Bias-Variance Tradeoff

UNIVERSITY of WASHINGTON

Optimal Prediction

Goal: Predict $Y \in \mathbb{R}^d$ **given** $X \in \mathbb{R}^d$ **if** $(X, Y) \sim P_{XY}$

Find function η that minimizes

$$\mathbb{E}_{XY}[(Y - \eta(X))^2] = \mathbb{E}_X\left[\mathbb{E}_{Y|X}[(Y - \eta(x))^2 | X = x]\right]$$

(Hint: for any x, $\eta(x) = c_x$ where c_x minimizes $\mathbb{E}_{Y|X}[(Y - c_x)^2 | X = x]$)

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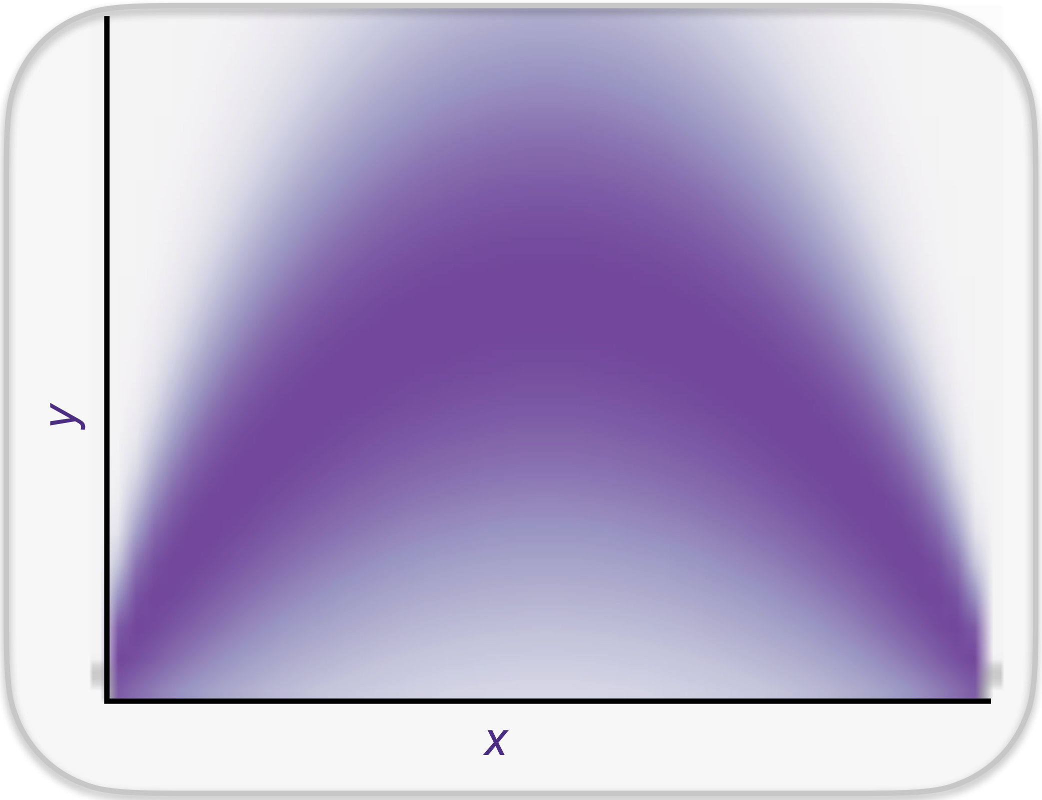
$$\begin{aligned} 0 &= \frac{d}{dc_x}\mathbb{E}_{Y|X}[(Y - c_x)^2 | X = x] \\ &= \mathbb{E}_{Y|X}[\frac{d}{dc_x}(Y - c_x)^2 | X = x] \\ &= \mathbb{E}_{Y|X}[-2(Y - c_x) | X = x] = -2\mathbb{E}_{Y|X}[Y | X = x] + 2c_x \end{aligned}$$

Squared Error Optimal Predictor: $\eta(x) = \mathbb{E}_{Y|X}[Y | X = x]$

Statistical Learning

$$\mathbb{E}_{XY}[(Y - \eta(X))^2]$$

$$P_{XY}(X = x, Y = y)$$



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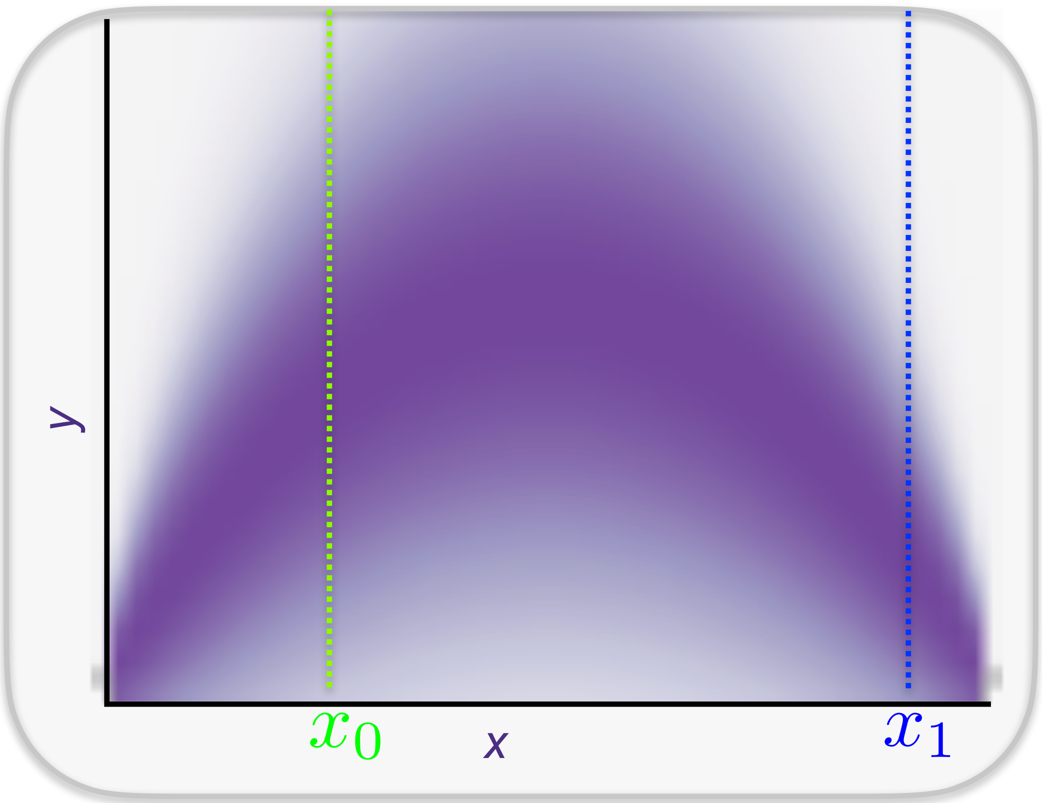
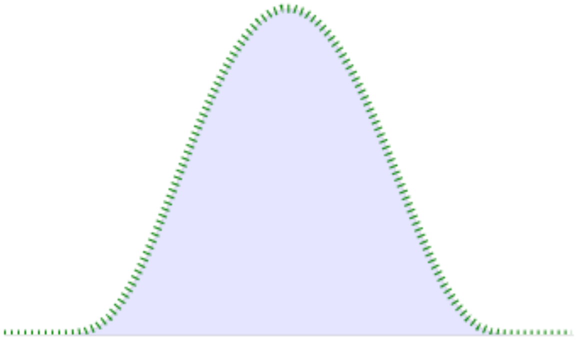


$$P_{XY}(Y=y|X=x_0)$$



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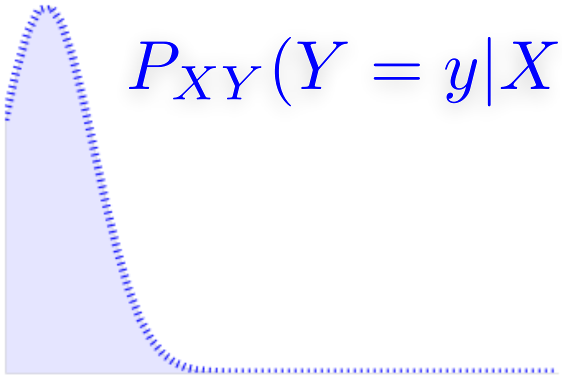

Statistical Learning

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Ideally, we want to find:

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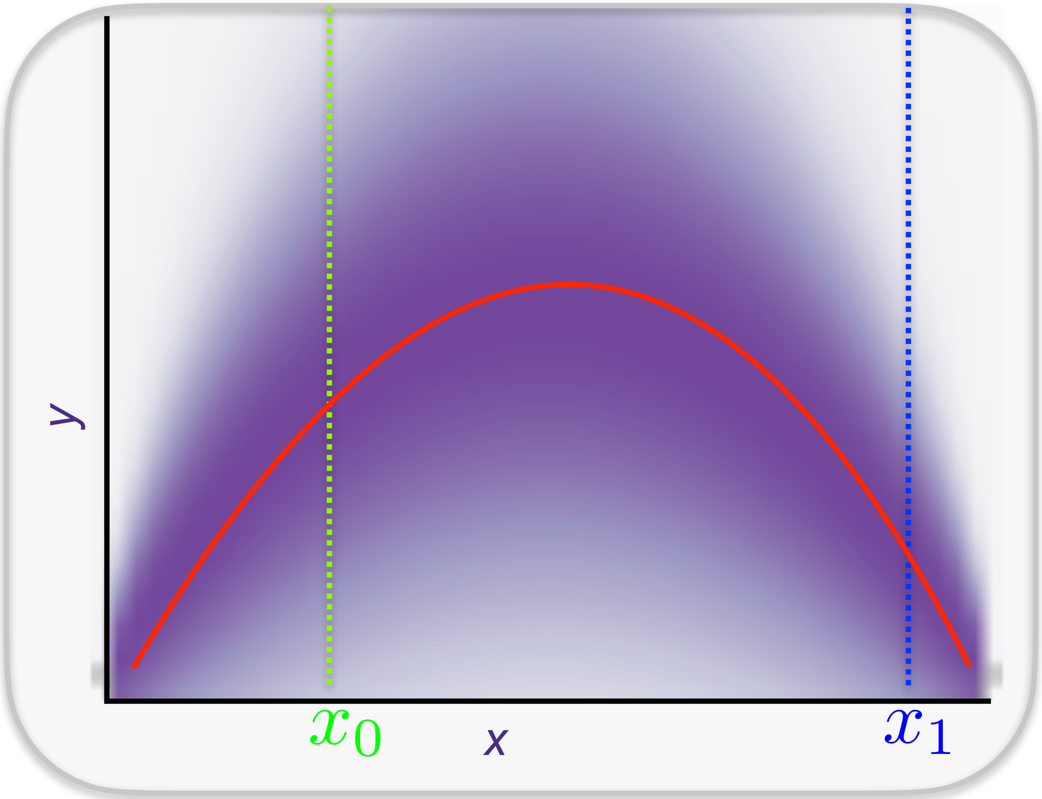

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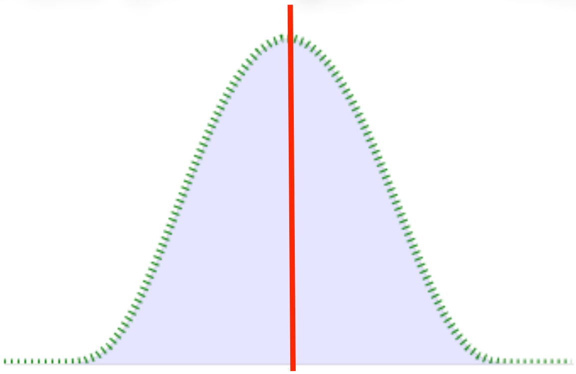

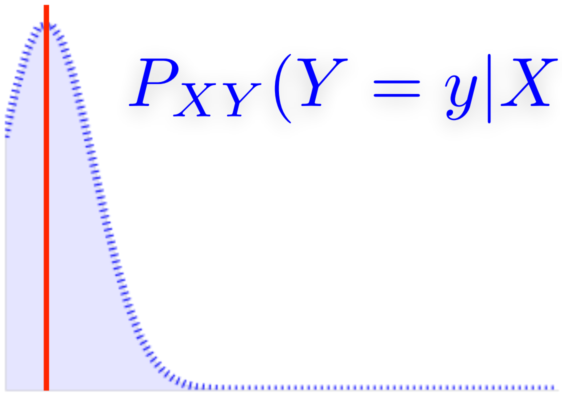

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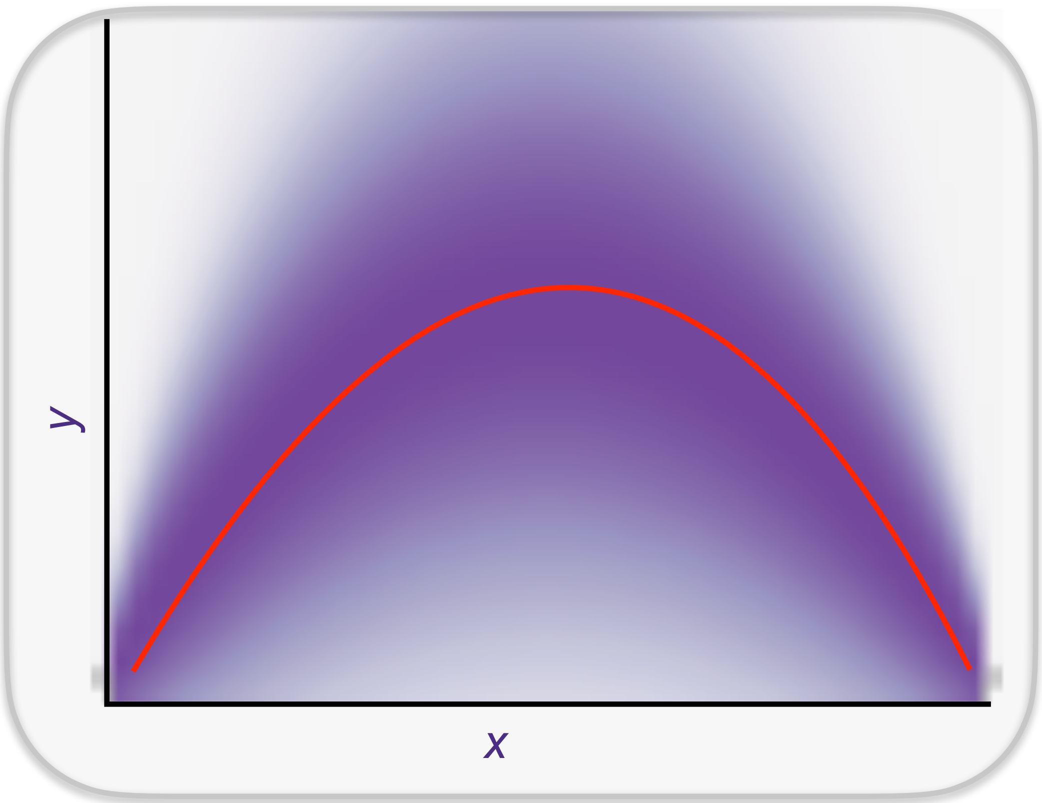

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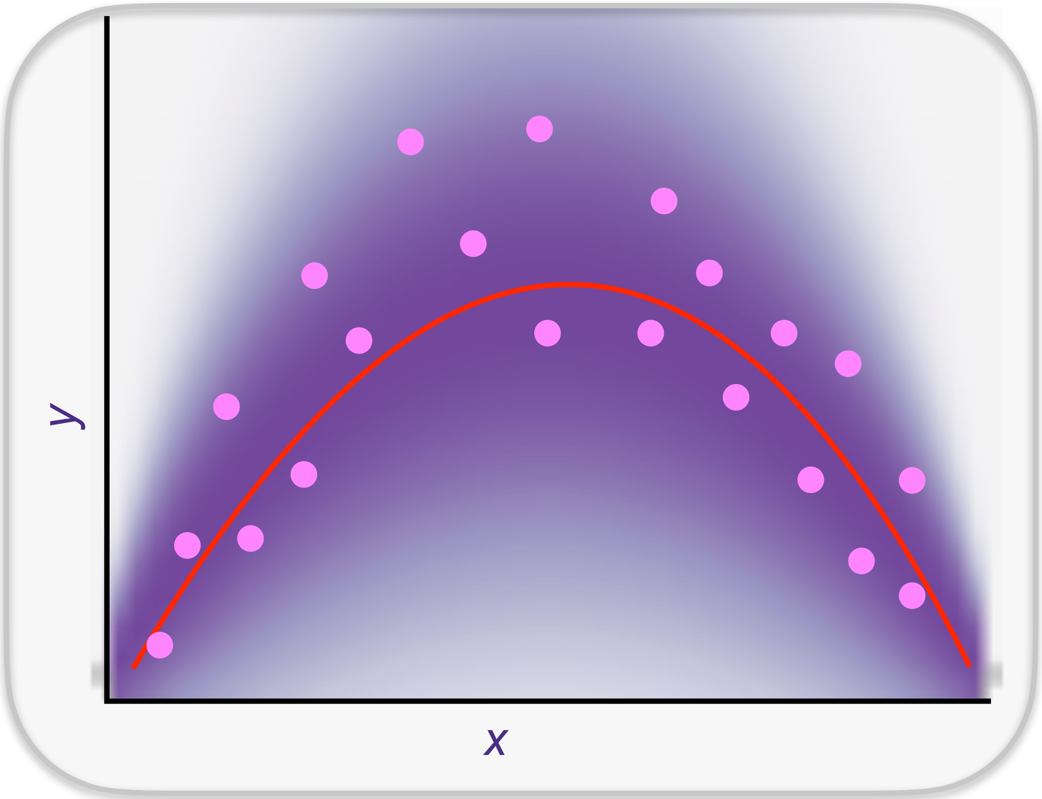

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But we only have samples:

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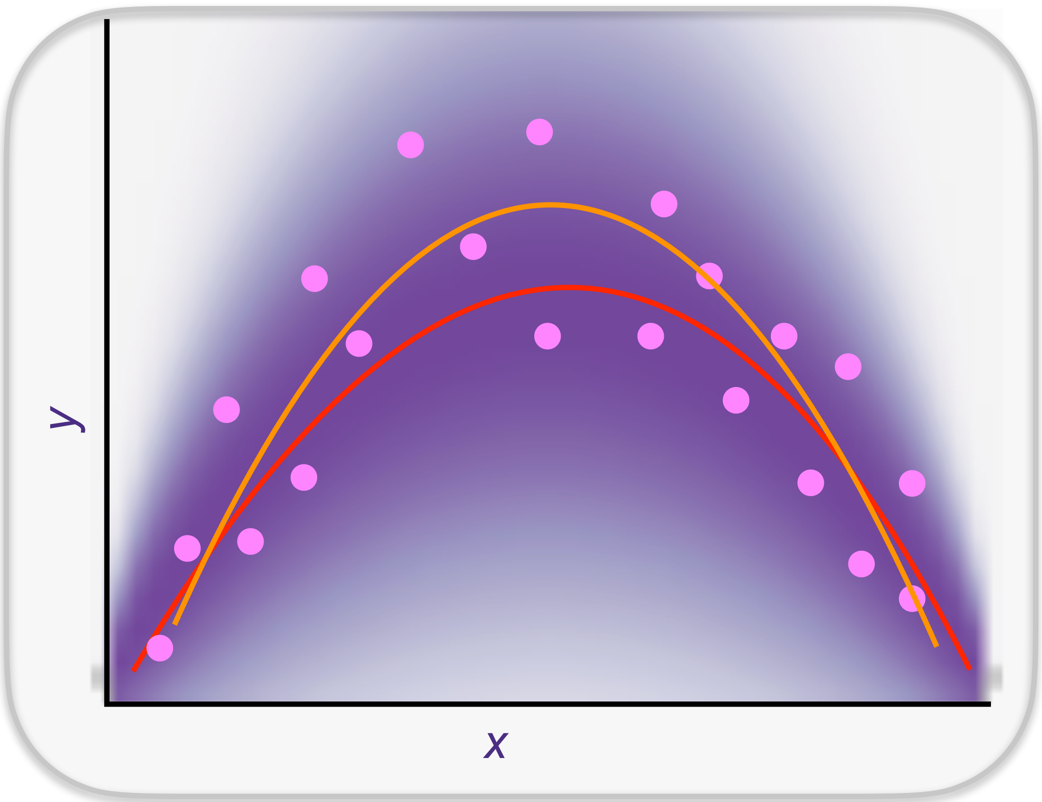

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and are restricted to a function class (e.g., linear) so we compute:

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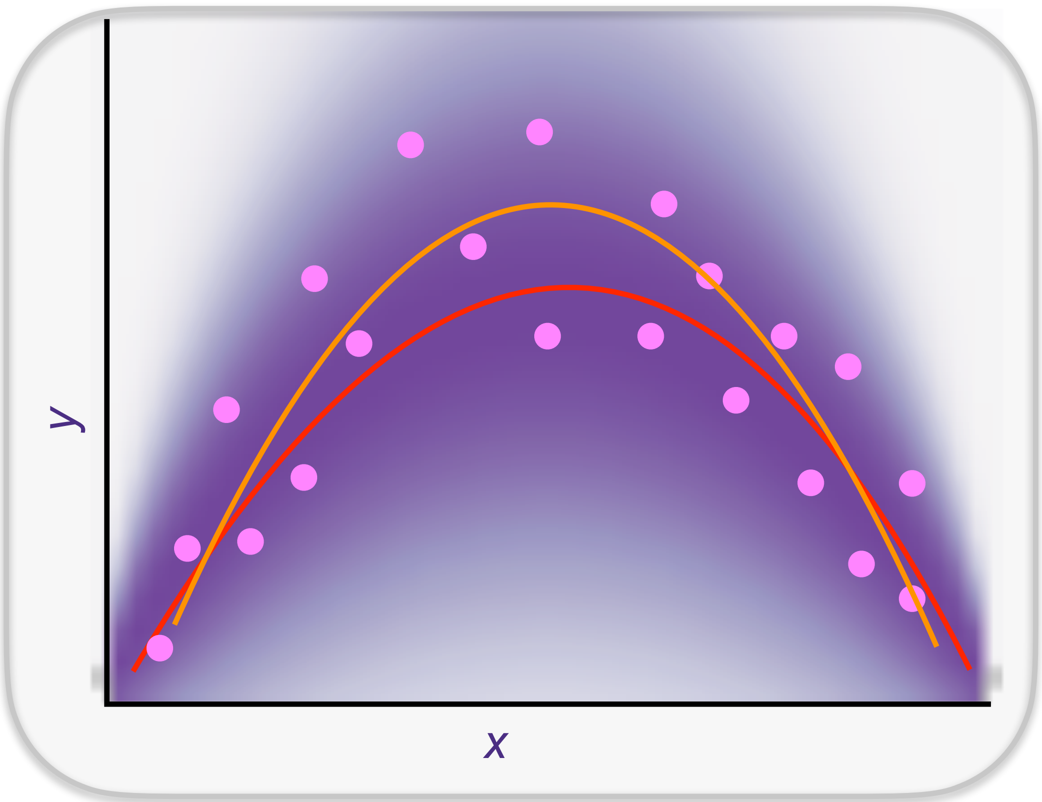

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We care about future predictions: $\mathbb{E}_{XY}[(Y - \widehat{f}(X))^2]$

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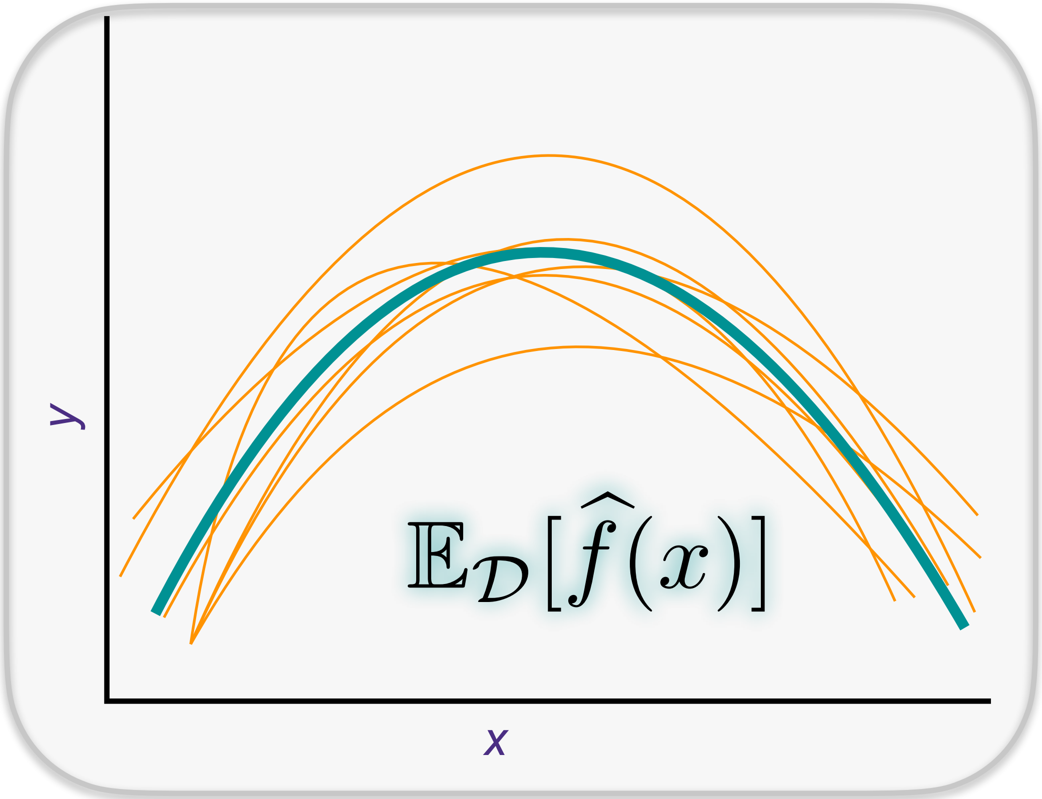

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Bias-Variance Tradeoff

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$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2]\big|X=x] = \mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \eta(x) + \eta(x) - \widehat{f}_{\mathcal{D}}(x))^2]\big|X=x]$$

Bias-Variance Tradeoff

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X=x] \qquad \widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$$

$$\begin{aligned}
\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y-\widehat{f}_{\mathcal{D}}(x))^2]\big|X=x] &= \mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y-\eta(x)+\eta(x)-\widehat{f}_{\mathcal{D}}(x))^2]\big|X=x] \\
&= \mathbb{E}_{Y|X}\Big[\mathbb{E}_{\mathcal{D}}[(Y-\eta(x))^2 + 2(Y-\eta(x))(\eta(x)-\widehat{f}_{\mathcal{D}}(x)) \\
&\quad + (\eta(x)-\widehat{f}_{\mathcal{D}}(x))^2]\big|X=x\Big] \\
&= \underbrace{\mathbb{E}_{Y|X}[(Y-\eta(x))^2\big|X=x]}_{\text{irreducible error}} + \underbrace{\mathbb{E}_{\mathcal{D}}[(\eta(x)-\widehat{f}_{\mathcal{D}}(x))^2]}_{\text{learning error}}
\end{aligned}$$

irreducible error
Caused by stochastic label noise

learning error
Caused by either using too "simple" of a model or not enough data to learn the model accurately

Bias-Variance Tradeoff

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$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

$$\mathbb{E}_{\mathcal{D}}[(\eta(x) - \widehat{f}_{\mathcal{D}}(x))^2] = \mathbb{E}_{\mathcal{D}}[(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] + \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

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$$\underline{\mathbb{E}_{\mathcal{D}}[(\eta(x) - \widehat{f}_{\mathcal{D}}(x))^2]} = \mathbb{E}_{\mathcal{D}}[(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] + \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

$$= \mathbb{E}_{\mathcal{D}}[(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2 + 2(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))$$

$$+ (\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

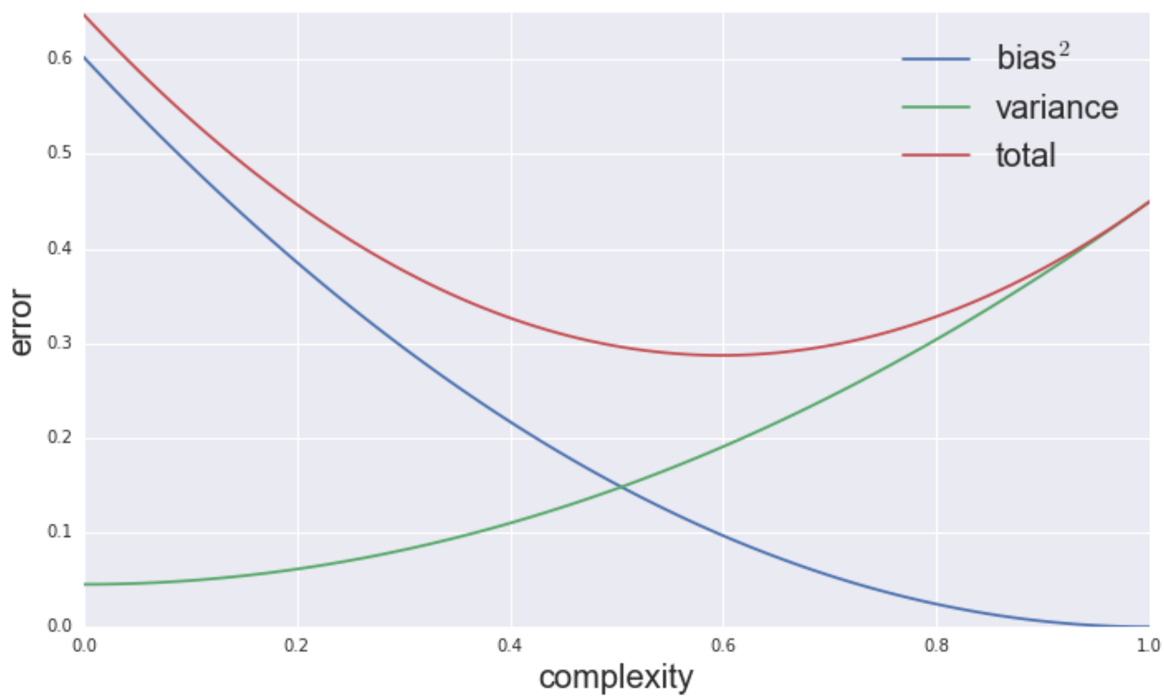
$$= \underline{(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2} + \underline{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]}$$

biased squared **variance**

Bias-Variance Tradeoff

$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2] \big| X = x] = \underbrace{\mathbb{E}_{Y|X}[(Y - \eta(x))^2 \big| X = x]}_{\text{irreducible error}}$$

$$+ \underbrace{(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2}_{\text{biased squared}} + \underbrace{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]}_{\text{variance}}$$



Overfitting

Bias-Variance Tradeoff

- Choice of hypothesis class introduces learning bias
  - More complex class → less bias
  - More complex class → more variance
- But in practice??

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  - More complex class → less bias
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- But in practice??
- Before we saw how increasing the feature space can increase the complexity of the learned estimator:

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_3 \subset \ldots$$

$$\widehat{f}_{\mathcal{D}}^{(k)} = \arg\min_{f \in \mathcal{F}_k} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

Complexity grows as k grows

Training set error as a function of model complexity

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TRAIN error:

$$\mathcal{D} \stackrel{i.i.d.}{\sim} P_{XY}$$

$$\frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - \widehat{f}_{\mathcal{D}}^{(k)}(x_i))^2$$

TRUE error:

$$\mathbb{E}_{XY}[(Y - \widehat{f}_{\mathcal{D}}^{(k)}(X))^2]$$

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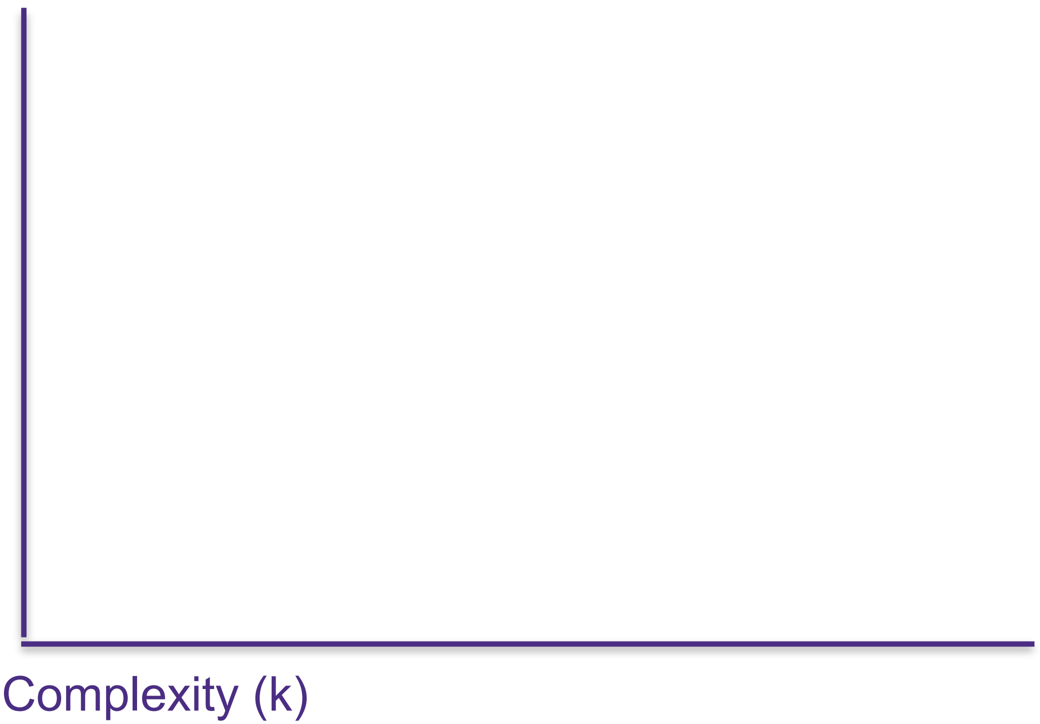

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TRUE error:

$$\mathbb{E}_{XY}[(Y - \widehat{f}_{\mathcal{D}}^{(k)}(X))^2]$$

TEST error:

$$\mathcal{T} \overset{i.i.d.}{\sim} P_{XY}$$

$$\frac{1}{|\mathcal{T}|} \sum_{(x_i, y_i) \in \mathcal{T}} (y_i - \widehat{f}_{\mathcal{D}}^{(k)}(x_i))^2$$

$$\boxed{\text{Important: } \mathcal{D} \cap \mathcal{T} = \emptyset}$$

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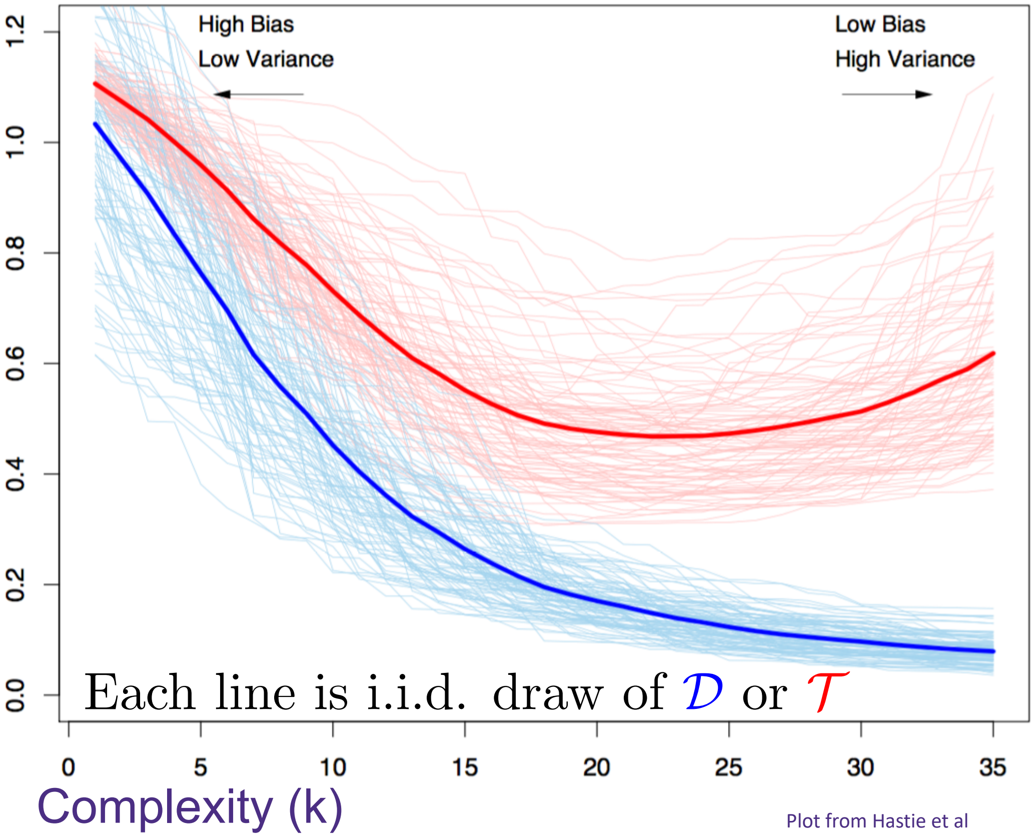

Plot from Hastie et al

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TRAIN error is **optimistically biased** because it is evaluated on the data it trained on. **TEST error** is **unbiased** only if *T* is never used to train the model or even pick the complexity k.

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Test set error

- Given a dataset, randomly split it into two parts:
  - Training data: $\mathcal{D}$
  - Test data: $\mathcal{T}$

$$\boxed{\text{Important: } \mathcal{D} \cap \mathcal{T} = \emptyset}$$

- Use training data to learn predictor
  - e.g., $\frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - \widehat{f}^{(k)}_{\mathcal{D}}(x_i))^2$
  - use training data to pick complexity k

- Use test data to report predicted performance

$$\frac{1}{|\mathcal{T}|} \sum_{(x_i, y_i) \in \mathcal{T}} (y_i - \widehat{f}^{(k)}_{\mathcal{D}}(x_i))^2$$

How many points do I use for training/testing?

> **Very hard question to answer!**
  - **Too few training points, learned model is bad**
  - **Too few test points, you never know if you reached a good solution**

> **Bounds, such as Hoeffding's inequality can help:**

$$P(|\ \widehat{\theta} - \theta^*\ | \geq \epsilon) \quad \leq \quad 2e^{-2N\epsilon^2}$$

> **More on this later the quarter, but still hard to answer**

> **Typically:**
  - **If you have a reasonable amount of data 90/10 splits are common**
  - **If you have little data, then you need to get fancy (e.g., bootstrapping)**