FIT2086 Lecture 12 Revision

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House Keeping

- Assignment #2
 - Everyone did well
 - From Clayton cohort:
 - Wanshu Li and Alex Hughes got 30/30 after bonus marks
 - Mukund Premkumar got 30/30 before bonus marks well done!
- Assignment #3
 - Due this coming Sunday
 - Submit one PDF file and appropriate R files
- Subject Evaluation of Teaching and Units (SETU)
 - Those who have not yet done so, can you please fill out the SETU feedback
 - Greatly appreciated!

- On completion of this unit, students should be able to:
 - perform exploratory data analysis with descriptive statistics on given datasets; √
 - ② construct models for inferential statistical analysis; √
 - ullet produce models for predictive statistical analysis; \checkmark
 - perform fundamental random sampling, simulation and hypothesis testing for required scenarios; √
 - implement a model for data analysis through programming and scripting; √
 - 6 interpret results for a variety of models. √

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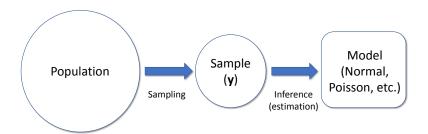
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Revision from Lecture 1



- Population: A large collection of objects or items with measureable attributes
- Sample: A finite number of recordings of attributes of items from a population
- Model: A mathematical or algorithmic description of the population learned/inferred from the sample



Revision from Lecture 2 (1)

- $\mathbb{P}(X = x, Y = y)$ is joint probability of X = x and Y = y.
 - Sum-rule (marginal probability):

$$\mathbb{P}(X=x) = \sum_{y} \mathbb{P}(X=x, Y=y)$$

Conditional probability

$$\mathbb{P}(X = x \mid Y = y) = \frac{\mathbb{P}(X = x, Y = y)}{\mathbb{P}(Y = y)}$$

• Cumulative distribution function (for ordered *x*):

$$\mathbb{P}(X \le x) = \sum_{x \le x} \mathbb{P}(X = x)$$

• Also: $\mathbb{P}(X > x) = 1 - \mathbb{P}(X \le x)$.



Revision from Lecture 2 (2)

• Let $\mathbb{P}(X = x) \equiv p(x)$; expectation and variance of f(X):

$$\begin{split} & \mathbb{E}\left[f(X)\right] &= \sum_{x} p(x) f(x) \\ & \mathbb{V}\left[f(X)\right] &= \mathbb{E}\left[\left(X - \mathbb{E}\left[f(X)\right]\right)^{2}\right] \end{split}$$

with integral replacing sum for continuous RVs.

- Some useful rules:
 - $\mathbb{E}\left[f(X) + g(Y)\right] = \mathbb{E}\left[f(X)\right] + \mathbb{E}\left[g(Y)\right]$
 - $\bullet \ \mathbb{E}\left[cf(X)\right] = c\mathbb{E}\left[f(X)\right]$
 - $\bullet \ \mathbb{V}\left[cf(X)\right] = c^2 \mathbb{V}\left[f(X)\right]$
- ullet If X, Y are independent RVs
 - $\mathbb{E}\left[f(X)g(Y)\right] = \mathbb{E}\left[f(X)\right]\mathbb{E}\left[g(Y)\right]$
 - $\bullet \ \mathbb{V}\left[f(X)+g(Y)\right]=\mathbb{V}\left[f(X)\right]+\mathbb{V}\left[g(Y)\right]$



Revision from Lecture 2 (3)

- Parametric distributions as models of populations
- Normal distribution; $X \in \mathbb{R}$, $X \sim N(\mu, \sigma^2)$

$$\mathbb{E}\left[X\right] = \mu, \quad \mathbb{V}\left[X\right] = \sigma^2$$

• Bernoulli distribution; $X \in \{0,1\}$, $X \sim \mathrm{Be}(\theta)$

$$\mathbb{E}[X] = \theta, \quad \mathbb{V}[X] = \theta(1 - \theta)$$

 \bullet Binomial distribution; $X \in \{0,1,\ldots,n\}$, $X \sim \mathrm{Bin}(\theta,n)$

$$\mathbb{E}[X] = n\theta, \quad \mathbb{V}[X] = n\theta(1-\theta)$$

• Poisson distribution; $X \in \{0, 1, 2, ...\}$, $X \sim Poi(\lambda)$

$$\mathbb{E}[X] = \lambda, \quad \mathbb{V}[X] = \lambda$$



Revision from Lecture 3 (1)

- We looked at problem of parameter estimation
- Method of maximum likelihood

$$\hat{\theta}_{\mathrm{ML}} = \arg\max_{\boldsymbol{\theta}} \{ p(\mathbf{y} \,|\, \boldsymbol{\theta}) \}$$

Maximum likelihood estimators for the normal

$$\hat{\mu}_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} y_i, \quad \hat{\sigma}_{\text{ML}} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu}_{\text{ML}})^2}$$

Maximum likelihood estimator for Poisson

$$\hat{\lambda}_{\mathrm{ML}} = \frac{1}{n} \sum_{i=1}^{n} y_i$$

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Revision from Lecture 3 (2)

- Sampling distributions of estimators
- Bias and variance of an estimator

$$b_{\theta}(\hat{\theta}) = \mathbb{E}\left[\hat{\theta}\right] - \theta, \ \operatorname{Var}_{\theta}(\hat{\theta}) = \mathbb{V}\left[\hat{\theta}\right]$$

Mean squared error of an estimator

$$MSE_{\theta}(\hat{\theta}) = b_{\theta}^{2}(\hat{\theta}) + Var_{\theta}(\hat{\theta})$$

• If Y_1, \ldots, Y_n have $\mathbb{E}\left[Y_i\right] = \mu$ and $\mathbb{V}\left[Y_i\right] = \sigma^2$ then

$$b_{\mu}(\bar{Y}) = 0$$
, $\operatorname{Var}_{\mu}(\bar{Y}) = \frac{\sigma^2}{n}$, $\operatorname{MSE}_{\mu}(\bar{Y}) = \frac{\sigma^2}{n}$

• An estimator $\hat{\theta}$ is consistent if

$$b_{\theta}(\hat{\theta}) \to 0, \quad \text{Var}_{\theta}(\hat{\theta}) \to 0,$$

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, $\operatorname{Var}_{\theta}(\hat{\theta}) \to 0$,

as $n \to \infty$ for all θ .



Example: ML Estimation of a Poisson (1)

• Recall the Poisson distribution with rate λ :

$$p(y \mid \lambda) = \frac{\lambda \exp(-y\lambda)}{y!}.$$

• If $\mathbf{y} = (y_1, \dots, y_n)$ are n integers, then the likelihood for a Poisson model is

$$p(\mathbf{y} \mid \lambda) = \prod_{i=1}^{n} p(y_i \mid \lambda)$$

$$= \left(\frac{\lambda \exp(-y_1 \lambda)}{y_1!}\right) \cdot \left(\frac{\lambda \exp(-y_2 \lambda)}{y_2!}\right) \cdots \left(\frac{\lambda \exp(-y_n \lambda)}{y_n!}\right)$$

$$= \frac{\lambda^n \exp(-\lambda \sum_{i=1}^n y_i)}{\prod_{i=1}^n y_i!}$$

by $e^a e^b = e^{a+b}$ and independence of y_1, \ldots, y_n .

Example: ML Estimation of a Poisson (2)

The negative log-likelihood is then

$$L(\mathbf{y} \mid \lambda) = -n \log \lambda + \lambda \sum_{i=1}^{n} y_i + \sum_{i=1}^{n} \log y_i!$$

 \bullet To find the ML estimator of λ we need to minimise $L(\mathbf{y}\,|\,\lambda)$, or equivalently solve

$$\frac{dL(\mathbf{y} \mid \lambda)}{d\lambda} = 0,$$

for λ .

Example: ML Estimation of a Poisson (3)

The derivative is given by

$$\frac{dL(\mathbf{y}\mid\lambda)}{d\lambda} = -\frac{n}{\lambda} + \sum_{i=1}^{n} y_{i} \tag{1}$$

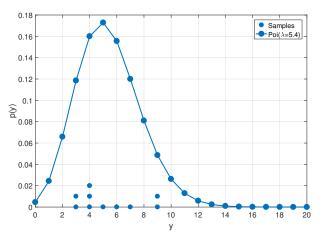
where we use $d \log x/dx = 1/x$

ullet Setting (1) to zero and solving for λ yields

$$\hat{\lambda} = \frac{1}{n} \sum_{i=1}^{n} y_i$$

So, the ML estimator for the Poisson rate is the sample mean.
 ⇒ this is not always the case!

Example: ML Estimation of a Poisson (4)



Data samples and the Poisson distribution fitted by maximum likelihood with $\hat{\lambda}=5.4$. Samples were $\mathbf{y}=(7,9,3,5,3,4,4,9,4,6)$.

Revision from Lecture 4

• Central limit theorem: if Y_1,\ldots,Y_n are RVs with $\mathbb{E}\left[Y_i\right]=\mu$ and $\mathbb{V}\left[Y_i\right]=\sigma^2$ then

$$\sum_{i=1}^{n} Y_i \stackrel{d}{\to} N\left(n\mu, n\sigma^2\right)$$

• Implies distribution of the sample mean \bar{Y} for Y_1,\ldots,Y_n with $\mathbb{E}\left[Y_i\right]=\mu$ and $\mathbb{V}\left[Y_i\right]=\sigma^2$ satisfies

$$\bar{Y} \stackrel{d}{\to} N\left(\mu, \frac{\sigma^2}{n}\right)$$

Confidence Intervals

 \bullet An interval estimator returns an interval of plausible values for a population parameter θ

Confidence Intervals

We use the method of confidence intervals.

We say the interval estimator $(\hat{\theta}_{\alpha}^{-}(\mathbf{y}), \hat{\theta}_{\alpha}^{+}(\mathbf{y}))$ generates a $100(1-\alpha)$ -percent confidence interval, for $\alpha \in (0,1)$, if

$$\mathbb{P}\left(\theta \in (\hat{\theta}_{\alpha}^{-}(\mathbf{y}), \ \hat{\theta}_{\alpha}^{+}(\mathbf{y}))\right) = 1 - \alpha,$$

where the probability is with respect to all the different samples ${\bf y}$ we could draw from our population.

• $100(1-\alpha)\%$ confidence intervals: cover the true population parameter for 95% of possible samples we could draw from our population



CI for Normal Mean, Known Variance

• Assuming the population is normally distributed with (unknown) mean μ and (known) variance σ^2 , these results yield the following 95% confidence interval for $\hat{\mu}_{\rm ML} \equiv \bar{Y}$,

$$\left(\hat{\mu}_{\mathrm{ML}} - 1.96 \frac{\sigma}{\sqrt{n}}, \ \hat{\mu}_{\mathrm{ML}} + 1.96 \frac{\sigma}{\sqrt{n}}\right)$$

• More generally, a $100(1-\alpha)\%$ confidence interval is given by:

$$\left(\hat{\mu}_{\mathrm{ML}} - z_{\alpha/2} \frac{\sigma}{\sqrt{n}}, \ \hat{\mu}_{\mathrm{ML}} + z_{\alpha/2} \frac{\sigma}{\sqrt{n}}\right)$$

where $z_{\alpha/2}$ is the $100(1-\alpha/2)$ percentile of the unit normal:

- for $\alpha = 0.05$, $z_{0.025} = Q(p = 0.975) \approx 1,96$;
- for $\alpha = 0.01$, $z_{0.005} = Q(p = 0.995) \approx 2.576$;
- for general α , use $Q(p=1-\alpha/2)$

where $Q(\cdot)$ is the quantile function for the unit normal



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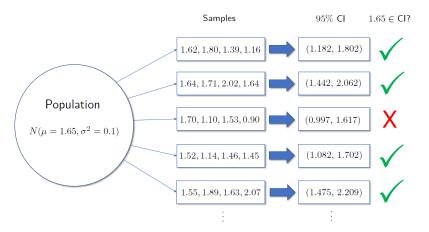
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CI for Normal Mean, Known Variance (2)



Cartoon showing multiple samples drawn from a $N(\mu=1.65,\sigma^2=0.1)$ population, along with the 95% confidence intervals for each sample. 5% of possible samples will result in CIs that <u>do not</u> include $\mu=1.65$.

Example: Normal Mean, Known Variance (1)

• Example: We have the following samples of body mass index taken people with diabetes from the Pima ethnic group

$$\mathbf{y} = (53.2, 33.6, 36.6, 42.0, 33.3, 37.8, 31.2, 43.4)$$

- Imagine we are given a value for the population variance of 43.75 which has been estimated by another, very large study of people from the Pima group.
- \bullet Task: Estimate the BMI of diabetic Pima people and construct a 95% CI
- Our best guess at the population mean BMI for Pima people with diabetes is

$$\hat{\mu}_{\rm ML} = 38.88$$



Example: Normal Mean, Known Variance (2)

 \bullet Our 95% CI is then

$$\left(38.88 - 1.96\sqrt{43.75/8}, 38.88 + 1.96\sqrt{43.75/8}\right)$$

which is equal to

In words, we summarise our analysis by:

"The estimated mean BMI of people from the Pima ethnic group with diabetes (sample size n=8) is $38.88\,kg/m^2$. We are 95% confident the population mean BMI for this group is between $34.3\,kg/m^2$ and $43.75\,kg/m^2$."

CI for Normal Mean, Unknown Variance

- Let us make our assumptions more realistic
 - $Y_1, \ldots, Y_n \sim N(\mu, \sigma^2)$ with both μ and σ^2 unknown.
- ullet We can instead estimate σ^2 and use the Student-t distribution

$$\left(\hat{\mu}_{\mathrm{ML}} - t_{\alpha/2, n-1} \frac{\hat{\sigma}_u}{\sqrt{n}}, \ \hat{\mu}_{\mathrm{ML}} + t_{\alpha/2, n-1} \frac{\hat{\sigma}_u}{\sqrt{n}}\right)$$

which achieves $100(1-\alpha)\%$ coverage if population is Gaussian

- $\hat{\sigma}_u^2$ is the unbiased estimate of variance from our sample
- Here, $t_{\alpha/2}$ is the $100(1-\alpha/2)$ -th percentile of the standard Student t-distribution with n-1 degrees of freedom
- To compare with normal percentiles, recall $z_{0.025} = 1.96$;
 - for n = 3, $t_{0.025,2} \approx 4.3$;
 - for n = 6, $t_{0.025,5} \approx 2.57$;
 - for n = 11, $t_{0.025,10} \approx 2.22$;



CI for Difference of Normal Means

- ullet We have two samples \mathbf{y}_A and \mathbf{y}_B
 - Wish to get confidence interval for $\mu_A \mu_B$ (i.e., the difference in population means)
- Instead, let us assume μ_A , μ_B , σ_A^2 , σ_B^2 are all unknown
- Let $\hat{\sigma}_A^2$ and $\hat{\sigma}_B^2$ be unbiased estimates of the variance in sample A and B, respectively
- Then the following interval:

$$\left(\hat{\mu}_{A} - \hat{\mu}_{B} - z_{\alpha/2}\sqrt{\frac{\hat{\sigma}_{A}^{2}}{n_{A}} + \frac{\hat{\sigma}_{B}^{2}}{n_{B}}}, \quad \hat{\mu}_{A} - \hat{\mu}_{B} + z_{\alpha/2}\sqrt{\frac{\hat{\sigma}_{A}^{2}}{n_{A}} + \frac{\hat{\sigma}_{B}^{2}}{n_{B}}}\right)$$

is an approximate $100(1-\alpha)\%$ confidence interval for $\hat{\mu}_A - \hat{\mu}_B$, with the approximation getting better for increasing n_A and n_B .



Revision from Lecture 5

Hypothesis testing; test null hypothesis vs alternative

 H_0 : null hypothesis

٧S

 H_A : alternative hypothesis

- A test-statistic measures how different our observed sample is from the null hypothesis
- ullet A p-value quantifies the evidence against the null hypothesis
- A *p*-value is the probability of seeing a sample that results in a test statistic as extreme, or more extreme, than the one we observed, just by chance <u>if the null was true</u>.

Testing μ with known variance

- Assume population follows normal distribution with unknown mean and known variance σ^2 ; testing inequality of μ
 - First calculate the ML estimate of the mean/sample mean

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} y_i$$

2 Then calculate the z-score

$$z_{\hat{\mu}} = \frac{\hat{\mu} - \mu_0}{(\sigma/\sqrt{n})}$$

3 Then calculate the *p*-value:

$$p = \left\{ \begin{array}{ll} 2 \, \mathbb{P}(Z < -|z_{\hat{\mu}}|)) & \quad \text{if } H_0 : \mu = \mu_0 \text{ vs } H_A : \mu \neq \mu_0 \\ 1 - \mathbb{P}(Z < z_{\hat{\mu}}) & \quad \text{if } H_0 : \mu \leq \mu_0 \text{ vs } H_A : \mu > \mu_0 \\ \mathbb{P}(Z < z_{\hat{\mu}}) & \quad \text{if } H_0 : \mu \geq \mu_0 \text{ vs } H_A : \mu < \mu_0 \end{array} \right..$$

where $Z \sim N(0,1)$



Example: Testing if $\mu = \mu_0$ (1)

- For US women aged between 20 to 34 years of age, the population body mass index (BMI) has
 - ullet an approximate mean of $26.8kg/m^2$; and
 - an approximate standard deviation of $4.5kg/m^2$.

(Source: Center for Disease Control)

 We have BMI measured on a sample of women aged 20-34 from the Pima ethnic group, without diabetes:

$$\mathbf{y} = (46.8, 27.8, 32.5, 39.5, 32.8, 31.0, 26.2, 20.8)$$

 Using this data, can we say whether women aged 20-34 in this Pima cohort have the same average BMI as the general US population?

Example: Testing if $\mu = \mu_0$ (2)

- We want to test:
 - $H_0: \mu=26.8$ vs $H_A: \mu \neq 26.8$, μ is the population mean BMI of Pima women aged 20-34.
- ullet The estimated mean $\hat{\mu}$ from our sample is

$$\hat{\mu} = 32.175$$

• From this we can calculate the z-score as

$$z_{\hat{\mu}} = \frac{32.175 - 26.8}{(4.5/\sqrt{8})} = 3.3784$$

This yields a p-value of

$$1 - \mathbb{P}(-z_{\hat{\mu}} < Z < z_{\hat{\mu}}) = 2 * pnorm(-abs(3.3784))$$

= 7.29×10^{-4}



Example: Testing if $\mu = \mu_0$ (3)

- How to interpret?
- A p-value of 7.29×10^{-4} can be interpreted as follows: If the null was true, i.e., Pima ethnic women aged 20-34 have the same BMI as the average US woman aged 20-34, then the chance of observing a sample with as an extreme, or more extreme, difference from the null as the one that we saw would be less than 1/1371.
- So quite unlikely to happen just by vagaries of sampling
 ⇒ strong evidence against the null.

Testing μ with unknown variance

• Then our test statistic is a *t*-score

$$t_{\hat{\mu}} = \frac{\hat{\mu} - \mu_0}{(\hat{\sigma}/\sqrt{n})}$$

where the unknown population σ is replaced with our estimate

• If the null was true, then

$$t_{\hat{\mu}} \sim \mathrm{T}(n-1)$$

where $\mathrm{T}(d)$ denotes a standard t-distribution with d degrees-of-freedom

The p-value is then

$$p = \left\{ \begin{array}{ll} 2 \, \mathbb{P}(T < -|t_{\hat{\mu}}|)) & \text{if } H_0 : \mu = \mu_0 \text{ vs } H_A : \mu \neq \mu_0 \\ 1 - \mathbb{P}(T < t_{\hat{\mu}}) & \text{if } H_0 : \mu \leq \mu_0 \text{ vs } H_A : \mu > \mu_0 \\ \mathbb{P}(T < t_{\hat{\mu}}) & \text{if } H_0 : \mu \geq \mu_0 \text{ vs } H_A : \mu < \mu_0 \end{array} \right..$$

where $T \sim T(n-1)$.



Testing difference of means, unknown variances

- ullet If we relax assumption that $\sigma_x^2=\sigma_y^2$ things get hard
- An approximate p-value can be computed by substituting estimates $\hat{\sigma}_x^2$ and $\hat{\sigma}_y^2$ into the formulae for known variance
- This give us the test statistic

$$z_{(\hat{\mu}_x - \hat{\mu}_y)} = \frac{\dot{\mu}_x - \dot{\mu}_y}{\sqrt{\frac{\hat{\sigma}_x^2}{n_x} + \frac{\hat{\sigma}_y^2}{n_y}}}$$

which is approximately N(0,1) for large samples.

We can then find approximate p-values using:

$$p \approx \left\{ \begin{array}{ll} 2 \, \mathbb{P}(Z < -|z_{(\hat{\mu}_x - \hat{\mu}_y)}|) & \quad \text{if } H_0 : \mu = \mu_0 \text{ vs } H_A : \mu \neq \mu_0 \\ 1 - \mathbb{P}(Z < z_{(\hat{\mu}_x - \hat{\mu}_y)}) & \quad \text{if } H_0 : \mu \leq \mu_0 \text{ vs } H_A : \mu > \mu_0 \\ \mathbb{P}(Z < z_{(\hat{\mu}_x - \hat{\mu}_y)}) & \quad \text{if } H_0 : \mu \geq \mu_0 \text{ vs } H_A : \mu < \mu_0 \end{array} \right. .$$

 More exact but complicated procedures exist; t.test() in R implements some of these



Revision from Lecture 6

- Imagine we have measured p+1 variables on n individuals (people, objects, things)
- ullet We would like to predict one of the variables using the remaining p variables
- If the variable we are predicting is categorical, we are performing classification
 - Example: predicting if someone has diabetes from medical measurements.
- If the variable we are predicting is numerical, we are performing regression
 - Example: Predicting the quality of a wine from chemical and seasonal information.

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Revision from Lecure 6 (1)

Linear regression

$$\mathbb{E}[Y_i] = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \dots + \beta_p x_{i,p}$$

- ullet eta_0 is the intercept (value of $\mathbb{E}\left[Y\right]$ when all predictors are zero)
- ullet eta_j is a coefficient (change in $\mathbb{E}\left[Y\right]$ per unit change in $x_{j,i}$)
- Residuals (errors)

$$e_i = y_i - \beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \dots - \beta_p x_{i,p}$$

Residual sum-of-squares

$$RSS(\beta_0, \beta_1, \dots, \beta_p) = \sum_{i=1}^n e_i^2$$

• Least-squares estimates linear model by finding $\beta_0,\beta_1,\ldots,\beta_p$ that minimise the RSS



Revision from Lecure 6 (2)

• R² measure of goodness-of-fit

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}$$

where TSS is the sum of squared errors for the mean model

- Sometimes our predictors are categorical variables
 - We turn them into K-1 new predictors (indicator variables)
- Sometimes predictor-target relationship is nonlinear
 - Nonlinear transformations of our variables can help
 - Polynomial transformations offer general purpose nonlinear fits
 - ullet We turn our variable into q new variables of the form:

$$x_{i,j} \Rightarrow x_{i,j}, x_{i,j}^2, x_{i,j}^3, \dots, x_{i,j}^q$$

Revision from Lecture 7 (1)

- ullet We also have p predictor variables X_1,\dots,X_p
- ullet We can build a classifier for Y using our predictors

$$P(y | x_1, x_2, \dots, x_p) = \frac{P(y, x_1, \dots, x_p)}{P(x_1, \dots, x_p)}$$

 Naïve Bayes assumes predictors are conditionally independent, given the value of the target

$$P(x_1,...,x_p | y) = \prod_{j=1}^p P(x_j | y)$$

Naïve Bayes classifier:

$$P(y | x_1, \dots, x_p) = \frac{\prod_{j=1}^p P(x_j | y) P(y)}{P(x_1, \dots, x_p)}$$

Revision from Lecture 7 (2)

A logistic regression models the conditional log-odds as

$$\log \left(\frac{\mathbb{P}(Y_i = 1 \mid x_{i,1}, \dots, x_{i,p})}{\mathbb{P}(Y_i = 0 \mid x_{i,1}, \dots, x_{i,p})} \right) = \beta_0 + \sum_{j=1}^p \beta_j x_{i,j} \equiv \eta_i$$

Logistic regression model of conditional probability

$$\mathbb{P}(Y_i = 1 \mid x_{i,1}, \dots, x_{i,p}) = \frac{1}{1 + \exp(-\eta_i)}$$

- Estimated using maximum likelihood
- Performance measures for classification
 - Classification error
 - Sensitivity and specificity
 - Area-under-the-curve (AUC)
 - Logarithmic loss



Revision from Lecture 8 (1)

- How many predictors should we include in our linear model?
- Underfitting
 - Omitting important predictors
 - Leads to systematic error ("bias") in predicting the target
- Overfitting
 - Including spurious predictors
 - Leads our model to "learn" noise and random variation
- Methods to trade off bias and variance
 - Hypothesis testing $\beta_j = 0$ vs $\beta_j \neq 0$
 - Multiple hypothesis testing problem, Bonferroni
 - Penalized likelihood likelihood plus complexity penalty
 - · AIC, KIC, BIC, RIC
 - Cross-validation



Revision from Lecture 8 (2)

- All-subsets selection:
 - Try all combination of predictors to model with smallest model selection criterion score
- Forward selection algorithm:
 - Start with the empty model;
 - Find the predictor that reduces info criterion by most
 - If no predictor improves model, end.
 - 4 Add this predictor to the model
 - Seturn to Step 2
- Backwards selection is related algorithm
 - Start with the full model and remove predictors

Revision from Lecture 8 (3)

- Statistical instability;
 - Small changes in data \Rightarrow big changes in model
- Ridge regression, squared penalty on coefficients

$$(\hat{\beta}_0, \hat{\beta}_{\lambda}) = \underset{\beta_0, \beta}{\operatorname{arg\,min}} \left\{ \operatorname{RSS}(\beta_0, \beta) + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$

Lasso regression, absolute penalty on coefficients

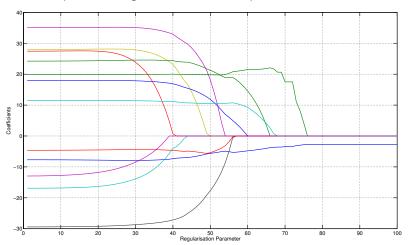
$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}}_{\lambda}) = \underset{\beta_0, \boldsymbol{\beta}}{\operatorname{arg\,min}} \left\{ \operatorname{RSS}(\beta_0, \boldsymbol{\beta}) + \lambda \sum_{j=1}^p |\beta_j| \right\}$$

- Lasso can estimate coefficients to be zero, ridge cannot
- ullet Vary λ to get a "path" of different complexity models
 - $\lambda=0$ most complex, $\lambda=\infty$ least complex
- Use cross validation to choose a good λ



Lasso Regression (3)

• Example lasso regression coefficient path



Revision from Lecture 9 (1)

- Machine learning methods
- Cross validation for model selection
 - Withhold data to estimate prediction error
 - K-fold CV divides data up into K equal sized groups
 - ullet Train on K-1 folds, predict on the remaining fold
- Decision Trees
 - Split the data up by asking questions of the predictors
 - Number of leaves determines complexity of tree
 - Easy to interpret, flexible
- Methods for learning trees
 - Greedy growing of trees find best split at each step
 - Backwards pruning of large tree
 - Use CV to select number of leaves in the tree

Revision from Lecture 9 (2)

- Trees have low bias, high variance
- One solution: random forests
 - Grow many trees with guided random search
 - Aggregate predictions from the trees
 - Stable, low variance, but loses interpretability
- k-nearest neighbours (kNN) methods
 - Assume individuals similar in predictors are similar in targets
 - ullet Find k "most similar" individuals in data to new individual
 - Use their targets to predict target for new individual
- Use CV to select k, other tuning parameters

K-fold Cross Validation

- ullet Outer loop: try different model complexities γ
 - For i=1 to m
 - $oldsymbol{0}$ Partition data into K equal sized, disjoint subsets

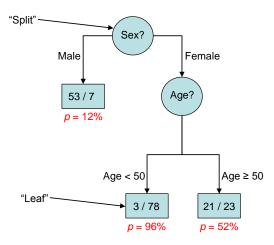
$$\mathbf{y}^{(1)}, \mathbf{y}^{(2)}, \mathbf{y}^{(3)}, \dots, \mathbf{y}^{(K)}$$

- $\bullet \quad \text{For } k = 1 \text{ to } K$
 - **1** Fit model $\mathcal{M}(\gamma)$ to all $\mathbf{y}^{(i)}$ except for i=k
 - ② Use fitted model to predict onto $\mathbf{y}^{(k)}$
 - 3 Calculate and accumulate prediction errors
- ② Average all m accumulated prediction errors
- Once this is done, we have CV errors for each complexity γ \Rightarrow choose the γ with the smallest estimated error
- ullet The larger the m, the more stable the estimates (but slower)

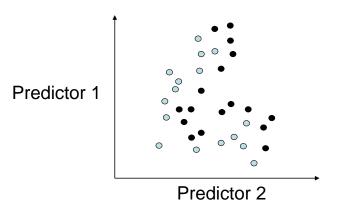


Decision Trees

• Example tree: predicting high blood pressure

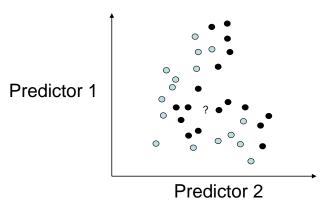


k-Nearest Neighbours Example 1 (1)



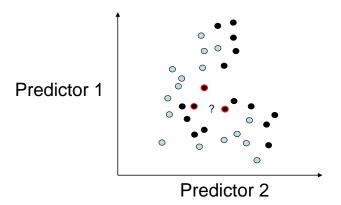
Example data set: black are individuals with disease, blue are those without

k-Nearest Neighbours Example 1 (2)



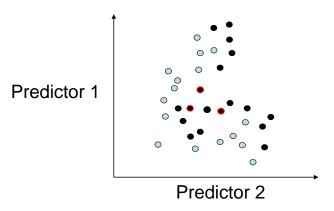
We want to predict the disease status of the individual marked with a "?" using a k nearest neighbour method with k=3 neighbours

k-Nearest Neighbours Example 1 (3)



We find the closest k=3 individuals

k-Nearest Neighbours Example 1 (4)



They all have the disease, so we predict that our new individual will also have the disease

Revision from Lecture 10 (1)

- Unsupervised Learning
- ullet n individuals, q attributes
 - No "target"; instead, discover structure inherent in data
- Clustering
 - ullet Model the population as K distinct sub-populations
 - ullet Learn both K and the subpopulation parameters
- *k*-means clustering algorithm
 - Allocate individuals to closest clusters
 - Re-estimate cluster centres
 - Iterate until convergence

Revision from Lecture 10 (2)

Mixture modelling

 Models data as a mixture of probability distributions (subpopulations)

$$p(y_{i,j}) = \sum_{k=1}^{K} \alpha_k p(y_{i,j} \mid \boldsymbol{\theta}_{k,j})$$

- Each subpopulation characterised by distributions
- "Soft" assignment of individuals to classes
- Intrinsic classification

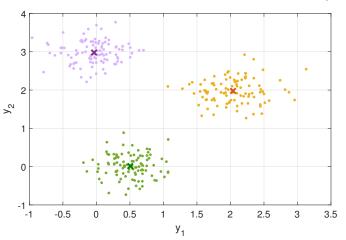
Matrix completion

- Missing entries in our data matrix
- Try to estimate the values of the missing data
- Applications: imputation, recommender systems
- Mixture modelling approach, k-NN approaches



K-means Clustering

• Find the centroids that minimise within-cluster sum-of-squares



Summary

- I have put some links up in Lecture 12 to books/book chapters you can read if you want to learn more about data science
- FIT3154 Advanced data analysis is a good follow up if you enjoyed this
 - More focus on machine learning, including neural networks/deep learning
- Good luck in the exam!