

Displays for Statistics 5401

Lecture 33

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Class Web Page

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You get canonical variables from the multistandardized $\tilde{\mathbf{x}}^{(1)} = \Sigma_{11}^{-1/2}(\mathbf{x}^{(1)} - \boldsymbol{\mu}^{(1)})$ and $\tilde{\mathbf{x}}^{(2)} = \Sigma_{22}^{-1/2}(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})$ using left and right singular vectors \mathbf{l}_j and \mathbf{r}_j of

$$\tilde{\boldsymbol{\rho}}_{12} = \text{corr}[\tilde{\mathbf{x}}^{(1)}, \tilde{\mathbf{x}}^{(2)}] = \Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1/2}.$$

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

- $z_j^{(1)} = \mathbf{l}_j^T \tilde{\mathbf{x}}^{(1)} = \mathbf{l}_j^T \Sigma_{11}^{-1/2}(\mathbf{x}^{(1)} - \boldsymbol{\mu}^{(1)})$
 $= \mathbf{u}_j^T (\mathbf{x}^{(1)} - \boldsymbol{\mu}^{(1)})$
 $= \mathbf{u}_j^T \mathbf{x}^{(1)} - \mathbf{u}_j^T \boldsymbol{\mu}^{(1)}$, where $\mathbf{u}_j = \Sigma_{11}^{-1/2} \mathbf{l}_j$
- $z_j^{(2)} = \mathbf{r}_j^T \tilde{\mathbf{x}}^{(2)} = \mathbf{r}_j^T \Sigma_{22}^{-1/2}(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})$
 $= \mathbf{v}_j^T (\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})$
 $= \mathbf{v}_j^T \mathbf{x}^{(2)} - \mathbf{v}_j^T \boldsymbol{\mu}^{(2)}$, where $\mathbf{v}_j = \Sigma_{22}^{-1/2} \mathbf{r}_j$

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 .

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Facts (easily checkable):

$$\Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \mathbf{u}_j = \tau_j^2 \Sigma_{11} \mathbf{u}_j = \theta_j \Sigma_{11} \mathbf{u}_j$$

$$\Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \mathbf{v}_j = \tau_j^2 \Sigma_{22} \mathbf{v}_j = \theta_j \Sigma_{22} \mathbf{v}_j$$

- Coefficient vector \mathbf{u}_j for $z_j^{(1)}$ is a eigenvector of $\Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$ relative to Σ_{11}
- Coefficient vector \mathbf{v}_j for $z_j^{(2)}$ is a eigenvector of $\Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$ relative to Σ_{22}

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

Usually, the canonical variables are defined as

$$z_j^{(1)} = \mathbf{u}_j^T \mathbf{x}^{(1)} = (\Sigma_{11}^{-1/2} \mathbf{l}_j)^T \mathbf{x}^{(1)}$$

$$z_j^{(2)} = \mathbf{v}_j^T \mathbf{x}^{(2)} = (\Sigma_{22}^{-1/2} \mathbf{r}_j)^T \mathbf{x}^{(2)}$$

without subtracting means. These differ only by constants $\mathbf{u}_j^T \boldsymbol{\mu}^{(1)}$ and $\mathbf{v}_j^T \boldsymbol{\mu}^{(2)}$ from the previous definition, and

$$\mathbf{u}_j^T \boldsymbol{\mu}^{(1)} = E[z_j^{(1)}], \quad \mathbf{v}_j^T \boldsymbol{\mu}^{(2)} = E[z_j^{(2)}]$$

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

You define

- *sample* canonical correlations $\hat{\tau}_j$
- pairs of sample canonical variables $\hat{z}_j^{(1)}$ and $\hat{z}_j^{(2)}$

in a similar way, starting with \mathbf{S} instead of Σ .

Continue with analysis of artificial data:

```
Cmd> s <- tabs(scores,covar:T)
Cmd> J1 <- run(3); J2 <- run(4,7) # selectors for variables
Cmd> s11 <- s[J1,J1]; s22 <- 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 $\hat{\tau}_j$ from SVD of correlation matrix of multi-standardized data:

```
Cmd> tauhat <- svd(cor(scores[,J1] %*% solve(cholesky(s11)),\
scores[,J2] %*% solve(cholesky(s22)))[J1,J2])
Cmd> tauhat^2 # same as tauhatsq
(1) 0.83093 0.030001 0.0089408 0
```

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 linear features $\mathbf{u}^T \mathbf{x}^{(1)}$ and $\mathbf{v}^T \mathbf{x}^{(2)}$ and try to find \mathbf{u} and \mathbf{v} to maximize (make as large as possible)

$$\begin{aligned} \rho^2[\mathbf{u}^T \mathbf{x}^{(1)}, \mathbf{v}^T \mathbf{x}^{(2)}] &= \frac{\text{Cov}[\mathbf{u}^T \mathbf{x}^{(1)}, \mathbf{v}^T \mathbf{x}^{(2)}]^2}{V[\mathbf{u}^T \mathbf{x}^{(1)}]V[\mathbf{v}^T \mathbf{x}^{(2)}]} \\ &= \frac{(\mathbf{u}^T \Sigma_{12} \mathbf{v})^2}{(\mathbf{u}^T \Sigma_{11} \mathbf{u})(\mathbf{v}^T \Sigma_{22} \mathbf{v})} \end{aligned}$$

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

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

If $\hat{\lambda}_j$ are the sample eigenvalues of \mathbf{H} relative to \mathbf{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)
Cmd> lambdahat
(1) 4.9149 0.030929 0.0090215 1.2698e-15
Cmd> lambdahat[run(3)]/(1 + lambdahat[run(3)])
(1) 0.83093 0.030001 0.0089408 thetahat = tauhat^2
Cmd> tauhatsq[run(3)]
(1) 0.83093 0.030001 0.0089408
```

The correlation canonical variables $\hat{z}_j^{(1)}$ and $\hat{z}_j^{(2)}$ 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.

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

- $\mathbf{u} = \mathbf{u}_1$, where $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_p$ are the **relative eigenvectors** of $\Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$ relative to Σ_{11} (both $p \times p$), with corresponding *relative eigenvalues* $\theta_1 \geq \theta_2 \geq \dots \geq \theta_p$.
- $\mathbf{v} = \mathbf{v}_1$, where $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_p$ are the **relative eigenvectors** of $\Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$ relative to Σ_{22} (both $q \times q$), with corresponding *relative eigenvalues* $\theta_1 \geq \theta_2 \geq \dots \geq \theta_q$.

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

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

That is

$$\max_{\mathbf{u}, \mathbf{v}} \rho^2[\mathbf{u}^T \mathbf{x}^{(1)}, \mathbf{v}^T \mathbf{x}^{(2)}] = \rho^2[\mathbf{u}_1^T \mathbf{x}^{(1)}, \mathbf{v}_1^T \mathbf{x}^{(2)}] = \theta_1$$

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

With the usual normalization for \mathbf{u}_1 ,

$$V[\mathbf{u}_1^T \mathbf{x}^{(1)}] = \mathbf{u}_1^T \Sigma_{11} \mathbf{u}_1 = 1$$

and

$$V[\mathbf{v}_1^T \mathbf{x}^{(2)}] = \mathbf{v}_1^T \Sigma_{22} \mathbf{v}_1 = 1.$$

and

$$\text{Cov}[\mathbf{u}_1^T \mathbf{x}^{(1)}, \mathbf{v}_1^T \mathbf{x}^{(2)}] = \tau_1 = \sqrt{\theta_1}.$$

Similarly

$$z_j^{(1)} = \mathbf{u}_j^T \mathbf{x}^{(1)}, \quad j = 1, \dots, \min(p, q)$$

$$z_j^{(2)} = \mathbf{v}_j^T \mathbf{x}^{(2)}$$

have $\text{Corr}[z_j^{(1)}, z_j^{(2)}] = \tau_j = \sqrt{\theta_j}$.

$z_j^{(1)}$ and $z_j^{(2)}$ have the largest squared correlation of any linear combinations uncorrelated with $z_k^{(1)}$ and $z_k^{(2)}$, $k < j$

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

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

$$\tau_i = \text{corr}[z_i^{(1)}, z_i^{(2)}], \quad i = 1, \dots, s.$$

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

- $\mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21}$ relative to \mathbf{S}_{11}
- $\mathbf{S}_{21} \mathbf{S}_{11}^{-1} \mathbf{S}_{12}$ relative to \mathbf{S}_{22} .

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

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

$$\mathbf{z} = [z_1^{(1)}, z_2^{(1)}, z_3^{(1)}, z_1^{(2)}, z_2^{(2)}, z_3^{(2)}, z_4^{(2)}]^T$$

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.

```
Cmd> eigs21 <- releigen(s12 %*% solve(s22) %*% s21, s11)
Cmd> eigs12 <- releigen(s21 %*% solve(s11) %*% s12, s22)
Cmd> uhat <- eigs21$vectors; vhat <- eigs12$vectors

Cmd> list(uhat, vhat)
uhat      REAL    3    3
vhat      REAL    4    4

Cmd> sqrt(eigs21$values) # canonical correlations
(1)  0.91156  0.17321  0.094556

Cmd> sqrt(eigs12$values[run(3)]) # canonical correlations
(1)  0.91156  0.17321  0.094556

Cmd> Z1 <- x1 %*% uhat; Z2 <- x2 %*% vhat
```

Z1 and Z2 contain canonical variables computed using relative eigenvectors.

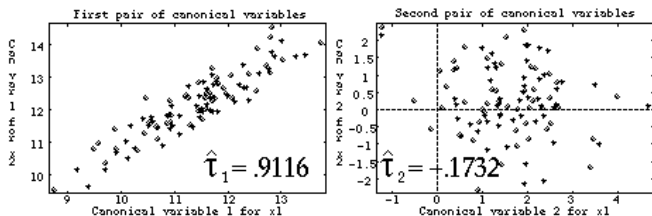
```
Cmd> print(format="7.4f", cor(Z1, Z2))
MATRIX:
(1,1)  1.0000 -0.0000 -0.0000: 0.9116  0.0000 -0.0000  0.0000
(2,1) -0.0000  1.0000 -0.0000: -0.0000 -0.1732 -0.0000 -0.0000
(3,1) -0.0000 -0.0000  1.0000: 0.0000  0.0000  0.0946 -0.0000
(4,1)  0.9116 -0.0000  0.0000: 1.0000  0.0000  0.0000 -0.0000
(5,1)  0.0000 -0.1732  0.0000: 0.0000  1.0000 -0.0000 -0.0000
(6,1) -0.0000 -0.0000  0.0946: 0.0000 -0.0000  1.0000  0.0000
(7,1)  0.0000 -0.0000 -0.0000: -0.0000 -0.0000  0.0000  1.0000
```

What do you do with canonical variables?

One thing to do is to make scatter plots of $\hat{z}_j^{(2)}$ vs $\hat{z}_j^{(1)}$.

```
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.

In terms of the canonical correlations and the matrix $\mathbf{S}_{11}^{-1}\mathbf{S}_{12}\mathbf{S}_{22}^{-1}\mathbf{S}_{21}$

<p>Hotelling's trace</p> $\sum \hat{\lambda}_i = \sum \hat{\theta}_i / (1 - \hat{\theta}_i)$ $= \text{tr}(\mathbf{E}_{1,2}^{-1} \mathbf{H}_{1,2})$ $= \text{tr}((\mathbf{S}_{11} - \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})$ $= \text{tr}((\mathbf{I}_p - \mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})^{-1} \mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})$
<p>LR test</p> $1 / \prod (1 + \hat{\lambda}_i) = \prod (1 - \hat{\theta}_i)$ $= \det(\mathbf{E}_{1,2}) / \det(\mathbf{H}_{1,2} + \mathbf{E}_{1,2})$ $= \det(\mathbf{I}_p - \mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})$
<p>Pillai's trace</p> $\sum \hat{\lambda}_i / (1 + \hat{\lambda}_i) = \sum \hat{\theta}_i$ $= \text{tr}\{(\mathbf{H}_{1,2} + \mathbf{E}_{1,2})^{-1} \mathbf{H}_{1,2}\}$ $= \text{tr}(\mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21})$

In these equations you can replace \mathbf{S}_{11} by \mathbf{S}_{22} and $\mathbf{S}_{11}^{-1}\mathbf{S}_{12}\mathbf{S}_{22}^{-1}\mathbf{S}_{21}$ by $\mathbf{S}_{22}^{-1}\mathbf{S}_{21}\mathbf{S}_{11}^{-1}\mathbf{S}_{12}$

The $\hat{\theta}_i$ have the same information as the eigenvalues $\hat{\lambda}_1, \hat{\lambda}_2, \dots$ of \mathbf{H} relative to \mathbf{E} that appear in the multivariate regression tests of $\boldsymbol{\rho}_{12} = \mathbf{0}$.

$\hat{\theta}_i = \hat{\lambda}_i / (1 + \hat{\lambda}_i)$	$\hat{\lambda}_i = \hat{\theta}_i / (1 - \hat{\theta}_i)$
--	---

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

The regression hypothesis and error matrices are

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

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

So $\hat{\lambda}_i$ is the i^{th} 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 $H_0: \boldsymbol{\rho}_{12} = \mathbf{0}$ is true,

$$\{\hat{\lambda}_i\} = \{\hat{\theta}_i / (1 - \hat{\theta}_i)\}$$

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

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 \mathbf{A} and \mathbf{B} such that

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

is as large as possible

2. Describe the pattern of correlation among $k > 2$ sets of variables $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(k)}$. One possibility would be to find vectors $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k$ that minimize $\det(\mathbf{R}_0)$, where \mathbf{R}_0 is the correlation matrix of $\mathbf{u}_1'\mathbf{x}^{(1)}, \mathbf{u}_2'\mathbf{x}^{(2)}, \dots, \mathbf{u}_k'\mathbf{x}^{(k)}$.

Since $\det(\mathbf{R}_0) = 1 - \rho^2[\mathbf{u}_1'\mathbf{x}^{(1)}, \mathbf{u}_2'\mathbf{x}^{(2)}]$ when $k = 2$, this leads to the ordinary canonical correlations when there are $k = 2$ groups of variables..

The classification problem

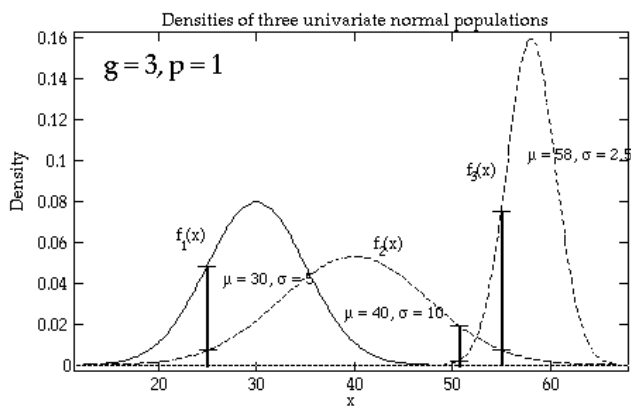
Situation: You have data \mathbf{x} (1 or several variables) on an individual that is known to belong to one of g distinct populations $\pi_1, \pi_2, \dots, \pi_g$.

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

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

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 .

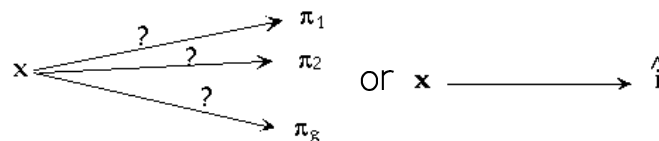
Here are densities for three $p=1$ populations with normal distributions.



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 .

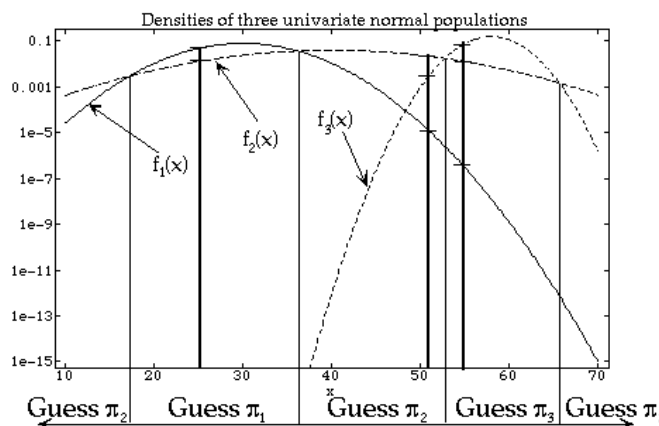
More formally, suppose

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



Here \hat{i} is the guessed index of the population chosen.

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

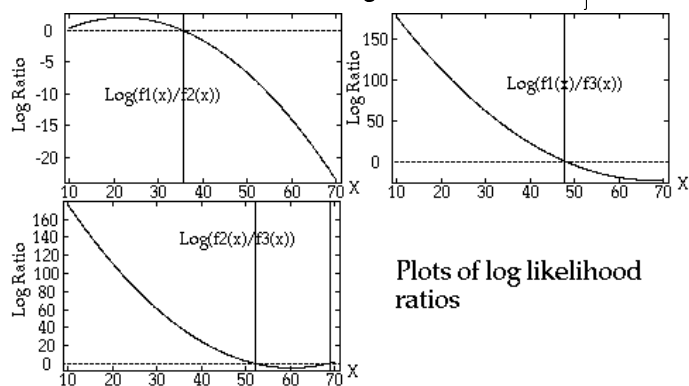


The extra vertical lines are where the densities intersect.

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 $f_j(x)/f_k(x)$ are informative for deciding between π_j and π_k .



Plots of log likelihood ratios

The 0 line is the line of equal likelihood. These let you choose between π_j and π_k

- When $10 < x < 35$, you would probably assign x to π_1 (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_3 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_2 from consideration and never pick π_2 .