Generalized Linear Regression and Bias-Variance Tradeoffs

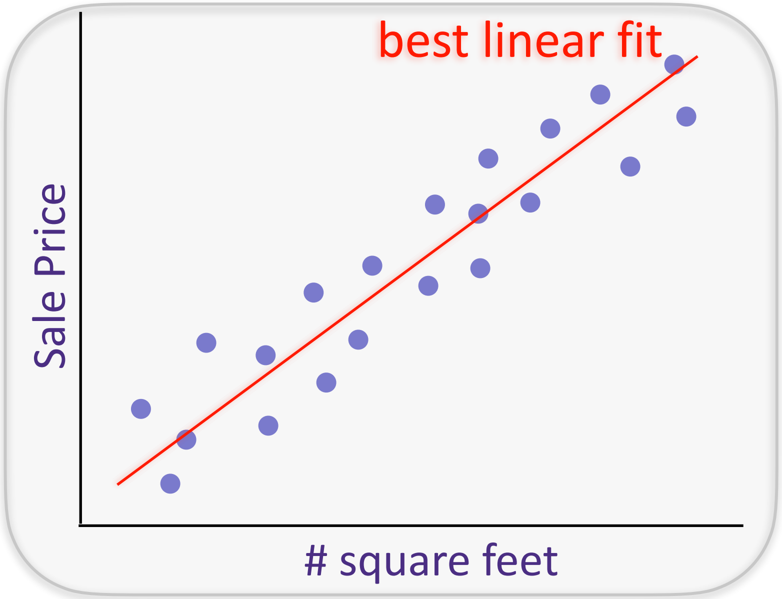
UNIVERSITY of WASHINGTON

The regression problem

Given past sales data on zillow.com, predict:

y* = House sale price *from

***x* = {# sq. ft., zip code, date of sale, etc.}**



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

Hypothesis: linear

$$y_i \approx x_i^T w$$

Loss: least squares

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

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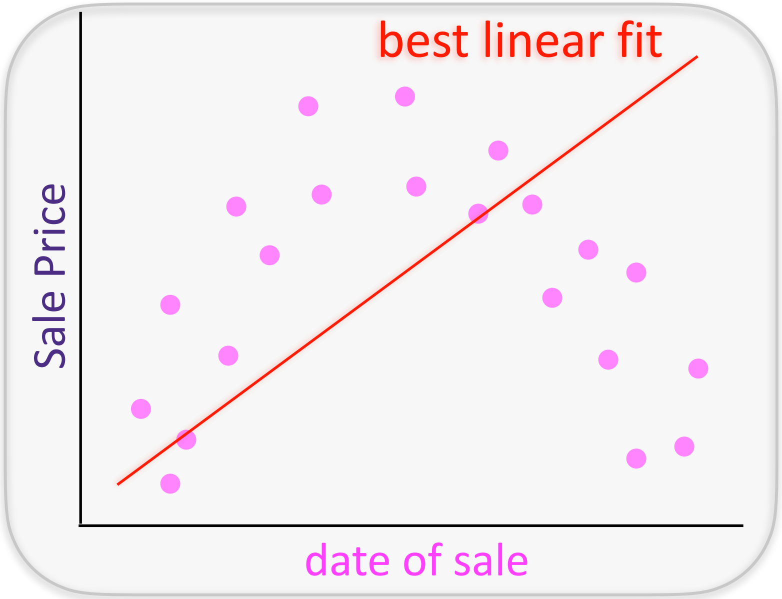

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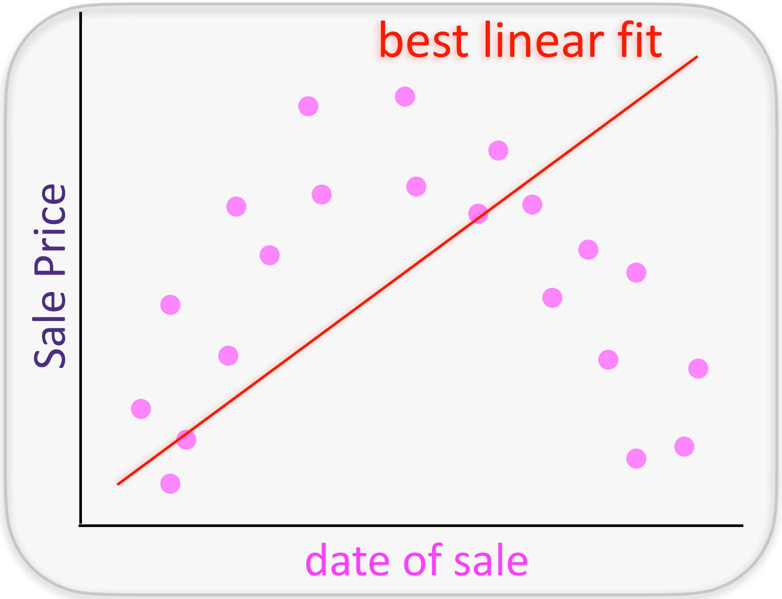

Best linear model of data of sale is a very poor fit!

Either because date of sale doesn't predict price well, or…

… because the relationship isn't linear.

Process

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

Quadratic Regression

Given past sales data on zillow.com, predict:

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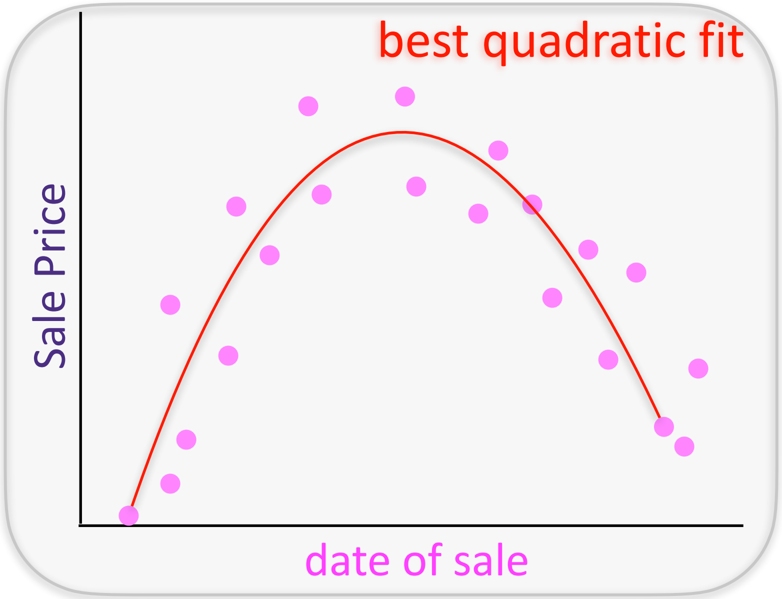

Training Data: $\{(x_i, y_i)\}_{i=1}^n$ $\quad x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$

$$y_i \approx \sum_{j=1}^d x_{i,j} w_{j,1} + x_{i,j}^2 w_{j,2}$$

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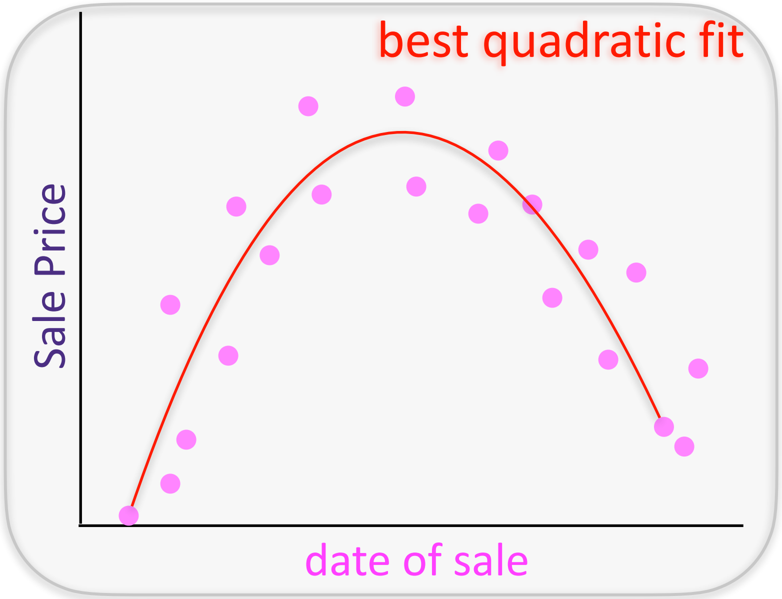

Training Data: $\{(x_i, y_i)\}_{i=1}^n$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

Hypothesis: quadratic

$$y_i \approx \sum_{j=1}^d x_{i,j} w_{j,1} + x_{i,j}^2 w_{j,2}$$

Polynomial regression

Given past sales data on zillow.com, predict:

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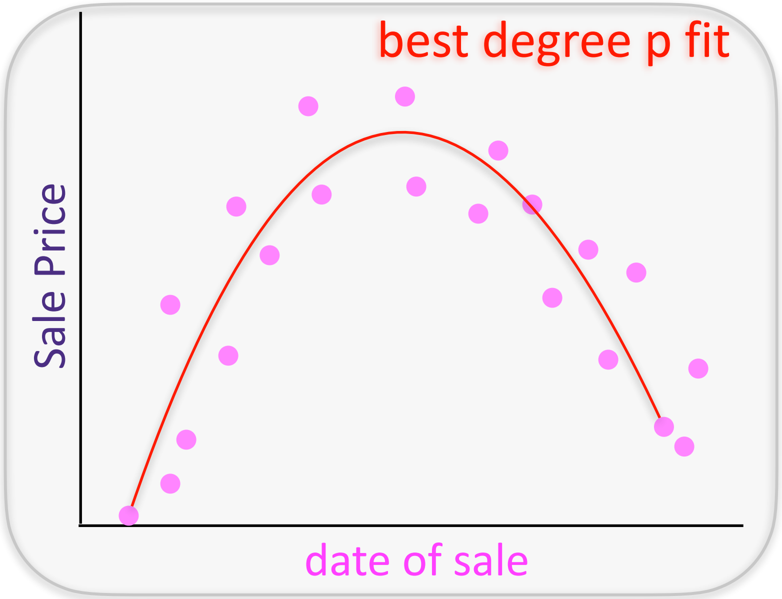

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$x_i \in \mathbb{R}^d$
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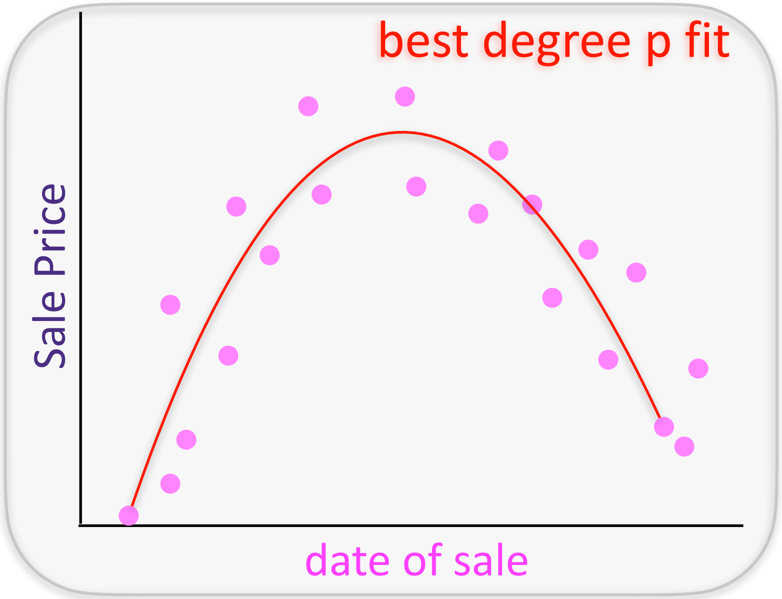

Training Data: $\{(x_i, y_i)\}_{i=1}^n$ $\quad x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$

Hypothesis:

degree p polynomial

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Generalized linear regression

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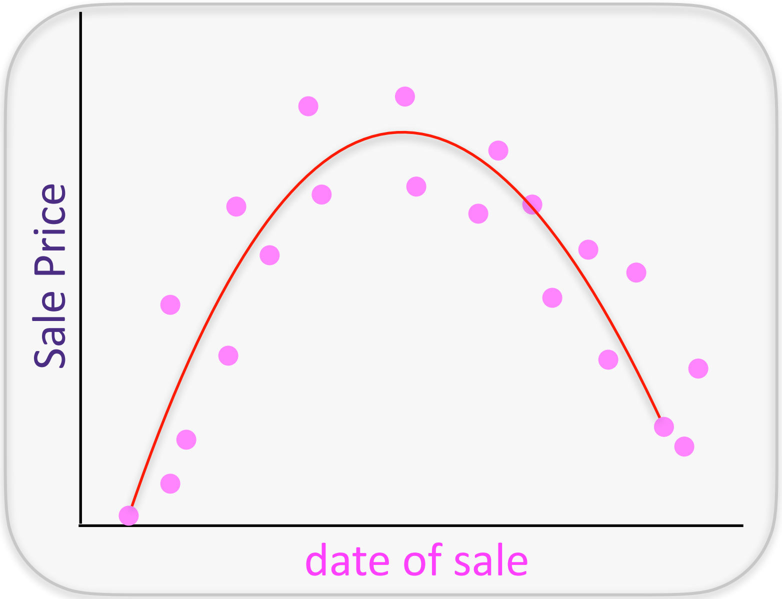

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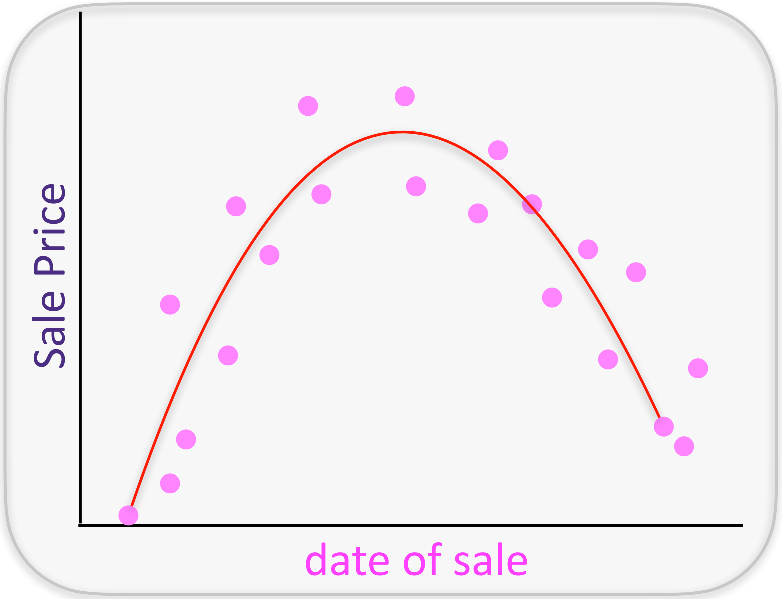

Training Data: $\{(x_i, y_i)\}_{i=1}^n$ $\quad x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$

Hypothesis:

generalized linear fn of x

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Loss: least squares

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

Transformed data:

$h : \mathbb{R}^d \to \mathbb{R}^p$ maps original features to a rich, possibly high-dimensional space

in d=1: $$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ \vdots \\ h_p(x) \end{bmatrix} = \begin{bmatrix} x \\ x^2 \\ \vdots \\ x^p \end{bmatrix}$$

for d>1, generate

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$$\{u_j\}_{j=1}^p \subset \mathbb{R}^d$$

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for d>1, generate

$$\{u_j\}_{j=1}^p \subset \mathbb{R}^d$$

$$h_j(x) = \frac{1}{1 + \exp(u_j^T x)}$$

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

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$$h_j(x) = (u_j^T x)^2$$

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$$h_j(x) = \cos(u_j^T x)$$

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

Hypothesis: linear in h

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

The regression problem

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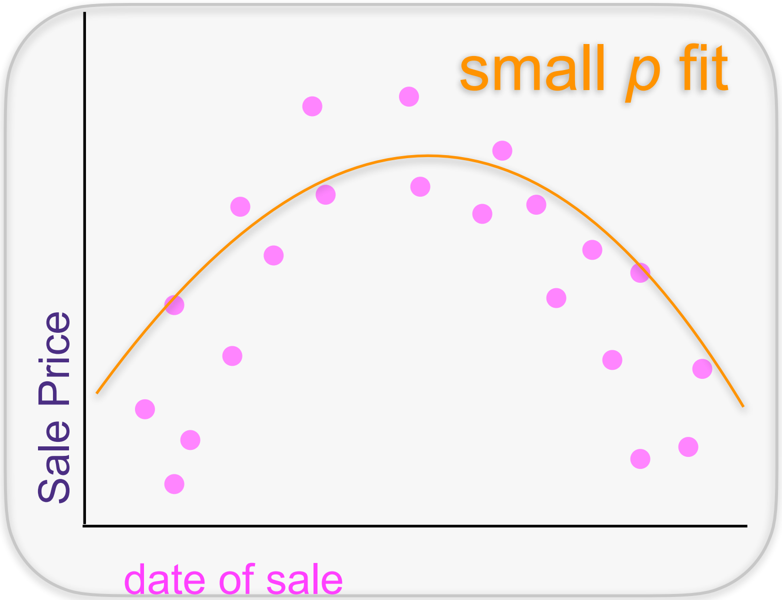

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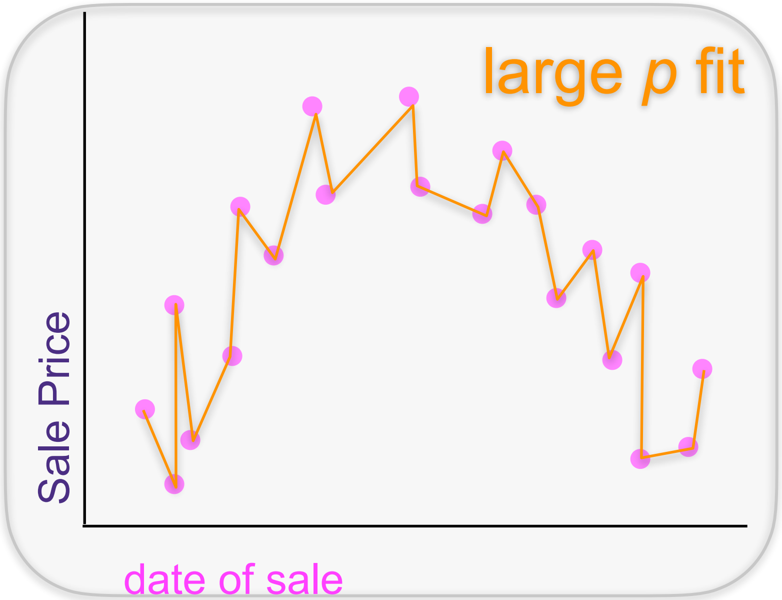

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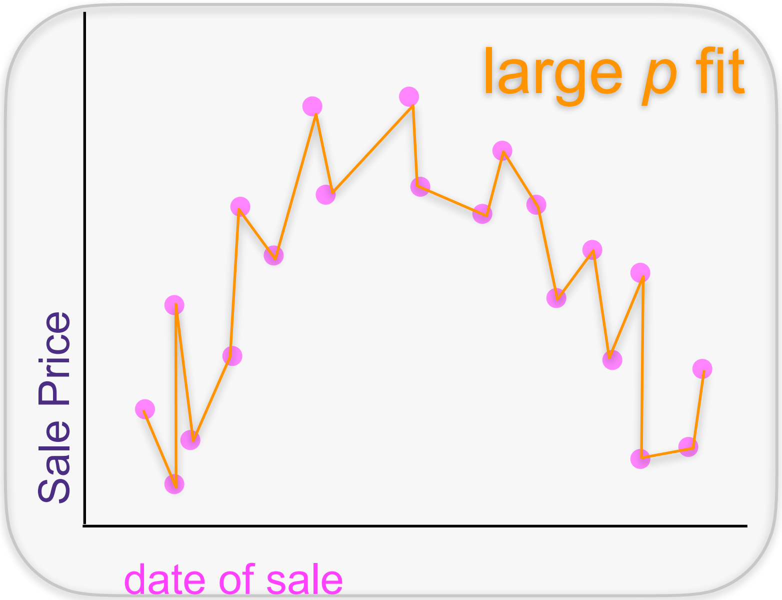
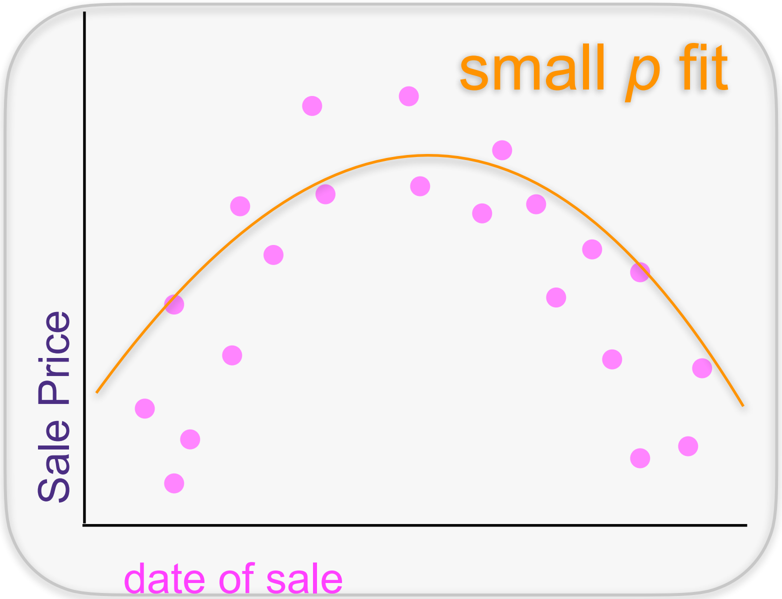
Which is better?

A: large p



B: small p



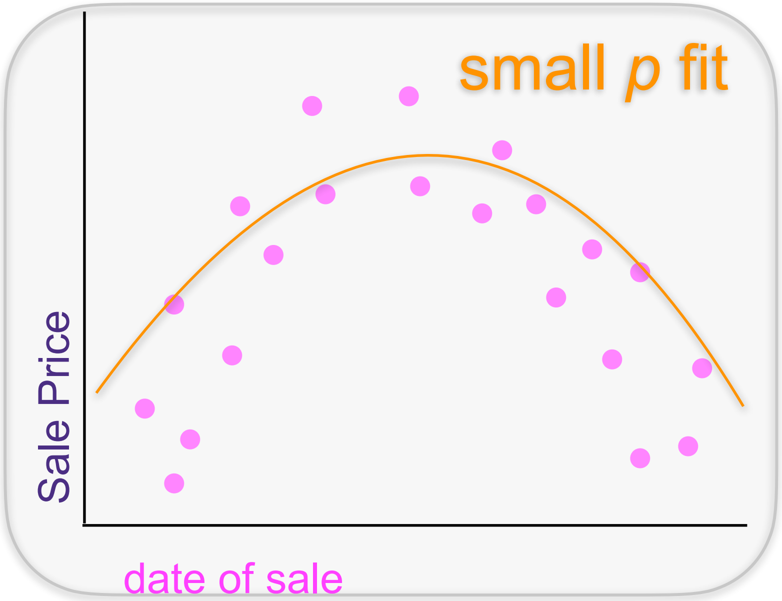
Bias-Variance Tradeoff

What is our goal, anyway?

What do these two graphs imply?

A: large p

B: small p



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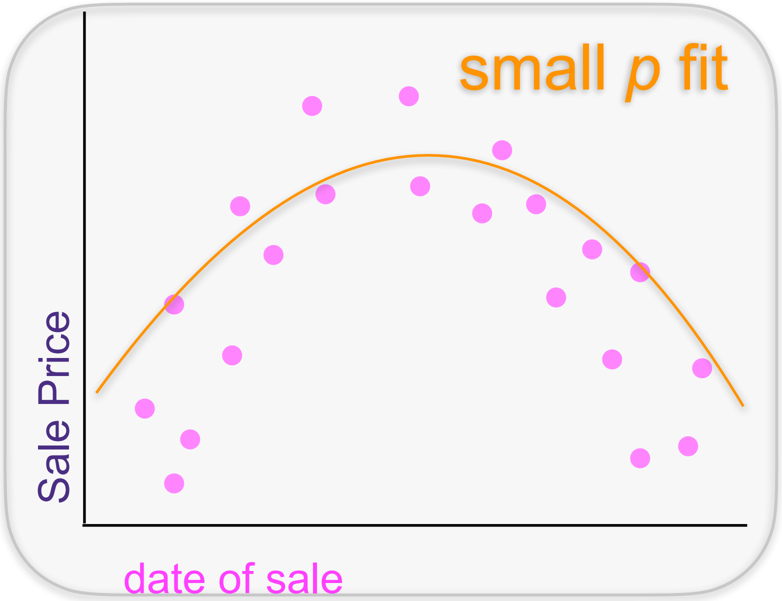

Least squares loss is 0 on training data

What do these two graphs imply?

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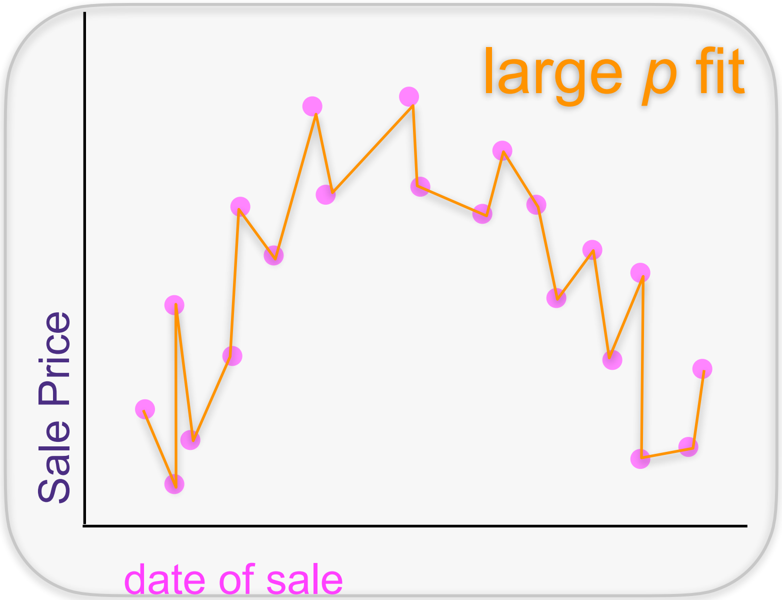
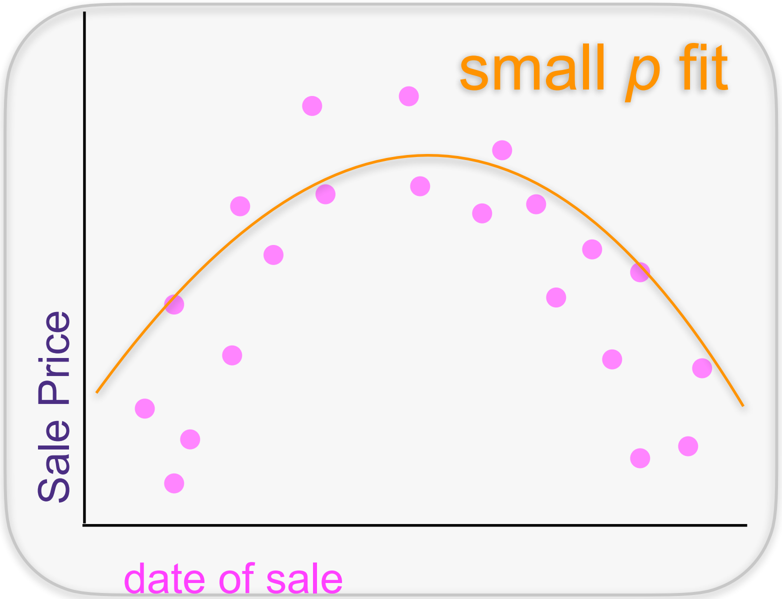


Least squares loss is 0 on training data

B: small p

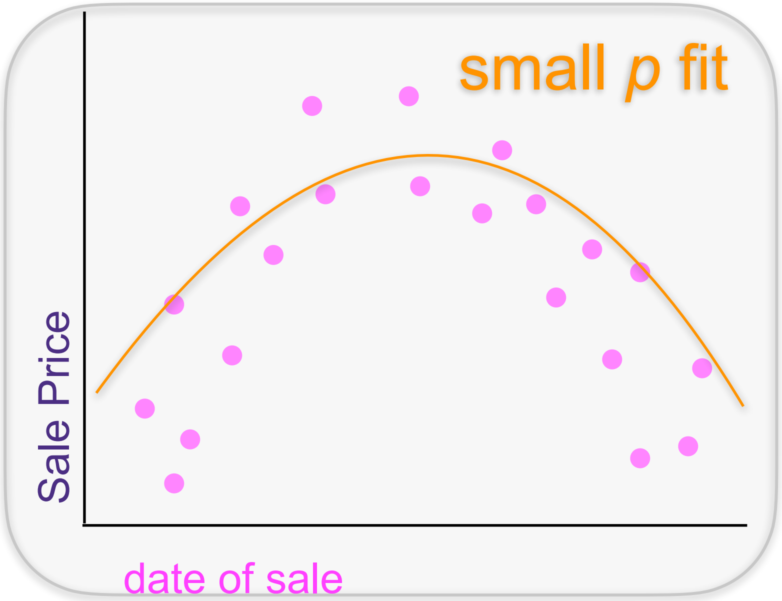


Least squares loss is > 0 on training data

What do these two graphs imply?

A: large p

B: small p



Least squares loss is 0 on training data

Least squares loss is > 0 on training data

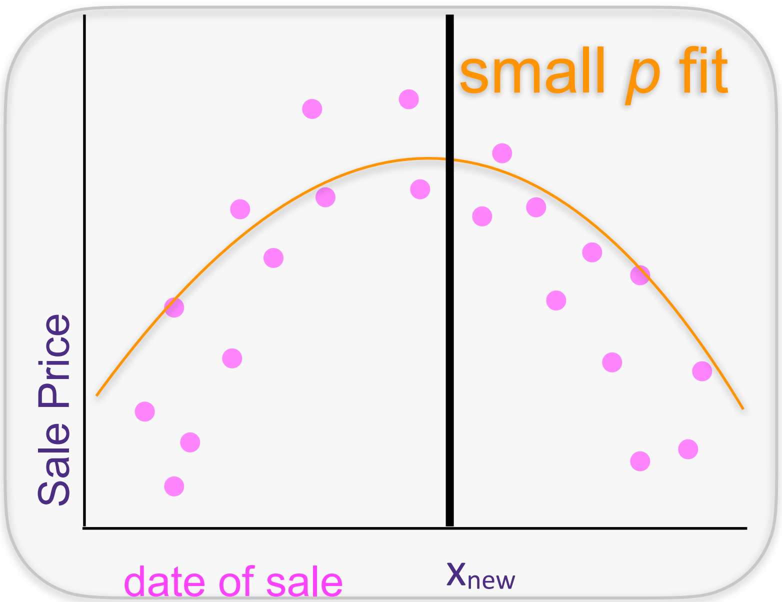
Least squares **training error** is lower on A than B

Predicting sale price for a new house: A vs B

Our goal is to predict prices for new houses

A: large p

B: small p



that "look like" the houses in our training data

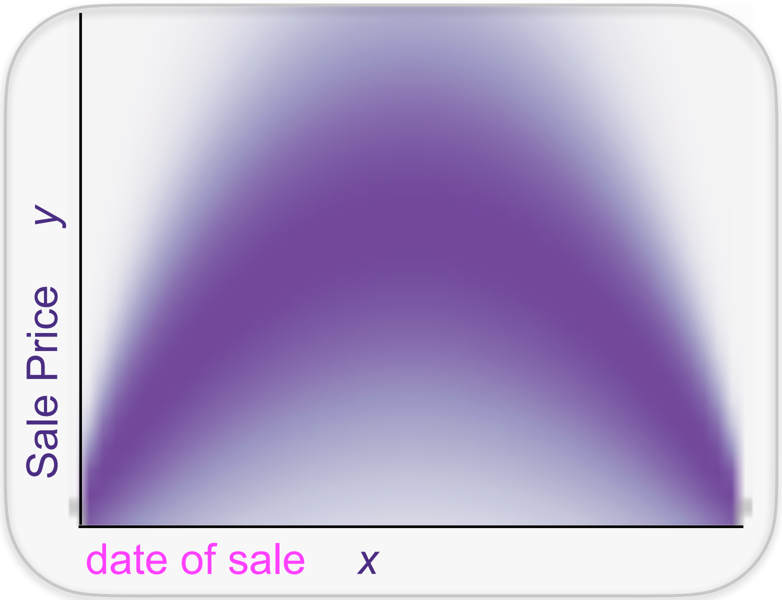
What do we mean by “look like”?

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

This will work best if our training data
came from the same distribution…

What do we mean by “look like”?

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



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Statistical Learning

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

Goal: Predict Y given X

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Find a function η that minimizes

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

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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

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

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

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

Statistical Learning

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

Goal: Predict Y given X

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

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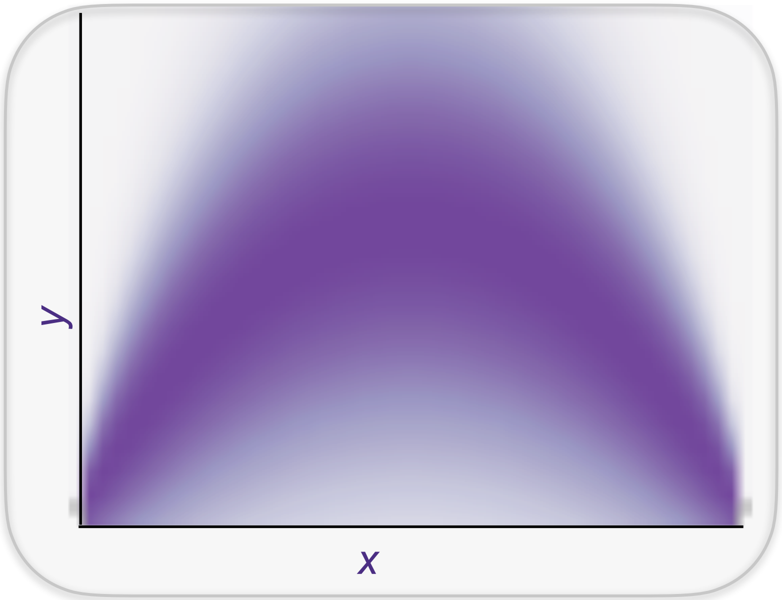

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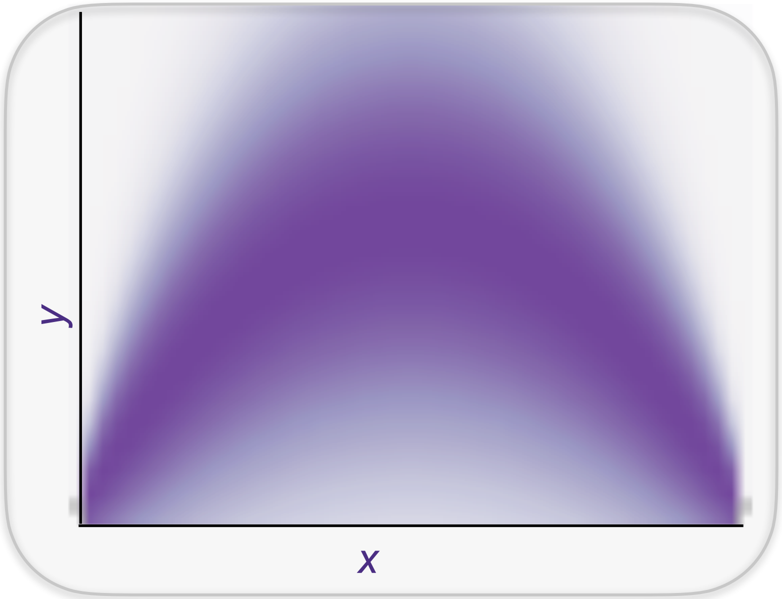

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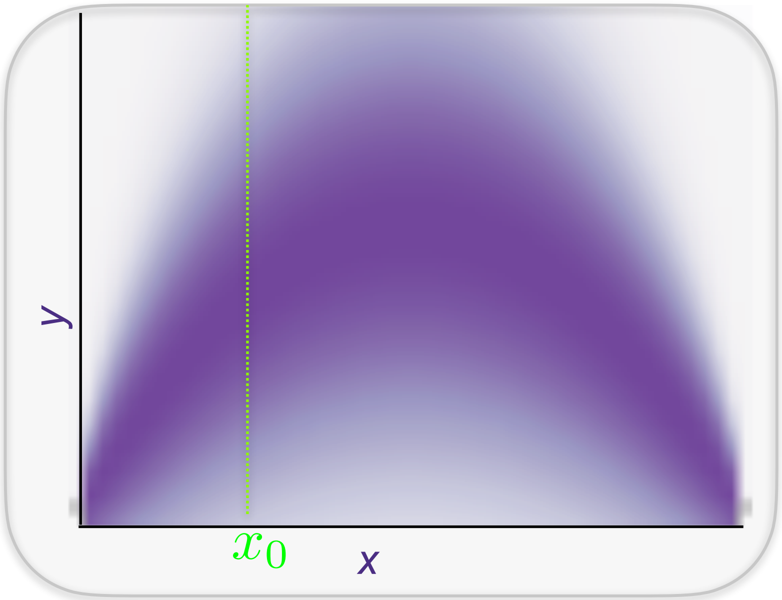

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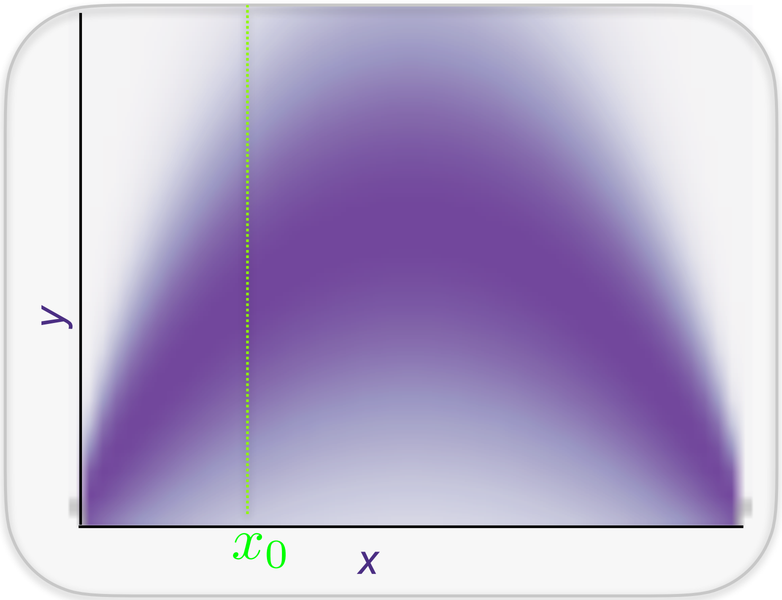
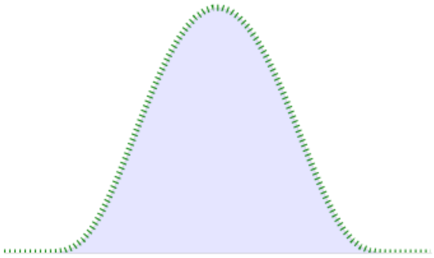


$$P_{XY}(Y = y | X = x_0)$$



Statistical Learning

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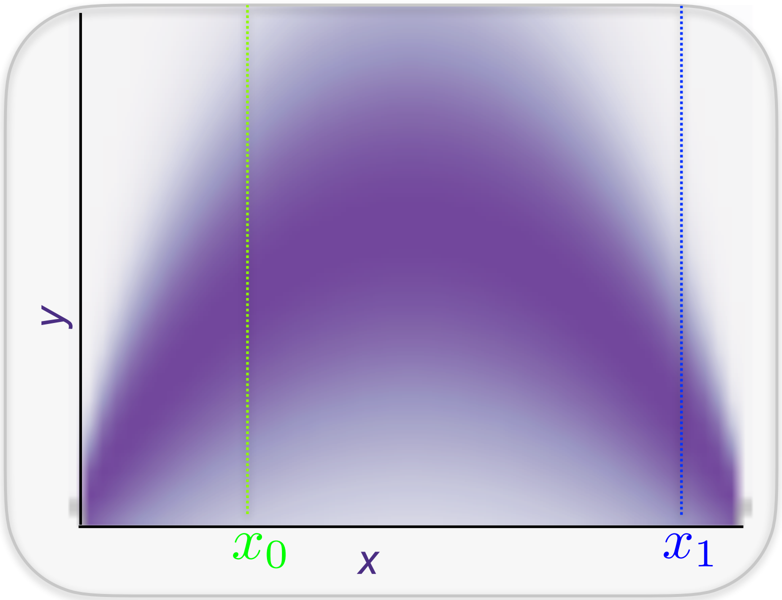
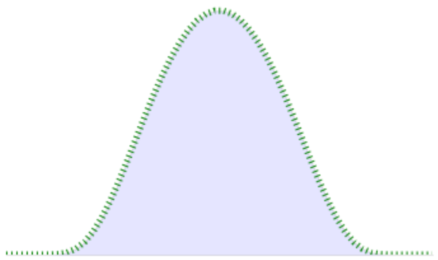


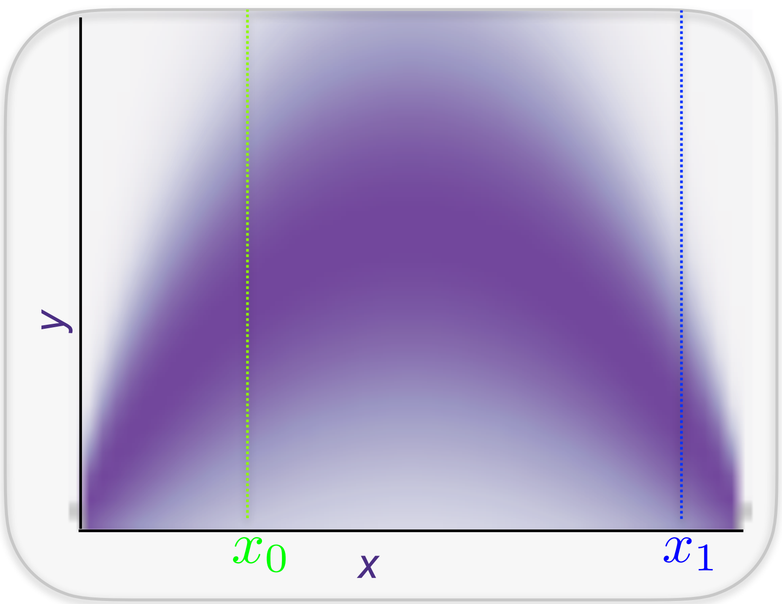
$P_{XY}(Y = y | X = x_0)$



Statistical Learning

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

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



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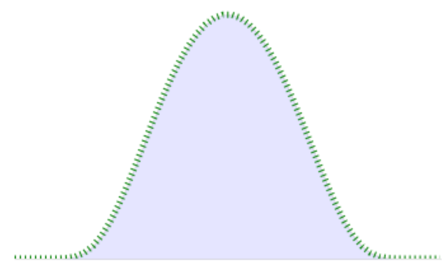
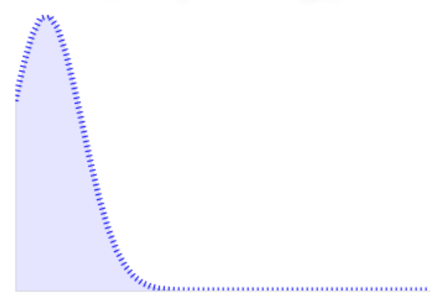


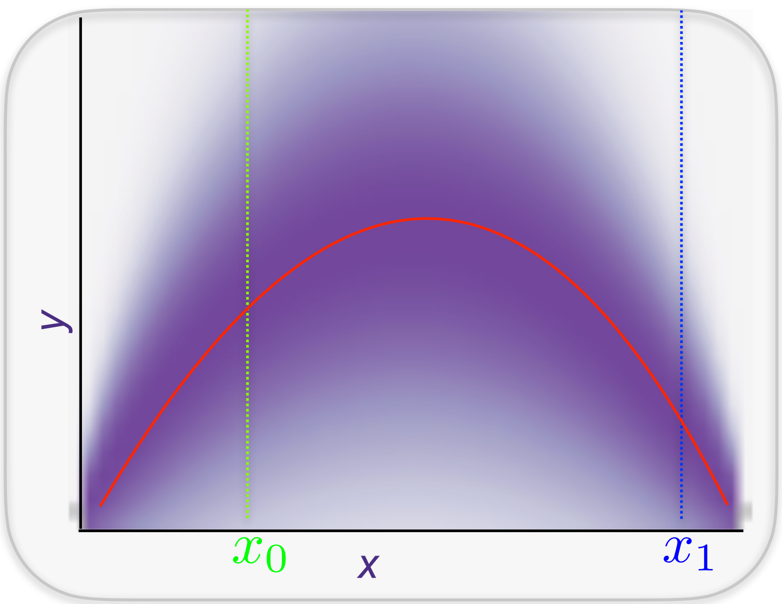
$P_{XY}(Y = y | X = x_1)$



Statistical Learning

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

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



Ideally, we want to find:

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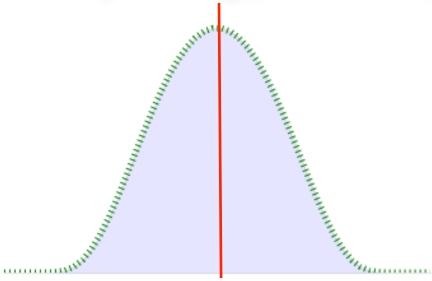
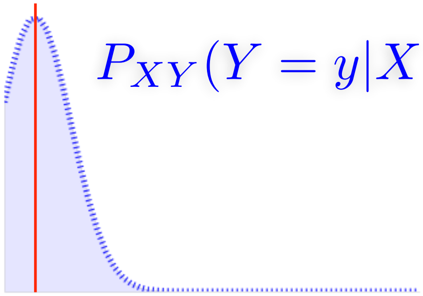
$P_{XY}(Y=y|X=x_0)$





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Statistical Learning

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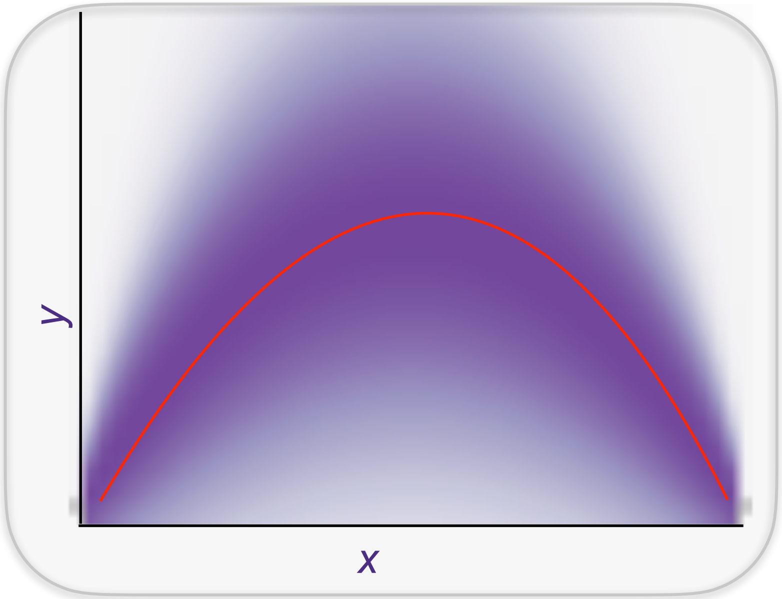

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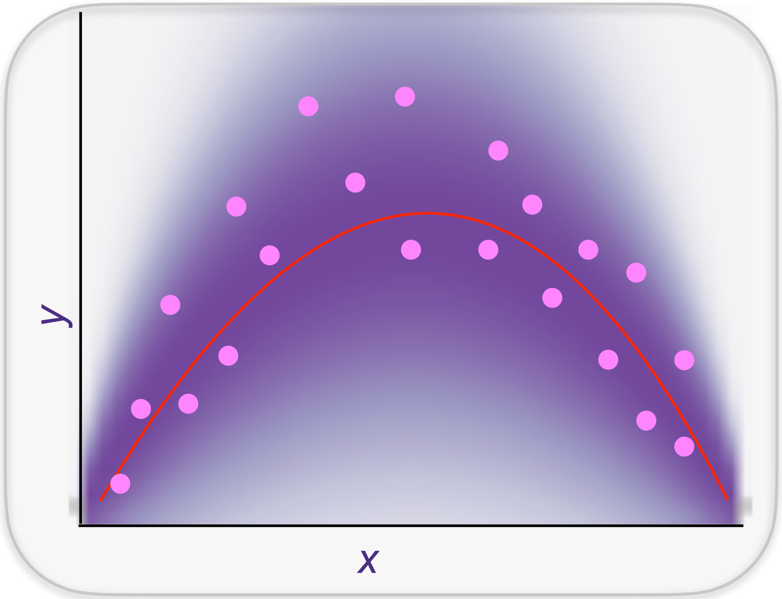

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But we only have samples:

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

Statistical Learning

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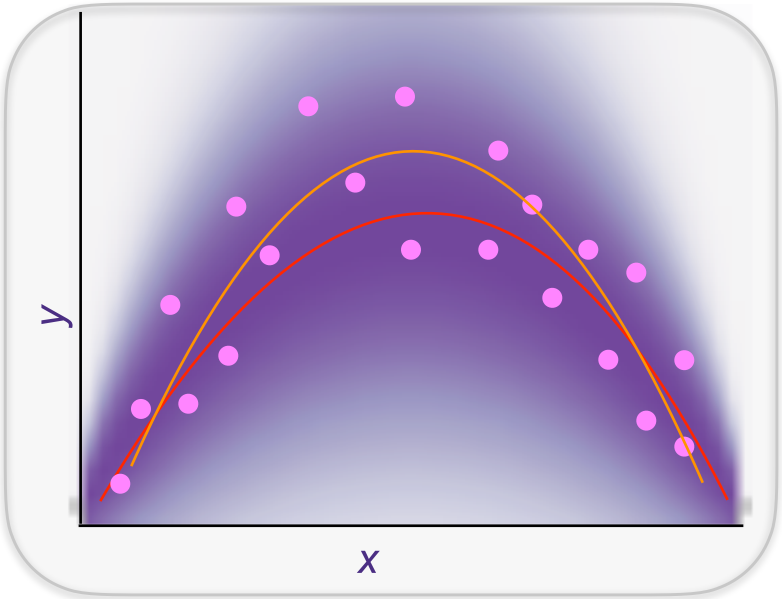

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Statistical Learning

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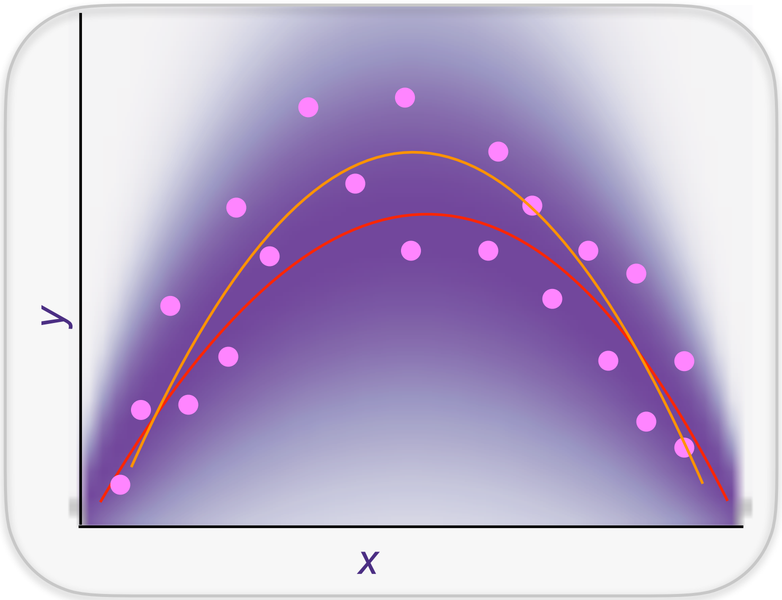

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We care about future predictions: $\mathbb{E}_{XY}[(Y - \widehat{f}(X))^2]$

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 $\widehat{f}$

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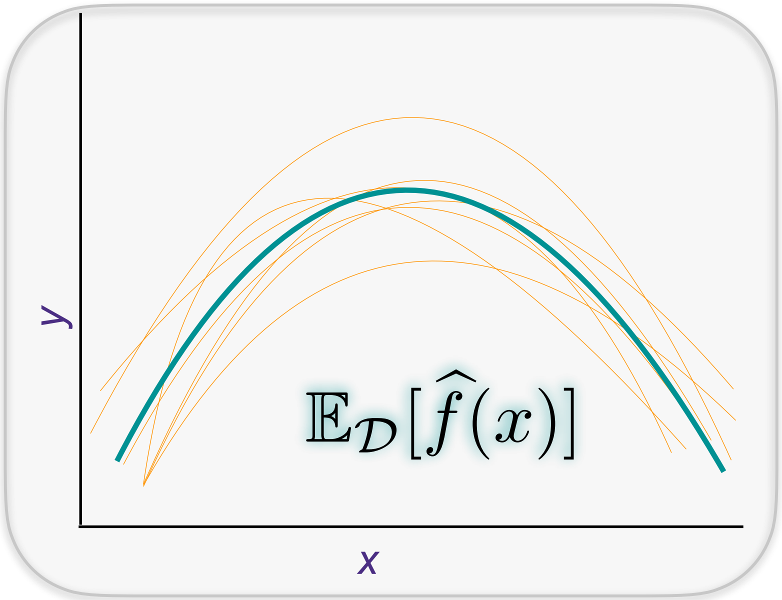

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Bias-Variance Tradeoff

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

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

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

Bias-Variance Tradeoff

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

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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

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

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

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

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

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

Bias-Variance Tradeoff

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$$\begin{aligned}
\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)) \\
&\quad + (\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2] \\
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Bias-Variance Tradeoff

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bias squared

Bias-Variance Tradeoff

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bias squared   variance

Bias-Variance Tradeoff

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

irreducible error

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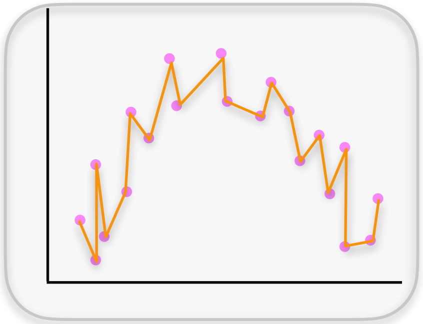
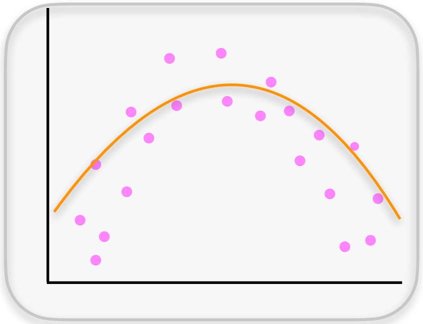
bias squared





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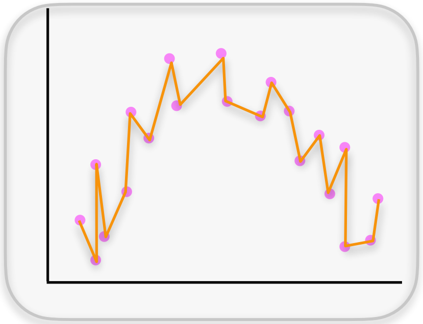
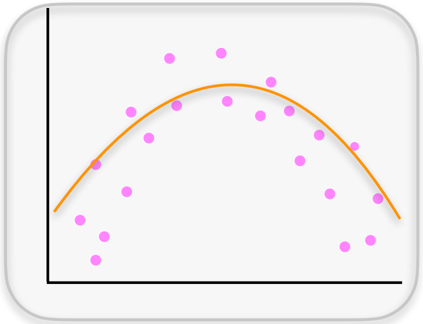
bias squared **variance**





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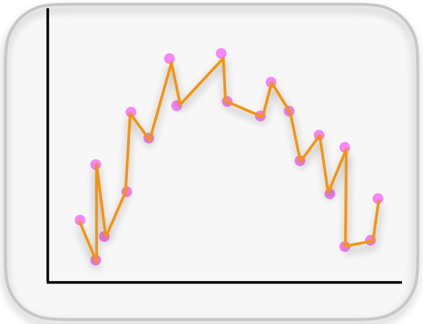

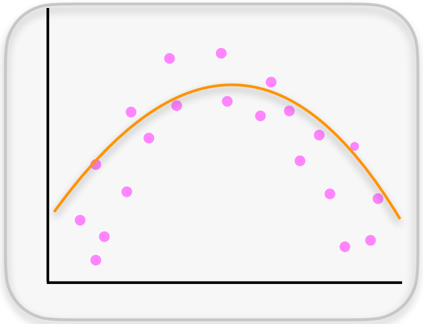

If we re-drew our data, what the LS training error estimator look like for generalized linear functions in small p/large p dimensions?

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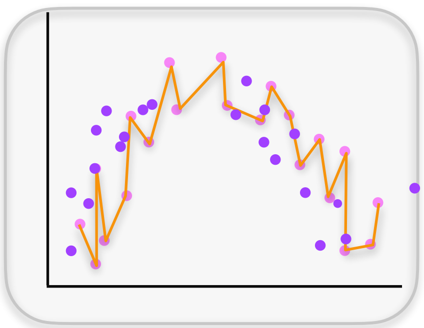

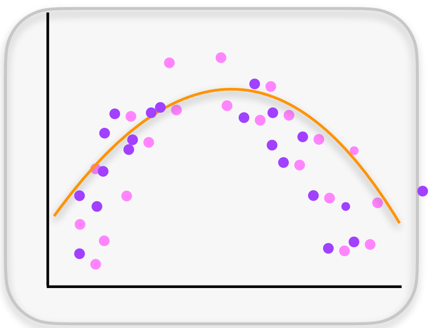

If we re-drew our data, what the LS training error estimator look like for generalized linear functions in small p/large p dimensions?

Bias-Variance Tradeoff

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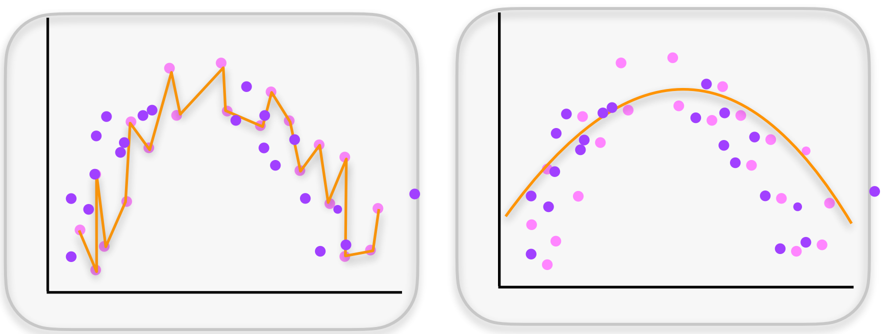

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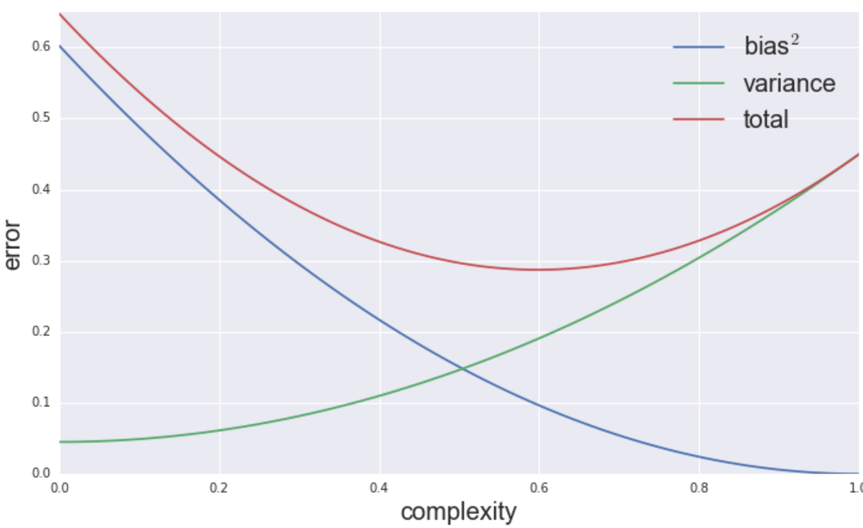

Example: Linear LS

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

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

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

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

$$\widehat{f}_{\mathcal{D}}(x) =$$

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

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

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

irreducible error

Example: Linear LS

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

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

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

irreducible error

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irreducible error

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

bias squared

Example: Linear LS: compute bias

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

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bias squared

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

variance

Example: Linear LS

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

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variance

Example: Linear LS

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variance

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$$= \sigma^2 x^T(\mathbf{X}^T\mathbf{X})^{-1}x$$

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$$= \sigma^2 x^T(\mathbf{X}^T\mathbf{X})^{-1}x$$

$$= \sigma^2 \text{Trace}((\mathbf{X}^T\mathbf{X})^{-1}xx^T)$$

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$$\mathbb{E}_{X=x}\Big[$$

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

irreducible error

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

bias squared

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

variance