Applied Statistics

Week 6 - Multivariate Analysis

This week

• Monday:

• Intro to Multivariate analysis - Fisher discriminant/Iris data

• Tuesday:

• Working on project two

• Friday:

• A peek into more involved Multivariate techniques / machine learning

- You want to figure out a method s.t. you are 95% sure a person is male:
- Easy: Gather height data from 10000 people, Estimate cut with 95% purity



- You want to figure out a method s.t. you are 95% sure a person is male:
- Your friend now gives you shoe size data as well:
 - More information: Better separation
 - Cut on both observables?





ple e a person is male:

- You want to figure out a method s.t. you are 95% sure a person is male:
- Your friend now gives you shoe size data as well:
 - Look at observable correlations







- You want to figure out a method s.t. you are 95% sure a person is male:
- Your friend now gives you shoe size data as well:





Promising!



- You want to figure out a method s.t. you are 95% sure a person is male:
- Add weight, etc. to your data.
 - Not intuitive how to define cut in N dimensions.
- Moreover, you are going to run out of statistics very fast if you try to populate an N dimensional histogram. size
 - 10 bins in 9 dimensions will require $>10^9$ entries...
- Introduce the Fisher discriminant
- But first a short word on separation



Shoe

Male Female Cut?

Height

Separation of data

- Separation a Null and and Alternative Hypothesis
 - In general: Null is what you are 'testing'. Alternative is what you are comparing to.
 - Example below is trying to keep as much Null as possible.



Null is true	Null is false
I-α Correct	β Type II error
α Type I error	Ι-β Correct

Reality

Separation of data

- Separation a Null and and Alternative Hypothesis
- As always, there does not exist a general measure of separation.



Multivariate Analysis

- Given a vector of data **x**, construct a test statistic to distinguish two hypotheses: H_{Null} and $H_{Alt:}$
- Optimal: The Likelihood Ratio.

Discriminating function

Test statistic
$$\longrightarrow t(\mathbf{x}) = \frac{f(\mathbf{x}|H_{Null})}{f(\mathbf{x}|H_{Alt})}$$

Vector of measurements $x = (x_1, ..., x_N)$

The value of the test statistic for a series of measurement can then be compared to what you know from simulation, or data of known outcome. This should tell you the probability that Null can describe your observations.

- Most real life cases, f can not be determined analytically.
- known type (H_{Null}/H_{Alt})
- criteria: Multivariate Analysis.

Estimated from simulation or data of

Can in general be N dimensional

Instead of populating histograms with many dimensions. Create an effective form of f and optimize under some

• Idea: Construct t as a linear combination of **x**:

$$t(\mathbf{x}) = \sum_{i=1}^{N} a_i x_i = a^T x$$

- We just need to figure out what a is.
- Goal is to construct them s.t. we have the maximal separation between the functions:

 $g(t|H_{Null}) \qquad g(t|H_{Alt})$

• This requires a bit of Linear Algebra



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g(t)

• Start by calculating mean and covariance for Null and Alt:

$$(\mu_k)_i = \int x_i f(x|H_k) dx_1 \dots dx_N$$
$$(V_k)_{ij} = \int (x - \mu_k)_i (x - \mu_k)_j f(x|H_k) dx_1 \dots dx_N$$

• Similarly, we can calculate the mean and variance of t:

$$\tau_k = \int tg(t|H_k)dt = a^T \mu_k$$
$$\Sigma_k^2 = \int (t - \tau_k)^2 g(t|H_k)dt = a^T V_k a$$

• k's indicate Null or Alt, i's/j's are measurement indices



• Find a s.t. the following separation is optimized:

$$J(a) = \frac{(\tau_{Null} - \tau_{Alt})^2}{\Sigma_{Null}^2 + \Sigma_{Alt}^2}$$

- Derive and set equal to zero:
 - Go trough rather lengthy derivation (see link)...Turns out it is useful to define:

$$W_{ij} = (V_{Null} + V_{Alt})_{ij}$$

• Resulting in a should be proportional to:

$$a \propto W^{-1}(\mu_{Null} - \mu_{Alt})$$



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Formal derivation can be found here: http://www.csd.uwo.ca/~olga/Courses/CS434a_541a/Lecture8.pdf

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The Fisher Discriminant - Summary

- In order to construct the linear discriminant:
- Calculate means from 'training' data sample: $(\mu_k)_i = \int x_i f(x|H_k) dx_1 \dots dx_N$
- Calculate covariance matrices: $(V_k)_{ij} = \int (x \mu_k)_i (x \mu_k)_j f(x|H_k) dx_1 \dots dx_N$
- Sum and invert covariance matrices: $W_{ij} = (V_{Null} + V_{Alt})_{ij}$
- a can now be calculated from this: $a \propto W^{-1}(\mu_{Null} \mu_{Alt})$
- Finally the Fisher discriminant can be calculated: $t(\mathbf{x}) = \sum_{i=1}^{N} a_i x_i = a^T x$



The Fisher Discriminant - Summary

• Having constructed the 'optimal' observable, it is always worthwhile looking back and see what was assumed.



- Needs linearly correlated left/right separated data.
- That being said, the (relative) simplicity of the method makes it useful in a large variety of real life experiments.

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MVA summary

- In a perfect world, it would be possible to calculate the Likelihood ratio between any Null and Alternative hypothesis.
- Ratio can be tried to be estimated by histograms. I.e. using simulation or data, gathered before the experiment.
- As the number of factors that influence the likelihood grow, this becomes more and more unreasonable. Required statistics grow as res^{Dimension}.







- Todays exercise:
 - Construct discriminant for data set that originally inspired Fisher.
 - Data: Measurements of Irises picked by Fisher's friend Anderson on the Gaspe peninsula...



Iris Virginica



Iris Setosa

Iris Versicolor





Multivariate Analysis

• Next time:

- Elaborate on separation measures: More applicable tools for real life analysis
- Introduce tools (superficially) that can handle more complex examples.
- Risk factors contributing to heart disease, based on data collected in South Africa.

