

# Introduction to Statistical Learning

Gaurav Sood

Spring 2015

## Two paradigms of learning

## Two paradigms of learning

- Supervised Learning

## Two paradigms of learning

- Supervised Learning
  - When getting labels (predictions) is expensive

# Two paradigms of learning

- Supervised Learning

- When getting labels (predictions) is expensive
  - Get labels for a small set of data

# Two paradigms of learning

- Supervised Learning

- When getting labels (predictions) is expensive
- Get labels for a small set of data
- Estimate relationship between  $Y$  and  $X$

# Two paradigms of learning

## – Supervised Learning

- When getting labels (predictions) is expensive
- Get labels for a small set of data
- Estimate relationship between  $Y$  and  $X$
- Predict labels of unseen data

# Two paradigms of learning

## – Supervised Learning

- When getting labels (predictions) is expensive
- Get labels for a small set of data
- Estimate relationship between  $Y$  and  $X$
- Predict labels of unseen data
- Labels and cost function *supervise* dimension reduction



# Two paradigms of learning

## – Supervised Learning

- When getting labels (predictions) is expensive
- Get labels for a small set of data
- Estimate relationship between  $Y$  and  $X$
- Predict labels of unseen data
- Labels and cost function *supervise* dimension reduction

## – Unsupervised Learning

# Two paradigms of learning

## – Supervised Learning

- When getting labels (predictions) is expensive
- Get labels for a small set of data
- Estimate relationship between  $Y$  and  $X$
- Predict labels of unseen data
- Labels and cost function *supervise* dimension reduction

## – Unsupervised Learning

- Find vectors similar to each other, maximize differences across

# Two paradigms of learning

## – Supervised Learning

- When getting labels (predictions) is expensive
- Get labels for a small set of data
- Estimate relationship between  $Y$  and  $X$
- Predict labels of unseen data
- Labels and cost function *supervise* dimension reduction

## – Unsupervised Learning

- Find vectors similar to each other, maximize differences across
- Find rows similar to each other, maximize differences across

How to learn from data?

$$- Y = f(X) + \epsilon$$

## How to learn from data?

- $Y = f(X) + \epsilon$
- How do we estimate  $f(X)$ ?

## How to learn from data?

- $Y = f(X) + \epsilon$
- How do we estimate  $f(X)$ ?
- If similar  $x$ , similar  $y$

## How to learn from data?

- $Y = f(X) + \epsilon$
- How do we estimate  $f(X)$ ?
- If similar  $x$ , similar  $y$
- Function: value of  $y$  same as that of the nearest neighbor

## How to learn from data?

- $Y = f(X) + \epsilon$
- How do we estimate  $f(X)$ ?
- If similar  $x$ , similar  $y$
- Function: value of  $y$  same as that of the nearest neighbor
- Question and a concern



## How to learn from data?

- $Y = f(X) + \epsilon$
- How do we estimate  $f(X)$ ?
- If similar  $x$ , similar  $y$
- Function: value of  $y$  same as that of the nearest neighbor
- Question and a concern
  - What do we mean by nearest?

## How to learn from data?

- $Y = f(X) + \epsilon$
- How do we estimate  $f(X)$ ?
- If similar  $x$ , similar  $y$
- Function: value of  $y$  same as that of the nearest neighbor
- Question and a concern
  - What do we mean by nearest?
  - Wouldn't it depend on what  $x$  are observed?

What do we mean by nearest?

What do we mean by nearest?

- Euclidean distance: If  $p$  and  $q$  are two  $n$  dimensional vectors

$$d_e(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

What do we mean by nearest?

- Euclidean distance: If  $p$  and  $q$  are two  $n$  dimensional vectors

$$d_e(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

- Some issues:

What do we mean by nearest?

- Euclidean distance: If  $p$  and  $q$  are two  $n$  dimensional vectors

$$d_e(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

- Some issues:
  - Not all features on the same scale

What do we mean by nearest?

- Euclidean distance: If  $p$  and  $q$  are two  $n$  dimensional vectors

$$d_e(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

- Some issues:
  - Not all features on the same scale
  - Features may be correlated with each other

## What do we mean by nearest?

- Euclidean distance: If  $p$  and  $q$  are two  $n$  dimensional vectors

$$d_e(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

- Some issues:
  - Not all features on the same scale
  - Features may be correlated with each other
- Mahalanobis distance between two vectors:  
Say  $S$  is the covariance matrix

$$d_m(\vec{p}, \vec{q}) = \sqrt{(\vec{p} - \vec{q})' S^{-1} (\vec{p} - \vec{q})}$$



## What do we mean by nearest?

- Euclidean distance: If  $p$  and  $q$  are two  $n$  dimensional vectors

$$d_e(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2}$$

- Some issues:

- Not all features on the same scale
- Features may be correlated with each other

- Mahalanobis distance between two vectors:

Say  $S$  is the covariance matrix

$$d_m(\vec{p}, \vec{q}) = \sqrt{(\vec{p} - \vec{q})' S^{-1} (\vec{p} - \vec{q})}$$

- For Boolean, Jaccard distance:

$$d_j(p, q) = \frac{|p \cup q| - |p \cap q|}{|p \cup q|}$$

Applications: Recommender systems, finding similar

## Learning from data

$$- Y = f(X) + e$$

## Learning from data

- $Y = f(X) + e$
- Problem formulated as a regression function

## Learning from data

- $Y = f(X) + e$
- Problem formulated as a regression function

## Learning from data

- $Y = f(X) + e$
- Problem formulated as a regression function
  - $E(Y|X)$

## Learning from data

- $Y = f(X) + e$
- Problem formulated as a regression function
  - $E(Y|X)$
  - $f(x) = E(Y|x = x)$

## Learning from data

- $Y = f(X) + e$
- Problem formulated as a regression function
  - $E(Y|X)$
  - $f(x) = E(Y|x = x)$
- Nearest neighbour averaging
  - $\hat{f}(x) = E[Y|X \in N(x)]$

## Learning from data

- $Y = f(X) + e$
- Problem formulated as a regression function
  - $E(Y|X)$
  - $f(x) = E(Y|x = x)$
- Nearest neighbour averaging
  - $\hat{f}(x) = E[Y|X \in N(x)]$
- Great when small  $p$ , large  $N$



## Curse of Dimensionality

$$- \hat{f}(x) = E[Y|X \in N(x)]$$

## Curse of Dimensionality

- $\hat{f}(x) = E[Y|X \in N(x)]$
- Define neighborhood too tightly, nothing in there.

## Curse of Dimensionality

- $\hat{f}(x) = E[Y|X \in N(x)]$
- Define neighborhood too tightly, nothing in there.
- If we expand it, nearest neighbors can be far away

## Curse of Dimensionality

- $\hat{f}(x) = E[Y|X \in N(x)]$
- Define neighborhood too tightly, nothing in there.
- If we expand it, nearest neighbors can be far away
- How do we solve the problem?

## Curse of Dimensionality

- $\hat{f}(x) = E[Y|X \in N(x)]$
- Define neighborhood too tightly, nothing in there.
- If we expand it, nearest neighbors can be far away
- How do we solve the problem?
- One way: parametric and structural models
$$f(x) = \beta_0 + \beta_1 * X_1 + \beta_2 * X_2 + \dots \beta_p * X_p$$

How to expand the linear model?

- Simple polynomial transformations

## How to expand the linear model?

- Simple polynomial transformations
- Interactions

## How to expand the linear model?

- Simple polynomial transformations
- Interactions
- Step functions. E.g. transform education into  $k$  dummy variables.



## How to expand the linear model?

- Simple polynomial transformations
- Interactions
- Step functions. E.g. transform education into  $k$  dummy variables.
- More complicated basis functions:

## How to expand the linear model?

- Simple polynomial transformations
- Interactions
- Step functions. E.g. transform education into  $k$  dummy variables.
- More complicated basis functions:
  - Piecewise polynomial: takes differential polynomial for different regions (split by knots)

## How to expand the linear model?

- Simple polynomial transformations
- Interactions
- Step functions. E.g. transform education into  $k$  dummy variables.
- More complicated basis functions:
  - Piecewise polynomial: takes differential polynomial for different regions (split by knots)
  - Add constraint that there are no abrupt changes across regions.

## How to expand the linear model?

- Simple polynomial transformations
- Interactions
- Step functions. E.g. transform education into  $k$  dummy variables.
- More complicated basis functions:
  - Piecewise polynomial: takes differential polynomial for different regions (split by knots)
  - Add constraint that there are no abrupt changes across regions.
  - Add constraint that first and second derivatives are the same. (For cubic splines.)

## How to expand the linear model?

- Simple polynomial transformations
- Interactions
- Step functions. E.g. transform education into  $k$  dummy variables.
- More complicated basis functions:
  - Piecewise polynomial: takes differential polynomial for different regions (split by knots)
  - Add constraint that there are no abrupt changes across regions.
  - Add constraint that first and second derivatives are the same. (For cubic splines.)
  - Add boundary constraint: linear before 1st knot or after last knot. (Natural spline.)

Error

## Error

- Reducible error:

$$\text{Var}(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$

## Error

- Reducible error:

$$\text{Var}(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$

- Bias-Variance tradeoff



## Error

- Reducible error:  
$$Var(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$
- Bias-Variance tradeoff
- As flexibility increases,  $Var(\hat{f})$  increases  
Model goes after each wrinkle in the training data

## Error

- Reducible error:  
$$Var(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$
- Bias-Variance tradeoff
- As flexibility increases,  $Var(\hat{f})$  increases  
Model goes after each wrinkle in the training data
- Say we have estimated the ideal function  $\hat{f}(X)$

## Error

- Reducible error:  
$$\text{Var}(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$
- Bias-Variance tradeoff
- As flexibility increases,  $\text{Var}(\hat{f})$  increases  
Model goes after each wrinkle in the training data
- Say we have estimated the ideal function  $\hat{f}(X)$
- Ideal w.r.t a loss function, e.g., average squared error:  $(Y - \hat{Y})^2$

## Error

- Reducible error:  
$$\text{Var}(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$
- Bias-Variance tradeoff
- As flexibility increases,  $\text{Var}(\hat{f})$  increases  
Model goes after each wrinkle in the training data
- Say we have estimated the ideal function  $\hat{f}(X)$
- Ideal w.r.t a loss function, e.g., average squared error:  $(Y - \hat{Y})^2$
- Ideal still leaves some error (irreducible error):
  - $\epsilon = Y - \hat{f}(x)$

# Error

- Reducible error:  
$$Var(\hat{f}) + [\text{Bias}(E[\hat{f}(x) - f(x)])]^2$$
- Bias-Variance tradeoff
- As flexibility increases,  $Var(\hat{f})$  increases  
Model goes after each wrinkle in the training data
- Say we have estimated the ideal function  $\hat{f}(X)$
- Ideal w.r.t a loss function, e.g., average squared error:  $(Y - \hat{Y})^2$
- Ideal still leaves some error (irreducible error):
  - $\epsilon = Y - \hat{f}(x)$
  - $E[(Y - \hat{f}(X))^2 | X = x] = (f(x) - \hat{f}(X))^2 + Var(\epsilon)$

# Evaluating Models

# Evaluating Models

- Deviance
  - Deviance  $\propto$   $-\text{Log-Likelihood}$

# Evaluating Models

- Deviance

- Deviance  $\propto -\text{Log-Likelihood}$
  - Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$



# Evaluating Models

- Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)

# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

# Evaluating Models

- Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

- AIC

# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

## – AIC

- Deviance + 2 \* df

# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

## – AIC

- Deviance +  $2 * \text{df}$
- In-sample - Out of sample Deviance  $\sim 2 * \text{df}$

# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

## – AIC

- Deviance +  $2 * \text{df}$
- In-sample - Out of sample Deviance  $\sim 2 * \text{df}$
- AIC  $\sim$  Out of sample Deviance

# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

## – AIC

- Deviance +  $2 * \text{df}$
- In-sample - Out of sample Deviance  $\sim 2 * \text{df}$
- AIC  $\sim$  Out of sample Deviance
- AIC overfits in high dimensions ( $\text{df} \sim n$ ).

# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

## – AIC

- Deviance + 2 \* df
- In-sample - Out of sample Deviance  $\sim$  2 \* df
- AIC  $\sim$  Out of sample Deviance
- AIC overfits in high dimensions (df  $\sim$  n).
- $\text{AICc} = \text{Deviance} + 2 * \text{df} * \frac{n}{n - \text{df} - 1}$



# Evaluating Models

## – Deviance

- Deviance  $\propto$   $-\text{Log-Likelihood}$
- Likelihood:  $p(y_1|x_1) \times p(y_2|x_2) \times \dots \times p(y_n|x_n)$
- $\hat{\beta}$  maximize Likelihood (or minimize Deviance)
- $R^2 = \frac{\text{Deviance of Fitted Model}}{\text{Deviance of Null Model}}$

## – AIC

- Deviance +  $2 * df$
- In-sample - Out of sample Deviance  $\sim 2 * df$
- AIC  $\sim$  Out of sample Deviance
- AIC overfits in high dimensions ( $df \sim n$ ).
- $AIC_c = \text{Deviance} + 2 * df * \frac{n}{n-df-1}$
- BIC = Deviance +  $df * \log(n)$
- BIC underfits when large  $n$ .

# Evaluating Classification Models

		<b>Observed</b>	
		true	false
<b>Predicted</b>	true	true positive	false positive
	false	false negative	true negative

# Evaluating Classification Models

		<b>Observed</b>	
		true	false
<b>Predicted</b>	true	true positive	false positive
	false	false negative	true negative

- Confusion matrix,  $c^2 - c$  total possible errors

## Evaluating Classification Models

		<b>Observed</b>	
		true	false
<b>Predicted</b>	true	true positive	false positive
	false	false negative	true negative

- Confusion matrix,  $c^2 - c$  total possible errors
- Accuracy:  $\frac{TP+TN}{TP+TN+FP+FN}$

# Evaluating Classification Models

		<b>Observed</b>	
		true	false
<b>Predicted</b>	true	true positive	false positive
	false	false negative	true negative

- Confusion matrix,  $c^2 - c$  total possible errors
- Accuracy:  $\frac{TP+TN}{TP+TN+FP+FN}$
- Error Rate:  $\frac{FP+FN}{TP+TN+FP+FN}$

# Evaluating Classification Models

		<b>Observed</b>	
		true	false
<b>Predicted</b>	true	true positive	false positive
	false	false negative	true negative

- Confusion matrix,  $c^2 - c$  total possible errors
- Accuracy:  $\frac{TP+TN}{TP+TN+FP+FN}$
- Error Rate:  $\frac{FP+FN}{TP+TN+FP+FN}$
- Sensitivity, TPR:  $\frac{TP}{TP+FN}$

# Evaluating Classification Models

		Observed	
		true	false
Predicted	true	true positive	false positive
	false	false negative	true negative

- Confusion matrix,  $c^2 - c$  total possible errors
- Accuracy:  $\frac{TP+TN}{TP+TN+FP+FN}$
- Error Rate:  $\frac{FP+FN}{TP+TN+FP+FN}$
- Sensitivity, TPR:  $\frac{TP}{TP+FN}$
- Specificity, FPR:  $\frac{TN}{FP+TN}$

# Evaluating Classification Models

		<b>Observed</b>	
		true	false
<b>Predicted</b>	true	true positive	false positive
	false	false negative	true negative

- Confusion matrix,  $c^2 - c$  total possible errors
- Accuracy:  $\frac{TP+TN}{TP+TN+FP+FN}$
- Error Rate:  $\frac{FP+FN}{TP+TN+FP+FN}$
- Sensitivity, TPR:  $\frac{TP}{TP+FN}$
- Specificity, FPR:  $\frac{TN}{FP+TN}$
- BER:  $\frac{1}{2}(TPR + TNR)$



## Evaluating Classification Models

- ROC: TPR Vs. FPR

## Evaluating Classification Models

- ROC: TPR Vs. FPR
- Precision: fraction of retrieved instances that are relevant

$$\frac{TP}{TP+FP}$$

## Evaluating Classification Models

- ROC: TPR Vs. FPR
- Precision: fraction of retrieved instances that are relevant

$$\frac{TP}{TP+FP}$$

- Recall: fraction of relevant instances that are retrieved

$$\frac{TP}{TP+FN}$$

# Evaluating Classification Models

- ROC: TPR Vs. FPR
- Precision: fraction of retrieved instances that are relevant

$$\frac{TP}{TP+FP}$$

- Recall: fraction of relevant instances that are retrieved

$$\frac{TP}{TP+FN}$$

- $F_1$ :  $2 \frac{\text{precision} * \text{recall}}{\text{precision} + \text{recall}}$

# Evaluating Classification Models

- ROC: TPR Vs. FPR
- Precision: fraction of retrieved instances that are relevant

$$\frac{TP}{TP+FP}$$

- Recall: fraction of relevant instances that are retrieved

$$\frac{TP}{TP+FN}$$

- $F_1$ :  $2 \frac{\text{precision} * \text{recall}}{\text{precision} + \text{recall}}$
- $F_\beta$ :  $(1 + \beta^2) \frac{\text{precision} * \text{recall}}{\beta^2 \text{precision} + \text{recall}}$

## Out of Sample Error

- Another way to assess model error

## Out of Sample Error

- Another way to assess model error
- $R^2$  always increases with more covariates.

## Out of Sample Error

- Another way to assess model error
- $R^2$  always increases with more covariates.
- Or: As model complexity increases, training error goes down.



## Out of Sample Error

- Another way to assess model error
- $R^2$  always increases with more covariates.
- Or: As model complexity increases, training error goes down.
- But out of sample error goes down and then up.

## Out of Sample Error

- Another way to assess model error
- $R^2$  always increases with more covariates.
- Or: As model complexity increases, training error goes down.
- But out of sample error goes down and then up.
- Out of sample  $R^2$  can be worse than  $\bar{y}$ .

## Out of Sample Error

- Another way to assess model error
- $R^2$  always increases with more covariates.
- Or: As model complexity increases, training error goes down.
- But out of sample error goes down and then up.
- Out of sample  $R^2$  can be worse than  $\bar{y}$ .
- Use of out of sample error to prevent overfitting

## Out of Sample Error

- Another way to assess model error
- $R^2$  always increases with more covariates.
- Or: As model complexity increases, training error goes down.
- But out of sample error goes down and then up.
- Out of sample  $R^2$  can be worse than  $\bar{y}$ .
- Use of out of sample error to prevent overfitting
- Net prediction error on test set can vary a lot.

## A Clarification

# Error in thinking about errors

## Error in thinking about errors

- In sciences, 'data mining' is a dirty 'phrase'

## Error in thinking about errors

- In sciences, 'data mining' is a dirty 'phrase'
- Jealousy?



## Error in thinking about errors

- In sciences, 'data mining' is a dirty 'phrase'
- Jealousy?
- Evokes concerns about false positives . . .

## Error in thinking about errors

- In sciences, ‘data mining’ is a dirty ‘phrase’
- Jealousy?
- Evokes concerns about false positives . . .
- But ‘mining’ is by definition ‘the extraction of valuable [stuff]’

## Error in thinking about errors

- In sciences, ‘data mining’ is a dirty ‘phrase’
- Jealousy?
- Evokes concerns about false positives . . .
- But ‘mining’ is by definition ‘the extraction of valuable [stuff]’
- So – is more data worse?

## Error in thinking about errors

- In sciences, ‘data mining’ is a dirty ‘phrase’
- Jealousy?
- Evokes concerns about false positives . . .
- But ‘mining’ is by definition ‘the extraction of valuable [stuff]’
- So – is more data worse?
- Not quite

## Error in thinking about errors

- In sciences, ‘data mining’ is a dirty ‘phrase’
- Jealousy?
- Evokes concerns about false positives . . .
- But ‘mining’ is by definition ‘the extraction of valuable [stuff]’
- So – is more data worse?
- Not quite
- Larger  $n$  allows for more precise estimation of relationship

## False Positives

- Significance testing:

# False Positives

- Significance testing:
  - Say .05, 5% false positive rate

# False Positives

- Significance testing:
  - Say .05, 5% false positive rate
  - Assume independence, 1 of 20 false positive



# False Positives

- Significance testing:
  - Say .05, 5% false positive rate
  - Assume independence, 1 of 20 false positive
  - Say 100 vars, 5 true positives, all sig., 5% of 95  $\sim$  5. So 50% false discovery rate.

# False Positives

- Significance testing:
  - Say .05, 5% false positive rate
  - Assume independence, 1 of 20 false positive
  - Say 100 vars, 5 true positives, all sig., 5% of 95  $\sim$  5. So 50%  
false discovery rate.
- Fixes:

# False Positives

- Significance testing:
  - Say .05, 5% false positive rate
  - Assume independence, 1 of 20 false positive
  - Say 100 vars, 5 true positives, all sig., 5% of 95  $\sim$  5. So 50% false discovery rate.
- Fixes:
  - Familywise error rate (Bonferroni)

# False Positives

- Significance testing:
  - Say .05, 5% false positive rate
  - Assume independence, 1 of 20 false positive
  - Say 100 vars, 5 true positives, all sig., 5% of 95  $\sim$  5. So 50% false discovery rate.
- Fixes:
  - Familywise error rate (Bonferroni)
  - Optimization can be done w.r.t. to cost of false positive and negative  
e.g. Increase cut-off marks in exams, Breast Cancer

# False Positives

- Significance testing:
  - Say .05, 5% false positive rate
  - Assume independence, 1 of 20 false positive
  - Say 100 vars, 5 true positives, all sig., 5% of 95  $\sim$  5. So 50% false discovery rate.
- Fixes:
  - Familywise error rate (Bonferroni)
  - Optimization can be done w.r.t. to cost of false positive and negative
    - e.g. Increase cut-off marks in exams, Breast Cancer
  - False Discovery Rate

## False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

## False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

- Can't be known but we can produce cutoffs so  $E(FDP) < q$

## False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

- Can't be known but we can produce cutoffs so  $E(FDP) < q$
- Benjamini and Hochberg (1995):



## False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

- Can't be known but we can produce cutoffs so  $E(FDP) < q$
- Benjamini and Hochberg (1995):
  - Rank the  $n$   $p$ -values, smallest to largest,  $p_1 \dots p_n$ .

## False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

- Can't be known but we can produce cutoffs so  $E(FDP) < q$
- Benjamini and Hochberg (1995):
  - Rank the  $n$   $p$ -values, smallest to largest,  $p_1 \dots p_n$ .
  - $p$ -value cut-off =  $\max (p_k : p_k \leq \frac{qk}{n})$

## False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

- Can't be known but we can produce cutoffs so  $E(FDP) < q$
- Benjamini and Hochberg (1995):
  - Rank the  $n$   $p$ -values, smallest to largest,  $p_1 \dots p_n$ .
  - $p$ -value cut-off =  $\max (p_k : p_k \leq \frac{qk}{n})$
  - All  $p$ -values below that accepted

# False Discovery Rate

$$\text{False discovery Proportion} = \frac{\# \text{ of FP}}{\# \text{ of Sig. Results}}$$

- Can't be known but we can produce cutoffs so  $E(FDP) < q$
- Benjamini and Hochberg (1995):
  - Rank the  $n$   $p$ -values, smallest to largest,  $p_1 \dots p_n$ .
  - $p$ -value cut-off =  $\max (p_k : p_k \leq \frac{qk}{n})$
  - All  $p$ -values below that accepted
  - Caveat: Assumes independence

## Other Ways of Being Wrong

- Sampling

## Other Ways of Being Wrong

- Sampling
- Changing data generating process over time

## Other Ways of Being Wrong

- Sampling
- Changing data generating process over time
- Confounding variables ('data leakage')

## Other Ways of Being Wrong

- Sampling
- Changing data generating process over time
- Confounding variables ('data leakage')
- Coding and computational errors