# Common principal components

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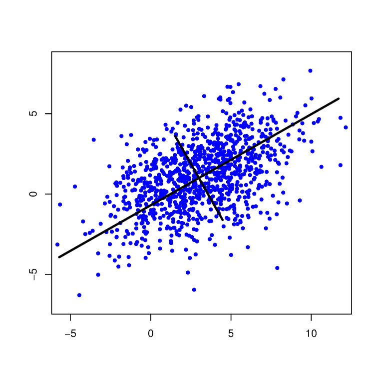
## Principal component analysis (PCA)

$$\mathbf{\Sigma} = \mathbf{B}\mathbf{\Lambda}\mathbf{B}'$$

Example:

$$\mathbf{\Sigma} = \begin{bmatrix} 0.87 & -0.49 \\ 0.49 & 0.87 \end{bmatrix} \begin{bmatrix} 10 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 0.87 & 0.49 \\ -0.49 & 0.87 \end{bmatrix}$$



## Common principal components (CPC)

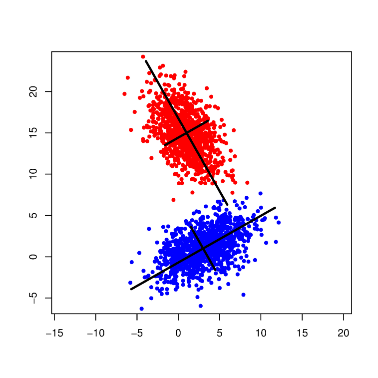
$$\mathbf{\Sigma}_1 = \mathbf{B}\mathbf{\Lambda}_1\mathbf{B}'$$

$$\mathbf{\Sigma}_2 = \mathbf{B}\mathbf{\Lambda}_2\mathbf{B}'$$

Example:

$$\mathbf{\Sigma}_1 = \begin{bmatrix} 0.87 & -0.49 \\ 0.49 & 0.87 \end{bmatrix} \begin{bmatrix} 10 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 0.87 & 0.49 \\ -0.49 & 0.87 \end{bmatrix}$$

$$\mathbf{\Sigma}_2 = \begin{bmatrix} 0.87 & -0.49 \\ 0.49 & 0.87 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 10 \end{bmatrix} \begin{bmatrix} 0.87 & 0.49 \\ -0.49 & 0.87 \end{bmatrix}$$



## Simultaneous diagonalisation algorithms

- Flury-Gautschi (FG), (Flury and Gautschi, 1986)

$$\phi\left(\boldsymbol{L}_1, \ldots, \boldsymbol{L}_k; n_1, \ldots, n_k\right) = \prod_{i=1}^{k} \frac{\left[\det\left(\operatorname{diag}\boldsymbol{L}_i\right)\right]^{n_i}}{\left[\det\left(\boldsymbol{L}_i\right)\right]^{n_i}} \tag{1}$$

- JADE package (Cardoso and Souloumiac, 1996)

$$\min\left(\sum_{i=1}^{k}\sum_{j=1}^{p}\sum_{\substack{h=1\\h\neq j}}^{p} l_{jhk}^2\right) \tag{2}$$

- Stepwise CPC (Trendafilov, 2010)
  - estimates eigenvectors sequentially
  - ensures common eigenvectors have same rank order in all groups

## The Vermont Oxford Network (VON) data

- Birth weight (kg)
- Apgar score at 1 min (0–10)
- Apgar score at 5 mins (0–10)
- Gestational age (weeks)
- Head circumference (cm)
- Temperature (°C)

Source: Wikipedia (https://en.wikipedia.org/wiki/Neonatal_intensive_care_unit)

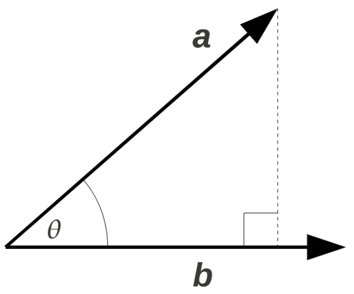
Regions:

- South Africa ($n_1 = 2921$)
- Namibia ($n_2 = 120$)

## AIC and Chi-square methods (Flury, 1988)

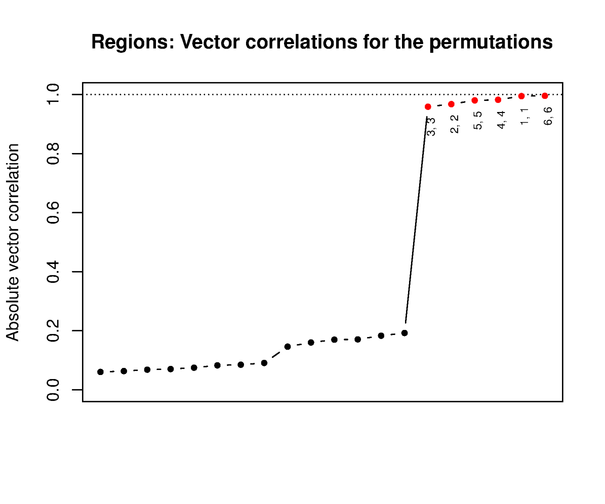
| **Model** | $\chi^2$ | **df** | $\frac{\chi^2}{\text{df}}$ | **AIC** |
|---|---|---|---|---|
| Equality | 5.99 | 1 | 5.99 | 85.77 |
| Proportionality | 10.09 | 5 | **2.02** | 81.78 |
| CPC | 2.06 | 1 | 2.06 | 81.69 |
| CPC(4) | 5.27 | 2 | 2.63 | 81.63 |
| CPC(3) | 12.87 | 3 | 4.29 | 80.37 |
| CPC(2) | 34.37 | 4 | 8.59 | 73.50 |
| CPC(1) | 15.13 | 5 | 3.03 | 47.13 |
| Heterogeneity | – | – | – | **42.00** |

## Vector correlations (Krzanowski, 1979)




$$\boldsymbol{a}'\boldsymbol{b} = \cos\theta$$

- Inspect *vector correlations* from pairwise combinations of all $p$ eigenvectors from the two groups.


Regions: Vector correlations for the permutations
Absolute vector correlation
0.0
0.2
0.4
0.6
0.8
1.0
3, 3
2, 2
5, 5
4, 4
1, 1
6, 6

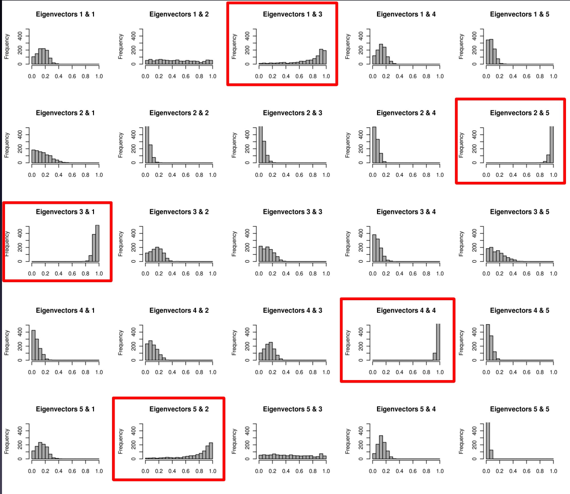
## Simulated CPC(5) data:

$k = 2$ groups

$p = 5$ variables

$n_1 = n_2 = 200$

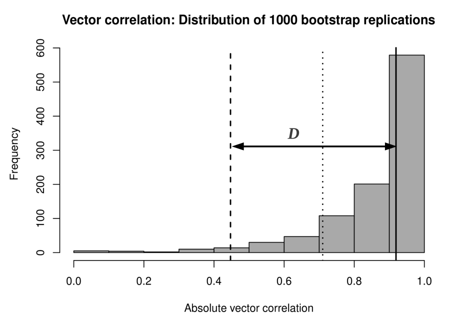
bootstrap reps $= 1000$



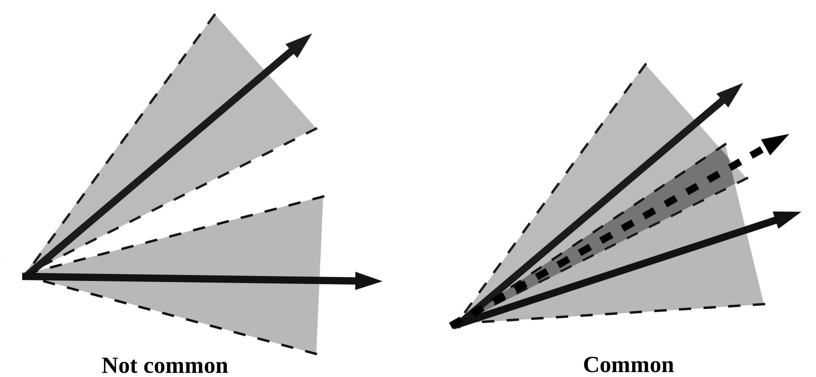
## Bootstrap vector correlation distribution (BVD)

Consider two eigenvectors to be common if:

1. median $> 0.71$
2. median $+ D \geq 1$



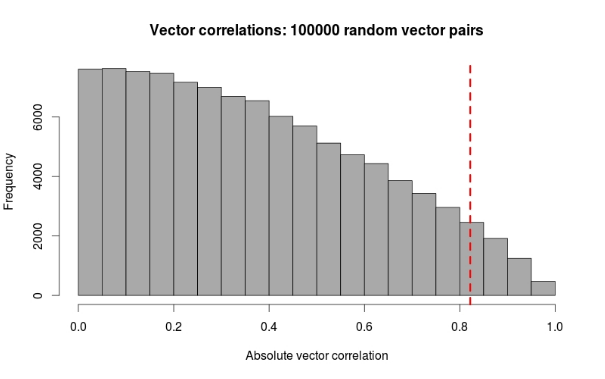
## Bootstrap confidence regions (BCR)



## Random vector correlations (RVC)

- adapted from Klingenberg and McIntyre (1998)

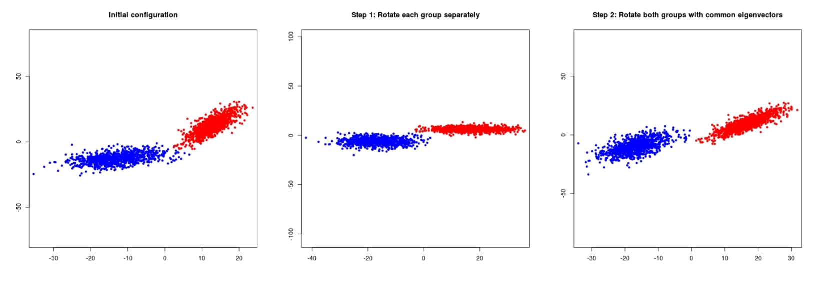
$$H_0: \text{ pair of eigenvectors are } \textit{not} \text{ common}$$



## Bootstrap hypothesis test (BootTest)

- adapted from Klingenberg (1996)

$$H_0 : \text{ pair of eigenvectors are common}$$




Twice rotated data for the $i^{th}$ group:

$$\boldsymbol{X}_i^\star = \boldsymbol{X}_i \boldsymbol{E}_i \boldsymbol{B}', \qquad i = 1, 2. \tag{3}$$

**Ensemble test**

Eigenvector pair considered equal (common) if majority vote of

- AIC
- BVD
- BCR
- RVC
- BootTest

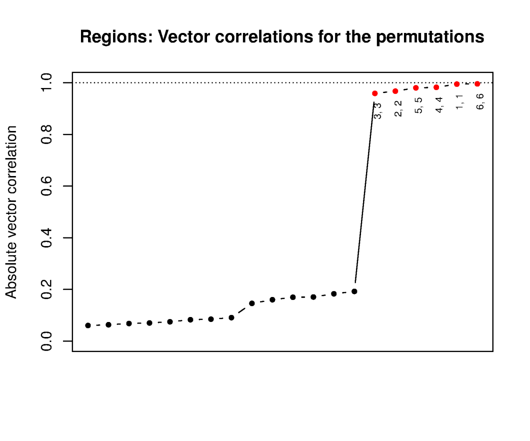
indicates it to be so.

## **Simulation results** ($p = 5$ variables)
Number of common eigenvectors correctly identified (%)

| | AIC | Chi$^2$ | BootTest | RVC | BVD | BCR | Ensemble |
|---|---|---|---|---|---|---|---|
| **Sample size** | | | | | | | |
| $n = 50$ | 33.1 | 27.0 | 26.1 | 30.0 | **33.9** | 25.6 | 32.5 |
| $n = 100$ | 34.2 | 30.7 | 26.4 | 32.2 | **36.1** | 29.4 | 35.0 |
| $n = 200$ | 43.1 | 28.1 | 33.1 | **47.2** | 44.4 | 35.3 | 46.1 |
| $n = 500$ | 43.3 | 34.8 | 46.1 | 53.3 | **56.4** | 49.4 | 54.2 |
| $n = 1000$ | 45.8 | 34.1 | 57.2 | 62.5 | 62.8 | 58.1 | **63.1** |
| **Distribution** | | | | | | | |
| Normal | 51.5 | 32.4 | 49.3 | 58.2 | **62.5** | 51.5 | 59.3 |
| Chi-squared | 43.5 | 34.2 | 39.5 | 52.0 | 51.0 | 42.7 | **52.5** |
| Multivariate $t$ | 24.7 | 26.2 | 24.5 | 25.0 | **26.7** | 24.5 | **26.7** |
| **Overall** | 39.9 | 31.0 | 37.8 | 45.1 | **46.7** | 39.6 | 46.2 |

## Application to the VON data (regions)

Ensemble test: 6 common eigenvectors



Covariance matrix estimators under the CPC model can:

- be less *biased* than when incorrectly assuming equality of the population covariance matrices, and
- be more *precise* than when incorrectly assuming that the population covariance matrices are unrelated.

## CPC estimator (Flury, 1988)

- $\boldsymbol{S}_i$ : unbiased sample covariance matrix estimator for $i^{th}$ group
- $\boldsymbol{B}$ : estimator of common eigenvector matrix

Estimator for $\boldsymbol{\Sigma}_i$ under the CPC model:

$$\boldsymbol{S}_{i(CPC)} = \boldsymbol{B}\boldsymbol{L}_i^0\boldsymbol{B}', \tag{4}$$

where

$$\boldsymbol{L}_i^0 = \text{diag}(\boldsymbol{B}'\boldsymbol{S}_i\boldsymbol{B}). \tag{5}$$

**Regularised CPC estimator**

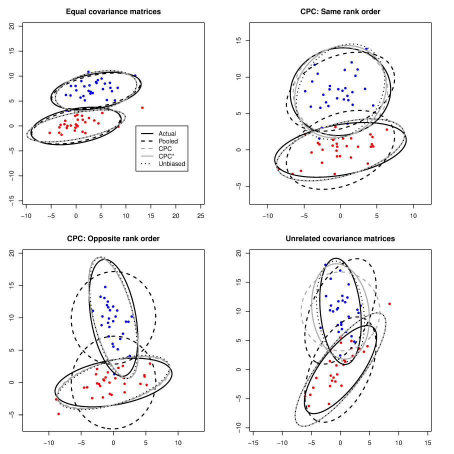
$$\boldsymbol{S}^{\star}_{i(CPC)} = \alpha_i \boldsymbol{S}_i + (1 - \alpha_i)\boldsymbol{S}_{i(CPC)}, \tag{6}$$

where $\alpha_i \in [0; 1]$ is the shrinkage intensity parameter.

Use cross-validation to find the value for $\alpha_i$ minimising a modified version of the Frobenius matrix norm on the training and validation samples.

## Covariance matrix shapes (95% confidence ellipses)

$k = 2$ populations, $p = 2$ variables



## Simulation results

Mean standardised modified Frobenius values (smaller is better):

| | Unbiased | CPC | CPC$^\star$ | Pooled |
|---|---|---|---|---|
| Full CPC | 0.269 | 0.372 | **0.192** | 0.792 |
| Half of eigenvectors common | 0.271 | 0.337 | **0.194** | 0.789 |
| Few common eigenvectors | 0.262 | 0.318 | **0.196** | 0.794 |
| Unrelated covariance matrices | 0.259 | 0.294 | **0.195** | 0.798 |

## VON data: Namibia ($n_2 = 120$)

$$S_2 = \begin{bmatrix} 0.87 & 0.62 & 0.45 & 3.02 & 3.39 & \mathbf{0.04} \\ 0.62 & 4.48 & 2.30 & 3.31 & 2.88 & \mathbf{-0.08} \\ 0.45 & 2.30 & 2.18 & 2.75 & 2.21 & \mathbf{-0.04} \\ 3.02 & 3.31 & 2.75 & 15.37 & 13.45 & \mathbf{-0.31} \\ 3.39 & 2.88 & 2.21 & 13.45 & 15.70 & \mathbf{0.05} \\ 0.04 & -0.08 & -0.04 & -0.31 & 0.05 & 0.50 \end{bmatrix}$$

$$S^{\star}_{2(\text{CPC})} = \begin{bmatrix} 0.87 & 0.57 & 0.44 & 3.16 & 3.30 & \mathbf{0.13} \\ 0.57 & 4.15 & 2.25 & 2.92 & 2.58 & \mathbf{0.07} \\ 0.44 & 2.25 & 2.31 & 2.45 & 2.02 & \mathbf{0.09} \\ 3.16 & 2.92 & 2.45 & 15.98 & 13.46 & \mathbf{0.21} \\ 3.30 & 2.58 & 2.02 & 13.46 & 15.22 & \mathbf{0.40} \\ 0.13 & 0.07 & 0.09 & 0.21 & 0.40 & 0.58 \end{bmatrix}$$

**CPC discriminant analysis**

Allocate a new observation, $x_{\text{new}}$, to the first group if

$$-\frac{1}{2}\boldsymbol{x}'_{\text{new}}(\boldsymbol{S}^{-1}_{1(\text{CPC})}-\boldsymbol{S}^{-1}_{2(\text{CPC})})\boldsymbol{x}_{\text{new}}+(\bar{\boldsymbol{x}}'_1\boldsymbol{S}^{-1}_{1(\text{CPC})}-\bar{\boldsymbol{x}}'_2\boldsymbol{S}^{-1}_{2(\text{CPC})})\boldsymbol{x}_{\text{new}} \geq c, \tag{7}$$

where

$$c = \frac{1}{2}\ln\left(\frac{|\boldsymbol{S}_{1(\text{CPC})}|}{|\boldsymbol{S}_{2(\text{CPC})}|}\right) + \frac{1}{2}(\bar{\boldsymbol{x}}'_1\boldsymbol{S}^{-1}_{1(\text{CPC})}\bar{\boldsymbol{x}}_1 - \bar{\boldsymbol{x}}'_2\boldsymbol{S}^{-1}_{2(\text{CPC})}\bar{\boldsymbol{x}}_2), \tag{8}$$

otherwise allocate it to the second group.

## Simulation results

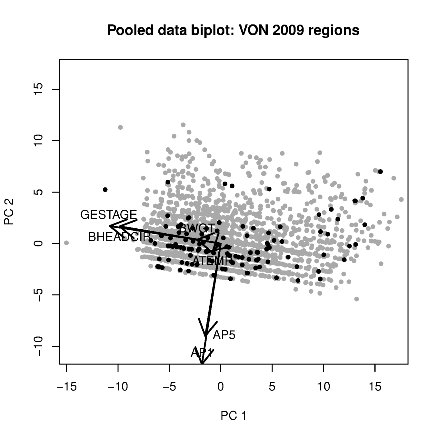
$n_1 = n_2$, $k = 2$ multivariate normal populations, $p = 10$ variables

| | | Misclassification error (%) | | | |
|---|---|---|---|---|---|
| **Structure** | $n_i$ | QDA | CPC | CPC$^\star$ | LDA |
| $\mathbf{\Sigma}_1 = \mathbf{\Sigma}_2$ | 50 | 37.79 | 31.65 | 31.67 | **30.68** |
| | 100 | 34.01 | 29.25 | 29.53 | **28.44** |
| | 200 | 31.27 | 28.25 | 28.35 | **27.70** |
| CPC | 50 | 22.96 | **16.50** | 16.81 | 30.43 |
| (similar | 100 | 18.12 | **14.93** | 15.08 | 28.80 |
| rank orders) | 200 | 15.89 | **14.13** | 14.26 | 27.49 |
| CPC | 50 | 3.31 | **2.15** | 2.22 | 21.55 |
| (Opposite | 100 | 2.41 | **1.95** | 1.97 | 18.31 |
| rank orders) | 200 | 1.99 | **1.84** | 1.85 | 16.56 |
| Unrelated | 50 | 8.66 | 8.14 | **6.94** | 32.94 |
| covariance | 100 | 5.85 | 7.15 | **5.57** | 30.80 |
| matrices | 200 | **4.89** | 6.95 | 4.92 | 29.76 |

## **VON data: Regions** (6 common eigenvectors)

Misclassification errors:

- QDA $= 25.2\%$
- LDA $= 25.4\%$
- CPC $= 21.2\%$
- CPC$^\star$ $= 22.9\%$

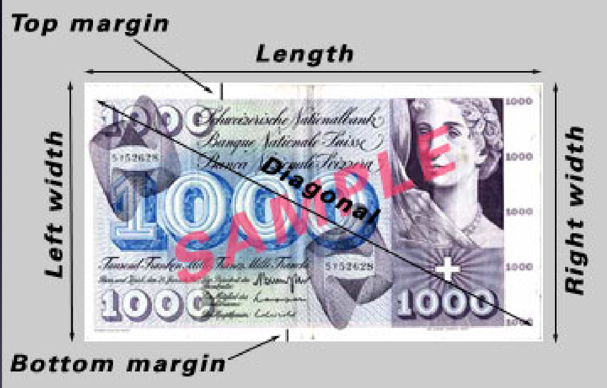


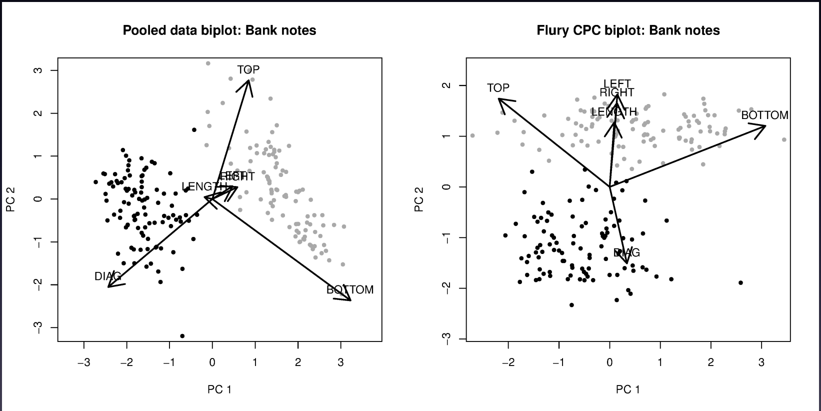
**Biplots for grouped data**

- overall quality of display
- *between-group* variation
- *within-group* variation
- representation of *variables*
    - adequacy
    - mean standard predictive error (MSPE), (Rui Alves, 2012)
- representation of *observations*
    - sample predictivities (Gower et al., 2011)

## Swiss bank notes (Flury, 1988)

Genuine notes ($n_1 = 100$), Forged notes ($n_2 = 100$)




Pooled data biplot: Bank notes
TOP
LENGTH
LEFT
RIGHT
DIAG
BOTTOM
PC 1
PC 2
Flury CPC biplot: Bank notes
TOP
LEFT
RIGHT
LENGTH
BOTTOM
DIAG
PC 1
PC 2

## Quality measures for 2D biplot of Bank Notes data

| | Overall | Within | Between | MSPE | Sample predictivities |
|---|---|---|---|---|---|
| Pooled S | 0.42 | **0.72** | 0.21 | 0.80 | 0.35 |
| Pooled data | **0.88** | 0.70 | **1.00** | **0.44** | **0.85** |
| Flury | 0.65 | 0.70 | 0.61 | 0.75 | 0.62 |
| Stepwise CPC | 0.35 | 0.71 | 0.10 | 0.75 | 0.31 |
| JADE | 0.44 | 0.71 | 0.26 | 0.79 | 0.38 |

## CPC regression

$$Y = \beta_0 + \beta_1 Z_1 + \ldots + \beta_q Z_q + \epsilon, \qquad 1 \leq q \leq p, \tag{9}$$

where $Z_j$ is the $j^{th}$ common principal component,

$$Z_j = \mathsf{b}_{j1} X_{i1} + \mathsf{b}_{j2} X_{i2} + \cdots + \mathsf{b}_{jp} X_{ip}, \qquad j = 1, \ldots, p; i = 1, \ldots, k. \tag{10}$$

Add dummy variables to design matrix to indicate group membership: Allows fitting regression models with different intercepts and/or partial slopes for the different groups.

## CPC regression: Conclusions

- CPC and PC regression provide very similar fits
- regression on full set of CPCs gives same fit as OLS regression
- CPC is covariance matrix model: not aimed at predicting a response
- PLS regression will give better results than CPC

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