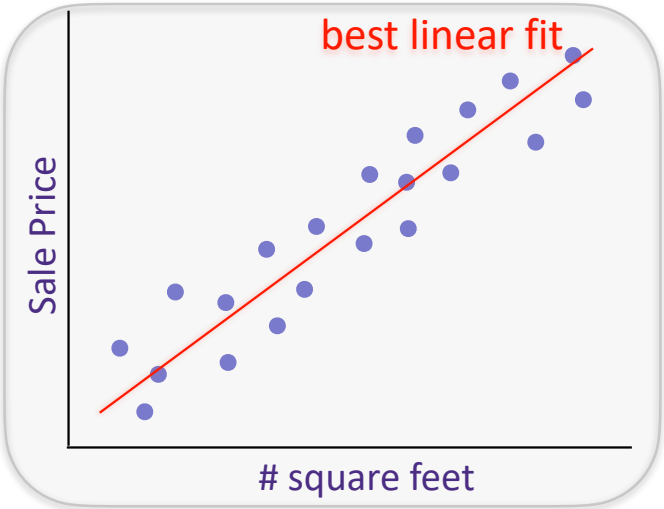
Generalized Linear Regression and Bias-Variance Tradeoffs

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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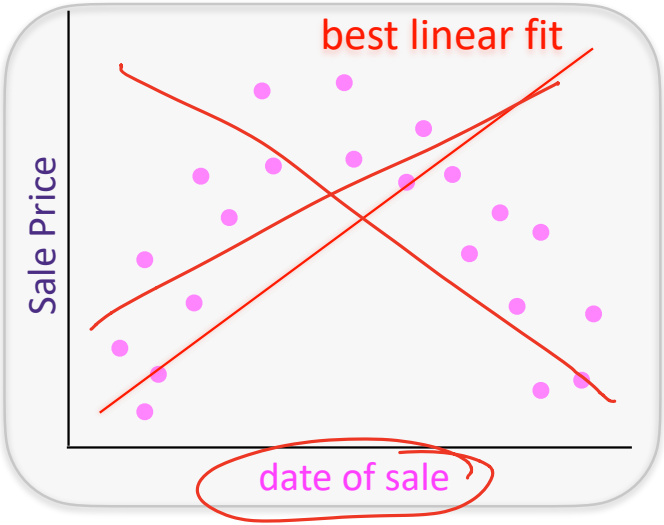

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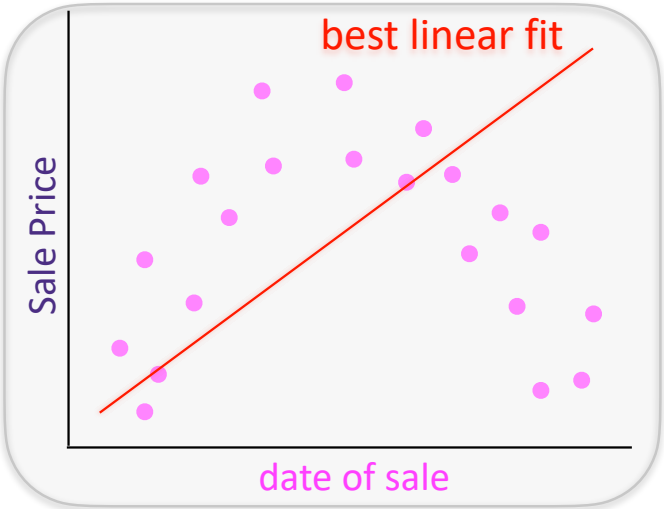

Best linear model of data of sale is a very poor fit!

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

… because the relationship isn't linear.

Process

Decide on a **model** → Quadratic fn, polynomial of degree p/...

Find the function which fits the data best

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

Use function to make prediction on new examples

Quadratic Regression

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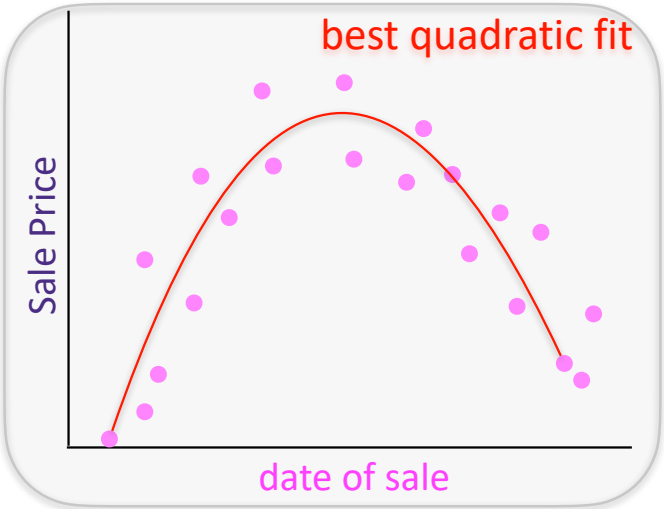

Training Data: $\{(x_i, y_i)\}_{i=1}^{n}$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

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

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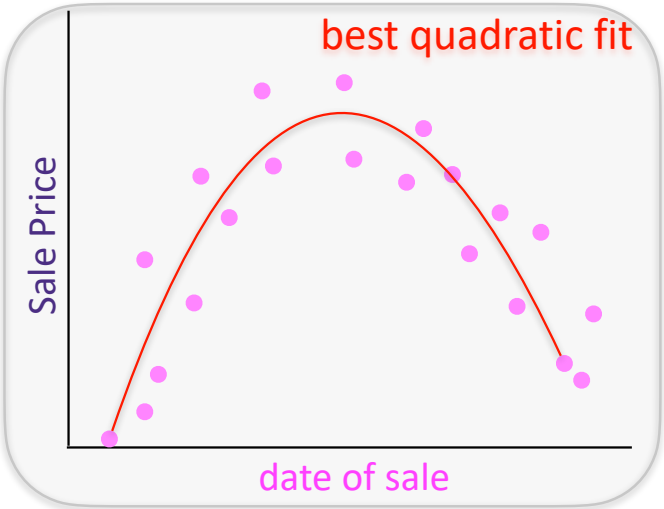

Training Data: $\{(x_i, y_i)\}_{i=1}^{n}$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

Hypothesis: quadratic (Model)

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

Polynomial regression

Given past sales data on zillow.com, predict:

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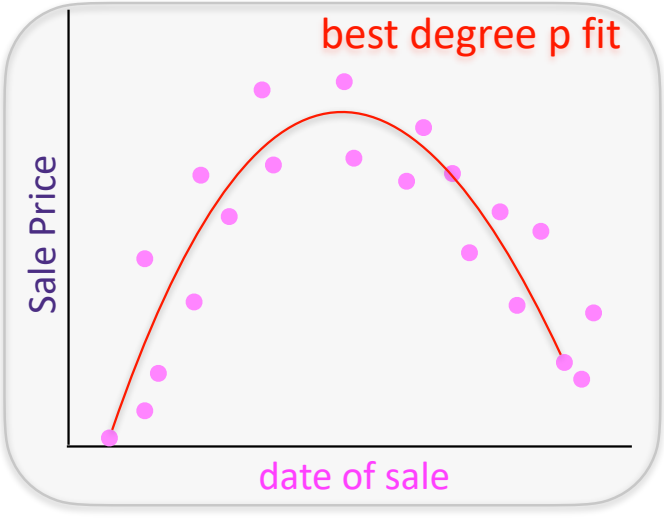

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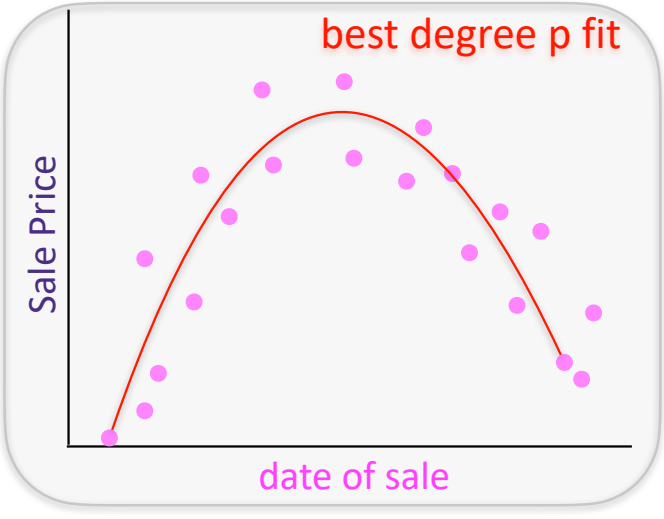

Training Data: $\{(x_i, y_i)\}_{i=1}^{n}$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

Hypothesis: / Model

degree p polynomial

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

Generalized linear regression

Given past sales data on zillow.com, predict:

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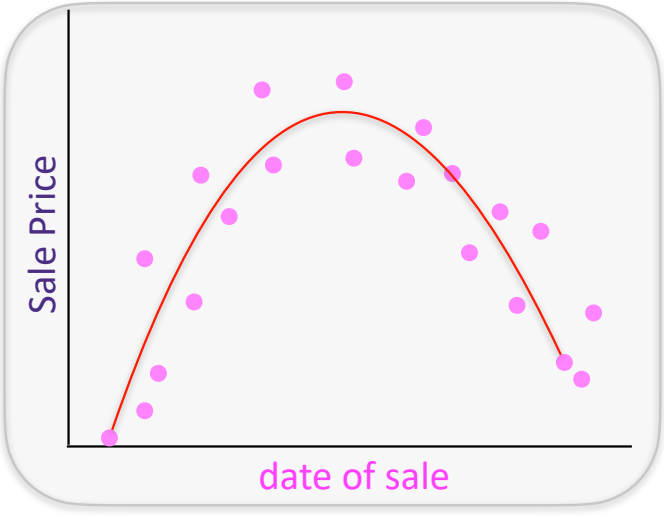

Training Data: $\{(x_i, y_i)\}_{i=1}^{n}$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

$$y_i \approx \sum_{\ell=1}^{p} h_\ell(x_i)^T w_\ell$$

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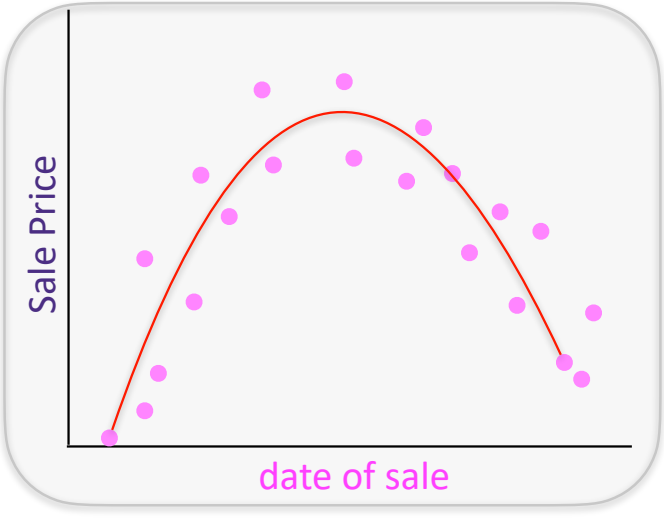

Training Data: $\{(x_i, y_i)\}_{i=1}^{n}$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$

Hypothesis:

generalized linear fn of x

$$y_i \approx \sum_{\ell=1}^{p} h_\ell(x_i)^T w_\ell$$

x_i: feature vector for house i

Process

Decide on a **model** → 

Find the function which fits the data best

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

Use function to make prediction on new examples

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

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

The regression problem

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

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

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

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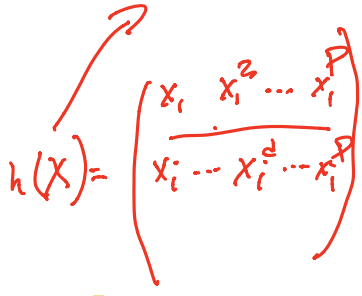

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$$h_j(x) = \frac{1}{1 + \exp(u_j^T x)}$$

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

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

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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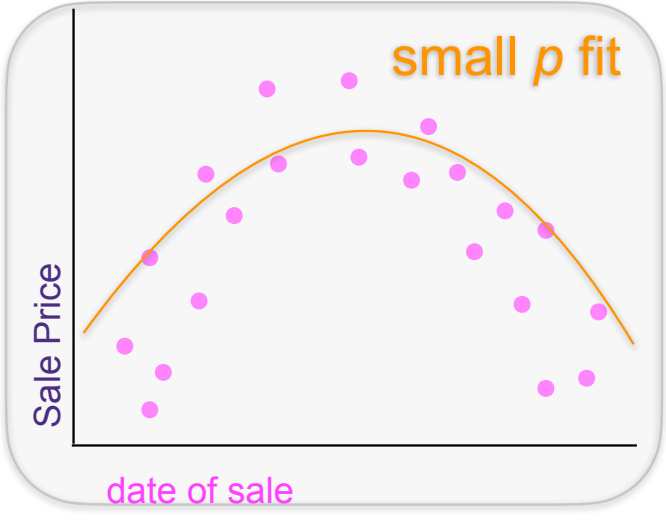

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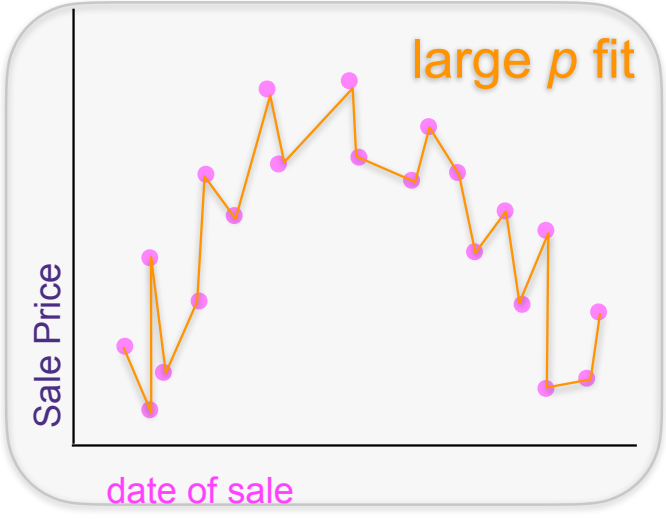

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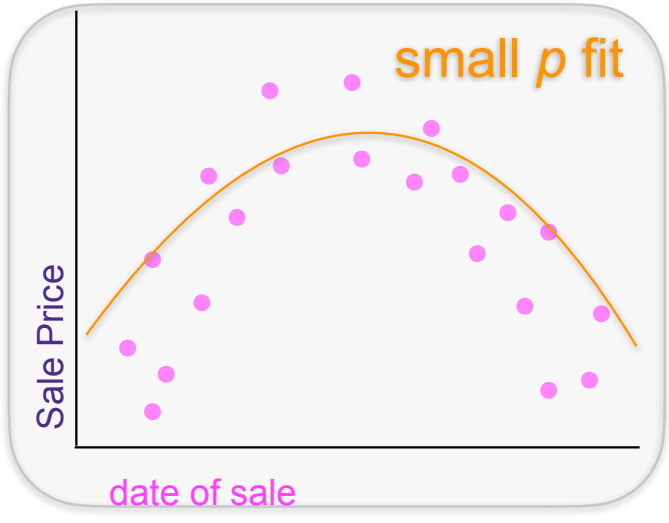
Which is better?

A: large p

B: small p



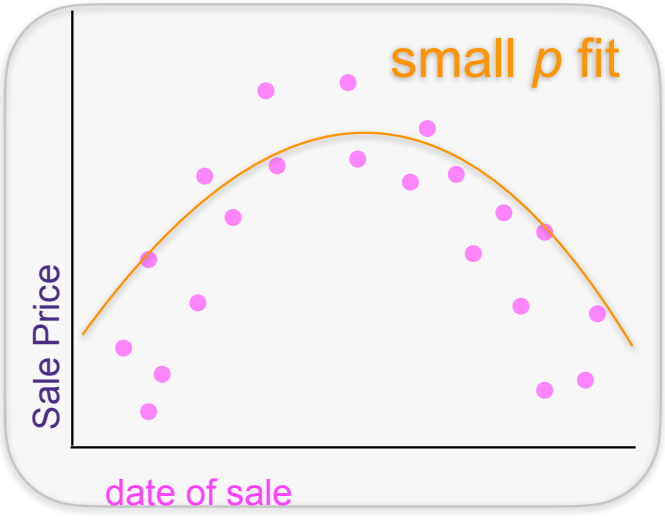
Bias-Variance Tradeoff

What is our goal, anyway?

What do these two graphs imply?

A: large p

B: small p



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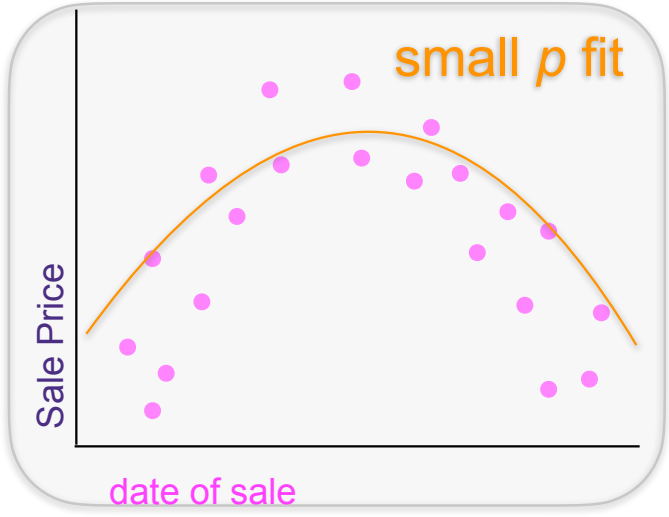


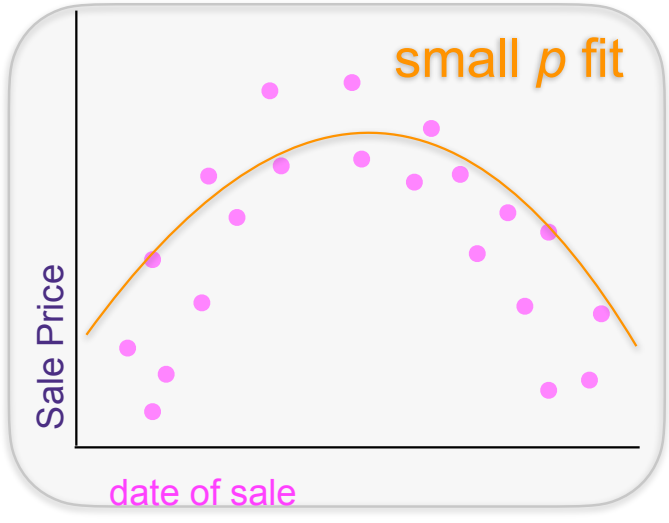
Least squares loss is 0 on training data

What do these two graphs imply?

A: large p

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?

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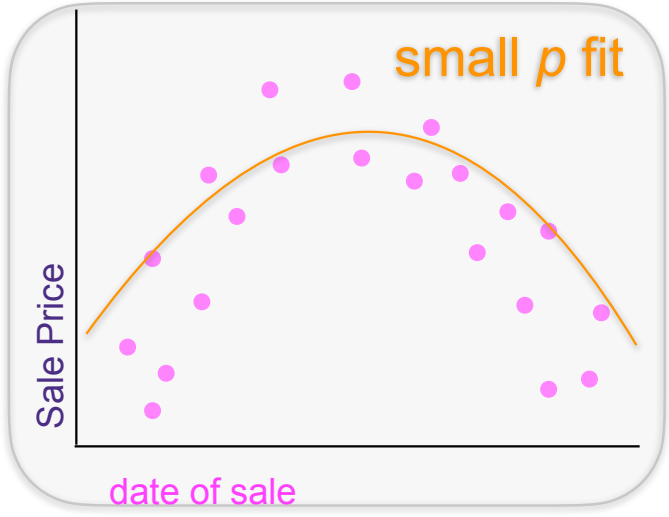
B: small p



Least squares loss is 0 on training data

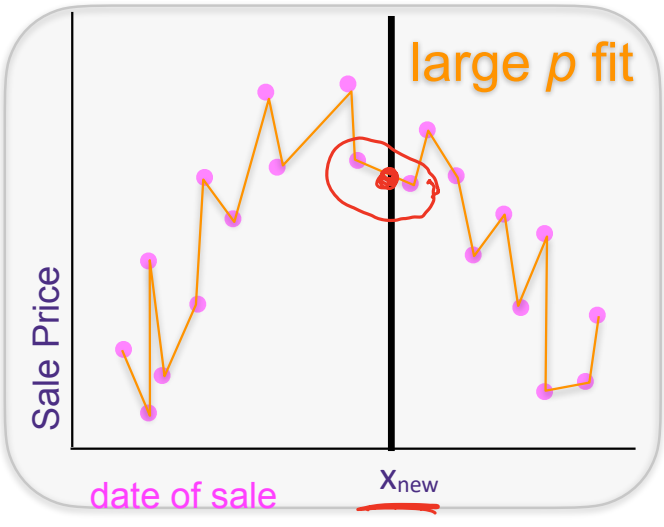
Least squares loss is > 0 on training data

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

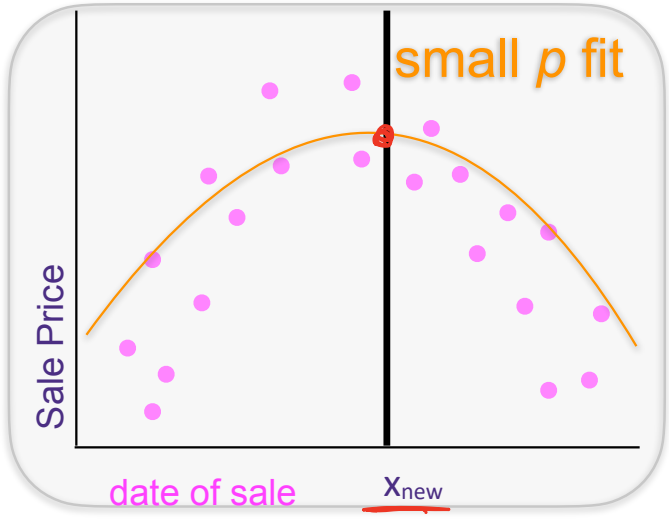
Predicting sale price for a new house: A vs B

Our goal is to predict prices for new houses

A: large p



B: small p



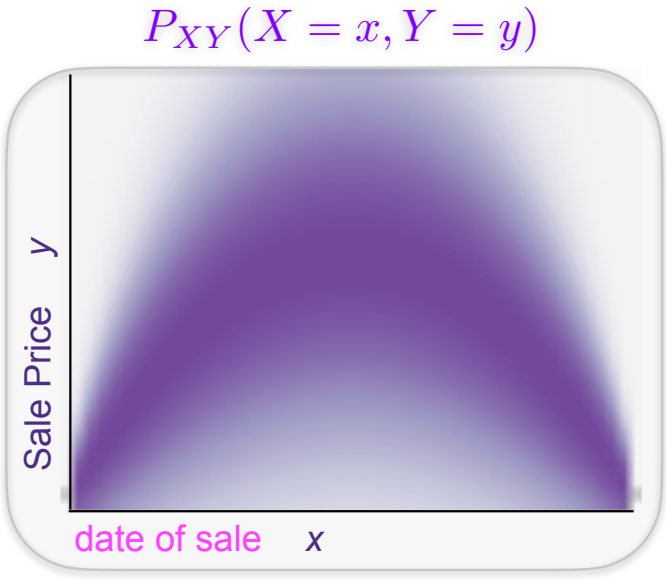
that "look like" the houses in our training data

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”?



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Statistical Learning

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

Goal: Predict Y given X

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

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Find a function η that minimizes our Loss

Statistical Learning

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

Goal: Predict Y given X

Find a function η that minimizes

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

(Least squares)

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

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

$Y \in [0, 1]$

Goal: Predict Y given X

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

$$\eta(x) = \arg\min_{c \in [0,1]} \mathbb{E}_{Y|X}[(Y - c)^2 | X = x] = \mathbb{E}_{Y|X}[Y | X = x]$$

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

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

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

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Statistical Learning

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Goal: Predict Y given X

Find a function η that minimizes

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

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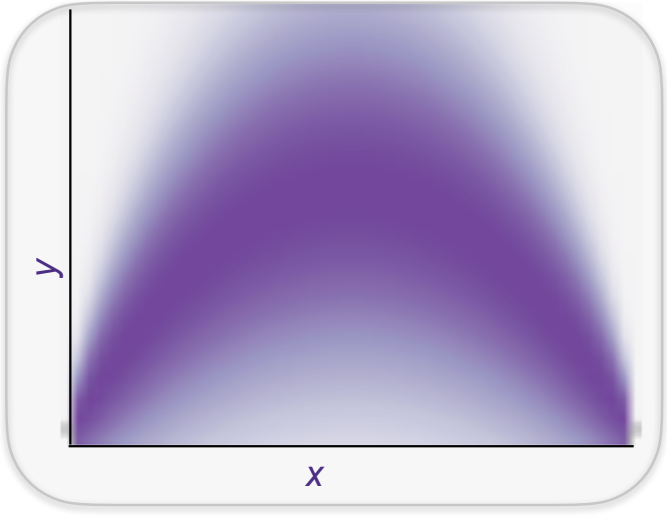
Statistical Learning

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

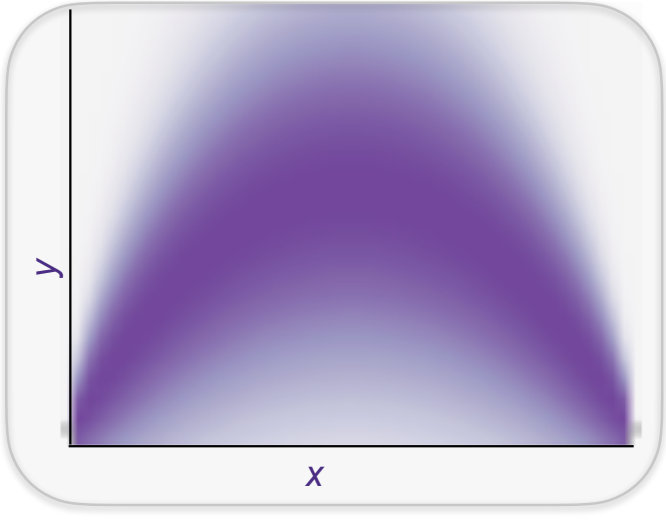
$P_{XY}(X = x, Y = y)$



Statistical Learning

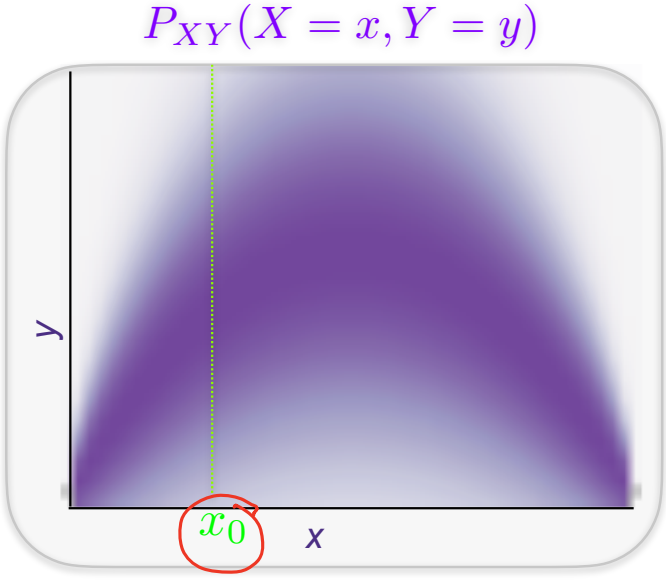
$$\mathbb{E}_{XY}[(Y - \eta(X))^2]$$

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



Statistical Learning

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



Statistical Learning

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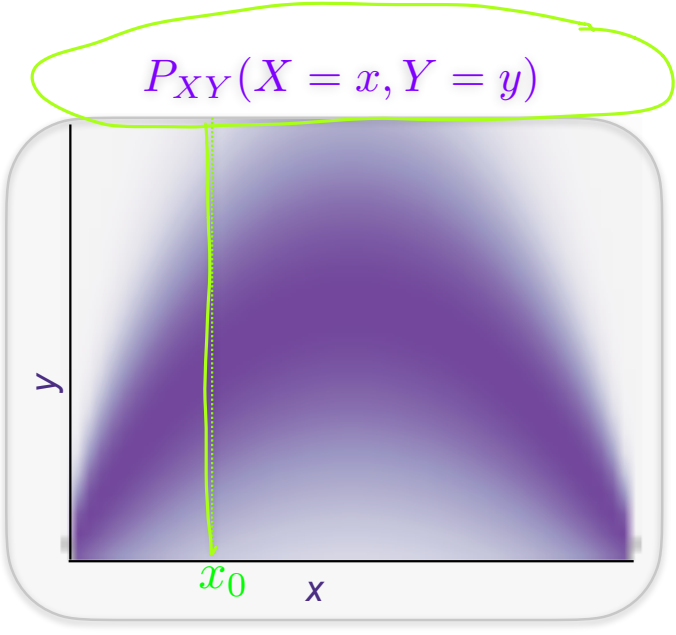
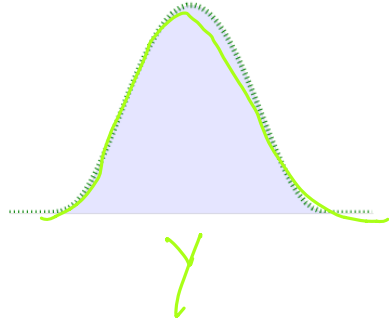


$$P_{XY}(Y = y|X = x_0)$$



Statistical Learning

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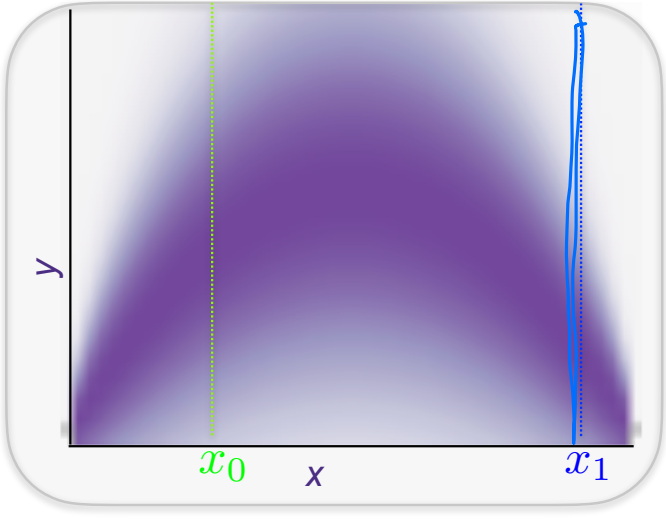

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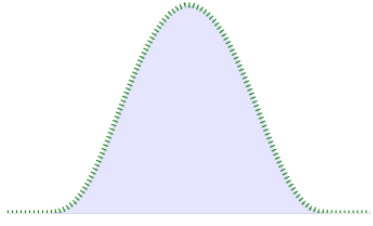

Statistical Learning

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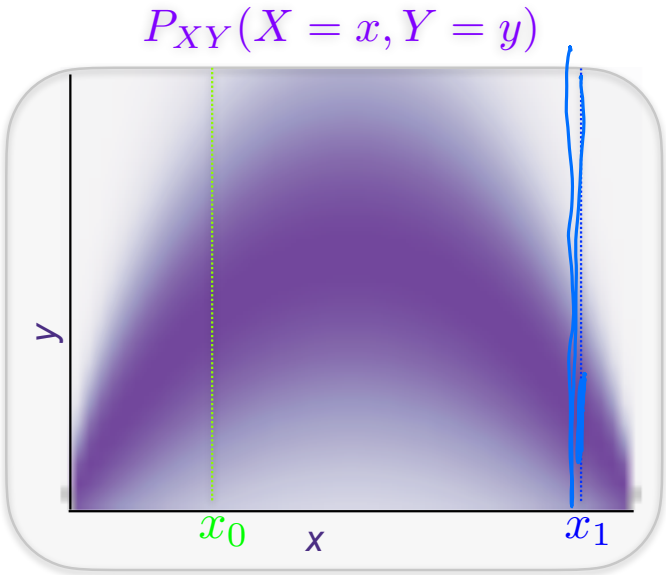

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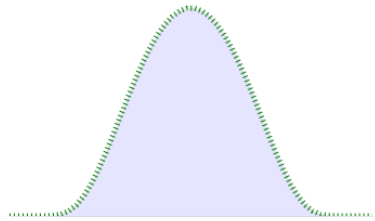
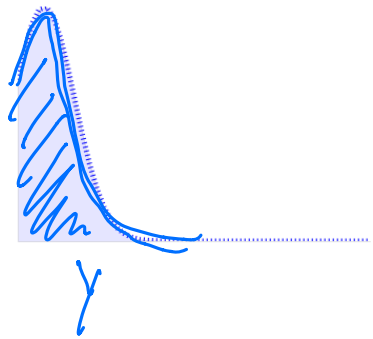
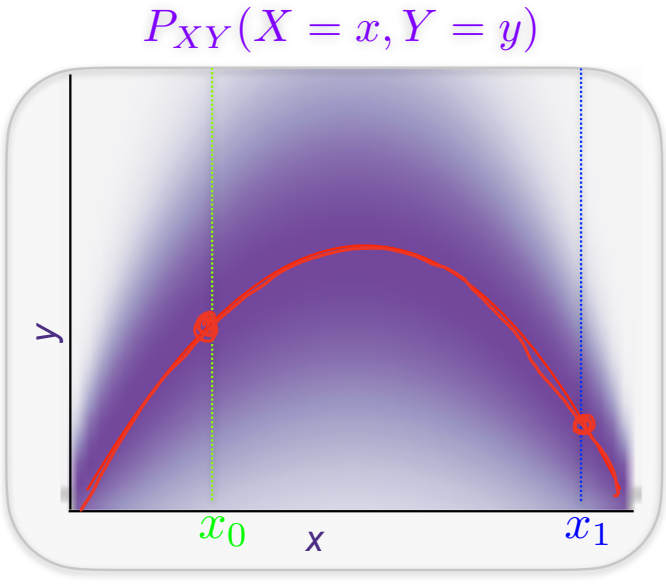


$P_{XY}(Y = y|X = x_1)$



Statistical Learning

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



Ideally, we want to find:

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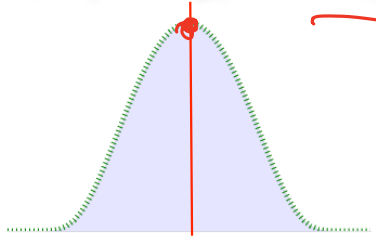
$P_{XY}(Y = y|X = x_0)$



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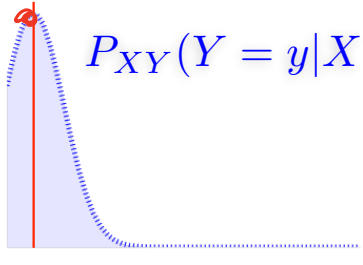
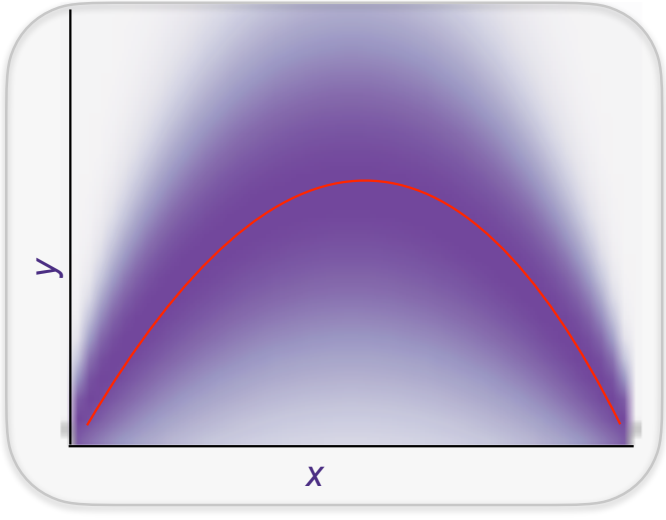


Statistical Learning

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



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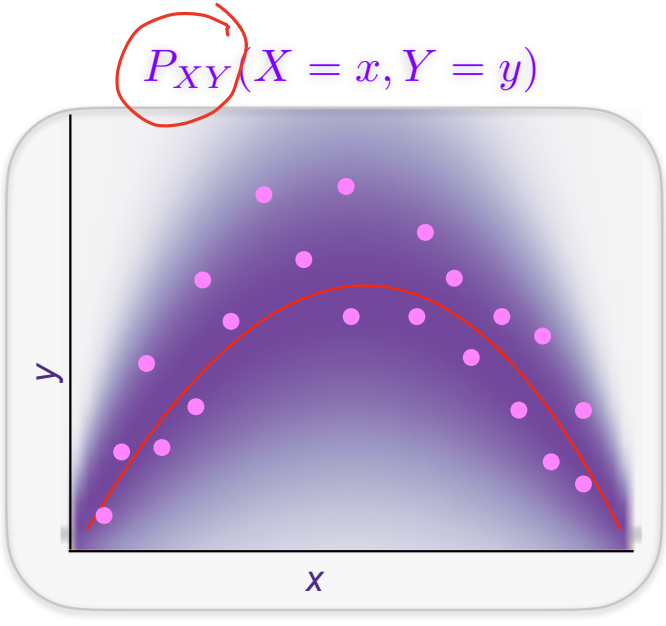
Statistical Learning



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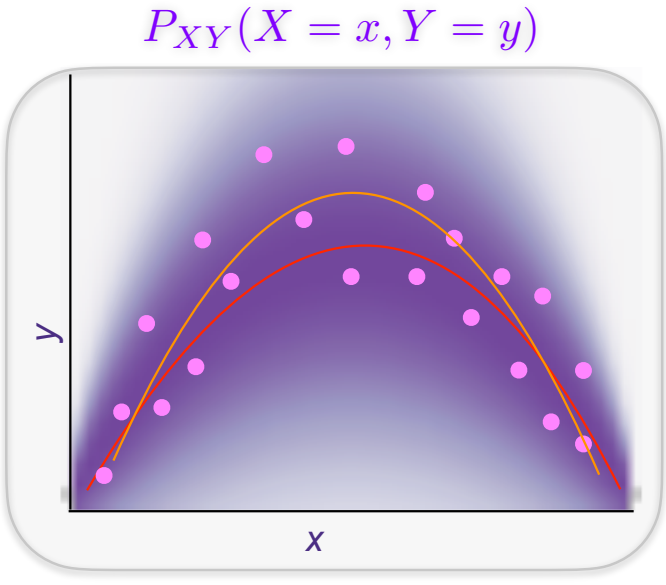
But we only have samples:

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

Statistical Learning



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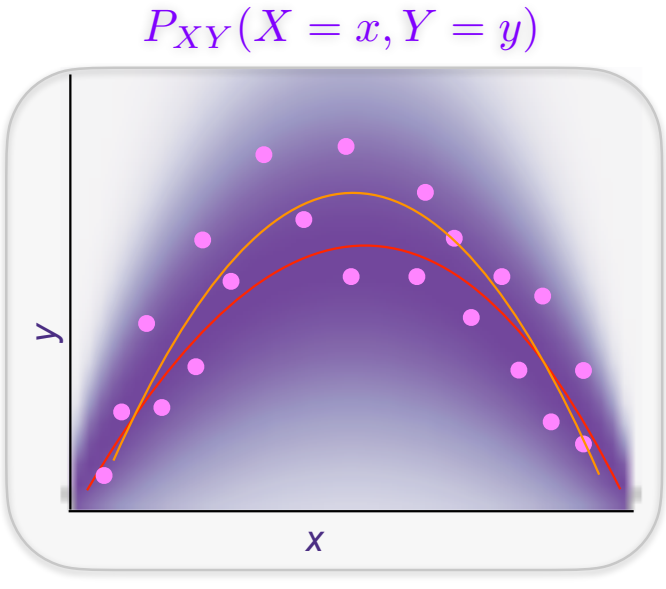
$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

$\mathcal{F}$: linear functions
quadratic functions

Statistical Learning



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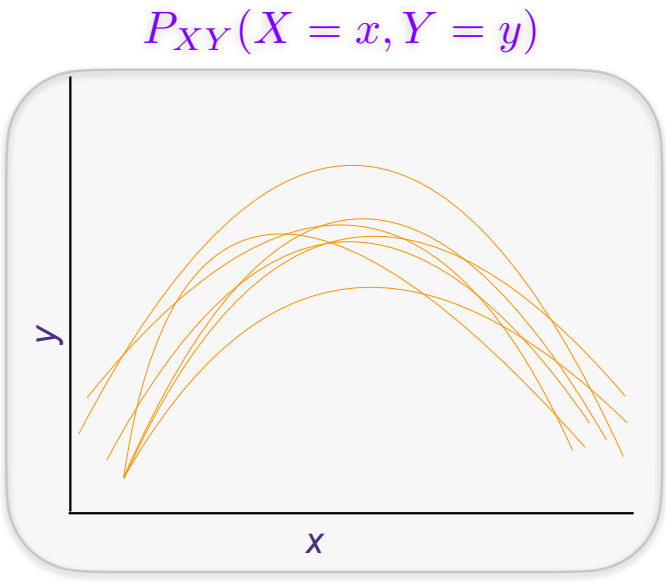
We care about future predictions: $\mathbb{E}_{XY}[(Y - \widehat{f}(X))^2]$

Statistical Learning



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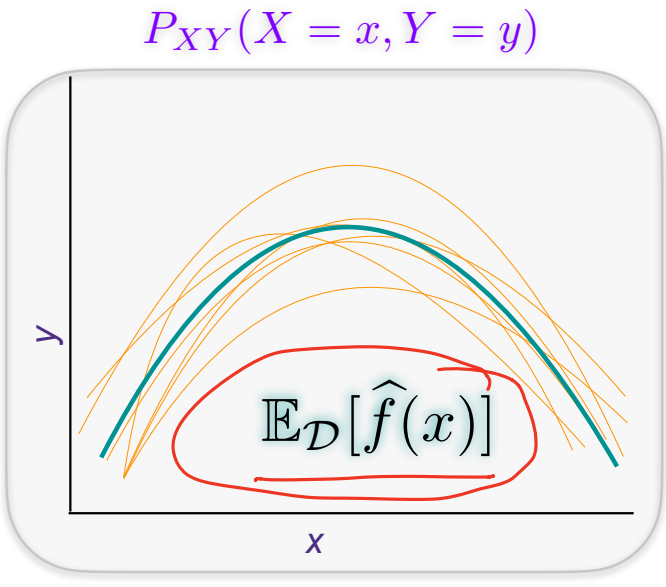
Each draw $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ results in different $\widehat{f}$

Statistical Learning



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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

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

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

Bias-Variance Tradeoff

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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

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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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Learning Error

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

CS

Bias-Variance Tradeoff

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Bias-Variance Tradeoff

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

Bias-Variance Tradeoff

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bias squared

Bias-Variance Tradeoff

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bias squared

variance

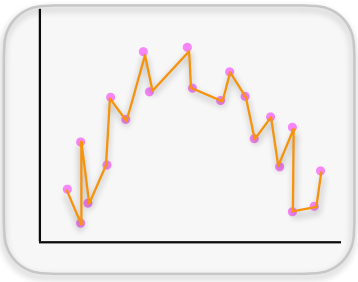
Bias-Variance Tradeoff

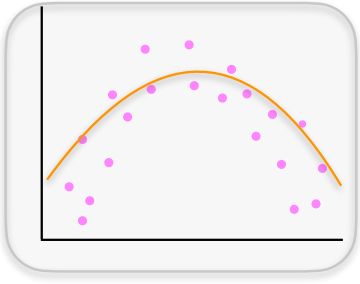
$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2] \big| X = x] = \mathbb{E}_{Y|X}[(Y - \eta(x))^2 \big| X = x]$$

irreducible error

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

bias squared





Bias-Variance Tradeoff

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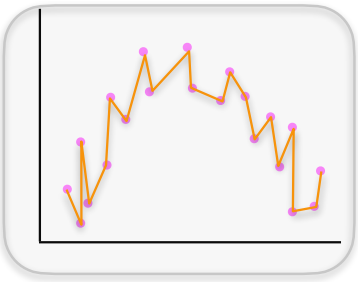
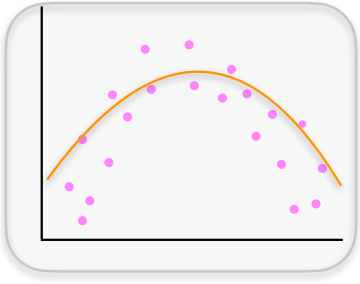
irreducible error

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

bias squared **variance**





Bias-Variance Tradeoff

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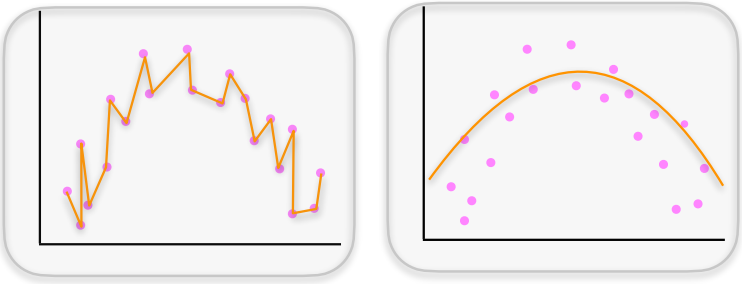

If we re-drew our data, what the LS training error estimator look like for generalized linear functions in small p/large p dimensions?

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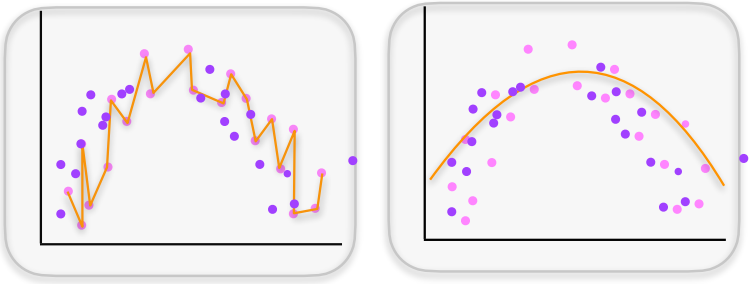


If we re-drew our data, what the LS training error estimator look like for generalized linear functions in small p/large p dimensions?

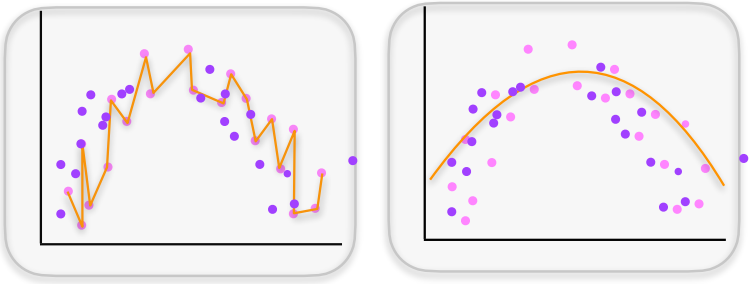
Bias-Variance Tradeoff

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

irreducible error

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

bias squared **variance**



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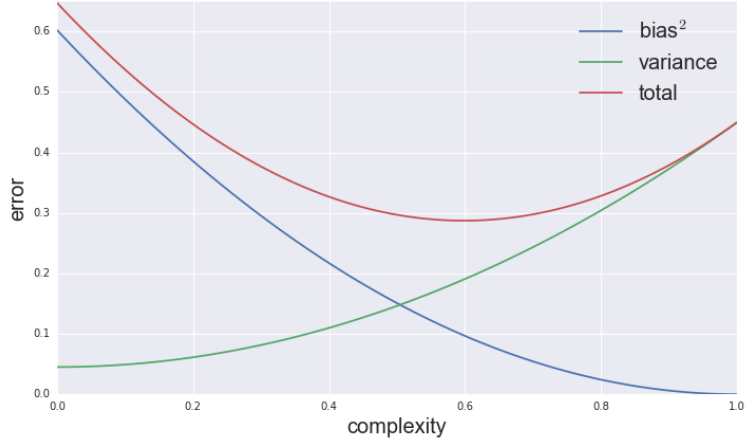

Example: Linear LS

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

if $\quad y_i = x_i^T w + \epsilon_i \quad$ 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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irreducible error

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

bias squared

Example: Linear LS: compute bias

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variance

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bias squared

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