Bias-Variance Tradeoff

CS229: Machine Learning
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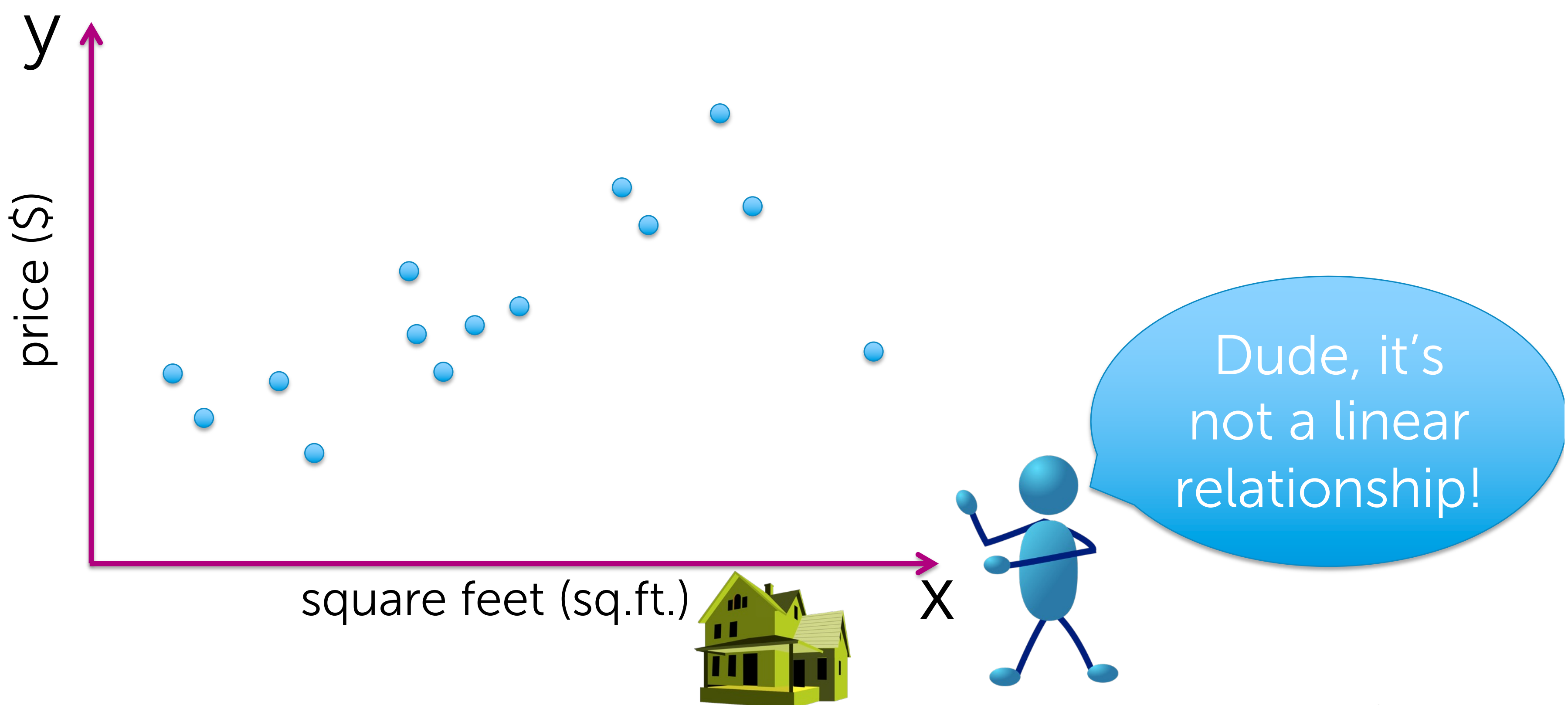
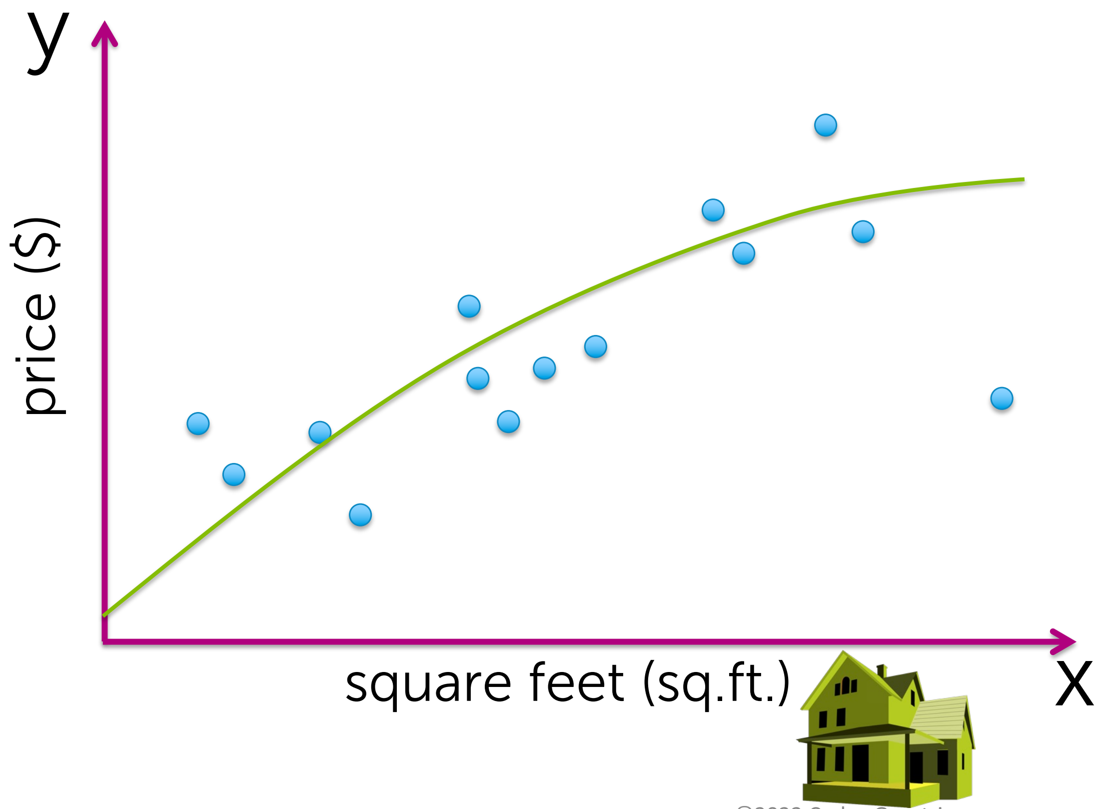
Slides include content developed by and co-developed with Emily Fox

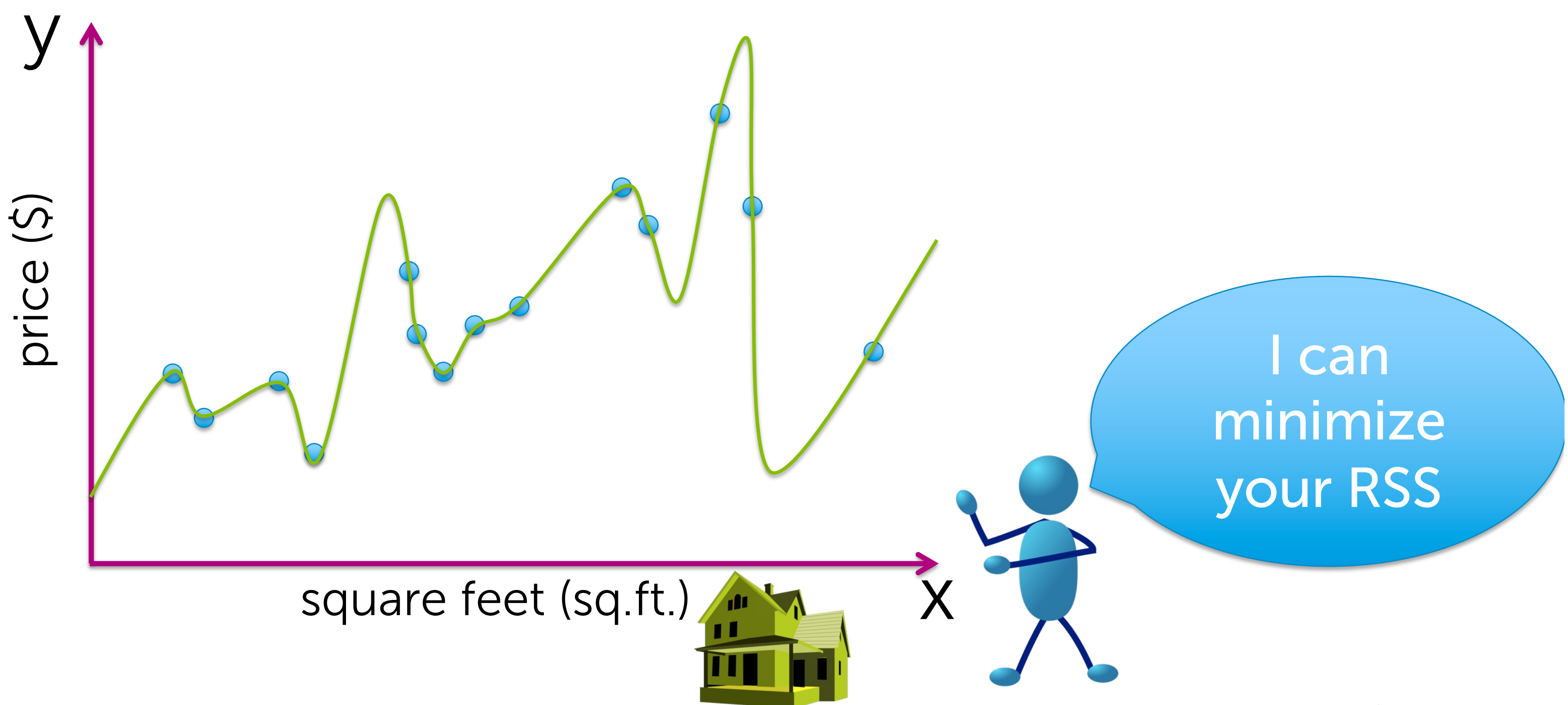
Fit data with a line or … ?



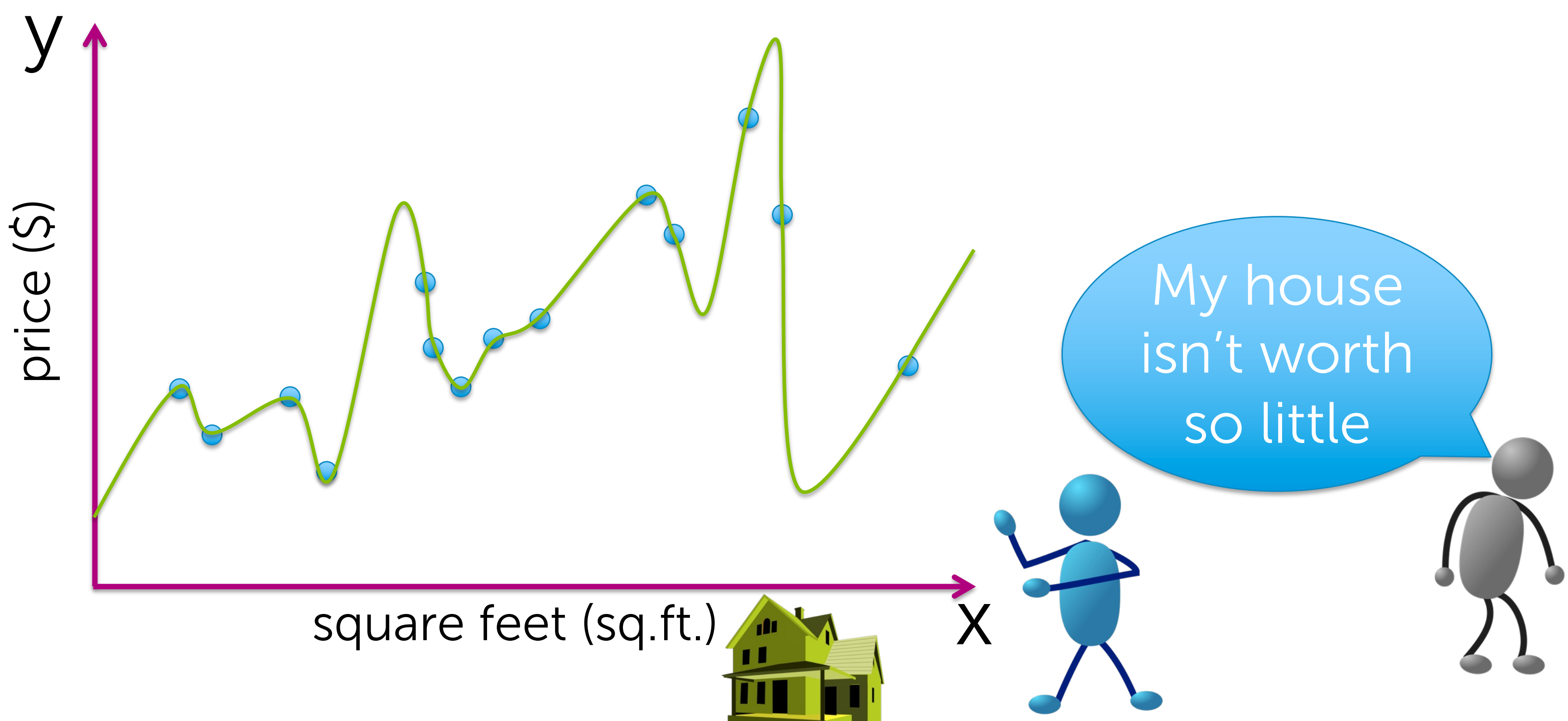
What about a quadratic function?



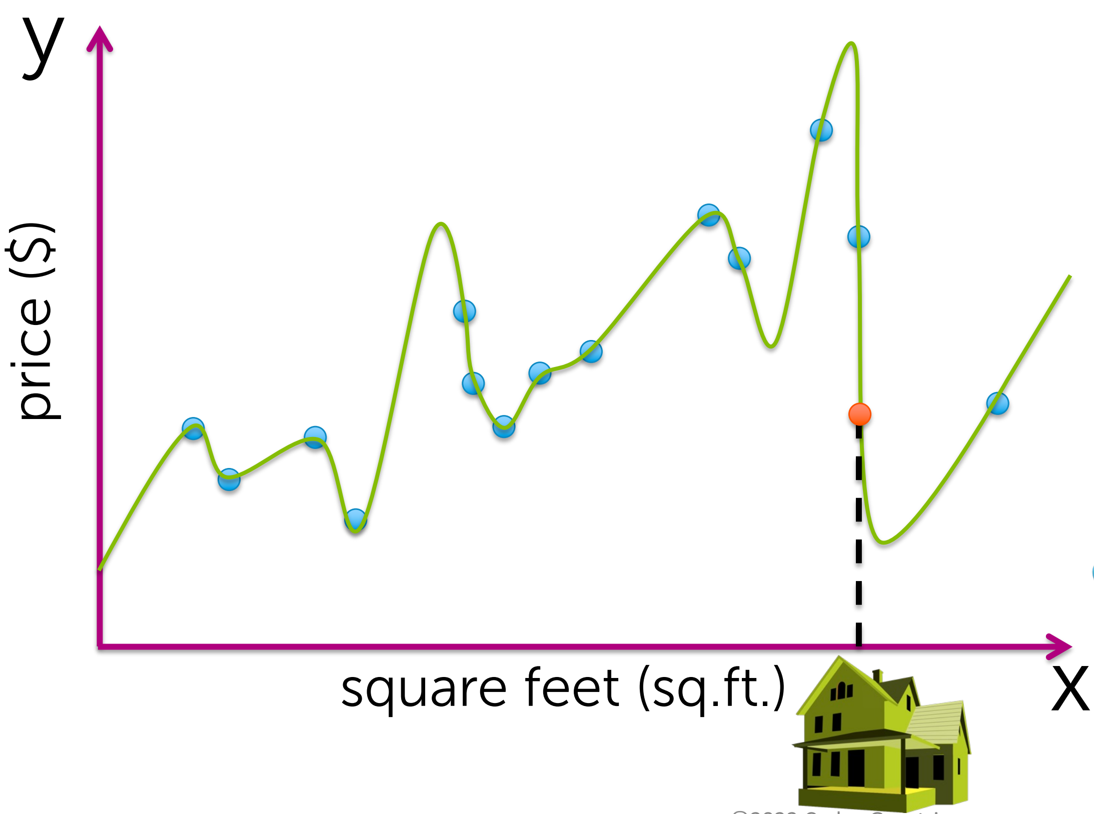
Even higher order polynomial



Do you believe this fit?



Do you believe this fit?



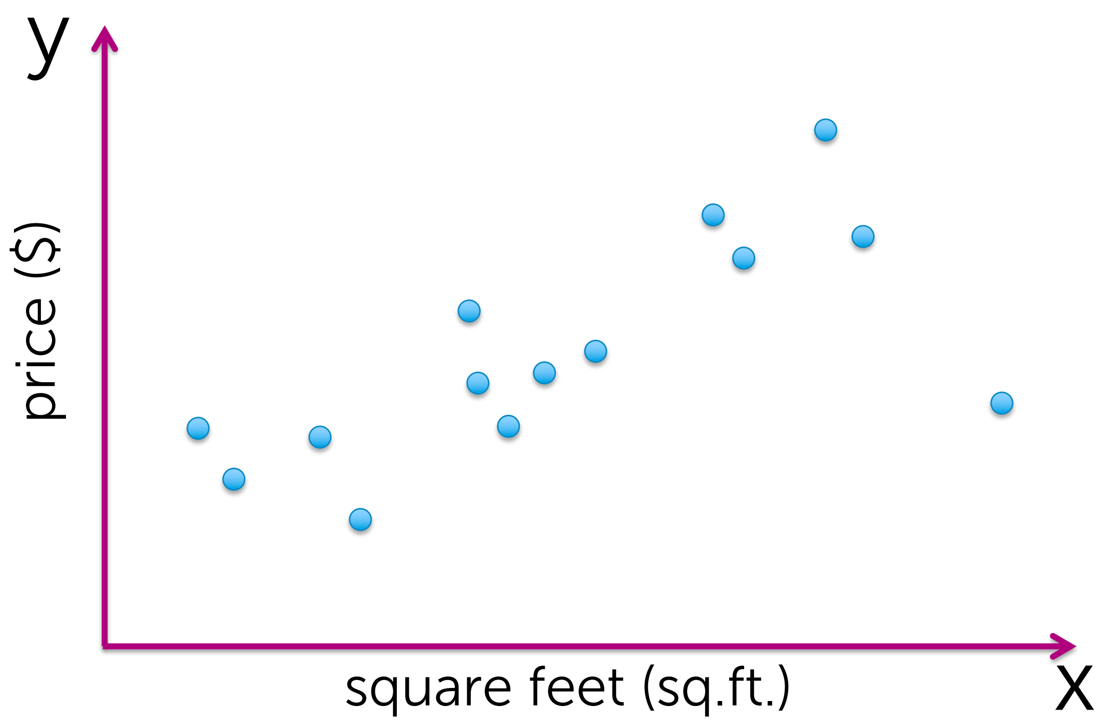
Minimizes RSS,
but bad predictions

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

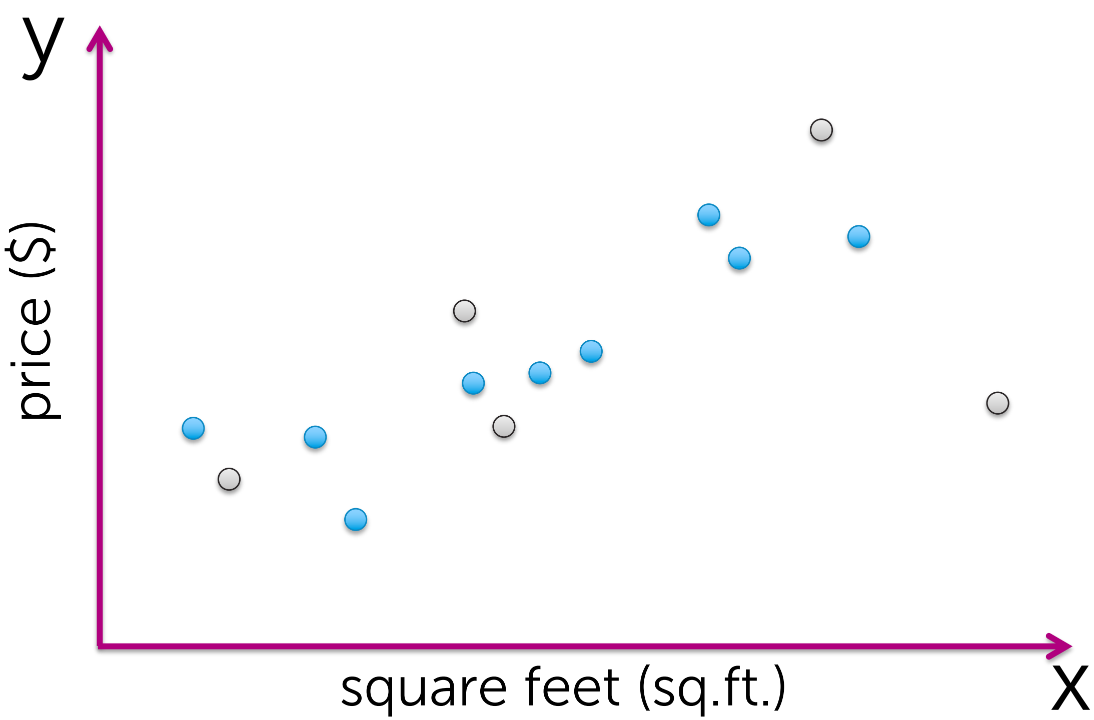
Assessing the loss

Assessing the loss
Part 1: Training error

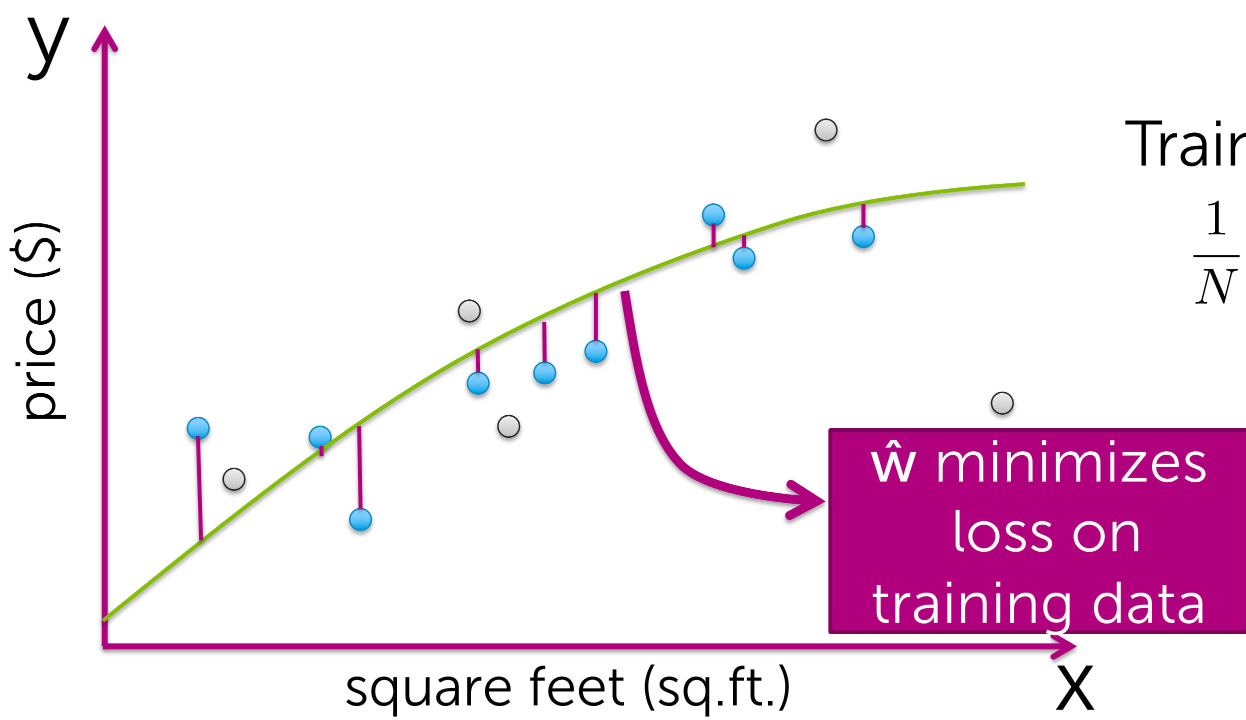
Define training data



Define training data



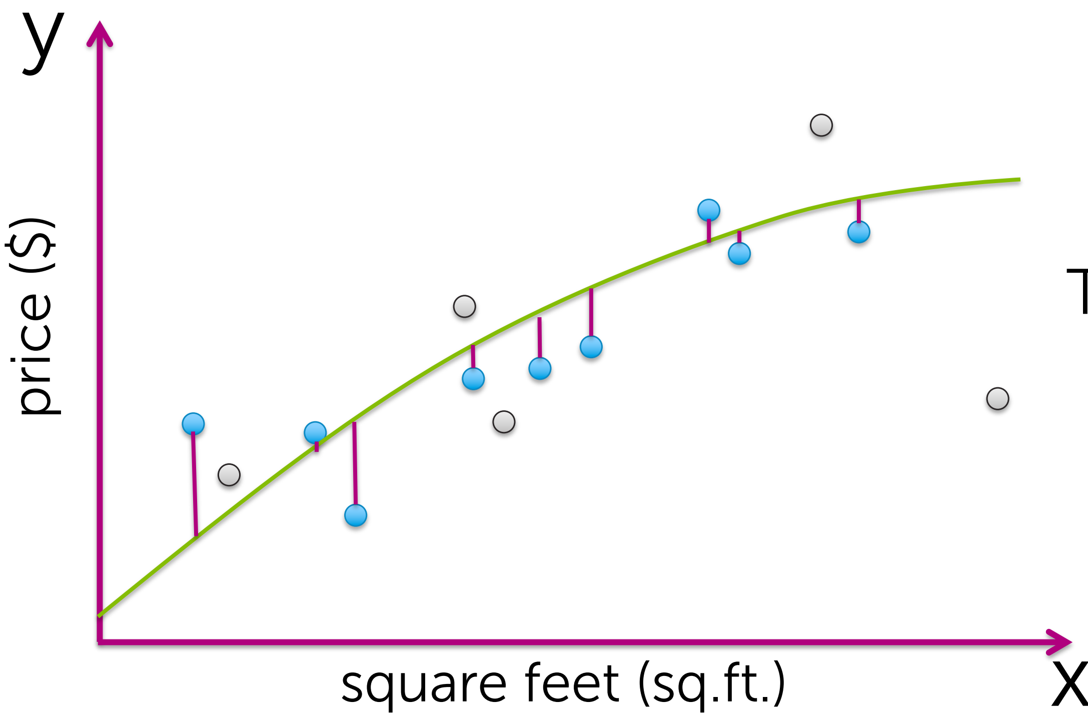
Example:
Fit quadratic to minimize RSS



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

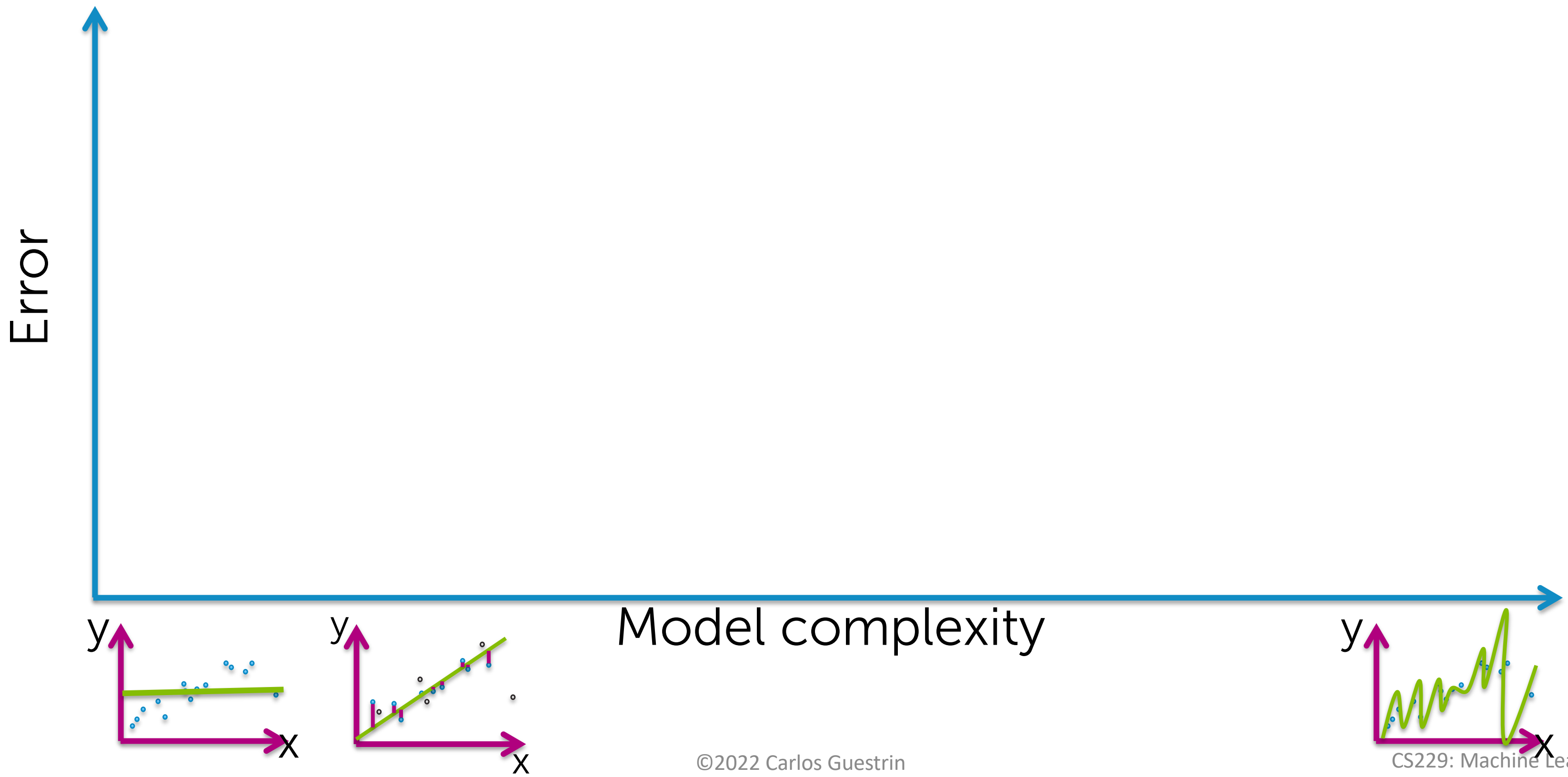
$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\hat{w}}(\mathbf{x}_i))^2$$

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]

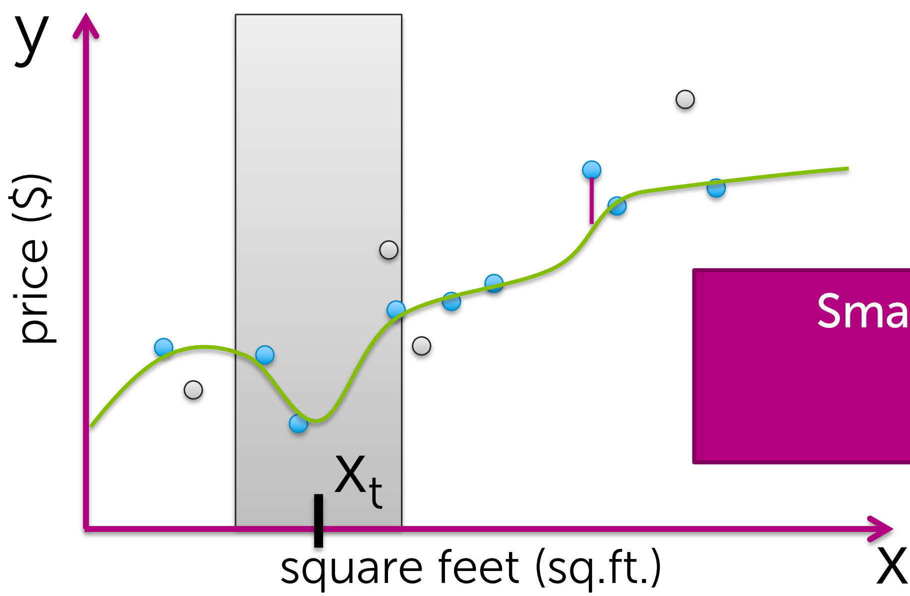
Training error vs. model complexity



Is training error a good measure of predictive performance?

Issue:

Training error is overly optimistic…ŵ was fit to training data



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

Assessing the loss
Part 2: Generalization (true) error

Generalization error

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

Lots of houses
in neighborhood,
but not in dataset

Generalization error definition

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

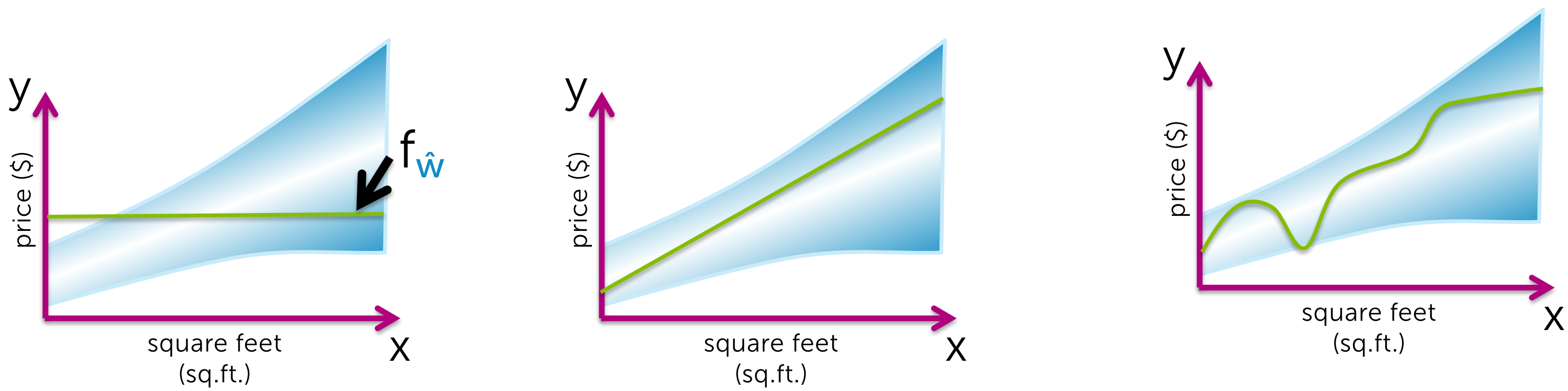
Formally:

average over all possible
($\mathbf{x}$,y) pairs weighted by
how likely each is

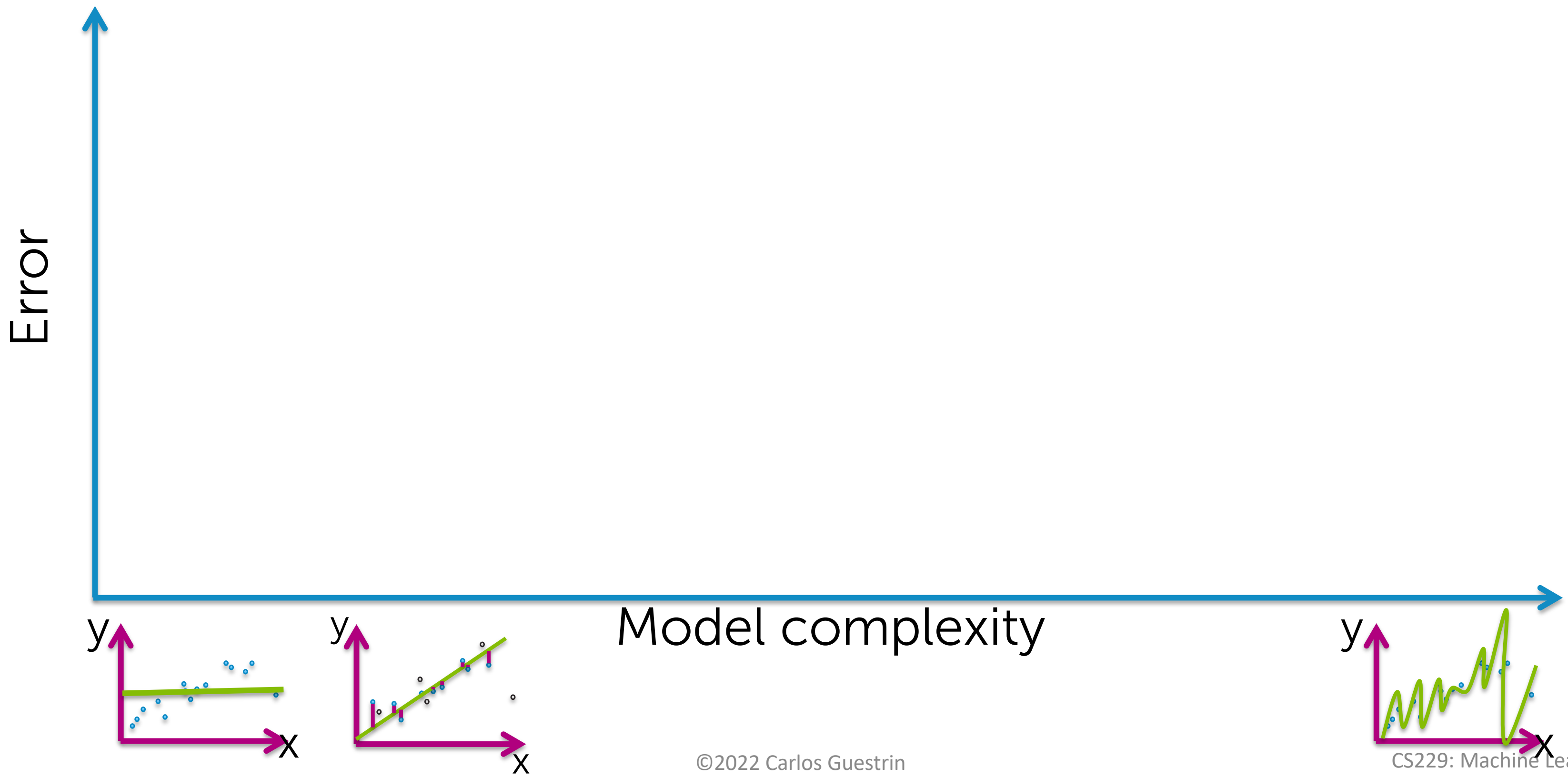
$$\text{generalization error} = E_{\mathbf{x},y}[L(y,f_{\hat{w}}(\mathbf{x}))]$$

fit using training data

Generalization error vs. model complexity



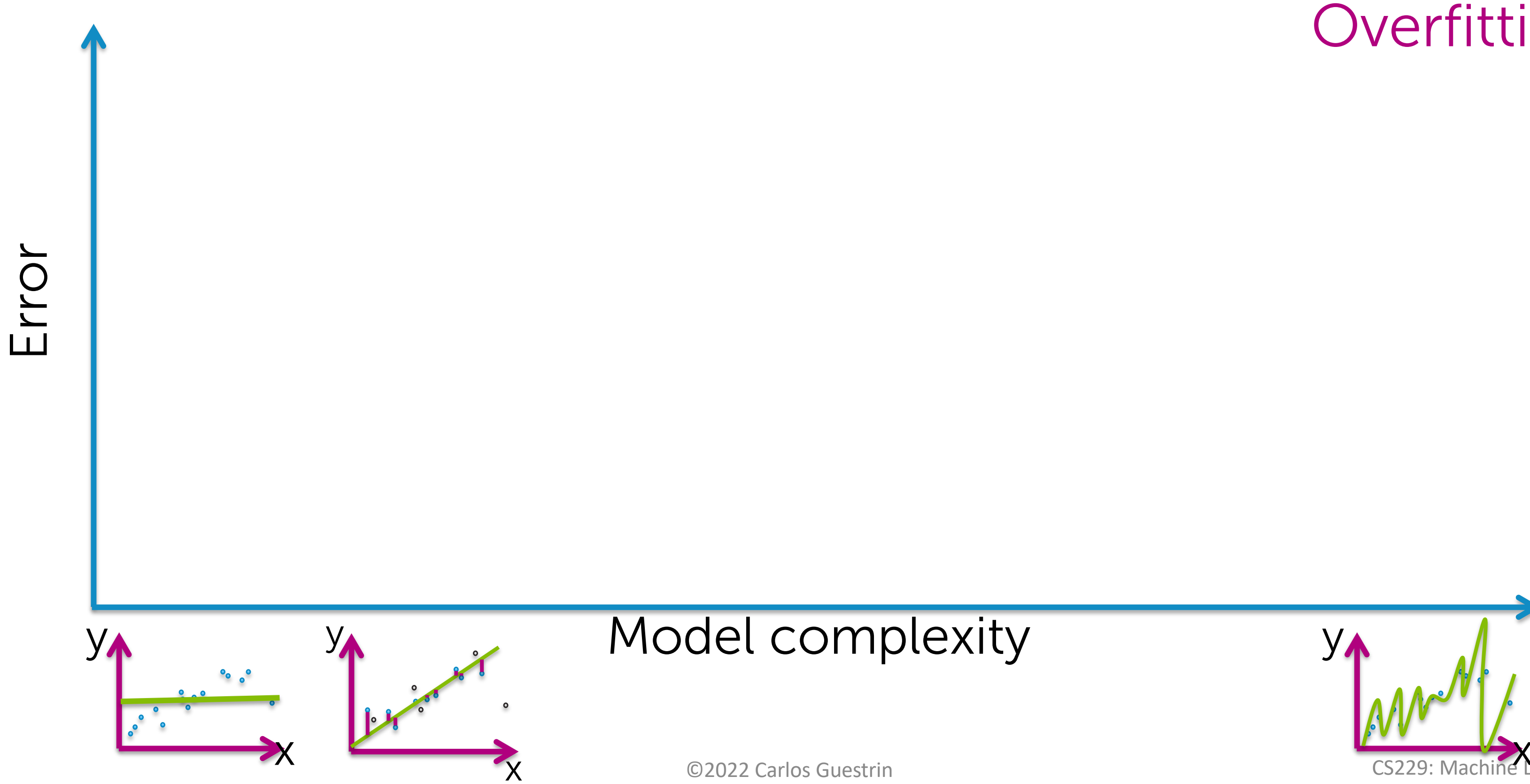
True error vs. model complexity



Assessing the loss
Part 3: Test error

Training, true, test error vs. model complexity

Overfitting if:



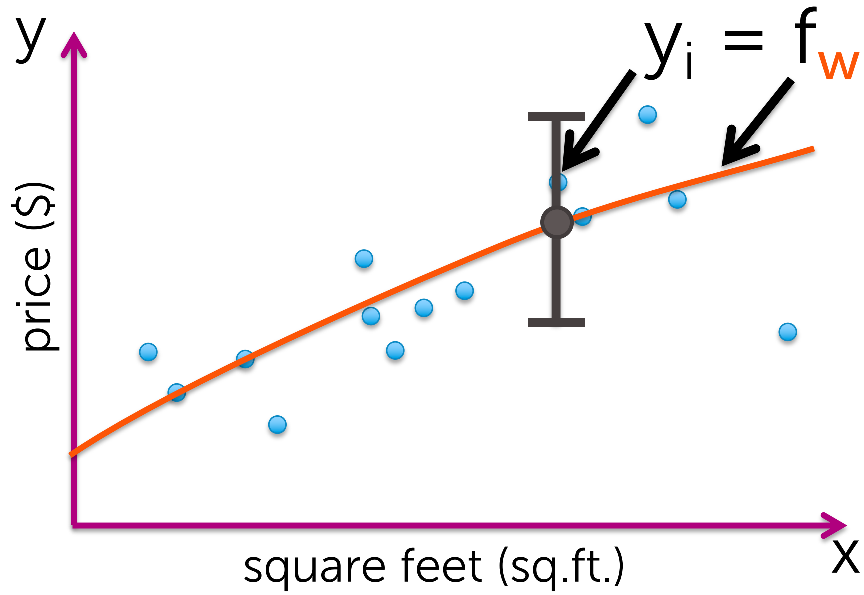
3 sources of error + the bias-variance tradeoff

3 sources of error

In forming predictions, there are 3 sources of error:

1. Noise
2. Bias
3. Variance

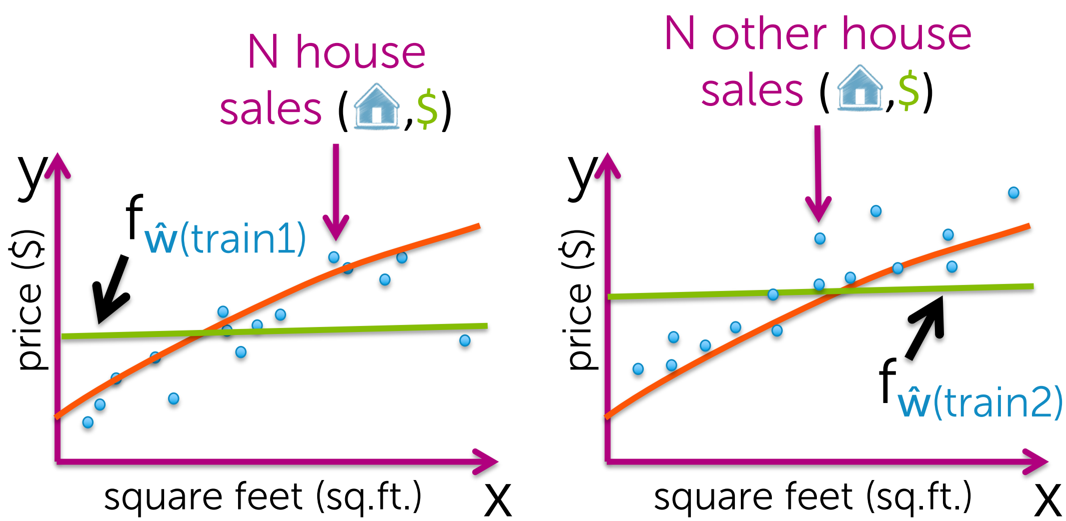
Data inherently noisy



$$y_i = f_{\mathbf{w}(\text{true})}(\mathbf{x}_i) + \varepsilon_i$$

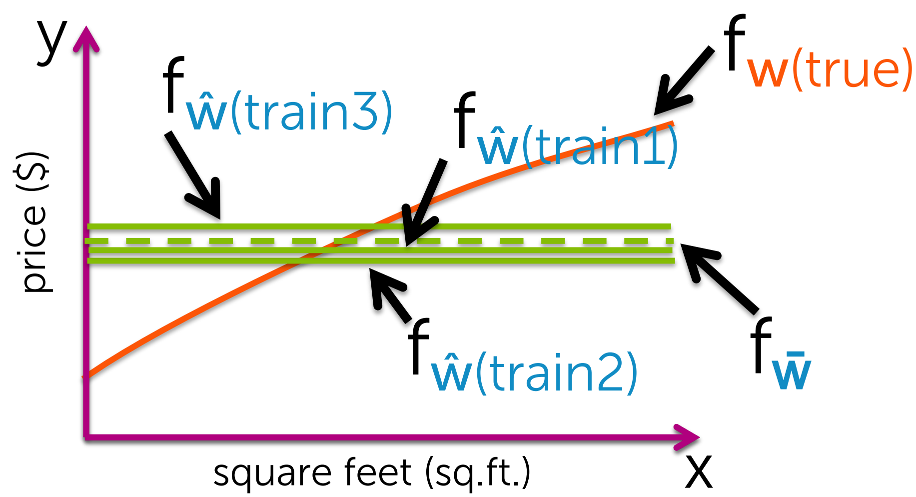
Bias contribution

Suppose we fit a constant function



Bias contribution

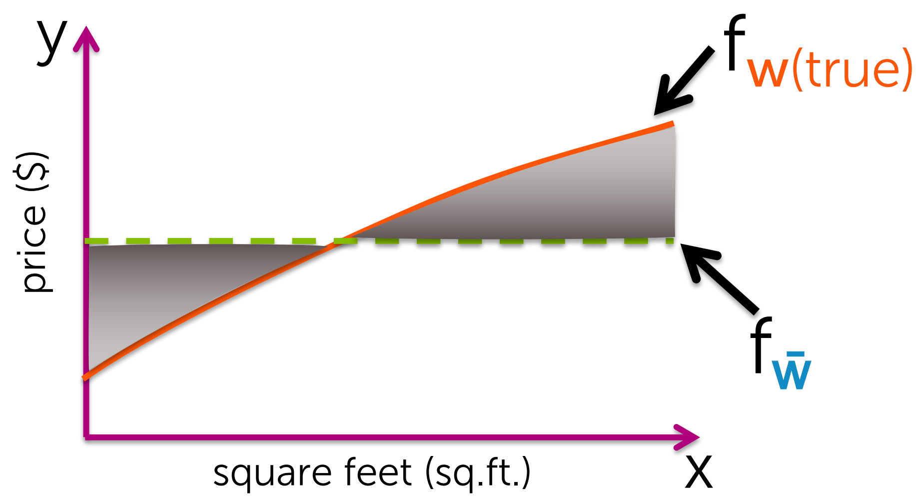
Over all possible size N training sets,
what do I expect my fit to be?



Bias contribution

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

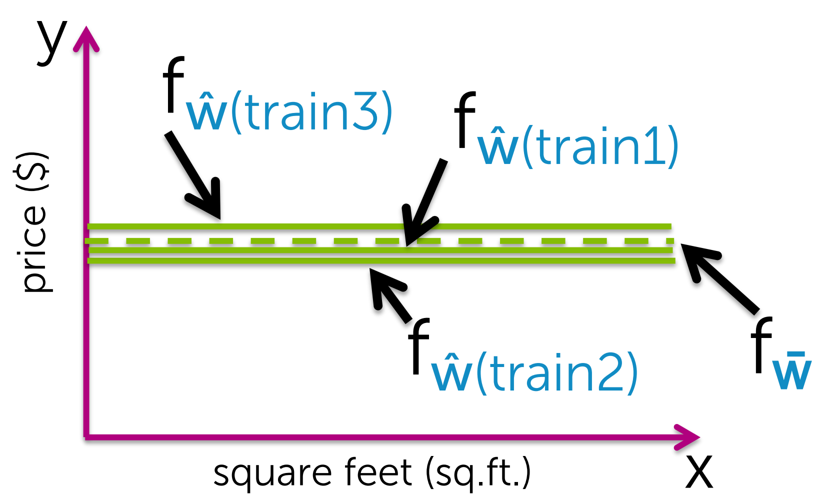
Is our approach flexible enough to capture $f_{w(true)}$?
If not, error in predictions.



low complexity →

Variance contribution

How much do specific fits vary from the expected fit?



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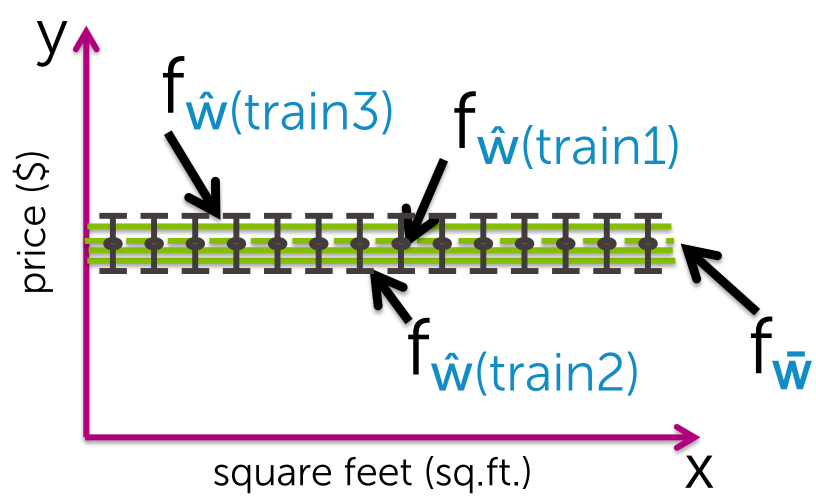
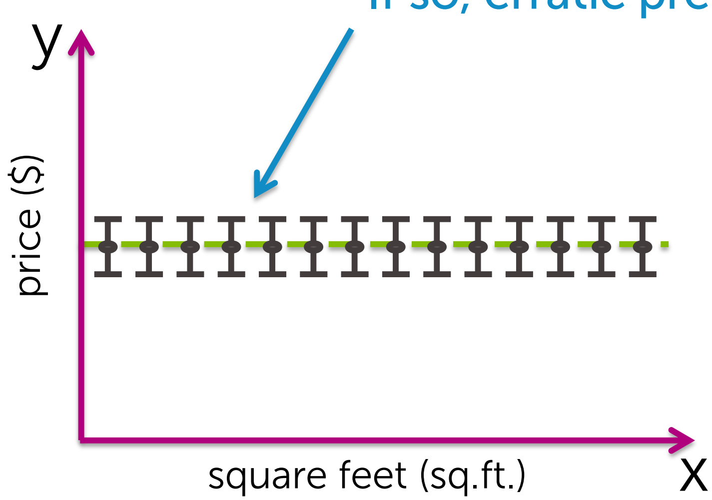


Variance contribution

How much do specific fits vary from the expected fit?

Can specific fits vary widely?

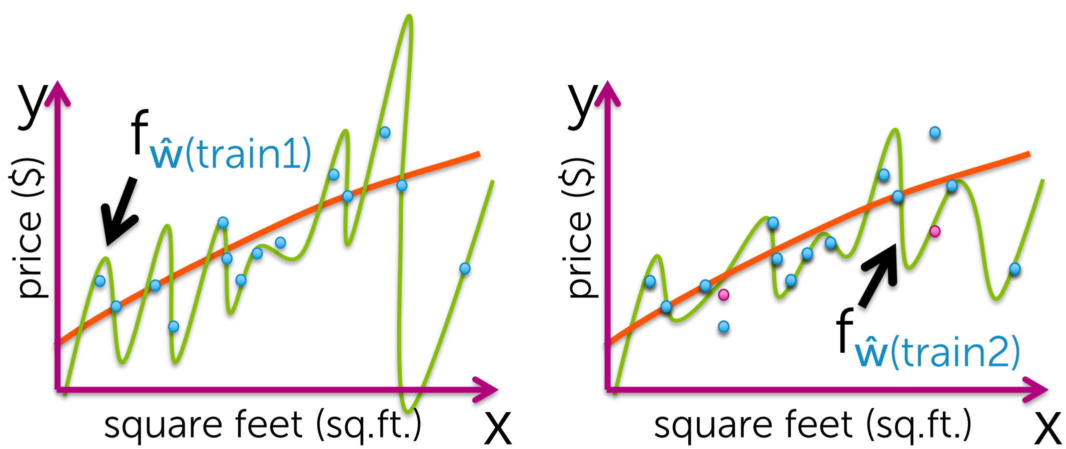
If so, erratic predictions



low complexity
→

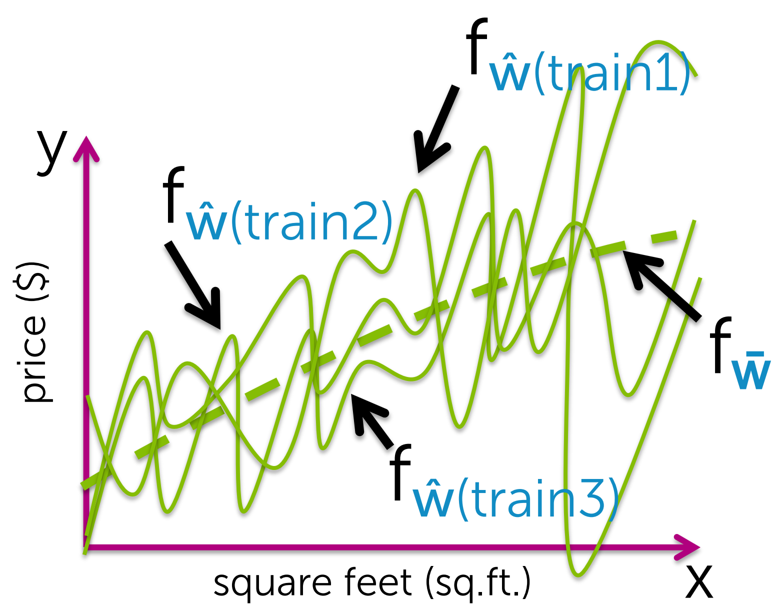
Variance of high-complexity models

Assume we fit a high-order polynomial

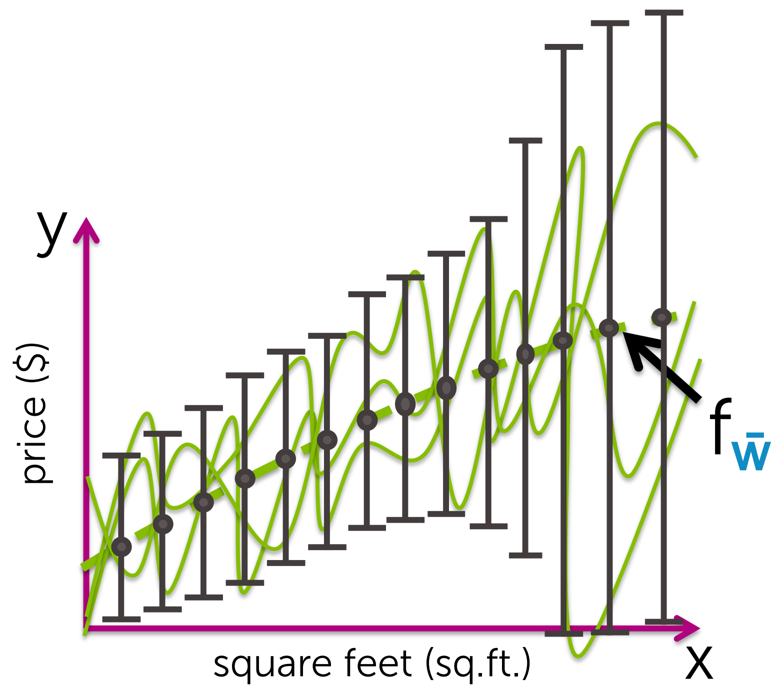


Variance of high-complexity models

Suppose we fit a high-order polynomial

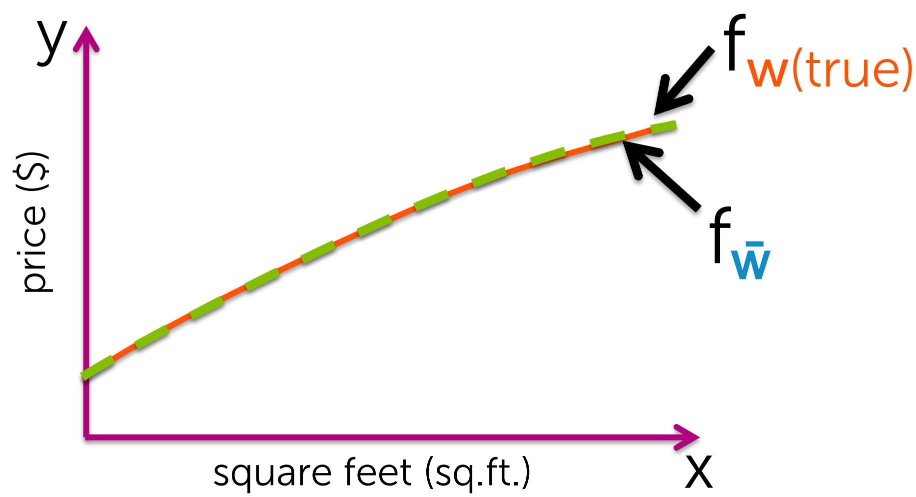


Variance of high-complexity models



high complexity
→

Bias of high-complexity models

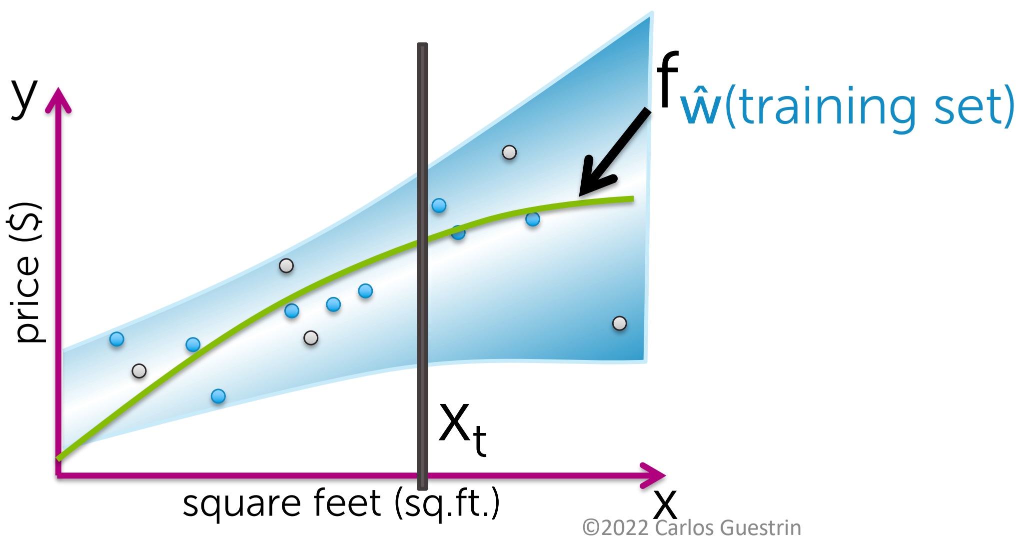


high complexity
→

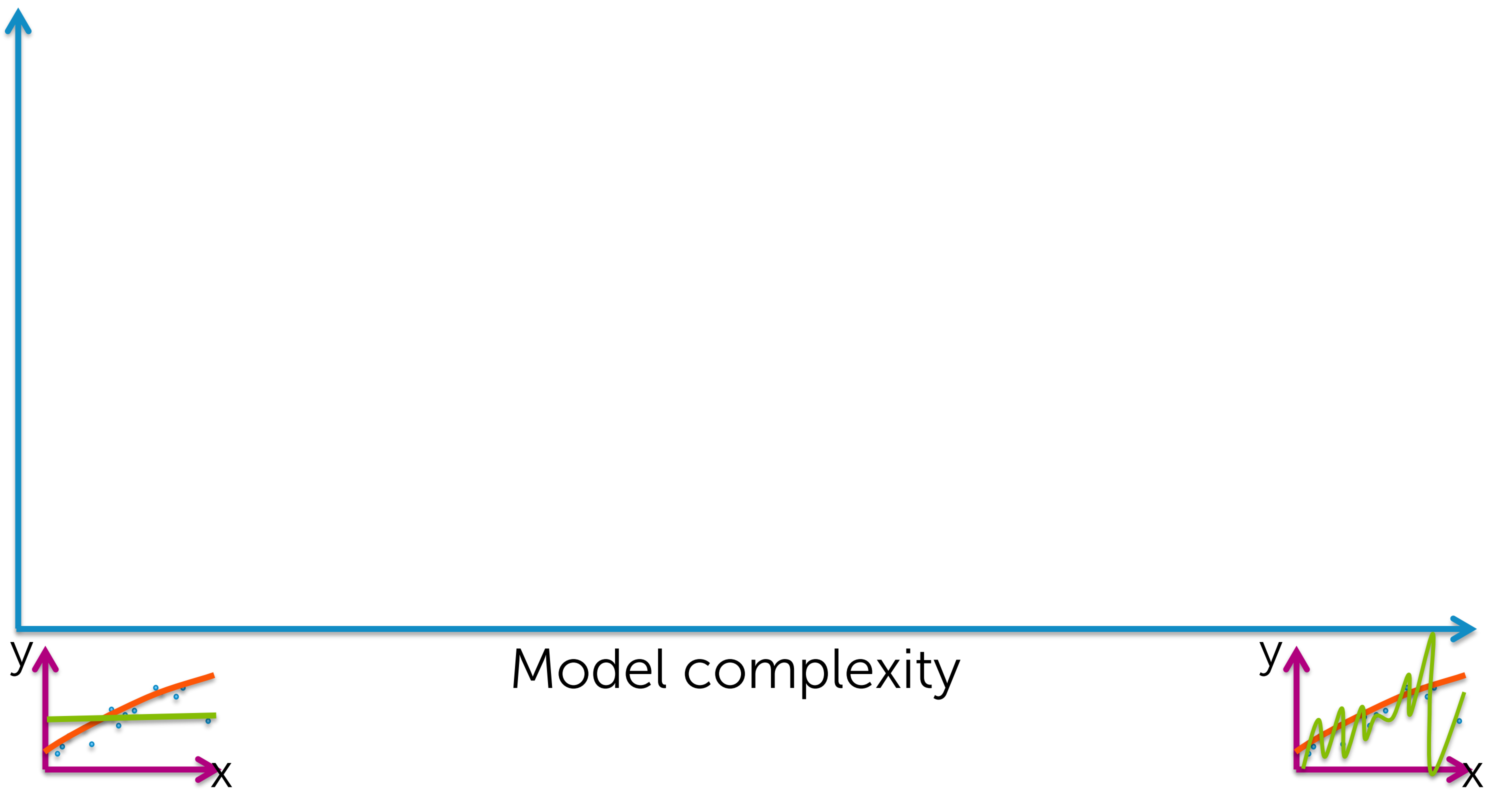
Sum of 3 sources of error

Average squared error at $\mathbf{x}_t$

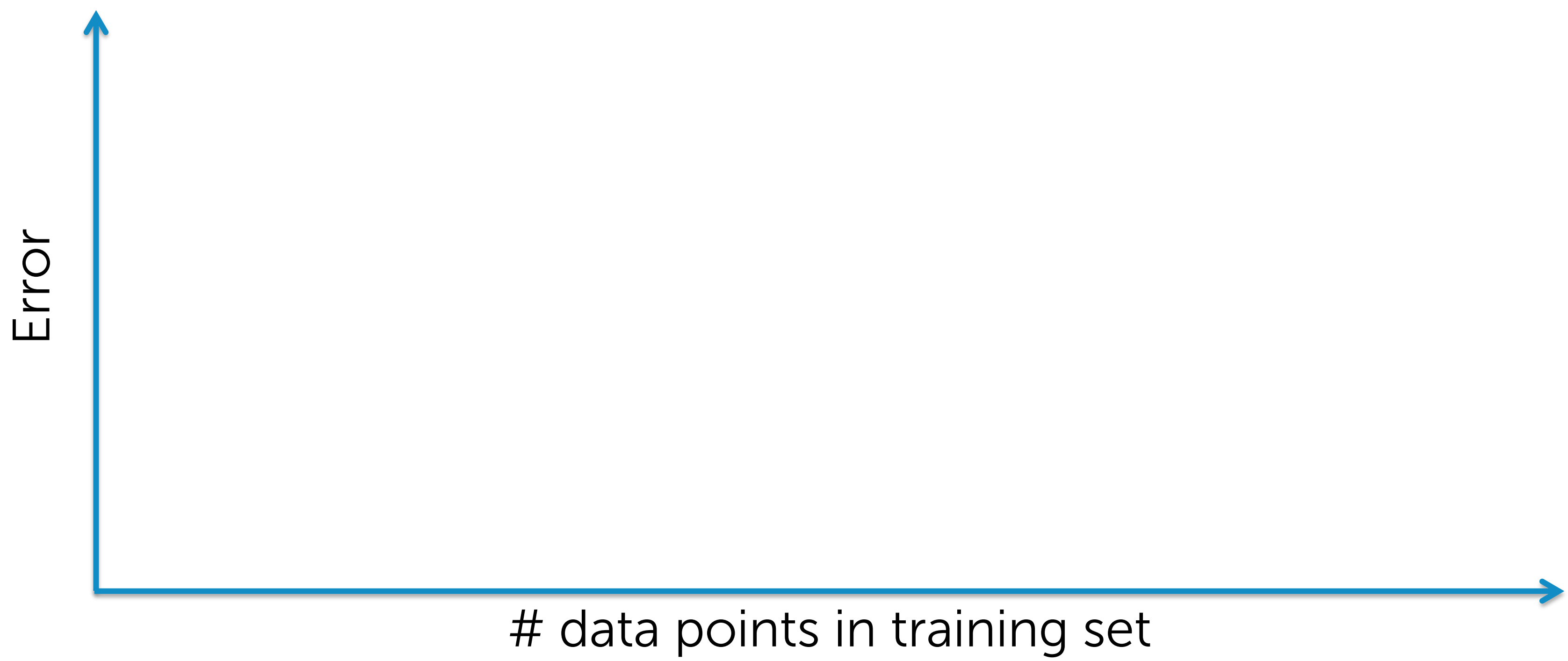
$$= \sigma^2 + [\text{bias}(f_{\hat{w}}(\mathbf{x}_t))]^2 + \text{var}(f_{\hat{w}}(\mathbf{x}_t))$$



Bias-variance tradeoff



Error vs. amount of data



Why 3 sources of error?
A formal derivation

Deriving expected prediction error

Expected prediction error

$= E_{train}$ [generalization error of $\hat{\mathbf{w}}$(train)]

$= E_{train}\left[E_{\mathbf{x},y}\left[L(y, f_{\hat{\mathbf{w}}(train)}(\mathbf{x}))\right]\right]$

1. Look at specific $\mathbf{x}_t$
2. Consider $L(y, f_{\hat{\mathbf{w}}}(\mathbf{x})) = (y - f_{\hat{\mathbf{w}}}(\mathbf{x}))^2$

Expected prediction error at $\mathbf{x}_t$

$= E_{train, y_t}\left[(y_t - f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t))^2\right]$

Simplifying Notation

- Expected prediction error at $\mathbf{x}_t$

  $= E_{train, y_t}\left[(y_t - f_{\hat{w}(train)}(\mathbf{x}_t))^2\right]$
- Simple (and abusive ☺) notation:
  - $y_t \rightarrow y$
  - $f_{w(true)}(\mathbf{x}_t) \rightarrow f$
  - $f_{\hat{w}(train)}(\mathbf{x}_t) \rightarrow \hat{f}$
  - $E_{train}\left[f_{\hat{w}(train)}(\mathbf{x}_t)\right] = f_{\bar{w}}(\mathbf{x}_t) \rightarrow \bar{f}$

Deriving expected prediction error

Expected prediction error at $\mathbf{x}_t$

$$= E_{\text{train},y_t}\left[(y_t - f_{\hat{w}(\text{train})}(\mathbf{x}_t))^2\right] = E_{\text{train}}\left[(y - \hat{f})^2\right] =$$

$$= E_{\text{train}}\left[((y - f) + (f - \hat{f}))^2\right]$$

Equating MSE with bias and variance

$$\mathrm{MSE}\left[f_{\hat{w}(\mathrm{train})}(\mathbf{x}_t)\right]$$

$$= \mathrm{E}_{\mathrm{train}}\left[(f - \hat{f})^2\right]$$

$$= \mathrm{E}_{\mathrm{train}}\left[((f - \bar{f}) + (\bar{f} - \hat{f}))^2\right]$$

Putting it all together

Expected prediction error at $\mathbf{x}_t$

$$= \sigma^2 + \text{MSE}\left[f_{\hat{w}}(\mathbf{x}_t)\right]$$

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

3 sources of error

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