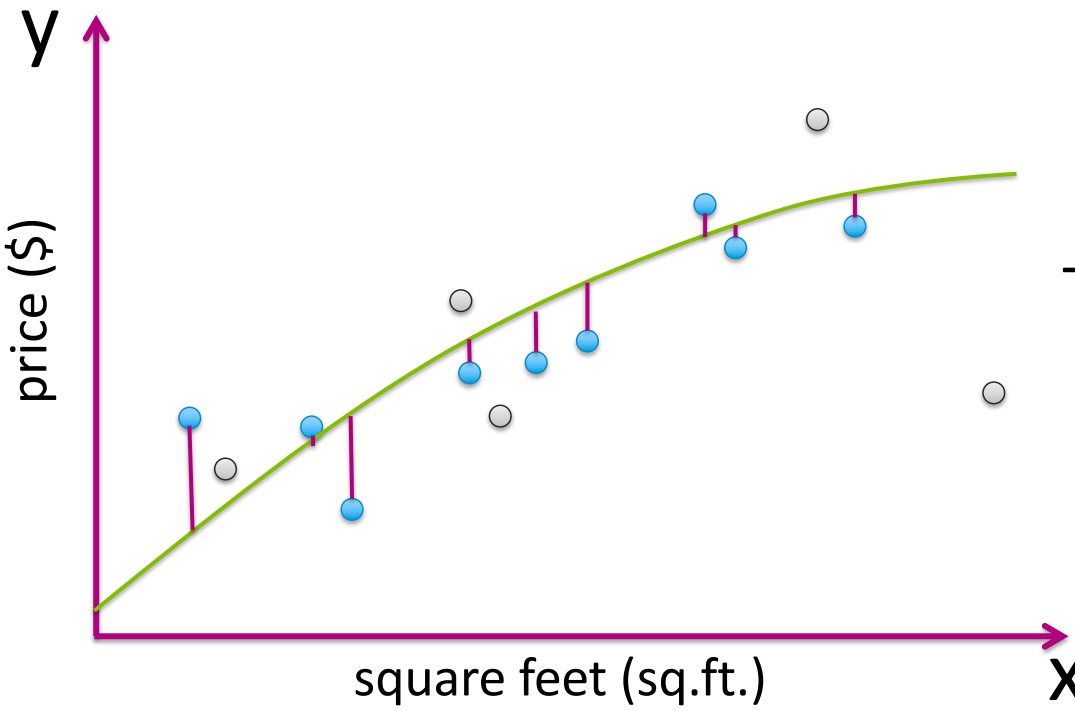
Example:

Use squared error loss $(y-f_{\hat{w}}(x))^2$



Training error ($\hat{w}$) = 1/N *

$[(\$_{\text{train 1}}-f_{\hat{w}}(\text{sq.ft.}_{\text{train 1}}))^2$

$+ (\$_{\text{train 2}}-f_{\hat{w}}(\text{sq.ft.}_{\text{train 2}}))^2$

$+ (\$_{\text{train 3}}-f_{\hat{w}}(\text{sq.ft.}_{\text{train 3}}))^2$

+ … include all training houses]

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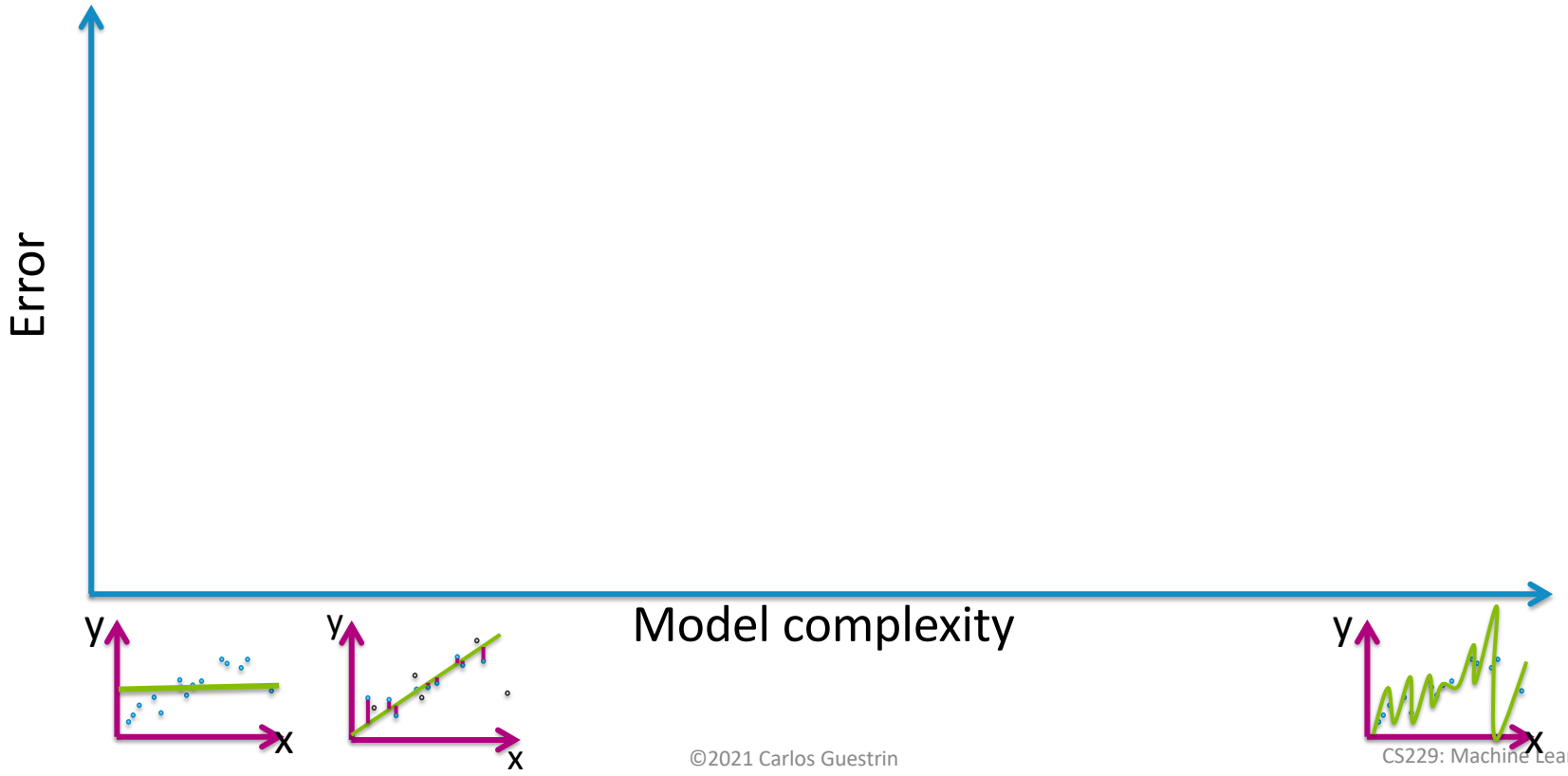
Training error vs. model complexity



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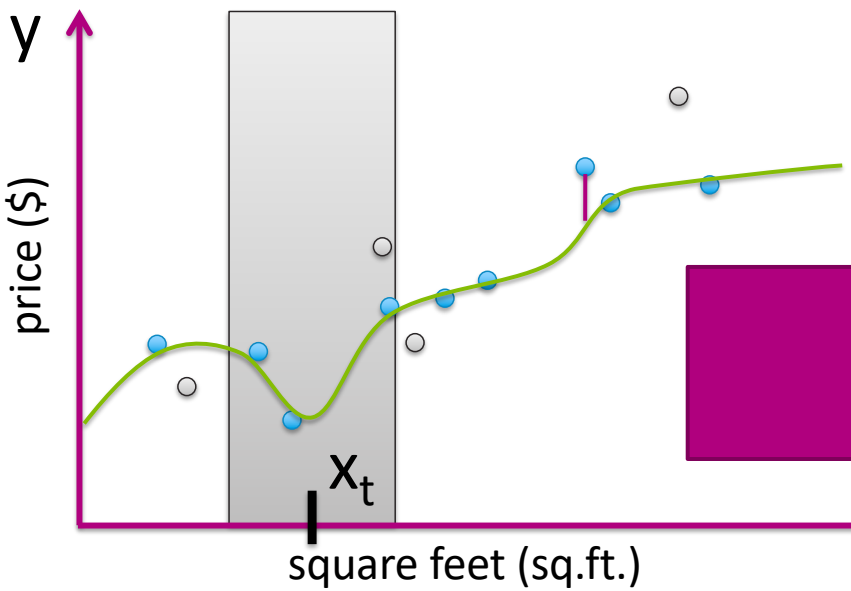
Is training error a good measure of predictive performance?

Issue:

Training error is overly optimistic…$\hat{w}$ was fit to training data



Small training error ≠ good predictions
(unless training data includes
everything you might ever see)

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Assessing the loss
Part 2: Generalization (true) error

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Generalization error

Really want estimate of loss over all possible (🏠,$) pairs

Lots of houses
in neighborhood,
but not in dataset

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Generalization error definition

Really want estimate of loss over all possible (,$) pairs

Formally:

average over all possible (x,y) pairs weighted by how likely each is

$$\text{generalization error} = E_{x,y}\left[L(y, f_{\hat{w}}(x))\right]$$

fit using training data

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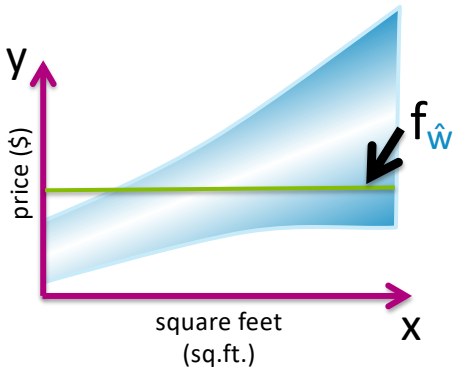
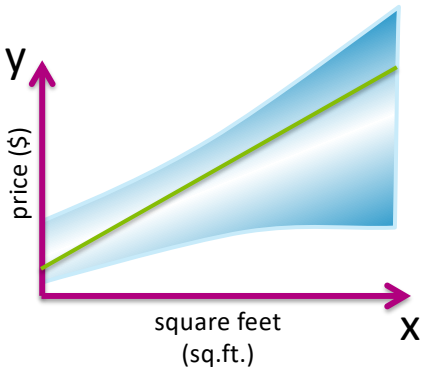
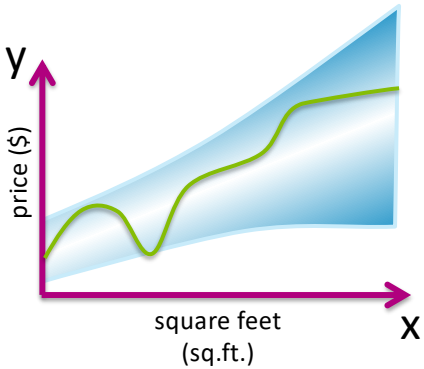
Generalization error vs. model complexity







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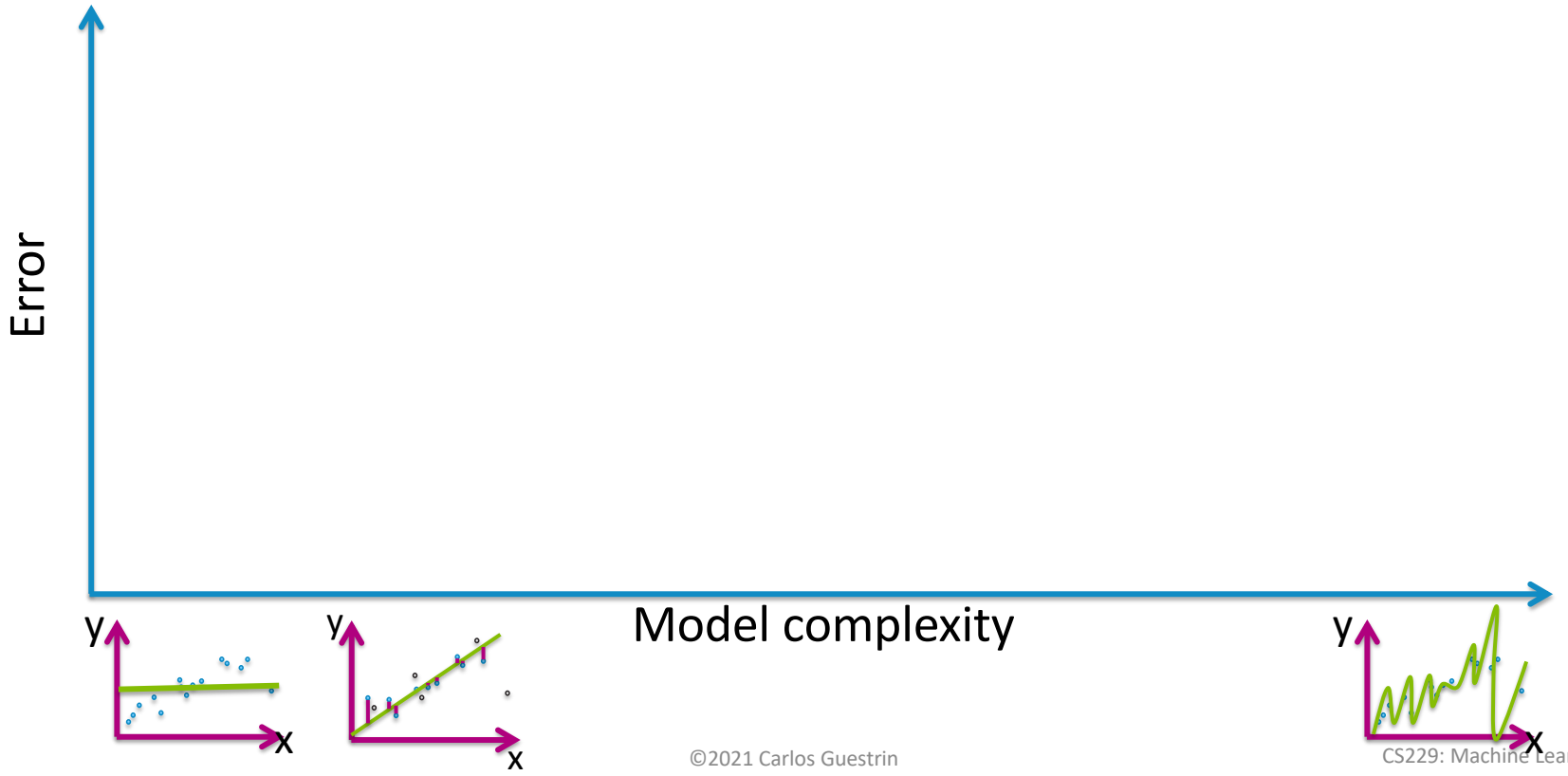
True error vs. model complexity



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Assessing the loss
Part 3: Test error

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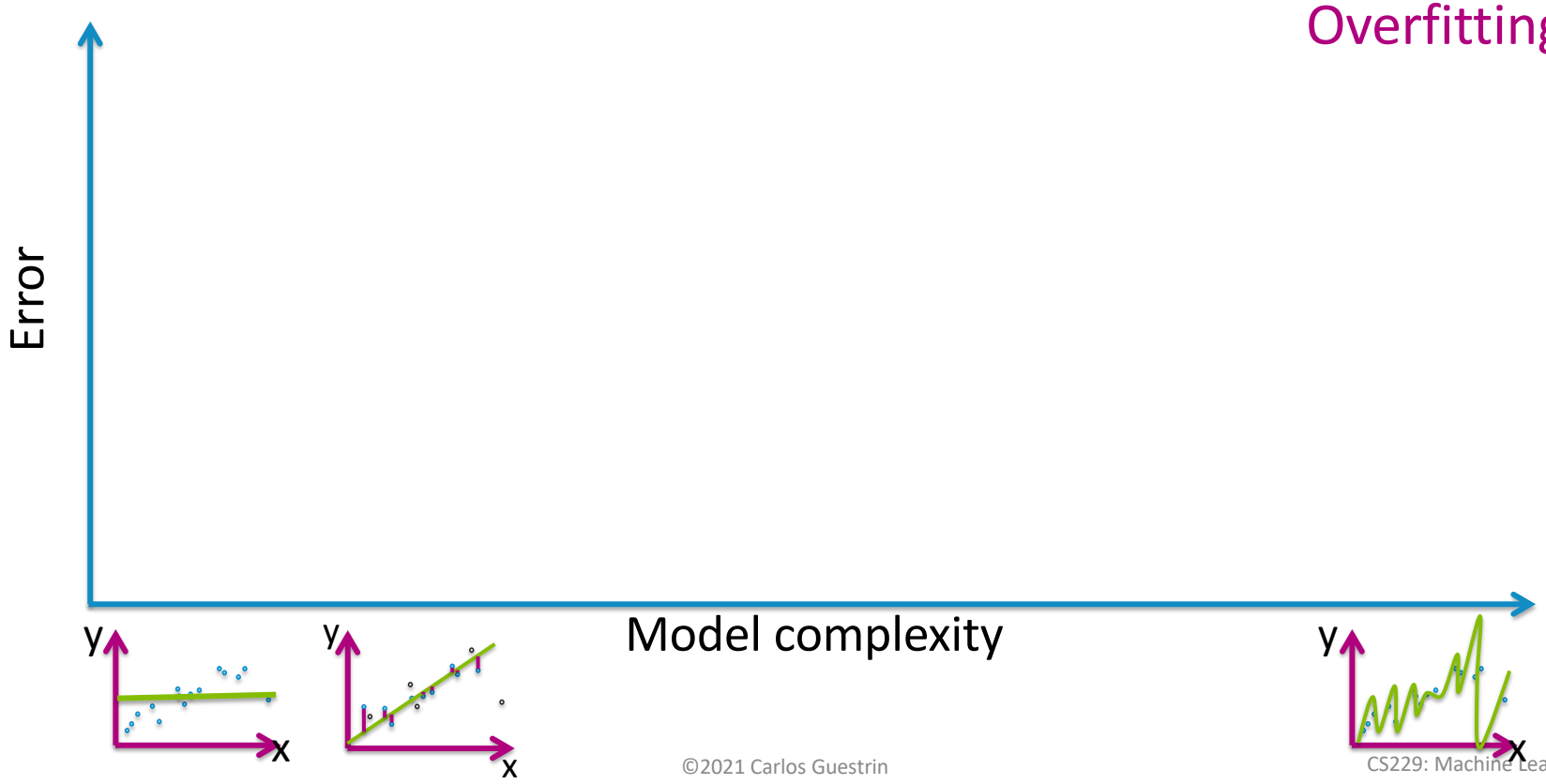
Training, true, test error vs. model complexity

Overfitting if:



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3 sources of error + the bias-variance tradeoff

3 sources of error

In forming predictions, there are 3 sources of error:

1. Noise
2. Bias
3. Variance

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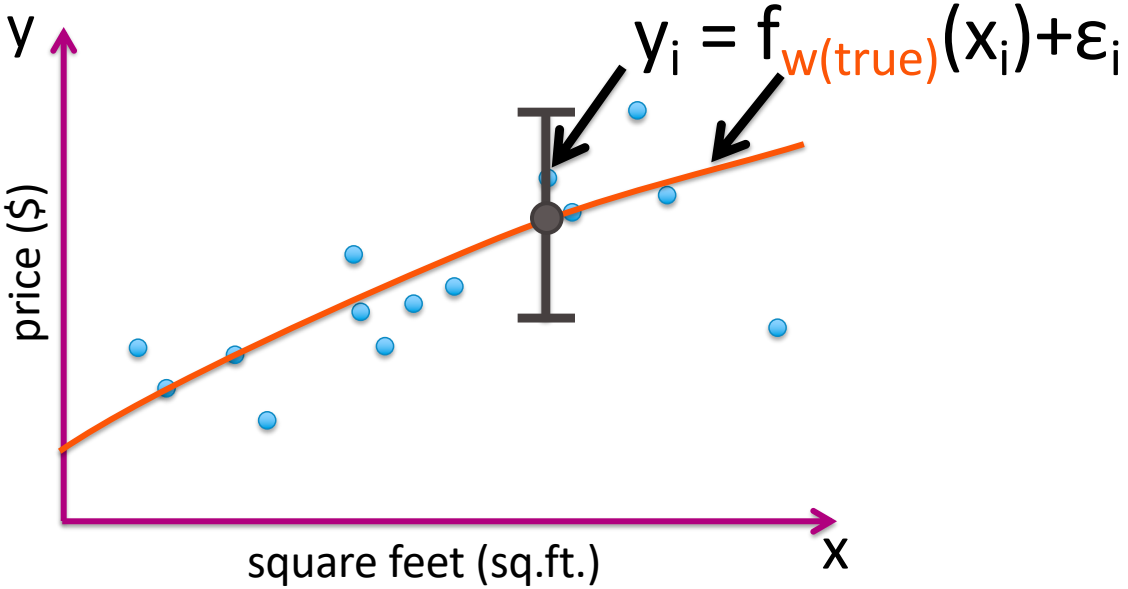
Data inherently noisy



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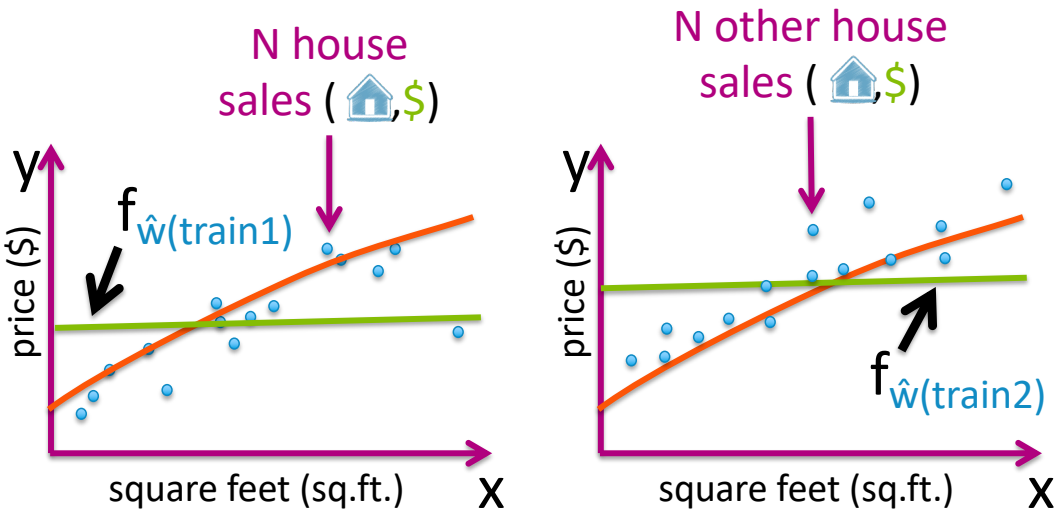
Bias contribution

Suppose we fit a constant function



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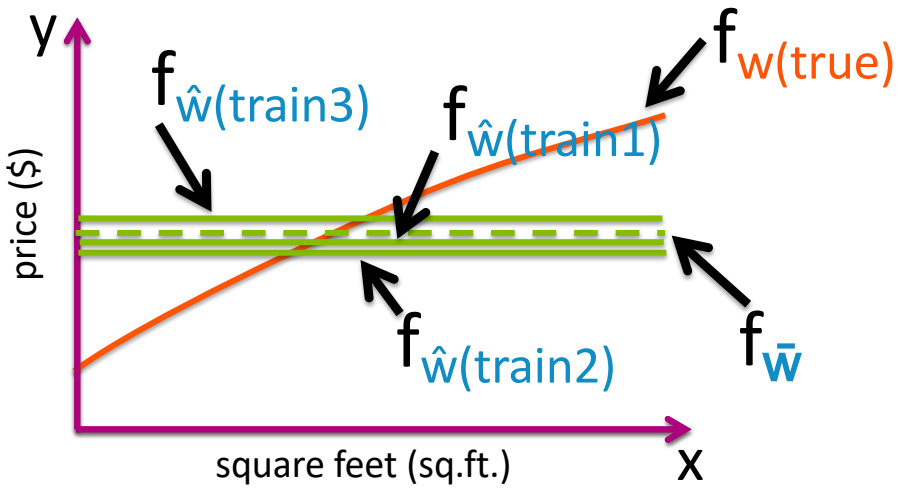
Bias contribution

Over all possible size N training sets,
what do I expect my fit to be?



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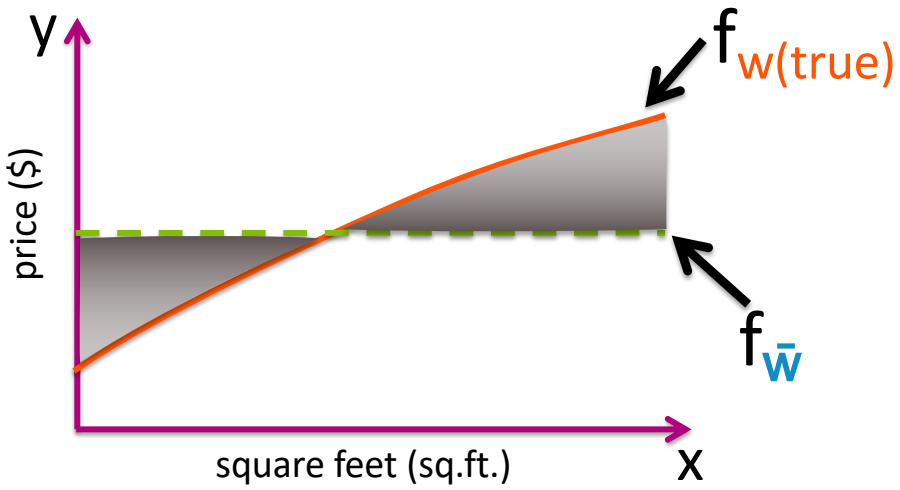
Bias contribution

$\text{Bias}(x) = f_{w(\text{true})}(x) - f_{\bar{w}}(x)$

← Is our approach flexible enough to capture $f_{w(\text{true})}$?
If not, error in predictions.



low complexity →

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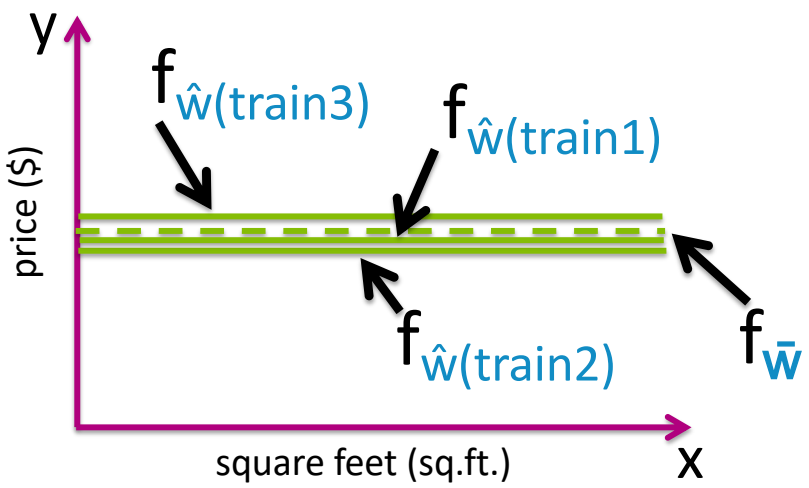
Variance contribution

How much do specific fits vary from the expected fit?



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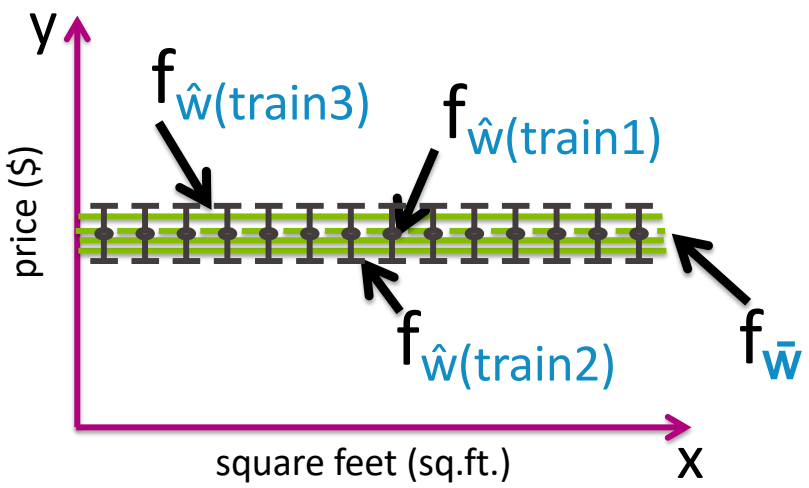

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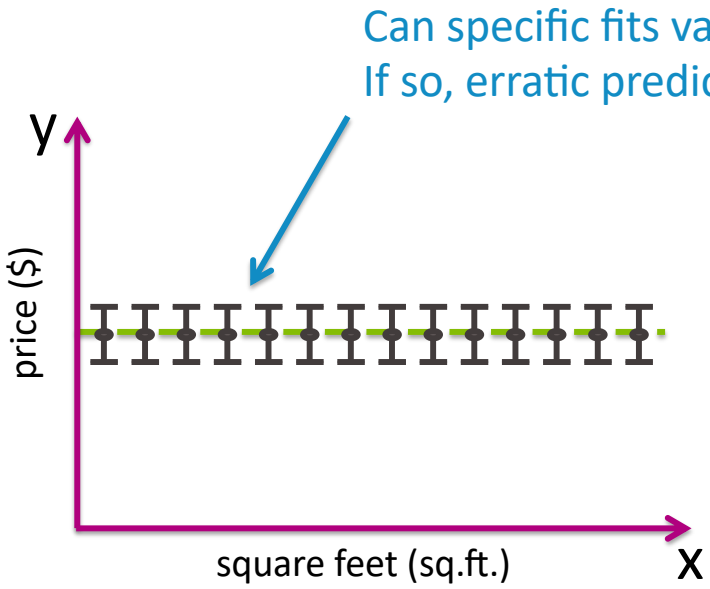

low complexity
→

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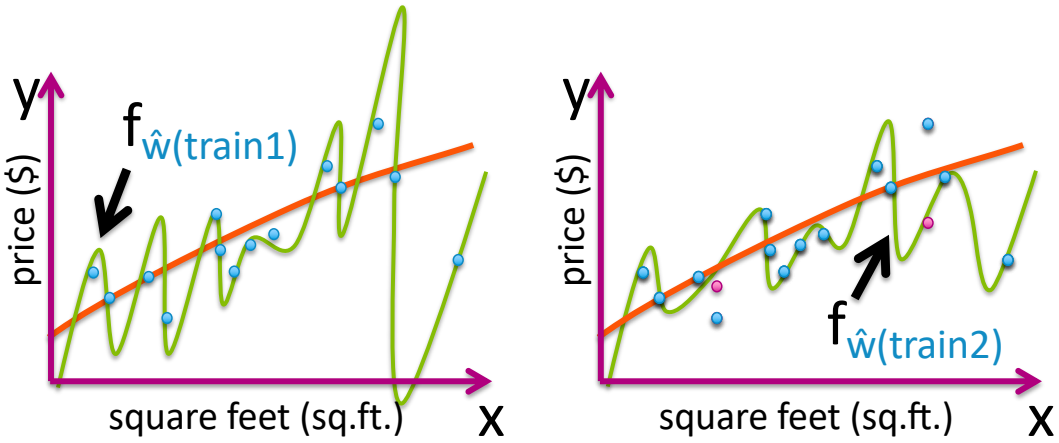
Variance of high-complexity models

Assume we fit a high-order polynomial



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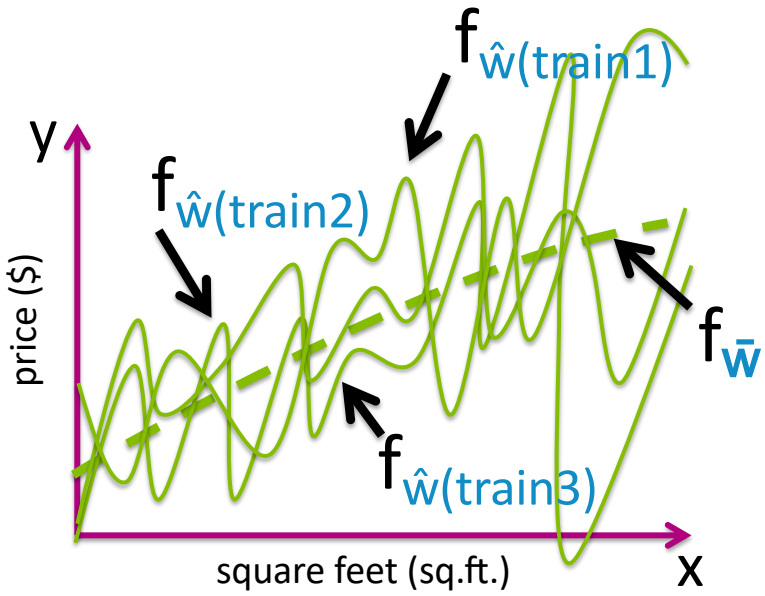
Variance of high-complexity models

Suppose we fit a high-order polynomial



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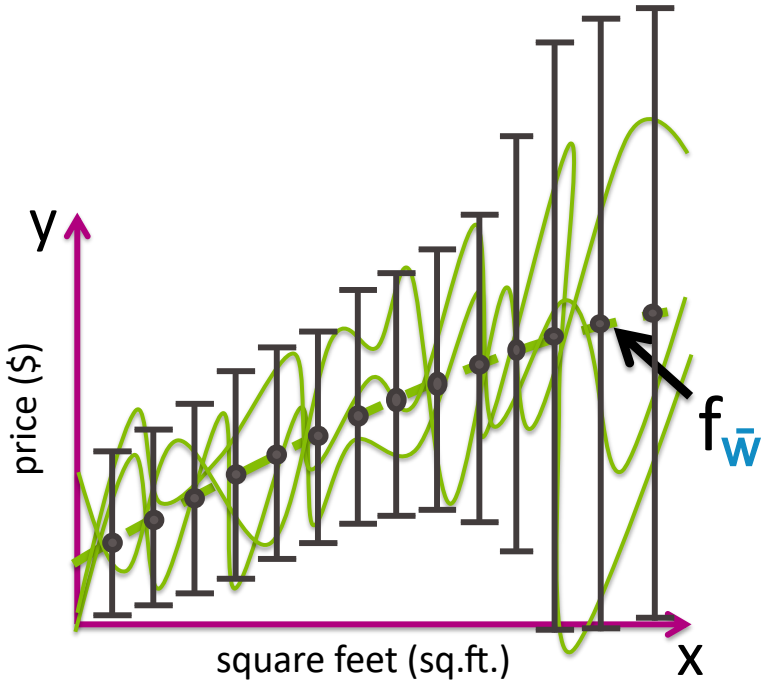
Variance of high-complexity models



high complexity
→

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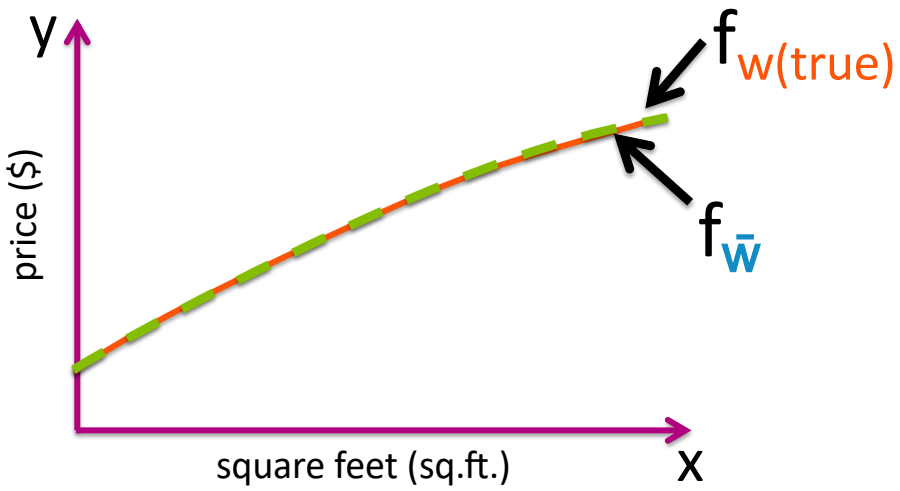
Bias of high-complexity models



high complexity
→

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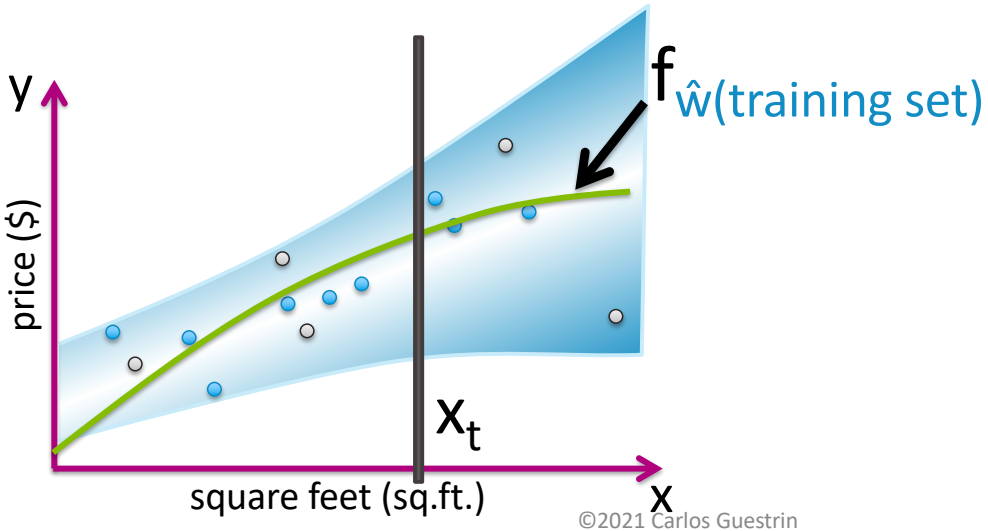
Sum of 3 sources of error

Average squared error at x_t

$$= \sigma^2 + [\text{bias}(f_{\hat{w}}(x_t))]^2 + \text{var}(f_{\hat{w}}(x_t))$$



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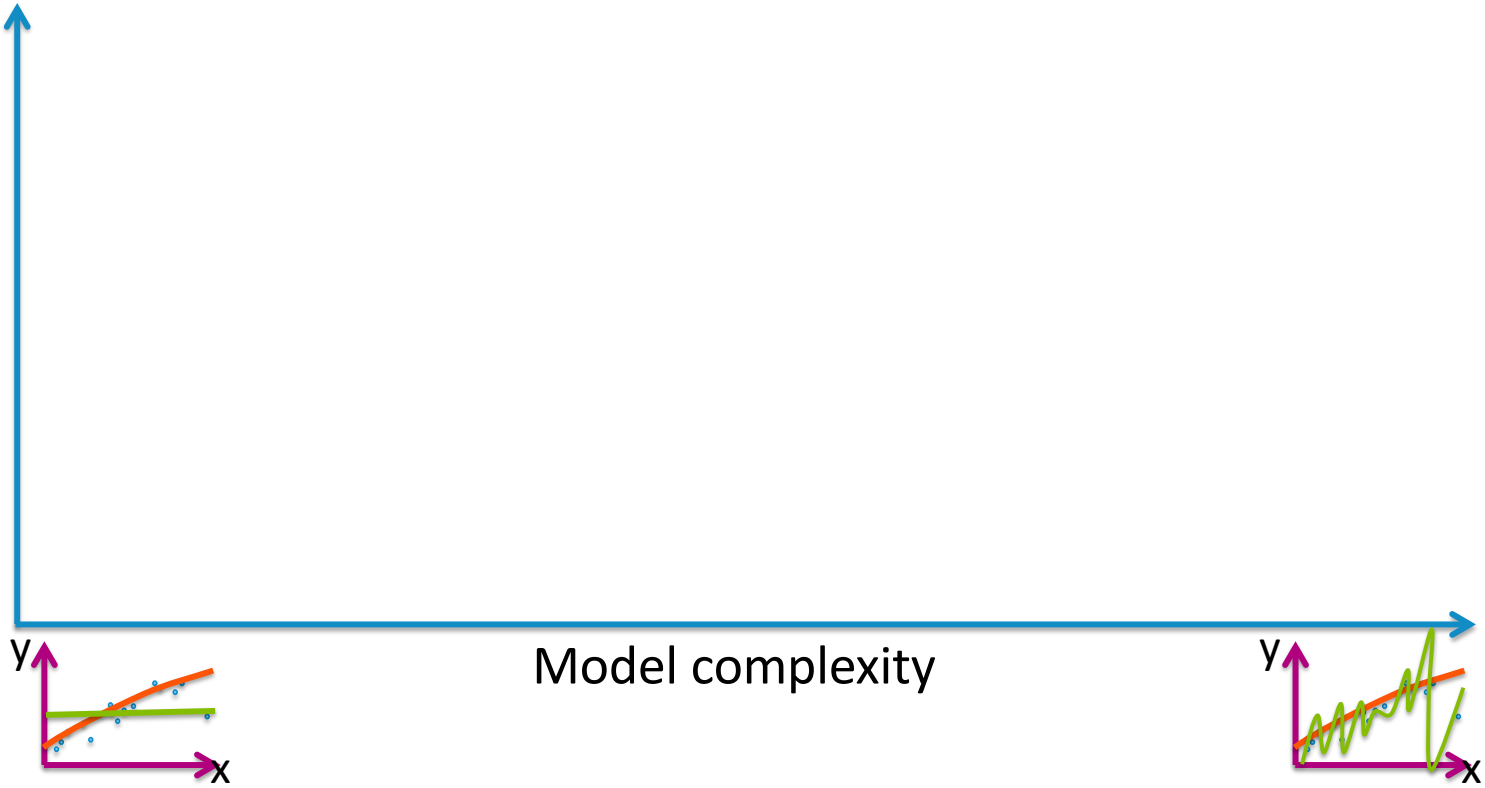
Bias-variance tradeoff



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Error vs. amount of data

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Summary of bias-variance tradeoff

What you can do now…

- Contrast relationship between model complexity and train, true and test loss
- Compute training and test error given a loss function for different model complexities
- List and interpret the 3 sources of avg. prediction error
  - Irreducible error, bias, and variance

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