Displays for Statistics 5401

Lecture 33

November 23, 2005

Christopher Bingham, Instructor 612-625-1024

Class Web Page

http://www.stat.umn.edu/~kb/classes/5401

Copyright© Christopher Bingham 2005

Statistics 5401 Lecture 33

You get canonical variables from the multistandardized $\widetilde{\mathbf{x}}^{(1)} = \Sigma_{11}^{-T/2} (\mathbf{x}^{(1)} - \boldsymbol{\mu}^{(1)})$ and $\widetilde{\mathbf{x}}^{(2)} = \Sigma_{22}^{-T/2} (\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})$ using left and right singular vectors \mathbf{l}_j and \mathbf{r}_j of $\widetilde{\boldsymbol{\rho}}_{12} = \text{corr}[\widetilde{\mathbf{x}}^{(1)}, \widetilde{\mathbf{x}}^{(2)}] = \Sigma_{11}^{-T/2} \Sigma_{12} \Sigma_{22}^{-1/2}$.

November 23, 2005

How do you get canonical variables directly from $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$, rather than from $\mathbf{\hat{x}}^{(1)}$ and $\mathbf{\hat{x}}^{(2)}$?

•
$$Z_{j}^{(1)} = \mathbf{l}_{j}^{T} \mathbf{\tilde{x}}^{(1)} = \mathbf{l}_{j}^{T} \mathbf{\Sigma}_{11}^{-T/2} (\mathbf{x}^{(1)} - \mathbf{\mu}^{(1)})$$

= $\mathbf{u}_{j}^{T} (\mathbf{x}^{(1)} - \mathbf{\mu}^{(1)})$
= $\mathbf{u}_{j}^{T} \mathbf{x}^{(1)} - \mathbf{u}_{j}^{T} \mathbf{\mu}^{(1)}$, where $\mathbf{u}_{j}^{T} = \mathbf{\Sigma}_{11}^{-1/2} \mathbf{l}_{j}^{T}$

•
$$Z_{j}^{(2)} = \mathbf{r}_{j}^{T} \mathbf{\tilde{X}}^{(2)} = \mathbf{r}_{j}^{T} \mathbf{\Sigma}_{22}^{-T/2} (\mathbf{X}^{(2)} - \boldsymbol{\mu}^{(2)})$$

= $\mathbf{v}_{j}^{T} (\mathbf{X}^{(2)} - \boldsymbol{\mu}^{(2)})$
= $\mathbf{v}_{j}^{T} \mathbf{X}^{(2)} - \mathbf{v}_{j}^{T} \boldsymbol{\mu}^{(2)}$, where $\mathbf{v}_{j} = \mathbf{\Sigma}_{22}^{-1/2} \mathbf{r}_{j}$

Thus you need to find \mathbf{u}_j and \mathbf{v}_j . Although they are defined using \mathbf{l}_j and \mathbf{r}_j , they can be computed directly from Σ .

Facts (easily checkable):

$$\begin{split} & \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\Sigma}_{21} \boldsymbol{u}_{j} = \boldsymbol{\tau}_{j}^{2} \boldsymbol{\Sigma}_{11} \boldsymbol{u}_{j} = \boldsymbol{\Theta}_{j} \boldsymbol{\Sigma}_{11} \boldsymbol{u}_{j} \\ & \boldsymbol{\Sigma}_{21} \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\Sigma}_{12} \boldsymbol{v}_{j} = \boldsymbol{\tau}_{j}^{2} \boldsymbol{\Sigma}_{22} \boldsymbol{v}_{j} = \boldsymbol{\Theta}_{j} \boldsymbol{\Sigma}_{22} \boldsymbol{v}_{j} \end{split}$$

- Coefficient vector \mathbf{u}_{j} for $z_{j}^{(1)}$ is a eigenvector of $\mathbf{\Sigma}_{12}\mathbf{\Sigma}_{22}^{-1}\mathbf{\Sigma}_{21}$ relative to $\mathbf{\Sigma}_{11}$
- Coefficient vector \mathbf{v}_{j} for $\mathbf{z}_{j}^{(2)}$ is a eigenvector of $\mathbf{\Sigma}_{21}\mathbf{\Sigma}_{11}^{-1}\mathbf{\Sigma}_{12}$ relative to $\mathbf{\Sigma}_{22}$

So you can find canonical variables by solving two <u>relative eigenvalue/vector</u> problems involving pieces of Σ .

Usually, the canonical variables are defined as

$$Z_{j}^{(1)} = \mathbf{U}_{j}^{\mathsf{T}} \mathbf{X}^{(1)} = (\mathbf{\Sigma}_{11}^{-1/2} \mathbf{Q}_{j})^{\mathsf{T}} \mathbf{X}^{(1)}$$

 $Z_{j}^{(2)} = \mathbf{V}_{j}^{\mathsf{T}} \mathbf{X}^{(1)} = (\mathbf{\Sigma}_{22}^{-1/2} \mathbf{r}_{j})^{\mathsf{T}} \mathbf{X}^{(2)}$

without subtracting means. These differ only by constants $\mathbf{u}_{_{j}}^{^{\mathsf{T}}}\boldsymbol{\mu}^{^{(1)}}$ and $\mathbf{v}_{_{j}}^{^{\mathsf{T}}}\boldsymbol{\mu}^{^{(1)}}$ from the previous definition, and

$$\mathbf{u}_{i}^{\mathsf{T}} \boldsymbol{\mu}^{(1)} = \mathsf{E}[z_{i}^{(1)}], \quad \mathbf{v}_{i}^{\mathsf{T}} \boldsymbol{\mu}^{(1)} = \mathsf{E}[z_{i}^{(2)}]$$

My examples have not, of course, had to do with <u>population</u> principal components, but rather with <u>sample</u> canonical correlations.

You define

- ullet sample canonical correlations $\hat{oldsymbol{arepsilon}}_{_{\mathbf{j}}}$
- ullet pairs of sample canonical variables $\hat{z_{\mathrm{j}}^{(1)}}$ and $\hat{z_{\mathrm{i}}^{(2)}}$

in a similar way, starting with ${\bf S}$ instead of ${\bf \Sigma}$.

Continue with analysis of artificial data:

```
Cmd> s <- tabs(scores,covar:T)</pre>
Cmd> J1 <- run(3); J2 <- run(4,7) # selectors for variables
Cmd> s11 \leftarrow s[J1,J1]; s22 \leftarrow s[J2,J2]
Cmd> s12 <- s[J1,J2]; s21 <- s12'
Cmd> tauhatsq <- releigenvals(s21 %*% solve(s11) %*% s12, s22)
Cmd> tauhatsq # squared canonical correlations
(1)
        0.83093
                    0.030001 0.0089408 6.5688e-18
```

Compute canonical correlations \hat{z}_i from SVD of correlation matrix of multistandardized data:

```
Cmd> tauhat <- svd(cor(scores[,J1] %*% solve(cholesky(s11)),\</pre>
           scores[,J2] %%*% solve(cholesky(s22)))[J1,J2])
Cmd> tauhat^2 # same as tauhatsq
                                                    0
        0.83093
                   0.030001
                               0.0089408
```

There is a close relationship between sample canonical correlations and relative eigenvalues from the <u>regression</u> approach discussed on Monday.

Lecture 33

If $\hat{\lambda_i}$ are the sample eigenvalues of ${f H}$ relative to E in either the multivariate regression of $\mathbf{x}^{(1)}$ on $\mathbf{x}^{(2)}$ or of $\mathbf{x}^{(2)}$ on $\mathbf{x}^{(1)}$, then

$$\hat{\tau}_{i} = \sqrt{\hat{\theta}_{i}} = \sqrt{\hat{\lambda}_{i}}/(1 + \hat{\lambda}_{i})$$

 $Cmd > manova("x2 = x1_1 + x1_2 + x1_3", silent:T)$ Cmd> h2 <- sum(SS[run(2,4),,]); e2 <- SS[5,,]Cmd> lambdahat <- releigenvals(h2,e2)</pre> Cmd> lambdahat 4.9149 0.030929 0.0090215 1.2698e-15 Cmd> lambdahat[run(3)]/(1 + lambdahat[run(3)]) 0.030001 0.0089408 thetahat = tauhat^2 Cmd> tauhatsq[run(3)] 0.83093 0.030001

The <u>correlation</u> canonical variables $\hat{z}_{i}^{(1)}$ and $\hat{z_i}^{(2)}$ are the same as the MANOVA canonical variables of regressions of $\mathbf{x}^{(1)}$ on $\mathbf{x}^{(2)}$ and of $\mathbf{x}^{(2)}$ on $\mathbf{x}^{(1)}$, except possibly for change of sign.

Alternative Approach: Find features or summaries of $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ that are highly correlated with each other.

This is the more traditional approach to canonical correlation.

We concentrate on <u>linear</u> features $\mathbf{u}^{\mathsf{T}}\mathbf{x}^{(1)}$ and $\mathbf{v}^{\mathsf{T}}\mathbf{x}^{(2)}$ and try to find \mathbf{u} and \mathbf{v} to maximize (make as large as possible)

$$\rho^{2}[\mathbf{u}^{\mathsf{T}}\mathbf{x}^{(1)}, \mathbf{v}^{\mathsf{T}}\mathbf{x}^{(2)}] = \frac{\mathsf{Cov}[\mathbf{u}^{\mathsf{T}}\mathbf{x}^{(1)}, \mathbf{v}^{\mathsf{T}}\mathbf{x}^{(2)}]^{2}}{\mathsf{V}[\mathbf{u}^{\mathsf{T}}\mathbf{x}^{(1)}]\mathsf{V}[\mathbf{v}^{\mathsf{T}}\mathbf{x}^{(2)}]}$$
$$= \frac{(\mathbf{u}^{\mathsf{T}}\boldsymbol{\Sigma}_{12}\mathbf{v})^{2}}{(\mathbf{u}^{\mathsf{T}}\boldsymbol{\Sigma}_{11}\mathbf{u})(\mathbf{v}^{\mathsf{T}}\boldsymbol{\Sigma}_{22}\mathbf{v})}$$

We work with ρ^2 because the sign of the correlation will be arbitrary.

I'll skip any derivation, but the solution can be stated using relative eigenvectors:

• $\mathbf{u} = \mathbf{u}_1$, where \mathbf{u}_1 , \mathbf{u}_2 , ..., \mathbf{u}_p are the relative eigenvectors of

 $\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$ relative to Σ_{11} (both p×p),

with corresponding relative eigenvalues $\theta_1 \geq \theta_2 \geq ... \geq \theta_p$.

• $\mathbf{v} = \mathbf{v}_1$, where \mathbf{v}_1 , \mathbf{v}_2 , ..., \mathbf{v}_p are the relative eigenvectors of

 $\Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}$ relative to Σ_{22} (both q×q),

with corresponding relative eigenvalues $\theta_1 \geq \theta_2 \geq ... \geq \theta_q$.

Furthermore the maximized value (<u>largest</u> squared correlation) is $\theta_1 = \tau_1^2$.

These are the same coefficient vectors from the first approach to canonical correlation.

That is

$$\max_{\mathbf{u}, \mathbf{v}} \rho^{2}[\mathbf{u}^{\mathsf{T}} \mathbf{x}^{(1)}, \mathbf{v}^{\mathsf{T}} \mathbf{x}^{(2)}] = \rho^{2}[\mathbf{u}_{1}^{\mathsf{T}} \mathbf{x}^{(1)}, \mathbf{v}_{1}^{\mathsf{T}} \mathbf{x}^{(2)}] = \Theta_{1}$$

Note: These θ_j 's are the same as before, that is $\theta_j = \tau_j^2$ where τ_j is a SV of $\widetilde{\Sigma}_{12}$.

With the usual normalization for \mathbf{u}_{1} ,

$$V[\mathbf{u}_{1}^{\mathsf{T}}\mathbf{x}^{(1)}] = \mathbf{u}_{1}^{\mathsf{T}}\mathbf{\Sigma}_{11}\mathbf{u}_{1} = 1$$

and

$$V[\mathbf{V}_1^\mathsf{T}\mathbf{X}^{(2)}] = \mathbf{V}_1^\mathsf{T}\mathbf{\Sigma}_{22}\mathbf{V}_1 = 1.$$

and

$$Cov[\mathbf{u}_{1}^{\mathsf{T}}\mathbf{x}^{(1)}, \mathbf{v}_{1}^{\mathsf{T}}\mathbf{x}^{(2)}] = \tau_{1} = \sqrt{\theta_{1}}.$$

Similarly

$$Z_{j}^{(1)} = \mathbf{u}_{j}^{\mathsf{T}} \mathbf{X}^{(1)}, \quad j = 1, ..., \min(p,q)$$

 $Z_{j}^{(2)} = \mathbf{v}_{j}^{\mathsf{T}} \mathbf{X}^{(2)}$

have $Corr[z_j^{(1)}, z_j^{(2)}] = \tau_j = \sqrt{\theta_j}$. $z_j^{(1)}$ and $z_j^{(2)}$ have the largest squared correlation of any linear combinations uncorrelated with $z_k^{(1)}$ and $z_k^{(2)}$, k < j

Here is what the correlation matrix (and variance matrix) of standardized canonical variables looks like when p = 4 and q = 3.

$$V[\mathbf{z}] = \begin{bmatrix} 1 & 0 & 0 & \sqrt{\theta_1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & \sqrt{\theta_2} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \sqrt{\theta_2} & 0 \\ \sqrt{\theta_1} & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \sqrt{\theta_2} & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\theta_3} & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{Z} = [Z_1^{(1)}, Z_2^{(1)}, Z_3^{(1)}, Z_1^{(2)}, Z_2^{(2)}, Z_3^{(2)}, Z_4^{(2)}]^T$$

There are only s = min(3,4) = 3 non-zero canonical correlations $\tau_1 = \sqrt{\theta_1}$, $\tau_2 = \sqrt{\theta_2}$ and $\tau_3 = \sqrt{\theta_3}$. Note that all correlations with $z_4^{(2)}$ are 0.

November 23, 2005

In general, there are $s = min(p,q) \underline{pairs}(z_j^{(1)}, z_j^{(2)})$ of canonical variables.

All the correlation between $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ is "concentrated" in

$$\tau_{i} = corr[z_{i}^{(1)}, z_{i}^{(2)}], i = 1, ..., s.$$

When $p \neq q$, there are |p - q| additional unpaired canonical variables that not correlated with anything and have no significance.

You define sample canonical correlations and correlation canonical variables the same way using the sample eigenvalues $\hat{\theta_i}$ = $\hat{\tau}_i^2$ and eigenvectors $\hat{\mathbf{u}}_i$ and $\hat{\mathbf{v}}_i$ of

- $S_{12}S_{22}^{-1}S_{21}$ relative to S_{11}
- $S_{21}S_{11}^{-1}S_{12}$ relative to S_{22} .

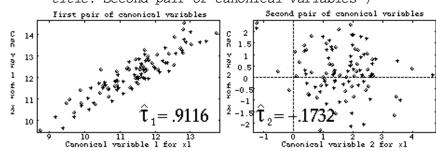
z1 and z2 contain canonical variables computed using relative eigenvectors.

What do you do with canonical variables? One thing to do is to make scatter plots of $\hat{z_i}^{(2)}$ vs $\hat{z_i}^{(1)}$.

Cmd> plot(Z1[,1],Z2[,1],xlab:"Canonical variable 1 for x1",\
 ylab:"Can var 1 for x2",\
 title:"First pair of canonical variables")

Cmd> plot(Z1[,2],Z2[,2],xlab:"Canonical variable 2 for x1",\ ylab:"Can var 2 for x2",\

title: "Second pair of canonical variables")



These are plots of $\hat{z_1}^{(2)}$ vs $\hat{z_1}^{(1)}$ (left) and $\hat{z_2}^{(2)}$ vs $\hat{z_2}^{(1)}$ (right).

And you can look at $\hat{\mathbf{u}}_{_{j}}$ and $\hat{\mathbf{v}}_{_{j}}$ to gain insight on what the canonical variables are made up from, much as you can do in MANOVA.

The $\hat{\theta_i}$ have the same information as the eigenvalues $\hat{\lambda}_1$, $\hat{\lambda}_2$, ... of **H** relative to **E** that appear in the multivariate regression tests of ρ_{12} = **0**.

$$\hat{\theta_i} = \hat{\lambda_i}/(1 + \hat{\lambda_i})$$
 $\hat{\lambda_i} = \hat{\theta_i}/(1 - \hat{\theta_i})$

Only s = min(p,q) of these are non-zero.

The regression hypothesis and error
matrices are

$$\mathbf{H}_{1.2} = \mathbf{f}_{e} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21}, \ \mathbf{E}_{1.2} = \mathbf{f}_{e} \mathbf{S}_{11} - \mathbf{H}_{1.2}, \ \mathbf{X}^{(1)} \ \text{on} \ \mathbf{X}^{(2)}$$

$$H_{2.1} = f_e S_{21} S_{11}^{-1} S_{12}, E_{2.1} = f_e S_{22} - H_{2.1}, \mathbf{x}^{(2)} \text{ on } \mathbf{x}^{(1)}$$

So $\hat{\lambda_i}$ is the ith eigenvalue of $\mathbf{H}_{1,2}$ relative to $\mathbf{E}_{1,2}$ or of $\mathbf{H}_{2,1}$ relative to $\mathbf{E}_{2,1}$

When
$$H_0$$
: $\rho_{12} = 0$ is true,
 $\{\hat{\lambda}_i\} = \{\hat{\theta}_i/(1 - \hat{\theta}_i)\}$

You can use any of the MANOVA tests based on relative eigenvalues.

In terms of the canonical correlations and the matrix $S_{11}^{-1}S_{12}S_{22}^{-1}S_{12}$

Hotelling's trace

$$\begin{split} & \sum \widehat{\lambda}_{i} = \sum \widehat{\theta}_{i} / (1 - \widehat{\theta}_{i}) \\ & = tr(\mathbf{E}_{1.2}^{-1} \mathbf{H}_{1.2}) \\ & = tr((\mathbf{S}_{11} - \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21}) \\ & = tr((\mathbf{I}_{D} - \mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})^{-1} \mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21}) \end{split}$$

IR test

$$1/\Pi(1 + \hat{\lambda}_{i}) = \Pi(1 - \hat{\theta}_{i})$$

$$= \det(\mathbf{E}_{1,2})/\det(\mathbf{H}_{1,2} + \mathbf{E}_{1,2})$$

$$= \det(\mathbf{I}_{D} - \mathbf{S}_{11}^{-1}\mathbf{S}_{12}\mathbf{S}_{22}^{-1}\mathbf{S}_{21})$$

Pillai's trace

$$\sum \hat{\lambda}_{i} / (1 + \hat{\lambda}_{i}) = \sum \hat{\theta}_{i}$$

$$= tr\{(H_{1.2} + E_{1.2})^{-1}H_{1.2}\}$$

$$= tr(S_{11}^{-1}S_{12}S_{22}^{-1}S_{21})$$

In these equations you can replace S_{11} by S_{22} and $S_{11}^{-1}S_{12}S_{22}^{-1}S_{21}$ by $S_{22}^{-1}S_{21}S_{11}^{-1}S_{12}$

Beyond Canonical Correlations

Here are two paths you might follow.

1. Use quadratic features instead of linear features. That is, try to find vectors \mathbf{u} and \mathbf{v} and symmetric matrices A and B such that

Corr[
$$\mathbf{u}'\mathbf{x}^{(1)} + \mathbf{x}^{(1)}'\mathbf{A}\mathbf{x}^{(1)}, \mathbf{v}'\mathbf{x}^{(2)} + \mathbf{x}^{(2)}'\mathbf{B}\mathbf{x}^{(2)}$$
] is as large as possible

2. Describe the pattern of correlation among k > 2 sets of variables $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$, ..., $\mathbf{x}^{(k)}$. One possibility would be to find vectors \mathbf{u}_{1} , \mathbf{u}_{2} , ... \mathbf{u}_{k} that minimize $\det(\mathbf{R}_{U})$, where R_{ij} is the correlation matrix of $\mathbf{U}_{1}'\mathbf{X}^{(1)}, \ \mathbf{U}_{2}'\mathbf{X}^{(2)}, \ ..., \ \mathbf{U}_{k}'\mathbf{X}^{(k)}.$

Since $det(\mathbf{R}_{11}) = 1 - \rho^{2}[\mathbf{u}_{1}'\mathbf{x}^{(1)},\mathbf{u}_{2}'\mathbf{x}^{(2)}]$ when k = 2, this leads to the ordinary canonical correlations when there are k = 2 groups of variables...

The classification problem

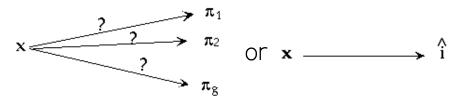
Situation: You have data \mathbf{x} (1 or several variables) on an individual that is known to belong to one of g distinct populations $\pi_1, \pi_2, ..., \pi_g$.

The *classification problem*: Find a "rule" or formula which uses \mathbf{x} to "guess" or "estimate" the population $\pi_{_{j}}$ the individual belongs to.

Example: When each population consists of patients with a particular <u>disease</u> and **x** contains an individual's <u>medical history</u> and test results, the classification problem would be to <u>diagnose</u> the correct disease from the information in **x**.

More formally, suppose

- You have a random vector x (the data)
 of p characteristics (variables).
- You know ${\bf x}$ has one of ${\bf g}$ densities $f_1({\bf x}), f_2({\bf x}), ..., f_g({\bf x}),$ where $f_j({\bf x})$ defines the distribution of ${\bf x}$ in population π_j .
- You seek a procedure or formula (a "rule") that maps x to a population.

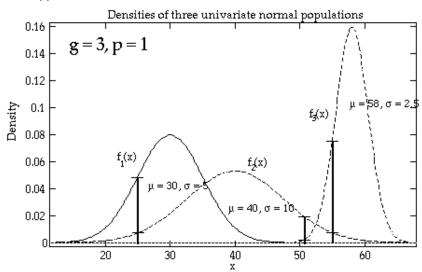


Here î is the guessed index of the population chosen.

Suppose the observed \mathbf{x} is much less likely to be observed in population π_1 (density $f_1(\mathbf{x})$) than in population π_2 (density $f_2(\mathbf{x})$). Then you might reasonably guess π_2 in preference to π_1 .

Statistics 5401

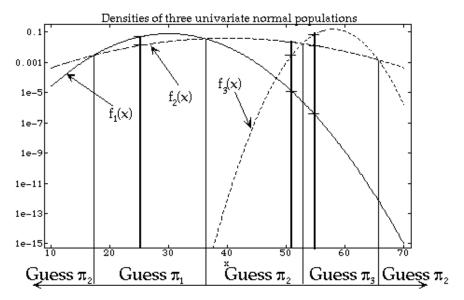
Here are densities for three p=1 populations with normal distributions.



When x = 25, you would choose π_1 over π_2 or π_3 ; when x = 51, you would choose π_2 ; when x = 55, you would choose π_3 .

It's often easier to compare densities when they are plotted in a log scale.

November 23, 2005

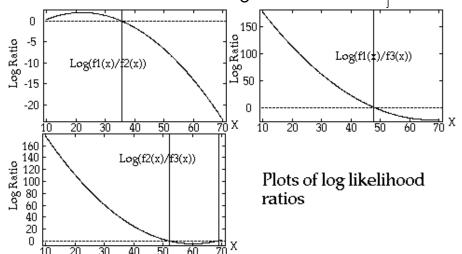


The extra vertical lines are where the densities intersect.

Under the graph is a sensible rule for picking one of these three populations - pick the population with largest density.

Near the boundary points you wouldn't be very sure about your decision based on this rule.

The logs of the ratios $f_i(x)/f_k(x)$ are informative for deciding between π_i and π_{ν} .



The O line is the line of equal likelihood. These let you choose between π_i and π_k

- When 10 < x < 35, you would probably assign x to π , (above 0 in top 2 plots)
- x near 45 you would assign x to π_2
- 60 < x < 70 you would assign x to π_3 .

It looks like for x < 10 and x > 70, you should prefer π_2 to π_1 and π_3 even though x is nearer to μ_1 or μ_2 than to μ_2 .

Effect of rarity

Suppose you knew, for example, that seeing any observation, regardless of value, from π_2 was extremely rare as compared to either π_1 or π_3 . Then this "obvious" way to guess a population might change.

In that case, you might classify a value of x = 45 as coming from π_1 , even though it would be an unlikely value to see from π_1 , just because it is unlikely to see any individual from π_{2} .

In the extreme, if the chance of seeing any individual from π_{2} was 1/1,000,000, for all practical purposes you can probably exclude π_{s} from consideration and never pick π_{2} .