Assessing Performance

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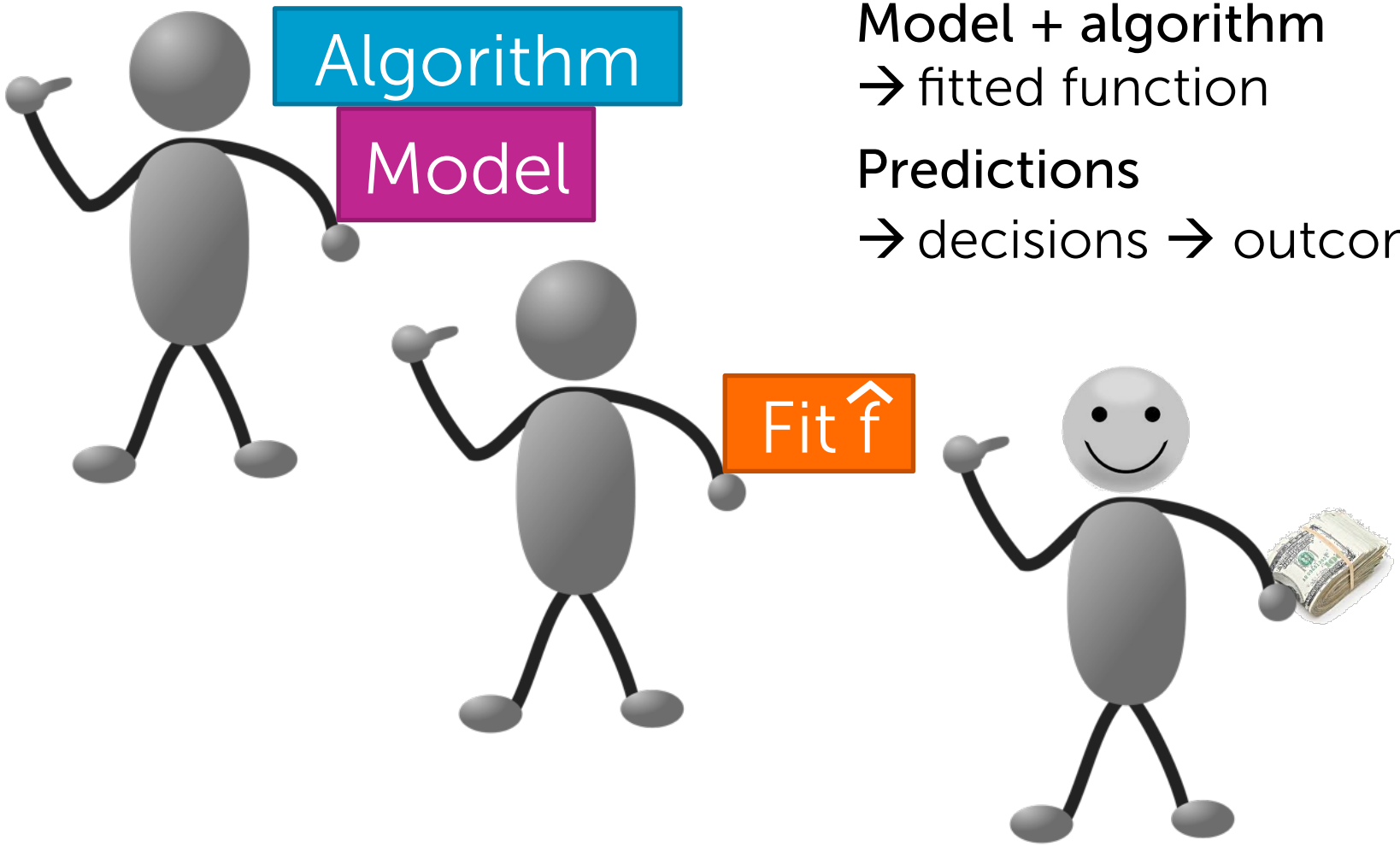
Make predictions, get $, right??



Model + algorithm
→ fitted function

Predictions
→ decisions → outcome

Or, how much am I losing?

Example: Lost $ due to inaccurate listing price

- Too low → low offers
- Too high → few lookers + no/low offers

How much am I losing compared to perfection?

Perfect predictions: Loss = 0

My predictions: Loss = ???

Measuring loss

Loss function:

$L(y, f_{\hat{w}}(\mathbf{x}))$

Cost of using $\hat{w}$ at x when y is true

actual value

$\hat{f}(\mathbf{x})$ = predicted value $\hat{y}$

Examples:

(assuming loss for underpredicting = overpredicting)

Absolute error: $L(y, f_{\hat{w}}(\mathbf{x})) = |y - f_{\hat{w}}(\mathbf{x})|$

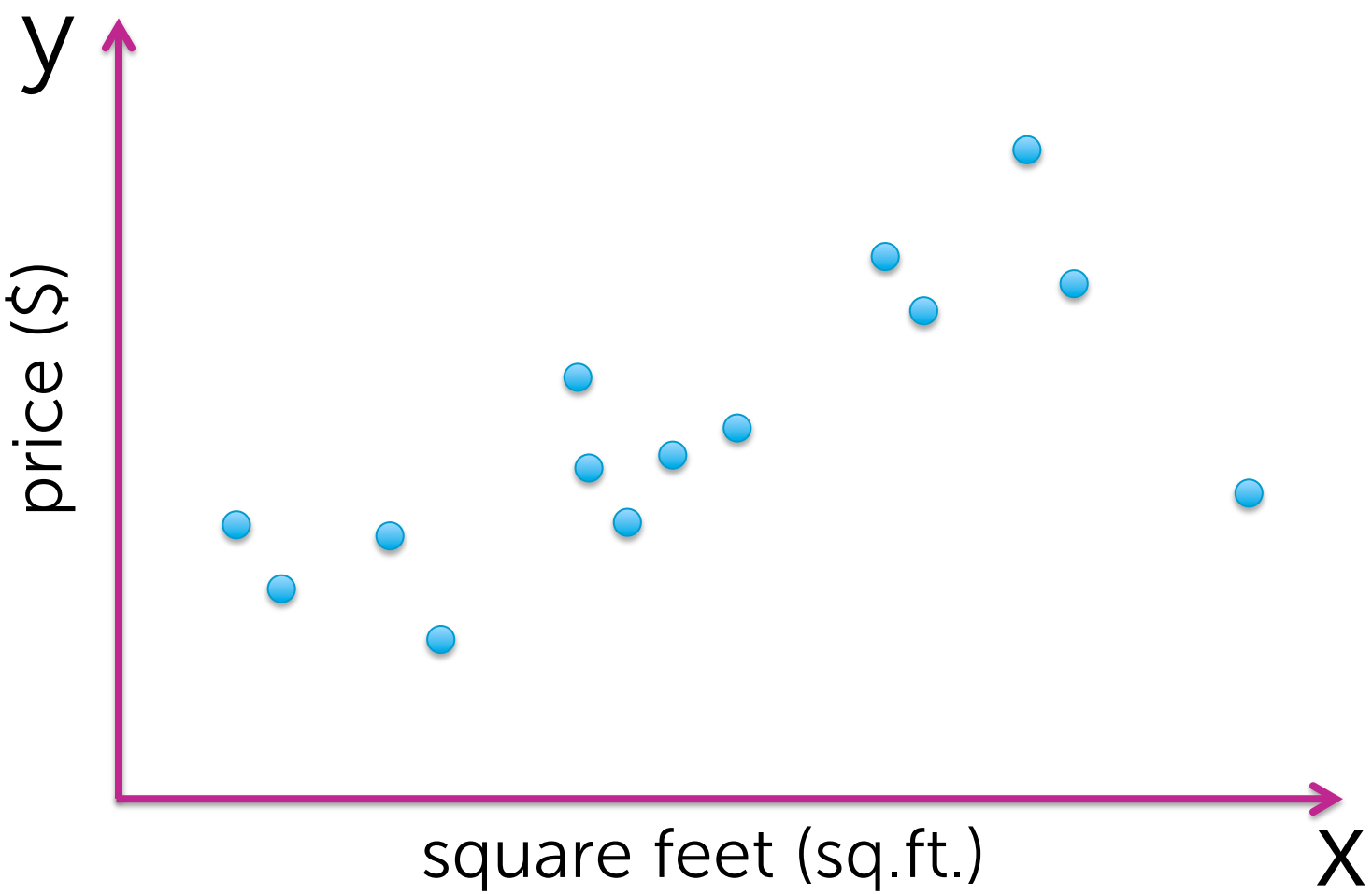
Squared error: $L(y, f_{\hat{w}}(\mathbf{x})) = (y - f_{\hat{w}}(\mathbf{x}))^2$

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

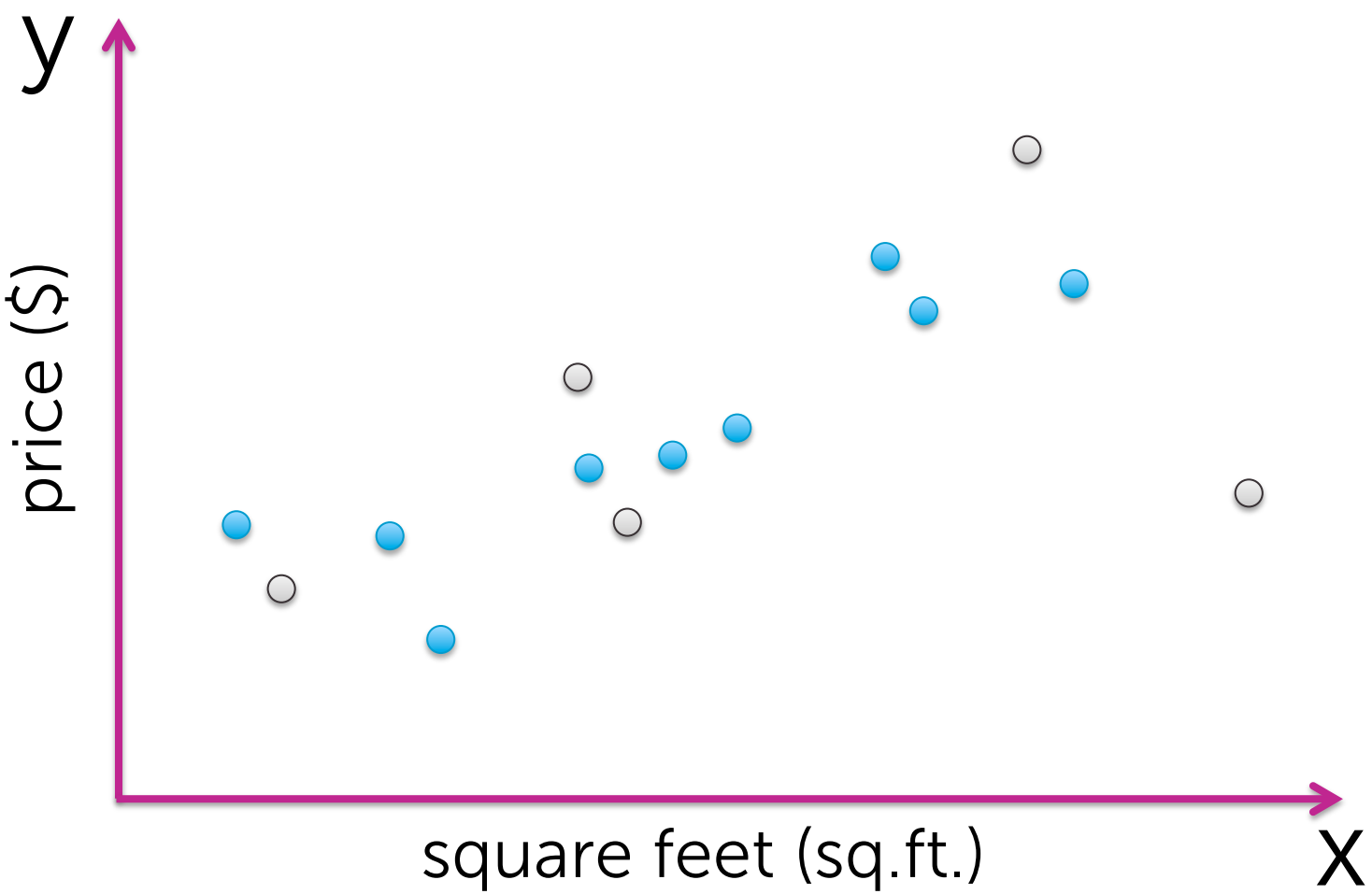
Assessing the loss

Assessing the loss
Part 1: Training error

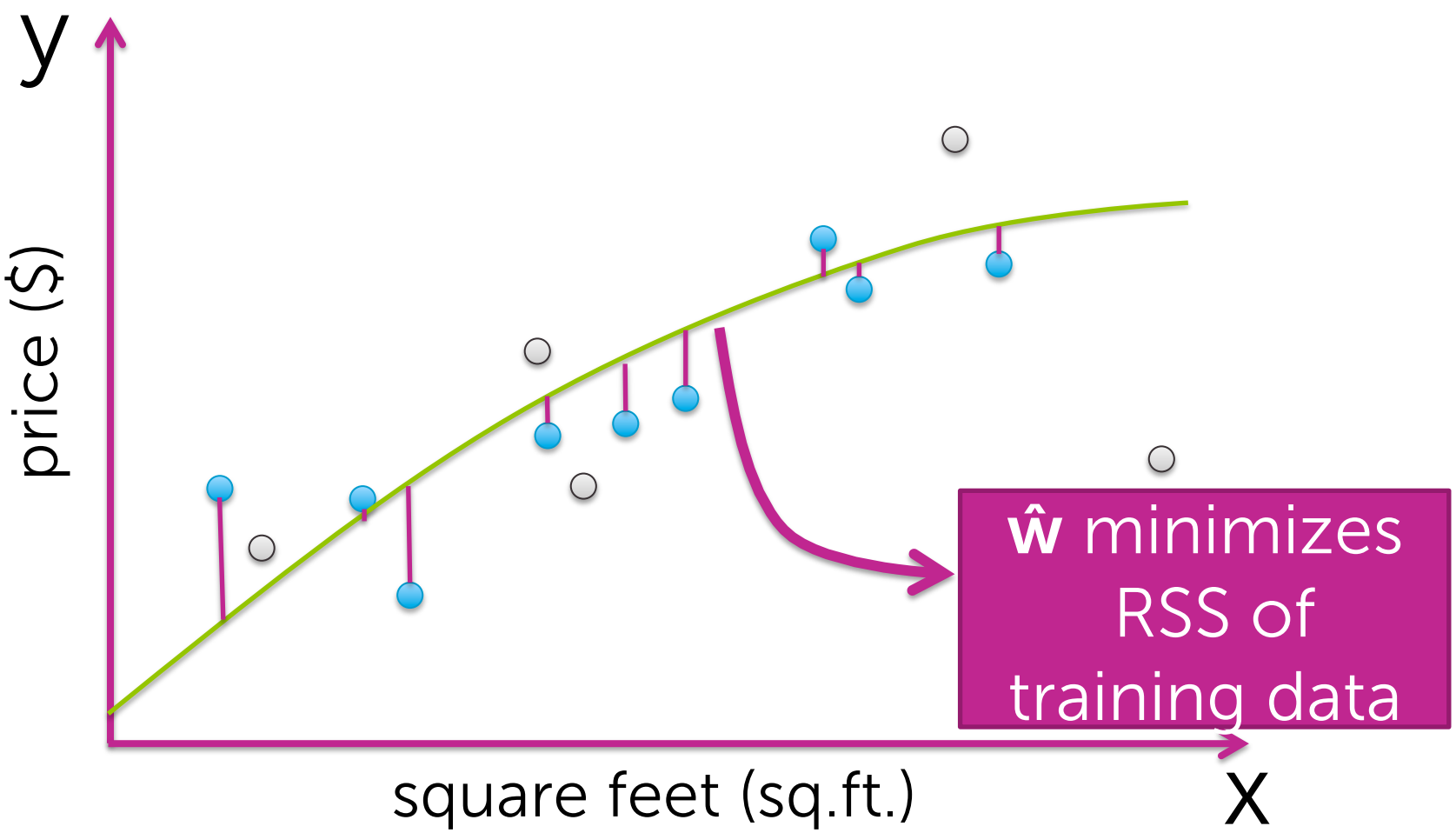
Define training data



Define training data



Example:
Fit quadratic to minimize RSS



Compute training error

1. Define a loss function $L(y, f_{\hat{\mathbf{w}}}(\mathbf{x}))$
   - E.g., squared error, absolute error,…

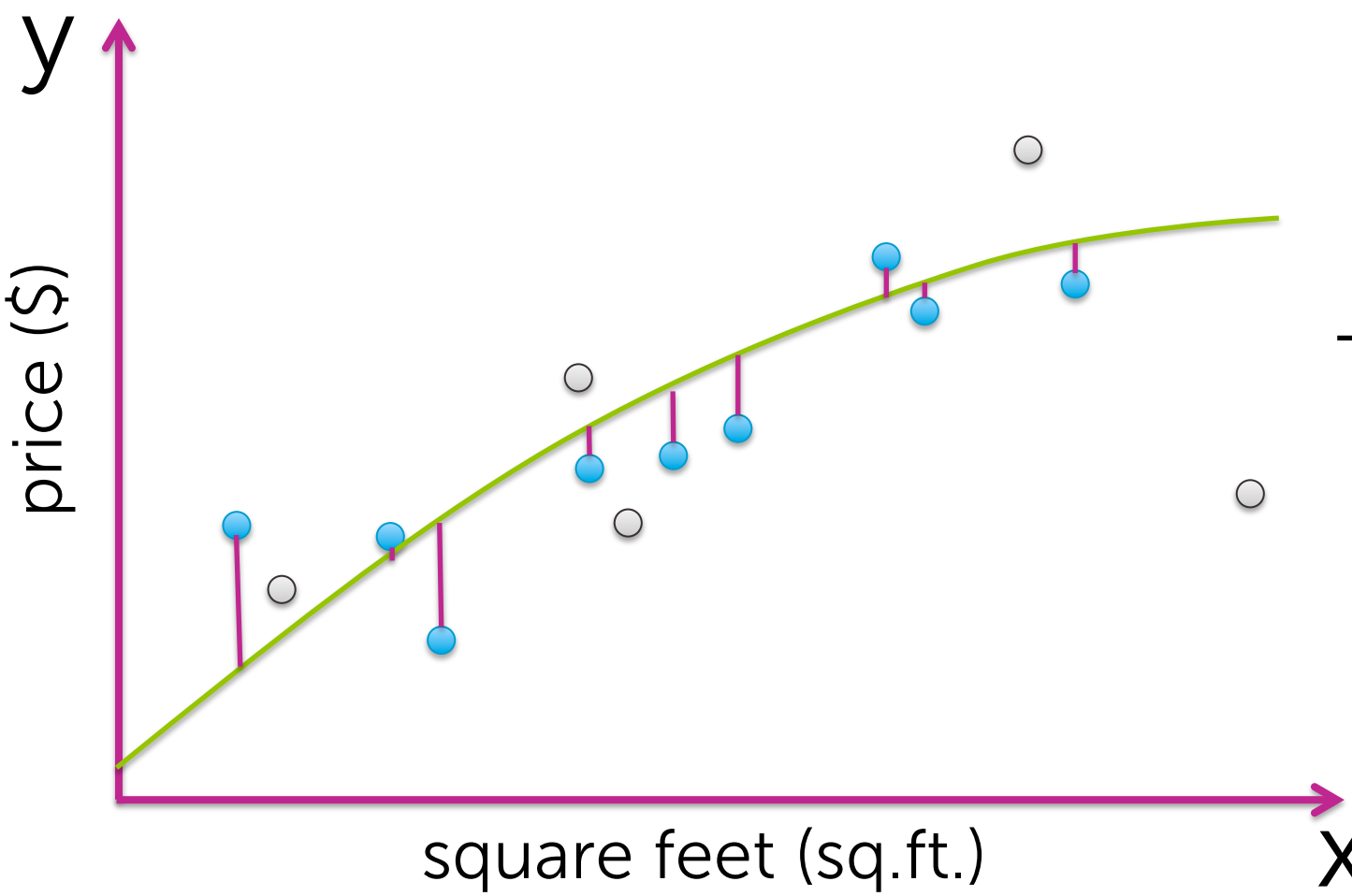
2. Training error

   = avg. loss on houses in training set

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

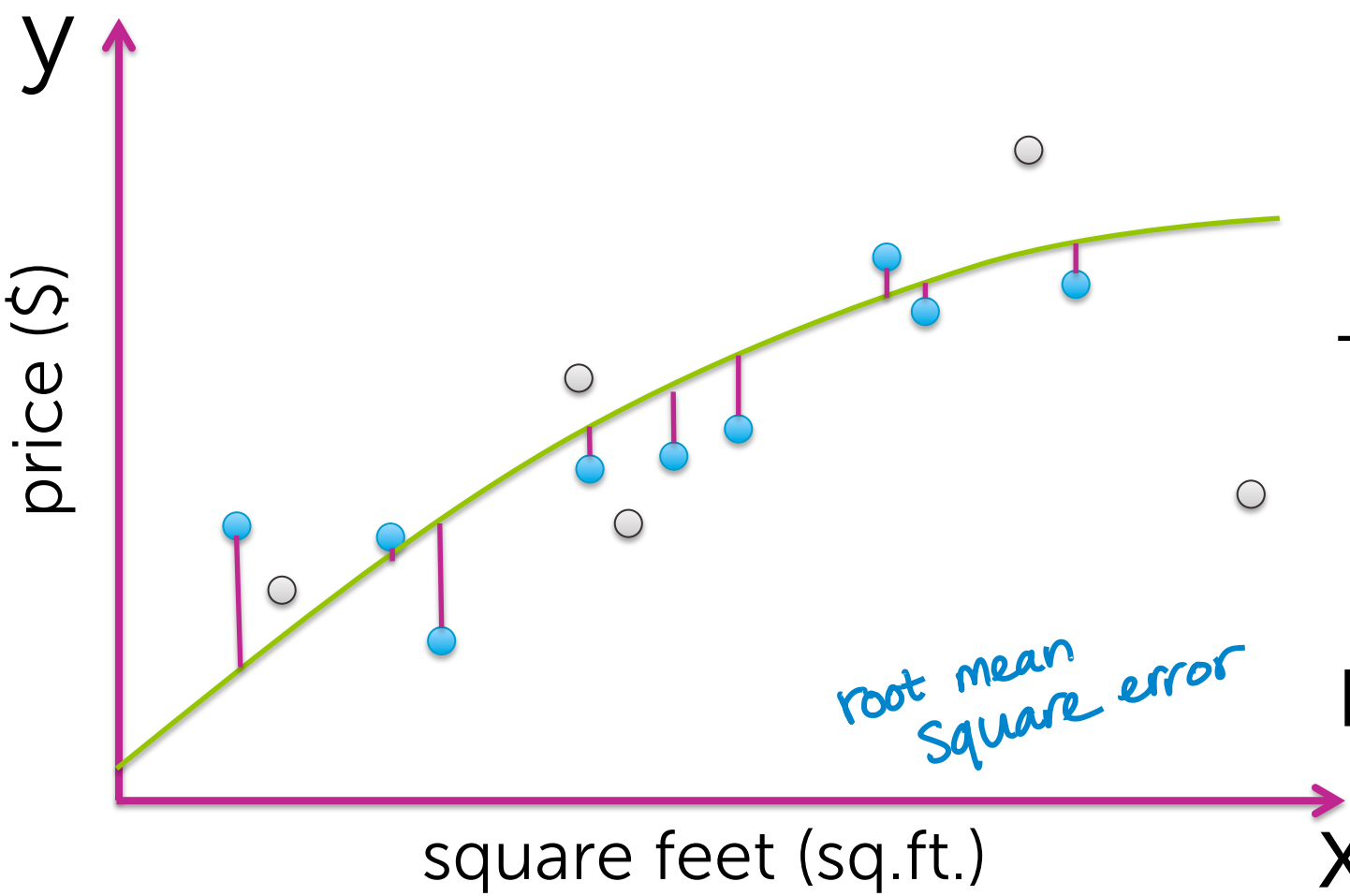
fit using training data

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



Training error ($\hat{w}$) = 1/N *
$[(\$_{train\ 1}-f_{\hat{w}}(sq.ft._{train\ 1}))^2$
$+ (\$_{train\ 2}-f_{\hat{w}}(sq.ft._{train\ 2}))^2$
$+ (\$_{train\ 3}-f_{\hat{w}}(sq.ft._{train\ 3}))^2$
+ … include all training houses]

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



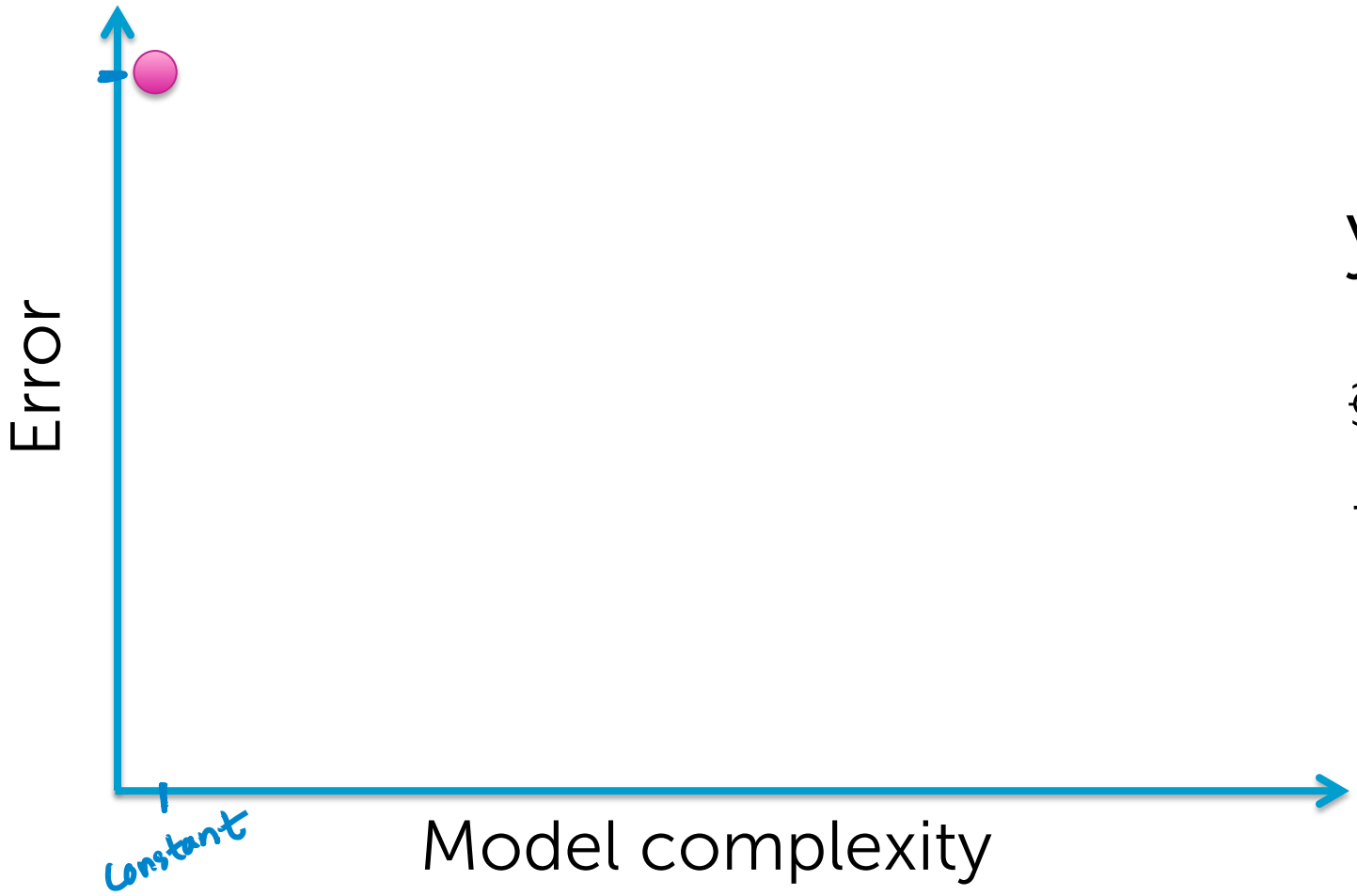
Training error ($\hat{w}$) =

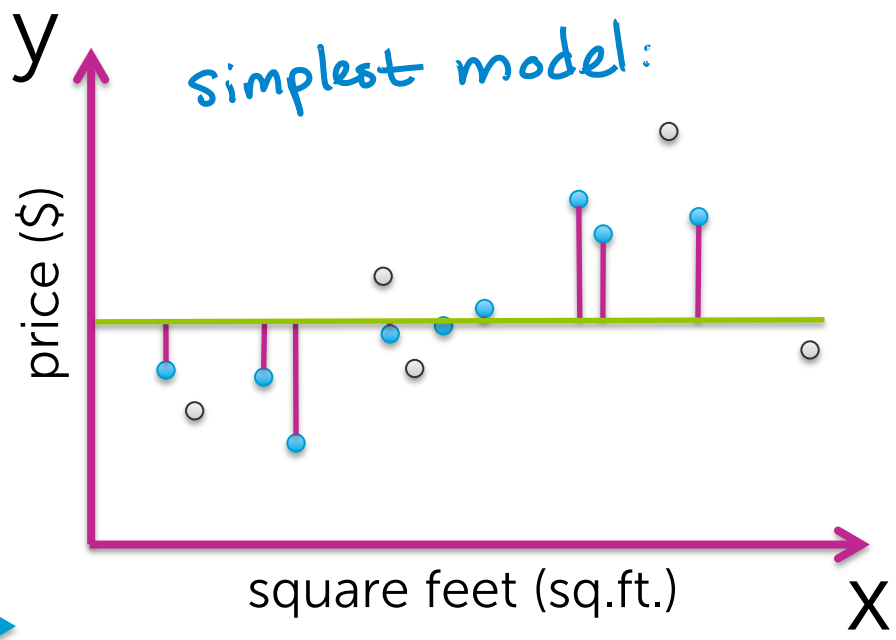
$$\frac{1}{N}\sum_{i=1}^{N}(y_i-f_{\hat{w}}(x_i))^2$$

RMSE =

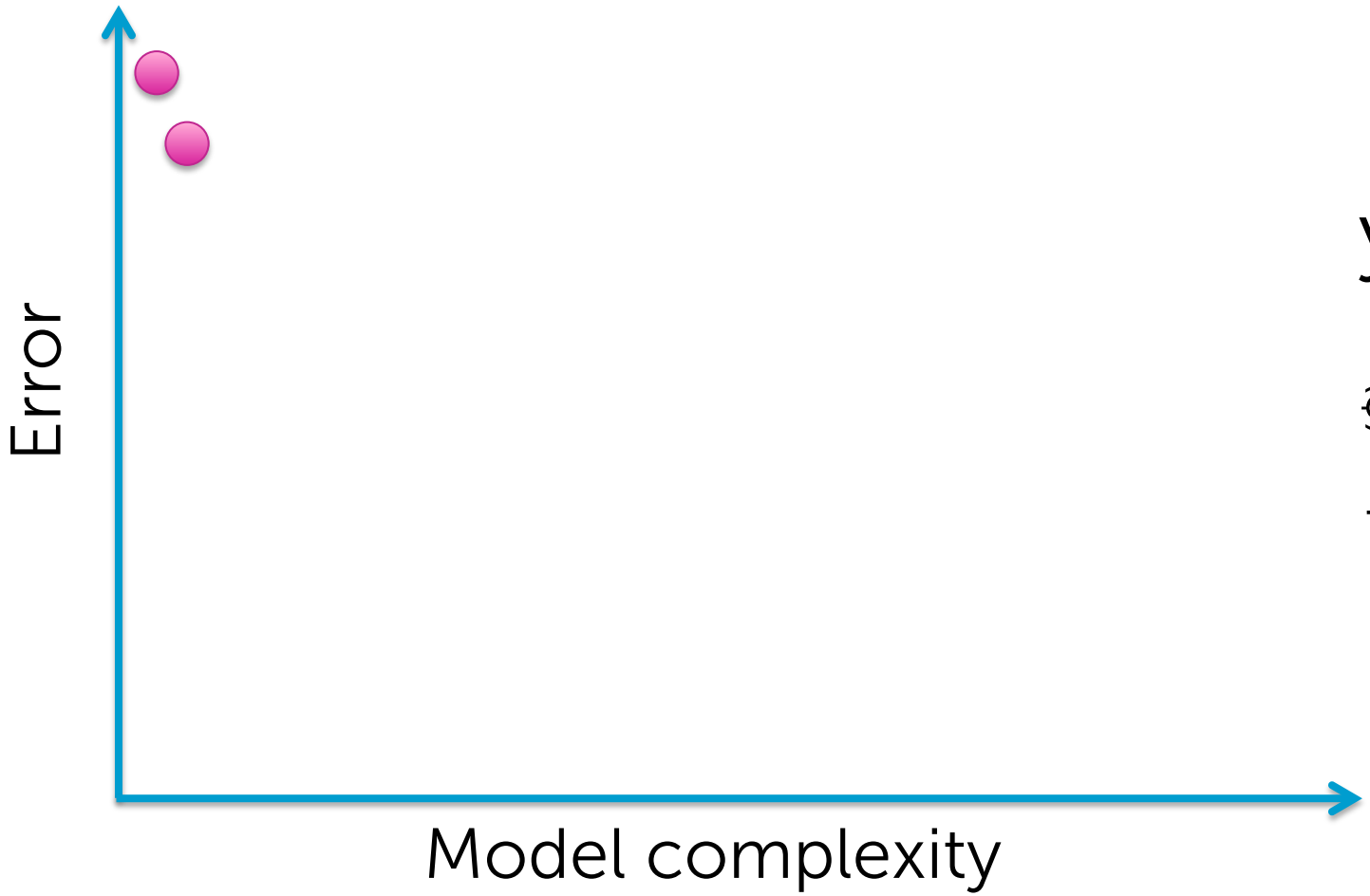
$$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i-f_{\hat{w}}(x_i))^2}$$

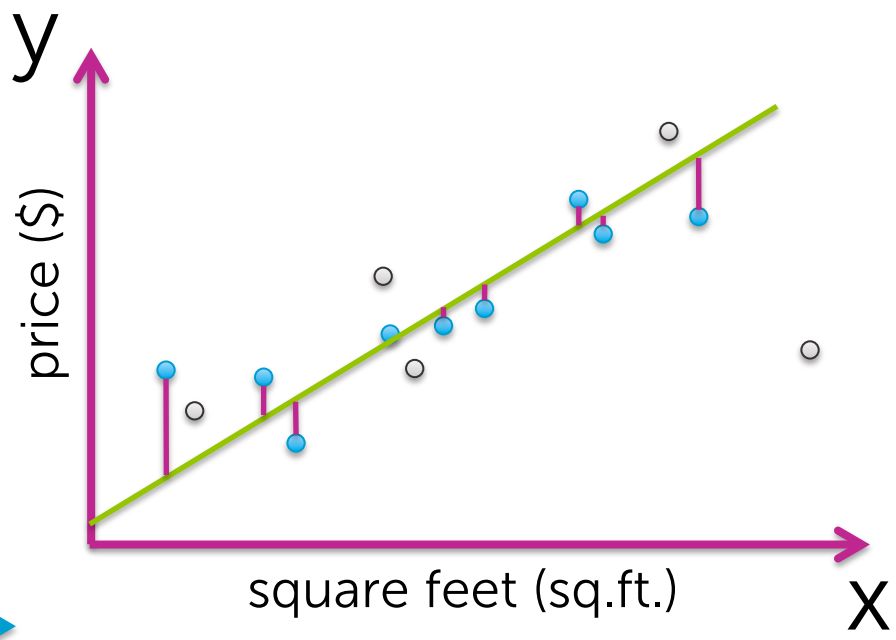
Training error vs. model complexity



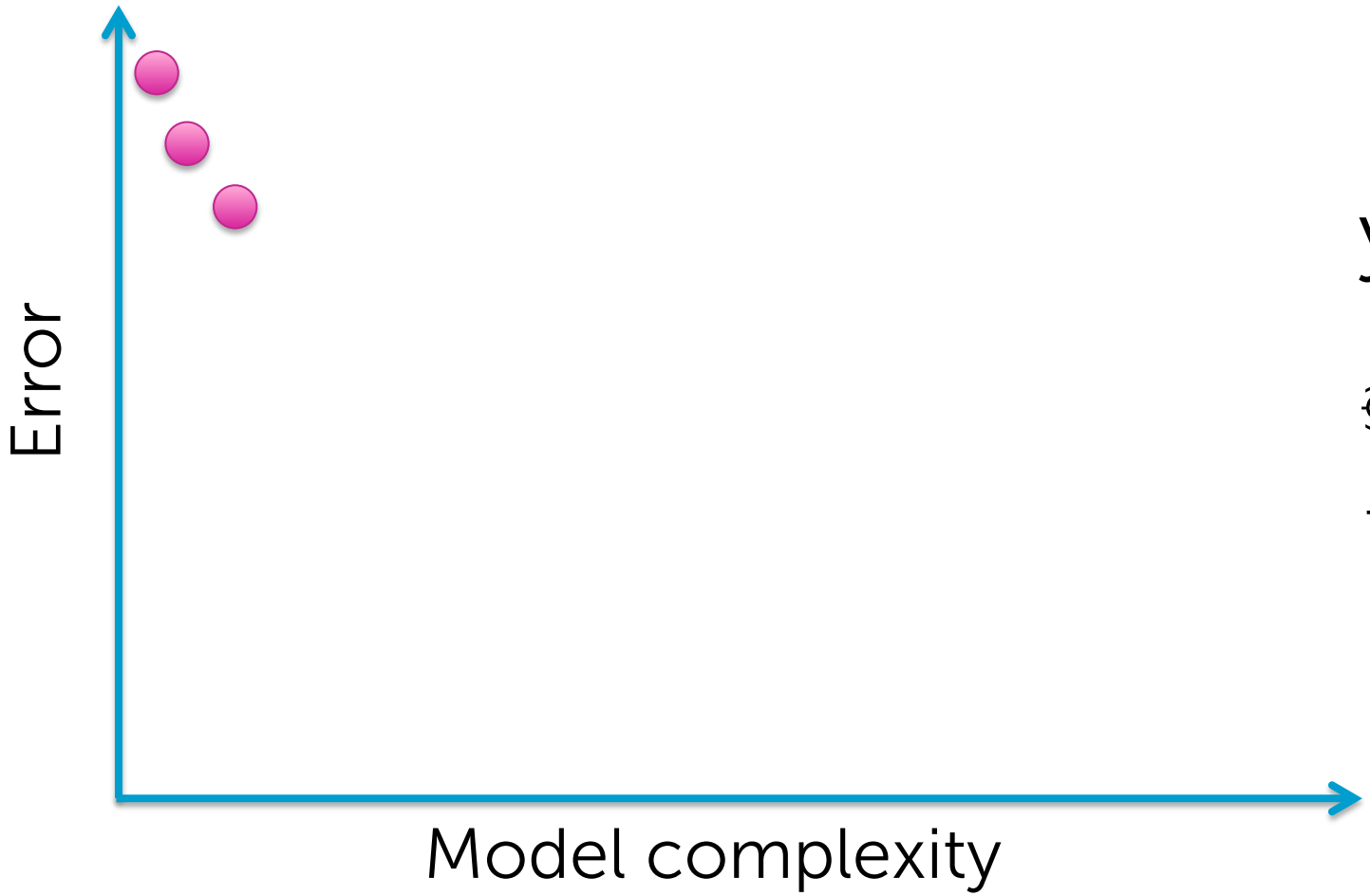


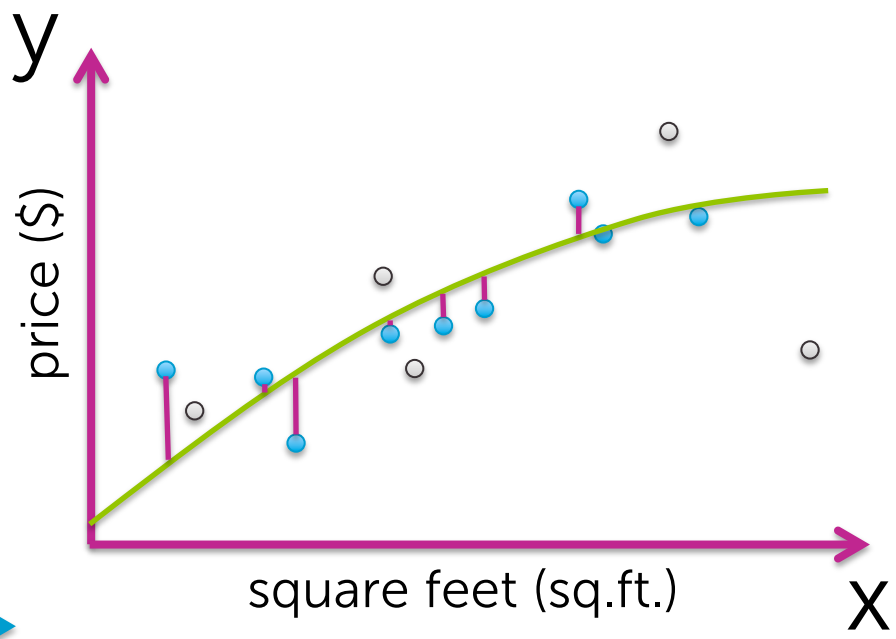
Training error vs. model complexity



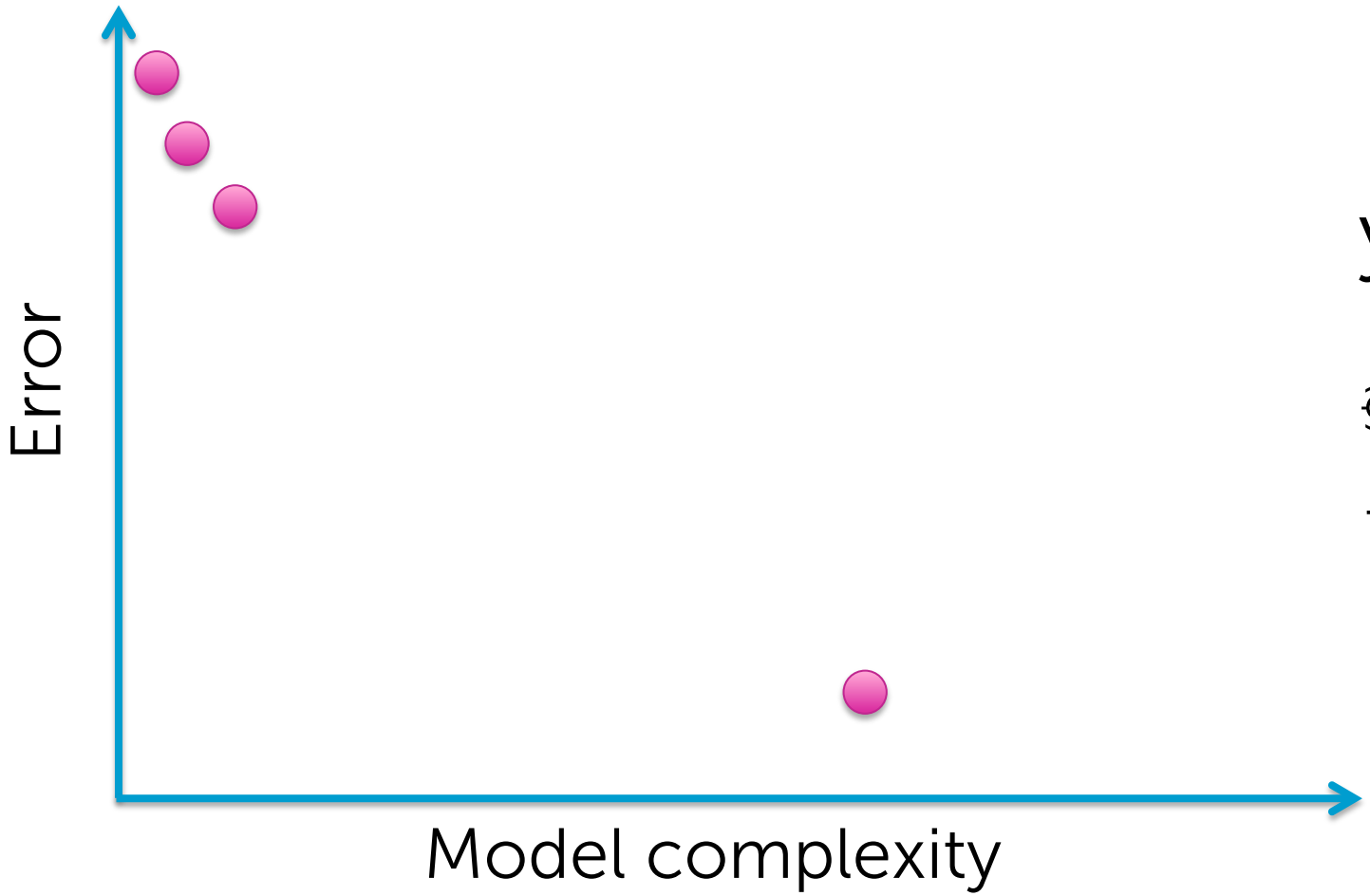


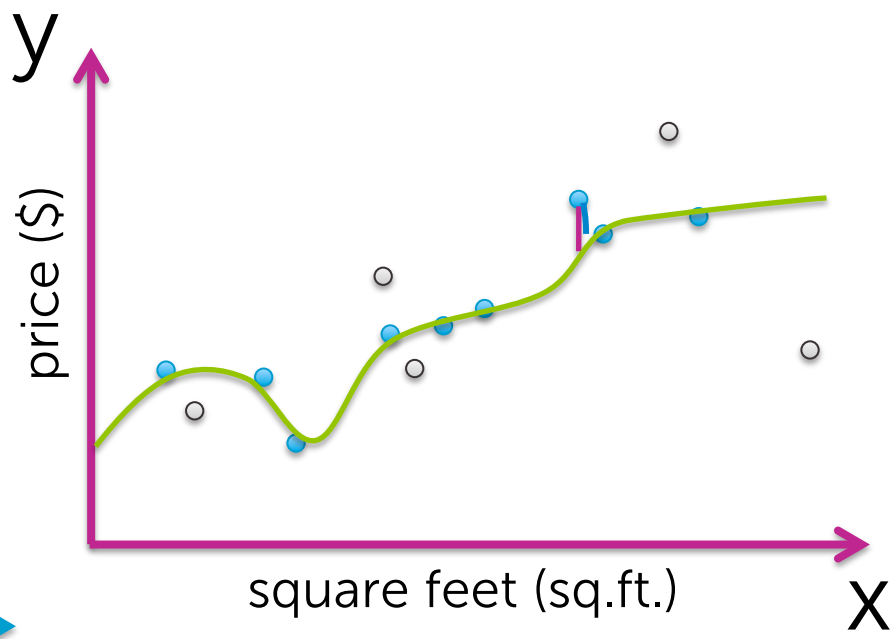
Training error vs. model complexity



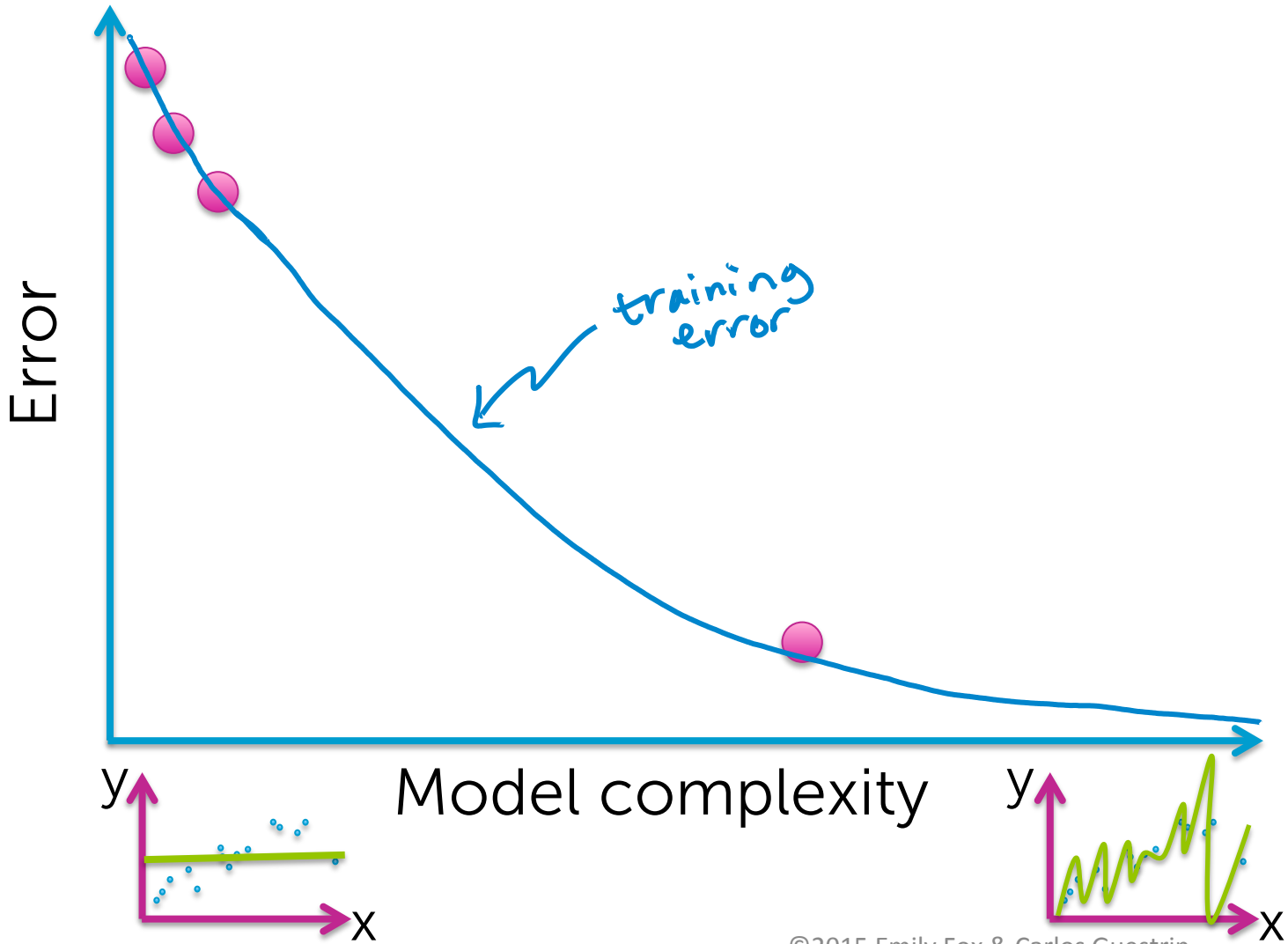


Training error vs. model complexity



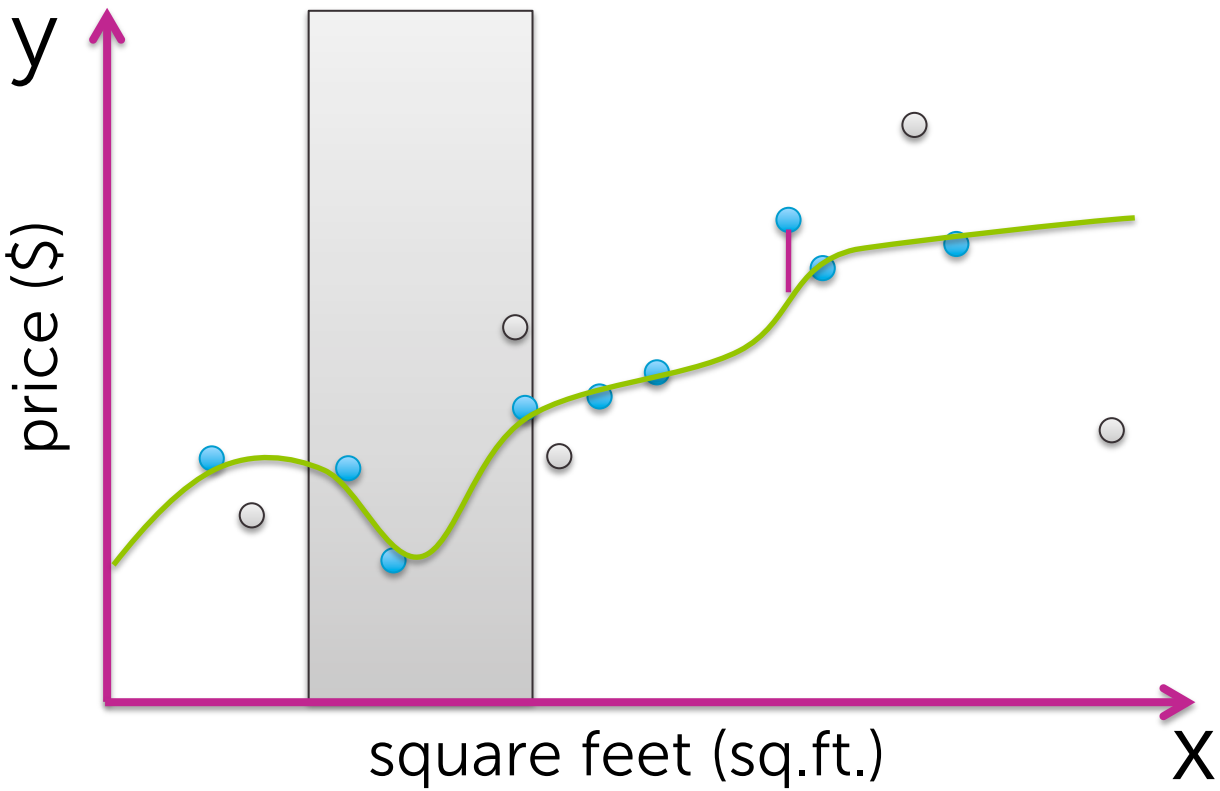


Training error vs. model complexity



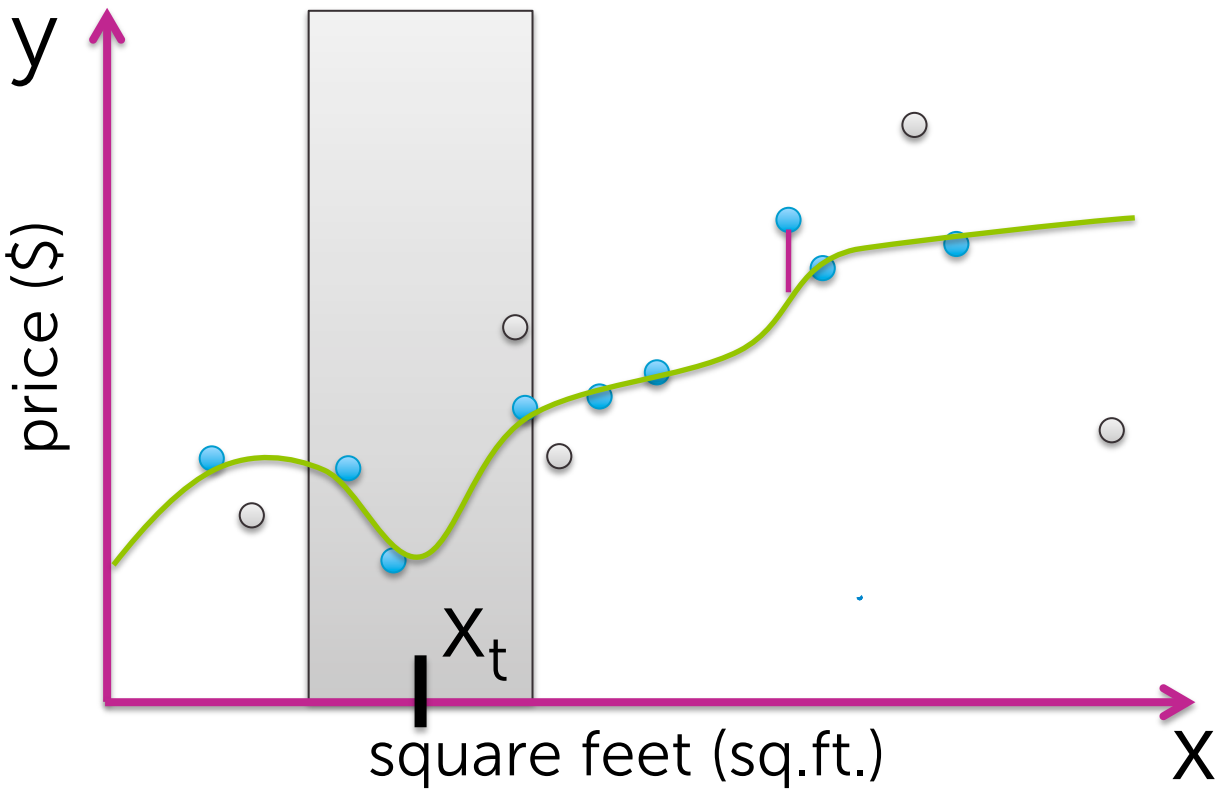
Is training error a good measure of predictive performance?

How do we expect to perform on a new house?



Is training error a good measure of predictive performance?

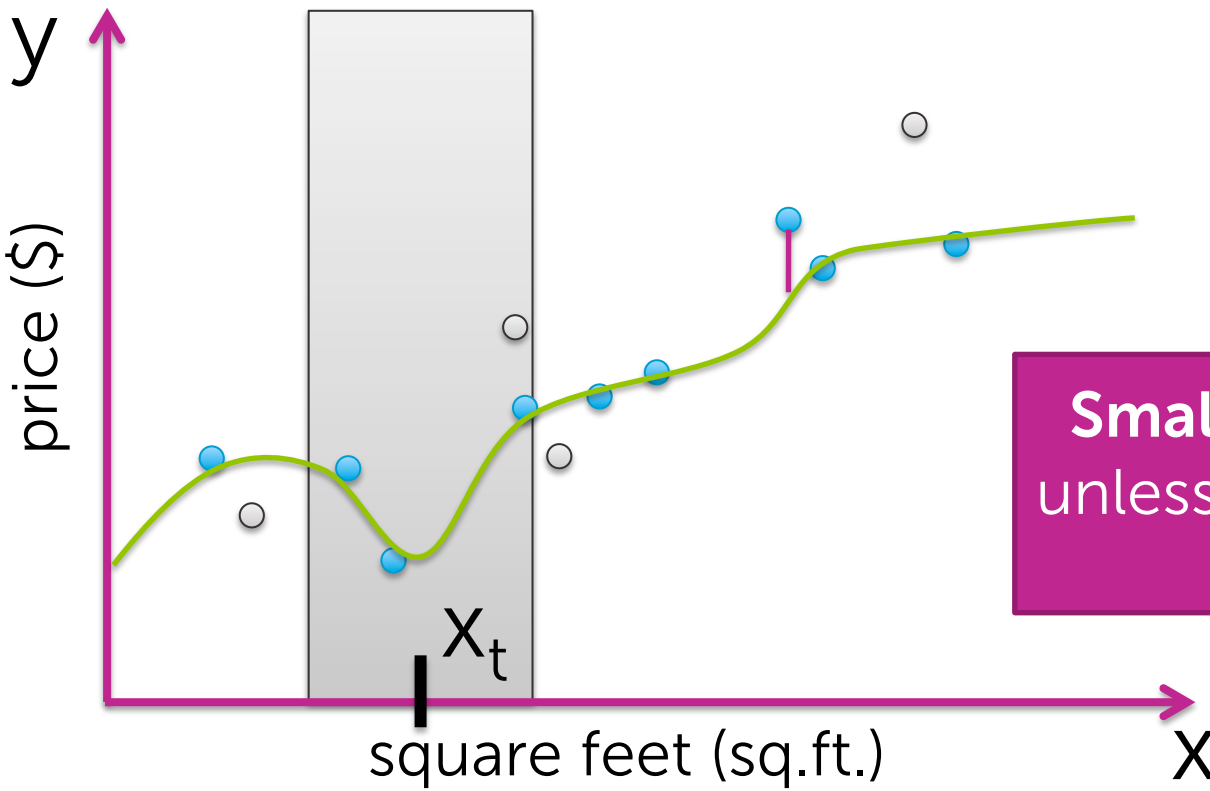
Is there something particularly bad about having x_t square feet???



Is training error a good measure of predictive performance?

Issue: Training error is overly optimistic

because $\hat{\mathbf{w}}$ 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

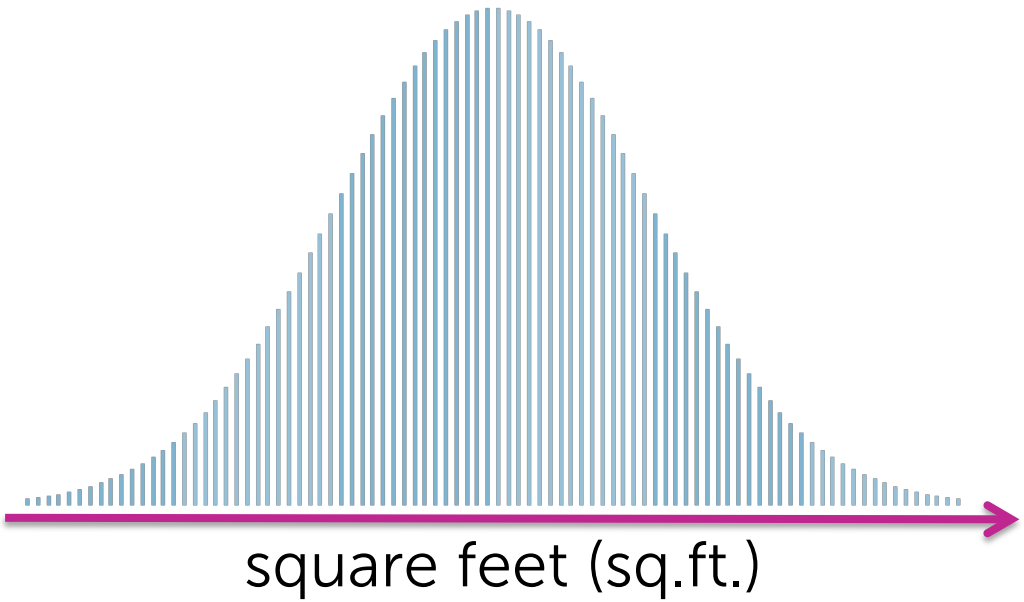
Generalization error

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

Lots of houses in neighborhood, but not in dataset

Distribution over houses

In our neighborhood, houses of what # sq.ft. () are we likely to see?



Distribution over sales prices

For houses with a given # sq.ft. (),
what house prices $ are we likely to see?

Generalization error definition

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

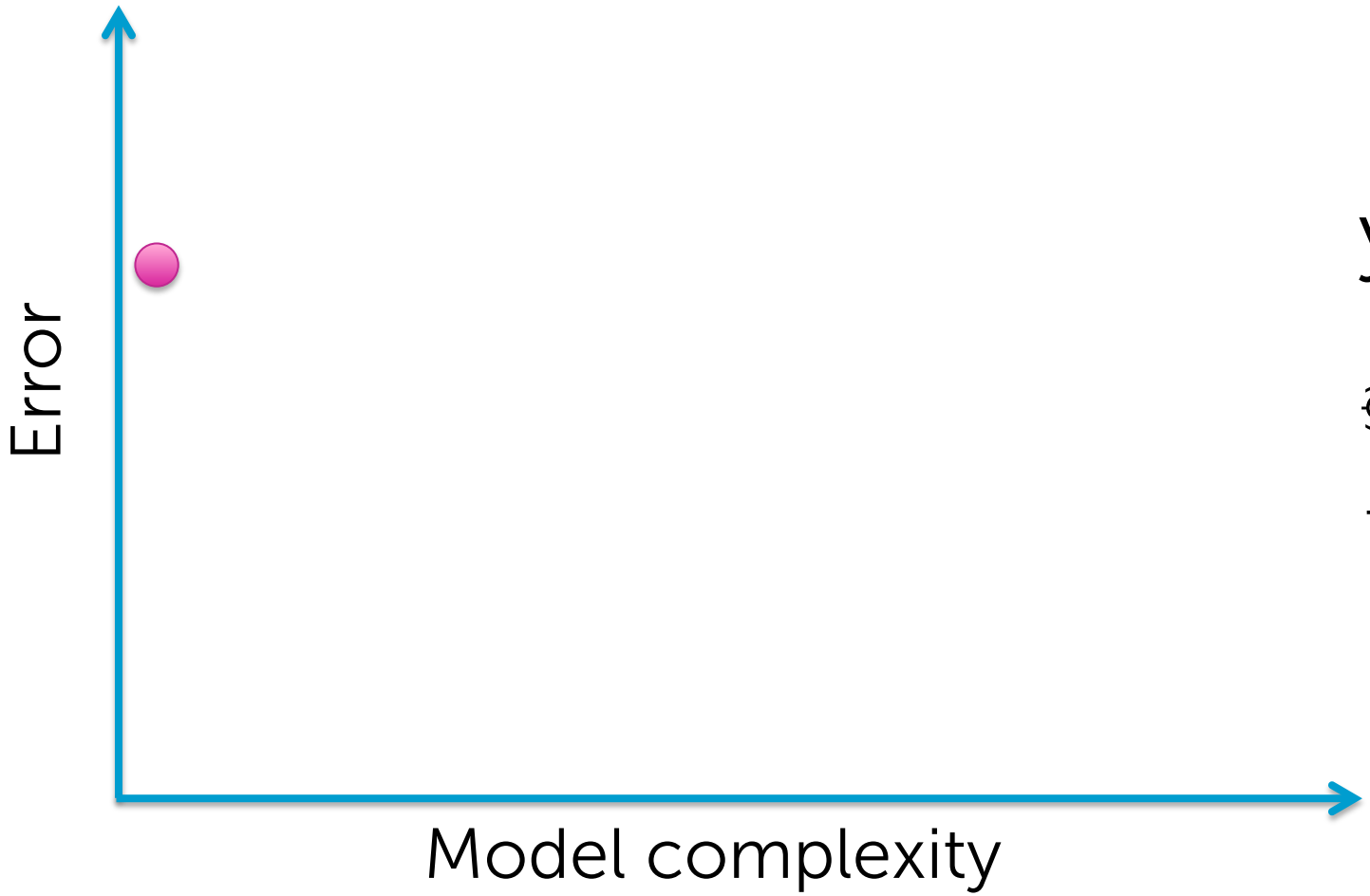
Formally:

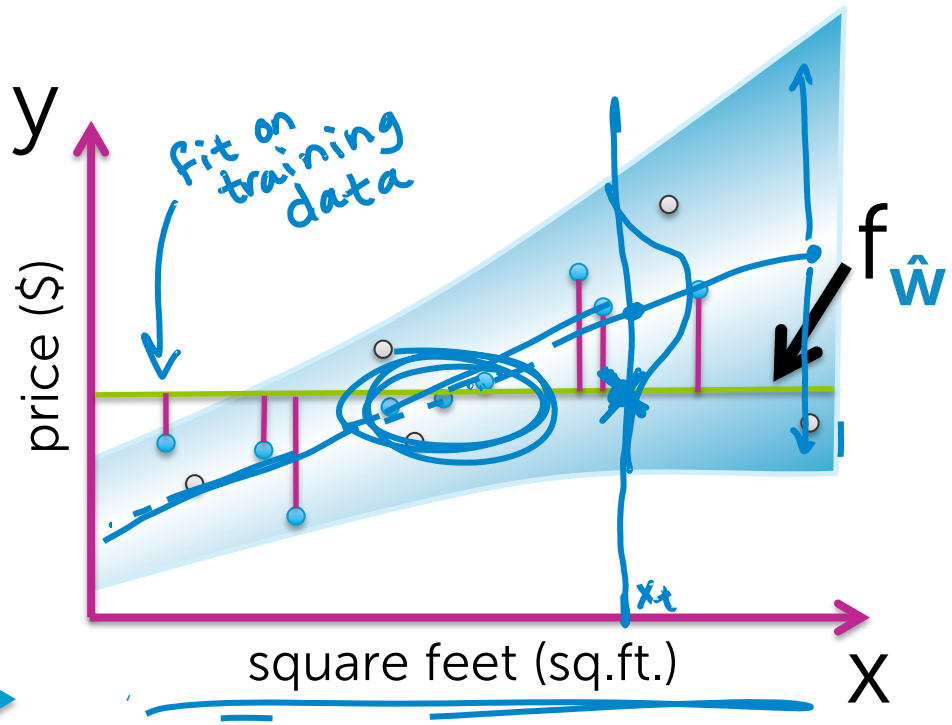
average over all possible (**x**,y) pairs weighted by how likely each is

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

fit using training data

Generalization error vs. model complexity





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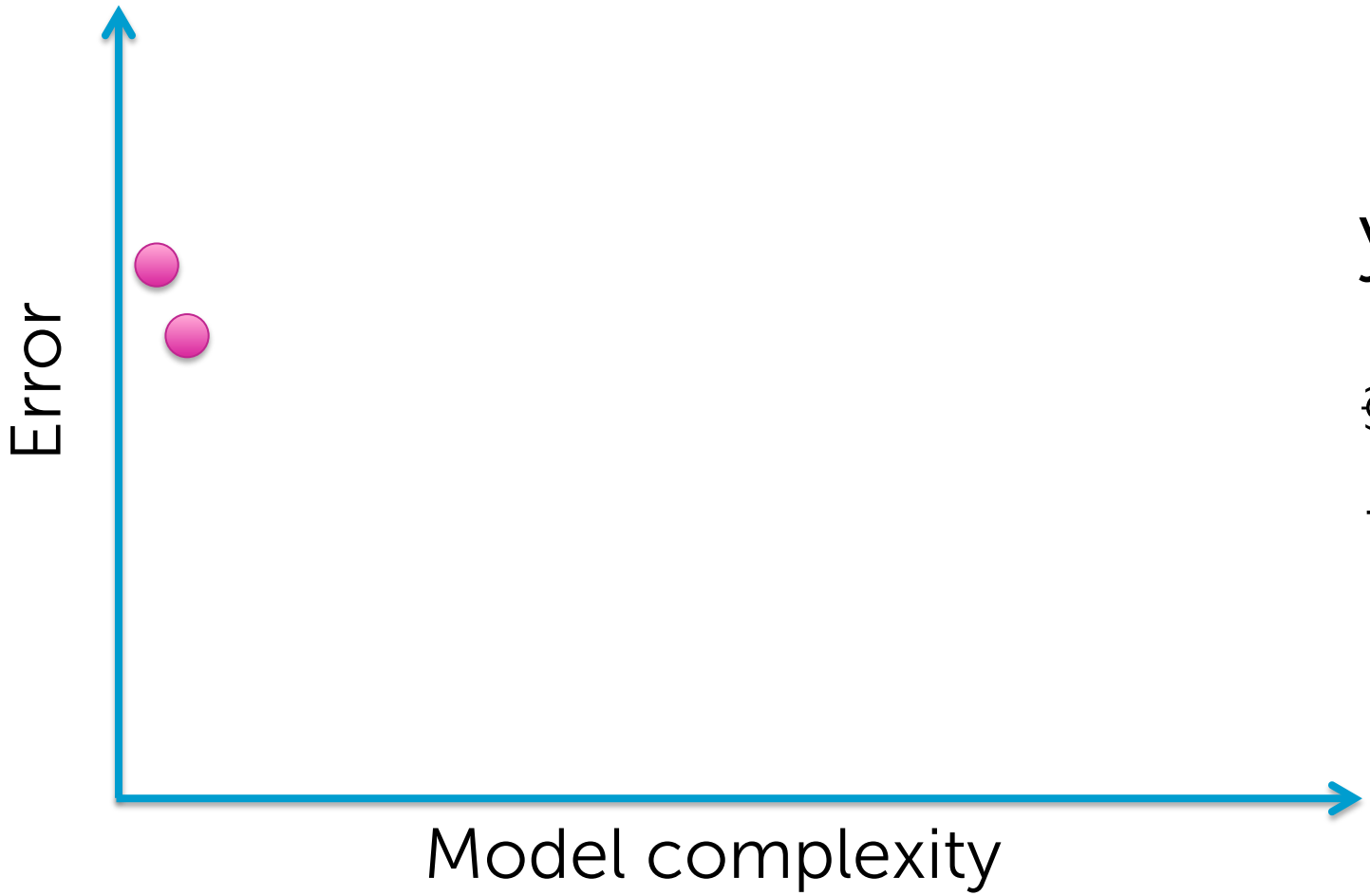

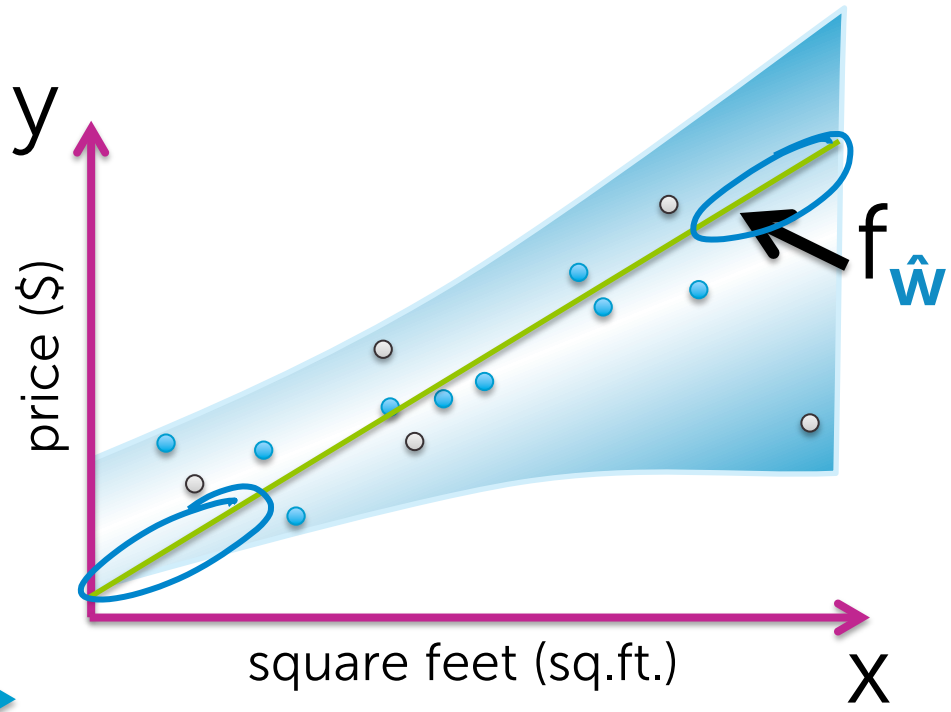

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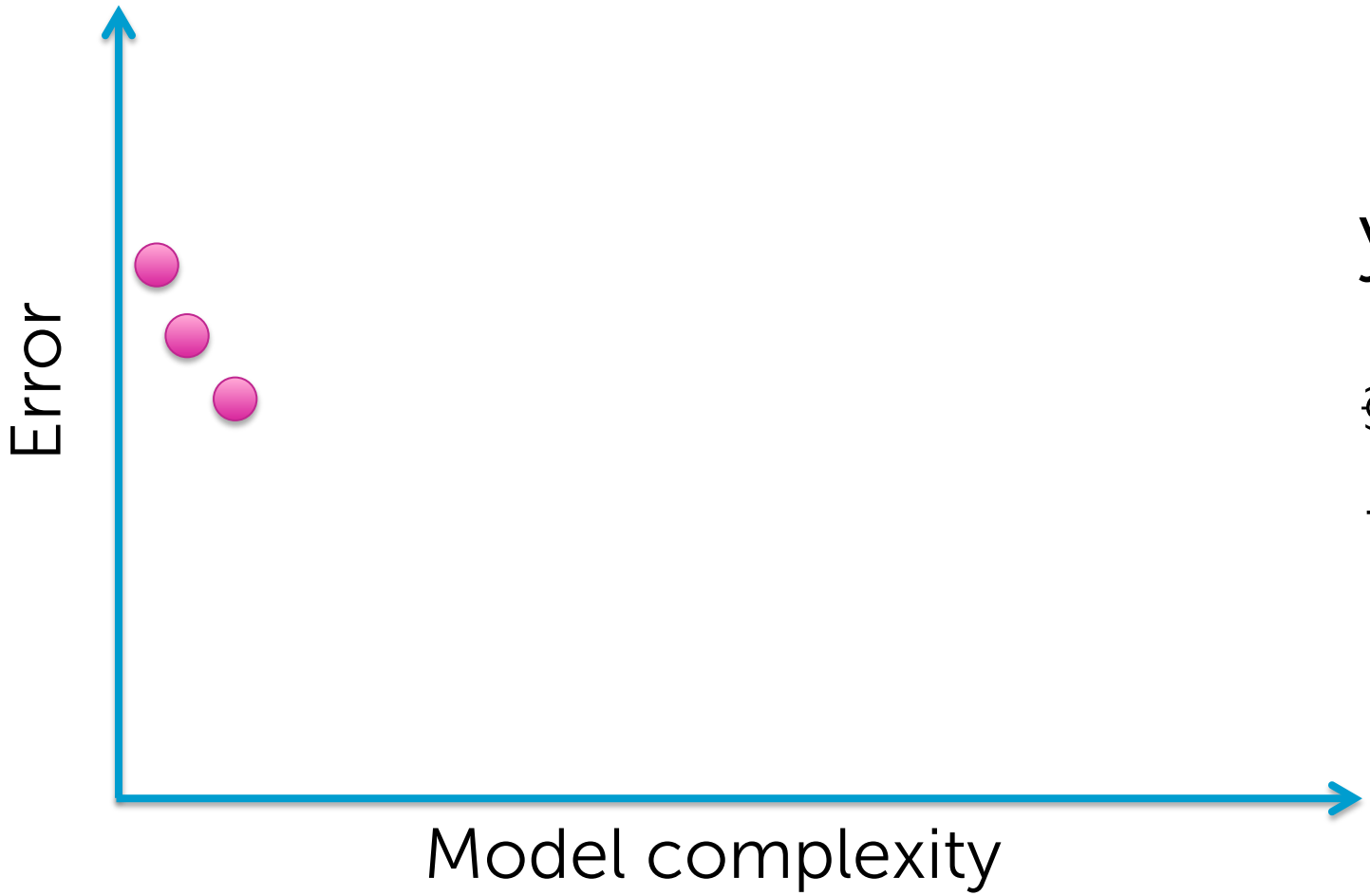

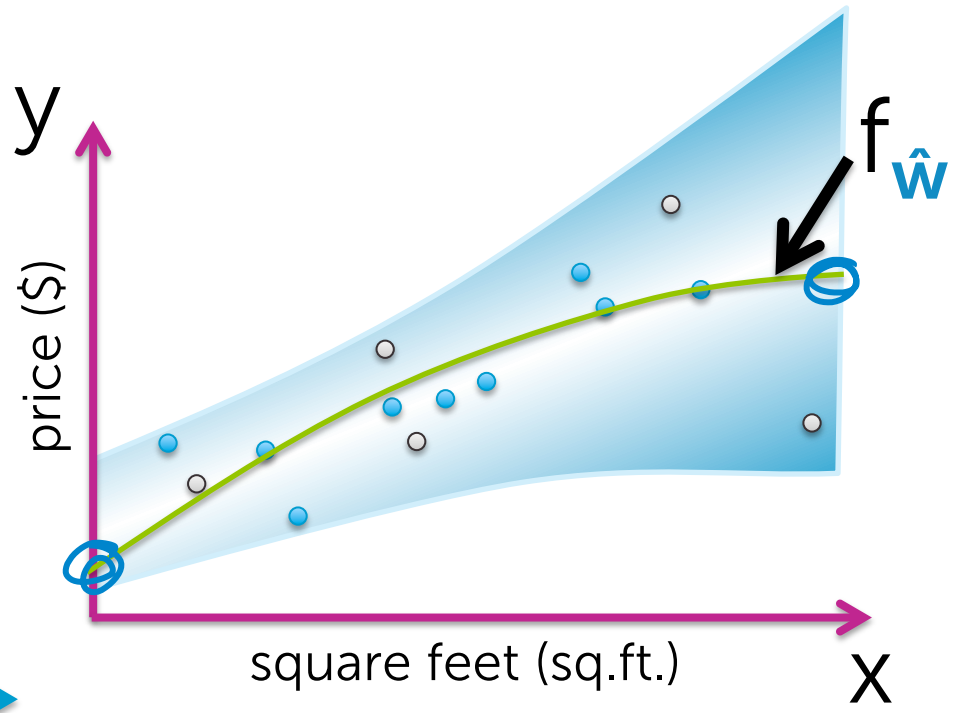

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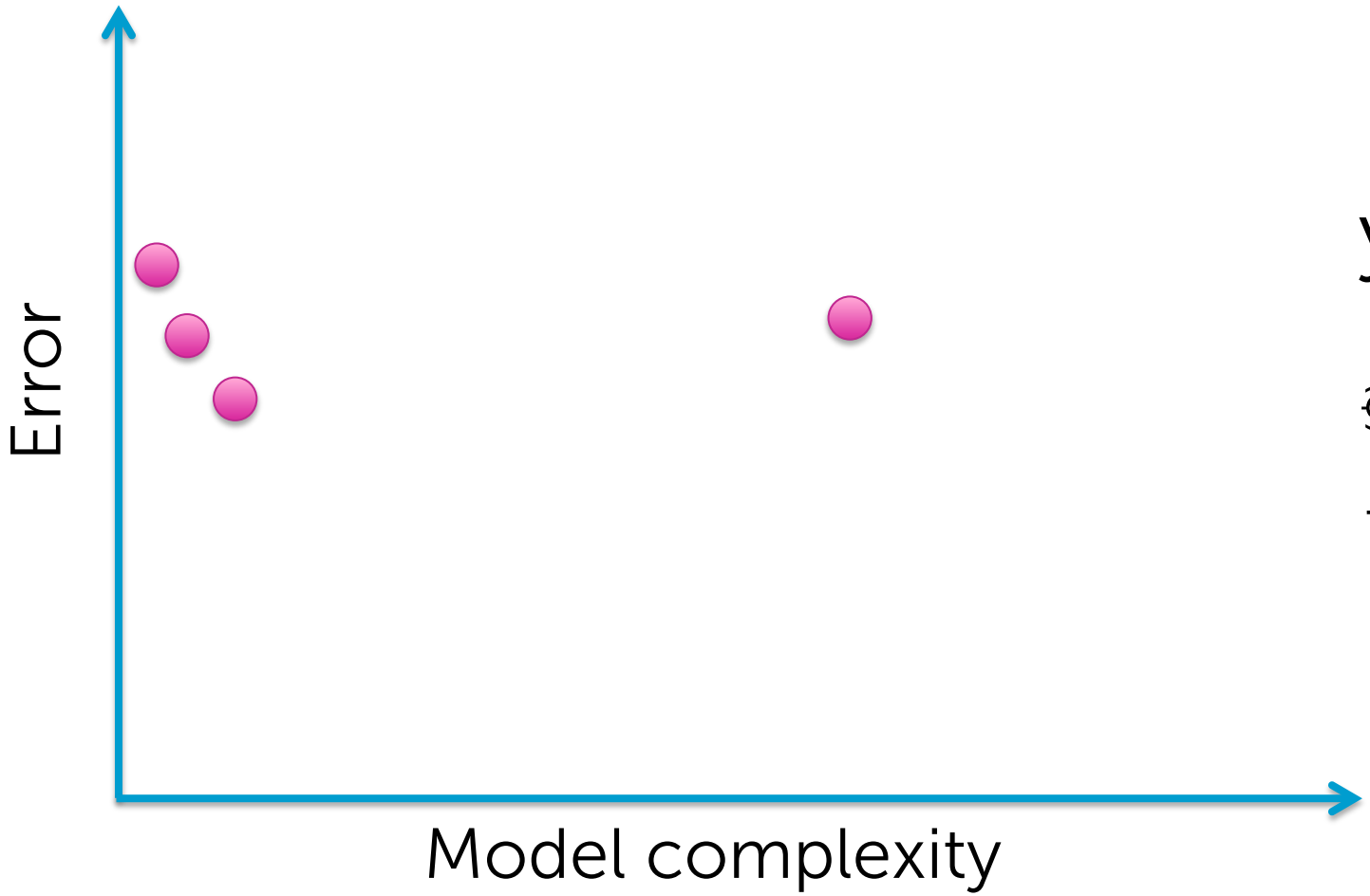
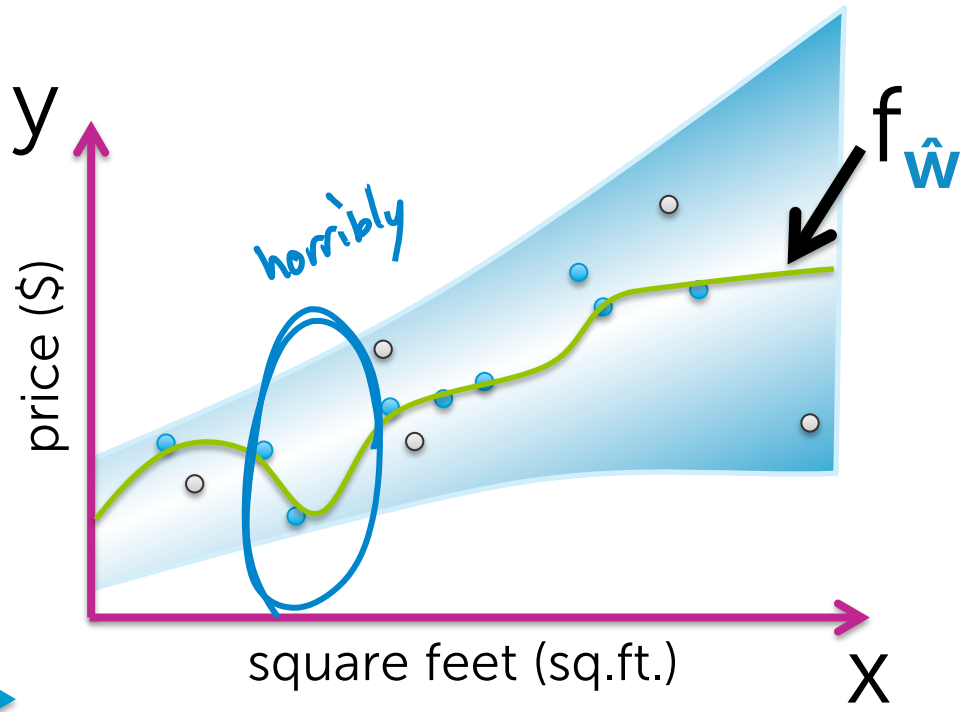
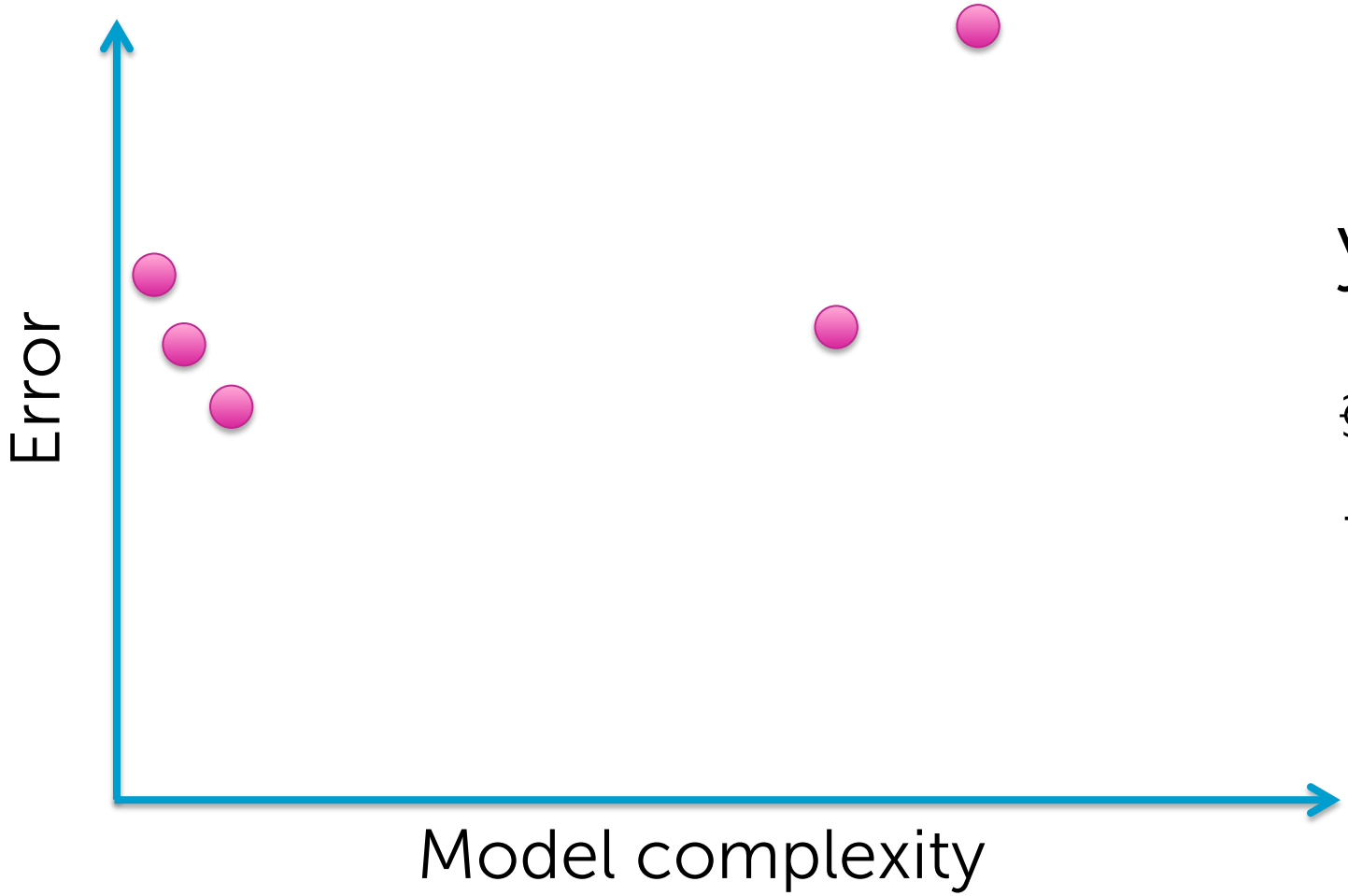
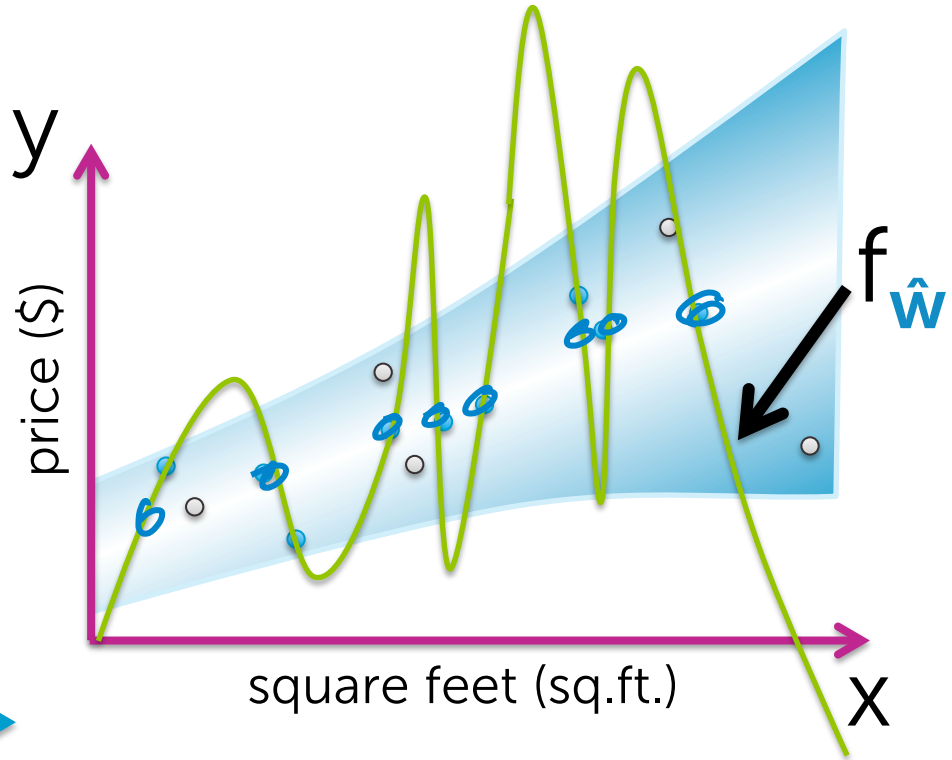


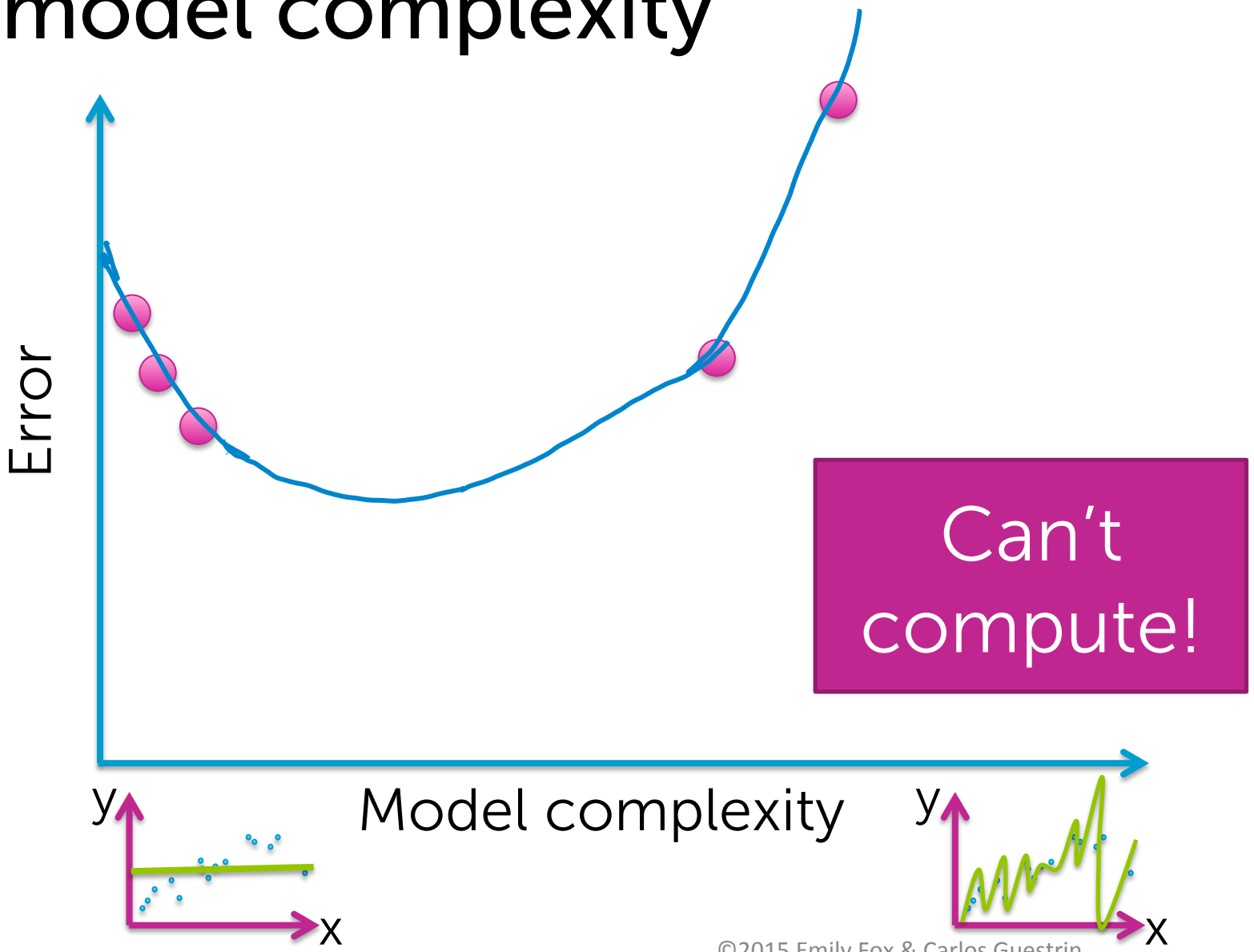


Generalization error vs. model complexity





Generalization error vs. model complexity



Can't compute!

Assessing the loss
Part 3: Test error

Approximating generalization error

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

Approximate by looking at houses not in training set

Forming a test set

Hold out some (🏠,$) that are *not* used for fitting the model

Training set

Test set

Forming a test set

Hold out some (🏠,$) that are *not* used for fitting the model

Proxy for "everything you might see"

Test set

Compute test error

Test error

= avg. loss on houses in test set

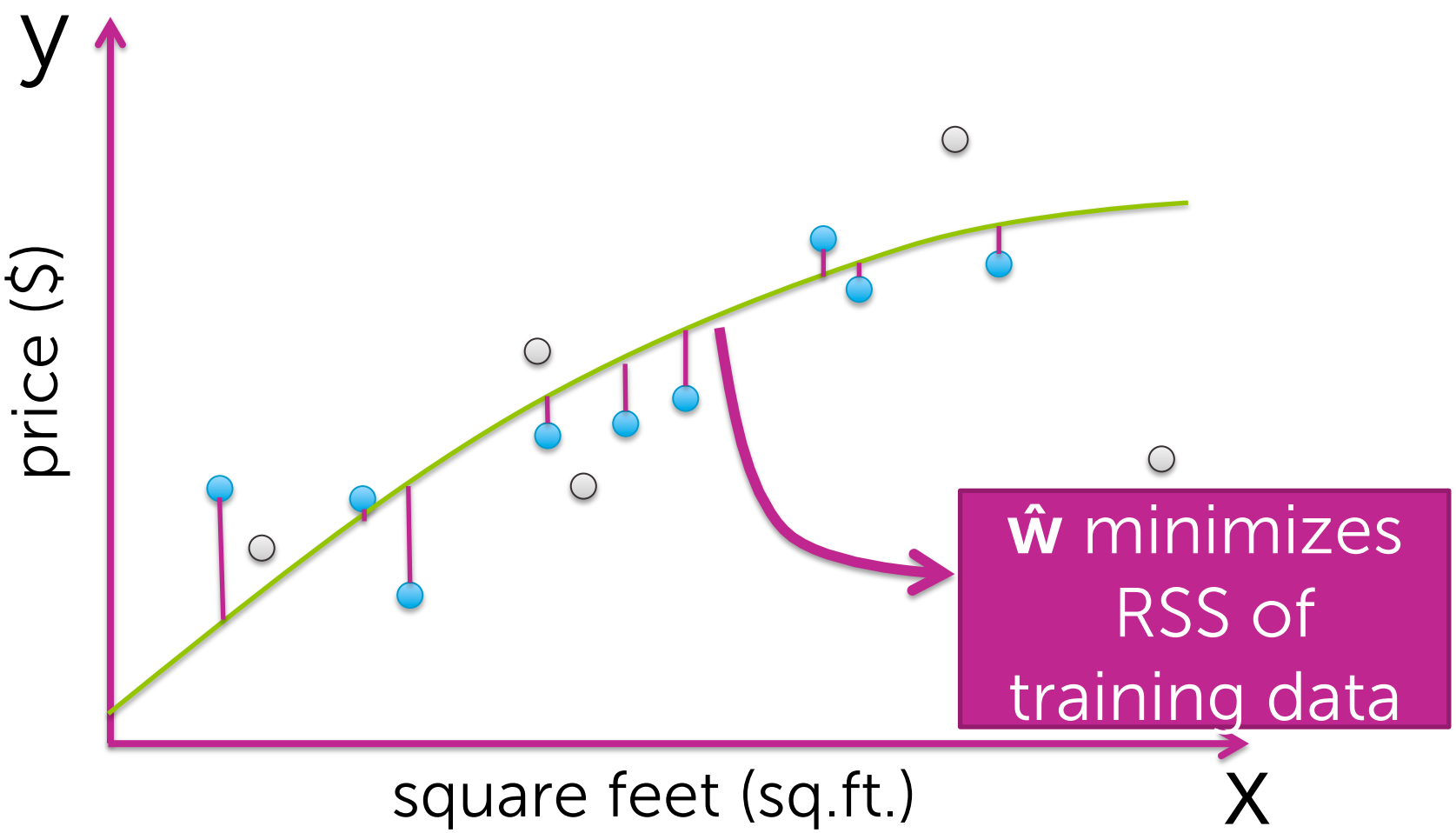
$$= \frac{1}{N_{test}} \sum_{i \text{ in test set}} L(y_i, f_{\hat{w}}(\mathbf{x}_i))$$

test points

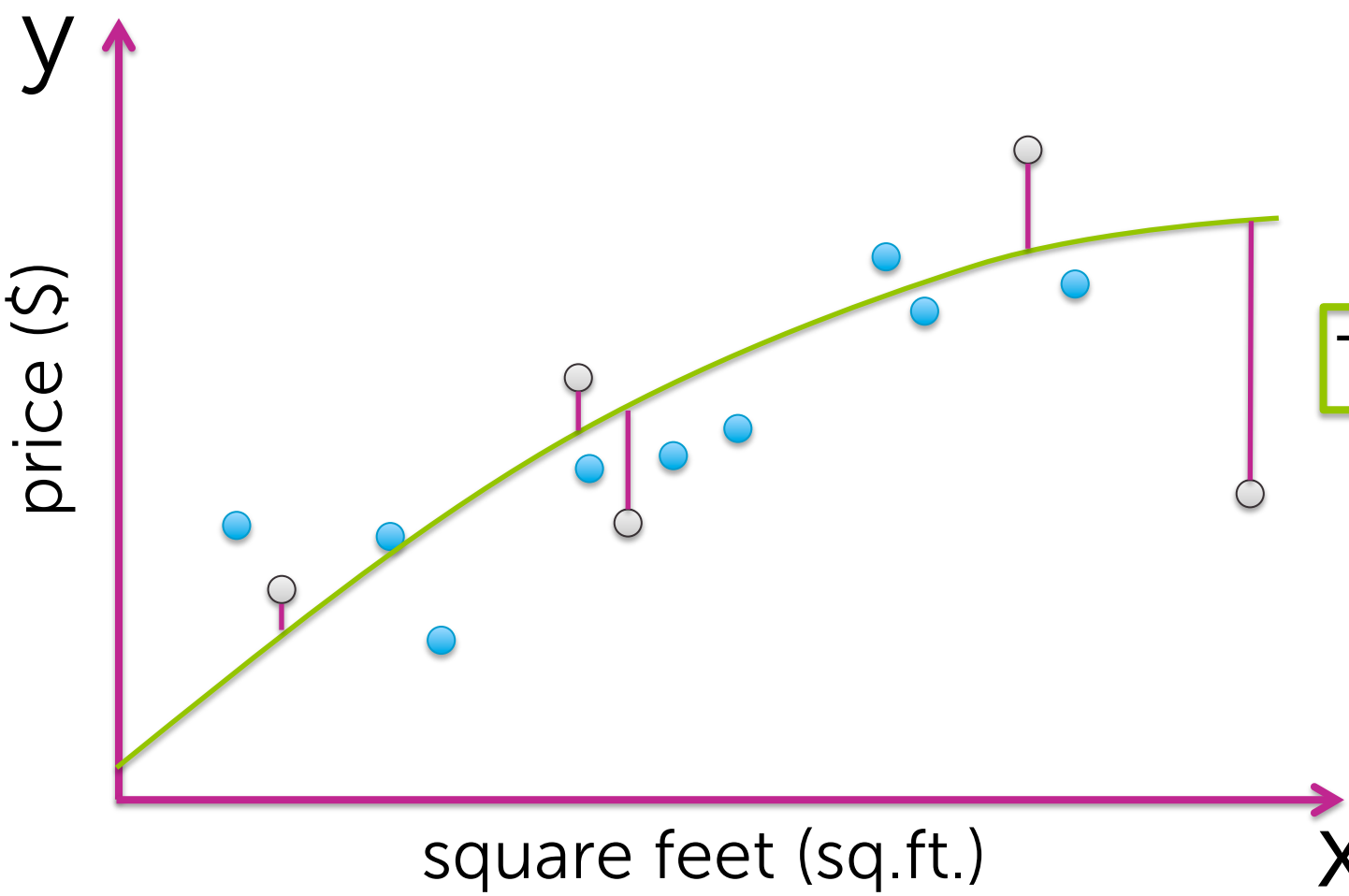
fit using training data

has never seen test data!

Example: As before, fit quadratic to training data

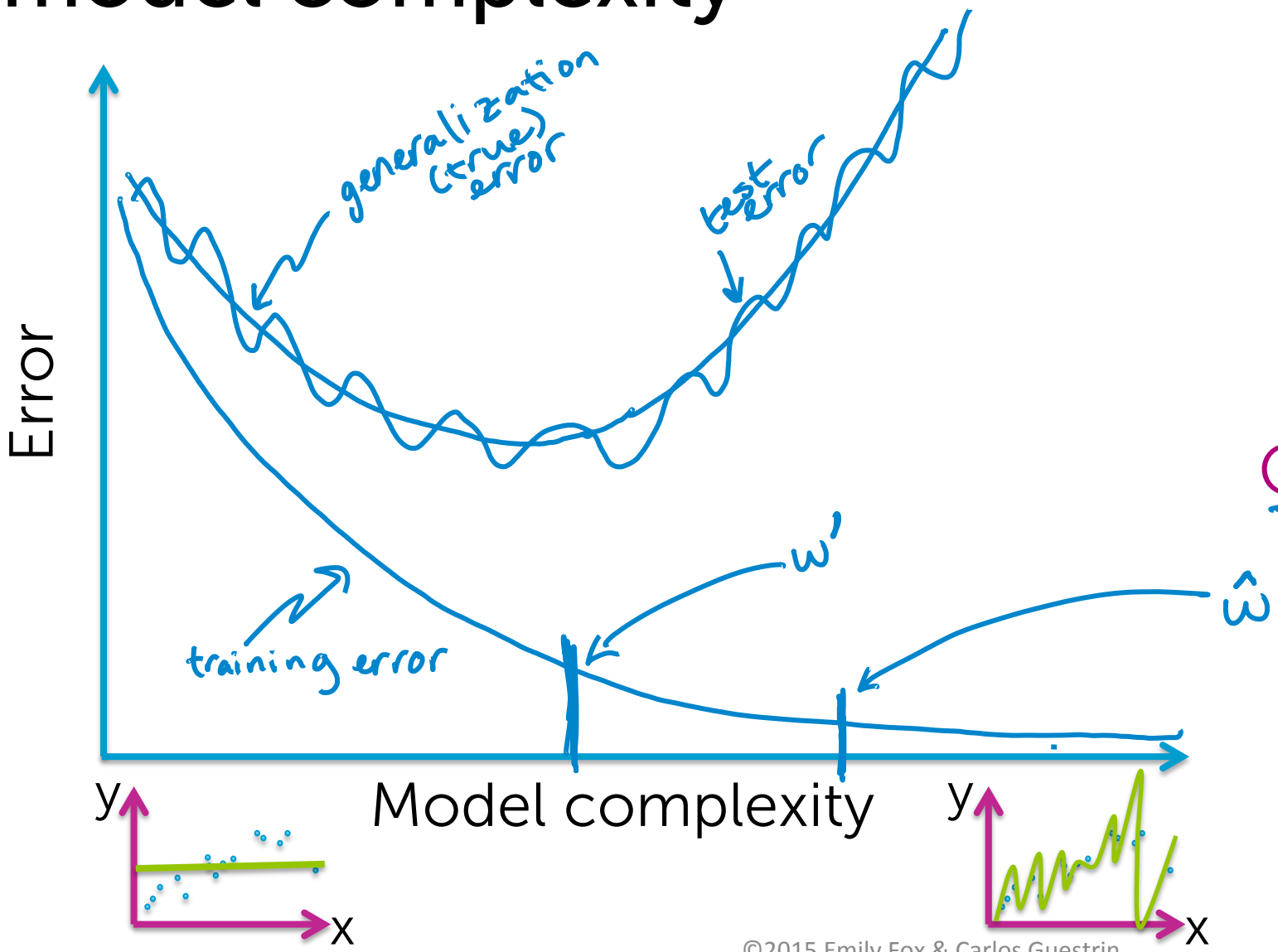


Example: As before, use squared error loss $(y-f_{\hat{w}}(x))^2$



Test error ($\hat{w}$) = 1/N *
$[(\$_{test\ 1}-f_{\hat{w}}(sq.ft._{test\ 1}))^2$
$+ (\$_{test\ 2}-f_{\hat{w}}(sq.ft._{test\ 2}))^2$
$+ (\$_{test\ 3}-f_{\hat{w}}(sq.ft._{test\ 3}))^2$
+ … include all test houses]

Training, true, & test error vs. model complexity



Overfitting if:

If there exists a model with estimated params w' such that

① training error($\hat{w}$) < training error(w')

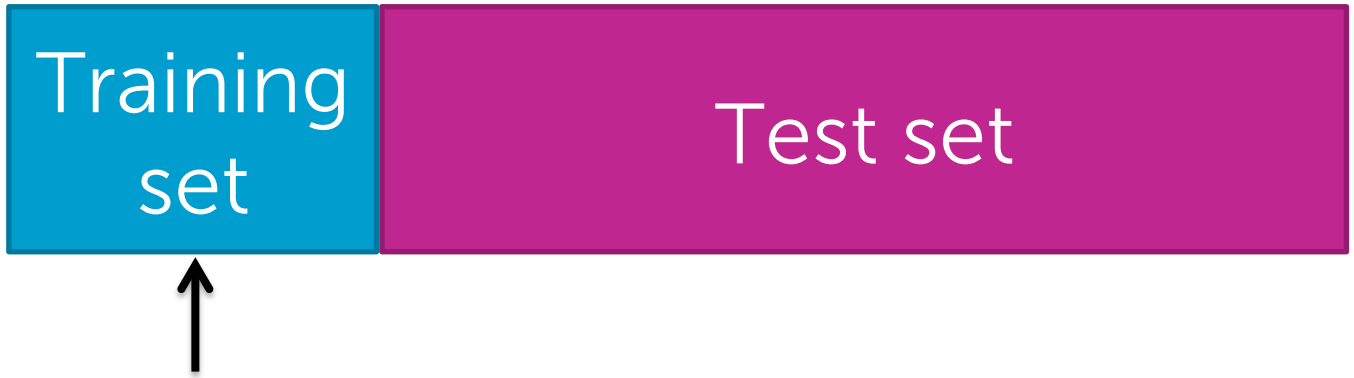
② true error($\hat{w}$) > true error(w')

Training/test split

Training/test splits

how many? vs. how many?

Training/test splits



Too few → $\hat{w}$ poorly estimated

Training/test splits

Too few → test error bad approximation of generalization error

Training/test splits

Typically, just enough test points to form a reasonable estimate of generalization error

If this leaves too few for training, other methods like **cross validation** (will see later…)

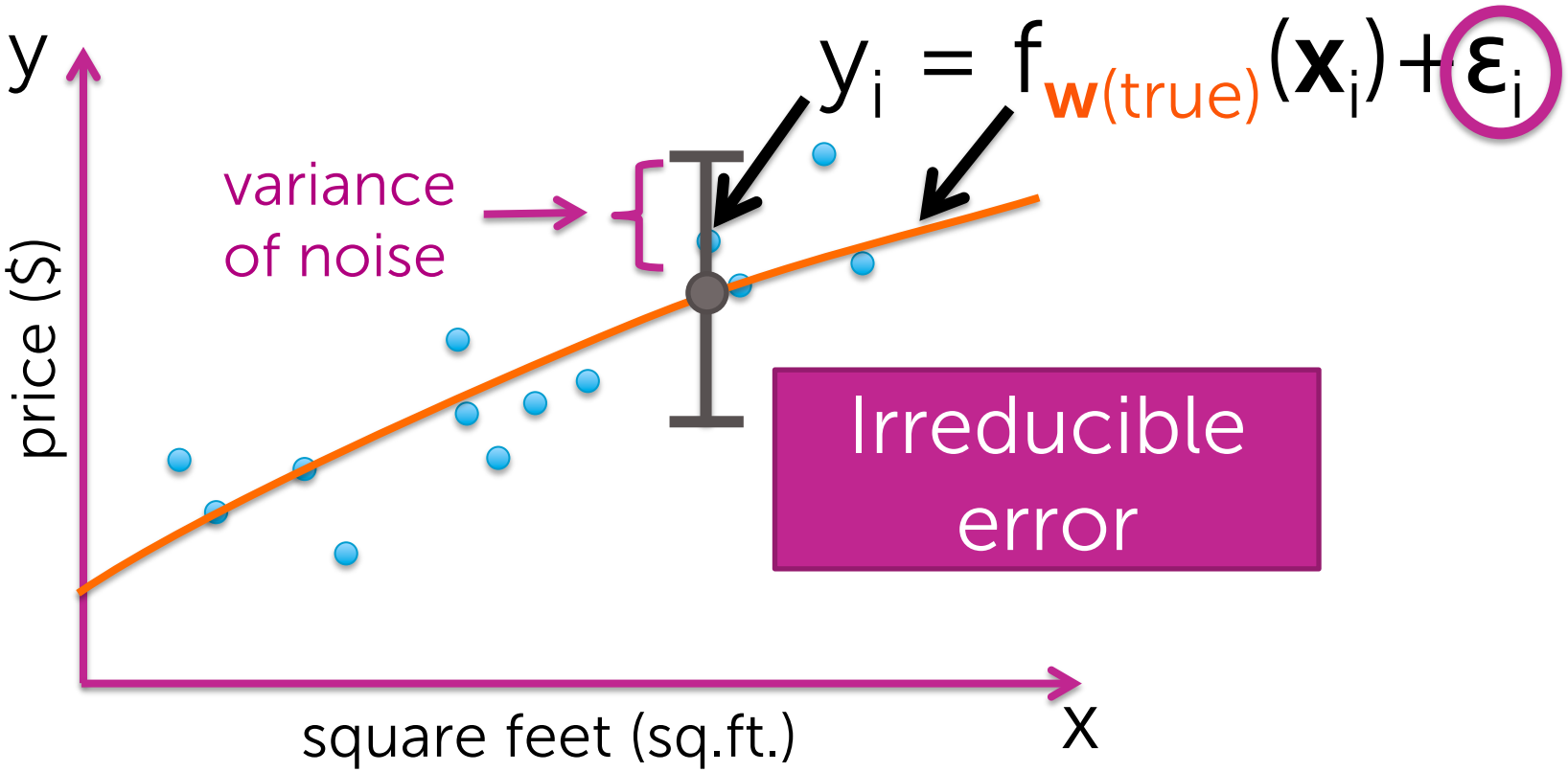
3 sources of error + the bias-variance tradeoff

3 sources of error

In forming predictions, there are 3 sources of error:

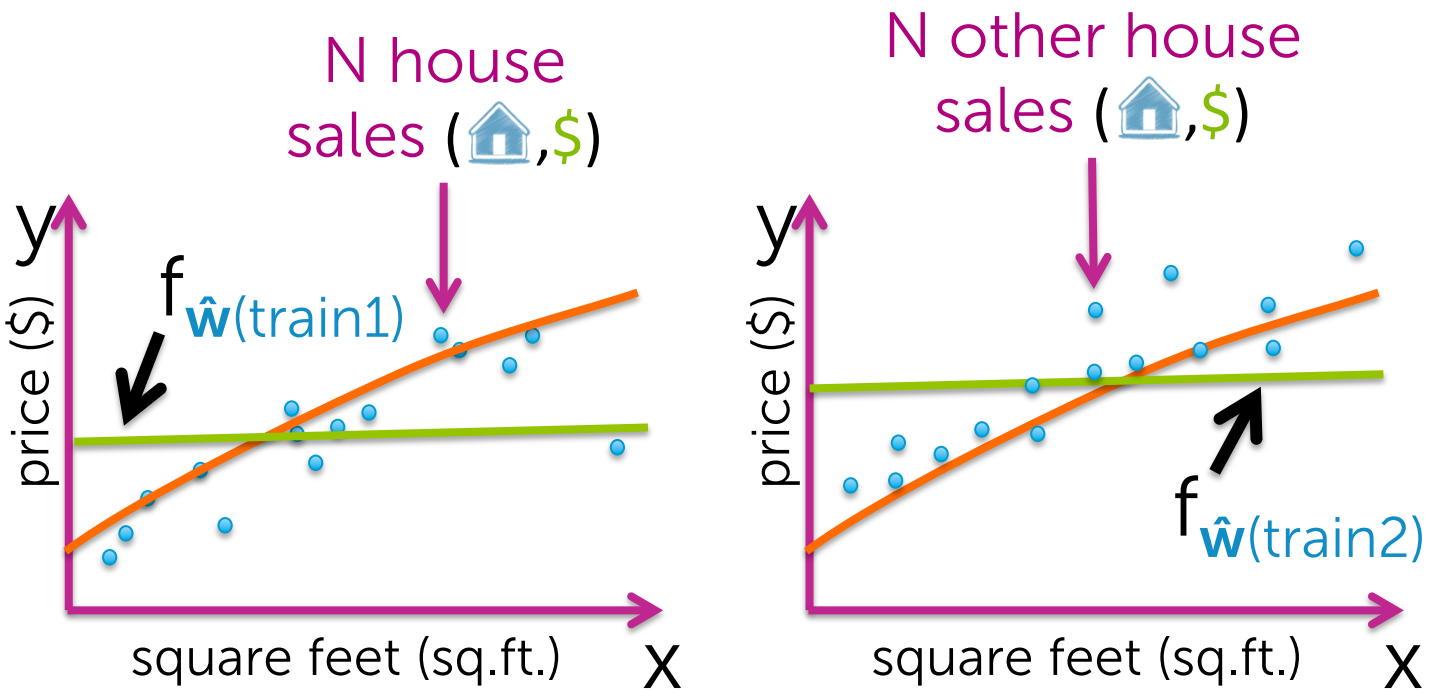
1. Noise
2. Bias
3. Variance

Data inherently noisy



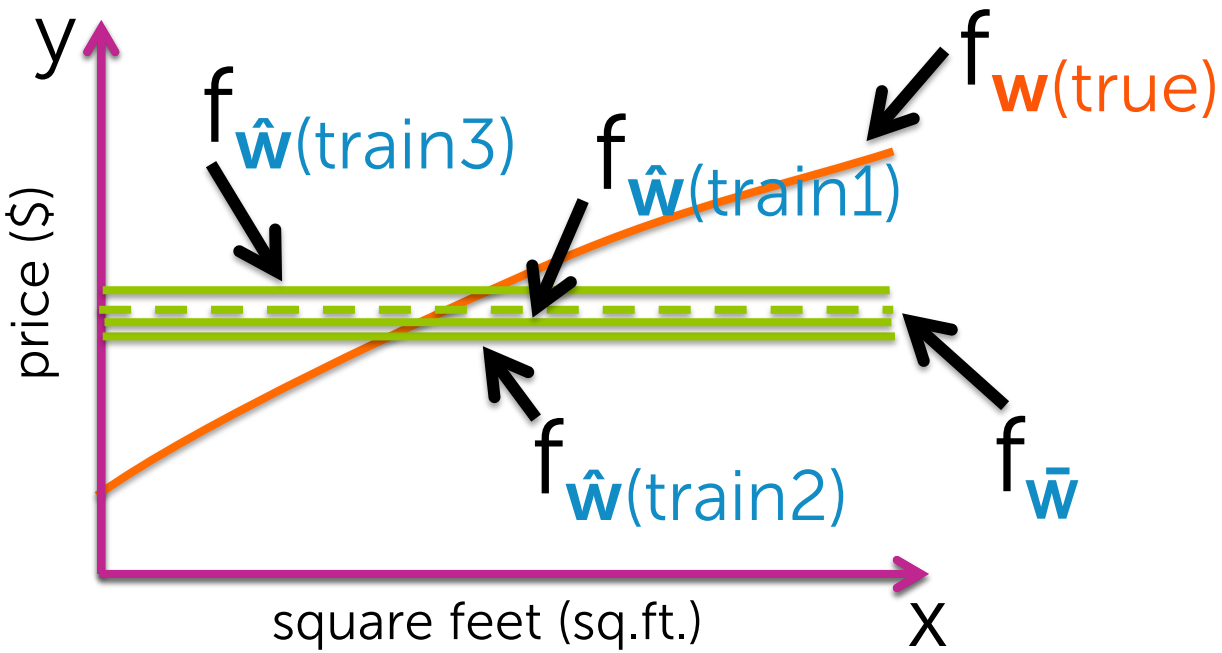
Bias contribution

Assume we fit a constant function



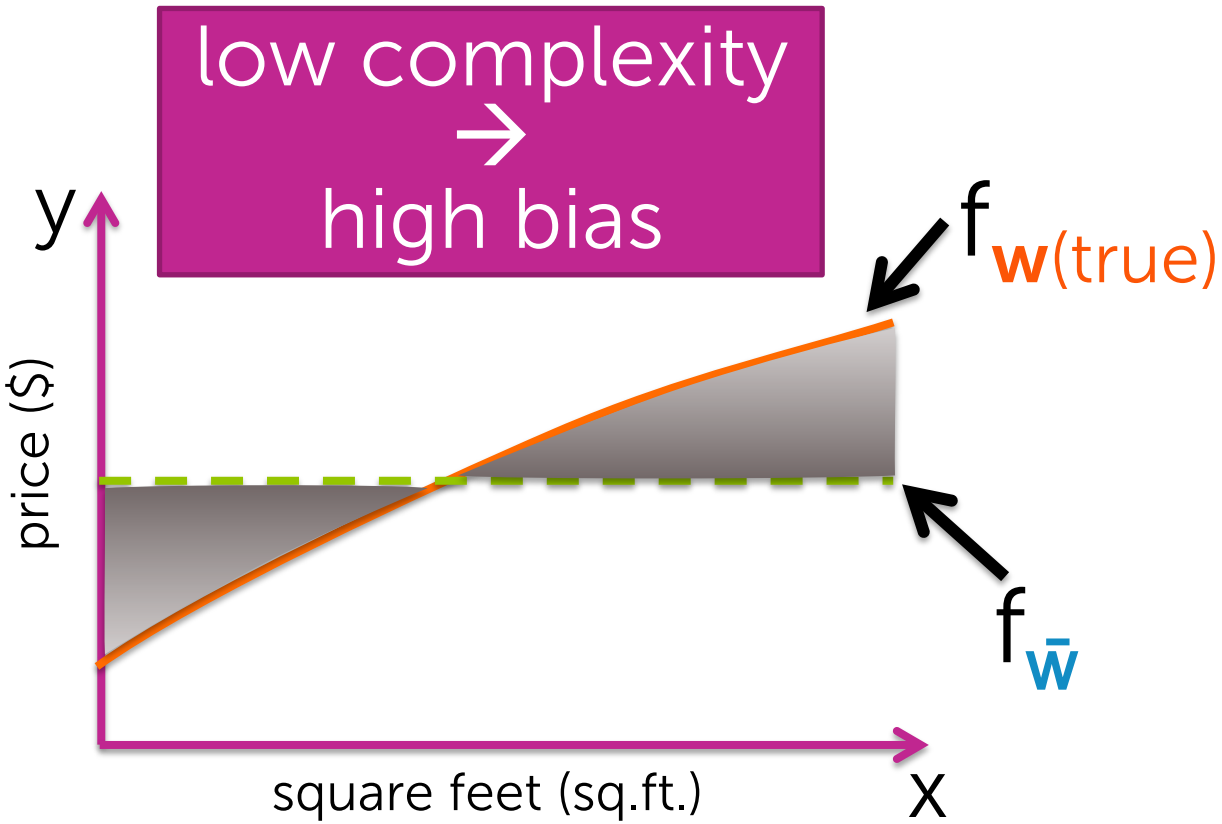
Bias contribution

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



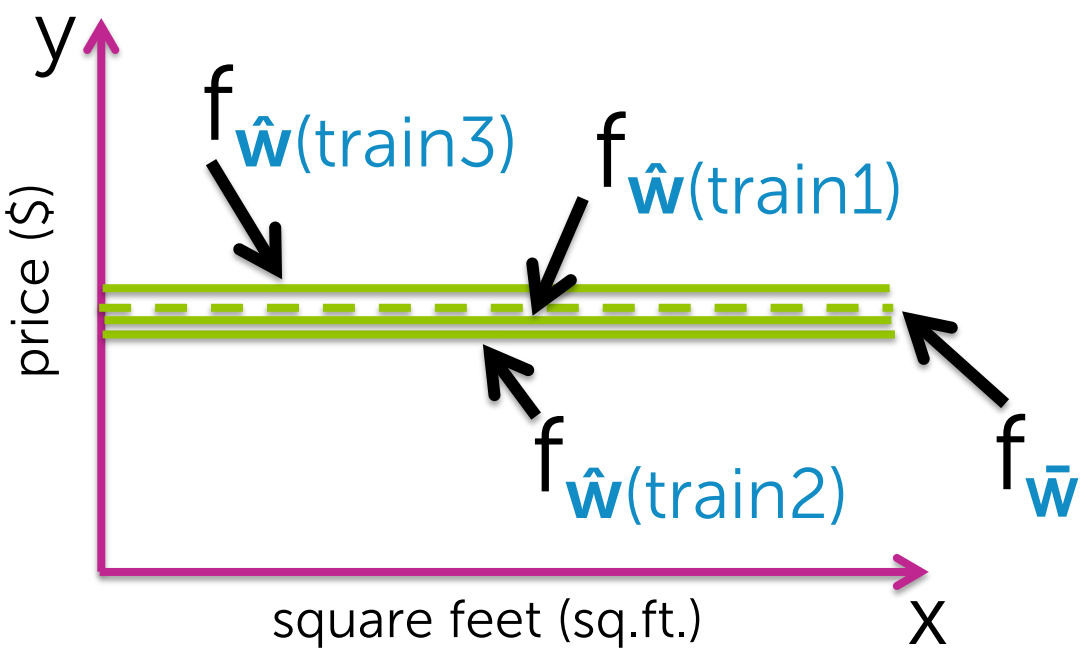
Bias contribution

$\text{Bias}(\mathbf{x}) = f_{\mathbf{w}(\text{true})}(\mathbf{x}) - f_{\bar{\mathbf{w}}}(\mathbf{x})$ ← Is our approach flexible enough to capture $f_{\mathbf{w}(\text{true})}$? **If not, error in predictions.**



Variance contribution

How much do specific fits vary from the expected fit?



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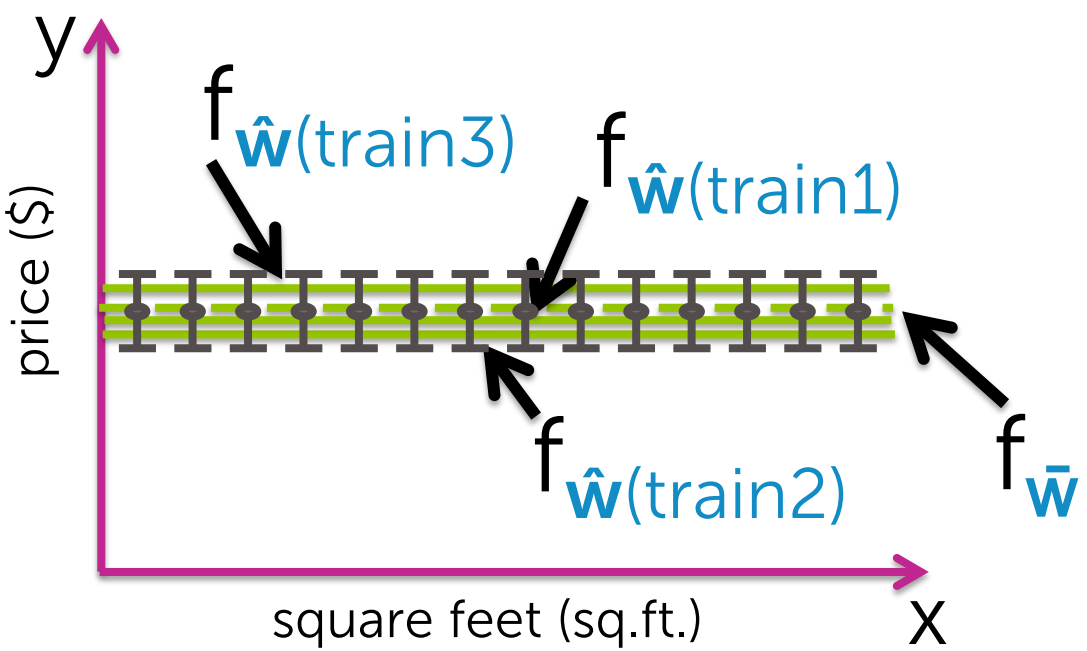

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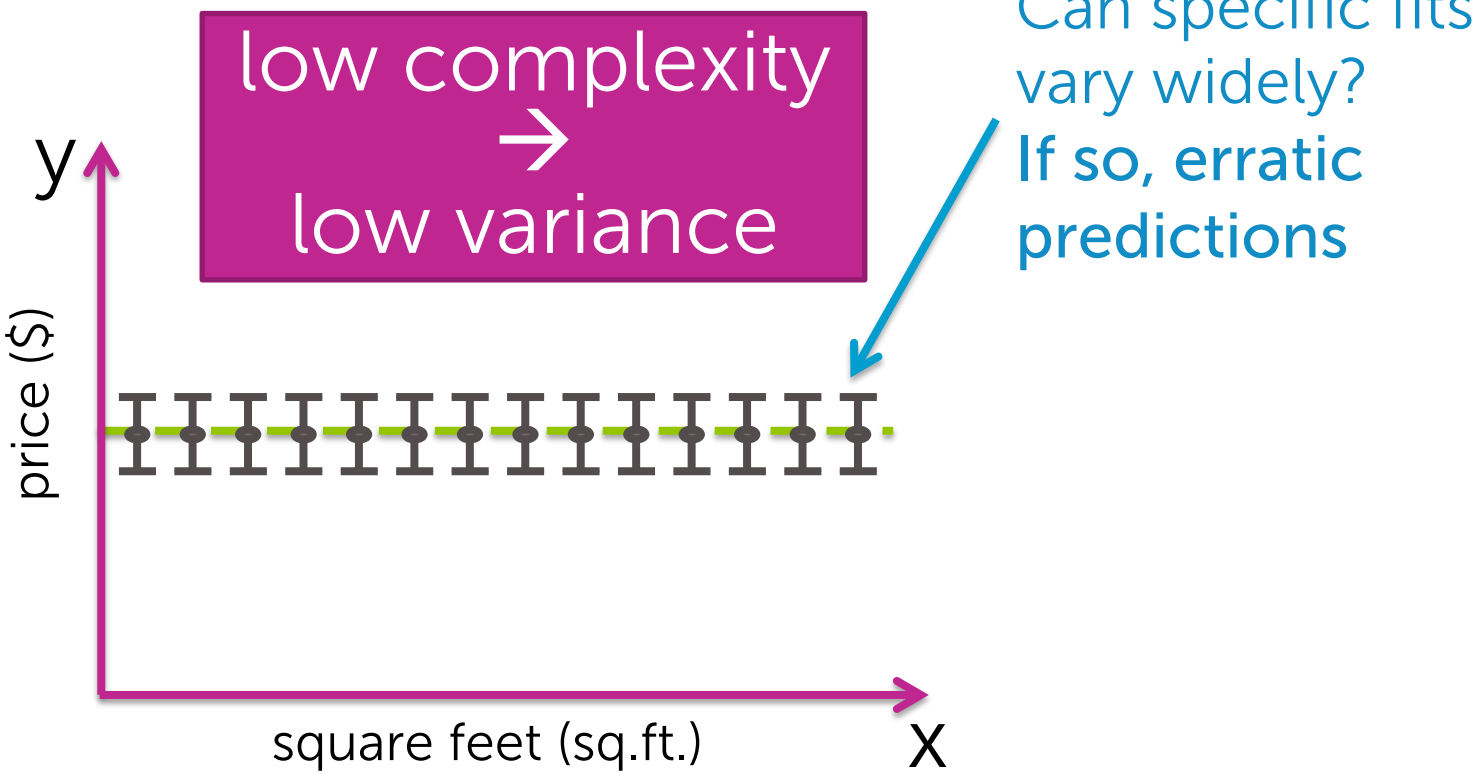
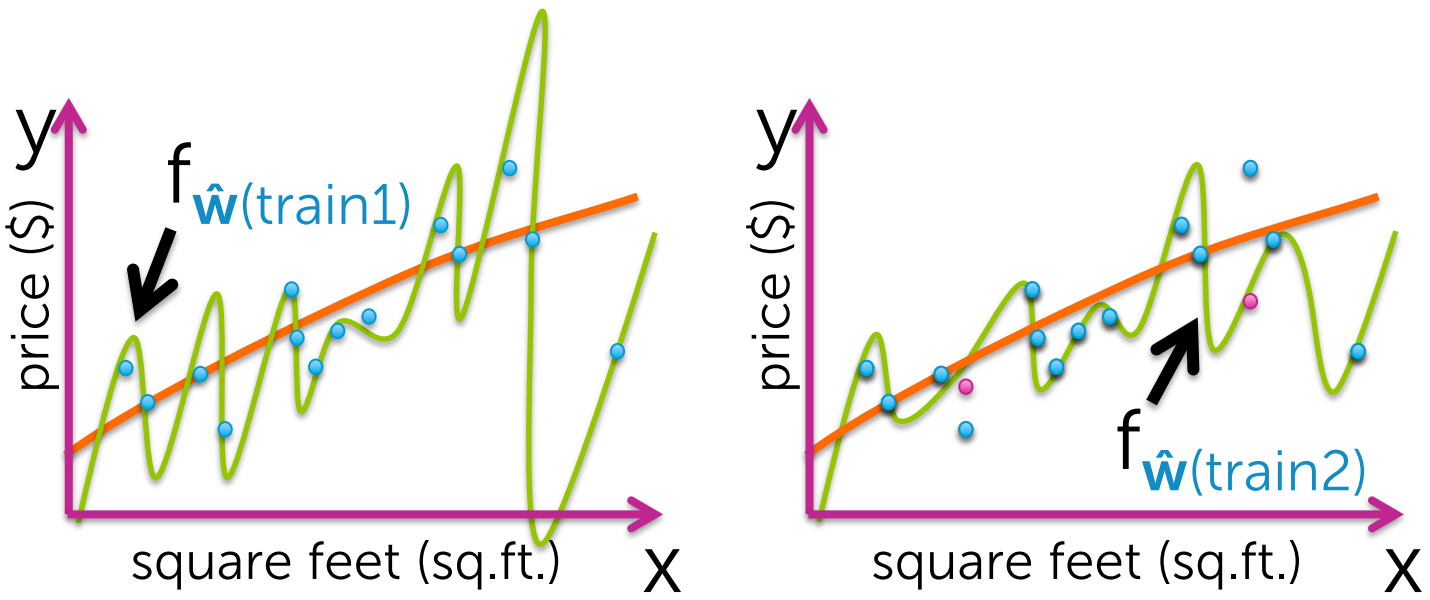


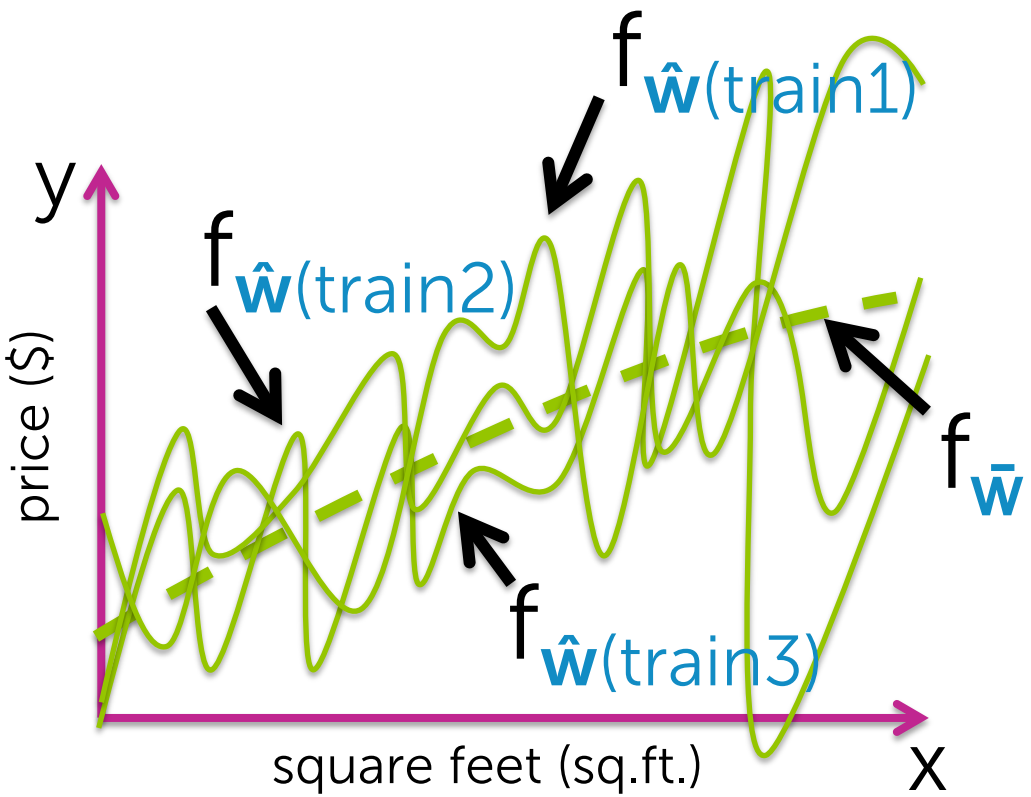
Variance of high-complexity models

Assume we fit a high-order polynomial

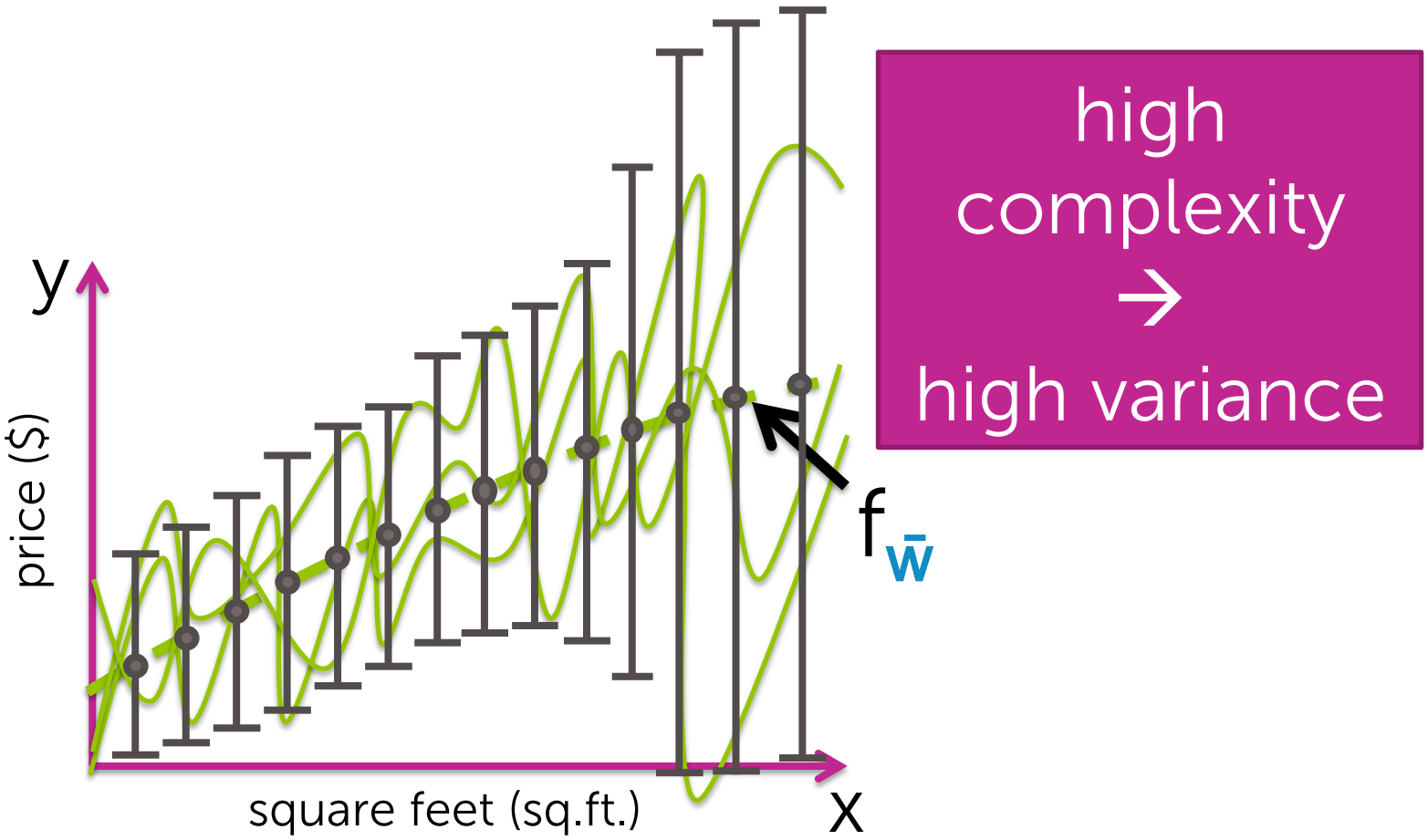


Variance of high-complexity models

Assume we fit a high-order polynomial



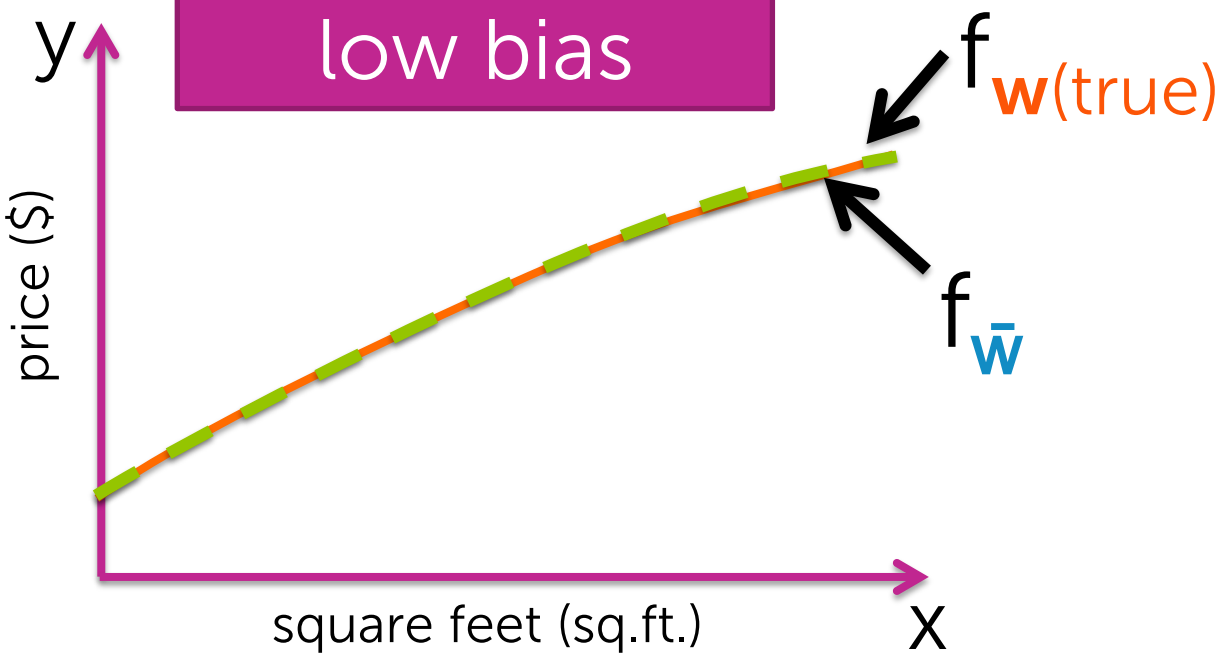
Variance of high-complexity models



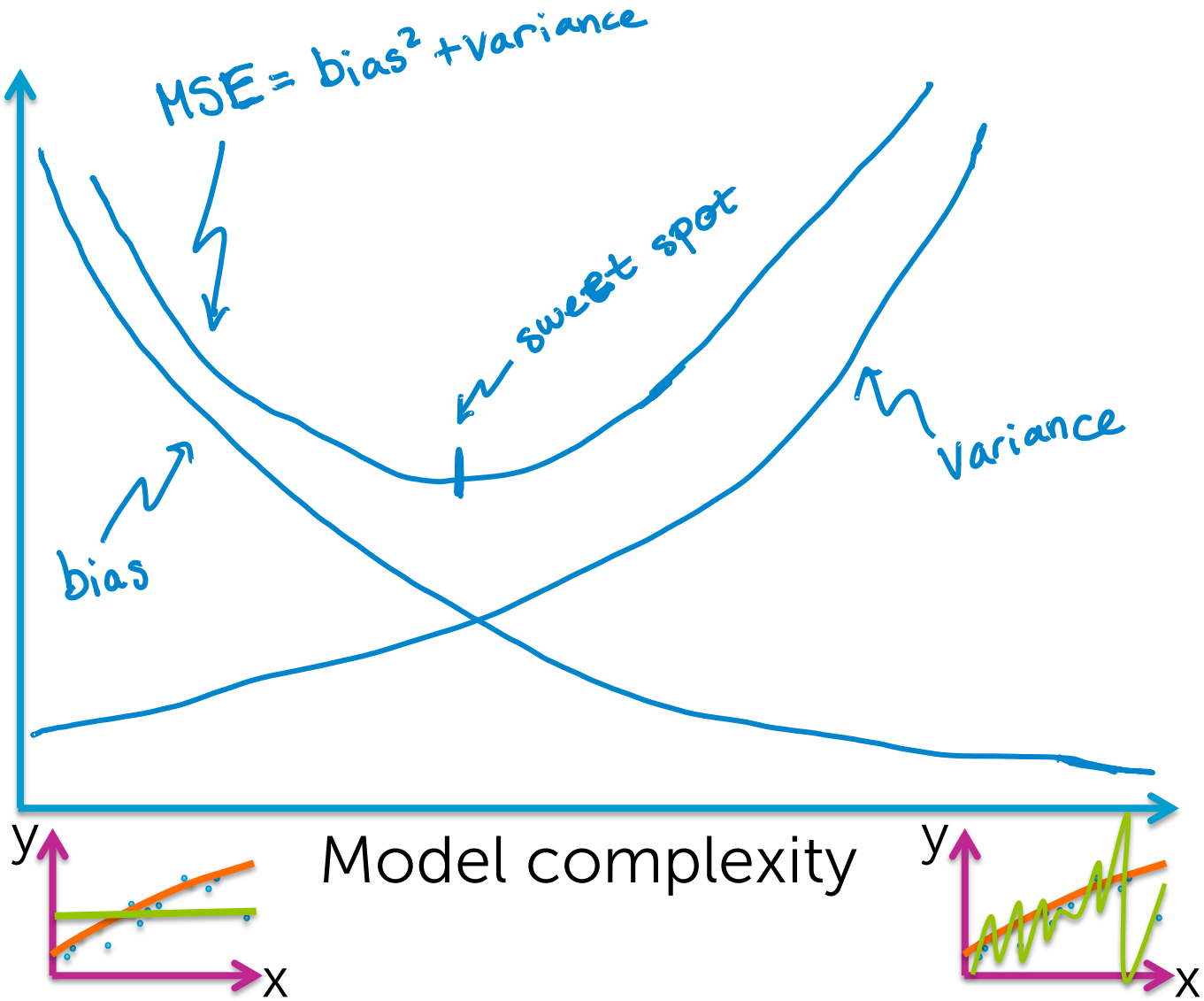
high complexity → high variance

Bias of high-complexity models

high complexity → low bias

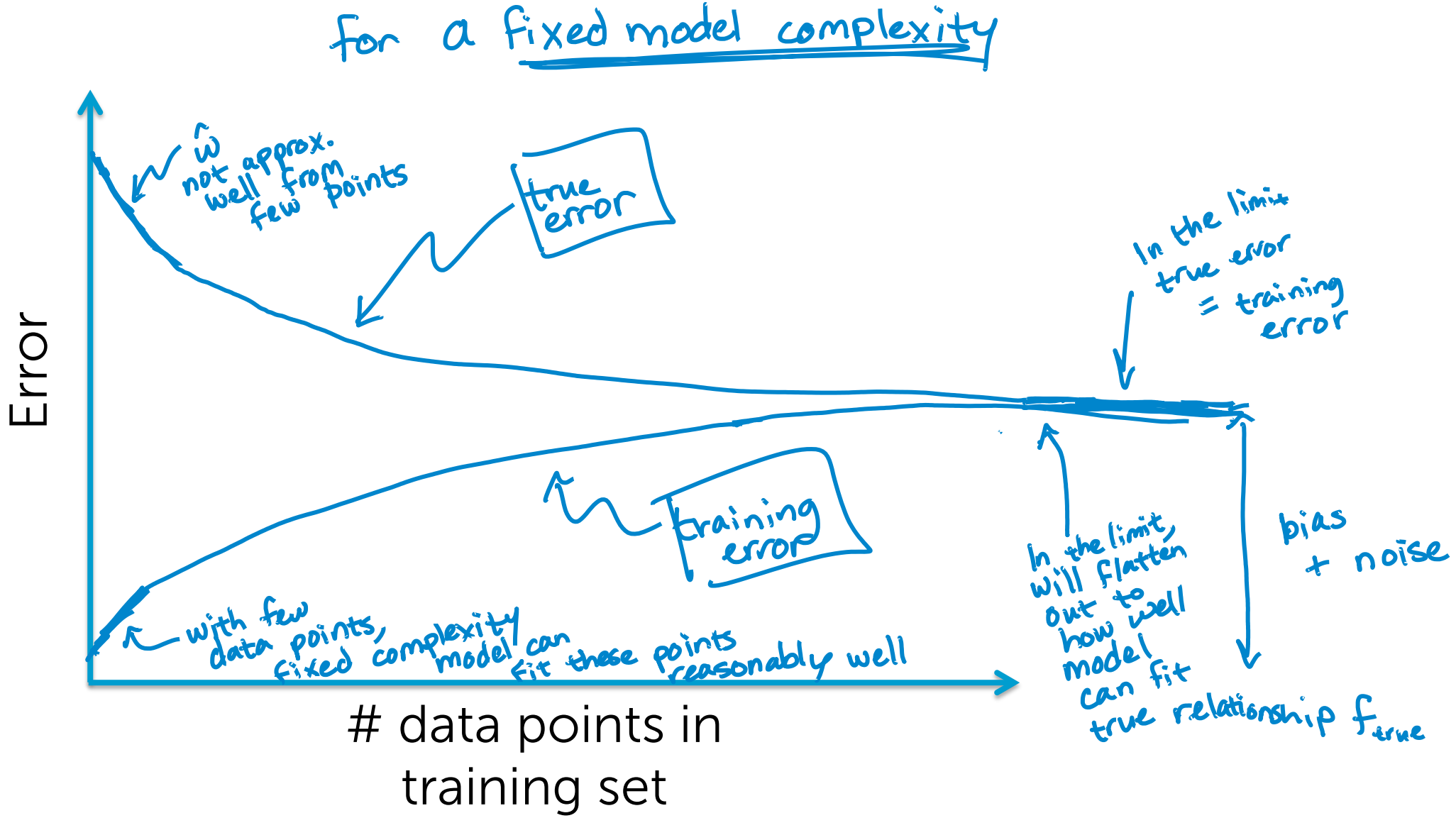


Bias-variance tradeoff



Just like with generalization error, we cannot compute bias and variance

Error vs. amount of data

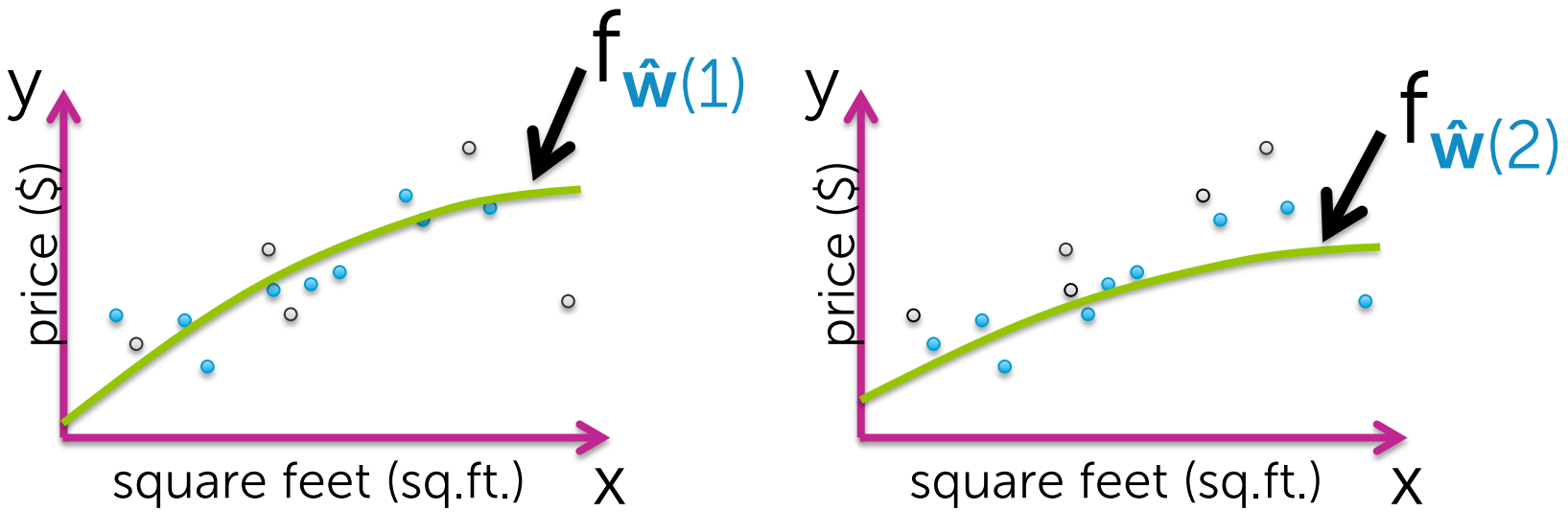


More in depth on the
3 sources of errors…

Accounting for training set randomness

Training set was just a random sample of N houses sold

What if N other houses had been sold and recorded?

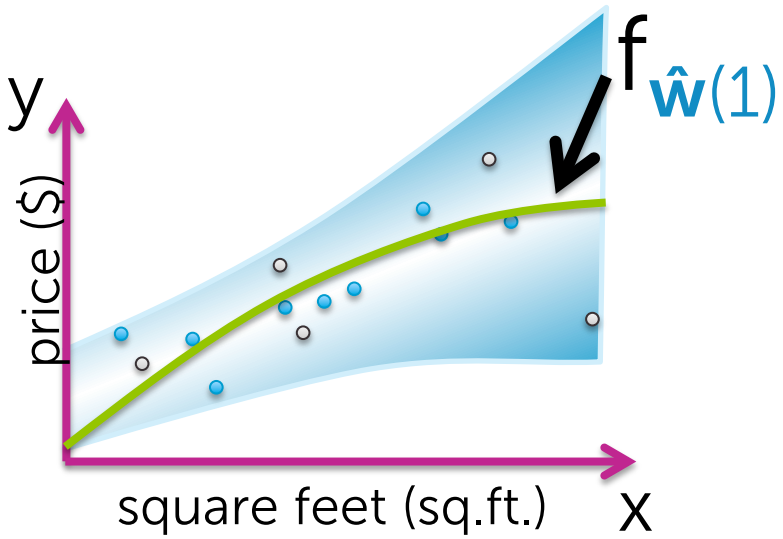


Accounting for training set randomness

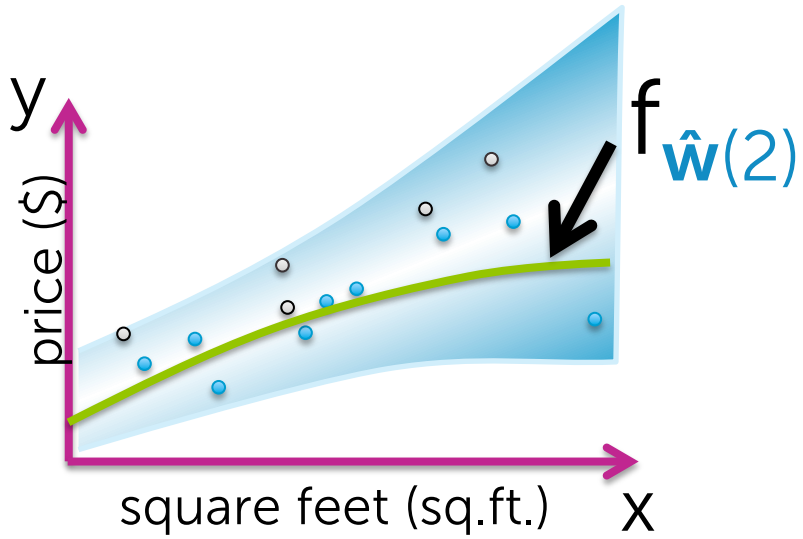
Training set was just a random sample of N houses sold

What if N other houses had been sold and recorded?

generalization error of $\hat{w}(1)$



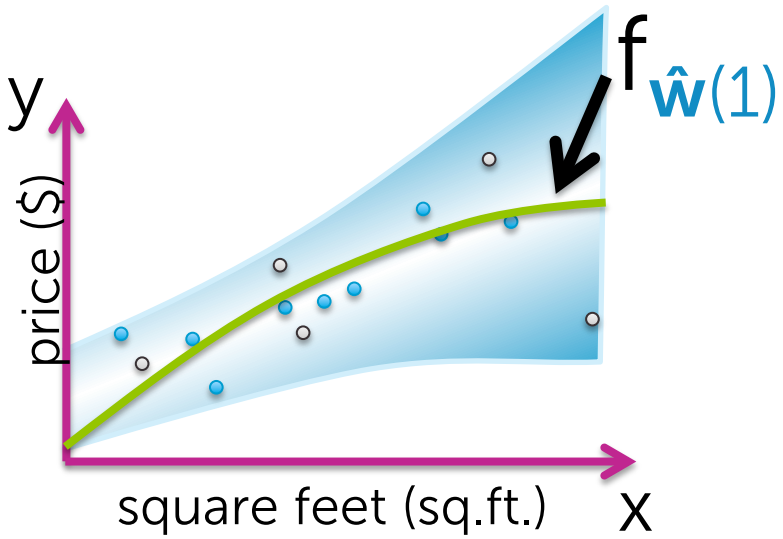
generalization error of $\hat{w}(2)$



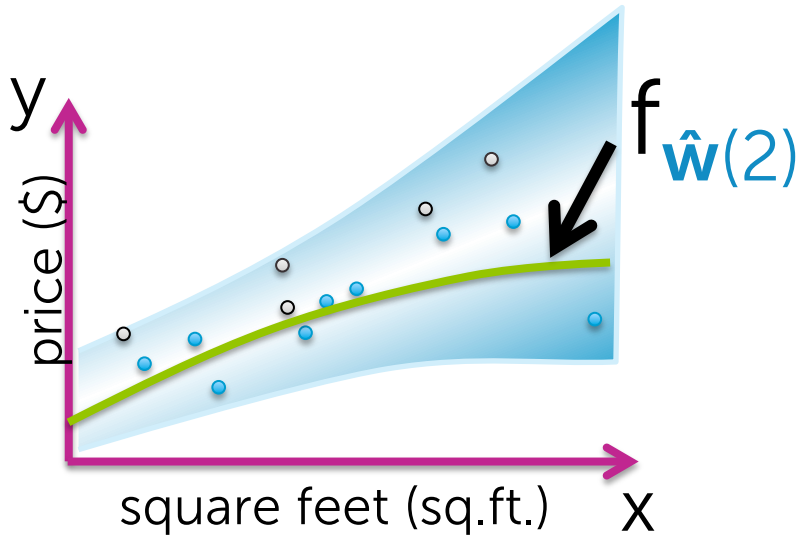
Accounting for training set randomness

Ideally, want performance averaged over all possible training sets of size N

generalization error of $\hat{\mathbf{w}}(1)$



generalization error of $\hat{\mathbf{w}}(2)$

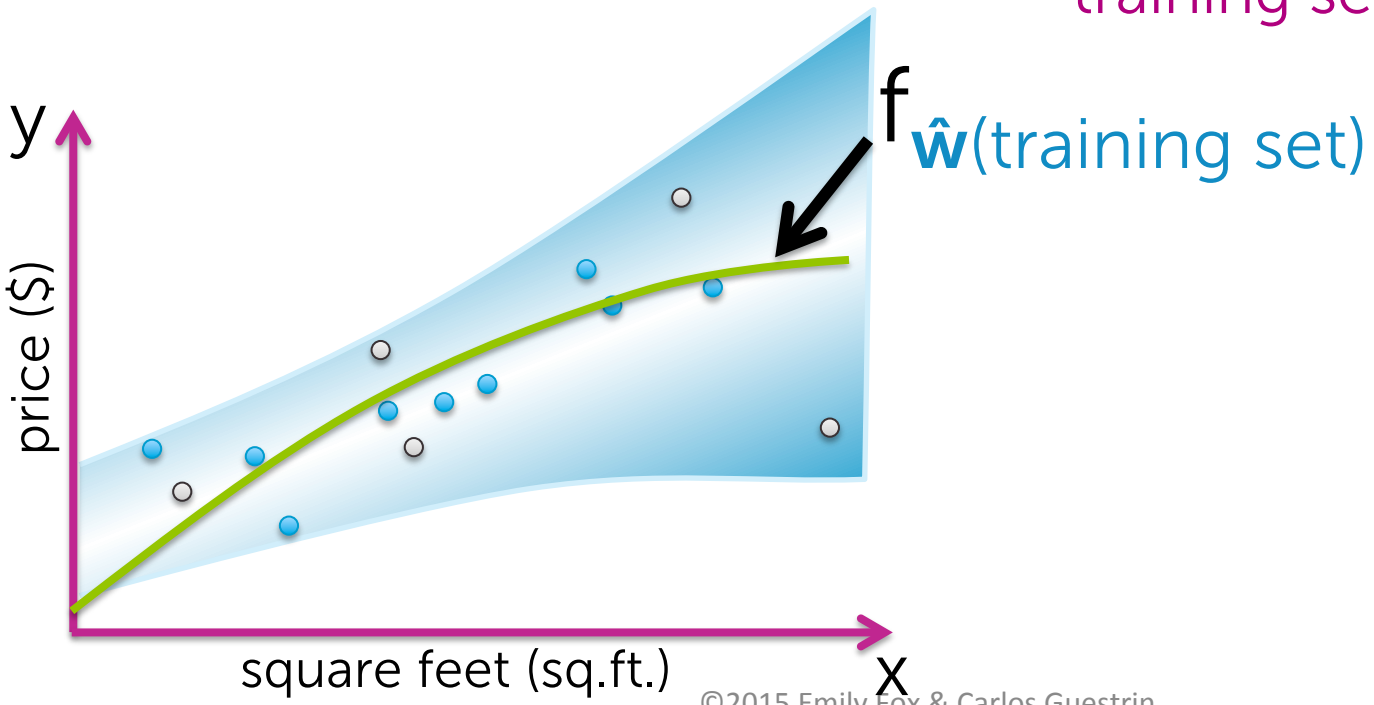


Expected prediction error

$E_{\text{training set}}$[generalization error of $\hat{\mathbf{w}}$(training set)]

averaging over all training sets (weighted by how likely each is)

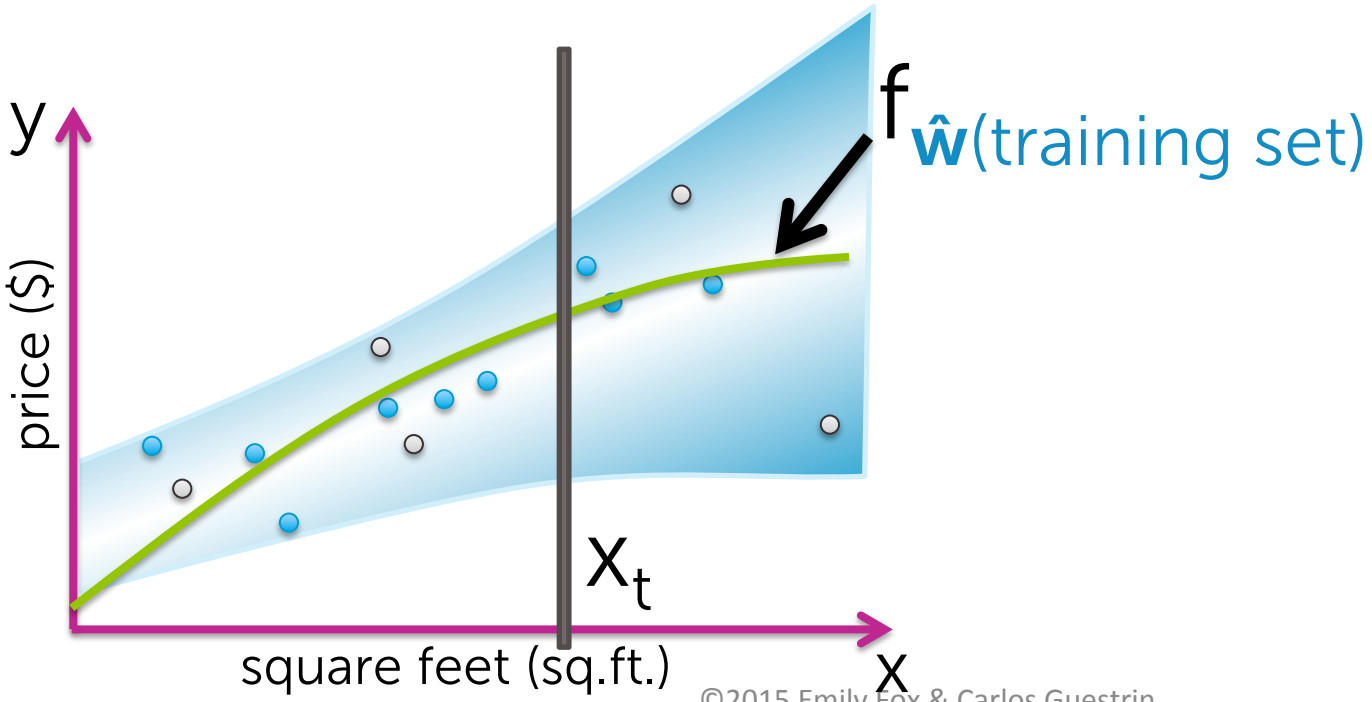
parameters fit on a specific training set



Prediction error at target input

Start by considering:

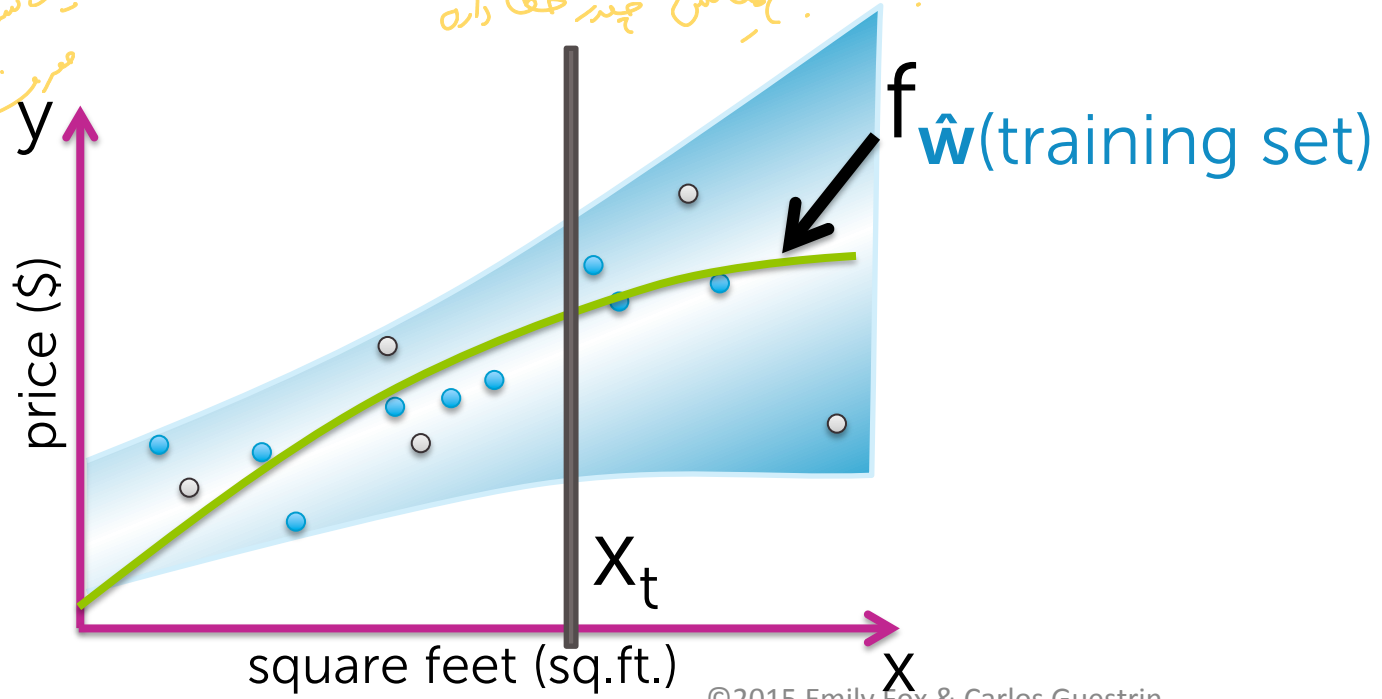
1. Loss at target $\mathbf{x}_t$ (e.g. 2640 sq.ft.)
2. Squared error loss $L(y, f_{\hat{\mathbf{w}}}(\mathbf{x})) = (y - f_{\hat{\mathbf{w}}}(\mathbf{x}))^2$



Sum of 3 sources of error

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

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



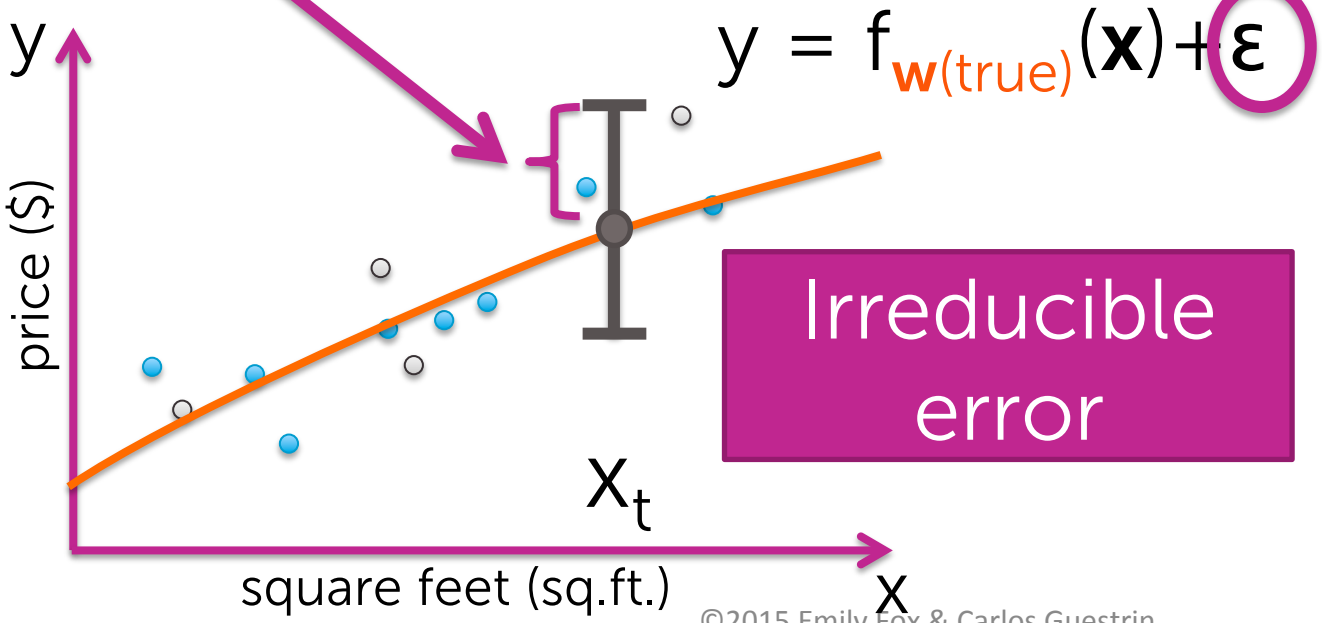
Error variance of the model

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

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

σ^2 = "variance"

$$y = f_{\mathbf{w}(\text{true})}(\mathbf{x}) + \varepsilon$$

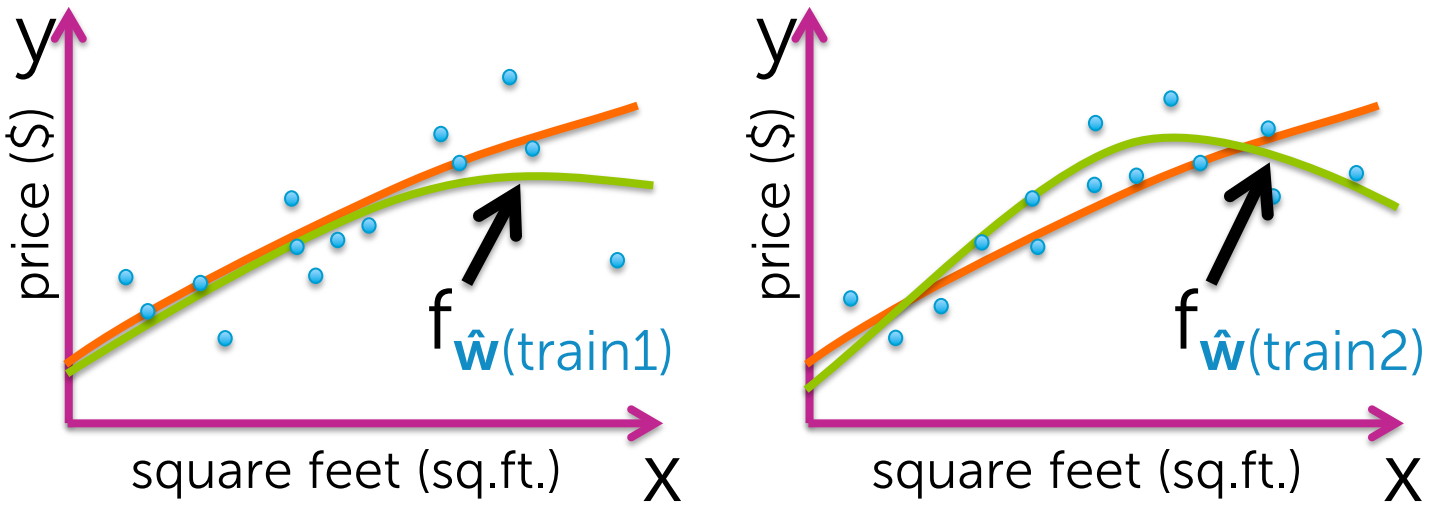


Irreducible error

Bias of function estimator

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

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



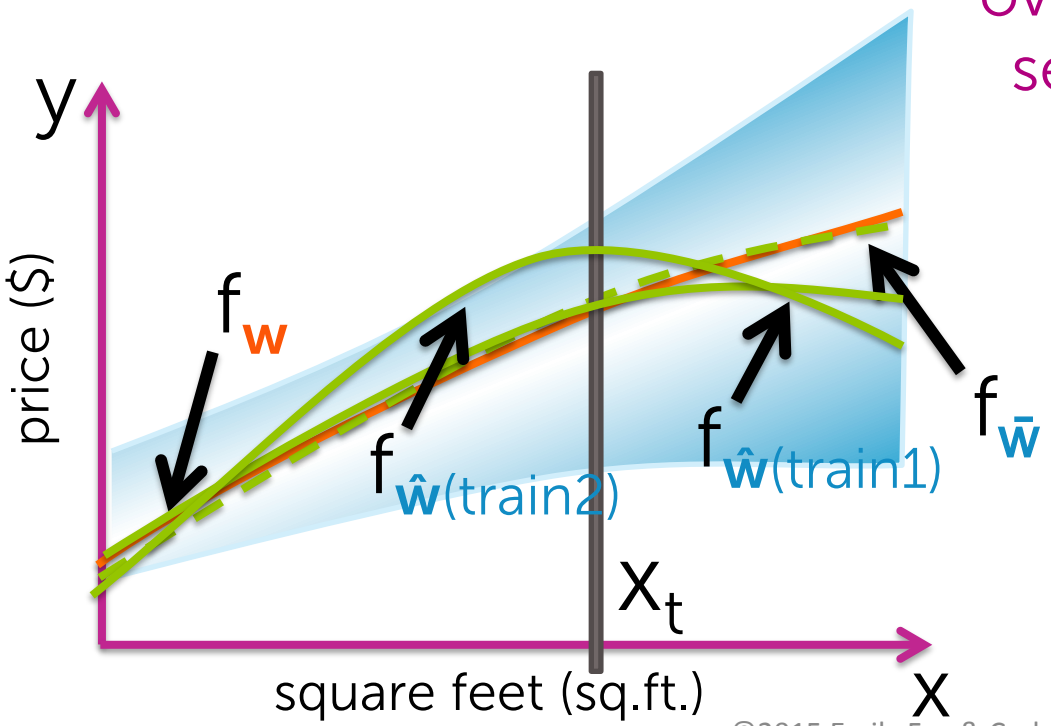
Bias of function estimator

Average estimated function = $f_{\bar{w}}(\mathbf{x})$

True function = $f_{\mathbf{w}}(\mathbf{x})$

$E_{train}[f_{\hat{\mathbf{w}}(train)}(\mathbf{x})]$

over all training sets of size N

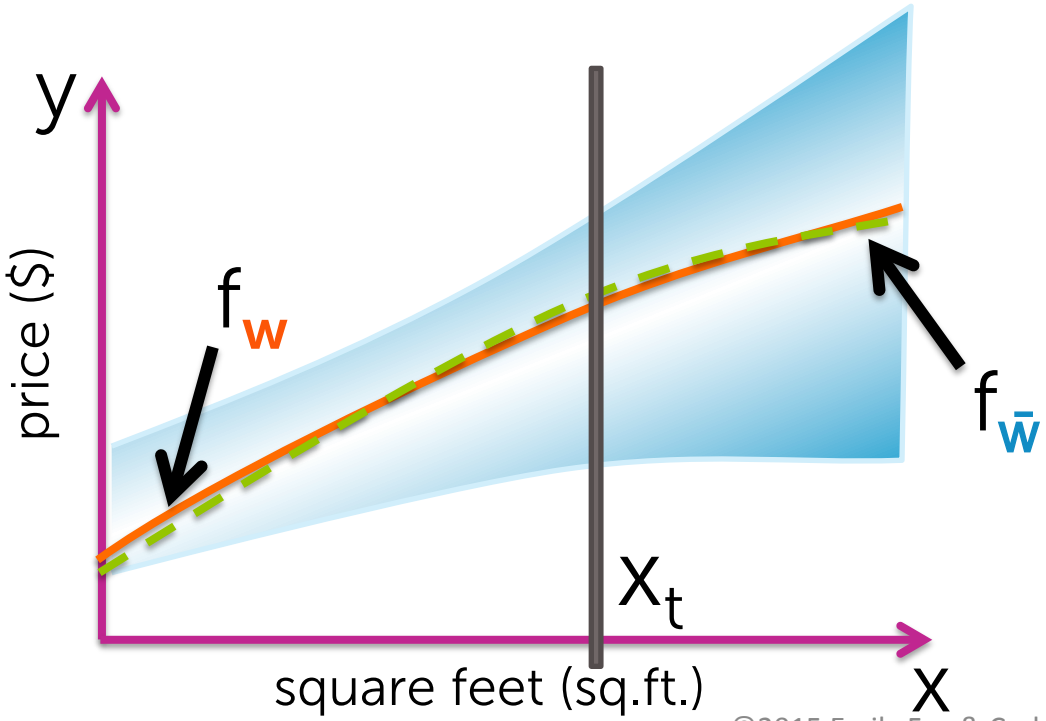


Bias of function estimator

Average estimated function = $f_{\bar{w}}(\mathbf{x})$

True function = $f_{w}(\mathbf{x})$

$$\text{bias}(f_{\hat{w}}(\mathbf{x}_t)) = f_{w}(\mathbf{x}_t) - f_{\bar{w}}(\mathbf{x}_t)$$



Bias of function estimator

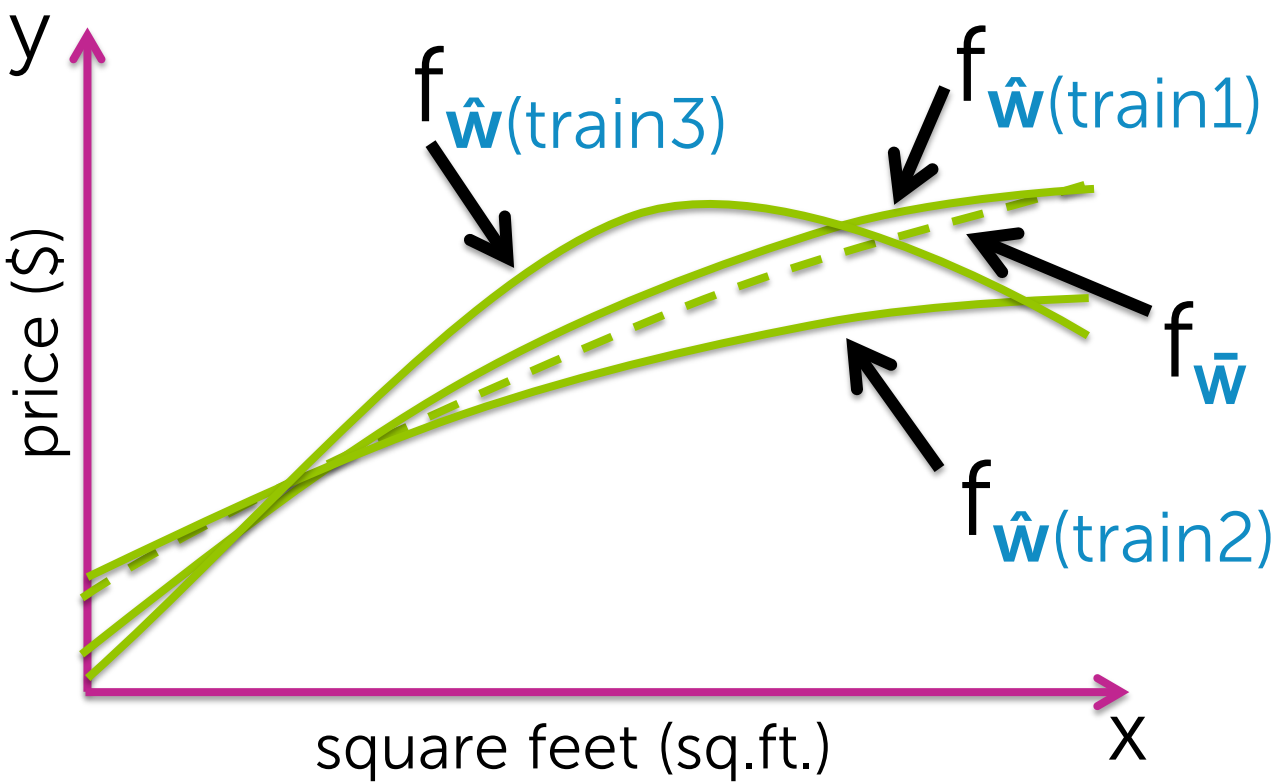
Average prediction error at $\mathbf{x}_t$

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

Variance of function estimator

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

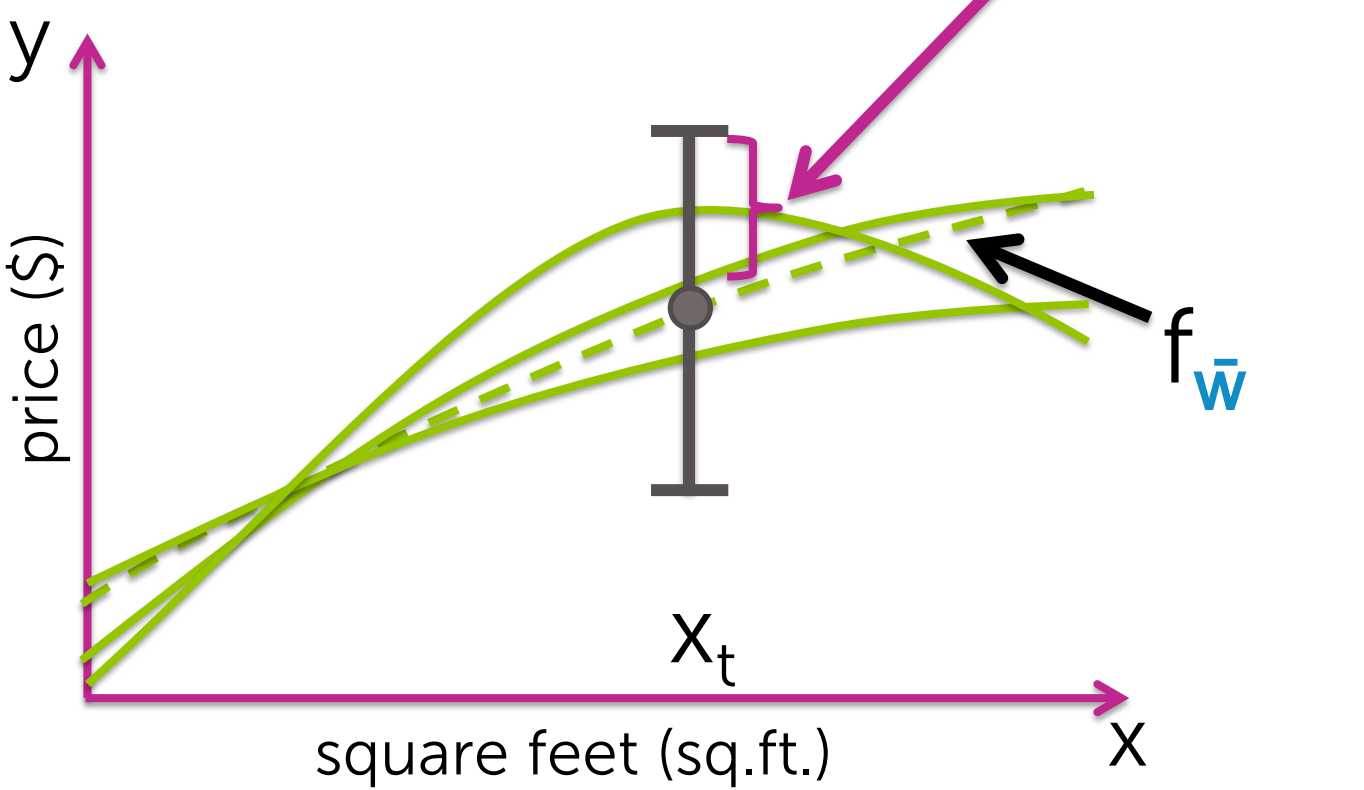
$$= \sigma^2 + [\text{bias}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t))]^2 + \text{var}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t))$$



Variance of function estimator

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

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



Variance of function estimator

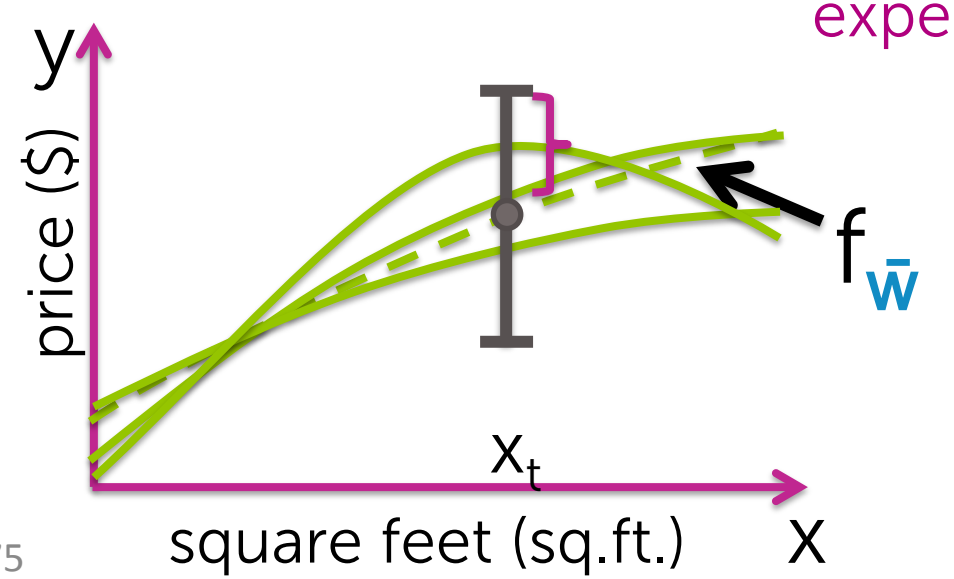
fit on a specific training dataset

what I expect to learn over all training sets

$$\text{var}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t)) = E_{\text{train}}[(f_{\hat{\mathbf{w}}(\text{train})}(\mathbf{x}_t) - f_{\bar{\mathbf{w}}}(\mathbf{x}_t))^2]$$

over all training sets of size N

deviation of specific fit from expected fit at $\mathbf{x}_t$



Why 3 sources of error?
A formal derivation

Deriving expected prediction error

Expected prediction error

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

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

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 $\mathbf{x}_t$

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

Deriving expected prediction error

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

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

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

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

$$= \sigma^2 + \text{MSE}(\hat{f})$$

Aside:

$$E[(a+b)^2] = E[a^2 + 2ab + b^2] = E[a^2] + 2E[ab] + E[b^2]$$

ind. r.v.s: $E[ab] = E[a]E[b]$

Shorthand: $y_t \to y$, $f_{w(true)} \to f$, $f_{\hat{w}(train)} \to \hat{f}$

Equating MSE with bias and variance

$$\text{MSE}\left[\underbrace{f_{\hat{\mathbf{w}}(\text{train})}(\mathbf{x}_t)}_{\hat{f}}\right]$$

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

shorthand new notation on this slide

$$= E_{\text{train}}\left[\left(\left(f_{\mathbf{w}(\text{true})}(\mathbf{x}_t) - f_{\bar{\mathbf{w}}}(\mathbf{x}_t)\right) + \underbrace{\left(f_{\bar{\mathbf{w}}}(\mathbf{x}_t) - f_{\hat{\mathbf{w}}(\text{train})}(\mathbf{x}_t)\right)}_{\bar{f}}\right)^2\right]$$

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

$E_{\text{train}}[\hat{f}]$

$(f-\bar{f})^2$ by definition $= \text{bias}^2(\hat{f})$

$(f-\bar{f})$ not a fcn of training data

$2(f-\bar{f})\,E_{\text{train}}[\bar{f}-\hat{f}]$

$\bar{f} - E_{\text{train}}[\hat{f}]$ by definition $= 0$

$E[(\hat{f}-\bar{f})^2] = \text{var}(\hat{f})$

$\hat{f}$: random function at x_t = random variable; $\bar{f}$: its mean

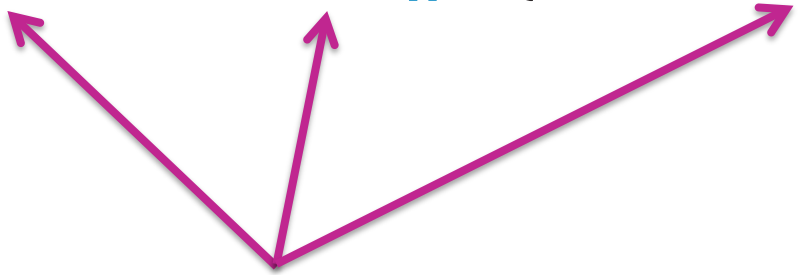
$$= \text{bias}^2(\hat{f}) + \text{Var}(\hat{f})$$

Putting it all together

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

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

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



3 sources of error

Summary of tasks

The regression/ML workflow

1. **Model selection**
   Often, need to choose tuning parameters λ controlling model complexity (e.g. degree of polynomial)

2. **Model assessment**
   Having selected a model, assess the generalization error

Hypothetical implementation

1. **Model selection**

For each considered model complexity λ :

i. Estimate parameters $\hat{\mathbf{w}}_\lambda$ on **training data**

ii. Assess performance of $\hat{\mathbf{w}}_\lambda$ on **test data**

iii. Choose λ^* to be λ with lowest test error

2. **Model assessment**

Compute test error of $\hat{\mathbf{w}}_{\lambda^*}$ (fitted model for selected complexity λ^*) to approx. generalization error

Hypothetical implementation

1. **Model selection**

For each considered model complexity λ :

i. Estimate parameters $\hat{\mathbf{w}}_\lambda$ on **training data**

ii. Assess performance of $\hat{\mathbf{w}}_\lambda$ on **test data**

iii. Choose λ^* to be λ with lowest test error

Overly optimistic!

2. **Model assessment**

Compute test error of $\hat{\mathbf{w}}_{\lambda^*}$ (fitted model for selected complexity λ^*) to approx. generalization error

Hypothetical implementation

Issue: Just like fitting $\hat{\mathbf{w}}$ and assessing its performance both on training data

- λ^* was selected to minimize test error (i.e., λ^* was fit on test data)
- If test data is not representative of the whole world, then $\hat{\mathbf{w}}_{\lambda^*}$ will typically perform worse than test error indicates

Practical implementation

Solution: Create two "test" sets!

1. Select λ^* such that $\hat{\mathbf{w}}_{\lambda^*}$ minimizes error on validation set
2. Approximate generalization error of $\hat{\mathbf{w}}_{\lambda^*}$ using test set

Practical implementation

fit $\hat{\mathbf{w}}_\lambda$

test performance of $\hat{\mathbf{w}}_\lambda$ to select λ^*

assess generalization error of $\hat{\mathbf{w}}_{\lambda^*}$

Typical splits

80%	10%	10%
50%	25%	25%

Summary of assessing performance

What you can do now…

- Describe what a loss function is and give examples
- Contrast training, generalization, and test error
- Compute training and test error given a loss function
- Discuss issue of assessing performance on training set
- Describe tradeoffs in forming training/test splits
- List and interpret the 3 sources of avg. prediction error
  - Irreducible error, bias, and variance
- Discuss issue of selecting model complexity on test data and then using test error to assess generalization error
- Motivate use of a validation set for selecting tuning parameters (e.g., model complexity)
- Describe overall regression workflow