COMS 4771
Introduction to Machine Learning

James McInerney

Adapted from slides by Nakul Verma

Announcements

- HW1:
  - Please submit as a group
  - Watch out for zero variance features (Q5)
- HW2 will be released soon

Last time...

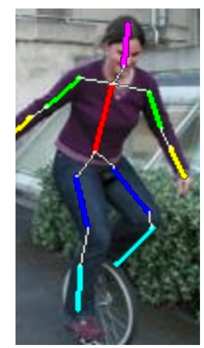
- Support Vector Machines
- Maximum Margin formulation
- Constrained Optimization
- Lagrange Duality Theory
- Convex Optimization
- SVM dual and Interpretation
- How get the optimal solution

Learning more Sophisticated Outputs

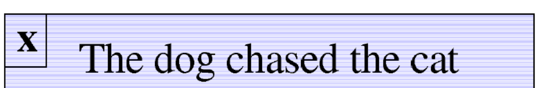
So far we have focused on classification $f : X \to \{1, \ldots, k\}$

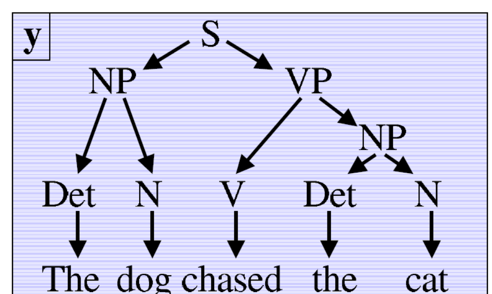
What about **other outputs**?

- $PM_{2.5}$ (pollutant) particulate matter exposure estimate:
  Input: # cars, temperature, etc. **Output:** 50 ppb
- Pose estimation



- Sentence structure estimate:





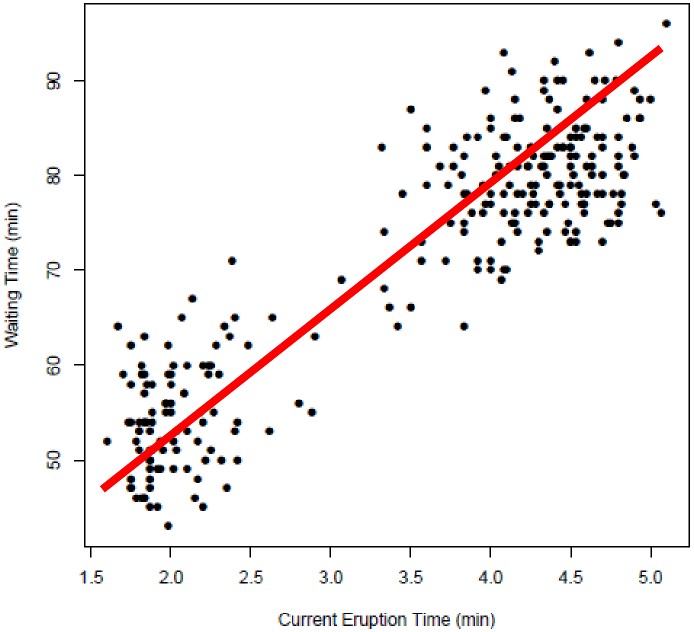
Regression

We'll focus on problems with real number outputs (regression problem):

$$f : X \to \mathbf{R}$$

Example:

Next eruption time of old faithful geyser (at Yellowstone)



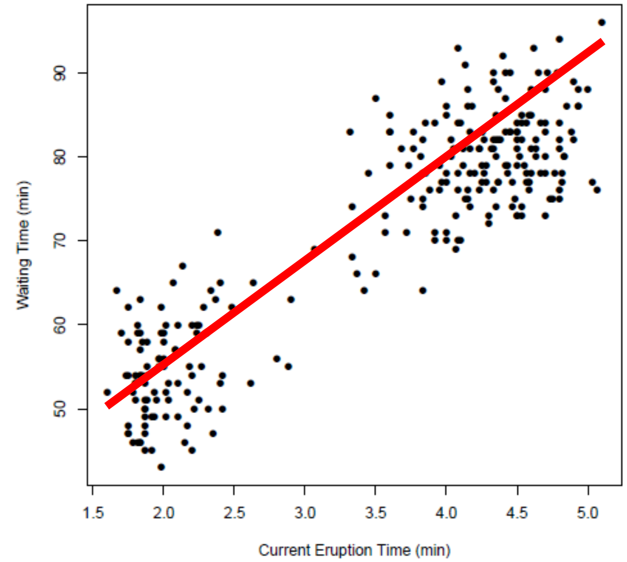
Regression Formulation for the Example

Given *x*, want to predict an estimate $\hat{y}$ of *y*, which minizes the discrepancy (*L*) between $\hat{y}$ and *y*.

$$L(\hat{y}; y) := |\hat{y} - y|$$ *Absolute error*

$$:= (\hat{y} - y)^2$$ *Squared error*

Loss



A **linear predictor** *f*, can be defined by the slope *w* and the intercept w_0 :

$$\hat{f}(\vec{x}) := \vec{w} \cdot \vec{x} + w_0$$

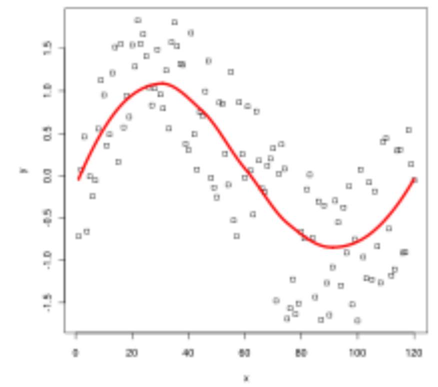
which minimizes the prediction loss.

$$\min_{w, w_0} \mathbb{E}_{\vec{x}, y} \left[L(\hat{f}(\vec{x}), y) \right]$$

How is this different from ***classification****?*

Parametric vs non-parametric Regression

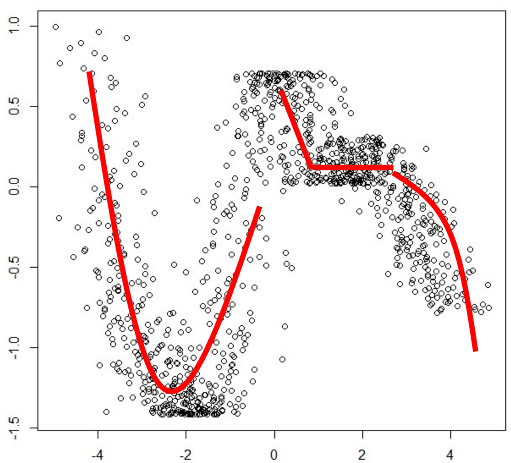
If we assume a particular form of the regressor:



Parametric regression

Goal: to learn the parameters which yield the minimum error/loss

If no specific form of regressor is assumed:



Non-parametric regression

Goal: to learn the predictor directly from the input data that yields the minimum error/loss

Linear Regression

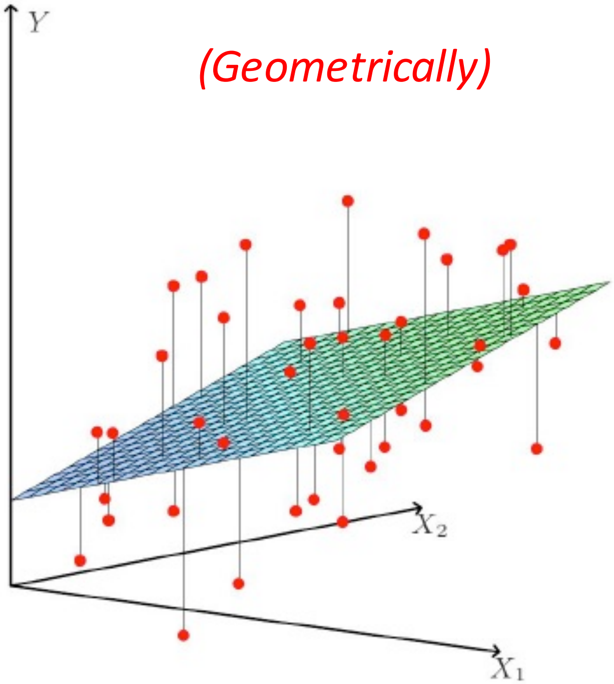
Want to find a **linear predictor** *f*, i.e., *w* (intercept w_0 absorbed via lifting):

$$\hat{f}(\vec{x}) := \vec{w} \cdot \vec{x}$$

which minimizes the prediction loss over the population.

$$\min_{\vec{w}} \mathbb{E}_{\vec{x},y}\left[L(\hat{f}(\vec{x}), y)\right]$$

(Geometrically)



We estimate the parameters by minimizing the corresponding loss on the training data:

$$\arg\min_{w} \frac{1}{n} \sum_{i=1}^{n} \left[L(\vec{w} \cdot \vec{x}_i, y_i)\right]$$

$$= \arg\min_{w} \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \vec{x}_i - y_i\right)^2$$

for squared error

Linear Regression: Learning the Parameters

Linear predictor with squared loss:

$$\arg\min_{w} \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \vec{x}_i - y_i\right)^2$$

$$= \arg\min_{w} \left\| \begin{pmatrix} \ldots\ x_1\ \ldots \\ \ldots\ x_i\ \ldots \\ \ldots\ x_n\ \ldots \end{pmatrix} \begin{bmatrix} \\ w \\ \\ \end{bmatrix} - \begin{bmatrix} y_1 \\ y_i \\ y_n \end{bmatrix} \right\|^2$$

$$= \arg\min_{w} \left\| X\vec{w} - \vec{y} \right\|_2^2$$

Unconstrained problem!

Can take the gradient and examine the stationary points!

Why need not check the second order conditions?

Linear Regression: Learning the Parameters

Best fitting *w*:

$$\frac{\partial}{\partial \vec{w}} \left\| X\vec{w} - \vec{y} \right\|^2 \quad = 2X^\top (X\vec{w} - \vec{y})$$

$$X^\top X \vec{w} = X^\top \vec{y}$$

At a stationary point

$$\Longrightarrow \quad \vec{w}_{\text{ols}} = (X^\top X)^\dagger X^\top \vec{y}$$

Pseudo-inverse

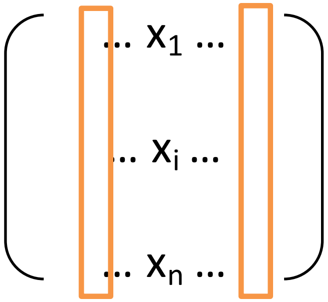
Also called the Ordinary Least Squares (OLS)

The solution is unique and stable when $X^T X$ is invertible

What is the interpretation of this solution?

Linear Regression: Geometric Viewpoint

Consider the ***column space*** view of data **X**:



$\ddot{x}_1, \ldots, \ddot{x}_d \in \mathbf{R}^n$

Find a *w*, such that the linear combination of ***minimizes***

$$\frac{1}{n}\left\|\vec{y} - \sum_{i=1}^{d} w_i \ddot{x}_i\right\|^2 \quad =: \text{residual}$$

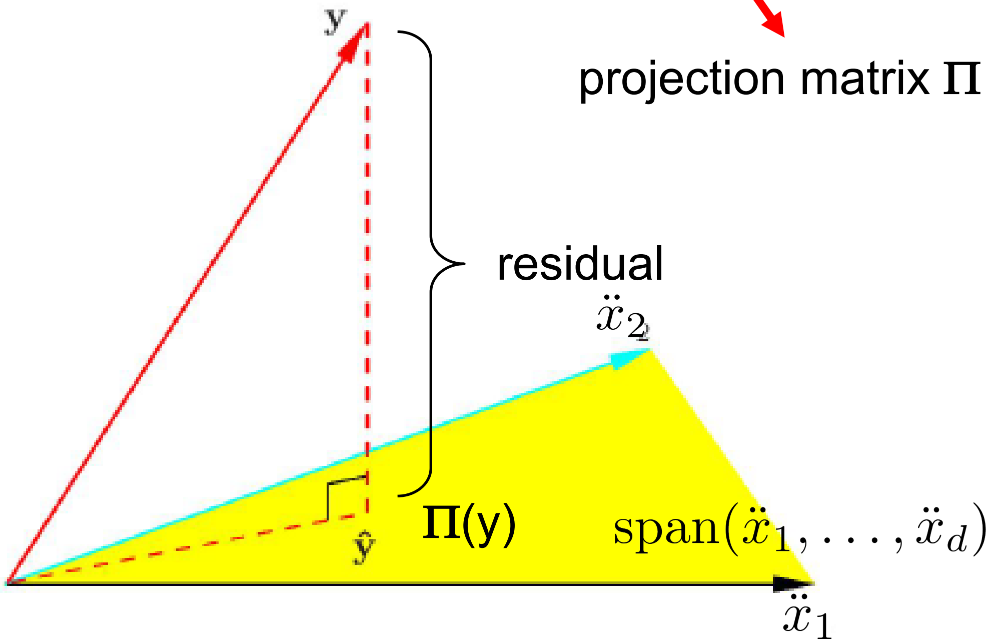
$$\hat{y} = X\vec{w}_{\text{ols}} = X(X^{\mathsf{T}}X)^{\dagger}X^{\mathsf{T}}\ \vec{y}$$

Say $\hat{y}$ is the ols solution, ie,

$$\hat{y} := X\vec{w}_{\text{ols}} = \sum_{i=1}^{d} w_{\text{ols},i}\ddot{x}_i$$

*Thus, $\hat{y}$ is the **orthogonal projection** of y onto the* $\text{span}(\ddot{x}_1, \ldots, \ddot{x}_d)$ *!*

w_{ols} *forms the **coefficients** of* $\hat{y}$



Linear Regression: Statistical Modeling View

Let's assume that data is **generated** from the following process:

- A example x_i is draw independently from the data space **X**

$$x_i \sim \mathcal{D}_X$$

- y_{clean} is computed as (w . x_i), from a fixed unknown w

$$y_{\text{clean}} := w \cdot x_i$$

- y_{clean} is corrupted from by adding independent Gaussian noise $N(0,\sigma^2)$

$$y_i := y_{\text{clean}} + \epsilon_i = w \cdot x_i + \epsilon_i \qquad \epsilon_i \sim N(0, \sigma^2)$$

- (x_i, y_i) is revealed as the i^{th} sample

$$(x_1, y_1), \ldots, (x_n, y_n) =: S$$

Linear Regression: Statistical Modeling View

How can we determine *w*, from Gaussian noise corrupted observations?

$$S = (x_1, y_1), \ldots, (x_n, y_n)$$

Observation:

$$y_i \sim w \cdot x_i + N(0, \sigma^2) = N(w \cdot x_i, \sigma^2)$$

How to estimate parameters of a Gaussian?

Let's try Maximum Likelihood Estimation!

parameter

$$\log \mathcal{L}(w|S)$$

$$= \sum_{i=1}^{n} \log p(y_i|w, x_i) = \sum_{i=1}^{n} -\frac{(y_i - x_i^\top w)^2}{2\sigma^2} + \text{constant}$$

ignoring terms independent of w

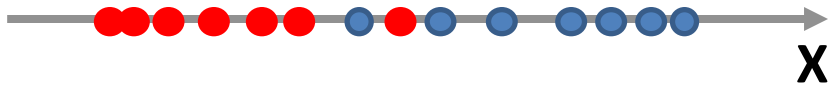
optimizing for w yields the same ols result!

What happens if we model each y_i with indep. noise of different variance?

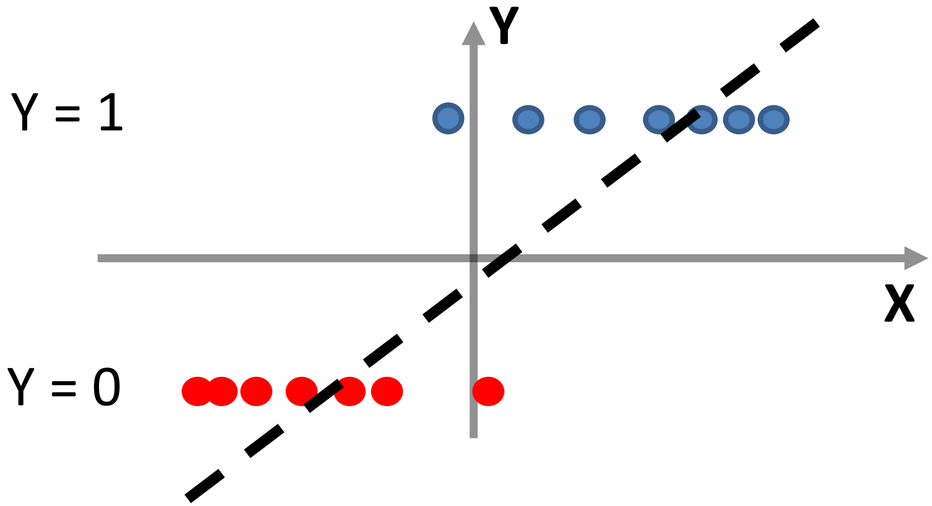
Linear Regression for Classification?

Linear regression seems general, can we use it to derive a binary classifier?

Let's study 1-d data:



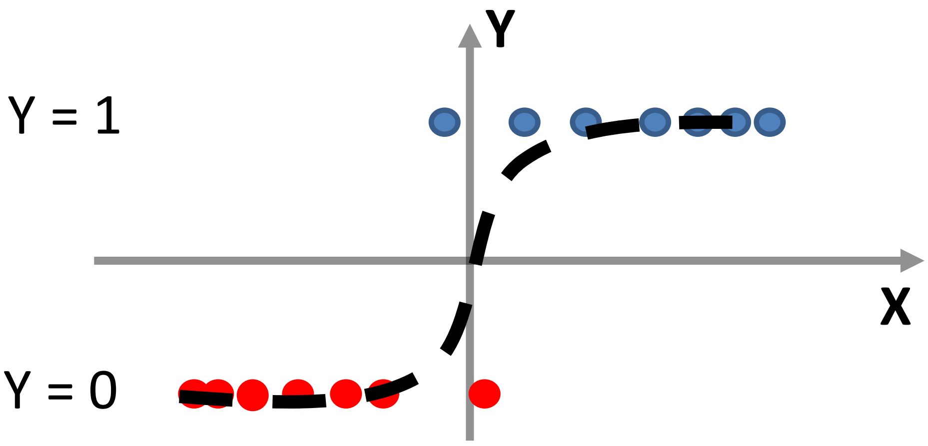
Problem #1: Where is y? for regression.



Problem #2: Not really linear!

*Perhaps it is linear in some **transformed** coordinates?*

Linear Regression for Classification



Sigmoid a better model!

$$\hat{y} = f(x) := \frac{1}{1 + e^{-w \cdot x}}$$

Binary predictor: $\mathrm{sign}(2f(x) - 1)$

Interpretation:

For an event that occurs with probability P, the ***odds*** of that event is:

$$\mathrm{odds}(P) := \frac{P}{1 - P}$$

For an event with P=0.9, odds = 9
But, for an event P=0.1, odds = 0.11
(very asymmetric)

Consider the "log" of the odds

$$\log(\mathrm{odds}(P)) := \mathrm{logit}(P) := \log\left(\frac{P}{1 - P}\right)$$

$$\mathrm{logit}(P) = -\mathrm{logit}(1 - P)$$

Symmetric!

Logistic Regression

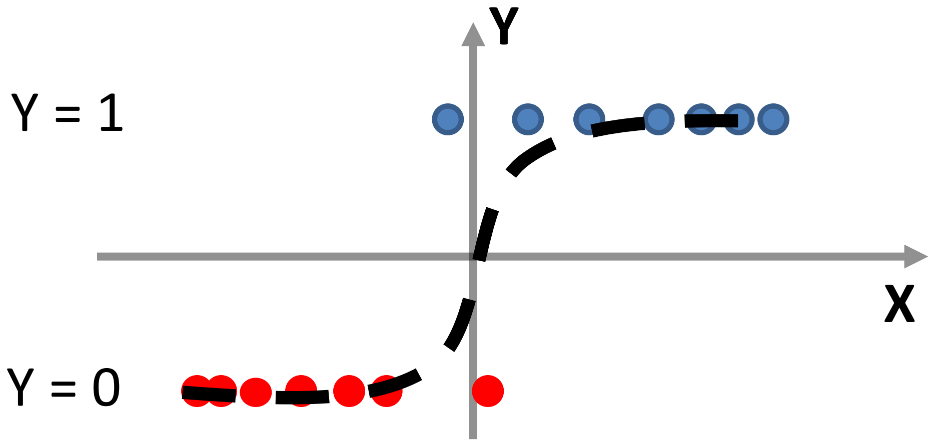
Model the log-odds or logit with linear function!

$$\text{logit}(P(x)) = \log\left(\frac{P(x)}{1-P(x)}\right) = w \cdot x$$

$$\frac{P(x)}{1-P(x)} = e^{w \cdot x}$$

$$P(x) = \frac{e^{w \cdot x}}{1+e^{w \cdot x}} \qquad = \frac{1}{1+e^{-w \cdot x}}$$

Sigmoid!



OK, we have a model, how do we learn the parameters?

Logistic Regression: Learning Parameters

Given samples $S = (x_1, y_1), \ldots, (x_n, y_n)$ ($y_i \in \{0,1\}$ binary)

$$\mathcal{L}(w|S) = \prod_{i=1}^{n} p(x_i)^{y_i}(1 - p(x_i))^{1-y_i}$$

Binomial

$$\log \mathcal{L}(w|S) = \sum_{i=1}^{n} y_i \log p(x_i) + (1 - y_i)\log(1 - p(x_i))$$

$$= \sum_{i=1}^{n} \log(1 - p(x_i)) + \sum_{i=1}^{n} y_i \log \frac{p(x_i)}{1 - p(x_i)}$$

Now, use logistic model!

$$= \sum_{i=1}^{n} -\log(1 + e^{w \cdot x_i}) + \sum_{i=1}^{n} y_i w \cdot x_i$$

Can take the derivative and analyze stationary points, unfortunately no closed form solution (use iterative methods like gradient descent to find the solution)

Linear Regression: Other Variations

Back to the ordinary least squares (ols):

$$\text{minimize} \;\; \|X\vec{w} - \vec{y}\|_2^2$$

$$\vec{w}_{\text{ols}} = (X^\top X)^\dagger X^\top \vec{y}$$

Often poorly behaved when $X^T X$ not invertible

Additionally how can we incorporate prior knowledge?

- perhaps want *w* to be sparse. *Lasso regression*
- perhaps want a simple *w*. *Ridge regression*

Ridge Regression

Objective

$$\text{minimize } \|X\vec{w} - \vec{y}\|^2 + \lambda\|\vec{w}\|^2$$

reconstruction error

'regularization' parameter

$$\vec{w}_{\text{ridge}} = (X^{\mathsf{T}}X + \lambda I)^{-1}X^{\mathsf{T}}\vec{y}$$

The 'regularization' helps avoid overfitting, and always resulting in a unique solution.

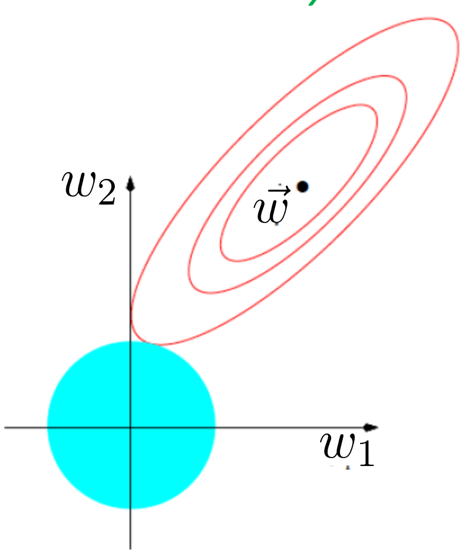
Geometrically:

Equivalent to the following optimization problem:

$$\text{minimize } \|X\vec{w} - \vec{y}\|^2$$

$$\text{such that } \|\vec{w}\|^2 \leq B$$

Why?



Lasso Regression

Objective

$$\text{minimize} \ \left\|X\vec{w}-\vec{y}\right\|^2 + \lambda\|\vec{w}\|_1$$

'lasso' penalty

$$\vec{w}_{\text{lasso}} = ?$$ *no closed form solution*

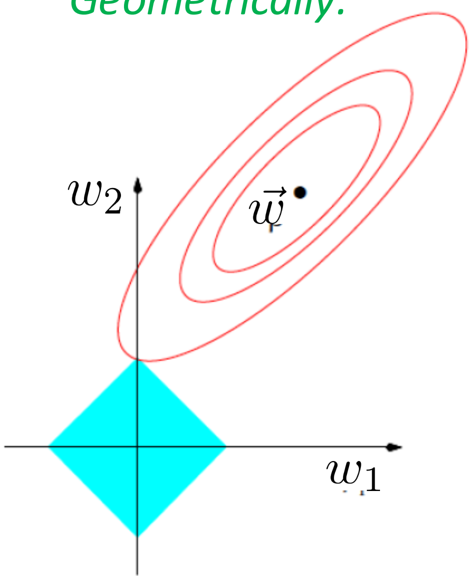
Lasso regularization encourages sparse solutions.

Geometrically:

Equivalent to the following optimization problem:

$$\text{minimize} \ \left\|X\vec{w}-\vec{y}\right\|^2$$
$$\text{such that} \ \left\|\vec{w}\right\|_1 \le B$$

Why?



How can we find the solution?

What About Optimality?

Linear regression (and variants) is great, but what can we say about the best possible estimate?

Can we construct an estimator for real outputs that ***parallels*** *Bayes classifier for discrete outputs?*

Optimal L_2 Regressor

Best possible regression estimate at *x*: $f^*(x) := \mathbb{E}[Y|X = x]$

Theorem: for any regression estimate *g*(*x*)

$$\mathbb{E}_{(x,y)}\big|f^*(x) - y\big|^2 \leq \mathbb{E}_{(x,y)}\big|g(x) - y\big|^2$$

Similar to Bayes classifier, but for regression.

Proof is straightforward…

Proof

$$f^*(x) := \mathbb{E}[Y|X = x]$$

Consider L_2 error of *g*(*x*)

$$\mathbb{E}|g(x) - y|^2 = \mathbb{E}|g(x) - f^*(x) + f^*(x) - y|^2$$

$$= \mathbb{E}|g(x) - f^*(x)|^2 + \mathbb{E}|f^*(x) - y|^2$$

Why?

Cross term:

$$2\mathbb{E}\left[(g(x) - f^*(x))(f^*(x) - y)\right]$$

$$= 2\mathbb{E}_x\left[\mathbb{E}_{y|x}\left[(g(x) - f^*(x))(f^*(x) - y) \mid X = x\right]\right]$$

$$= 2\mathbb{E}_x\left[(g(x) - f^*(x)) \cdot \mathbb{E}_{y|x}\left[(f^*(x) - y) \mid X = x\right]\right]$$

$$= 2\mathbb{E}_x\left[(g(x) - f^*(x))(f^*(x) - f^*(x))\right] = 0$$

Therefore $\mathbb{E}|g(x) - y|^2 = \int_x |g(x) - f^*(x)|^2 \mu(dx) + \mathbb{E}|f^*(x) - y|^2$

Which is minimized when g(x) = f(x)!*

■

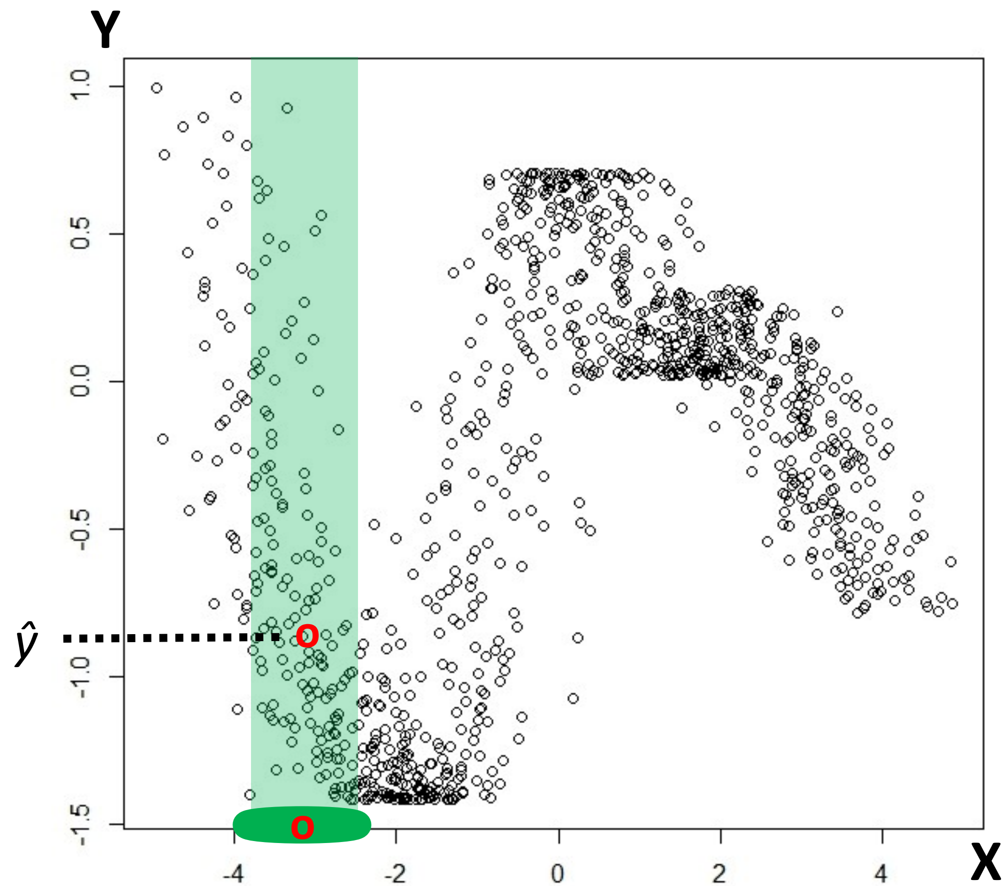
Non-parametric Regression

Linear regression (and variants) is great, but what if we don't know parametric form of the relationship between the independent and dependent variables?

How can we predict value of a new test point *x* ***without*** model assumptions?

Idea:

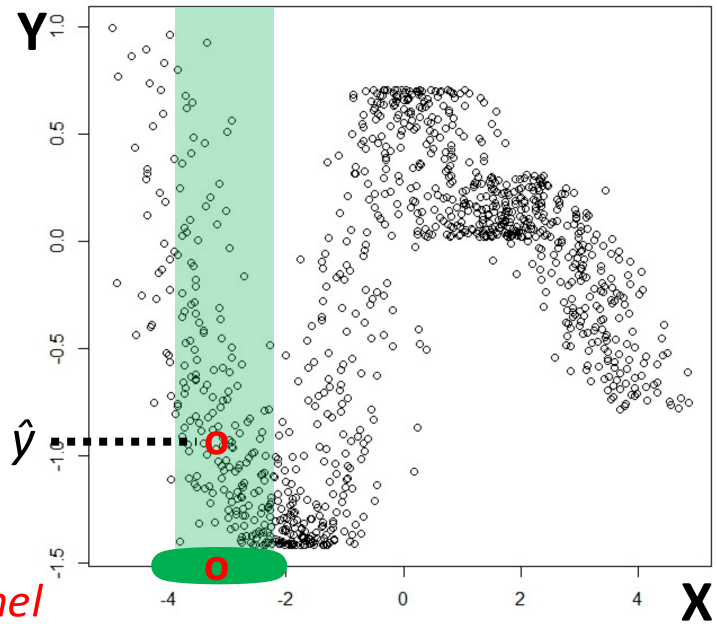
$\hat{y} = f(x) =$ *Average estimate **Y** of observed data in a local neighborhood **X** of x!*



Kernel Regression

$$\hat{y} = \hat{f}_n(x) := \sum_{i=1}^{n} w_i(x)\, y_i$$

Want weights that emphasize **local** observations



Consider example localization functions:

$$K_h(x, x') = e^{-\|x-x'\|^2/h}$$ *Gaussian kernel*

$$= \mathbf{1}\left[\|x - x'\| \leq h\right]$$ *Box kernel*

$$= \left[1 - (1/h)\|x - x'\|\right]_+$$ *Triangle kernel*

Then define:

$$w_i(x) := \frac{K_h(x, x_i)}{\sum_{j=1}^{n} K_h(x, x_j)}$$ *Weighted average*

Kernel Regression

$$\hat{y} = \hat{f}_n(x) := \sum_{i=1}^{n} \frac{K_h(x, x_i)}{\sum_{j=1}^{n} K_h(x, x_j)} \, y_i$$

Advantages:

- Does not assume any parametric form of the regression function.
- Kernel regression is consistent

Disadvantages:

- Evaluation time complexity: O(*dn*)
- Need to keep all the data around!

What We Learned…

- Linear Regression
- Parametric vs Nonparametric regression
- Logistic Regression for classification
- Ridge and Lasso Regression
- Kernel Regression

Questions?