Bias-Variance Tradeoff

Process

Collect a **data set**

Decide on a **model**

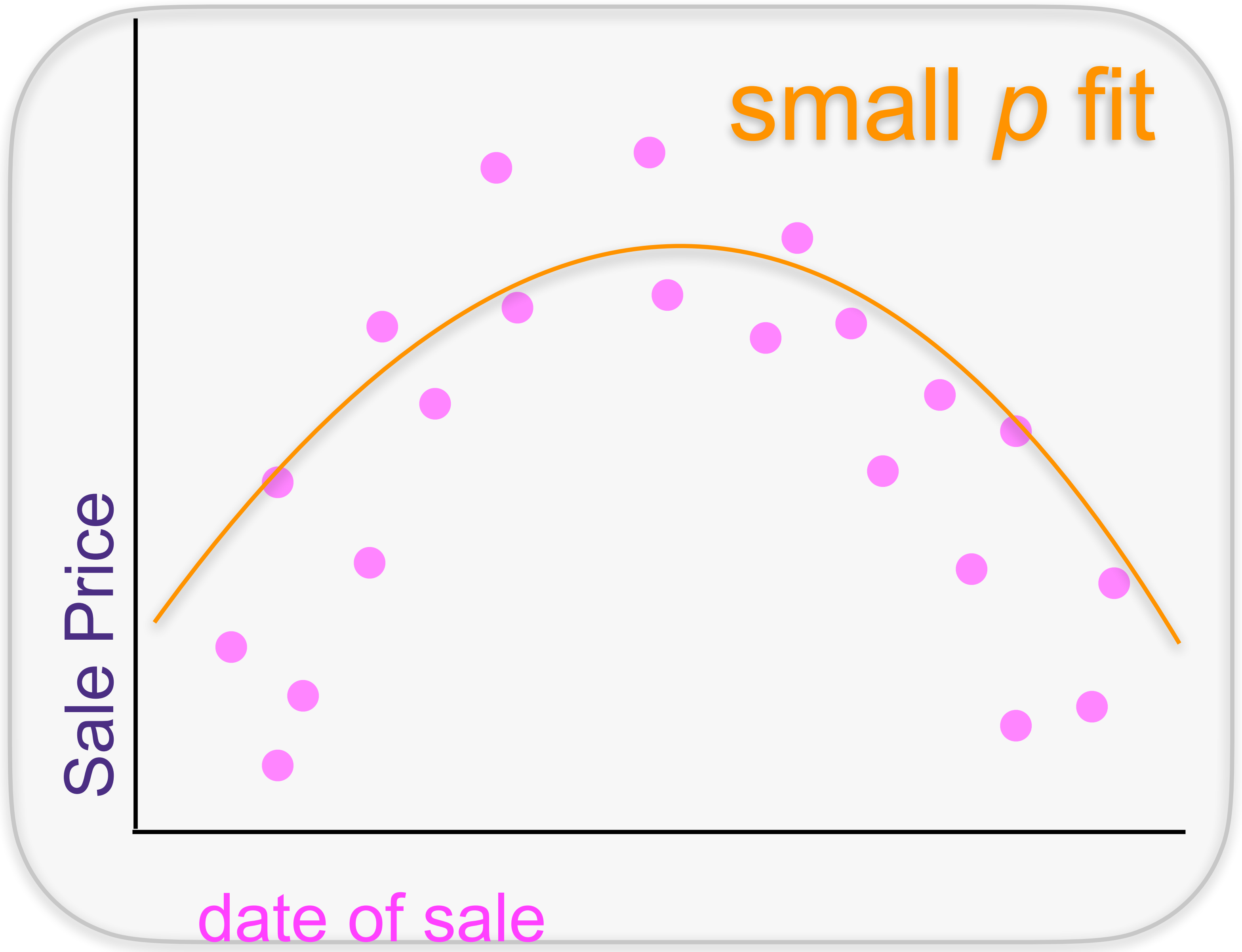
Find the function which fits the data best

- **Choose a loss function**
- **Pick the function which minimizes loss on data**

Use function to make prediction on new examples

The regression problem

Training Data: $\{(x_i, y_i)\}_{i=1}^n$ $\quad x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$



Transformed data:

$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ \vdots \\ h_p(x) \end{bmatrix}$$

Hypothesis: linear in h

$$y_i \approx h(x_i)^T w \quad w \in \mathbb{R}^p$$

Loss: least squares

$$\min_w \sum_{i=1}^n \left(y_i - h(x_i)^T w\right)^2$$

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Training Data: $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

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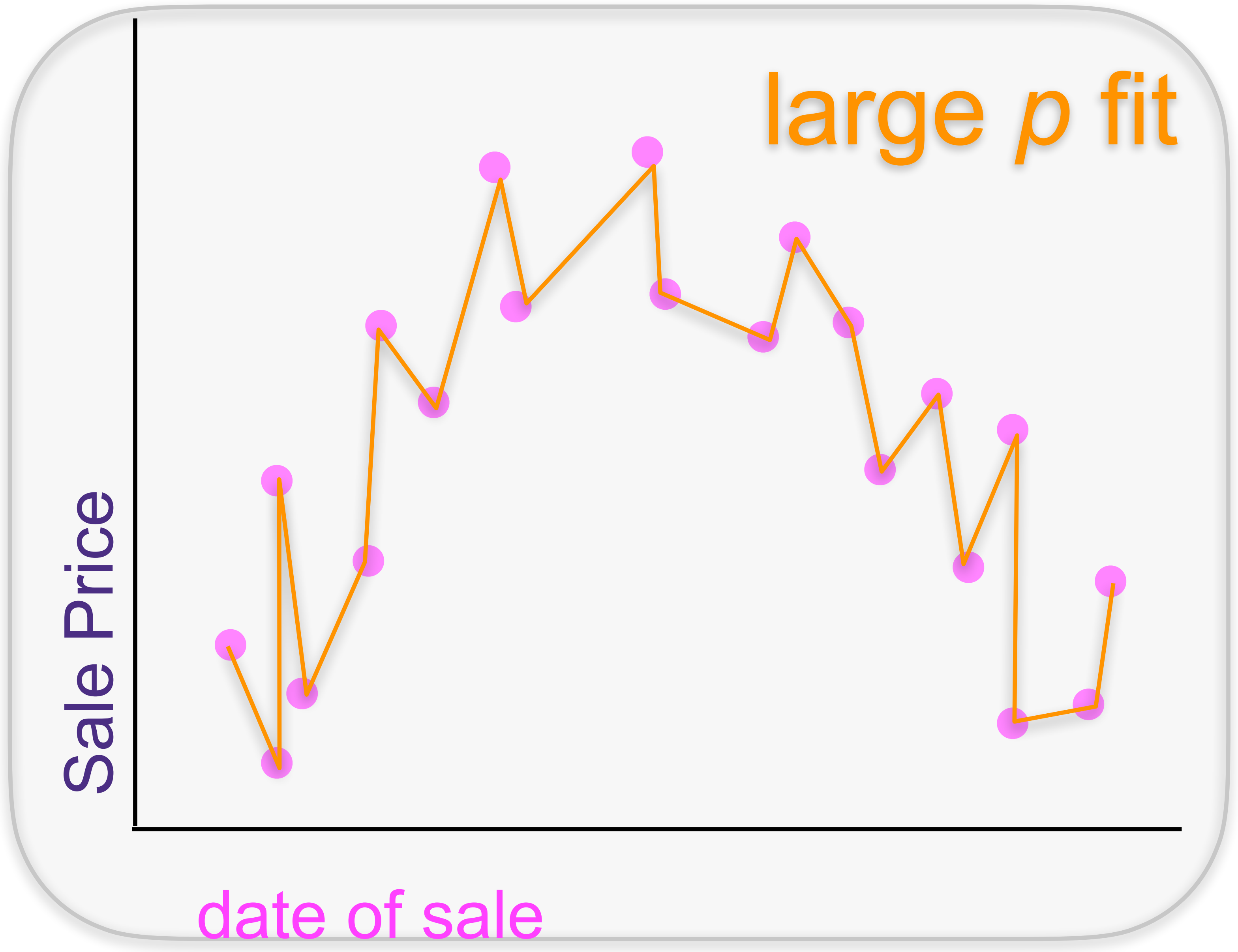

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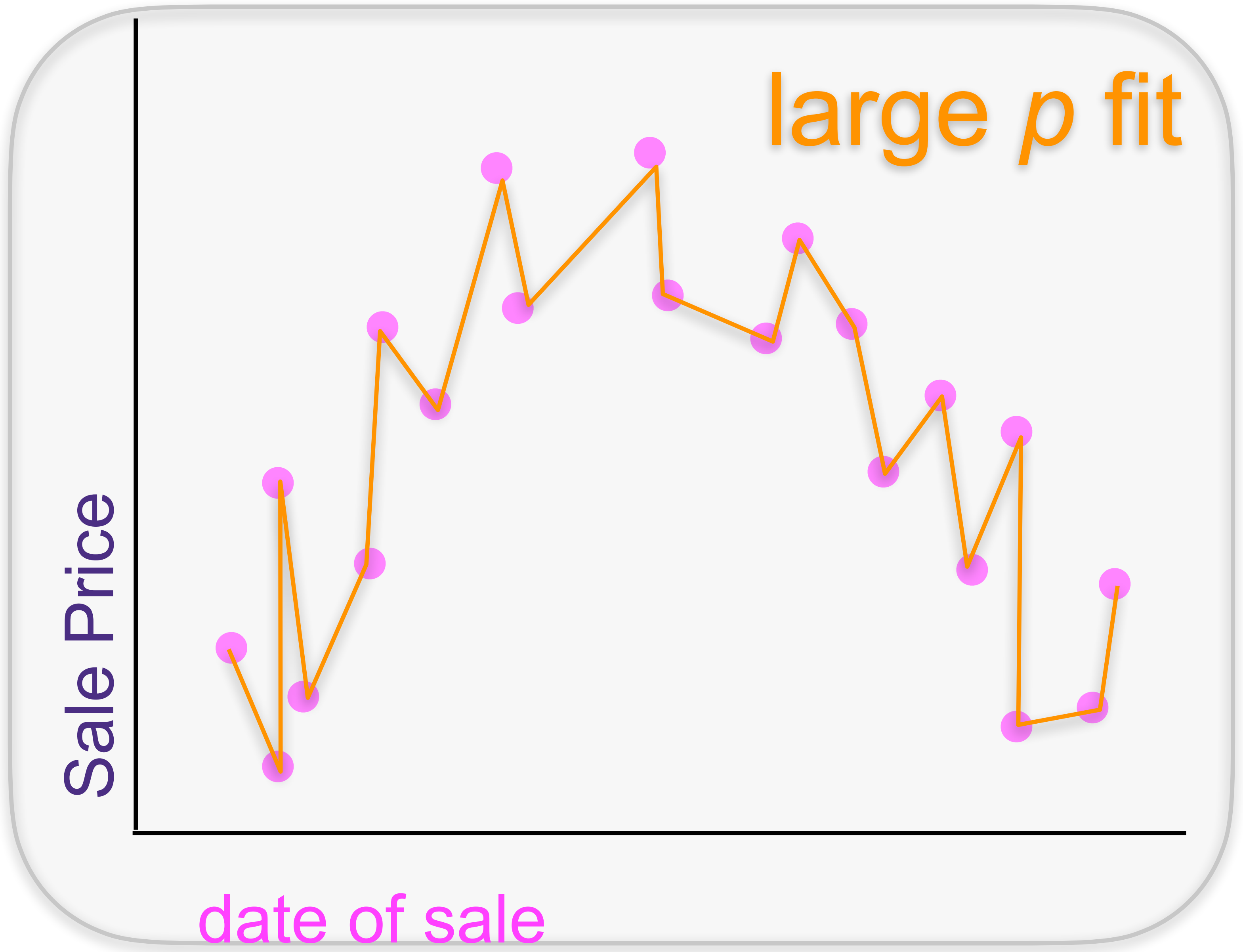
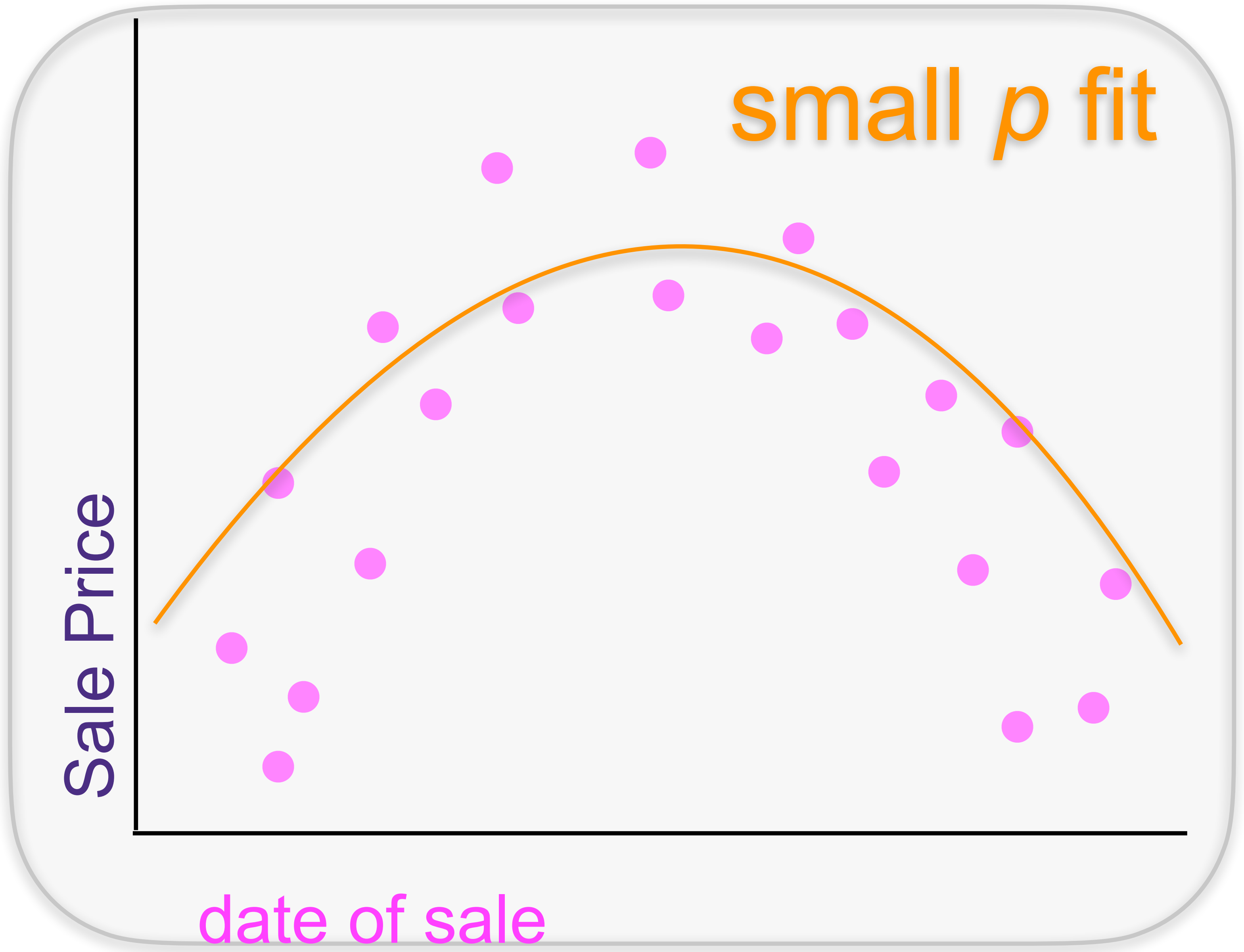
Which is better?

A: large p



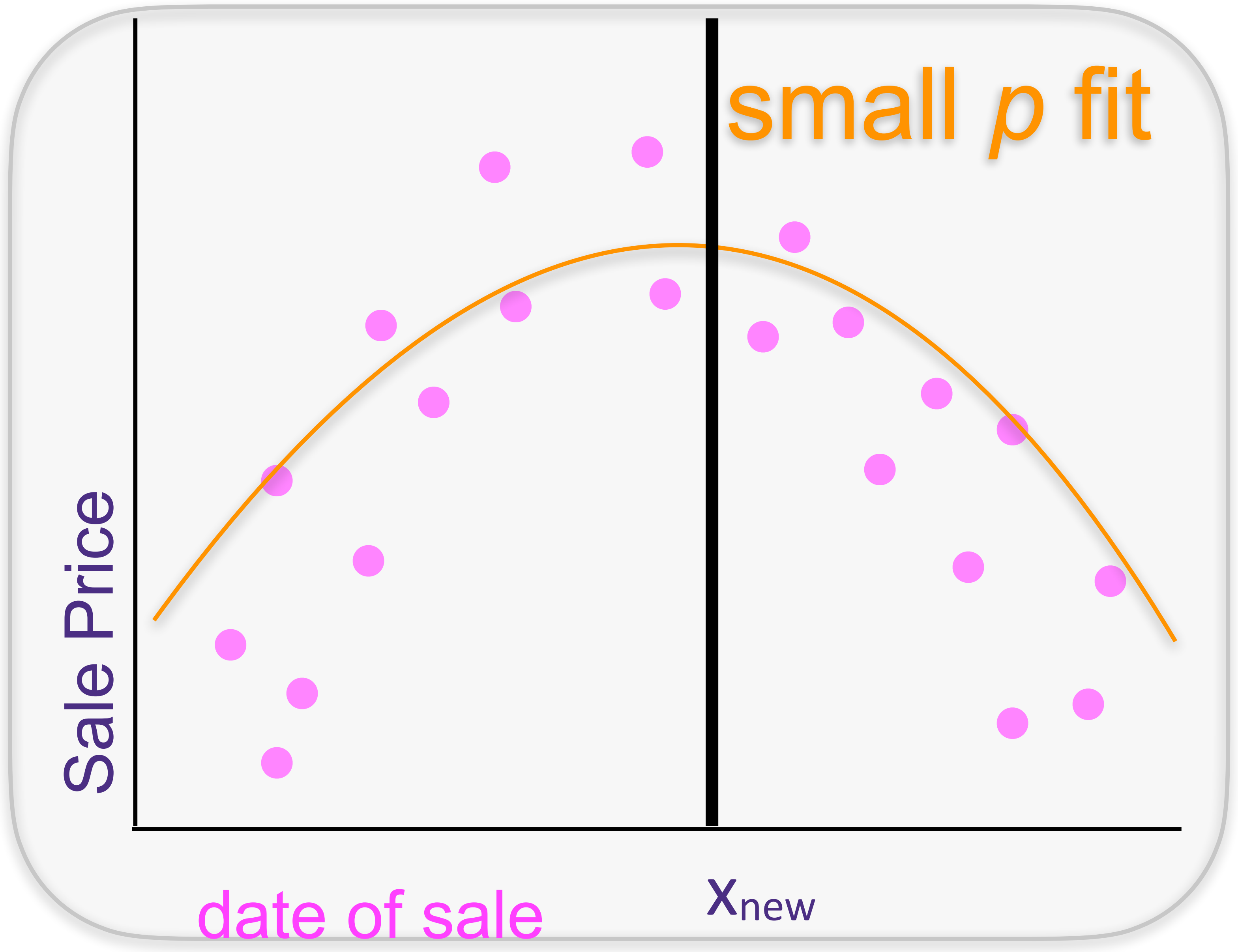
B: small p



Predicting sale price for a new house: A vs B

A: large p

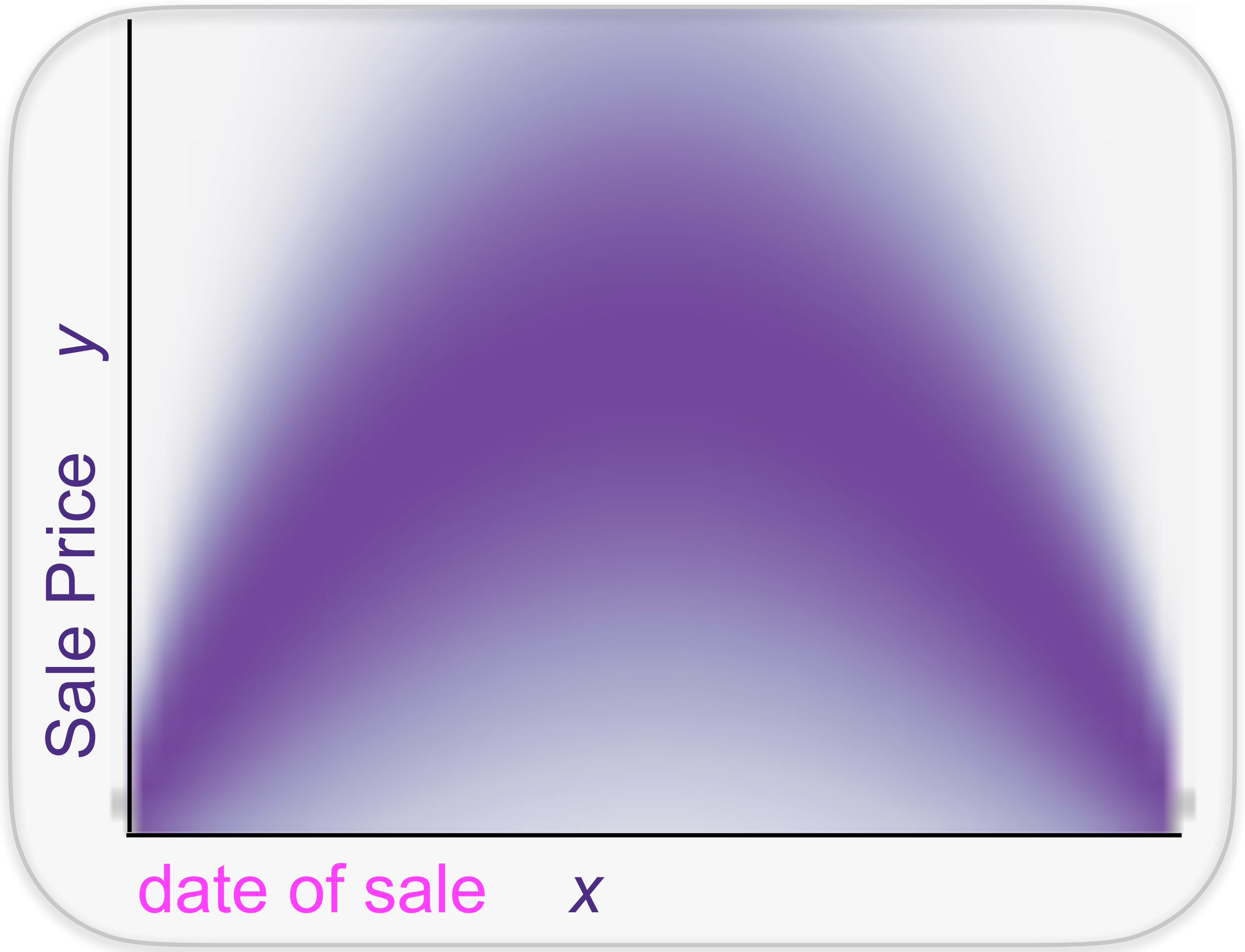
B: small p



Our goal is to predict prices for new houses

Average Accuracy

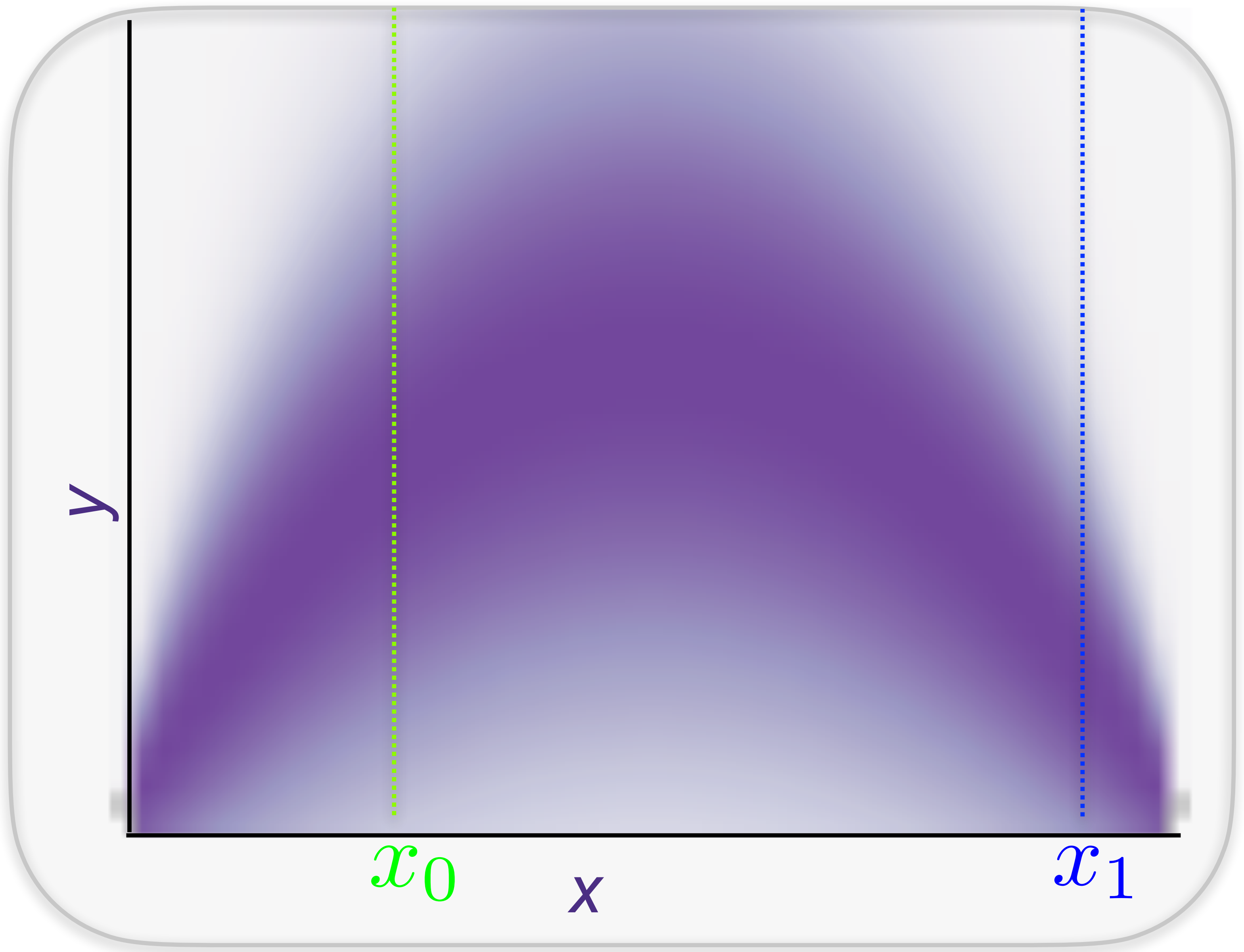
$$P_{XY}(X = x, Y = y)$$



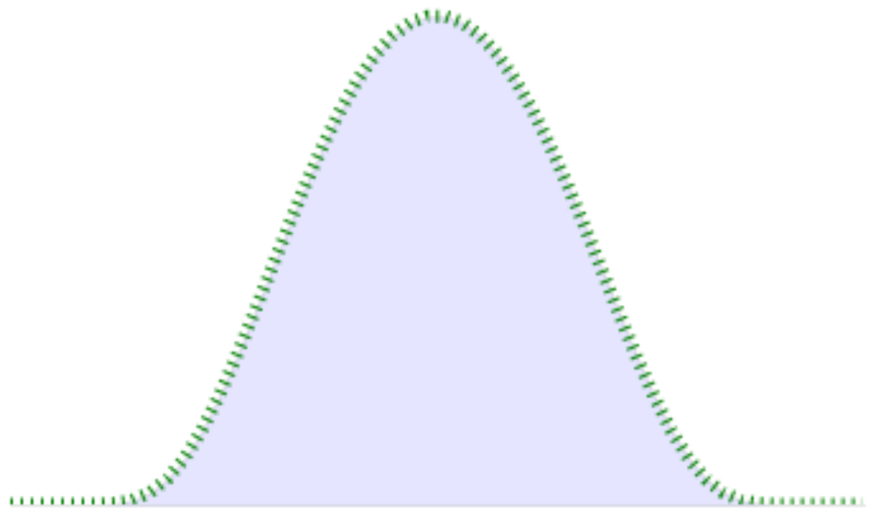
On *average* over a house
drawn from this distribution,
we want to make a good prediction.

Goal: predict future sale prices

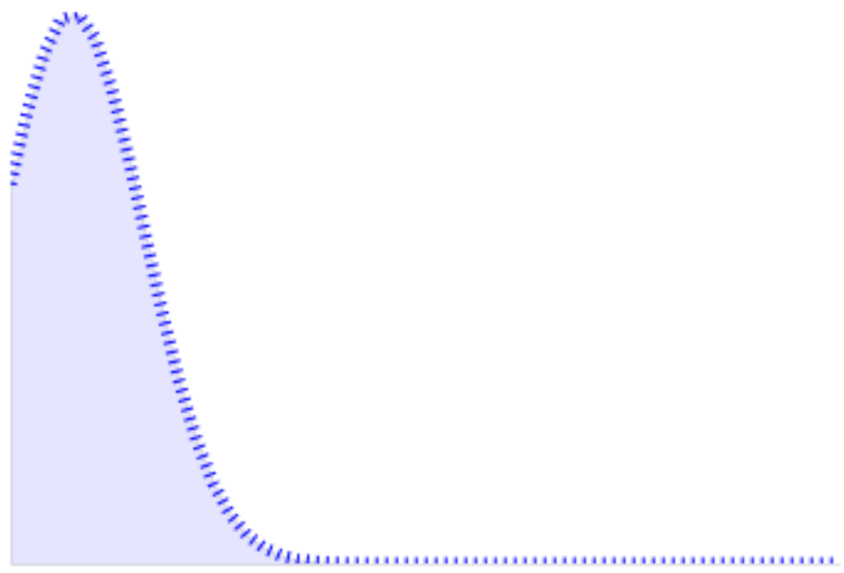
$$P_{XY}(X = x, Y = y)$$



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



$$P_{XY}(Y = y | X = x_1)$$



Statistical Learning

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

Goal: Predict Y given X

Find a function η that minimizes

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

Thus far, we've been using η which is a:
- Linear functions of X
- Degree p polynomials of X
- Linear "generalization" of X in p dimensions

Statistical Learning

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

Goal: Predict Y given X

Find a function η that minimizes

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

$$\eta(x) = \arg\min_c \mathbb{E}_{Y|X}[(Y - c)^2 | X = x] = \mathbb{E}_{Y|X}[Y | X = x]$$

Under LS loss, optimal predictor: $\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$

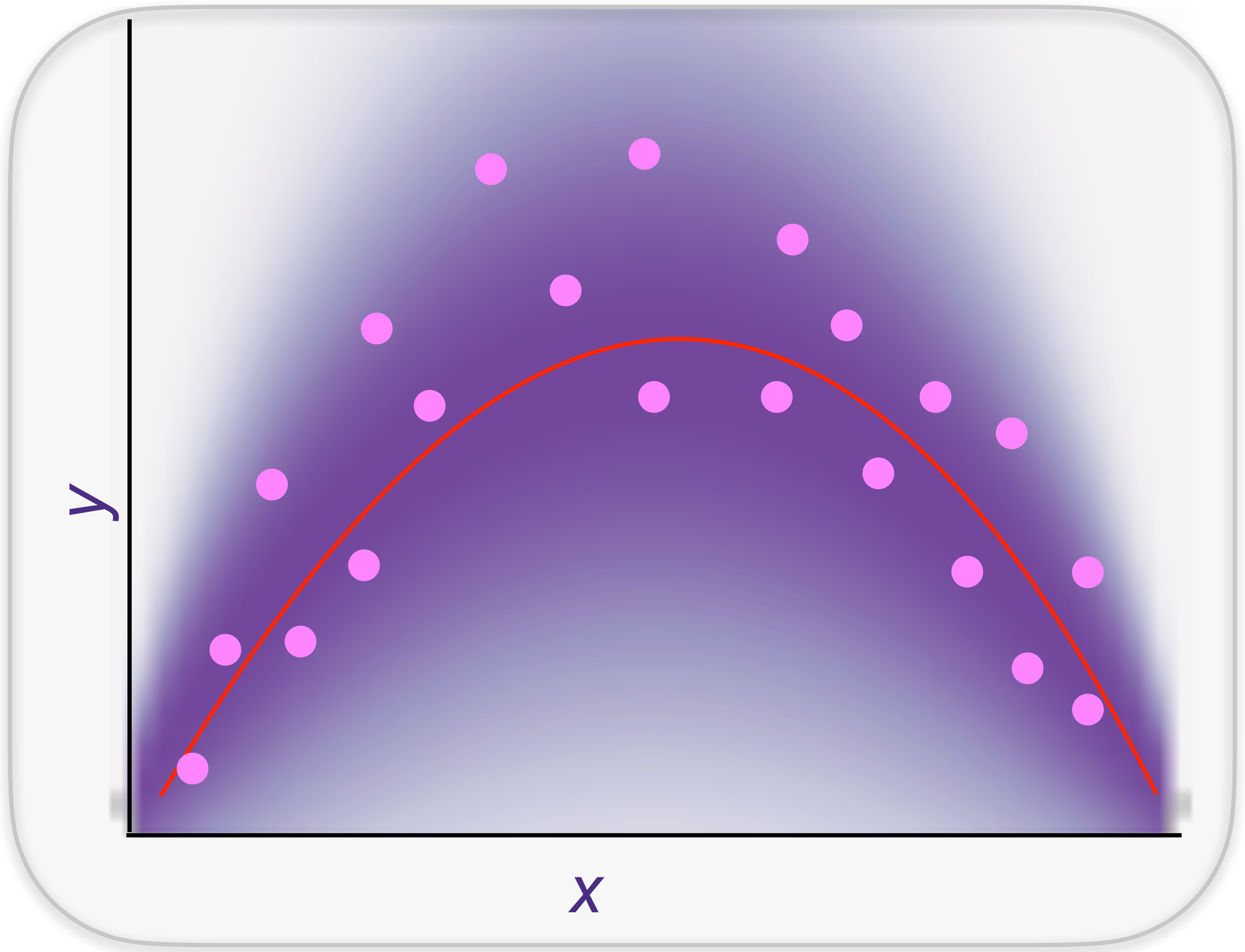
Optimal Prediction

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

Under LS loss, optimal predictor: $\eta(x) = \mathbb{E}_{Y|X}[Y|X=x]$

Statistical Learning

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



Ideally, we want to find:

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

But we only have samples:

$$(x_i, y_i) \overset{i.i.d.}{\sim} P_{XY} \quad \text{for } i = 1, \ldots, n$$

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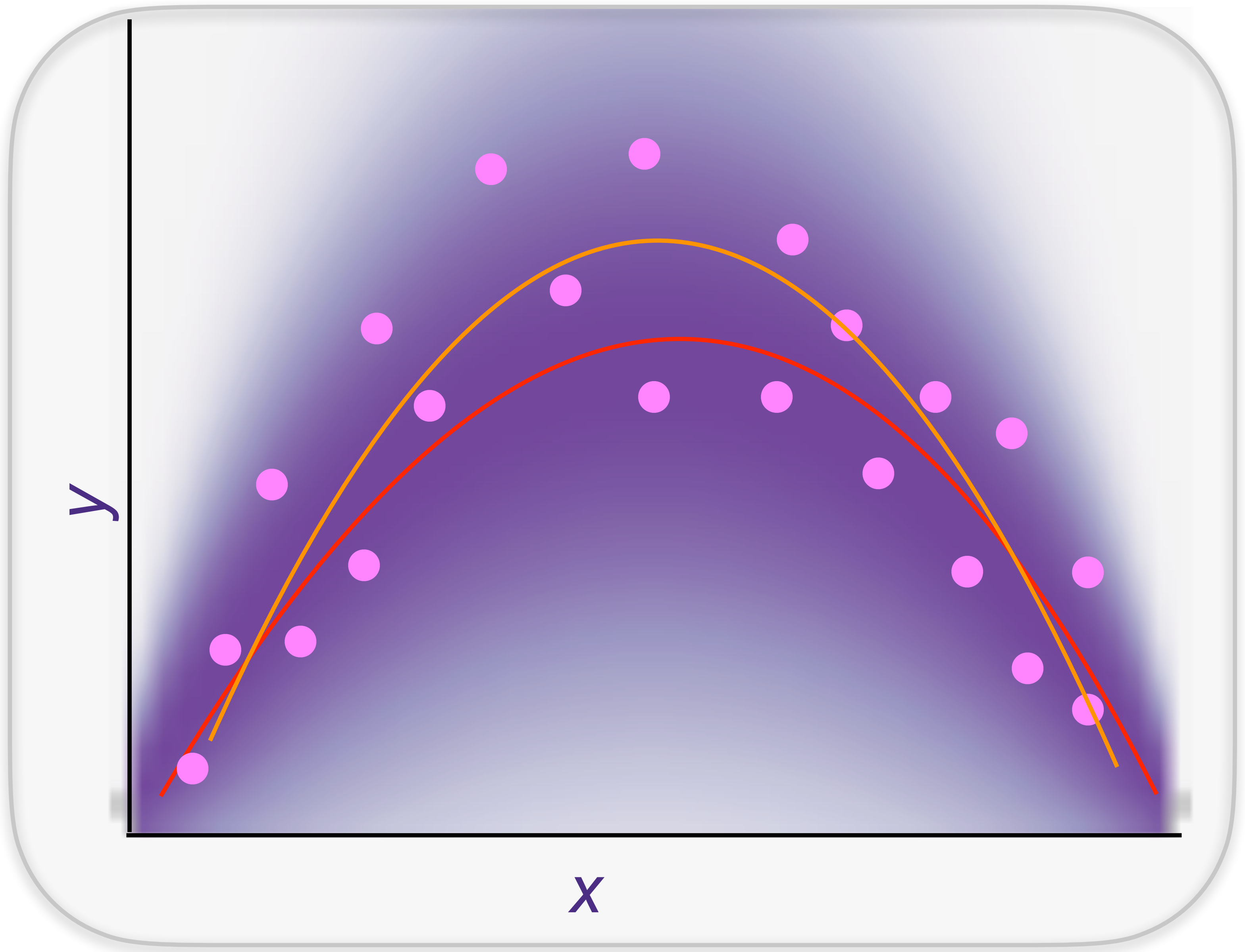

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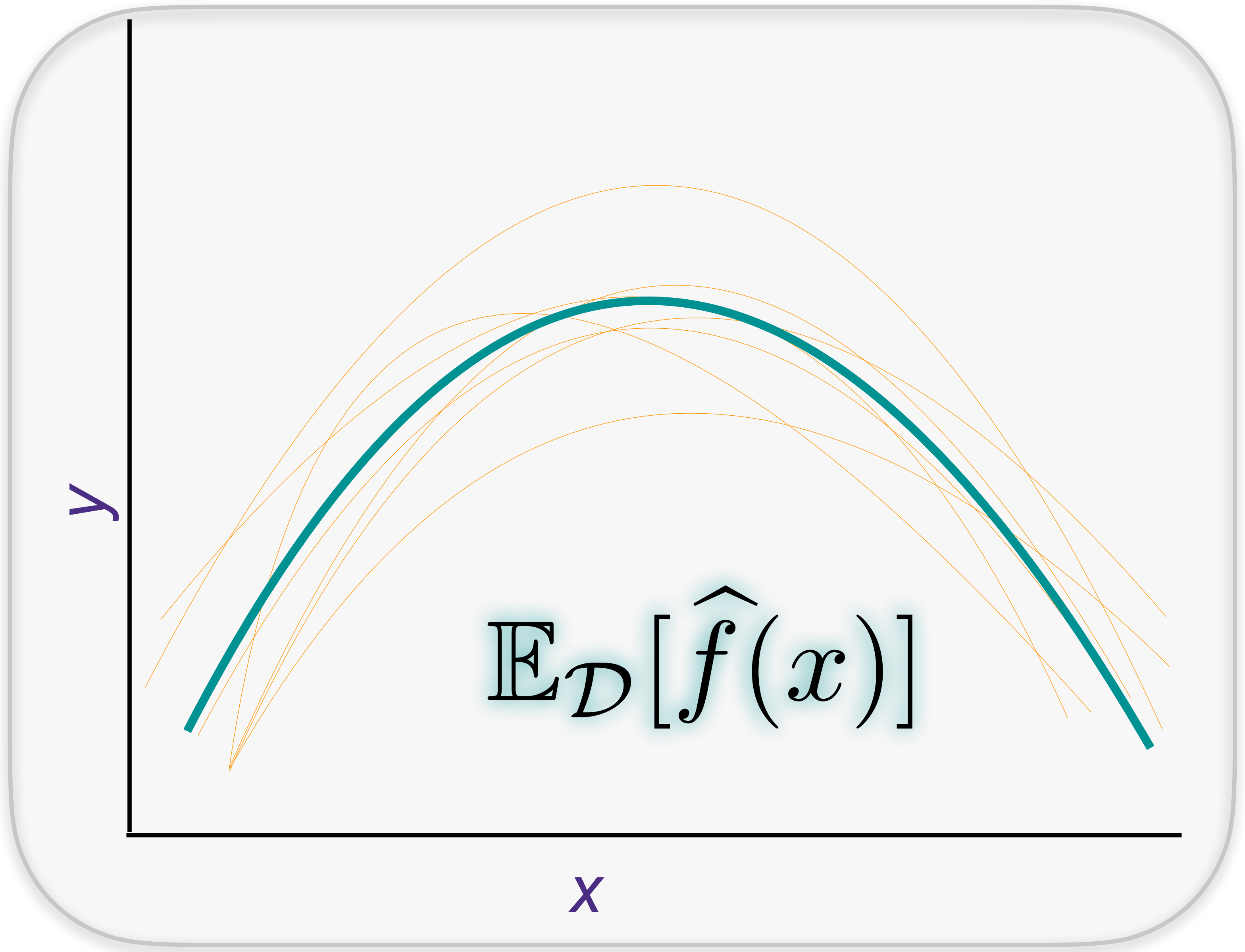
and are restricted to a function class (e.g., linear) so we compute:

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

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

Statistical Learning

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



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Each draw $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$ results in different $\widehat{f}$

Bias-Variance Tradeoff

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

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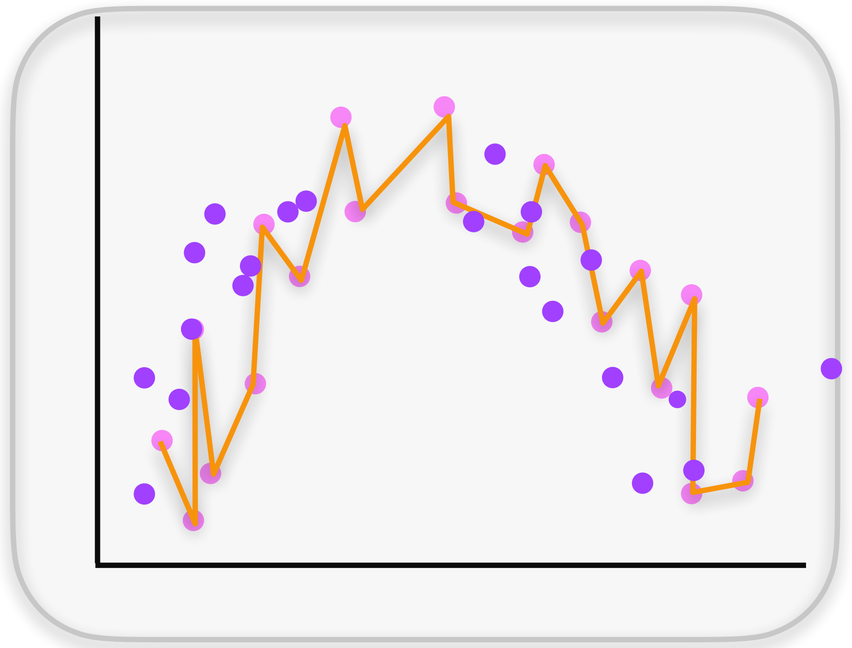
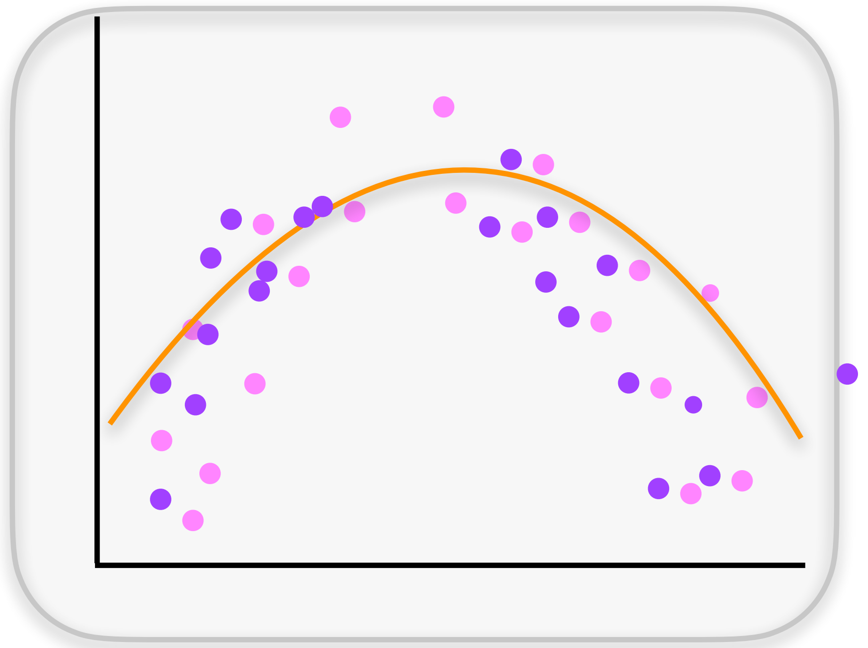
Bias-Variance Tradeoff

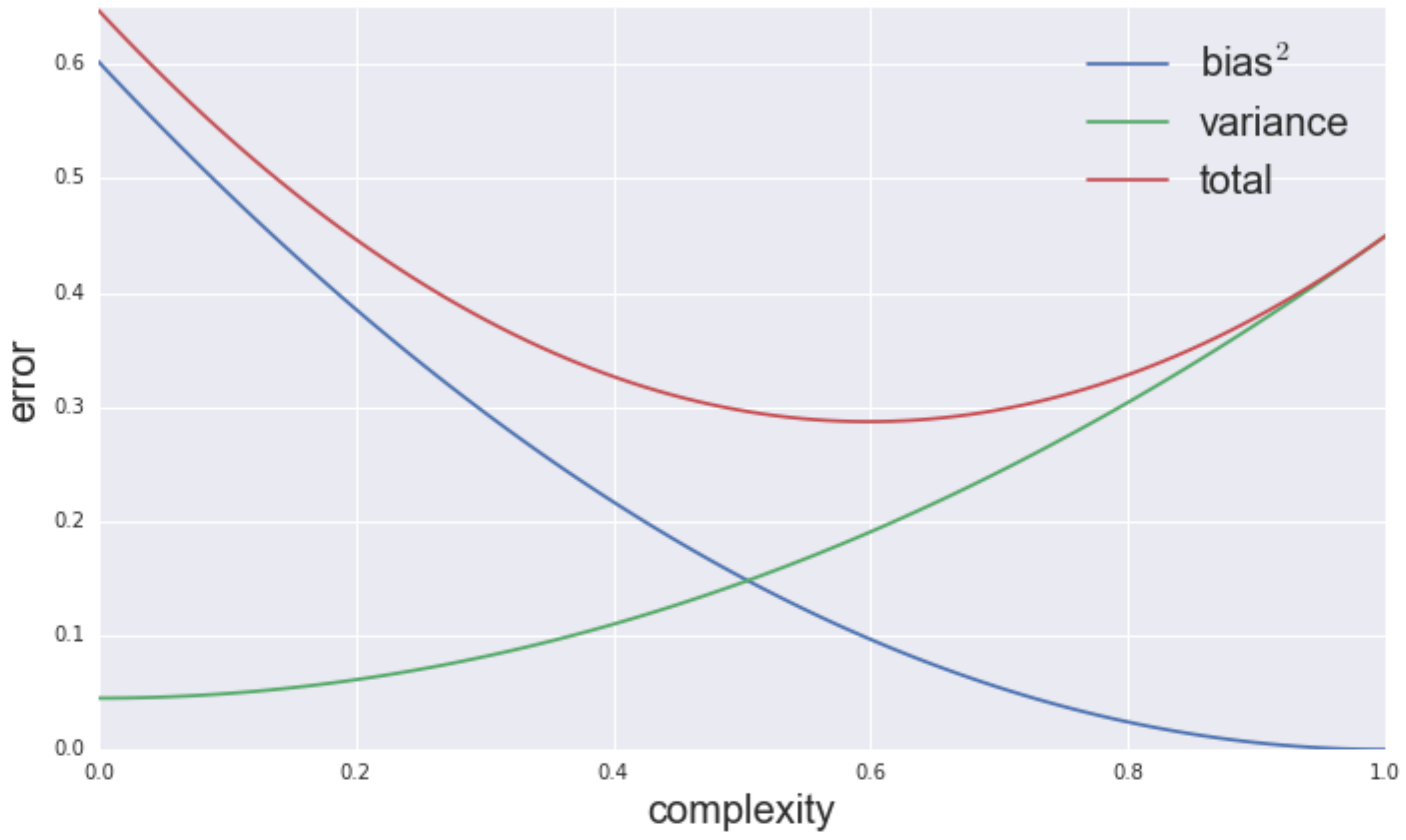
$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2] \big| X = x] = \underbrace{\mathbb{E}_{Y|X}[(Y - \eta(x))^2 \big| X = x]}_{\text{irreducible error}}$$

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





If we re-drew our data, what the LS training error estimator look like for generalized linear functions in small p/large p dimensions?



Bias-Variance Tradeoff

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

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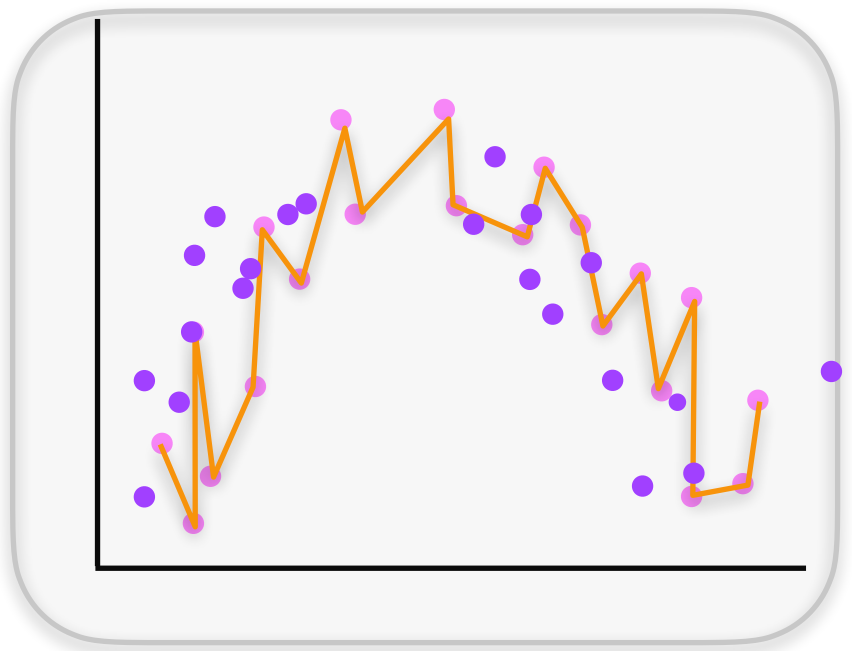

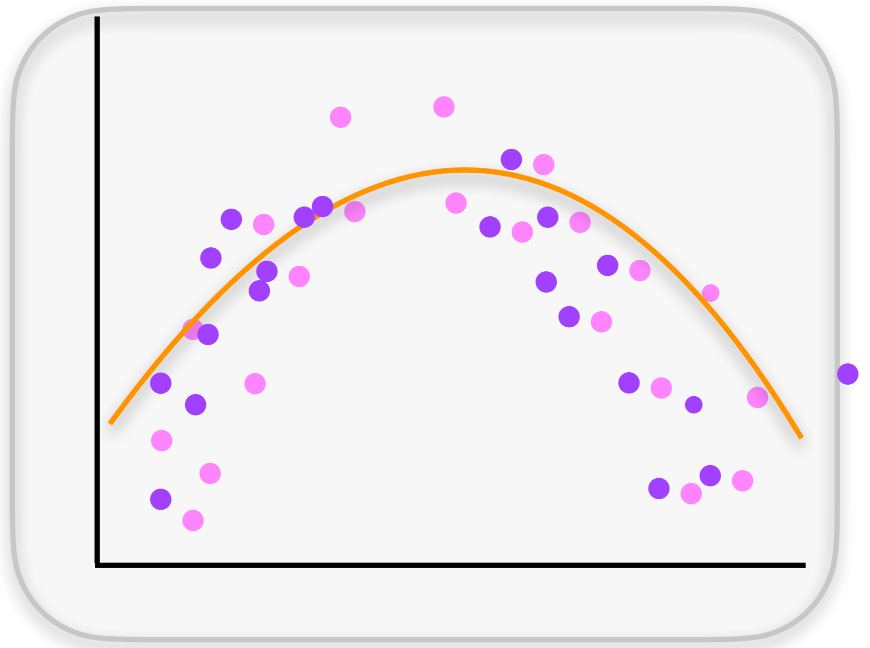

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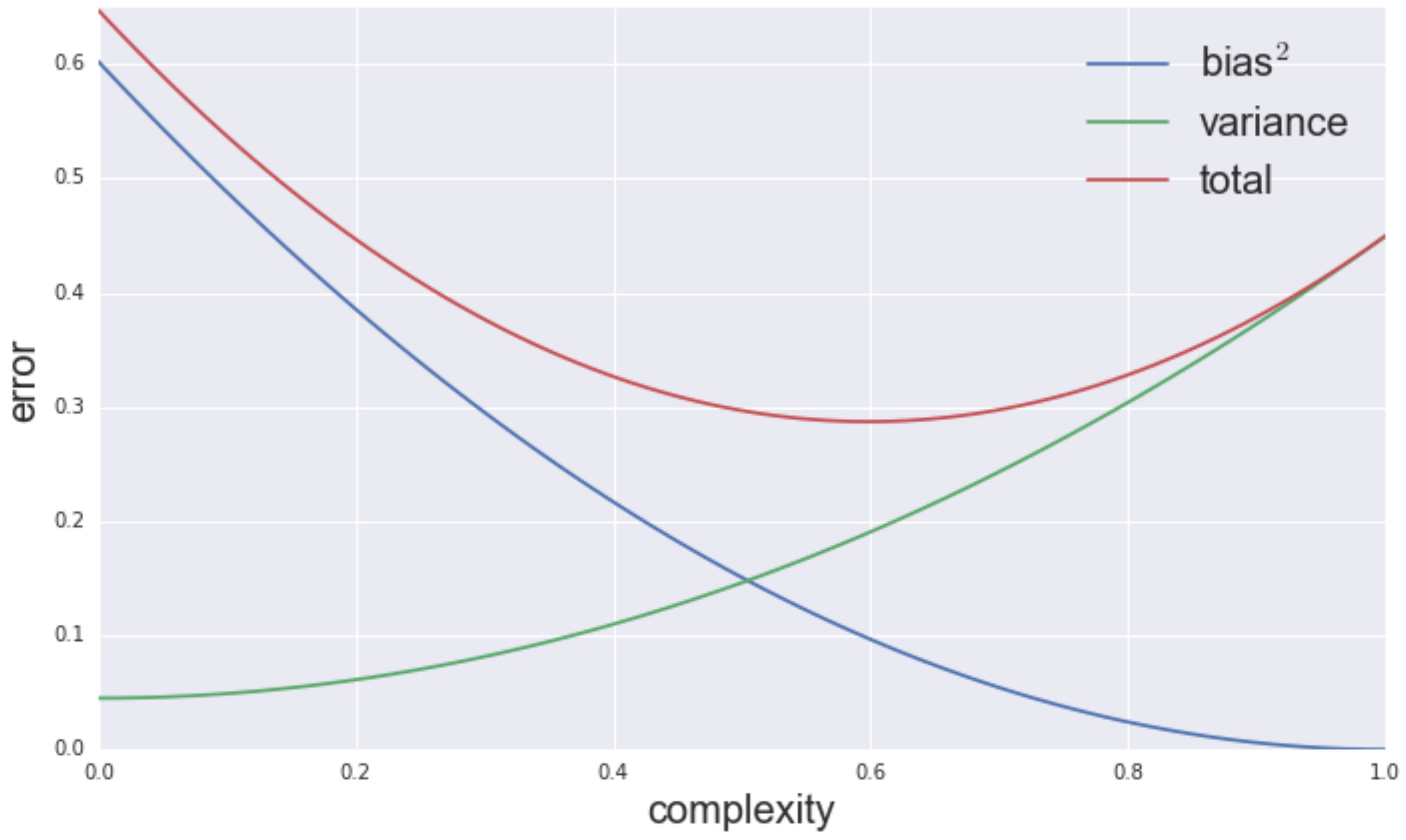

Example: Linear LS

$$\mathbf{Y} = \mathbf{X}w + \epsilon$$

$$\text{if} \quad y_i = x_i^T w + \epsilon_i \quad \text{and} \quad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$$

Example: Linear LS: compute bias

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$$\widehat{w}_{MLE} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = w + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

$$\widehat{f}_{\mathcal{D}}(x) = \widehat{w}^T x = w^T x + \epsilon^T \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1} x$$

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

Example: Linear LS: compute variance

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$$\underbrace{\mathbb{E}_{XY}[(Y - \eta(x))^2 | X = x]}_{\text{irreducible error}} = \sigma^2$$

$$\underbrace{(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2}_{\text{bias squared}} = 0$$

$$\mathbb{E}_{X=x}\Big[\underbrace{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]}_{\text{variance}}\Big] = \frac{p\sigma^2}{n}$$

Overfitting

Bias-Variance Tradeoff

> Choice of hypothesis class introduces learning bias
  - More complex class → less bias
  - More complex class → more variance

> But in practice??

Bias-Variance Tradeoff

> Choice of hypothesis class introduces learning 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

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

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TRAIN error:

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

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

TRUE error:

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

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TRUE error:

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TEST error:

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

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

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

Training set error as a function of model complexity

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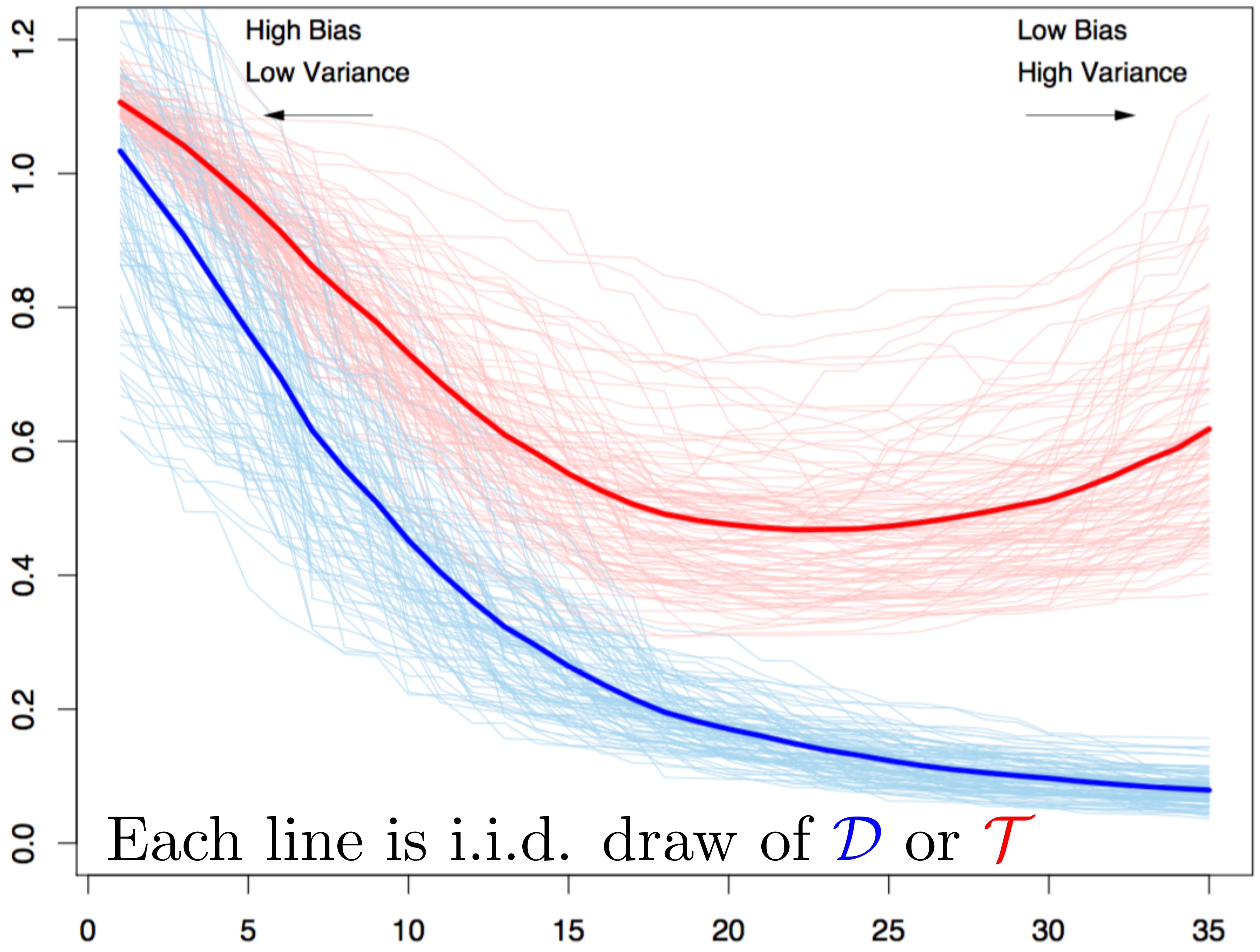

Complexity (k)

Plot from Hastie et al

TRAIN error:

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

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

TRUE error:

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

TEST error:

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

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

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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.

TRAIN error:

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TRUE error:

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TEST error:

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

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

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
- 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)