Bias-Variance Tradeoff

Overview of the second half the semester

1. A little bit Learning Theory

2. Make our linear models nonlinear (Kernel)

3. How to combine multiple classifiers into a stronger one (Bagging & Boosting)?

4. Intro of Neural Networks (old and new)

Objective

Understand Bias-Variance tradeoff — When and why your ML models work (or don't work)

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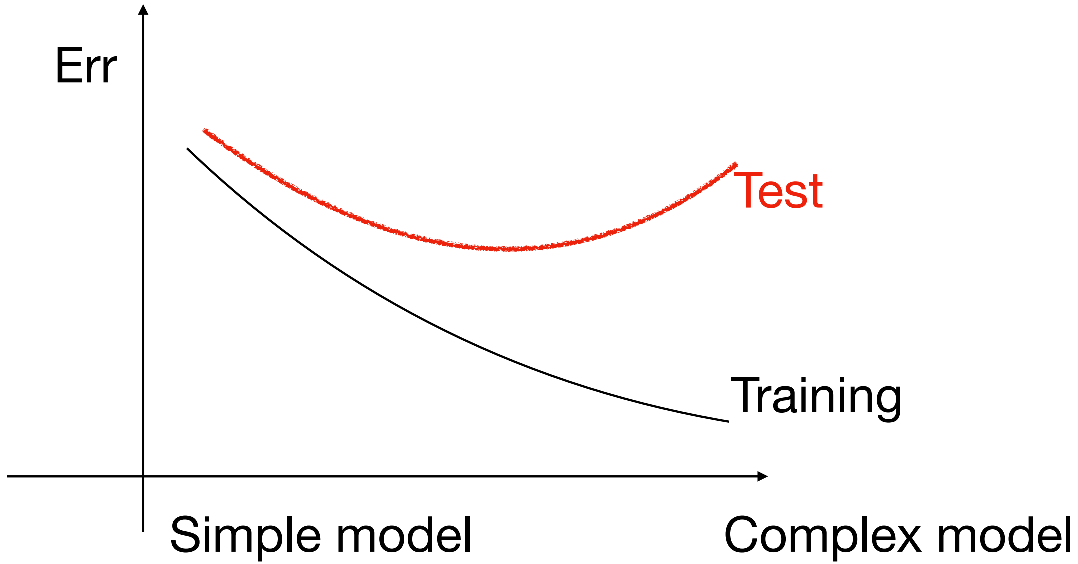
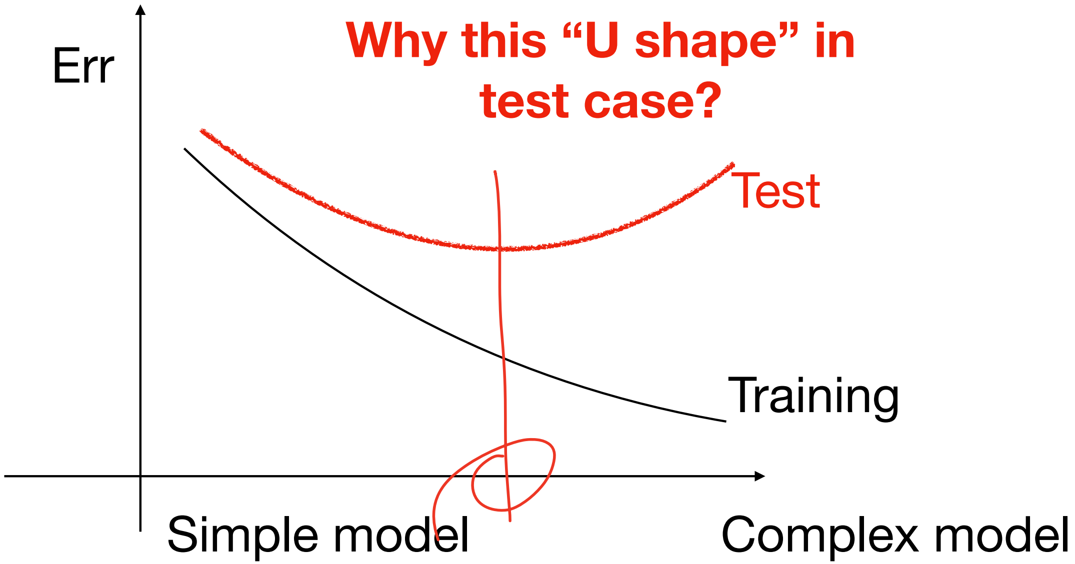


Objective

Understand Bias-Variance tradeoff — When and why your ML models work (or don't work)



Outline of Today

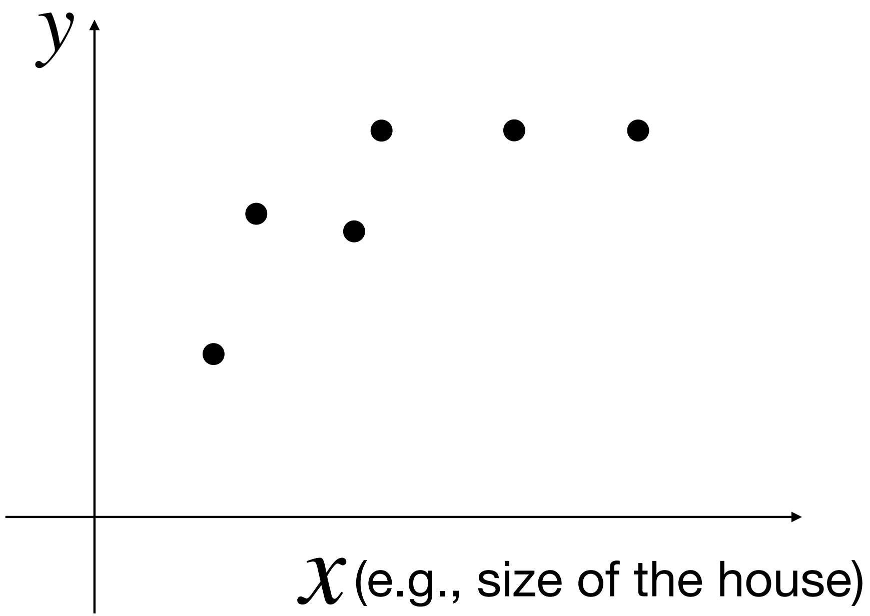
1. Intro on Underfitting/Overfitting and Bias/Variance

2. Derivation of the Bias-Variance Decomposition

Bayes optimal predictor

Consider regression problem w/ dataset $\mathscr{D} = \{x, y\}, (x, y) \sim P, x \in \mathbb{R}, y \in \mathbb{R}$

$\ell(h) = (h(x) - y)^2$



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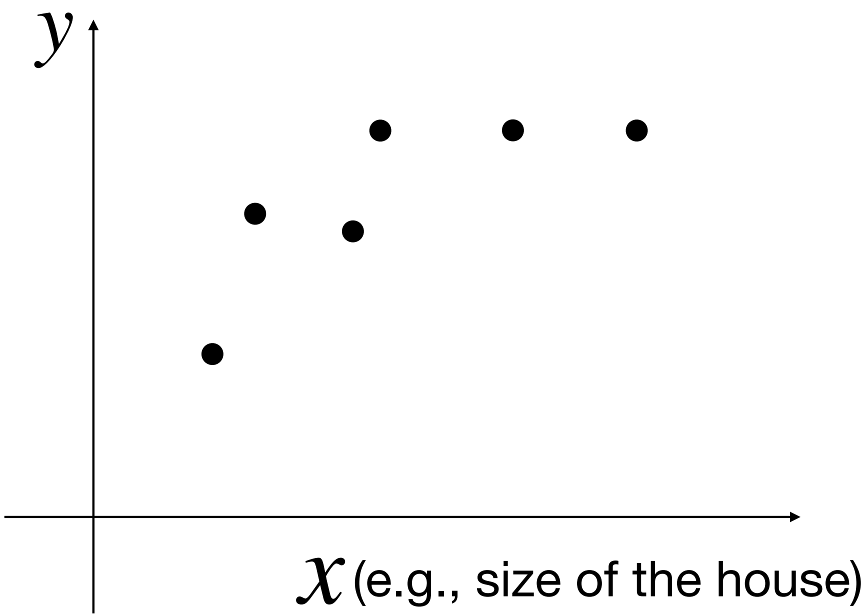

The Bayes optimal regressor:

$$\bar{y}(x) := \mathbb{E}[y \mid x]$$

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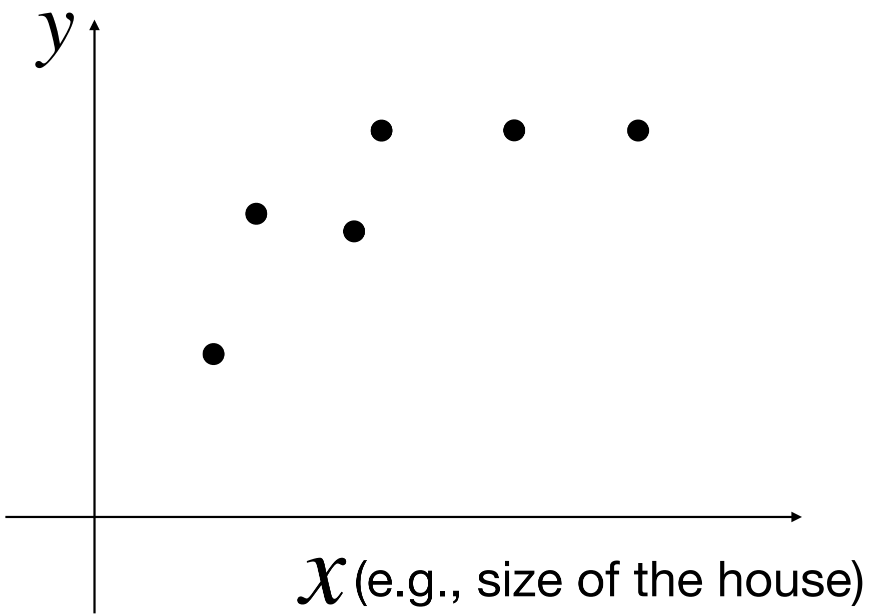

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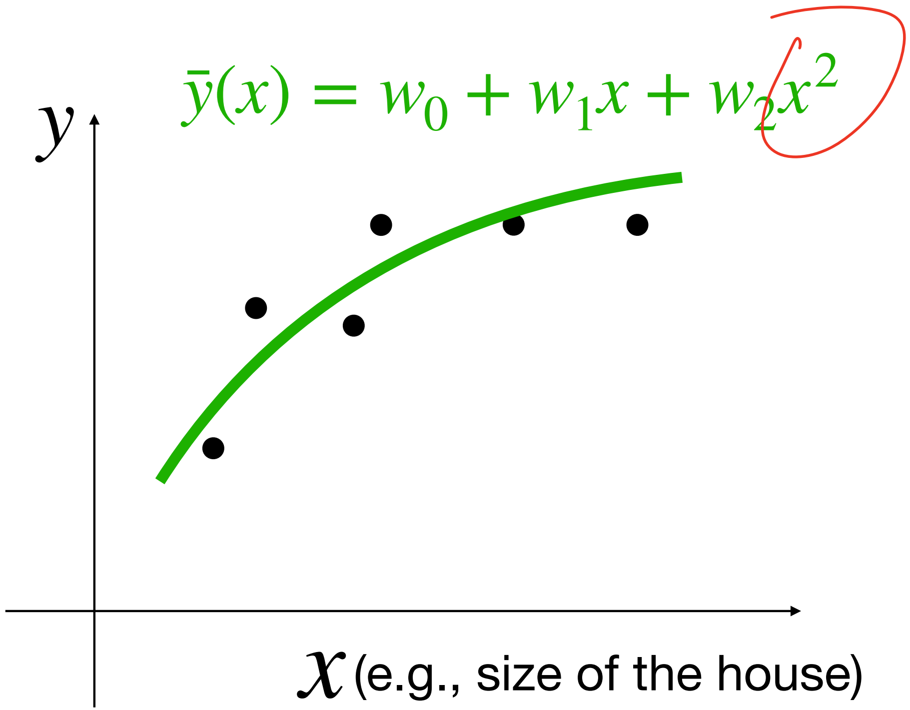

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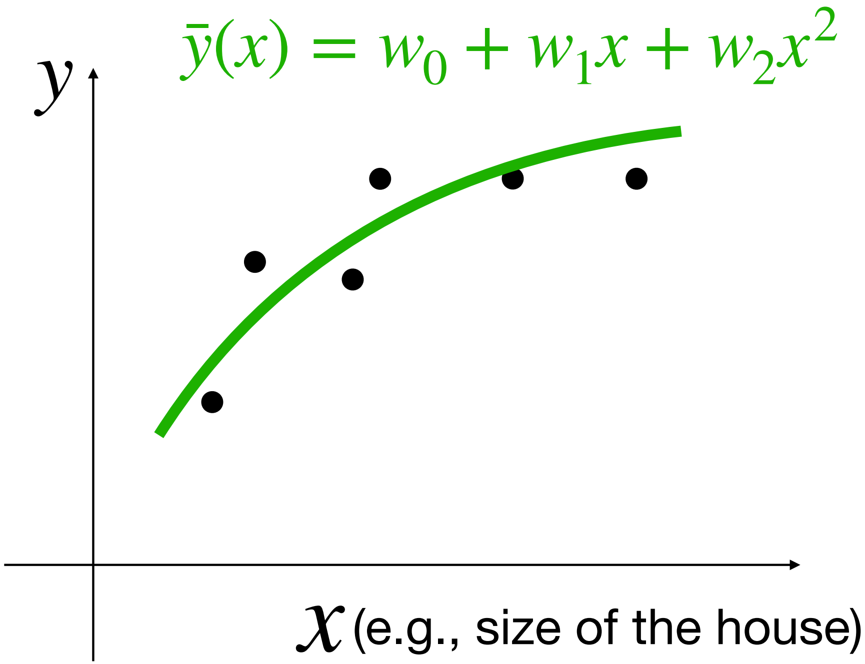
Underfitting



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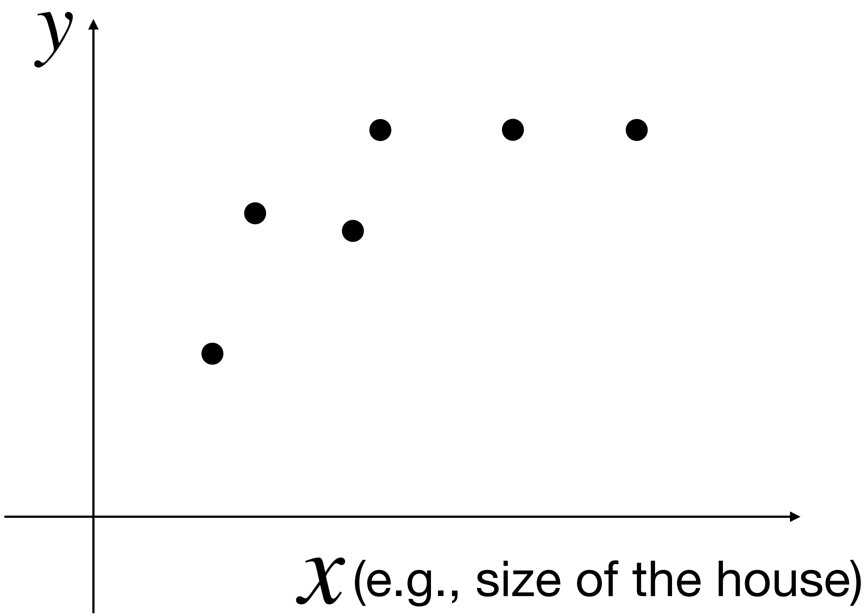

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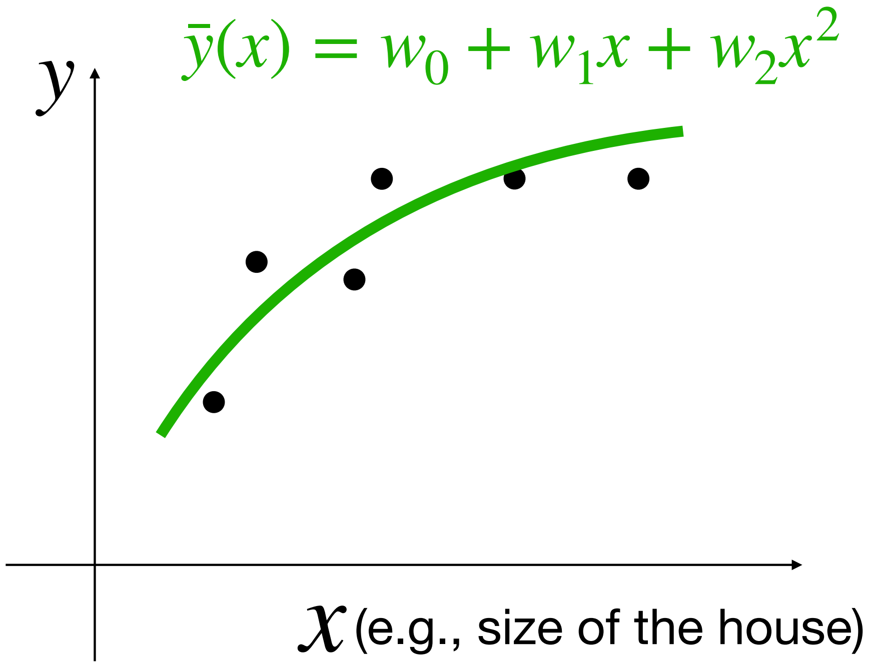

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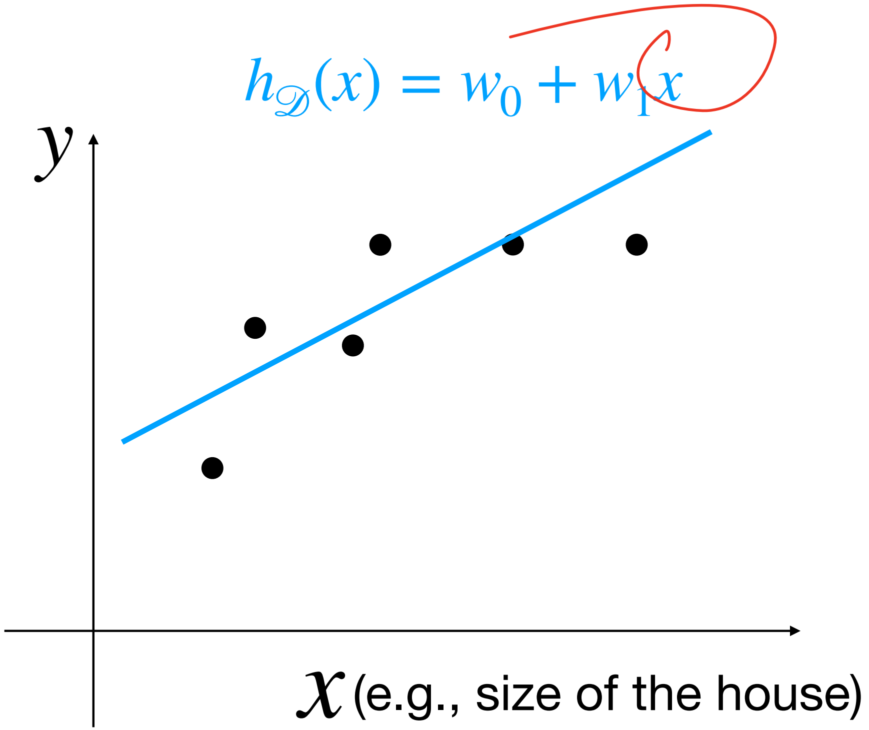

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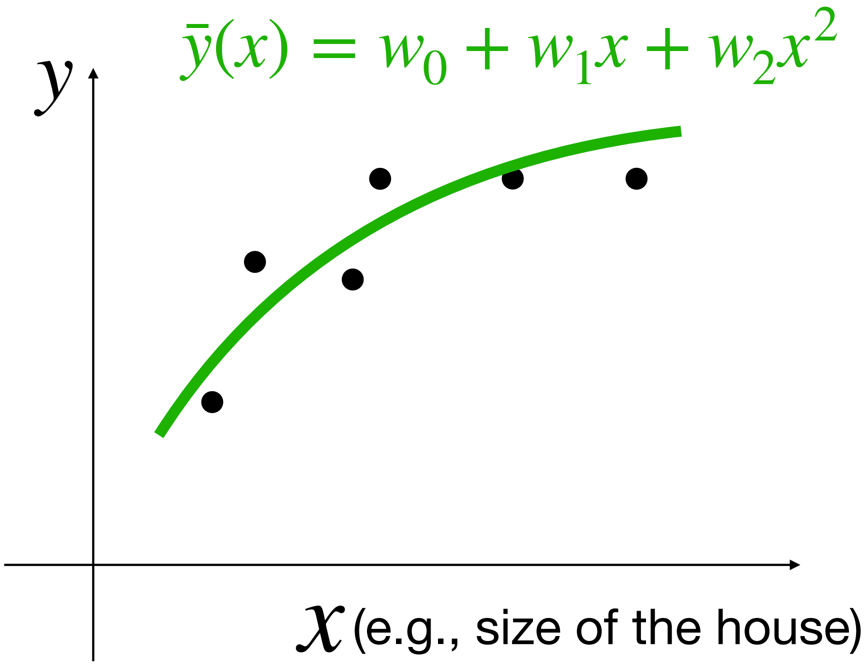

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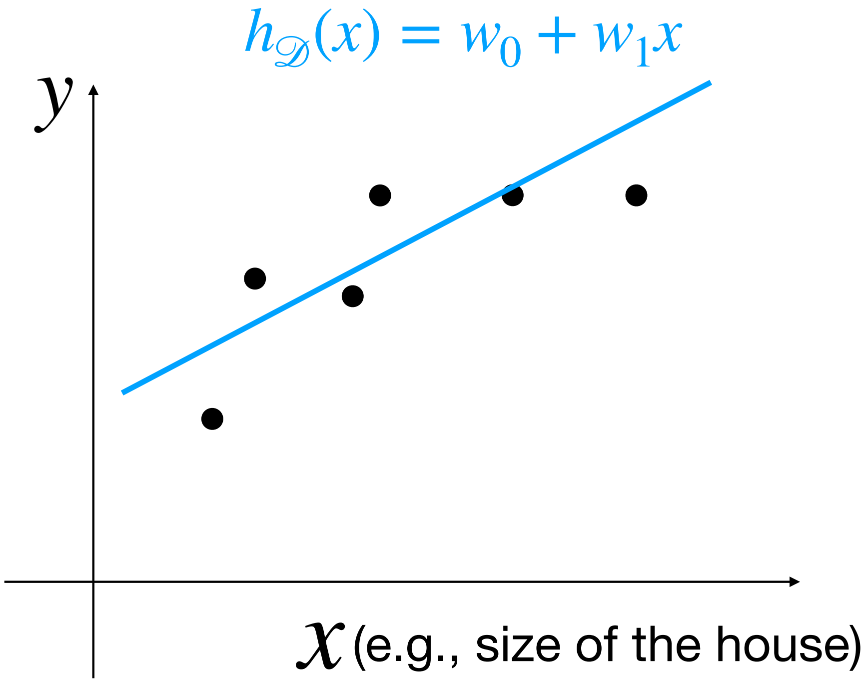
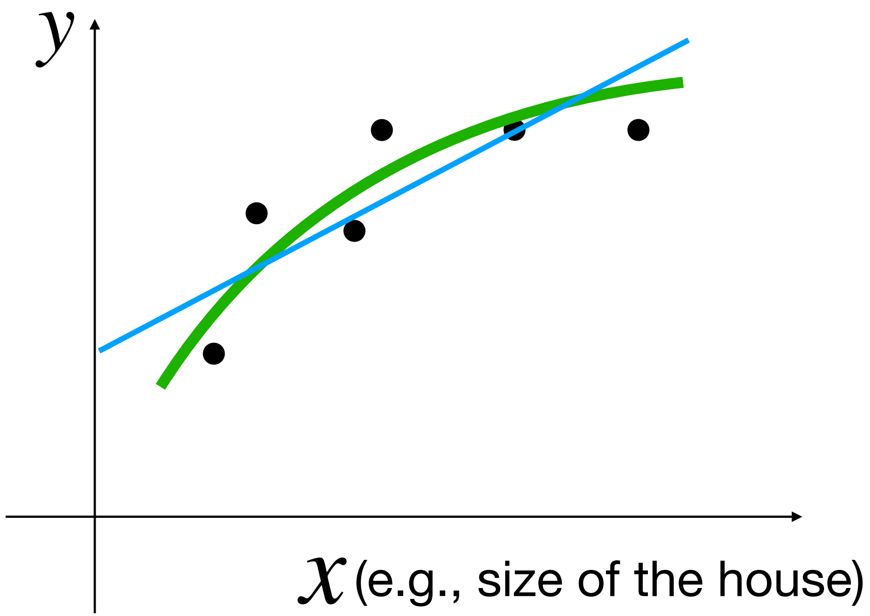


Underfitting

Underfitting

Just right versus Underfitting

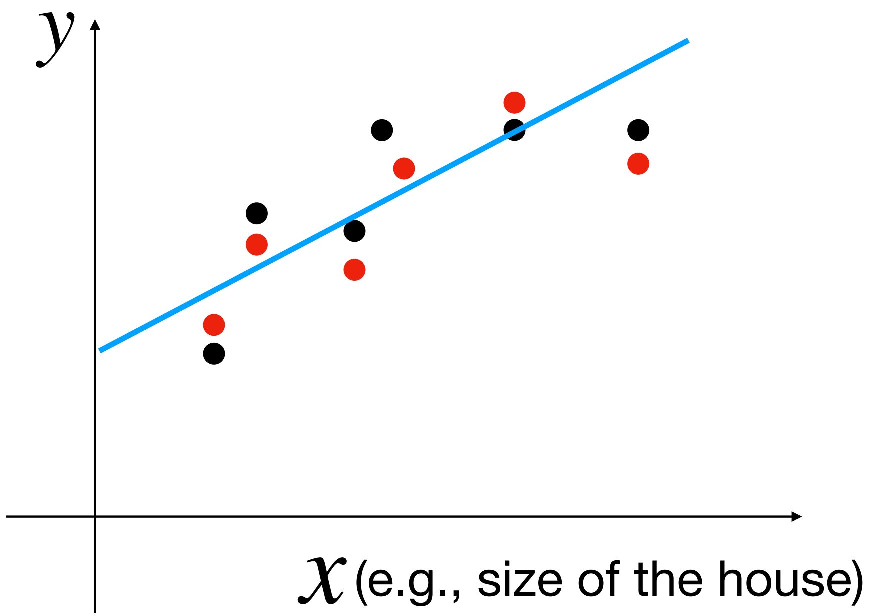


Bias:

Bias towards to linear models

Underfitting

Now let's redo linear regression on a different dataset $\mathscr{D}'$ (but from the same distribution)



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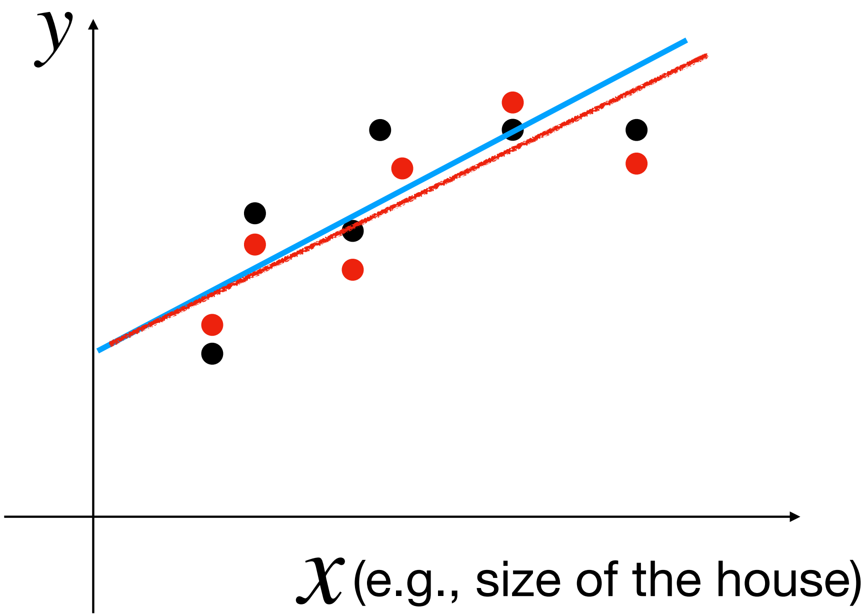

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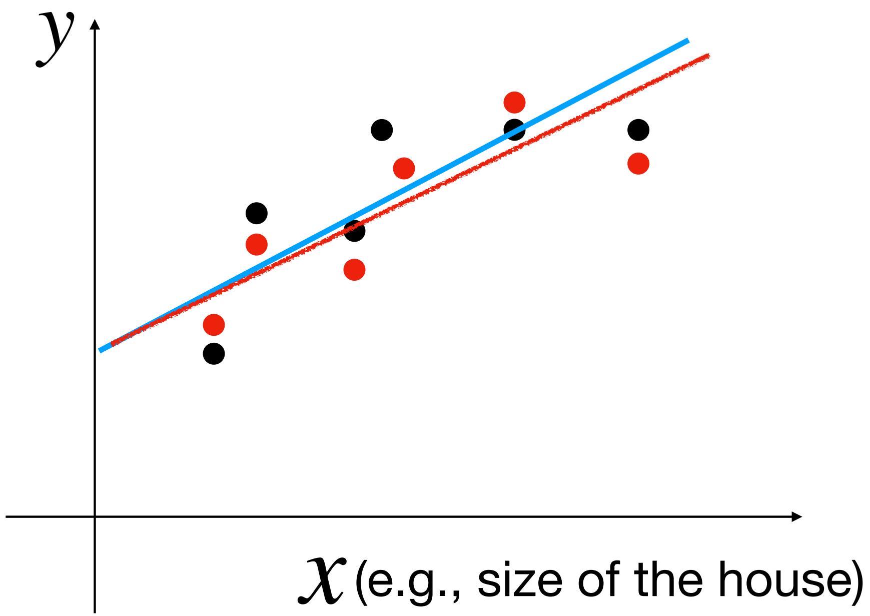

The new linear function does not differ too much from the old one

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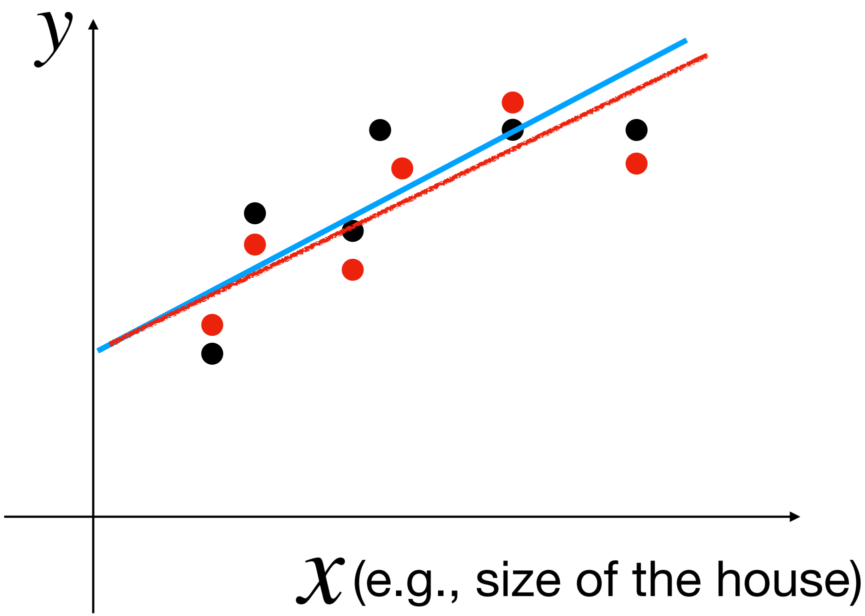

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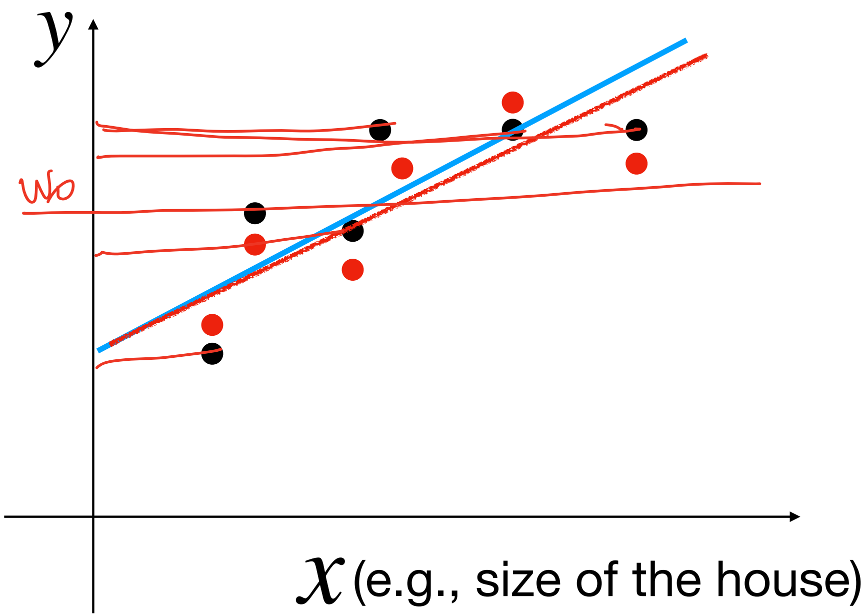

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Q: what happens when our linear predictor is $h(x) = w_0$?

$\hat{w_0} = \frac{1}{n} \sum_{i=1}^{n} y_i = \mathbb{E}_y[y]$

Summary on underfitting

1. Often our model is too simple, i.e.., we bias towards too simple models

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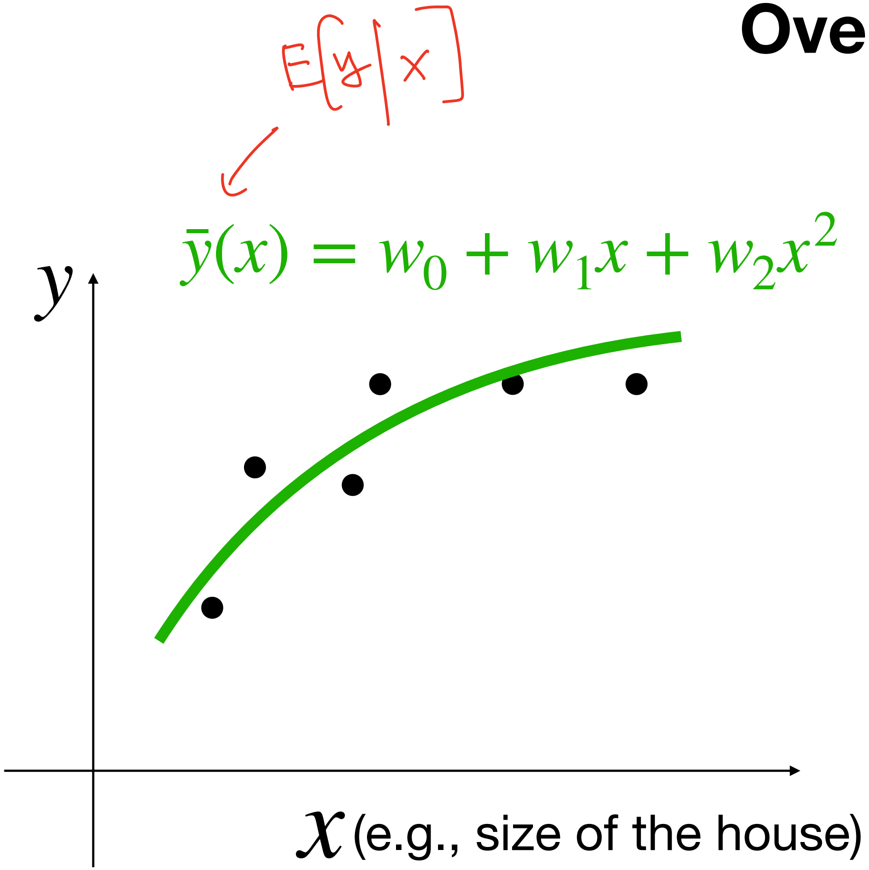
3. In this case, we have large bias, but low variance (think about the $h(x) = w_0$ case)

Overfitting



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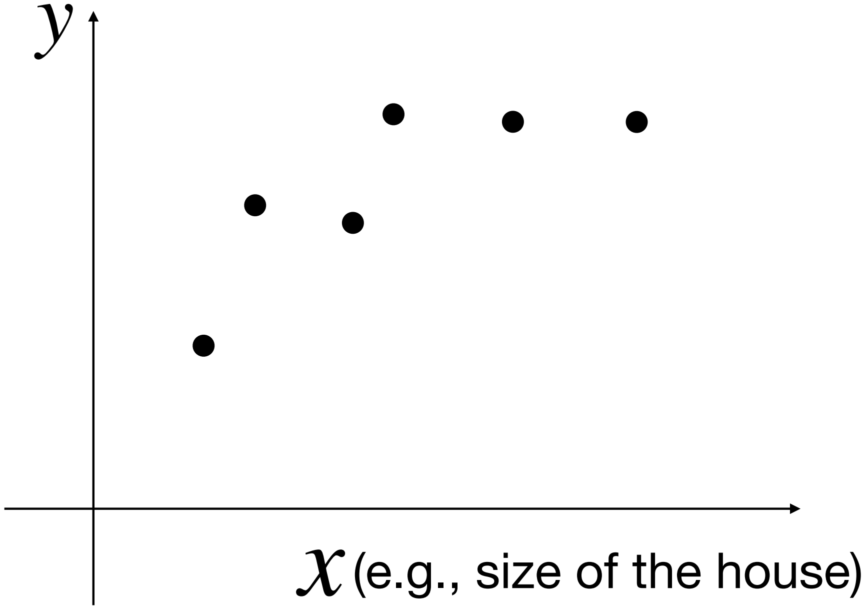
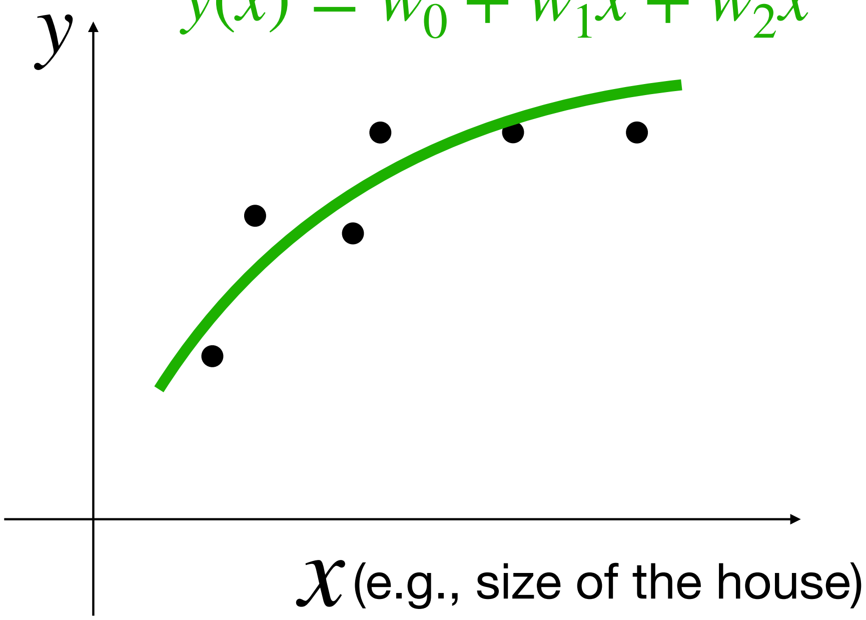


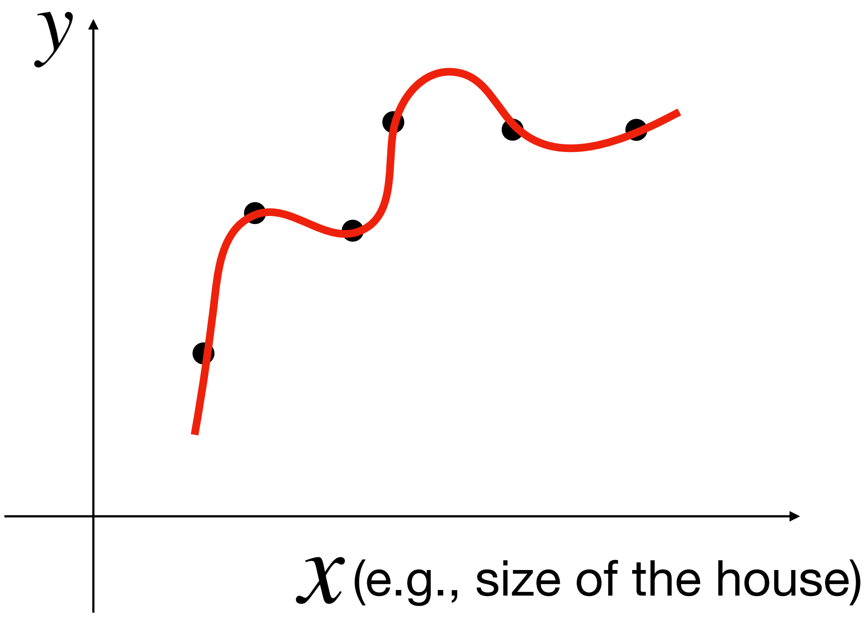
Overfitting

$$\bar{y}(x) = w_0 + w_1 x + w_2 x^2$$



(Just right)

$$h_{\mathcal{D}}(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_6 x^5$$



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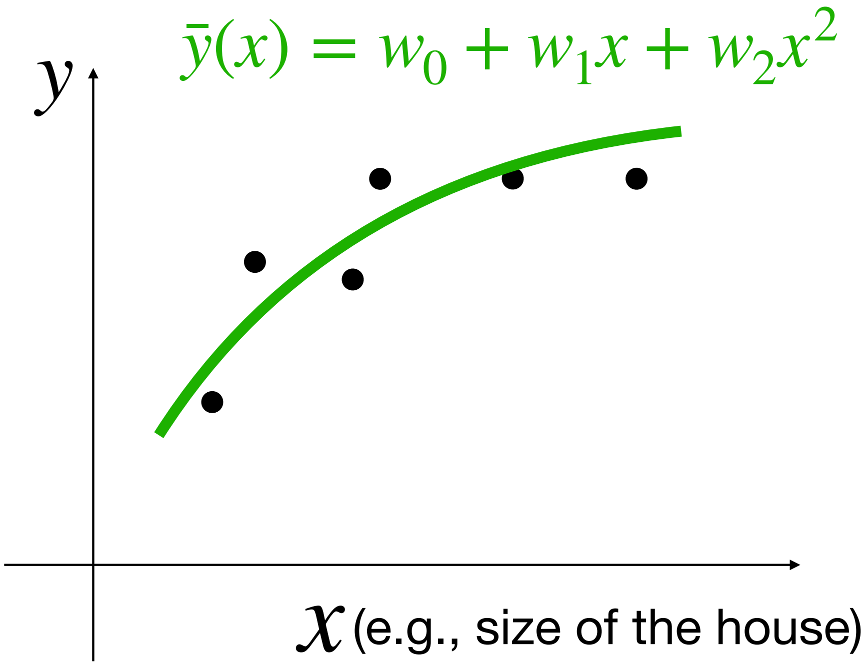

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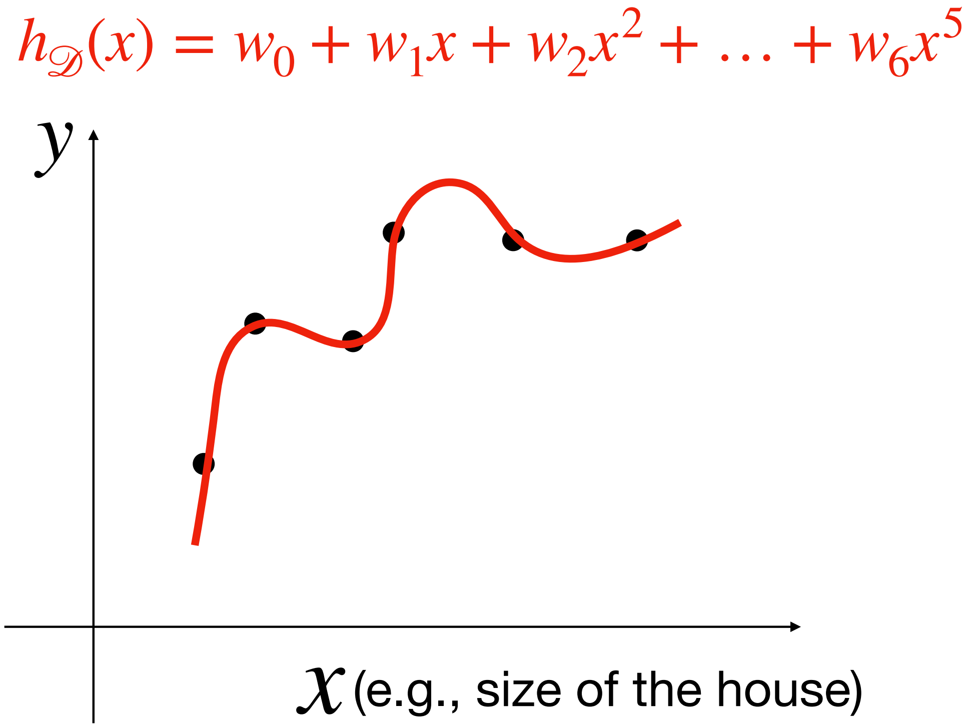

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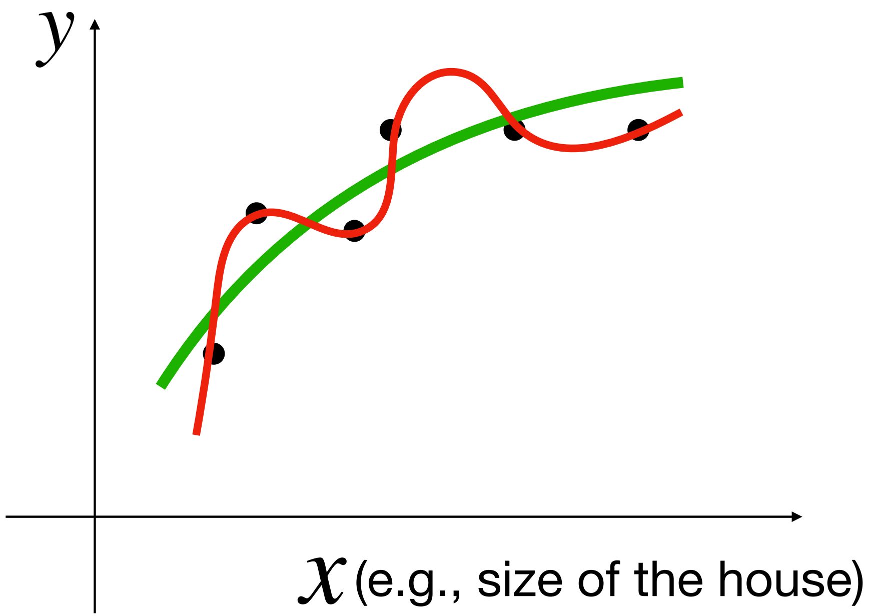
Just right versus Overfitting



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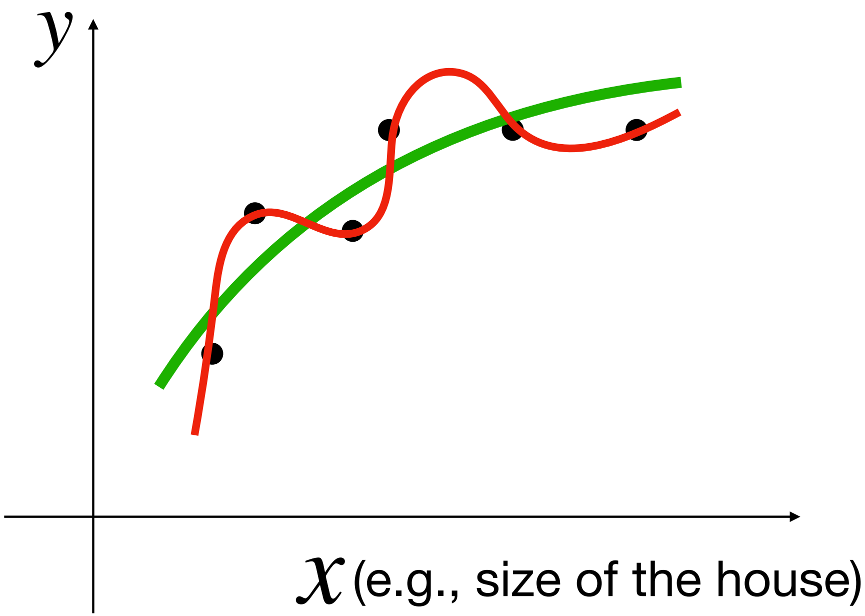
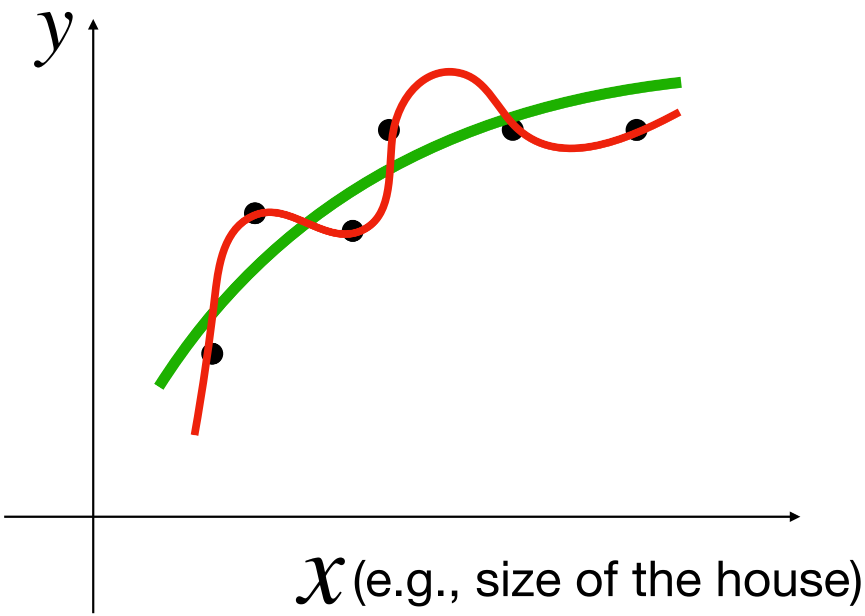


No strong bias:

Our hypothesis class is all polynomials up to 5-th order

Overfitting

Just right versus Overfitting



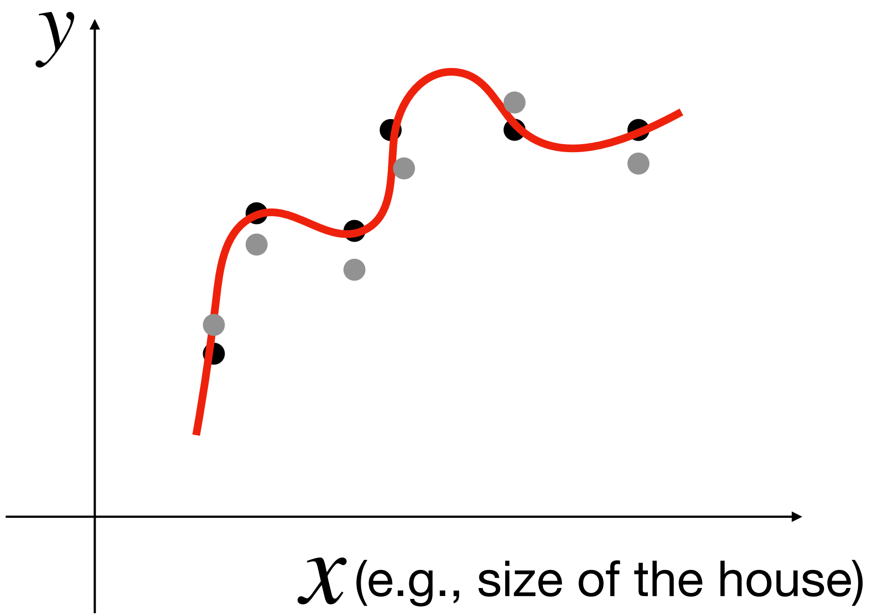
No strong bias:

Our hypothesis class is all polynomials up to 5-th order

i.e., a priori, no strong bias towards linear or quadratic, or cubic, etc

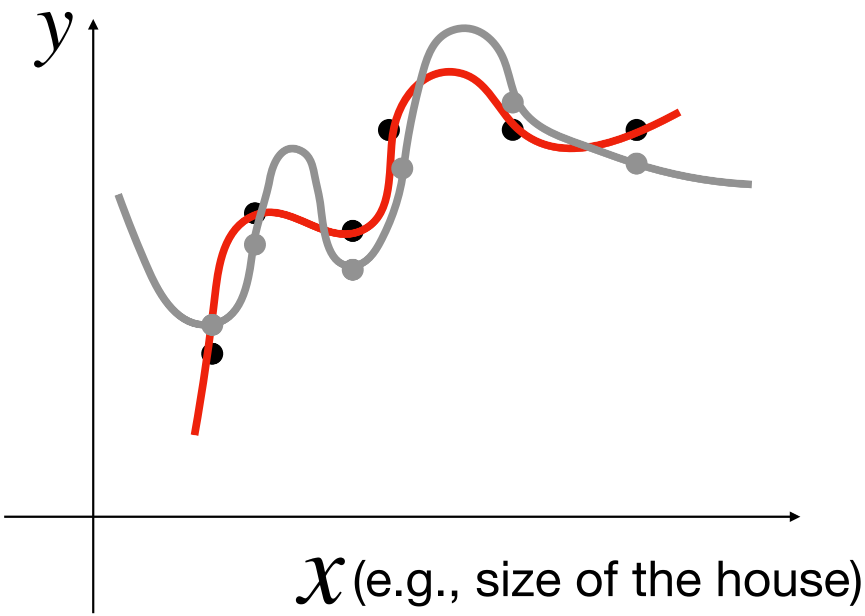
Overfitting

Redo the higher-order polynomial fitting on different dataset $\mathscr{D}'$



Overfitting

Redo the higher-order polynomial fitting on different dataset $\mathscr{D}'$



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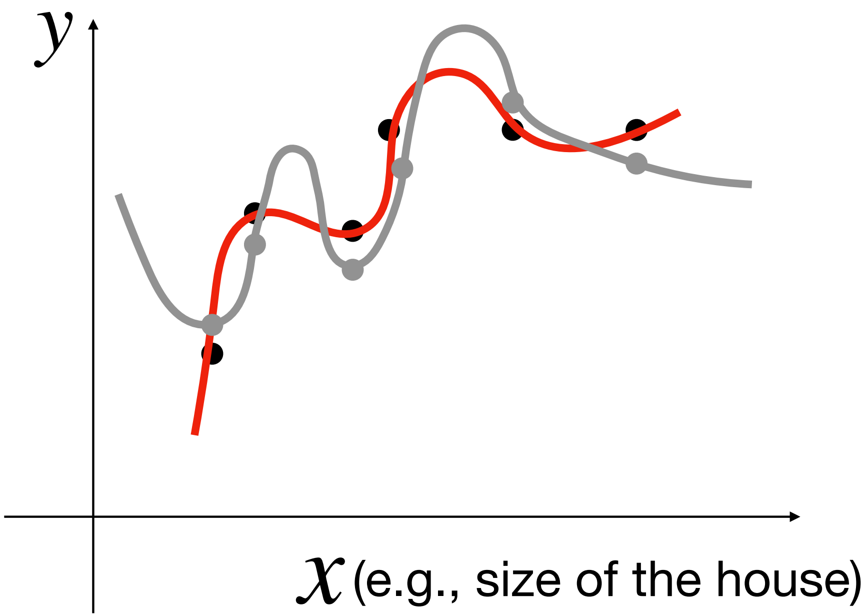

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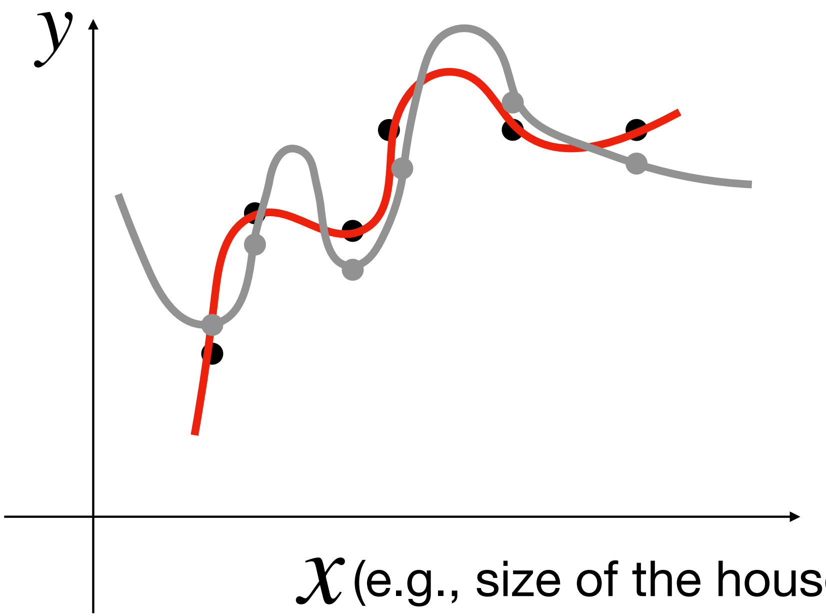

x (e.g., size of the house)

The new function can differ a lot from the old one

This is called high variance

Summary on Overfitting

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3. In this case, we have small bias, but large variance
(tiny change on the dataset cause large change in the fitted functions)

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1. Intro on Underfitting/Overfitting and Bias/Variance

2. Derivation of the Bias-Variance Decomposition

Generalization error

Given dataset $\mathscr{D}$, a hypothesis class $\mathscr{H}$, squared loss $\ell(h, x, y) = (h(x) - y)^2$, denote $h_{\mathscr{D}}$ as the ERM solution

$$h_D = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \left(h(x_i) - y_i\right)^2$$

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We are interested in the generalization error of $h_{\mathscr{D}}$:

$$\mathbb{E}_{\mathscr{D}} \mathbb{E}_{x,y \sim P} (h_{\mathscr{D}}(x) - y)^2$$

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$$\mathbb{E}_{\mathscr{D}}\mathbb{E}_{x,y\sim P}(h_{\mathscr{D}}(x) - y)^2$$

Q: how to estimate this in practice?

The expectation of our model $h_{\mathscr{D}}$

Since $h_{\mathscr{D}}$ is random, we consider its expected behavior:

$$\bar{h} := \mathbb{E}_{\mathscr{D}}\left[h_{\mathscr{D}}\right]$$

$D_1 \sim P, \quad D_2 \sim P, \quad \cdots \quad D_{10} \sim P$

LR: $\downarrow$ LR $\downarrow$ LR $\downarrow$

$\hat{w}_1 \quad \hat{w}_2 \quad \hat{w}_{10}$

$$\bar{w} = \sum_{i=1}^{10} \hat{w}_i / 10$$

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$$\hat{w}_1 \ldots \hat{w}_{10}$$

$$\bar{w}^T x = \frac{1}{10} \sum_{i=1}^{10} \hat{w}_i^T x$$

$$\min_{w_0} \sum_{i=1}^{n} (w_0 - y_i)^2 \qquad \hat{w}_0 \xrightarrow{LLN} \mathbb{E}_y[y]$$

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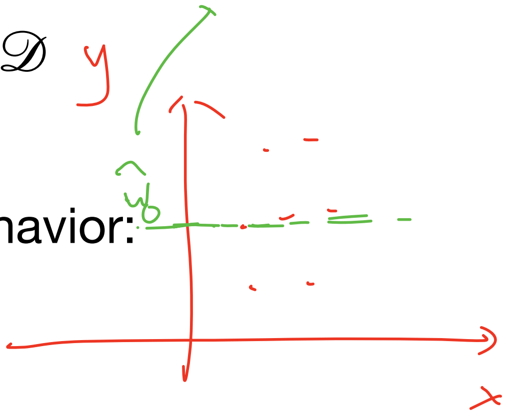

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A: $\bar{h}(x) = \mathbb{E}_y[y]$

Formal definition of Bias and Variance

$$\bar{h} := \mathbb{E}_{\mathcal{D}}\left[h_{\mathcal{D}}\right] \qquad \bar{y}(x) := \mathbb{E}[y \mid x]$$

Bayes opt

Bias^2: (squared)difference between $\bar{h}$ and the best $\bar{y}(x)$, i.e., $\mathbb{E}_x\left(\bar{y}(x) - \bar{h}(x)\right)^2$

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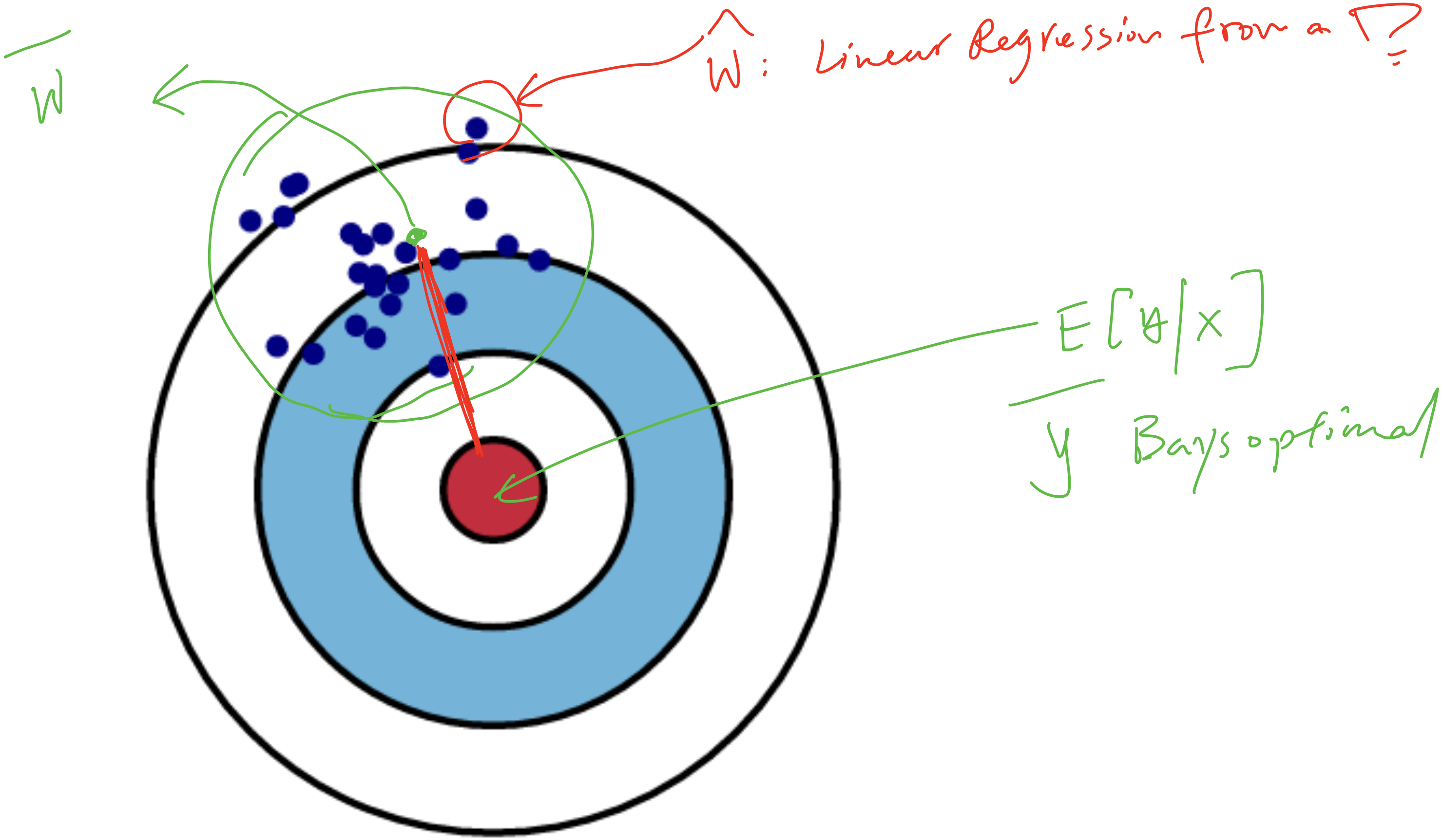
Variance: difference from $\bar{h}$ and $h_{\mathscr{D}}$, i.e., $\mathbb{E}_{\mathscr{D}}\mathbb{E}_x \left(h_{\mathscr{D}}(x) - \bar{h}(x)\right)^2$

Fluctuation of our random model around its mean

Bias-Variance illustration



Generalization error decomposition

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What we gonna show now:

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What we gonna show now:

$$\mathbb{E}_{\mathcal{D}}\mathbb{E}_{x,y\sim P}(h_{\mathcal{D}}(x) - y)^2$$

= **Bias**^{2} + **Variance** + Noise (unavoidable, independent of Algs/models)

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We will use the following trick twice: $(x-y)^2 = (x-z)^2 + (z-y)^2 + 2(x-z)(z-y)$

$(x - z + z - y)^2$

$\to \mathbb{E}_{D} \mathbb{E}_{xy}$

$\bar{h} = \mathbb{E}_{D}[h_D]$

$$\mathbb{E}(h_{\mathcal{D}}(x) - y)^2$$

$$= \mathbb{E}(h_{\mathcal{D}}(x) - \bar{h}(x) + \bar{h}(x) - y)^2$$

$\bar{h} = \mathbb{E}_{D}[h_D]$

$$\mathbb{E}(h_{\mathcal{D}}(x) - y)^2$$

$$= \mathbb{E}(\underbrace{h_{\mathcal{D}}(x) - \bar{h}(x)}_{①} + \underbrace{\bar{h}(x) - y}_{②})^2$$

$$= \underbrace{\mathbb{E}(h_{\mathcal{D}}(x) - \bar{h}(x))^2}_{①^2} + \underbrace{\mathbb{E}(\bar{h}(x) - y)^2}_{②^2} + 2\mathbb{E}_{\mathcal{D},x,y}\left[\underbrace{(h_{\mathcal{D}}(x) - \bar{h}(x))(\bar{h}(x) - y)}_{① \times ②}\right]$$

Var

$$\mathbb{E}(h_{\mathscr{D}}(x) - y)^2$$

$$= \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x) + \bar{h}(x) - y)^2$$

$$= \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - y)^2 + 2\mathbb{E}_{\mathscr{D},x,y}\left[(h_{\mathscr{D}}(x) - \bar{h}(x))(\bar{h}(x) - y)\right]$$

Def of $\bar{h}$:

$$\bar{h} = \mathbb{E}_{D}[h_D]$$

This term is zero since:

$$\mathbb{E}_{x,y,\mathscr{D}}\left[(h_{\mathscr{D}}(x) - \bar{h}(x))(\bar{h}(x) - y)\right]$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_{\mathscr{D}}(h_{\mathscr{D}}(x) - \bar{h}(x)) \cdot (\bar{h}(x) - y)\right]$$

$$= \mathbb{E}_{x,y}\left[(\bar{h}(x) - \bar{h}(x)) \cdot (\bar{h}(x) - y)\right]$$

$= 0$

Bias: $\bar{h} - \underbrace{E[y|x]}_{:=\bar{y}}$

$$\mathbb{E}(h_{\mathcal{D}}(x) - y)^2$$

$$-\bar{y}(x) + \bar{y}(x)$$

$$= \underbrace{\mathbb{E}(h_{\mathcal{D}}(x) - \bar{h}(x))^2}_{\text{Variance}} + \mathbb{E}(\bar{h}(x) - y)^2$$

$$\mathbb{E}(h_{\mathscr{D}}(x) - y)^2$$

$$= \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - y)^2$$

Variance

$$\mathbb{E}(h_{\mathscr{D}}(x) - y)^2$$

$$= \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - y)^2$$

Variance

$\bar{y}(x) = \mathbb{E}[y|x]$

$$\mathbb{E}(h_{\mathcal{D}}(x) - y)^2$$

$$= \mathbb{E}(\bar{h}(x) - \bar{y}(x) + \bar{y}(x) - y)^2$$

Complete square

$$= \mathbb{E}(h_{\mathcal{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - y)^2$$

Variance

$$\mathbb{E}(h_{\mathscr{D}}(x) - y)^2$$

$$= \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - y)^2$$

Variance

$$= \mathbb{E}(\bar{h}(x) - \bar{y}(x) + \bar{y}(x) - y)^2$$

$$= \mathbb{E}(\bar{h}(x) - \bar{y}(x))^2 + \mathbb{E}(\bar{y}(x) - y)^2$$

$$+ 2\mathbb{E}(\bar{h}(x) - \bar{y}(x))(\bar{y}(x) - y)$$

$\mathbb{E}(h_{\mathcal{D}}(x) - y)^2$

$= \mathbb{E}(h_{\mathcal{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - y)^2$

Variance

Bias^2

$= \mathbb{E}(\bar{h}(x) - \bar{y}(x) + \bar{y}(x) - y)^2$

$= \mathbb{E}(\bar{h}(x) - \bar{y}(x))^2 + \mathbb{E}(\bar{y}(x) - y)^2$

$+ 2\mathbb{E}(\bar{h}(x) - \bar{y}(x))(\bar{y}(x) - y)$

$\mathbb{E}_{x,y} := \mathbb{E}_{x} \mathbb{E}_{y|x}$

This term is zero since:

$= \mathbb{E}_x \left[(\bar{h}(x) - \bar{y}(x)) \cdot \mathbb{E}_{y|x}(\bar{y}(x) - y) \right]$

$= \mathbb{E}_x \left[(\bar{h}(x) - \bar{y}(x)) \cdot (\bar{y}(x) - \mathbb{E}_{y|x}[y]) \right] = 0$

$\mathbb{E}_{y|x}[y] := \bar{y}(x)$

Putting the derivations together, we arrive at:

$$\mathbb{E}(h_{\mathcal{D}}(x) - y)^2 = \mathbb{E}(h_{\mathcal{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - \bar{y}(x))^2 + \mathbb{E}(\bar{y}(x) - y)^2$$

Variance

Bias^2

Putting the derivations together, we arrive at:

$$\mathbb{E}(h_{\mathscr{D}}(x) - y)^2 = \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - \bar{y}(x))^2 + \mathbb{E}(\bar{y}(x) - y)^2$$

Variance

Bias^2

Noise

Putting the derivations together, we arrive at:

$$\mathbb{E}(h_{\mathscr{D}}(x) - y)^2 = \mathbb{E}(h_{\mathscr{D}}(x) - \bar{h}(x))^2 + \mathbb{E}(\bar{h}(x) - \bar{y}(x))^2 + \mathbb{E}(\bar{y}(x) - y)^2$$

Variance

Bias^2

Noise

Note that the noise term is independent of training algorithms / models