Department of Computer Science
UNIVERSITY OF COLORADO **BOULDER**

Regression

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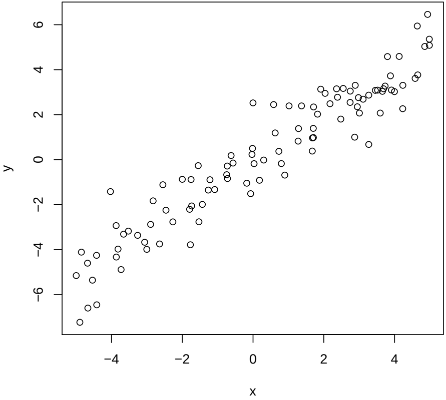
LECTURE 11

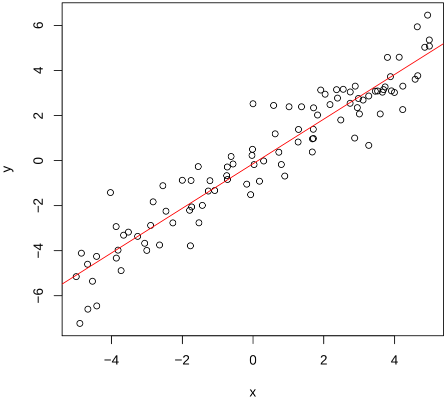
Slides adapted from Lauren Hannah

Linear Regression



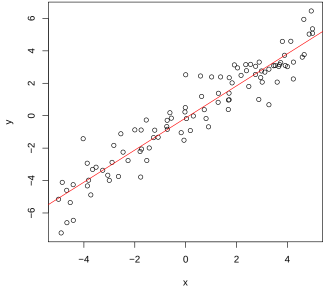
Data are the set of inputs and outputs, $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$

Linear Regression



In *linear regression*, the goal is to predict y from x using a linear function

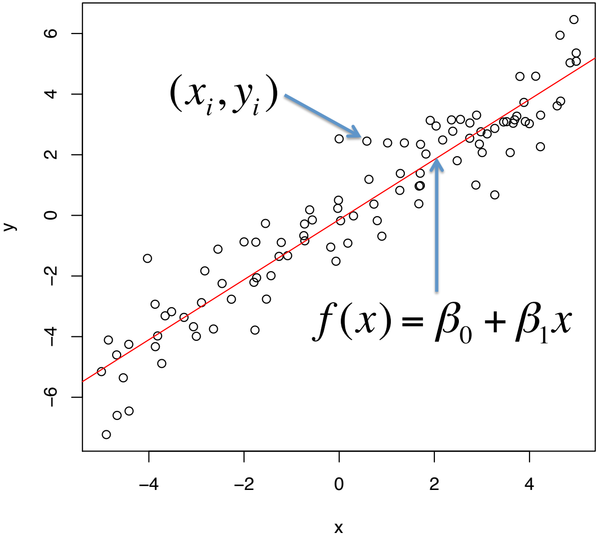
Linear Regression



Examples of linear regression:

- given a child's age and gender, what is his/her height?
- given unemployment, inflation, number of wars, and economic growth, what will the president's approval rating be?
- given a browsing history, how long will a user stay on a page?

Linear Regression



Multiple Covariates

Often, we have a vector of inputs where each represents a different *feature* of the data

$$\mathbf{x} = (x_1, \ldots, x_p)$$

The function fitted to the response is a linear combination of the covariates

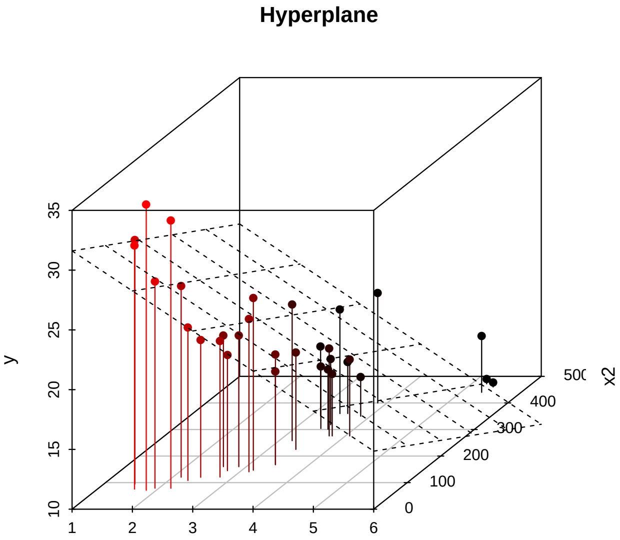
$$f(\mathbf{x}) = \beta_0 + \sum_{j=1}^{p} \beta_j x_j$$

Multiple Covariates

- Often, it is convenient to represent $\mathbf{x}$ as $(1, x_1, \dots, x_p)$
- In this case $\mathbf{x}$ is a vector, and so is β (we'll represent them in bold face)
- This is the dot product between these two vectors
- This then becomes a sum (this should be familiar!)

$$\beta \mathbf{x} = \beta_0 + \sum_{j=1}^{p} \beta_j x_j$$

Hyperplanes: Linear Functions in Multiple Dimensions

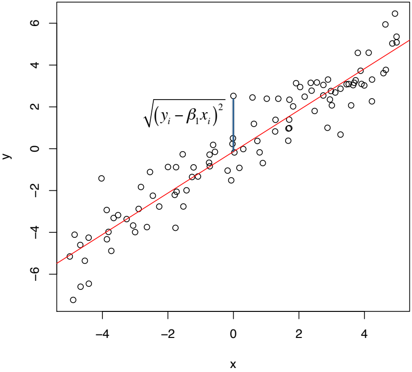


Covariates

- Do not need to be raw value of $x_1, x_2, \ldots$
- Can be any feature or function of the data:
  - Transformations like $x_2 = \log(x_1)$ or $x_2 = \cos(x_1)$
  - Basis expansions like $x_2 = x_1^2$, $x_3 = x_1^3$, $x_4 = x_1^4$, etc
  - Indicators of events like $x_2 = 1_{\{-1 \leq x_1 \leq 1\}}$
  - Interactions between variables like $x_3 = x_1 x_2$
- Because of its simplicity and flexibility, it is one of the most widely implemented regression techniques

Plan

Fitting a Linear Regression



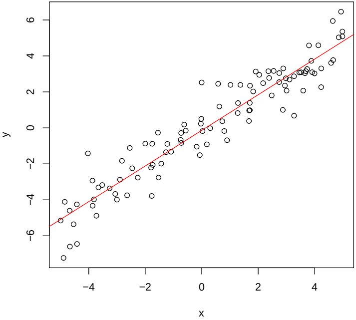
Idea: minimize the Euclidean distance between data and fitted line

$$RSS(\beta) = \frac{1}{2} \sum_{i=1}^{n} (y_i - \beta \mathbf{x}_i)^2$$

How to Find β

- Use calculus to find the value of β that minimizes the RSS
- The optimal value is

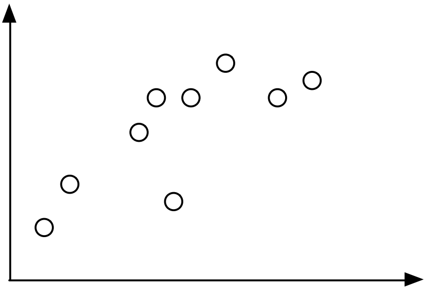
$$\hat{\beta} = \frac{\sum_{i=1}^{n} y_i x_i}{\sum_{i=1}^{n} x_i^2}$$



Prediction

- After finding $\hat{\beta}$, we would like to predict an output value for a new set of covariates
- We just find the point on the line that corresponds to the new input:

$$\hat{y} = \beta_0 + \beta_1 x \tag{1}$$



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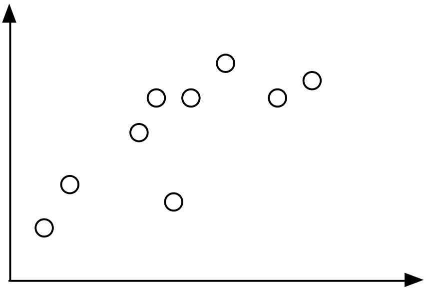
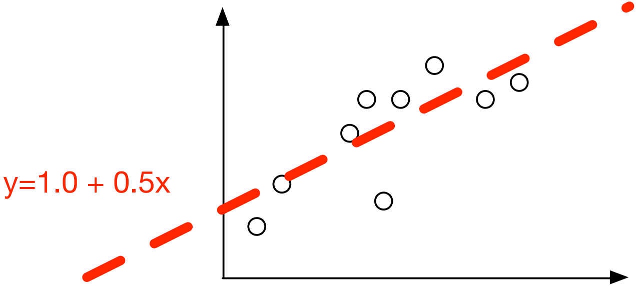


Prediction

- After finding $\hat{\beta}$, we would like to predict an output value for a new set of covariates
- We just find the point on the line that corresponds to the new input:

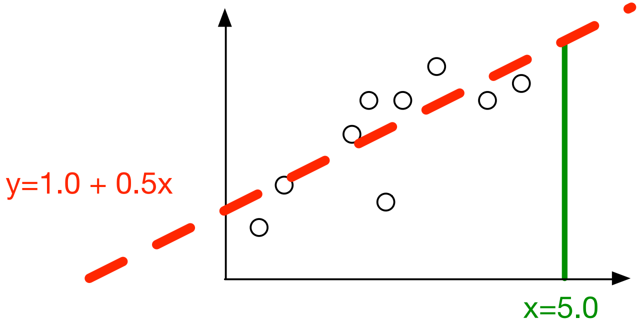
$$\hat{y} = 1.0 + 0.5x \tag{1}$$



Prediction

- After finding $\hat{\beta}$, we would like to predict an output value for a new set of covariates
- We just find the point on the line that corresponds to the new input:

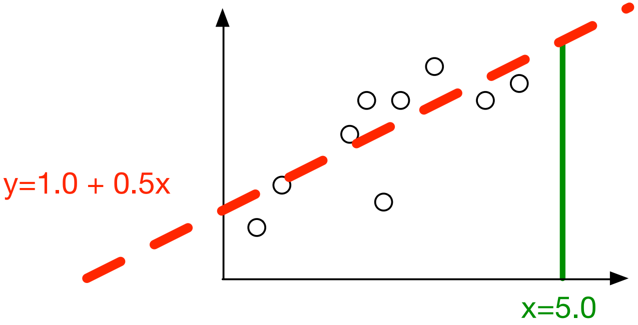
$$\hat{y} = 1.0 + 0.5 * 5 \tag{1}$$



Prediction

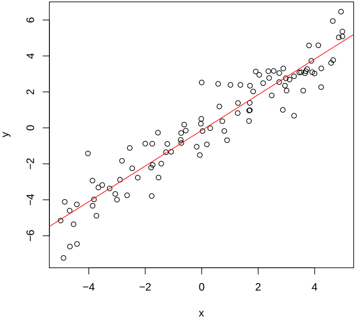
- After finding $\hat{\beta}$, we would like to predict an output value for a new set of covariates
- We just find the point on the line that corresponds to the new input:

$$\hat{y} = 3.5 \tag{1}$$



Probabilistic Interpretation

- Our analysis so far has not included any probabilities
- Linear regression does have a *probabilisitc* (probability model-based) interpretation

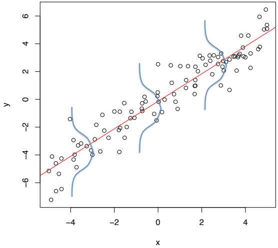


Probabilistic Interpretation

- Linear regression assumes that response values have a Gaussian distribution around the linear mean function,

$$Y_i \mid \mathbf{x}_i, \beta \sim N(\mathbf{x}_i \beta, \sigma^2)$$

- This is a *discriminative model*, where inputs x are not modeled



- Minimizing RSS is equivalent to maximizing conditional likelihood

Plan

Example: Old Faithful

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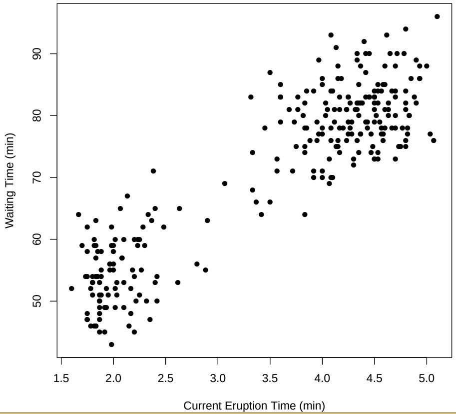
We will predict the time that we will have to wait to see the next eruption given the duration of the current eruption

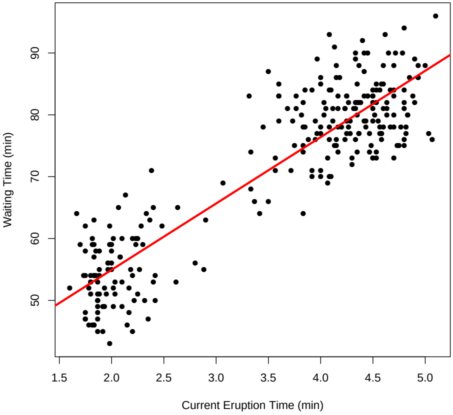


Example: Old Faithful

We can plot our data and make a function for new predictions

```
>  # Plot a line on the data
>  abline(fit.lm,col="red",lwd=3)
>
>  # Make a function for prediction
>  fit.lm$coefficients[1]
(Intercept)
     33.4744
>  fit.lm$coefficients[2]
eruptions
  10.72964
>  faithful.fit <- function(x) fit.lm$coefficients[1] +
fit.lm$coefficients[2]*x
>  x.pred <- c(2.0, 2.7, 3.8, 4.9)
>  faithful.fit(x.pred)
[1] 54.93368 62.44443 74.24703 86.04964
```

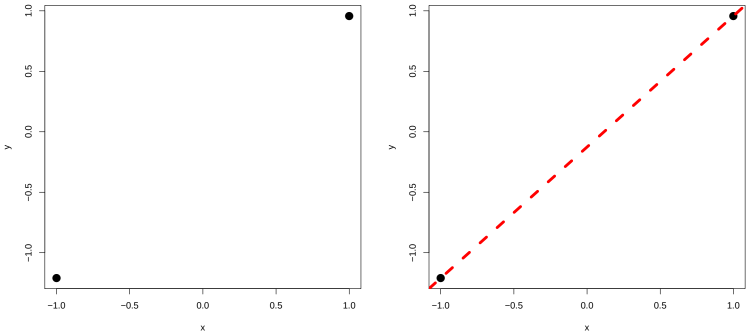
Example: Old Faithful



Plan

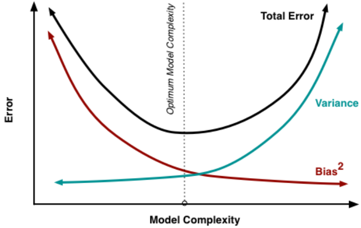
Multivariate Linear Regression

Example: $p = 1$, have 2 points



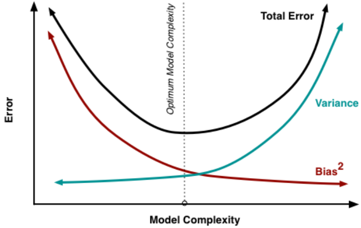
- Have $p+1$ or fewer points, line hits all (or p with mean 0 data)
- $\geq p+1$ (but still close to that number), line goes *close* to all points

Noise, Bias, Variance Tradeoff



- **Noise**: Lower bound on performance
- **Bias**: Error as a result as choosing the **wrong** model
- **Variance**: Variation due to training sample and randomization

Noise, Bias, Variance Tradeoff



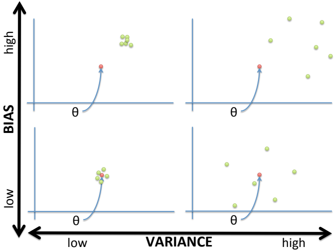
- **Noise**: Lower bound on performance
- **Bias**: Error as a result as choosing the **wrong** model
- **Variance**: Variation due to training sample and randomization

- No model is perfect
- More complex models are more susceptible to errors due to variance

Multivariate Linear Regression

Why linear regression:

- has few parameters to estimate (p)
- really restrictive model–low variance, higher bias



- *should be good for data with few observations, large number of covariates...*
- **... but we can't use it in this situation**

Multivariate Linear Regression

Idea: if we have a large number of covariates compared to observations, say $n < 2p$, **best to estimate most coefficients as 0!**

- not enough info to determine all coefficients
- try to estimate ones with strong signal
- set everything else to 0 (or close)

Coefficients of 0 may not be a bad assumption...

If we have 1,000s of coefficients, are they all equally important?

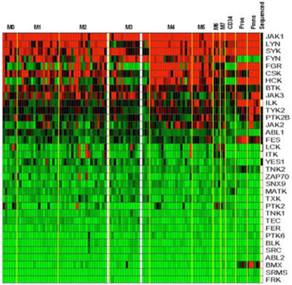
Gene Expression

Example: microarray gene expression data

- gene expression: want to measure the level at which information in a gene is used in the synthesis of a functional gene product (usually protein)
- can use gene expression data to determine subtype of cancer (e.g. which *type* of Lymphoma B?) or predict recurrence, survival time, etc
- problem: thousands of genes, hundreds of patients, $p > n$!

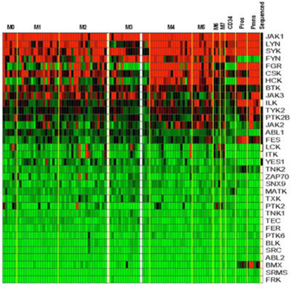
Intuition: only a handful of genes should affect outcomes

Gene Expression



- gene expression levels are continuous values
- data: observation i is gene expression levels from patient i, attached to outcome for patient (survival time)
- covariates: expression levels for p genes

Gene Expression



- collinearity: does it matter *which* gene is selected for *prediction*? No!
- overfitting: now fitting p' non-0 coefficients to n observations with $p' << n$ means less fitting of noise

Regularized Linear Regression

Regularization:

- still minimize the RSS
- place a *penalty* on large values for β_1, ..., β_p (why not β_0? can always easily estimate mean)
- add this penalty to the objective function
- solve for $\hat{\beta}$!

New objective function:

$$\hat{\beta} = \arg\min_{\beta} \frac{1}{2} \sum_{i=1}^{n} (y_i - \mathbf{x}_i \beta)^2 + \lambda \sum_{j=1}^{p} \mathrm{penalty}(\beta_j)$$

λ acts as a weight on penalty: low values mean few coefficients near 0, high values mean many coefficients near 0

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Regularized Linear Regression

Regularization: what is a good penalty function?

Same as penalties used to fit errors:

- Ridge regression (squared penalty):

$$\hat{\beta}^{Ridge} = \arg\min_{\beta} \frac{1}{2} \sum_{i=1}^{n} (y_i - \mathbf{x}_i \beta)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

- Lasso regression (absolute value penalty):

$$\hat{\beta}^{Lasso} = \arg\min_{\beta} \frac{1}{2} \sum_{i=1}^{n} (y_i - \mathbf{x}_i \beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

Comparing Ridge and Lasso

	Ridge	Lasso
Objective	$\frac{1}{2}\sum_{i=1}^{n}\left(y_i - \mathbf{x}_i\beta\right)^2 + \lambda\sum_{j=0}^{p}\beta_j^2$	$\frac{1}{2}\sum_{i=1}^{n}\left(y_i - \mathbf{x}_i\beta\right)^2 + \lambda\sum_{j=0}^{p}\lvert\beta_j\rvert$
Estimator	$\left(\mathbf{X}^T\mathbf{X} + \lambda I\right)^{-1}\mathbf{X}^T\mathbf{y}$	not closed form
Coefficients	most close to 0	most exactly 0
Stability	robust to changes in $\mathbf{X}$, $\mathbf{y}$	not robust to changes in $\mathbf{X}$, $\mathbf{y}$

Regularized linear regression is fantastic for low signal datasets or those with $p >> n$

- Ridge: good when many coefficients affect value but not large (gene expression)
- Lasso: good when you want an *interpretable* estimator

Choosing λ

Both Ridge and Lasso have a tunable parameter, λ

- use cross validation to find best λ

$$\hat{\lambda} = \arg\min_{\lambda} \sum_{i=1}^{n} \left(y_i - \mathbf{x}_i \hat{\beta}_{-i,\lambda} \right)^2$$

- try out many values
- see how well it works on "development" data

Plan

Regression

- Workhorse technique of data analysis
- Fundamental tool that we will use later for classification ("Logistic Regression")
- Important to understand interpretation of regression parameters