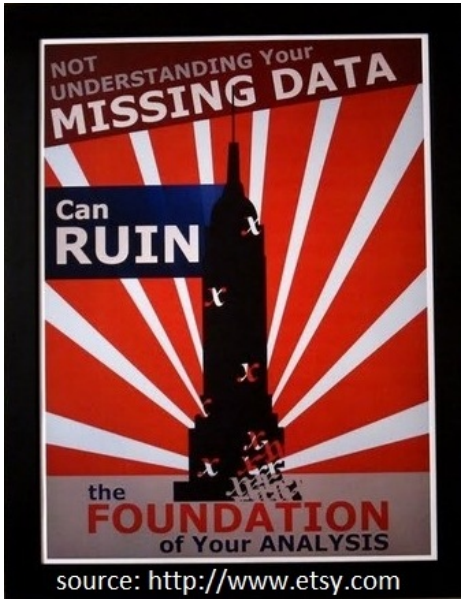
Handling missing values

Julie Josse
Polytechnique CMAP, INRIA



Palaiseau, 28 June 2018

Research activities

- Dimensionality reduction methods to visualize complex data (PCA based): multi-sources data, textual data, arrays
- Missing values - matrix completion
- Low rank estimation, selection of regularization parameters
- Fields of application: bio-sciences (agronomy, sensory analysis), health data (hospital APHP)
- R community: book R for Statistics, R foundation, R taskforce for women, R packages and JSS papers:

  FactoMineR explore continuous, categorical, multiple contingency tables (correspondence analysis), combine clustering and PC, ..
  MissMDA for single and multiple imputation, PCA with missing
  denoiseR to denoise data

Outline

⇒ Morning:

- overview of missing values problems
- single imputation with SVD methods

⇒ Afternoon:

- multiple imputation
- categorical, mixed data

⇒ Lecture notes + code available

Outline

1. Introduction
2. Single imputation with PCA
3. SI Practice
4. Single imputation for mixed variables
5. Multiple imputation for continuous data
6. Multiple imputation for categorical data
7. Conclusion
8. Distribution

Missing values

are everywhere: unanswered questions in a survey, lost data, damaged plants, machines that fail...

The best thing to do with missing values is not to have any" Gertrude Mary Cox.

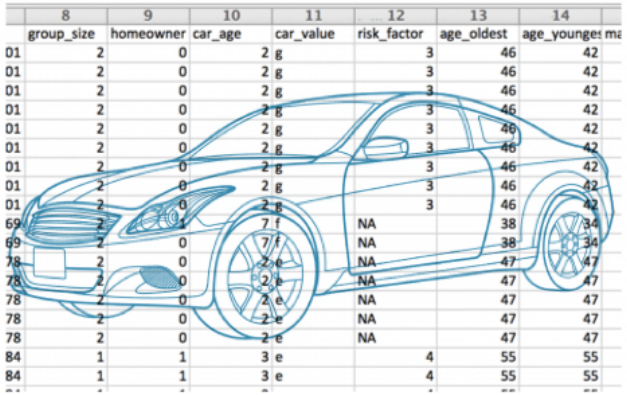
⇒ Still an issue in the "big data" area

Data integration: data from different sources

Kaggle

You can use any type of data to create a Kaggle competition, for example:

- **Numerical**
- Text
- Media
- Multiple formats



	8 group_size	9 homeowner	10 car_age	11 car_value	12 risk_factor	13 age_oldest	14 age_younges ma
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
01	2	0	2	g	3	46	42
69	2	0	7	f	NA	38	34
69	2	0	7	f	NA	38	34
78	2	0	2	e	NA	47	47
78	2	0	2	e	NA	47	47
78	2	0	2	e	NA	47	47
78	2	0	2	e	NA	47	47
78	2	0	2	e	NA	47	47
84	1	1	3	e	4	55	55
84	1	1	3	e	4	55	55

Allstate ran a competition to predict a customer's purchase based on a limited amount of shopping history data.

airbnb

Jobs • 1,429 teams

Airbnb New User Bookings

Wed 25 Nov 2015 — Thu 11 Feb 2016 (40 hours to go)

Predict in which country a new user will make his first booking:
age: 42.4 %
date first booking: 6.7 %
first affiliate tracked: 2.2 %
gender: 46 %

Public Assistance - Paris Hospitals

Traumabase: 15000 patients/ 250 variables

	Center	Accident	Age	Sex	Weight	Height	BMI	BP	SBP
1	Beaujon	Fall	54	m	85	NR	NR	180	110
2	Lille	Other	33	m	80	1.8	24.69	130	62
3	Pitie Salpetriere	Gun	26	m	NR	NR	NR	131	62
4	Beaujon	AVP moto	63	m	80	1.8	24.69	145	89
6	Pitie Salpetriere	AVP bicycle	33	m	75	NR	NR	104	86
7	Pitie Salpetriere	AVP pedestrian	30	w	NR	NR	NR	107	66
9	HEGP	White weapon	16	m	98	1.92	26.58	118	54
10	Toulon	White weapon	20	m	NR	NR	NR	124	73
11	Bicetre	Fall	61	m	84	1.7	29.07	144	105

.....

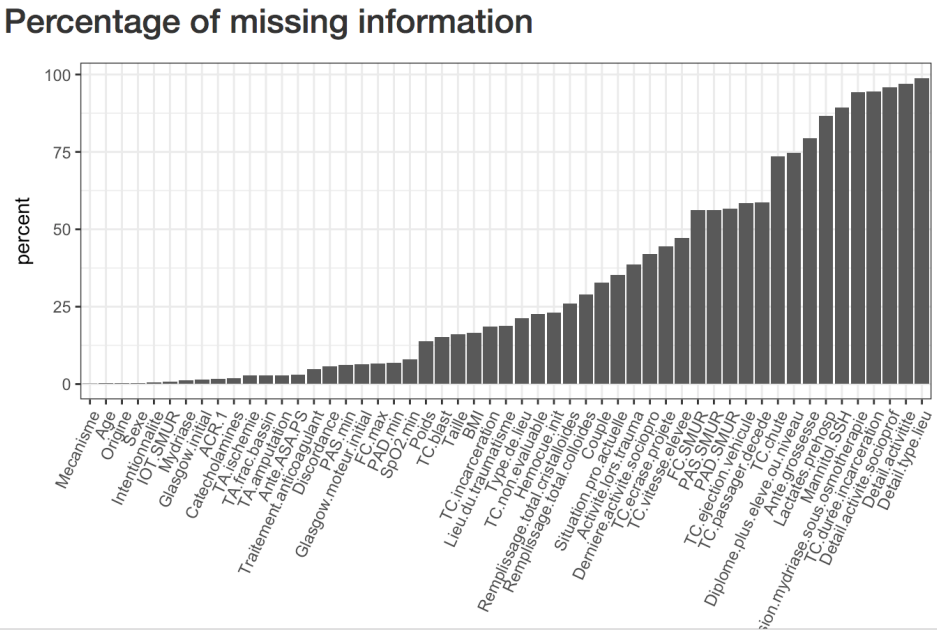
	SpO2	Temperature	Lactates	Hb	Glasgow	Transfusion	.....
1	97	35.6	<NA>	12.7	12	yes	
2	100	36.5	4.8	11.1	15	no	
3	100	36	3.9	11.4	3	no	
4	100	36.7	1.66	13	15	yes	
6	100	36	NM	14.4	15	no	
7	100	36.6	NM	14.3	15	yes	
9	100	37.5	13	15.9	15	yes	
10	100	36.9	NM	13.7	15	no	
11	100	36.6	1.2	14.2	14	no	

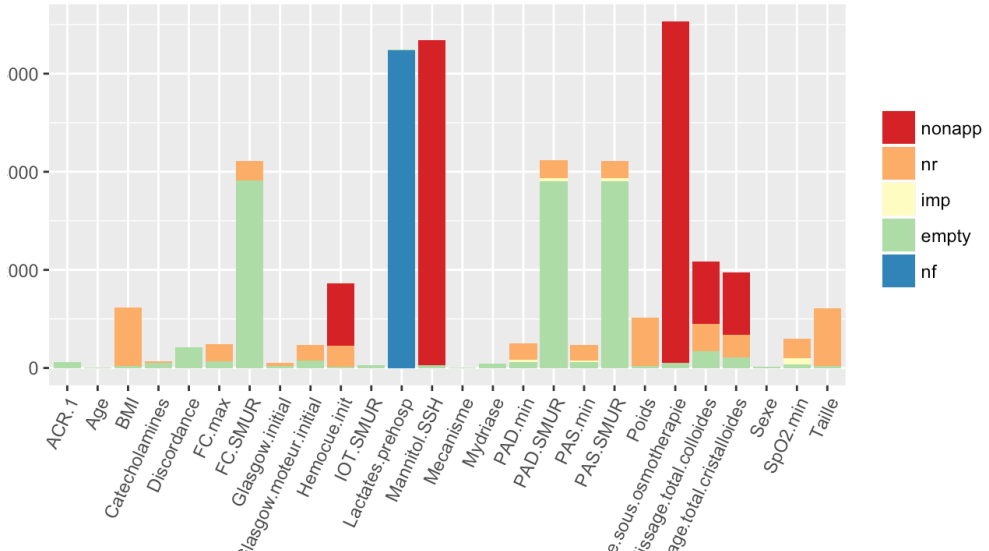
.....

$\Rightarrow$ Predict the Glasgow score, whether to start a blood transfusion, to administer fresh frozen plasma, etc...

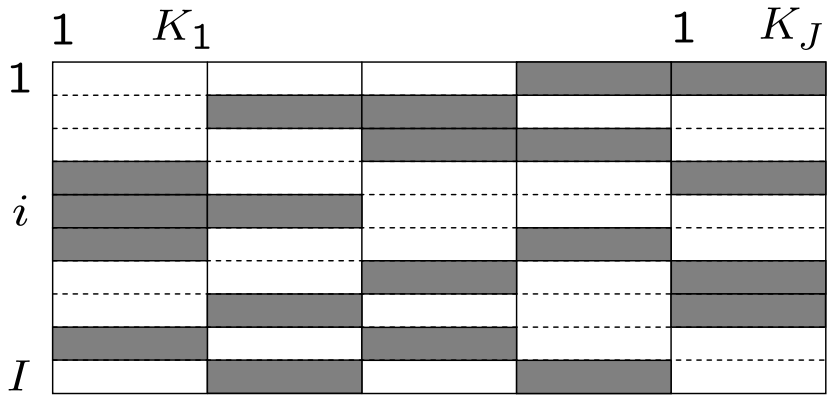
$\Rightarrow$ Logistic regressions/Random Forests with missing categorical/continuous values

Public Assistance - Paris Hospitals





Multi-blocks data set



L'OREAL: 100 000 women in different countries - 300 variables

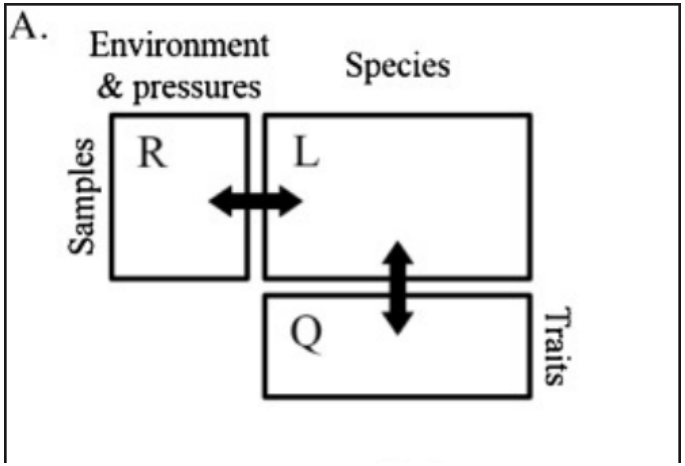
- Self-assessment questionnaire: life style, skin and hair characteristics, care and consumer habits
- Clinical assessments by a dermatologist: facial skin complexion, wrinkles, scalp dryness, greasiness
- Hair assessments by a hair dresser: abundance, volume, breakage, curliness
- Skin and hair photographs and measurements: sebum quantity, etc.

Contingency tables with side information

National agency for wildlife and hunting management (ONCFS)

Data: Water-bird count data, 1990-2016 from 722 wetland sites in 5 countries in North Africa

Sites and years infp: meteorological, geographical (altitude, long)



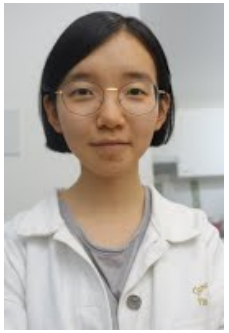
⇒ Aims: Assess the effect of time on species abundances

Monitor the population and assess wetlands conservation policies.

⇒ 70% of missing values in contingency tables

On going works

- François Husson (Agrocampus)
- Genevieve Robin, B. Narasimhan (Stanford): distributed matrix completion for multilevel medical data
- Genevieve Robin, R. Tibshirani (Stanford), E. Mouline, O. Klopp: imputation of multilevel tables with main effects
- Wei Jiang: glm with missing values and variable selection
- Erwan Scornet, N. Prost, S. Wager, G. Varoquaux (INRIA): random forest with missing values and causal inference



Ozone data set

	maxO3	T9	T12	T15	Ne9	Ne12	Ne15	Vx9	Vx12	Vx15	maxO3v
0601	NA	15.6	18.5	18.4	4	4	8	NA	-1.7101	-0.6946	84
0602	82	17	18.4	17.7	5	5	7	NA	NA	NA	87
0603	92	NA	17.6	19.5	2	5	4	2.9544	1.8794	0.5209	82
0604	114	16.2	NA	NA	1	1	0	NA	NA	NA	92
0605	94	17.4	20.5	NA	8	8	7	-0.5	NA	-4.3301	114
0606	80	17.7	NA	18.3	NA	NA	NA	-5.6382	-5	-6	94
0607	NA	16.8	15.6	14.9	7	8	8	-4.3301	-1.8794	-3.7588	80
0610	79	14.9	17.5	18.9	5	5	4	0	-1.0419	-1.3892	NA
0611	101	NA	19.6	21.4	2	4	4	-0.766	NA	-2.2981	79
0612	NA	18.3	21.9	22.9	5	6	8	1.2856	-2.2981	-3.9392	101
0613	101	17.3	19.3	20.2	NA	NA	NA	-1.5	-1.5	-0.8682	NA
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
0919	NA	14.8	16.3	15.9	7	7	7	-4.3301	-6.0622	-5.1962	42
0920	71	15.5	18	17.4	7	7	6	-3.9392	-3.0642	0	NA
0921	96	NA	NA	NA	3	3	3	NA	NA	NA	71
0922	98	NA	NA	NA	2	2	2	4	5	4.3301	96
0923	92	14.7	17.6	18.2	1	4	6	5.1962	5.1423	3.5	98
0924	NA	13.3	17.7	17.7	NA	NA	NA	-0.9397	-0.766	-0.5	92
0925	84	13.3	17.7	17.8	3	5	6	0	-1	-1.2856	NA
0927	NA	16.2	20.8	22.1	6	5	5	-0.6946	-2	-1.3681	71
0928	99	16.9	23	22.6	NA	4	7	1.5	0.8682	0.8682	NA
0929	NA	16.9	19.8	22.1	6	5	3	-4	-3.7588	-4	99
0930	70	15.7	18.6	20.7	NA	NA	NA	0	-1.0419	-4	NA

http://www.airbreizh.asso.fr/

Aim: regression with missing values

Some references

Schafer (1997),

Joseph L. Schafer

Little & Rubin (1987, 2002)

Roderick Little

Donald Rubin

Analysis of incomplete data - Statistical analysis with missing values

Suggested reading: chap 25 of Gelman & Hill (2006)

Andrew Gelman

Jennifer L. Hill

Data Analysis Using Regression and Multilevel/Hierarchical Models

Missing values problematic

A very simple way: deletion (default `lm` function in R)

Dealing with missing values depends on:

- the pattern of missing values
- the mechanism leading to missing values

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- the pattern of missing values
- the mechanism leading to missing values

$X = (X_{miss}, X_{obs})$. Let M with $M_{ik} = 1$ if X_{ik} is observed and 0 otherwise. M and X have distributions.

- MCAR: probability does not depend on any values $f(M|X_{obs}, X_{miss}; \phi) = f(M; |phi)$ each entry has the same probability to be observed
- MAR: probability may depend on values on other variables $f(M|X_{obs}, X_{miss}; \phi) = f(M|X_{obs}; \phi)$
- MNAR: probability depends on the value itself $f(M|X_{obs}, X_{miss}; \phi) = f(M|X_{miss}; \phi)$
  $\Rightarrow$ Ex, Age Income.

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  $\Rightarrow$ Ex, Age Income.

$\Rightarrow$ Assume MAR: ignore $f(M|X_{obs}, X_{miss}; \phi)$ when doing inference.

Ignorable

X has a density, parametrized by θ that we want to estimate
$f(X, M|\theta, \phi)$ the joint distribution
ML estimate:

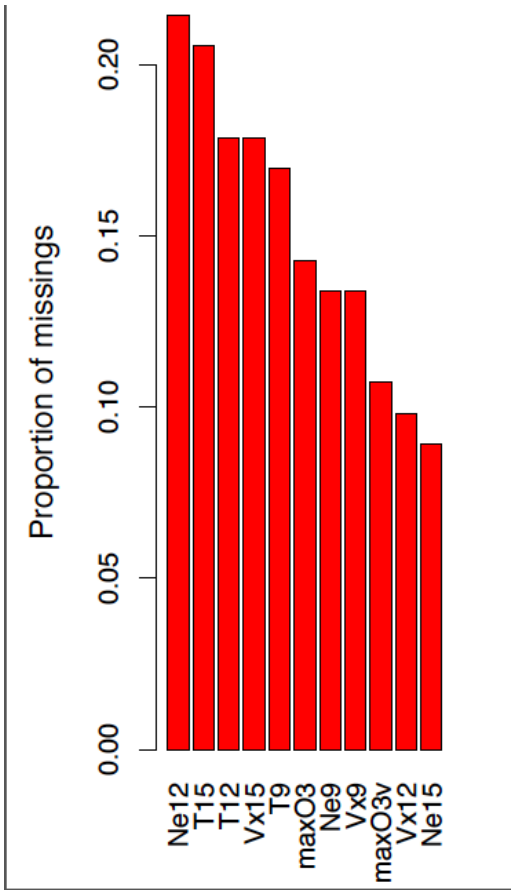
$$\begin{aligned} f(X_{\text{obs}}, M; \theta, \phi) &= \int f(X_{\text{obs}}, X_{\text{mis}}, M; \theta, \phi) dX_{\text{mis}} \\ &= \int f(X_{\text{obs}}, X_{\text{mis}}; \theta) f(M|X_{\text{obs}}, X_{\text{miss}}; \phi) dX_{\text{mis}}. \end{aligned}$$

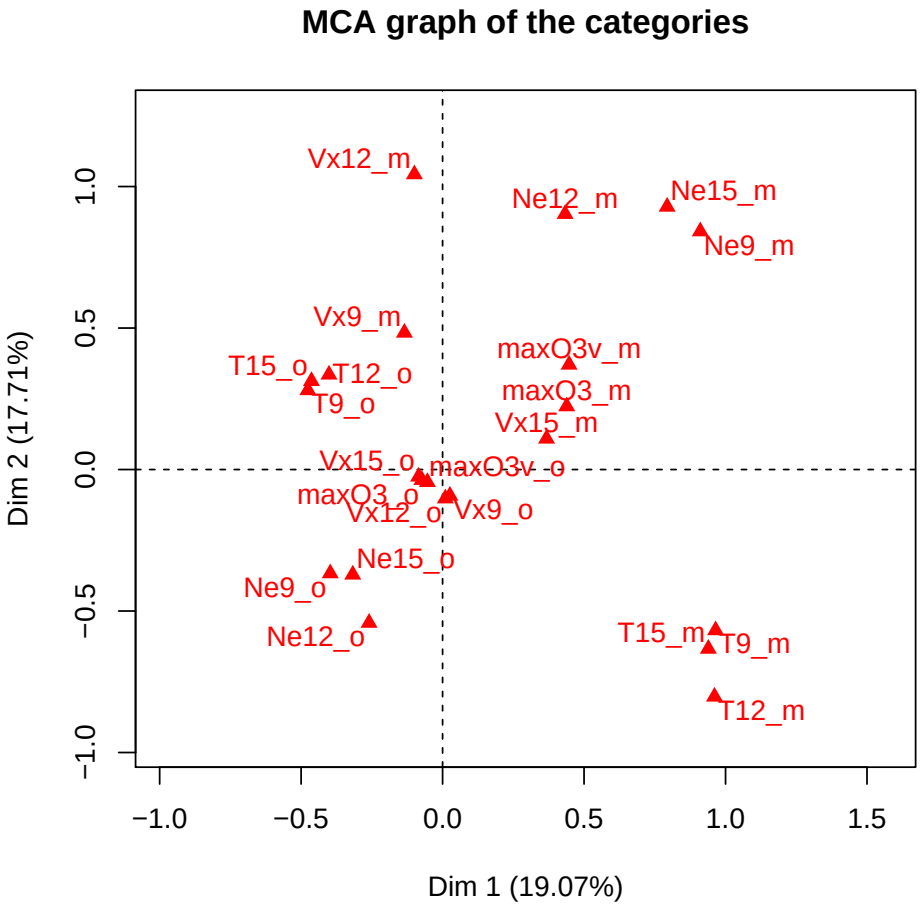
When MAR

$$\begin{aligned} f(X_{\text{obs}}, M; \theta, \phi) &= \int f(X_{\text{obs}}, X_{\text{mis}}; \theta) f(M|X_{\text{obs}}; \phi) dX_{\text{mis}}, \\ &= f(M|X_{\text{obs}}; \phi) \int f(X_{\text{obs}}, X_{\text{miss}}; \theta) dX_{\text{miss}}, \end{aligned}$$

$$f(X_{\text{obs}}, M; \theta, \phi) = f(M|X_{\text{obs}}; \phi) f(X_{\text{obs}}; \theta).$$

Visualization with Multiple Correspondence Analysis





Implemented in `VIM`, `naniar` (matthias Templ, Nick Tierney) - `FactoMineR` (YouTube)

Recommended methods

$\Rightarrow$ Modify the method, the estimation process to deal with missing values. Maximum likelihood: EM algorithm to obtain point estimates (+ other algorithms for their variability)

Expectation - Maximization (Dempster *et al.*, 1977)

$\Rightarrow$ Modify the estimation process (not always easy!)

Rationale to get ML estimates: max L_{obs} through max of L_{comp} of $X = (X_{obs}, X_{miss})$. Augment the data to simplify the problem.

E step (conditional expectation):

$$Q(\theta, \theta^{\ell}) = \int \ln(f(X;\theta)) f(X_{miss}|X_{obs};\theta^{\ell}) dX_{miss}$$

M step (maximization):

$$\theta^{\ell+1} = \text{argmax}_{\theta} Q(\theta, \theta^{\ell})$$

Result: when $\theta^{\ell+1}$ max $Q(\theta, \theta^{\ell})$ then $L(X_{obs}, \theta^{\ell+1}) \geq L(X_{obs}, \theta^{\ell})$.

Maximum likelihood approach

Ex: Hypothesis $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$

$\Rightarrow$ Point estimates with EM:

```
> library(norm)
> pre <- prelim.norm(as.matrix(don))
> thetahat <- em.norm(pre)
> getparam.norm(pre,thetahat)
```

Exercice: EM with bivariate data

Maximum likelihood approach

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Exercice: EM with bivariate data

$\Rightarrow$ Variances:

- Supplemented EM (Meng, 1991), Louis formulae
- Bootstrap approach:
  - Bootstrap rows: $X^1, \ldots, X^B$
  - EM algorithm: $(\hat{\mu}^1, \hat{\Sigma}^1), \ldots, (\hat{\mu}^B, \hat{\Sigma}^B)$

Maximum likelihood approach

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Other models: SAEM (SAEM for logistic regression)

Recommended methods

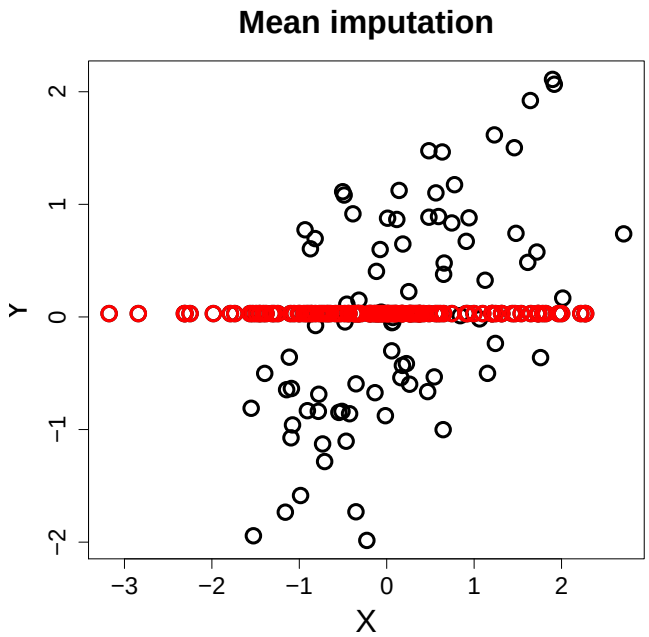
$\Rightarrow$ Modify the method, the estimation process to deal with missing values. Maximum likelihood: EM algorithm to obtain point estimates (+ other algorithms for their variability)

One specific algorithm for each statistical method...

$\Rightarrow$ Imputation (multiple) to get a completed data set on which you can perform any statistical method

Dealing with missing values

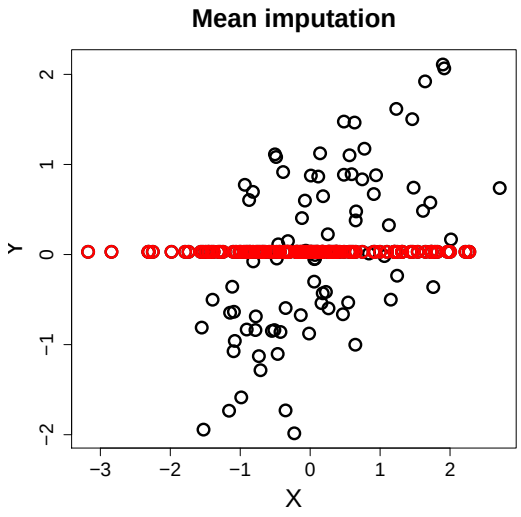
⇒ Imputation to get a completed data set



$\mu_y = 0$
$\sigma_y = 1$
$\rho = 0.6$

$\hat{\mu}_y = 0.01$
$\hat{\sigma}_y = 0.5$
$\hat{\rho} = 0.30$

Imputation with joint model with gaussian distribution



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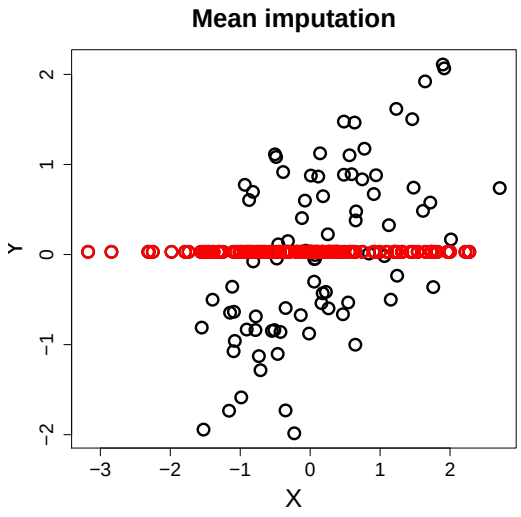
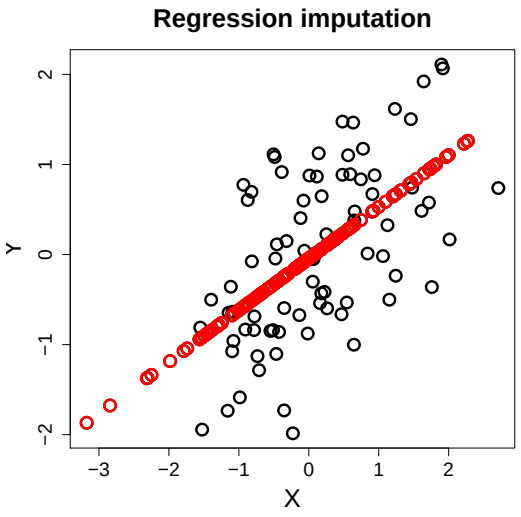
0.01
0.5
0.30

Imputation with joint model with gaussian distribution

- Impute by regression take into account the relationship: estimate β - impute $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \Rightarrow$ variance underestimated and correlation overestimated.





$\mu_y = 0$
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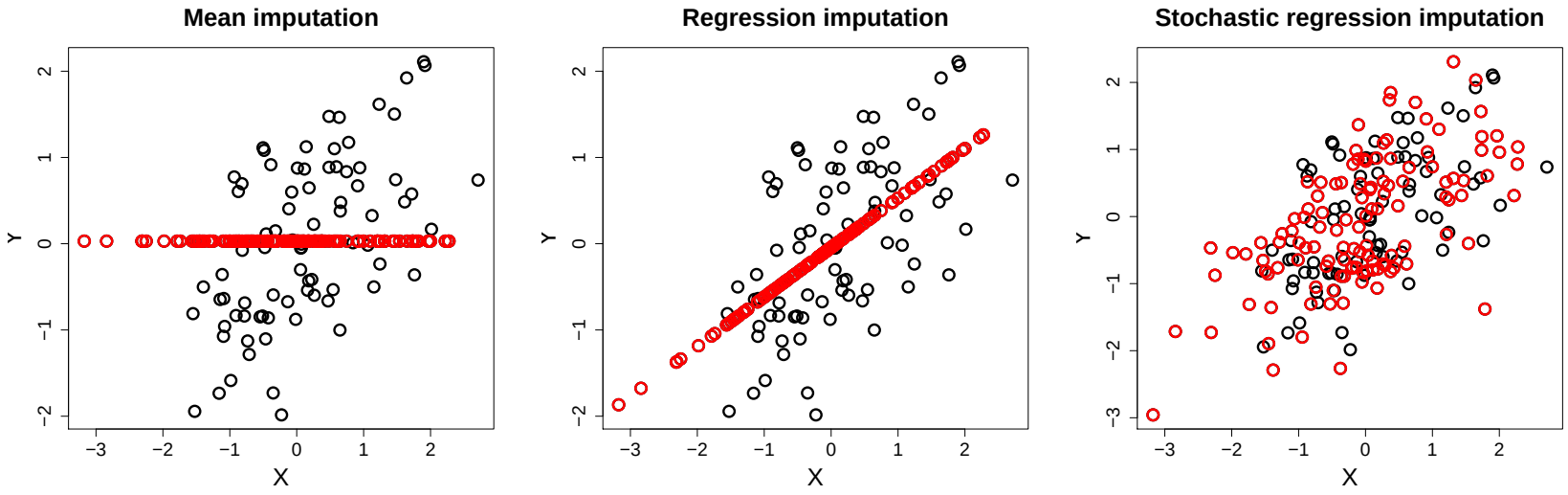
0.01
0.5
0.30

0.01
0.72
0.78

Imputation with joint model with gaussian distribution

- Impute by regression take into account the relationship: estimate β - impute $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \Rightarrow$ variance underestimated and correlation overestimated.
- Impute by stochastic reg: estimate β and σ - impute from the predictive $y_i \sim \mathcal{N}\left(x_i\hat{\beta}, \hat{\sigma}^2\right) \Rightarrow$ preserve distribution



	Mean imputation	Regression imputation	Stochastic regression imputation
$\mu_y = 0$	0.01	0.01	0.01
$\sigma_y = 1$	0.5	0.72	0.99
$\rho = 0.6$	0.30	0.78	0.59

Imputation with joint model with gaussian distribution

$\Rightarrow$ Hypothesis $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$

Bivariate case with missing values on $x_{.1}$ (stochastic regression): estimate β and σ - impute from the predictive $x_{i1} \sim \mathcal{N}\left(x_{i2}\hat{\beta}, \hat{\sigma}^2\right)$

Extension to the multivariate case:

- Estimate μ and Σ from an incomplete data with EM
- Impute by drawing from $\mathcal{N}\left(\hat{\mu}, \hat{\Sigma}\right) \Rightarrow$ equivalence conditional expectation and regression

```
> pre <- prelim.norm(as.matrix(don))
> thetahat <- em.norm(pre)
> rngseed(123)
> imp <- imp.norm(pre,thetahat,don)
# Same withres.amelia$imputations$imp1
```

Other single imputation methods

- k-nearest neighbor (package `class`, `FNN`)
- random forest (package `missForest`, Stekhoven & Bühlmann, 2011)
- based on Gaussian assumption (join/ conditional), packages `mice`, `Amelia`

⇒ van Buuren: http://www.stefvanbuuren.nl/mi/Software.html
⇒ R task View: Official Statistics & Survey Methodology
⇒ R miss-tatic

Outline

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2. Single imputation with PCA
3. SI Practice
4. Single imputation for mixed variables
5. Multiple imputation for continuous data
6. Multiple imputation for categorical data
7. Conclusion
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PCA (complete)

Find the subspace that best represents the data

Figure: Camel or dromedary?

$\Rightarrow$ Best approximation with projection
$\Rightarrow$ Best representation of the variability

PCA (complete)

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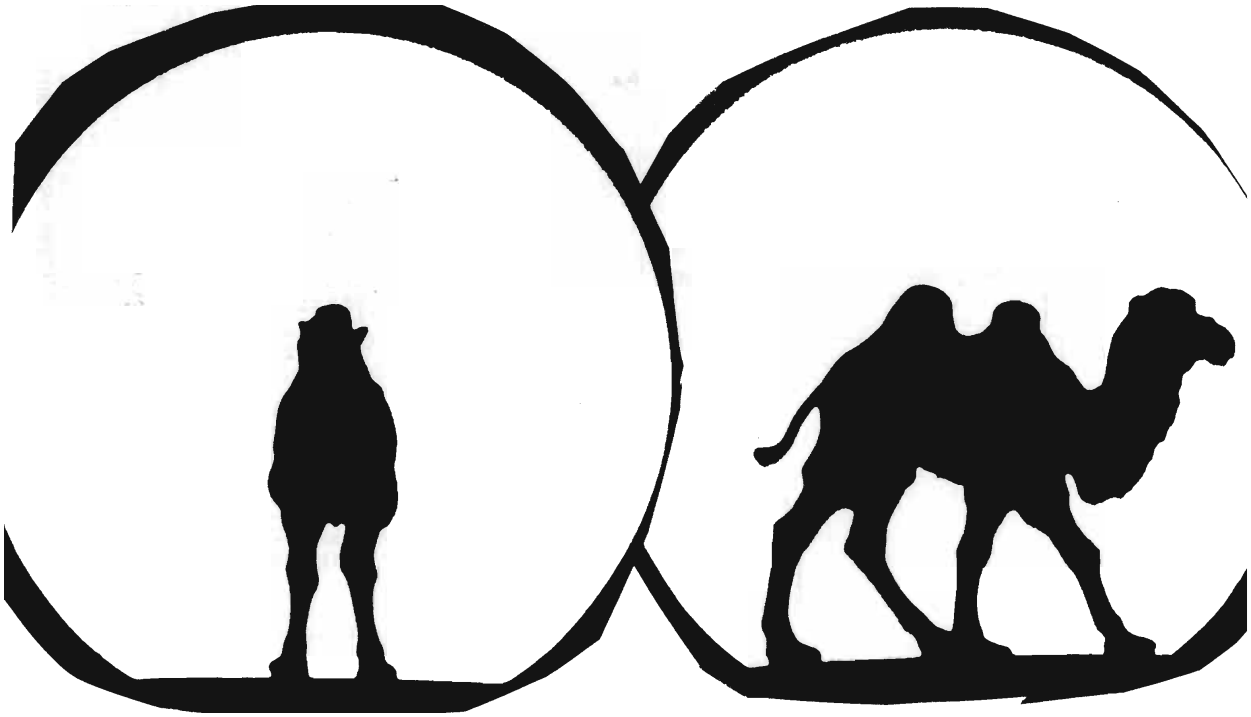


Figure: Camel or dromedary? source J.P. Fénelon

$\Rightarrow$ Best approximation with projection
$\Rightarrow$ Best representation of the variability

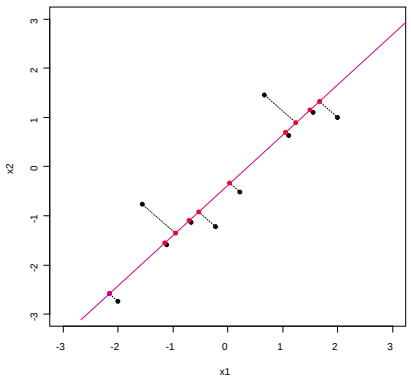
PCA reconstruction

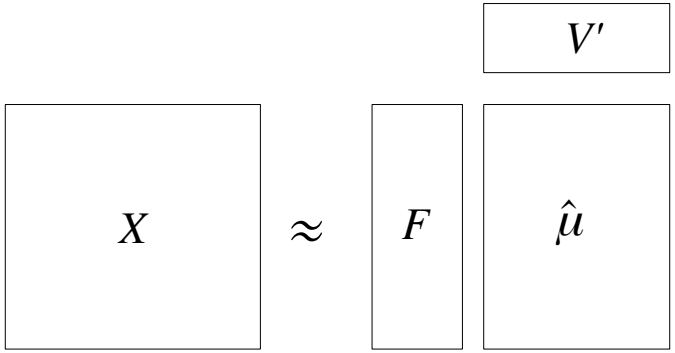
X

-2.00	-2.74
-1.56	-0.77
-1.11	-1.59
-0.67	-1.13
-0.22	-1.22
0.22	-0.52
0.67	1.46
1.11	0.63
1.56	1.10
2.00	1.00

$\hat{\mu}$

-2.16	-2.58
-0.96	-1.35
-1.15	-1.55
-0.70	-1.09
-0.53	-0.92
0.04	-0.34
1.24	0.89
1.05	0.69
1.50	1.15
1.67	1.33





$\Rightarrow$ Minimizes distance between observations and their projection

$\Rightarrow$ Approx $X_{n\times p}$ with a low rank matrix $S < p$ $\|A\|_2^2 = \mathrm{tr}(AA^\top)$:

$$\mathrm{argmin}_\mu \left\{ \|X - \mu\|_2^2 : \mathrm{rank}\,(\mu) \leq S \right\}$$

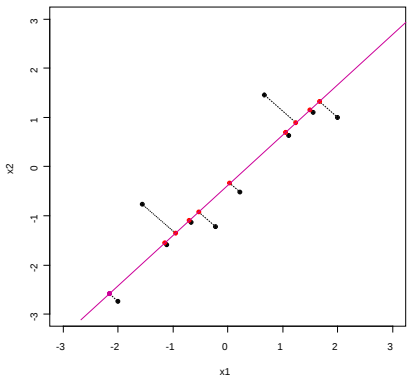
PCA reconstruction

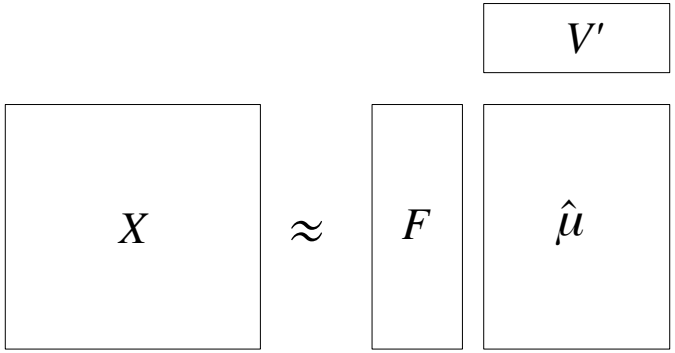
X

-2.00	-2.74
NA	-0.77
-1.11	-1.59
-0.67	-1.13
-0.22	NA
0.22	-0.52
0.67	1.46
NA	0.63
1.56	1.10
2.00	1.00

$\hat{\mu}$

-2.16	-2.58
-0.96	-1.35
-1.15	-1.55
-0.70	-1.09
-0.53	-0.92
0.04	-0.34
1.24	0.89
1.05	0.69
1.50	1.15
1.67	1.33





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SVD X: $\hat{\mu}^{\mathrm{PCA}} = U_{n\times S}\Lambda^{\frac{1}{2}}_{S\times S}V'_{p\times S}$ $\quad F = U\Lambda^{\frac{1}{2}}$ PC - scores

$= F_{n\times S}V'_{p\times S}$ $\quad V$ principal axes - loadings

Missing values in PCA

$\Rightarrow$ PCA: least squares

$$\text{argmin}_{\mu} \left\{ \|X_{n\times p} - \mu_{n\times p}\|_2^2 : \text{rank}\,(\mu) \leq S \right\}$$

$\Rightarrow$ PCA with missing values: weighted least squares

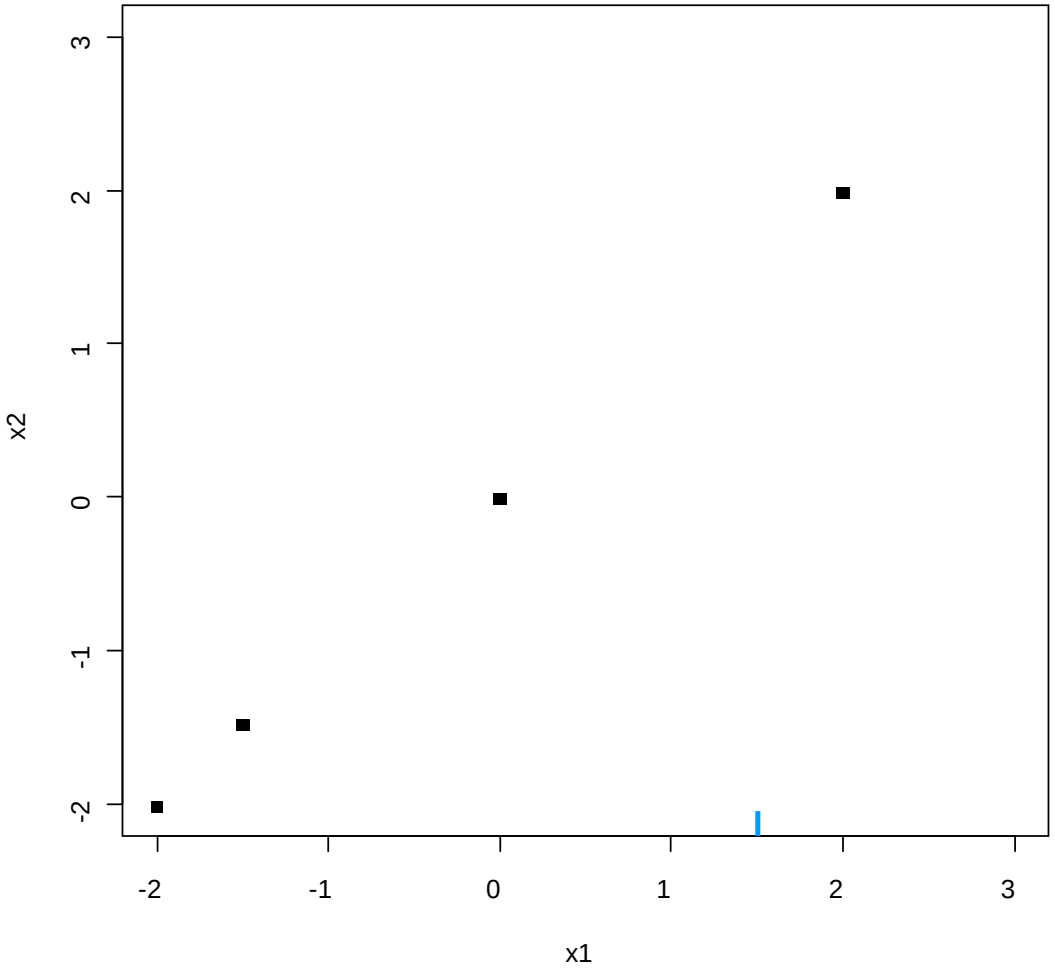
$$\text{argmin}_{\mu} \left\{ \| W_{n\times p} * (X - \mu)\|_2^2 : \text{rank}\,(\mu) \leq S \right\}$$

with $W_{ij} = 0$ if X_{ij} is missing, $W_{ij} = 1$ otherwise; $*$ elementwise multiplication

Many algorithms: weighted alternating least squares (Gabriel & Zamir, 1979); iterative PCA (Kiers, 1997)

Iterative PCA

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	NA
2.0	1.98



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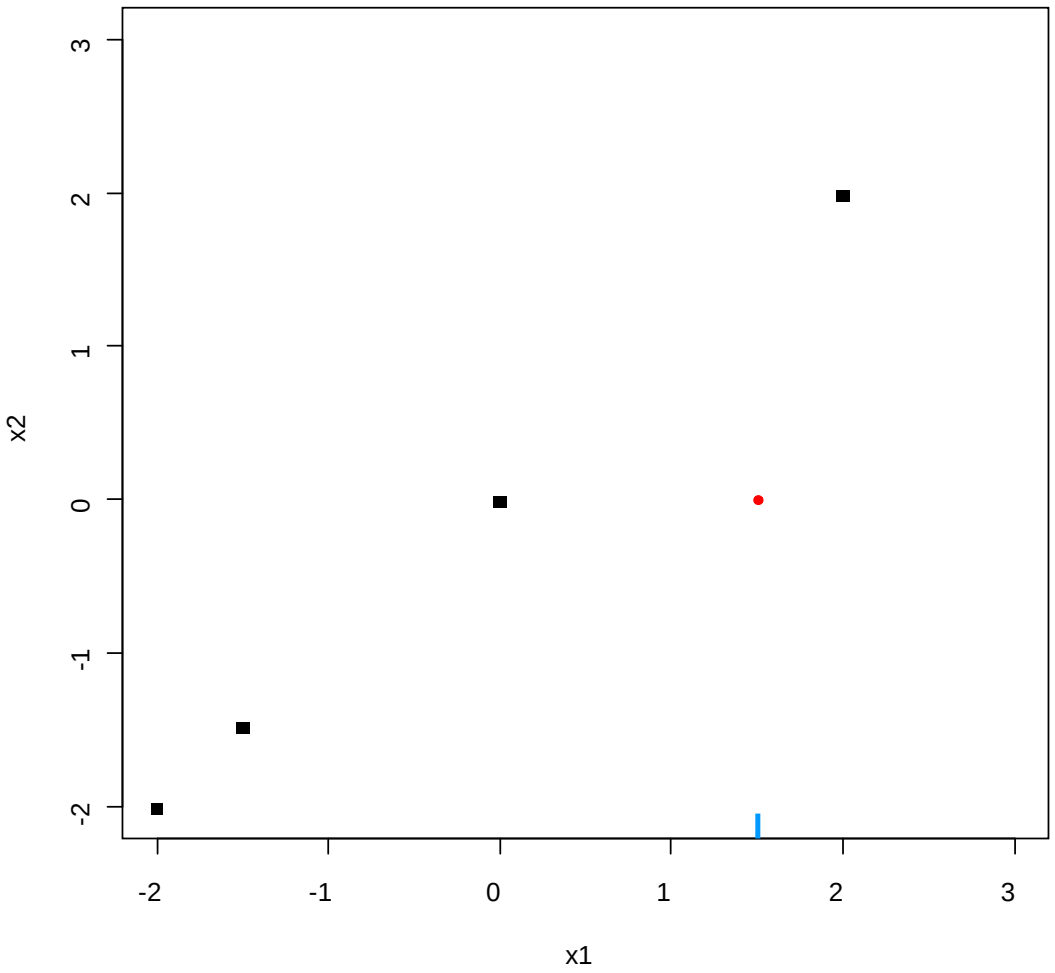

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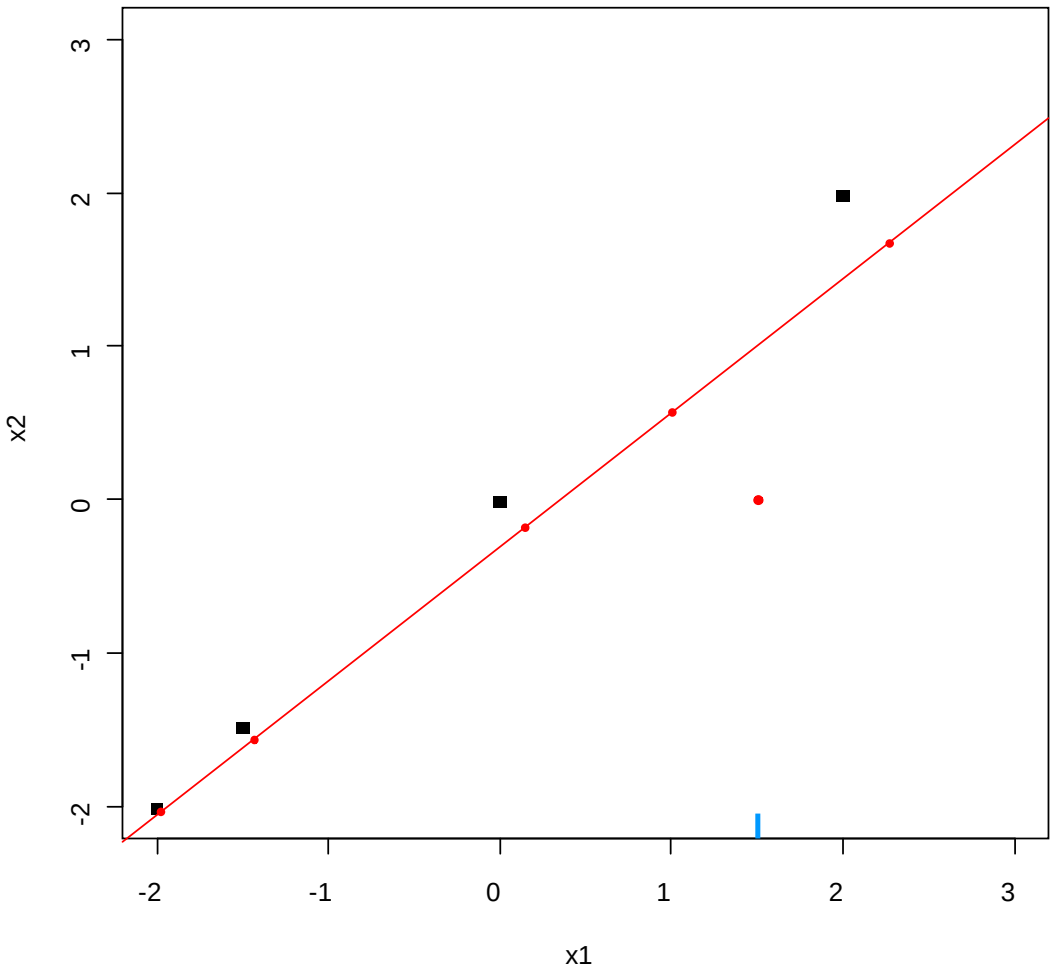
$\widehat{x1}$	$\widehat{x2}$
-1.98	-2.04
-1.44	-1.56
0.15	-0.18
1.00	0.57
2.27	1.67



PCA on the completed data set $\rightarrow (U^\ell, \Lambda^\ell, V^\ell)$;

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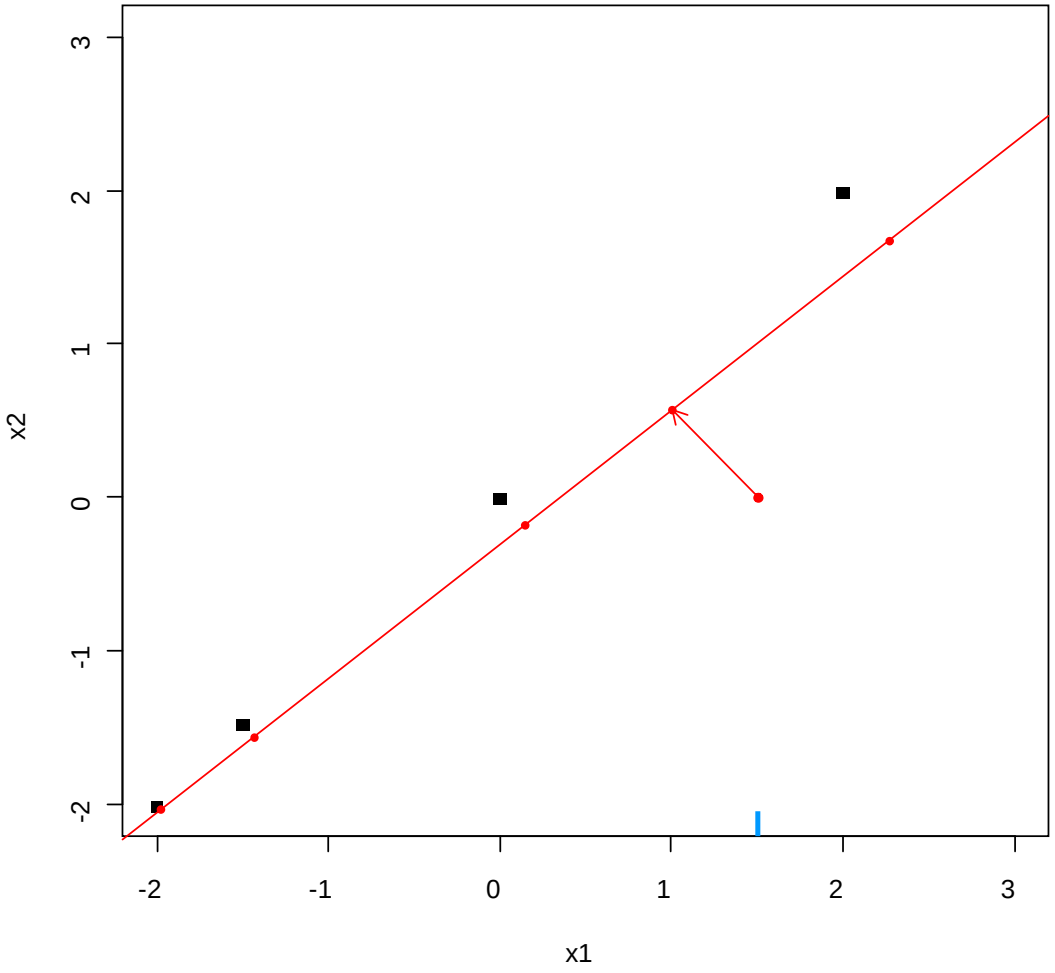

Missing values imputed with the fitted matrix $\hat{\mu}^\ell = U^\ell \Lambda^{1/2^\ell} V^{\ell\prime}$

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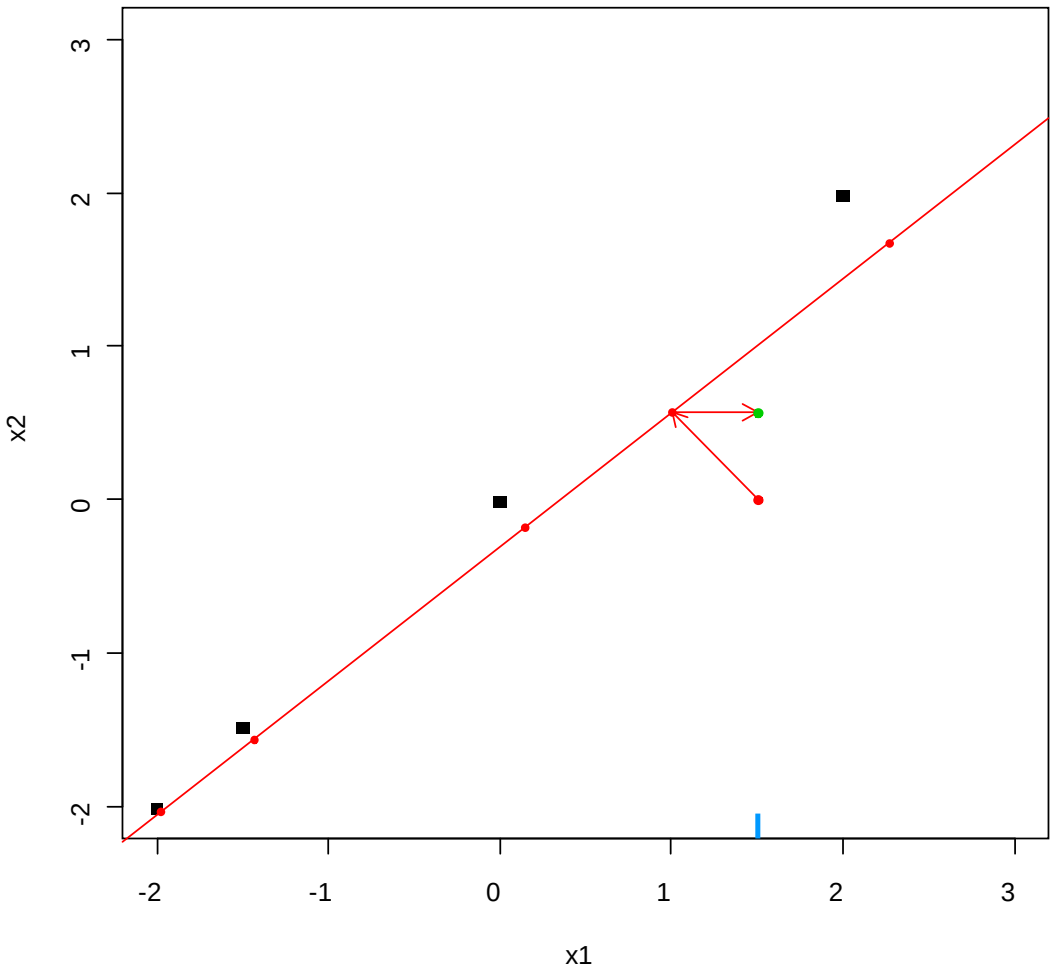

The new imputed dataset is $\hat{X}^{\ell} = W * X + (\mathbf{1} - W) * \hat{\mu}^{\ell}$

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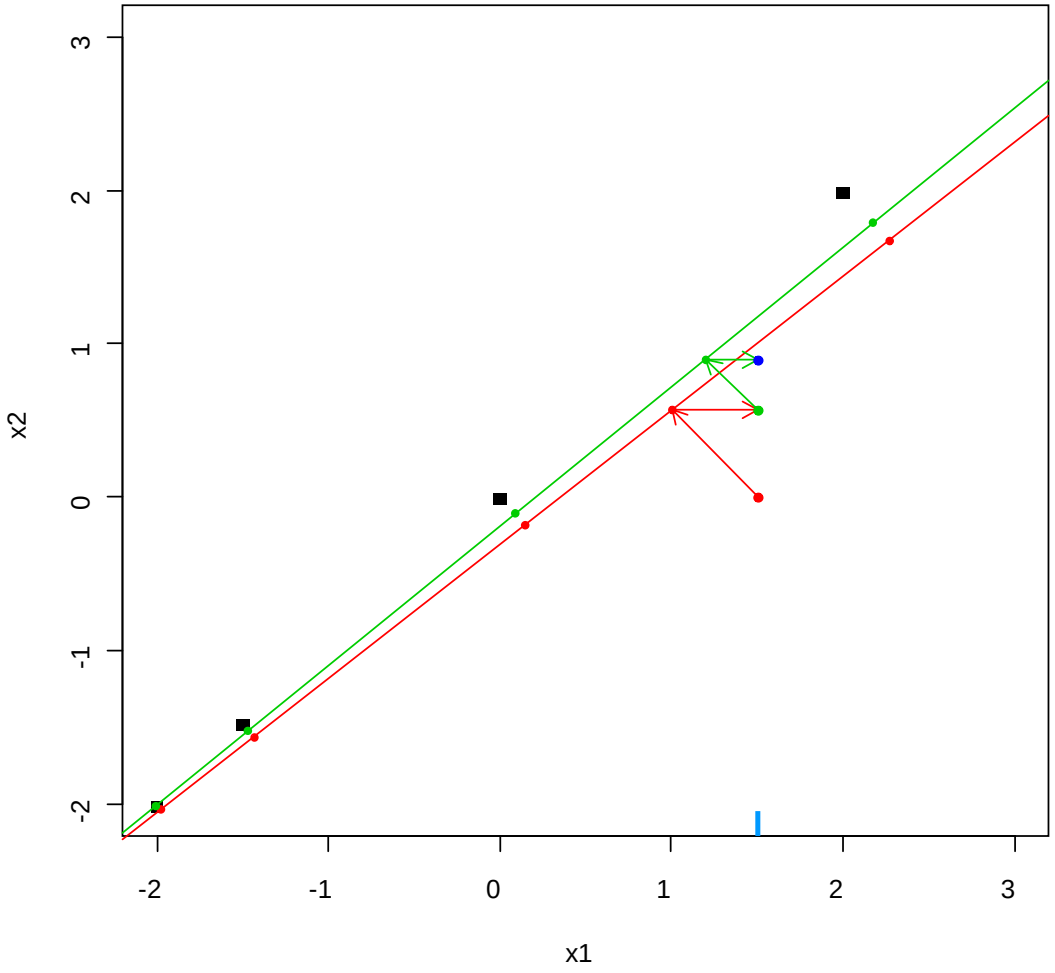

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$\hat{x1}$	$\hat{x2}$
-2.00	-2.01
-1.47	-1.52
0.09	-0.11
1.20	**0.90**
2.18	1.78

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-2.0	-2.01
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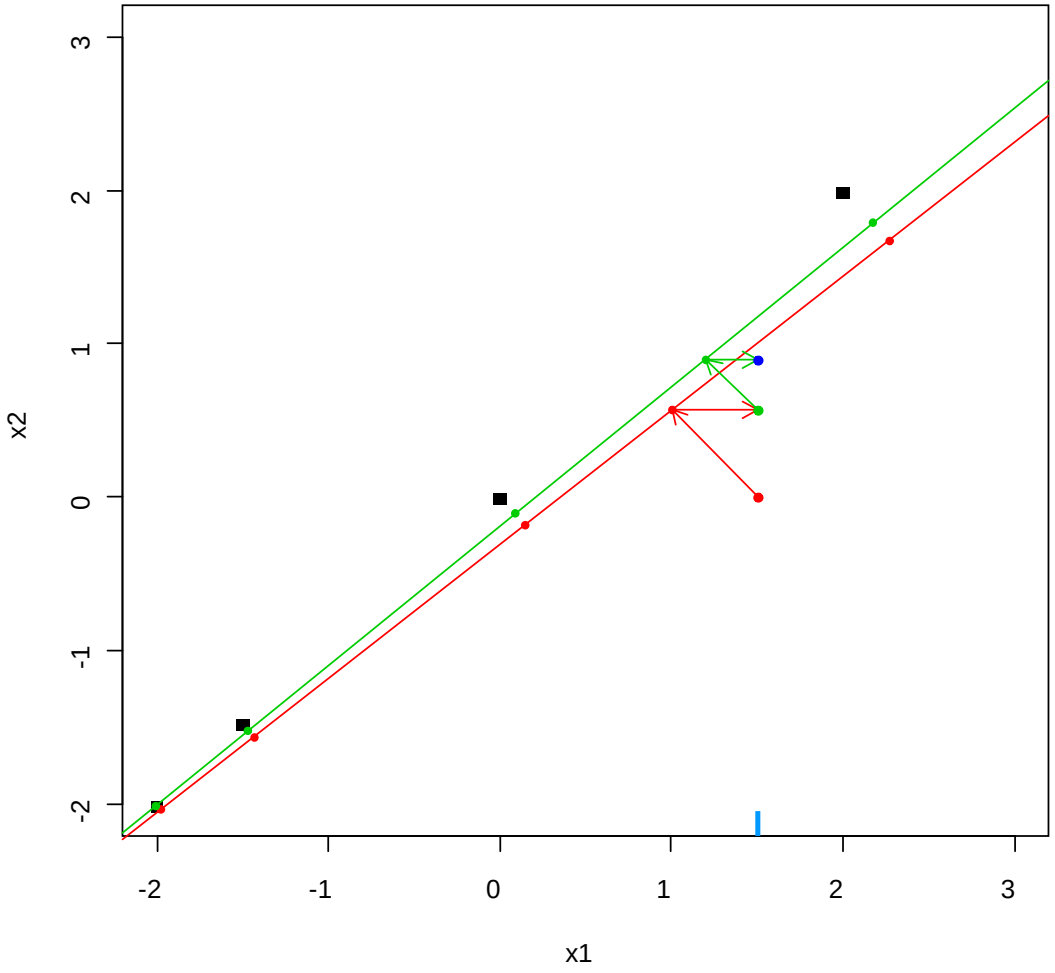

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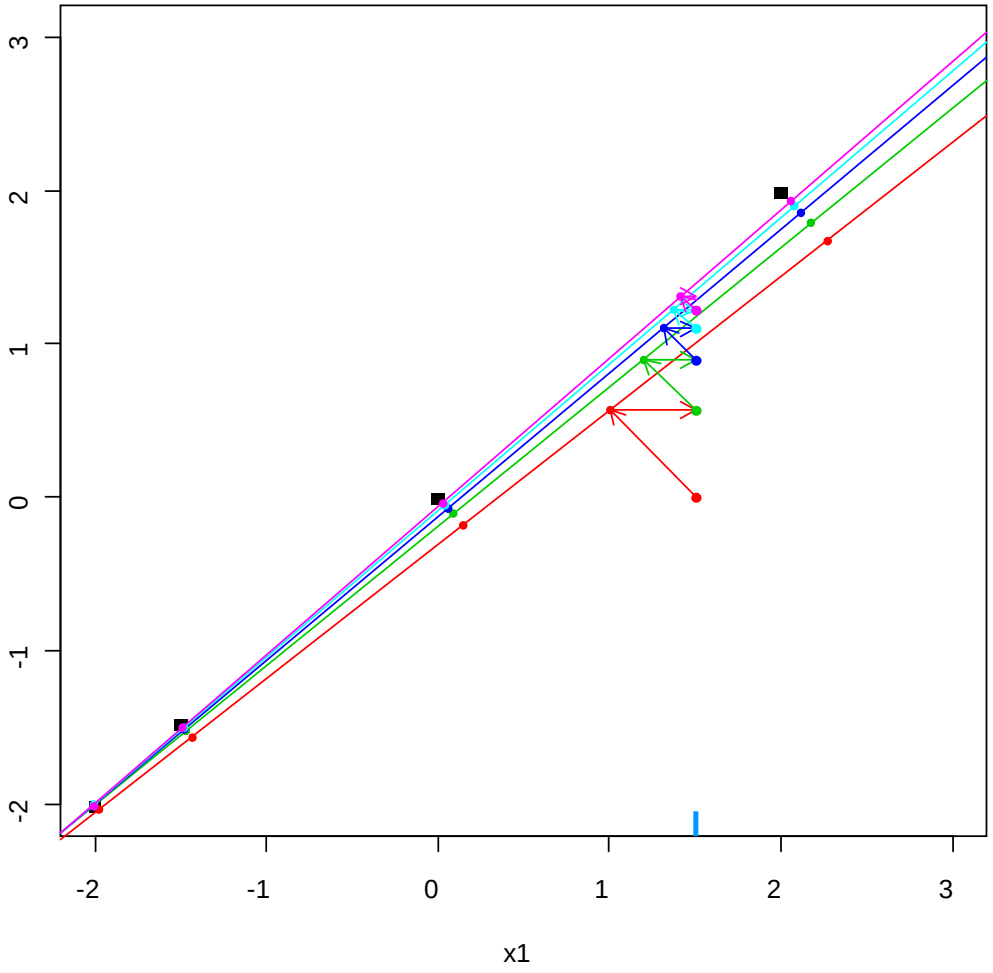

Steps are repeated until convergence

Iterative PCA

```
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-1.5 -1.48
 0.0 -0.01
 1.5    NA
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```

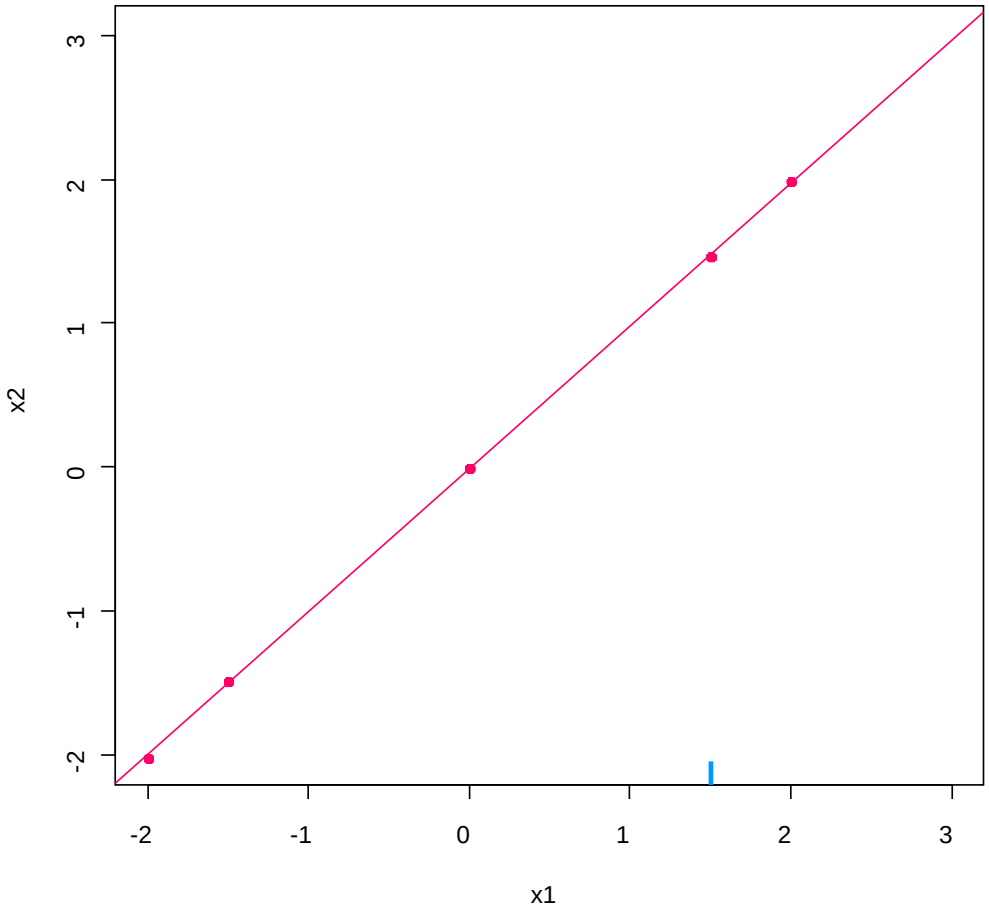


```
  x1    x2
-2.0 -2.01
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 0.0 -0.01
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```

PCA on the completed data set $\rightarrow (U^\ell, \Lambda^\ell, V^\ell)$

Missing values imputed with the fitted matrix $\hat{\mu}^\ell = U^\ell \Lambda^{1/2^\ell} V^{\ell\prime}$

Iterative PCA

1. initialization $\ell = 0$: X^0 (mean imputation)
2. step ℓ:
   (a) PCA on the completed data $\rightarrow (U^\ell, \Lambda^\ell, V^\ell)$;
   S dimensions kept
   (b) missing values are imputed with $(\hat{\mu}^S)^\ell = U^\ell \Lambda^{1/2^\ell} V^{\ell\prime}$
   the new imputed data is $\hat{X}^\ell = W * X + (\mathbf{1} - W) * (\hat{\mu}^S)^\ell$
3. steps of estimation and imputation are repeated

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$\Rightarrow$ $\hat{\mu}$ from incomplete data: EM algo

$X_{n\times p} = \mu + \varepsilon,\ \varepsilon_{ij} \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)\ x_{ij} = \sum_{s=1}^{S} \sqrt{\tilde{\lambda}_s} \tilde{u}_{is} \tilde{v}_{js} + \varepsilon_{ij}$

$\Rightarrow$ Reduction of the variability (imputation by $U\Lambda^{1/2}V'$)

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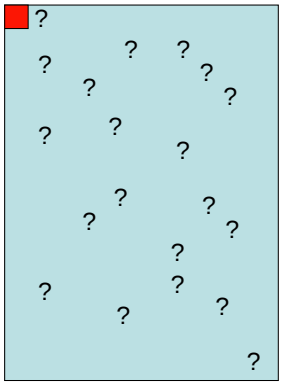
$\Rightarrow$ Reduction of the variability (imputation by $U\Lambda^{1/2}V'$)

$\Rightarrow$ Selecting S? Cross-validation

Cross-validation to select S



$\Rightarrow$ EM-CV (Bro *et al.* 2008)
$\Rightarrow$ $\text{MSEP}_S = \frac{1}{np}\sum_{i=1}^{n}\sum_{j=1}^{p}(X_{ij} - (\hat{\mu}_{ij}^{S})^{-ij})^2$
$\Rightarrow$ Computational costly

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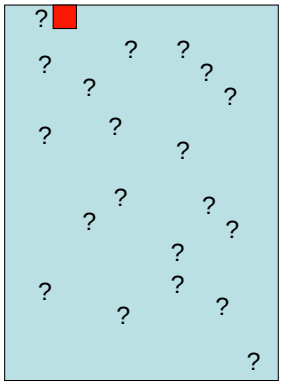

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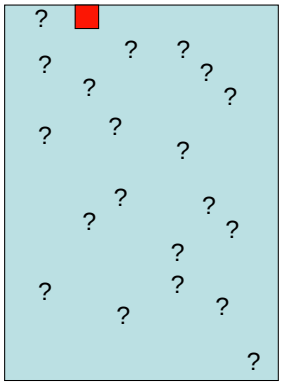

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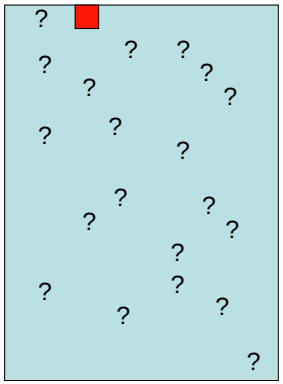

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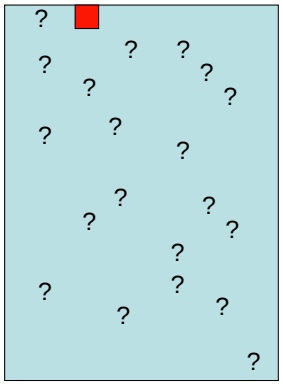
$\Rightarrow$ In regression $\hat{y} = Py$ (Craven & Whaba, 1979)

$$\hat{y}_i^{-i} - y_i = \frac{\hat{y}_i - y_i}{1 - P_{i,i}}$$

Cross-validation to select S



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$$\hat{y}_i^{-i} - y_i = \frac{\hat{y}_i - y_i}{1 - P_{i,i}}$$

$\Rightarrow$ Aim: write PCA as $\hat{\mu}^{(S)} = PX$

$$(\hat{\mu}_{ij}^S)^{-ij} - x_{ij} \simeq \frac{(\hat{\mu}_{ij}^S) - X_{ij}}{1 - P_{ij,ij}}$$

PCA as a smoother

2 projection matrices: $\|X_{n\times p} - F_{n\times S}V'_{S\times p}\|_2^2$

$$\begin{cases} V' = (F'F)^{-1}F'X & \Rightarrow P_F = F(F'F)^{-1}F' \\ F = XV(V'V)^{-1} & \Rightarrow P_V = V(V'V)^{-1}V' \end{cases}$$

$\hat{\mu}^S = FV' = XP_V = P_F X$

$\mathrm{vec}(\hat{\mu}^{(S)}) = P^{(S)}\mathrm{vec}(X) \quad P^{(S)}_{np\times np} = (P_V^{'} \otimes \mathbb{I}_n) + (\mathbb{I}_p^{'} \otimes P_F) - (P_V^{'} \otimes P_F)$

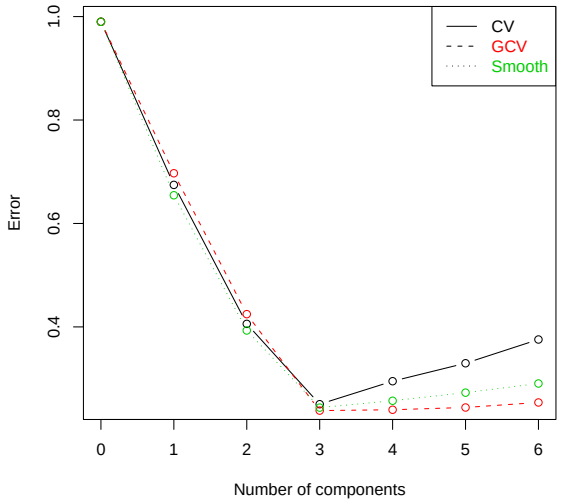
Pazman & Denis, 2002; Candes & Tao, 2009

$\Rightarrow$ Number of independent parameters:

$$\hat{\sigma}^2 = \frac{RSS}{\mathrm{tr}\left(\mathbb{I}_{np} - P^{(S)}\right)} = \frac{n\sum_{s=S+1}^{min(n,p)}\lambda_s}{np - (nS + pS - S^2)}$$

Cross-validation approximations

```
> nb <- estim_ncp(don)
> nb$criterion
        0         1         2         3         4         5
1.2884873 0.8069719 0.6400517 0.7045074 2.2257738 3.0274337
```



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Josse, J. & Husson, F. Selecting the number of components in PCA using cross-validation approximations. *Computational Statististics and Data Analysis*.

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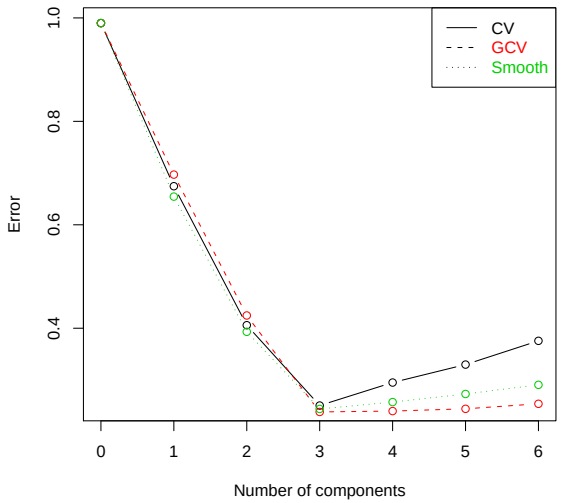

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$$\mathrm{GCV}_S = \frac{1}{np} \times \frac{\sum_{i,j}(X_{ij} - \hat{\mu}_{ij}^S))^2}{(1 - \mathrm{tr}(P^{(S)})/np)^2}$$

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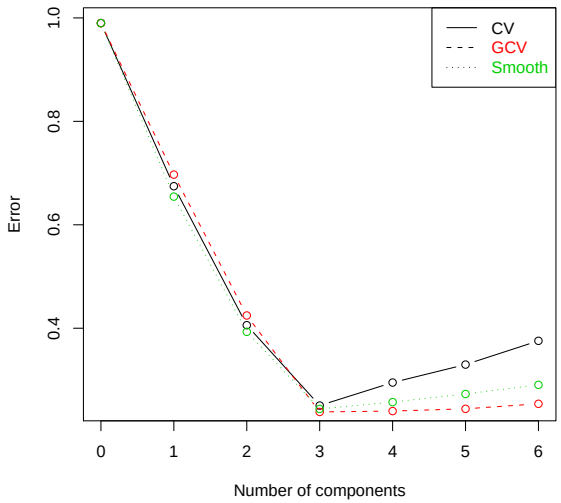

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$$\mathrm{GCV}_S = \frac{np\sum_{i,j}(X_{ij} - \hat{\mu}_{ij}^S))^2}{(np - \mathrm{tr}(P^{(S)}))^2}$$

$$\mathrm{GCV\ NA}_S = \frac{np\|W * (X - \hat{\mu}^S))\|_2^2}{(np - |NA| - (nS + pS - S^2))}$$

Josse, J. & Husson, F. Selecting the number of components in PCA using cross-validation approximations. *Computational Statistics and Data Analysis*.

Overfitting

Overfitting when:

- many parameters / the number of observed values (the number of dimensions S and of missing values are important)
- data are very noisy

$\Rightarrow$ Trust too much the relationship between variables

Remarks:

- missing values: special case of small data set
- iterative PCA: prediction method

Solution:
$\Rightarrow$ Shrinkage methods

Soft thresholding SVD

$\Rightarrow$ Init. - estimation - imputation steps.

The imputation step:

$$\hat{\mu}_{ij}^{\text{PCA}} = \sum_{s=1}^{S} \sqrt{\lambda_s} u_{is} v_{js}$$

is replaced by a "shrunk" imputation step:

Imputation: $\hat{\mu}_{ij}^{\text{Soft}} = \sum_{s=1}^{p} \left(\sqrt{\lambda_s} - \lambda\right)_+ u_{is} v_{js}$

$$X = \mu + \varepsilon \qquad \text{argmin}_\mu \left\{ \|W * (X - \mu)\|_2^2 + \lambda \|\mu\|_* \right\}$$

SoftImpute for large matrices. T. Hastie, R. Mazumber, 2015, Matrix Completion and Low-Rank SVD via Fast Alternating Least Squares. *JMLR*
Implemented in `softImpute` (CRAN)

$\Rightarrow$ Selecting λ?

Verbank, J. & Husson (2013); J. & Wager (2015), J. & Sardy (2014), Gavish & Donoho (2015), Matrix Completion with Nonconvex Regularization: Spectral Operators and Scalable Algorithms, Mazumder (2018). Other regularizations denoiseR

Regularized iterative PCA (Josse *et al.*, 2009)

$\Rightarrow$ Init. - estimation - imputation steps. In `missMDA` (Youtube)

The imputation step:

$$\hat{\mu}_{ij}^{\text{PCA}} = \sum_{s=1}^{S} \sqrt{\lambda_s} u_{is} v_{js}$$

is replaced by a "shrunk" imputation step (Efron & Morris 1972):

$$\hat{\mu}_{ij}^{\text{rPCA}} = \sum_{s=1}^{S} \left(\frac{\lambda_s - \hat{\sigma}^2}{\lambda_s} \right) \sqrt{\lambda_s} u_{is} v_{js} = \sum_{s=1}^{S} \left(\sqrt{\lambda_s} - \frac{\hat{\sigma}^2}{\sqrt{\lambda_s}} \right) u_{is} v_{js}$$

σ^2 small $\rightarrow$ regularized PCA $\approx$ PCA

σ^2 large $\rightarrow$ mean imputation

$$\hat{\sigma}^2 = \frac{RSS}{\text{ddl}} = \frac{n \sum_{s=S+1}^{p} \lambda_s}{np - p - nS - pS + S^2 + S} \qquad (X_{n \times p}; U_{n \times S}; V_{p \times S})$$

Properties

$\Rightarrow$ Very good quality of imputation. Imputation using similarities between individuals and relationship between variables. Popular in machine learning community with recommandation systems (Netflix: 99% missing).

Model makes sense: Data = structure of rank S + noise

(Udell & Townsend Nice Latent Variable Models Have Log-Rank, 2017)

- low noise: iterative PCA (tuning S: cross-validation, GCV)
- moderate noise: iterative regularized PCA (non-linear transformation, tuning σ, S)
- high noise (SNR low, S large): soft thresholding (tuning λ, σ)

Outline

1. Introduction
2. Single imputation with PCA
3. SI Practice
4. Single imputation for mixed variables
5. Multiple imputation for continuous data
6. Multiple imputation for categorical data
7. Conclusion
8. Distribution

Incomplete ozone

	O3	T9	T12	T15	Ne9	Ne12	Ne15	Vx9	Vx12	Vx15	O3v
0601	87	15.6	18.5	18.4	4	4	8	NA	-1.7101	-0.6946	84
0602	82	NA	18.4	17.7	5	5	7	NA	NA	NA	87
0603	92	NA	17.6	19.5	2	5	4	2.9544	1.8794	0.5209	82
0604	114	16.2	NA	NA	1	1	0	NA	NA	NA	92
0605	94	17.4	20.5	NA	8	8	7	-0.5	NA	-4.3301	114
0606	80	17.7	NA	18.3	NA	NA	NA	-5.6382	-5	-6	94
0607	NA	16.8	15.6	14.9	7	8	8	-4.3301	-1.8794	-3.7588	80
0610	79	14.9	17.5	18.9	5	5	4	0	-1.0419	-1.3892	NA
0611	101	NA	19.6	21.4	2	4	4	-0.766	NA	-2.2981	79
0612	NA	18.3	21.9	22.9	5	6	8	1.2856	-2.2981	-3.9392	101
0613	101	17.3	19.3	20.2	NA	NA	NA	-1.5	-1.5	-0.8682	NA
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
0919	NA	14.8	16.3	15.9	7	7	7	-4.3301	-6.0622	-5.1962	42
0920	71	15.5	18	17.4	7	7	6	-3.9392	-3.0642	0	NA
0921	96	NA	NA	NA	3	3	3	NA	NA	NA	71
0922	98	NA	NA	NA	2	2	2	4	5	4.3301	96
0923	92	14.7	17.6	18.2	1	4	6	5.1962	5.1423	3.5	98
0924	NA	13.3	17.7	17.7	NA	NA	NA	-0.9397	-0.766	-0.5	92
0925	84	13.3	17.7	17.8	3	5	6	0	-1	-1.2856	NA
0927	NA	16.2	20.8	22.1	6	5	5	-0.6946	-2	-1.3681	71
0928	99	16.9	23	22.6	NA	4	7	1.5	0.8682	0.8682	NA
0929	NA	16.9	19.8	22.1	6	5	3	-4	-3.7588	-4	99
0930	70	15.7	18.6	20.7	NA	NA	NA	0	-1.0419	-4	NA

Complete ozone

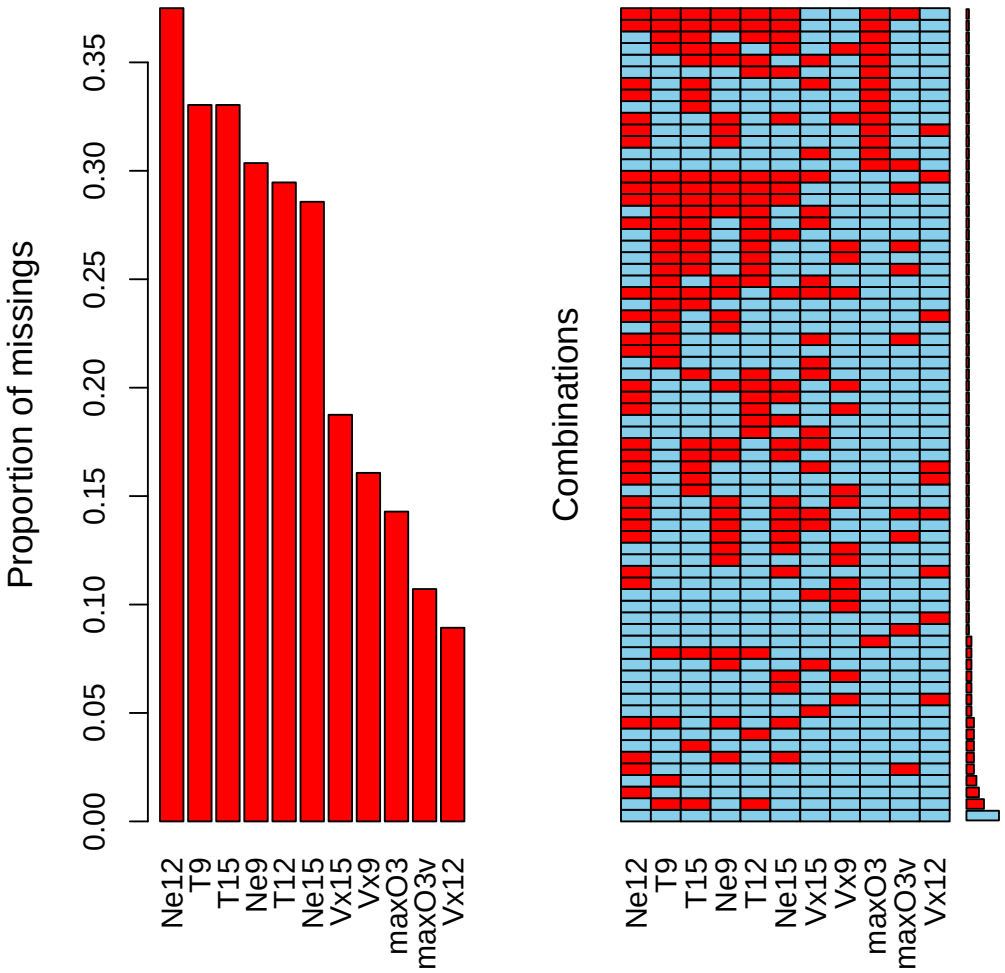
```
         maxO3     T9    T12    T15   Ne9  Ne12  Ne15    Vx9   Vx12   Vx15  maxO3v
20010601  87.000 15.600 18.500 20.471 4.000 4.000 8.000  0.695 -1.710 -0.695  84.000
20010602  82.000 18.505 20.870 21.799 5.000 5.000 7.000 -4.330 -4.000 -3.000  87.000
20010603  92.000 15.300 17.600 19.500 2.000 3.984 3.812  2.954  1.951  0.521  82.000
20010604 114.000 16.200 19.700 24.693 1.000 1.000 0.000  2.044  0.347 -0.174  92.000
20010605  94.000 18.968 20.500 20.400 5.294 5.272 5.056 -0.500 -2.954 -4.330 114.000
20010606  80.000 17.700 19.800 18.300 6.000 7.020 7.000 -5.638 -5.000 -6.000  94.000
20010607  79.000 16.800 15.600 14.900 7.000 8.000 6.556 -4.330 -1.879 -3.759  80.000
20010610  79.000 14.900 17.500 18.900 5.000 5.000 5.016  0.000 -1.042 -1.389  99.000
20010611 101.000 16.100 19.600 21.400 2.000 4.691 4.000 -0.766 -1.026 -2.298  79.000
20010612 106.000 18.300 22.494 22.900 5.000 4.627 4.495  1.286 -2.298 -3.939 101.000
20010613 101.000 17.300 19.300 20.200 7.000 7.000 3.000 -1.500 -1.500 -0.868 106.000
.....

20010915  69.000 17.100 17.700 17.500 6.000 7.000 8.000 -5.196 -2.736 -1.042  71.000
20010916  71.000 15.400 18.091 16.600 4.000 5.000 5.000 -3.830  0.000  1.389  69.000
20010917  60.000 15.283 18.565 19.556 4.000 5.000 4.000  0.000  3.214  0.000  71.000
20010918  42.000 14.091 14.300 14.900 8.000 7.000 7.000 -2.500 -3.214 -2.500  60.000
20010919  65.000 14.800 16.425 15.900 7.000 7.982 7.000 -4.341 -6.062 -5.196  42.000
20010920  71.000 15.500 18.000 17.400 7.000 7.000 6.000 -3.939 -3.064  0.000  65.000
20010924  76.000 13.300 17.700 17.700 5.631 5.883 5.453 -0.940 -0.766 -0.500  65.139
20010925  75.573 13.300 18.434 17.800 3.000 5.000 5.001  0.000 -1.000 -1.286  76.000
20010927  77.000 16.200 20.800 20.499 5.368 5.495 5.177 -0.695 -2.000 -1.473  71.000
20010928  99.000 18.074 22.169 23.651 3.531 3.610 3.561  1.500  0.868  0.868  93.135
20010929  83.000 19.855 22.663 23.847 5.374 5.000 3.000 -4.000 -3.759 -4.000  99.000
20010930  70.000 15.700 18.600 20.700 7.000 6.405 7.000 -2.584 -1.042 -4.000  83.000
```

```
> library(missMDA)
> res.comp <- imputePCA(ozo[, 1:11])
> res.comp$comp
```

Count missing values

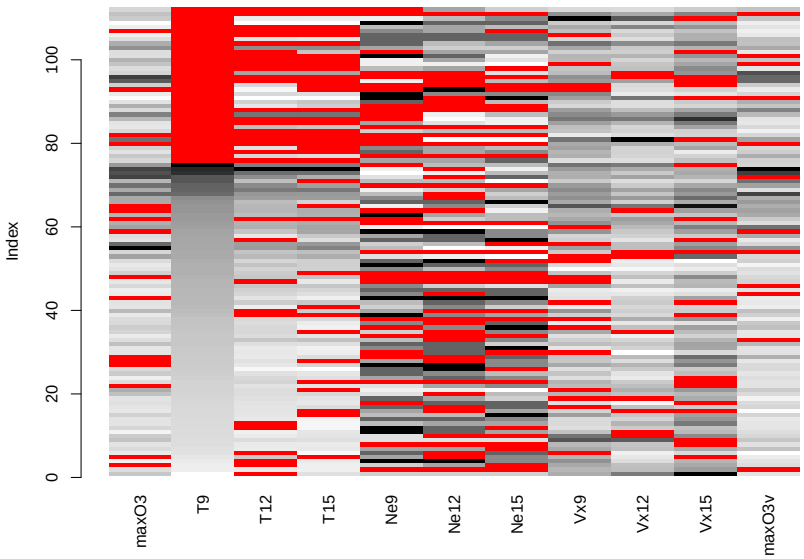
```
> library(missMDA)
> WindDirection <- ozo[,12]
> don <- ozo[,1:11]
> library(VIM)
> res <- summary(aggr(don, sortVar = TRUE))$combinations
> res[rev(order(res[, 2])),]

Variables sorted by
number of missings:                    Combinations Count    Percent
Variable      Count          0:0:0:0:0:0:0:0:0:0:0    13 11.6071429
    Ne12 0.37500000          0:1:1:1:0:0:0:0:0:0:0     7  6.2500000
      T9 0.33035714          0:0:0:0:0:1:0:0:0:0:0     5  4.4642857
     T15 0.33035714          0:1:0:0:0:0:0:0:0:0:0     4  3.5714286
     Ne9 0.30357143          0:1:0:0:1:1:1:0:0:0:0     3  2.6785714
     T12 0.29464286          0:0:1:0:0:0:0:0:0:0:0     3  2.6785714
    Ne15 0.28571429          0:0:0:1:0:0:0:0:0:0:0     3  2.6785714
    Vx15 0.18750000          0:0:0:0:1:1:1:0:0:0:0     3  2.6785714
     Vx9 0.16071429          0:0:0:0:0:1:0:0:0:0:1     3  2.6785714
   maxO3 0.14285714          0:1:1:1:1:0:0:0:0:0:0     2  1.7857143
  maxO3v 0.10714286          0:0:0:0:1:0:0:0:0:1:0     2  1.7857143
    Vx12 0.08928571          0:0:0:0:0:0:1:1:0:0:0     2  1.7857143
                             0:0:0:0:0:0:1:0:0:0:0     2  1.7857143
                             ......................    .  ...
```

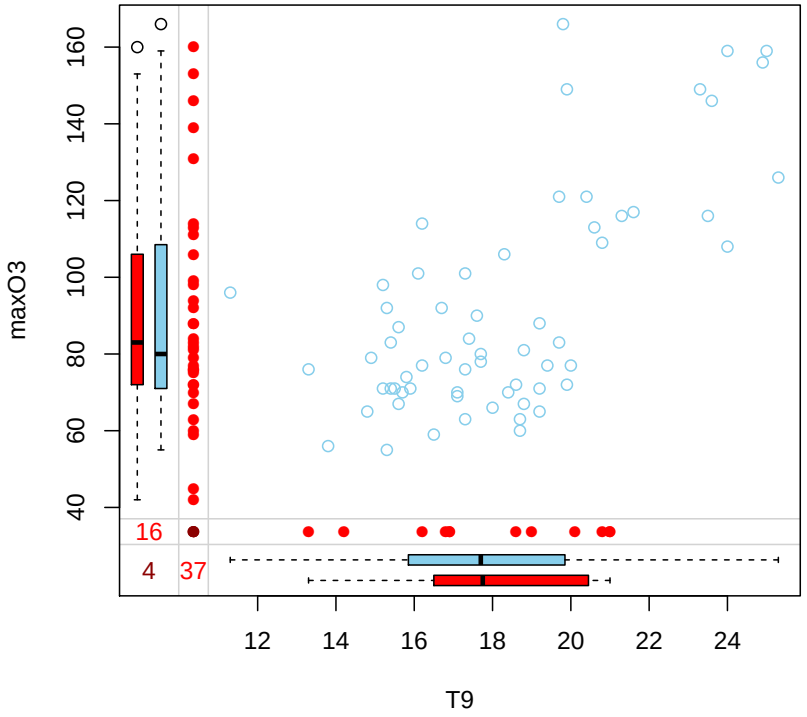
Pattern visualization




```
 #library(VIM)
> aggr(don, sortVar = TRUE)
```

Visualization





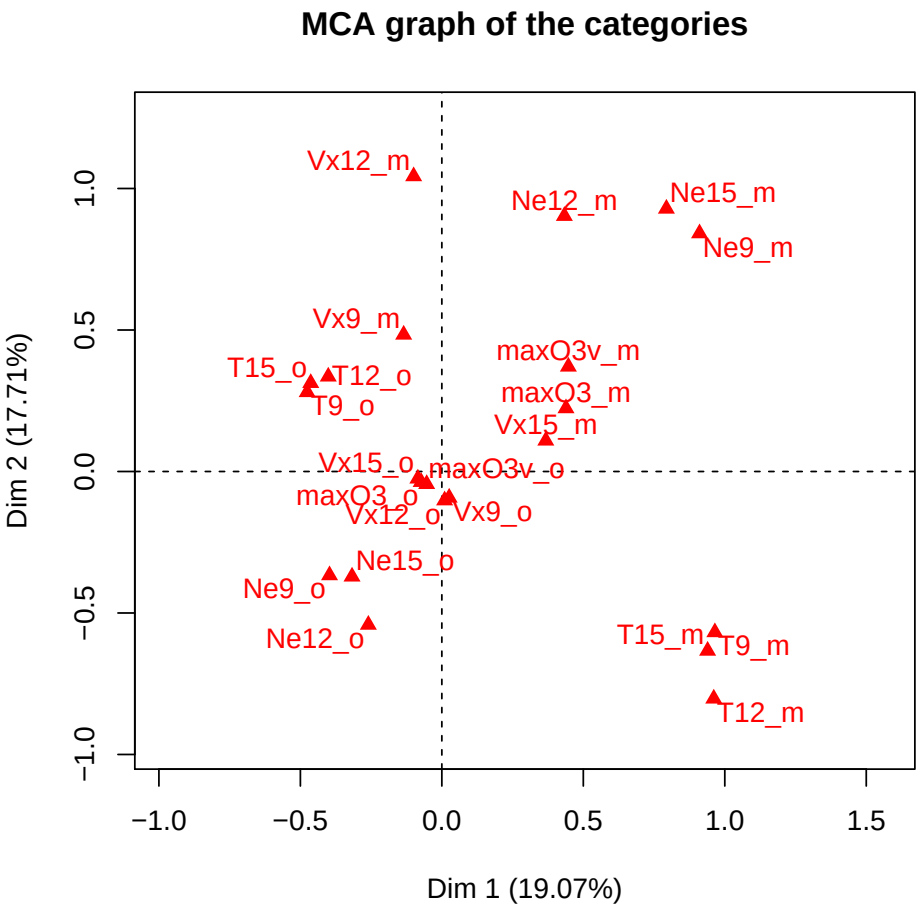

```
# library(VIM)
> matrixplot(don, sortby = 2)
> marginplot(don[ ,c("T9", "maxO3")])
```

Visualization with Multiple Correspondence Analysis

⇒ Create the missingness matrix

```
> mis.ind <- matrix("o", nrow = nrow(don), ncol = ncol(don))
> mis.ind[is.na(don)] = "m"
> dimnames(mis.ind) = dimnames(don)
> mis.ind

         maxO3 T9  T12 T15 Ne9 Ne12 Ne15 Vx9 Vx12 Vx15 maxO3v
20010601 "o"   "o" "o" "m" "o" "o"  "o"  "o" "o"  "o"  "o"
20010602 "o"   "m" "m" "m" "o" "o"  "o"  "o" "o"  "o"  "o"
20010603 "o"   "o" "o" "o" "o" "m"  "m"  "o" "m"  "o"  "o"
20010604 "o"   "o" "o" "m" "o" "o"  "o"  "m" "o"  "o"  "o"
20010605 "o"   "m" "o" "o" "m" "m"  "m"  "o" "o"  "o"  "o"
20010606 "o"   "o" "o" "o" "o" "m"  "o"  "o" "o"  "o"  "o"
20010607 "o"   "o" "o" "o" "o" "o"  "m"  "o" "o"  "o"  "o"
20010610 "o"   "o" "o" "o" "o" "o"  "m"  "o" "o"  "o"  "o"
```

Visualization with Multiple Correspondence Analysis

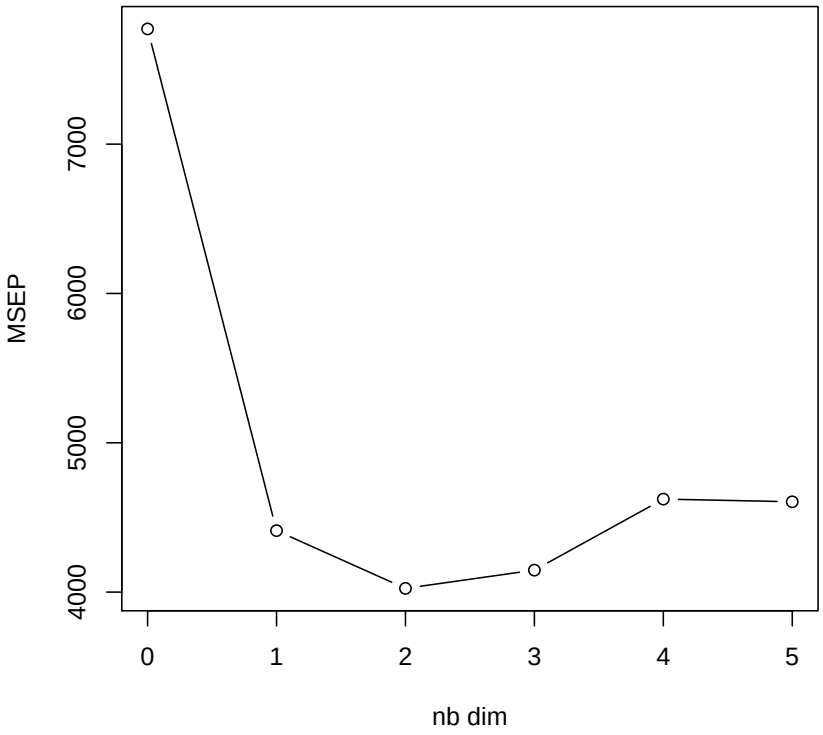



```
> library(FactoMineR)
> resMCA <- MCA(mis.ind)
> plot(resMCA, invis = "ind", title = "MCA graph of the categories")
```

Imputation with PCA in practice

⇒ Step 1: Estimation of the number of dimensions
(Cross Validation, Bro, 2008; GCV, Josse & Husson, 2011)

```
> library(missMDA)
> nb <- estim_ncpPCA(don, method.cv = "Kfold")
> nb$ncp    #2
> plot(0:5, nb$criterion, xlab = "nb dim", ylab ="MSEP")
```

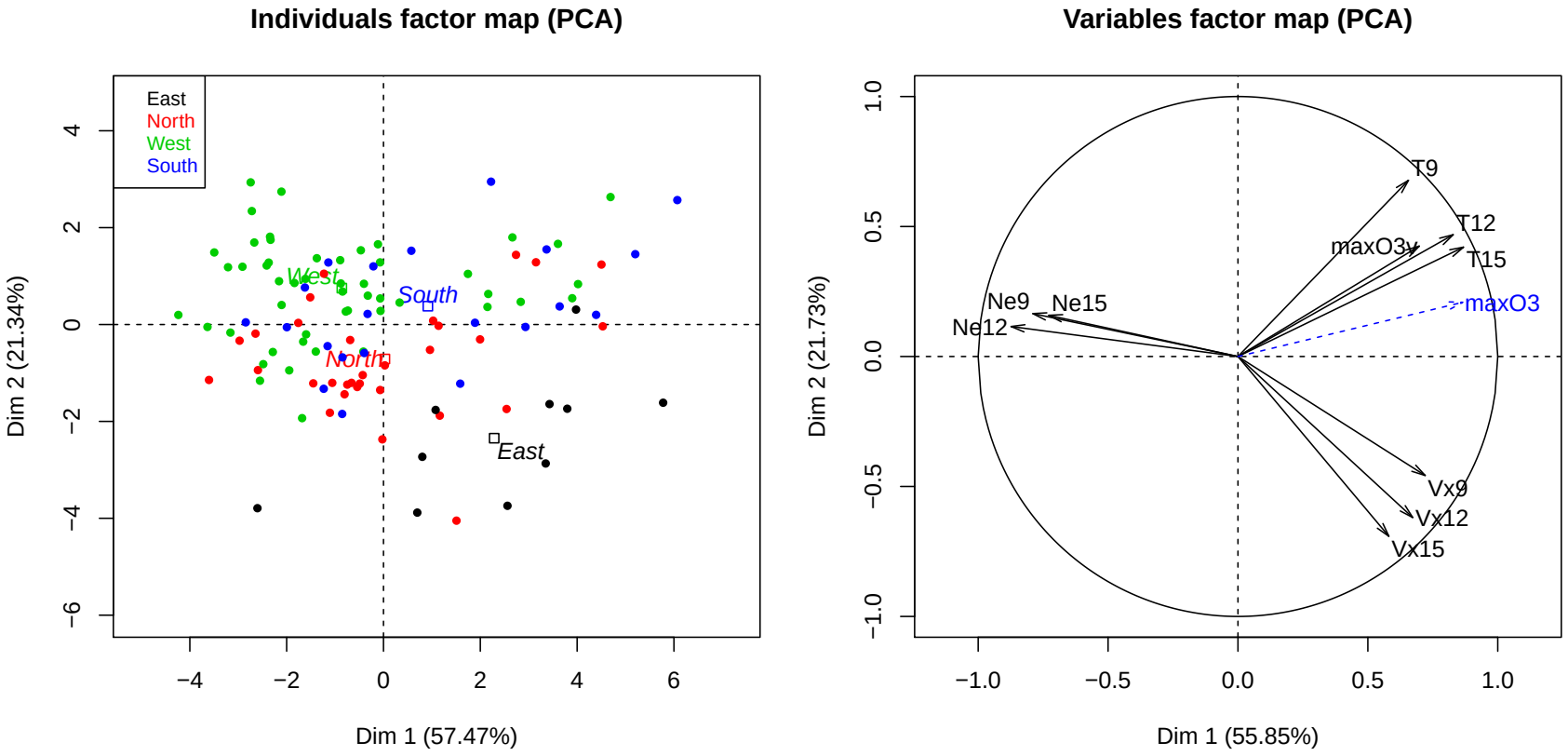


Imputation with PCA in practice

⇒ Step 2: Imputation of the missing values

```
> res.comp <- imputePCA(don, ncp = 2)
> res.comp$completeObs[1:3, ]
     maxO3    T9   T12   T15 Ne9 Ne12 Ne15   Vx9  Vx12  Vx15 maxO3v
0601    87 15.60 18.50 20.47   4 4.00 8.00  0.69 -1.71 -0.69     84
0602    82 18.51 20.88 21.81   5 5.00 7.00 -4.33 -4.00 -3.00     87
0603    92 15.30 17.60 19.50   2 3.98 3.81  2.95  1.97  0.52     82
```

Cherry on the cake: PCA on incomplete data!




```
> imp <- cbind.data.frame(res.comp$completeObs, ozo[, 12])
> res.pca <- PCA(imp, quanti.sup = 1, quali.sup = 12)
> plot(res.pca, hab = 12, lab = "quali"); plot(res.pca, choix = "var")
> res.pca$ind$coord #scores (principal components)
```

Imputation for continuous data

```
> library(softImpute)
> fit1 <- softImpute(XNA, rank = , lambda = )
> X.soft <- complete(XNA, fit1)

> library(denoiseR)
> adaNA <- imputeada(XNA,  gamma = 1) ## time consuming...
> X.ada <- adaNA$completeObs
```

An ecological data set

Glopnet data: 2494 species described by 6 quantitative variables

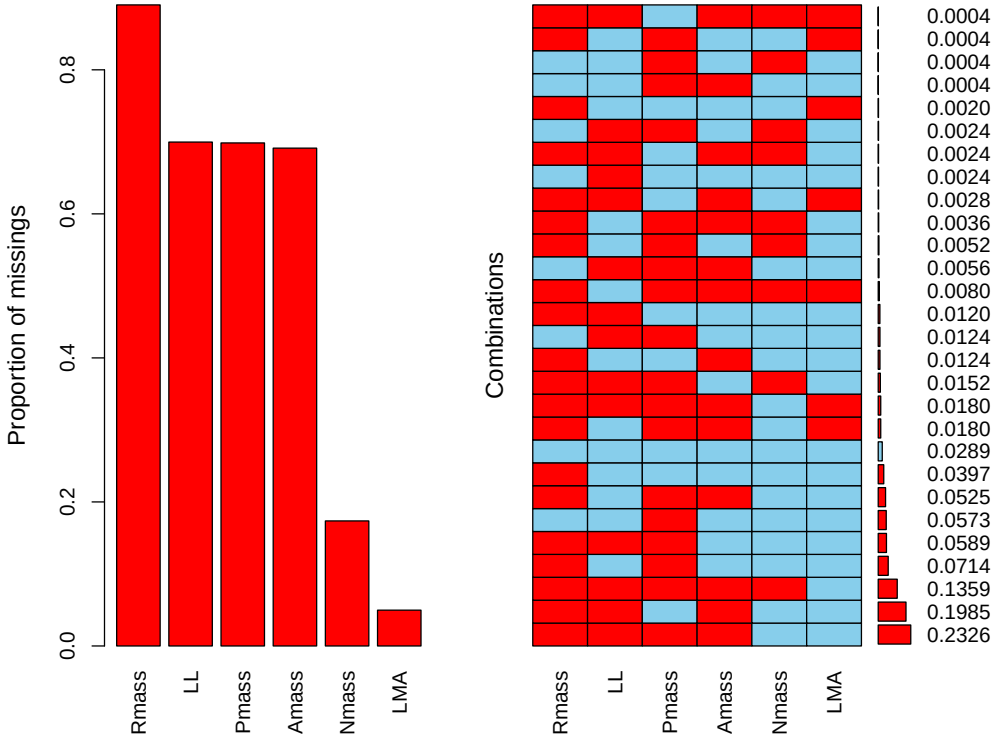
- LMA (leaf mass per area)
- LL (leaf lifespan)
- Amass (photosynthetic assimilation)
- Nmass (leaf nitrogen),
- Pmass (leaf phosphorus)
- Rmass (dark respiration rate)

and 1 categorical variable: the biome

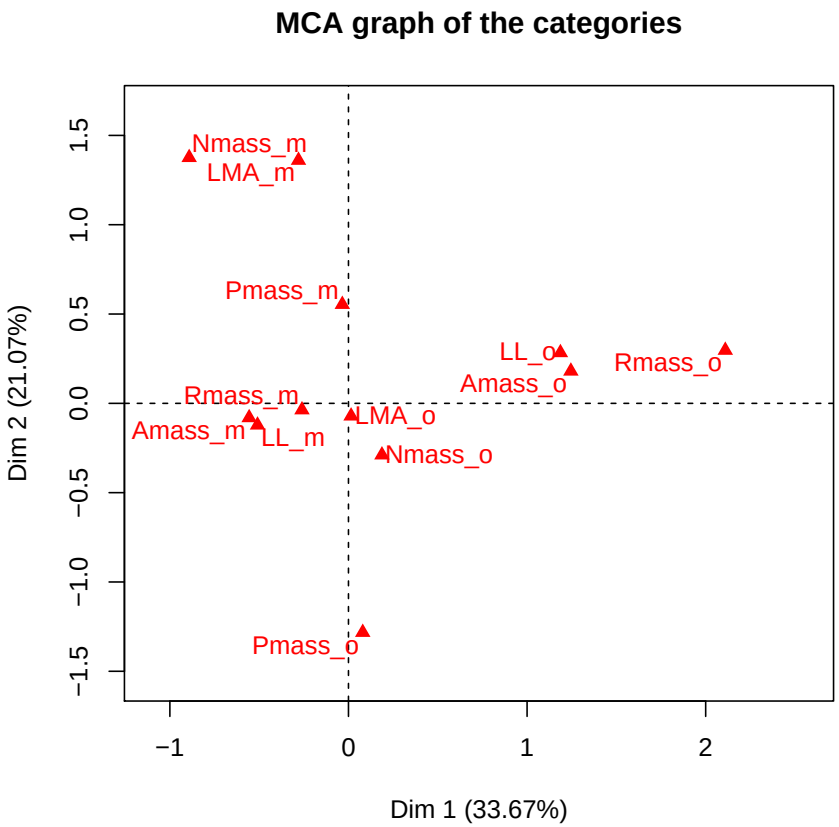
Reference: Wright IJ, et al. (2004) The worldwide leaf economics spectrum. Nature, 428:821.
`www.nature.com/nature/journal/v428/n6985/extref/nature02403-s2.xls`

An ecological data set

```
> sum(is.na(don))/(nrow(don)*ncol(don)) # 53% of missing values
[1] 0.5338145
> dim(na.omit(don))  ## Delete species with missing values
[1] 72  6            ## only 72 remaining species!

> library(VIM)
> aggr(don,numbers=TRUE,sortVar=TRUE)
```



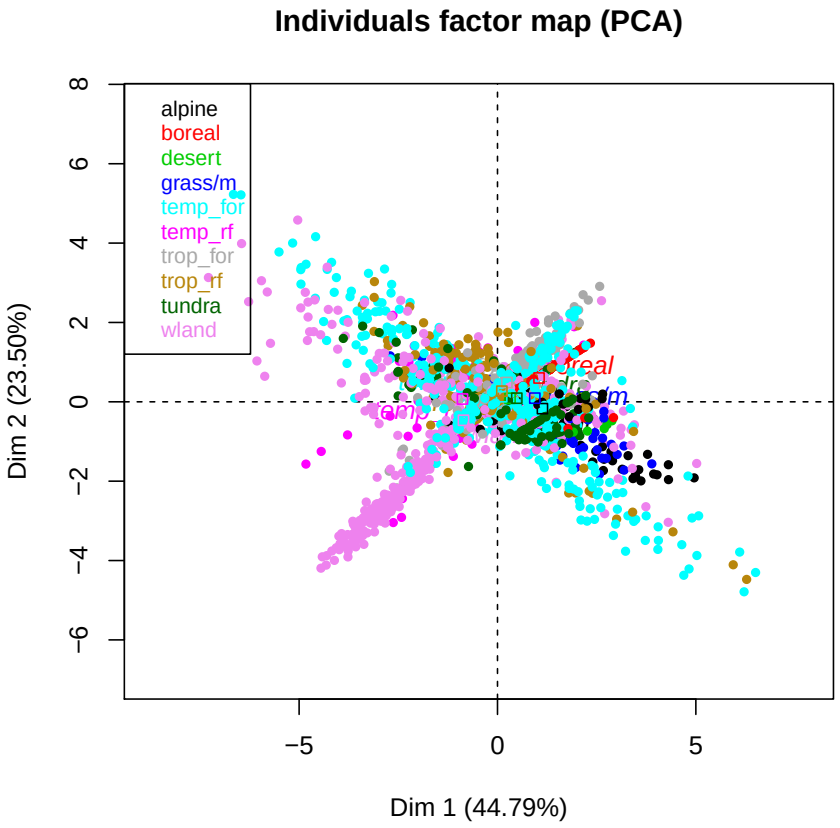
An ecological data set

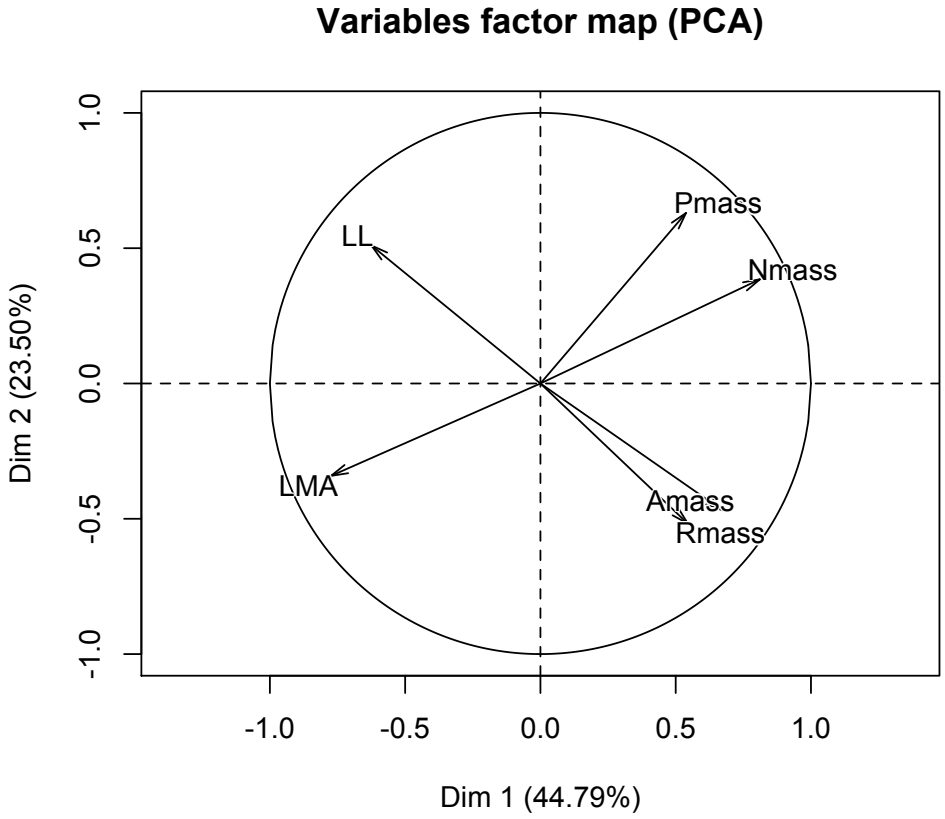



```
> mis.ind <- matrix("o",nrow=nrow(don),ncol=ncol(don))
> mis.ind[is.na(don)] <- "m"
> dimnames(mis.ind) <- dimnames(don)
> library(FactoMineR)
> resMCA <- MCA(mis.ind)
> plot(resMCA,invis="ind",title="MCA graph of the categories")
```

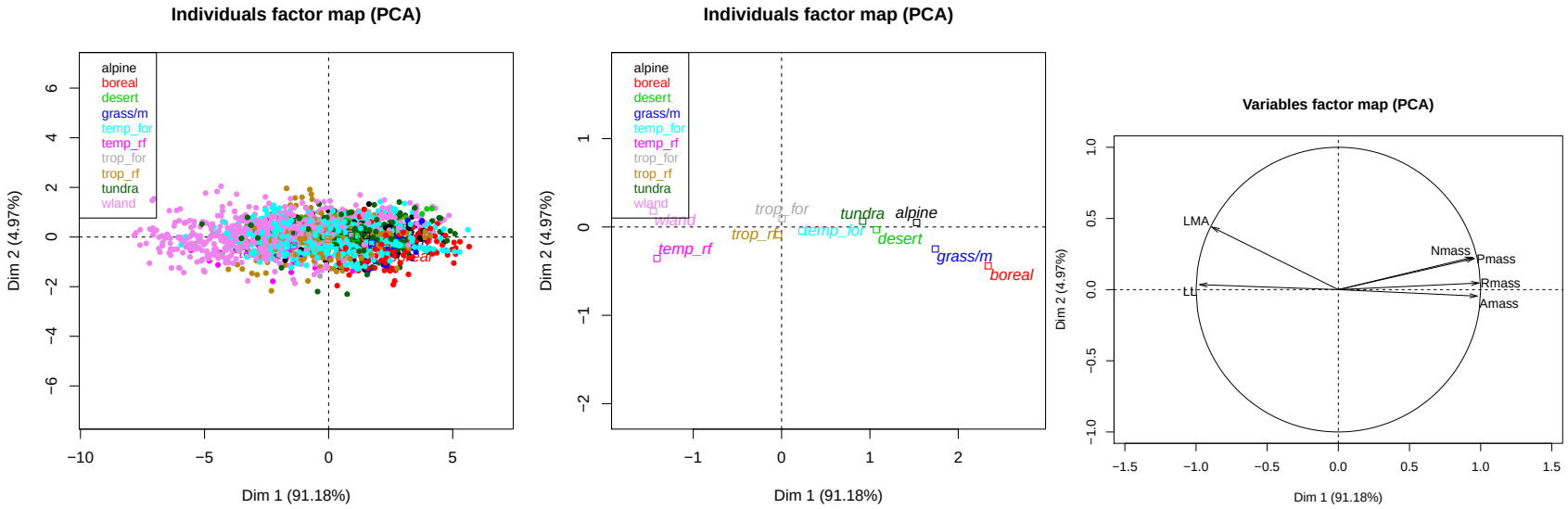
An ecological data set

What about mean imputation?





An ecological data set




```
> library(missMDA)
> nb <- estim_ncpPCA(don,method.cv="Kfold",nbsim=100)
> res.comp <- imputePCA(don,ncp=2)
> imp <- cbind.data.frame(res.comp$completeObs,tab.init[,1:4])
> res.pca <- PCA(imp,quanti.sup=1,quali.sup=12)
> plot(res.pca, hab=12, lab="quali"); plot(res.pca, choix="var")
> res.pca$ind$coord #scores (principal components)
```

Iterative Random Forests imputation

1. Initial imputation: mean imputation - random category
   Sort the variables according to the amount of missing values
2. Fit a RF X_j^{obs} on variables X_{-j}^{obs} and then predict X_j^{miss}
3. Cycling through variables
4. Repeat step 2.2 and 3 until convergence

- number of trees: 100
- number of variables randomly selected at each node $\sqrt{p}$
- number of iterations: 4-5

Implemented in the R package `missForest` (paper) `missForest`
(Daniel J. Stekhoven, Peter Buhlmann, 2011)

Missing At Random

	Feat1	Feat2	Feat3	Feat4	Feat5...
C1	1	1	1	1	1
C2	1	1	1	1	1
C3	2	2	2	2	2
C4	2	2	2	2	2
C5	3	3	3	3	3
C6	3	3	3	3	3
C7	4	4	4	4	4
C8	4	4	4	4	4
C9	5	5	5	5	5
C10	5	5	5	5	5
C11	6	6	6	6	6
C12	6	6	6	6	6
C13	7	7	7	7	7
C14	7	7	7	7	7
Igor	8	NA	NA	8	8
Frank	8	NA	NA	8	8
Bertrand	9	NA	NA	9	9
Alex	9	NA	NA	9	9
Yohann	10	NA	NA	10	10
Jean	10	NA	NA	10	10

Random Forests versus PCA

	Feat1	Feat2	Feat3	Feat4	Feat5
C1	1	1.0	1.00	1	1
C2	1	1.0	1.00	1	1
C3	2	2.0	2.00	2	2
C4	2	2.0	2.00	2	2
C5	3	3.0	3.00	3	3
C6	3	3.0	3.00	3	3
C7	4	4.0	4.00	4	4
C8	4	4.0	4.00	4	4
C9	5	5.0	5.00	5	5
C10	5	5.0	5.00	5	5
C11	6	6.0	6.00	6	6
C12	6	6.0	6.00	6	6
C13	7	7.0	7.00	7	7
C14	7	7.0	7.00	7	7
Igor	8	6.87	6.87	8	8
Frank	8	6.87	6.87	8	8
Bertrand	9	6.87	6.87	9	9
Alex	9	6.87	6.87	9	9
Yohann	10	6.87	6.87	10	10
Jean	10	6.87	6.87	10	10

$\Rightarrow$ with Random Forests

	Feat1	Feat2	Feat3	Feat4	Feat5
C1	1	1	1	1	1
C2	1	1	1	1	1
C3	2	2	2	2	2
C4	2	2	2	2	2
C5	3	3	3	3	3
C6	3	3	3	3	3
C7	4	4	4	4	4
C8	4	4	4	4	4
C9	5	5	5	5	5
C10	5	5	5	5	5
C11	6	6	6	6	6
C12	6	6	6	6	6
C13	7	7	7	7	7
C14	7	7	7	7	7
Igor	8	8	8	8	8
Frank	8	8	8	8	8
Bertrand	9	9	9	9	9
Alex	9	9	9	9	9
Yohann	10	10	10	10	10
Jean	10	10	10	10	10

$\Rightarrow$ with PCA

(Stekhoven, Buhlmann, 2011 - Bartlett, Carpenter, 2014)

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1. Introduction
2. Single imputation with PCA
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Categorical data

Survey data

```
region                     sex        age          year         edu         drunk        alcohol      gla
Ile de France      :8120   F:29776   18_25: 6920   2005:27907   E1:12684  0    :44237   <1/m :12889   0
Rhone Alpes        :5421   M:23165   26_34: 9401   2010:25034   E2:23521  1-2  : 4952   0    : 6133   0-2
Provence Alpes     :4116             35_44:10899                E3:6563   10-19:  839   1-2/m: 7583   10-
Nord Pas de Calais :3819             45_54: 9505                E4:10100  20-29:  212   1-2/w: 9526   3-4
Pays de Loire      :3152             55_64: 9503                NA:73     3-5  : 1908   3-4/w: 6815   5-6
Bretagne           :3038             65_+ : 6713                          30+  :  404   5-6/w: 3402   7-9
(Other)            :25275                                                 6-9  :  389   7/w  : 6593

binge                   Pbsleep                  Tabac
<2/m:10323              Never:20605              Frequent  : 9176
0   :34345              Often: 10172             Never     :39080
1/m : 6018              Rare :22134              Occasional: 4588
1/w : 1800              NA:  30                  NA:  97
7/w :  374
NA  :   81
```

INPES `http://www.inpes.sante.fr`

Principal components method: Multiple Correpondence Analysis
Single imputation based on MCA for categorical data

Multiple Correspondence Analysis (MCA)

$X_{n\times m}$ m categorical variables coded with indicator matrix A

$$X = \begin{array}{|c|c|c|} \hline y & \dots & attack \\ y & \dots & attack \\ y & \dots & attack \\ n & \dots & suicide \\ & & \\ & & \\ n & \dots & accident \\ n & \dots & suicide \\ \hline \end{array} \qquad A = \begin{array}{|cc|c|ccc|} \hline 1 & 0 & \dots & 1 & 0 & 0 \\ 1 & 0 & \dots & 1 & 0 & 0 \\ 1 & 0 & \dots & 1 & 0 & 0 \\ 0 & 1 & \dots & 0 & 1 & 0 \\ & & & & & \\ & & & & & \\ 0 & 1 & \dots & 0 & 0 & 1 \\ 0 & 1 & \dots & 0 & 1 & 0 \\ \hline \end{array} \qquad D_p = \begin{array}{|ccc|} \hline p_1 & & 0 \\ & \ddots & \\ 0 & & p_J \\ \hline \end{array}$$

For a category c, the frequency of the category: $p_c = n_c/n$.

A SVD on weighted matrix: $Z = \frac{1}{\sqrt{mn}}(A - 1p^T)D_p^{-1/2} = U\Lambda V'$

The PC ($F = U\Lambda^{1/2}$) satisfies: $\arg\max_{F_s\in\mathbb{R}^n} \quad \frac{1}{m}\sum_{j=1}^m \eta^2(F_s, X_j)$

$$\eta^2(F, X_j) = \frac{\sum_{c=1}^{C_j} n_c(F_{.c} - F_{..})^2}{\sum_{i=1}^n \sum_{c=1}^{C_j}(F_{ic})^2} = \frac{\text{RSS between}}{\text{RSS tot}}$$

Benzecri, 1973 :*"In data analysis the mathematical problems reduces to computing eigenvectors; all the science (the art) is in finding the right matrix to diagonalize"*

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

	V1	V2	V3	...	V14
ind 1	a	**NA**	g	...	u
ind 2	**NA**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**NA**		v
...	...	...	...		...
ind 1232	c	f	h		v

	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	**NA**	**NA**	1	0	...
ind 2	**NA**	**NA**	**NA**	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	**NA**	**NA**	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

```
library(missMDA); ?imputeMCA
```

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

1. initialization: imputation of the indicator matrix (proportion)

	V1	V2	V3	...	V14
ind 1	a	**NA**	g	...	u
ind 2	**NA**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**NA**		v
...	...	...	...		...
ind 1232	c	f	h		v

	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	0.41	0.59	1	0	...
ind 2	0.20	0.30	0.50	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	0.27	0.78	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

```
library(missMDA); ?imputeMCA
```

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

1. initialization: imputation of the indicator matrix (proportion)
2. iterate until convergence
   (a) estimation: MCA on the completed data $\rightarrow U, \Lambda, V$

	V1	V2	V3	...	V14
ind 1	a	**NA**	g	...	u
ind 2	**NA**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**NA**		v
...	...	...	...		...
ind 1232	c	f	h		v

	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	0.41	0.59	1	0	...
ind 2	0.20	0.30	0.50	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	0.27	0.78	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

```
library(missMDA); ?imputeMCA
```

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

1. initialization: imputation of the indicator matrix (proportion)
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   (a) estimation: MCA on the completed data $\rightarrow U, \Lambda, V$
   (b) imputation with the fitted matrix $\hat{\mu} = U_S \Lambda_S^{1/2} V_S'$

	V1	V2	V3	...	V14
ind 1	a	**NA**	g	...	u
ind 2	**NA**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**NA**		v
...	...	...	...		...
ind 1232	c	f	h		v

	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	0.65	0.35	1	0	...
ind 2	0.11	0.20	0.69	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	0.30	0.40	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

```
library(missMDA); ?imputeMCA
```

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

1. initialization: imputation of the indicator matrix (proportion)
2. iterate until convergence
   (a) estimation: MCA on the completed data $\rightarrow U, \Lambda, V$
   (b) imputation with the fitted matrix $\hat{\mu} = U_S \Lambda_S^{1/2} V_S'$
   (c) column margins are updated

	V1	V2	V3	...	V14
ind 1	a	**NA**	g	...	u
ind 2	**NA**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**NA**		v
...	...	...	...		...
ind 1232	c	f	h		v

	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	0.65	0.35	1	0	...
ind 2	0.11	0.20	0.69	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	0.30	0.40	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

```
library(missMDA); ?imputeMCA
```

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

1. initialization: imputation of the indicator matrix (proportion)
2. iterate until convergence
   (a) estimation: MCA on the completed data $\rightarrow U, \Lambda, V$
   (b) imputation with the fitted matrix $\hat{\mu} = U_S \Lambda_S^{1/2} V_S'$
   (c) column margins are updated

	V1	V2	V3	...	V14
ind 1	a	**NA**	g	...	u
ind 2	**NA**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**NA**		v
...	...	...	...		...
ind 1232	c	f	h		v

	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	**0.71**	**0.29**	1	0	...
ind 2	**0.12**	**0.29**	**0.59**	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	**0.37**	**0.63**	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

$\Rightarrow$ the imputed values can be seen as degree of membership

```
library(missMDA); ?imputeMCA
```

Regularized iterative MCA *(Chavent et al., 2012)*

Iterative MCA algorithm:

1. initialization: imputation of the indicator matrix (proportion)
2. iterate until convergence
   (a) estimation: MCA on the completed data $\rightarrow U, \Lambda, V$
   (b) imputation with the fitted matrix $\hat{\mu} = U_S \Lambda_S^{1/2} V_S'$
   (c) column margins are updated

	V1	V2	V3	...	V14
ind 1	a	**e**	g	...	u
ind 2	**c**	f	g		u
ind 3	a	e	h		v
ind 4	a	e	h		v
ind 5	b	f	h		u
ind 6	c	f	h		u
ind 7	c	f	**g**		v
...	...	...	...		...
ind 1232	c	f	h		v

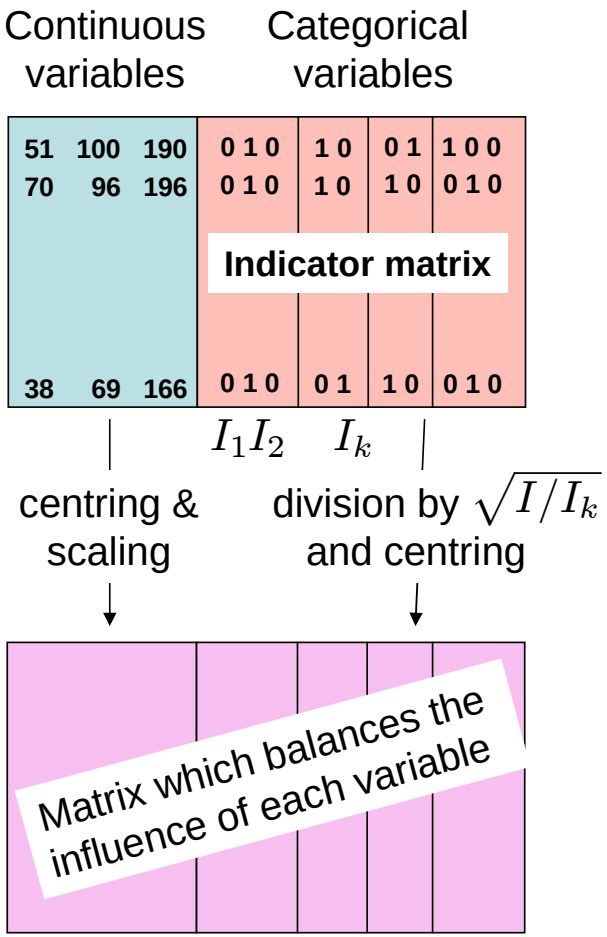
	V1_a	V1_b	V1_c	V2_e	V2_f	V3_g	V3_h	...
ind 1	1	0	0	**0.71**	**0.29**	1	0	...
ind 2	**0.12**	**0.29**	**0.59**	0	1	1	0	...
ind 3	1	0	0	1	0	0	1	...
ind 4	1	0	0	1	0	0	1	...
ind 5	0	1	0	0	1	0	1	...
ind 6	0	0	1	0	1	0	1	...
ind 7	0	0	1	0	1	**0.37**	**0.63**	...
...	...	...	...	...	...	...	...	...
ind 1232	0	0	1	0	1	0	1	...

Two ways to obtain categories: majority or draw

```
library(missMDA); ?imputeMCA
```

Principal component method for mixed data (complete)

Factorial Analysis on Mixed Data (Escofier, 1979), PCAMIX (Kiers, 1991)



A SVD is performed on the matrix X with the concatenation of the continuous variables and the indicator matrix which is centered and weighted by D_Σ, the diagonal matrix with the standard deviation and the weights $\sqrt{(n_c/n)}$.

Properties of the method

- The principal component F_s maximises:

$$\sum_{k=1}^{K_{cont}} r^2(F_s, v_k) + \sum_{q=1}^{Q_{cat}} \eta^2(F_s, v_q)$$

- The distance between individuals is:

$$d^2(i, l) = \sum_{k=1}^{K_{cont}} \frac{1}{\sigma_k}(x_{ik} - x_{lk})^2 + \sum_{q=1}^{Q} \sum_{c=1}^{c_q} \frac{1}{n_{c_q}}(x_{iq} - x_{lq})^2$$

Regularized iterative FAMD

1. Initialization: imputation mean (continuous) and proportion (dummy)
2. Iterate until convergence
   (a) estimation: FAMD on the completed data $\Rightarrow U, \Lambda, V$
   (b) imputation with the fitted matrix $\hat{\mu} = U_S \Lambda_S^{1/2} V_S'$
   (c) means, standard deviations and column margins are updated

age	weight	size	alcohol	sex	snore	tobacco
NA	100	190	NA	M	yes	no
70	96	186	1-2 gl/d	M	NA	<=1
NA	104	194	No	W	no	NA
62	68	165	1-2 gl/d	M	no	<=1

NA	100	190	NA	NA	NA	1	0	0	1	1	0	0
70	96	186	0	1	0	1	0	NA	NA	0	1	0
NA	104	194	1	0	0	0	1	1	0	NA	NA	NA
62	68	165	0	1	0	1	0	1	0	0	1	0

imputeAFDM

51	100	190	0.2	0.7	0.1	1	0	0	1	1	0	0
70	96	186	0	1	0	1	0	0.8	0.2	0	1	0
48	104	194	1	0	0	0	1	1	0	0.1	0.8	0.1
62	68	165	0	1	0	1	0	1	0	0	1	0

age	weight	size	alcohol	sex	snore	tobacco
51	100	190	1-2 gl/d	M	yes	no
70	96	186	1-2 gl/d	M	no	<=1
48	104	194	No	W	no	<=1
62	68	165	1-2 gl/d	M	no	<=1

$\Rightarrow$ Imputed values can be seen as degrees of membership

Simulation study

Several data sets

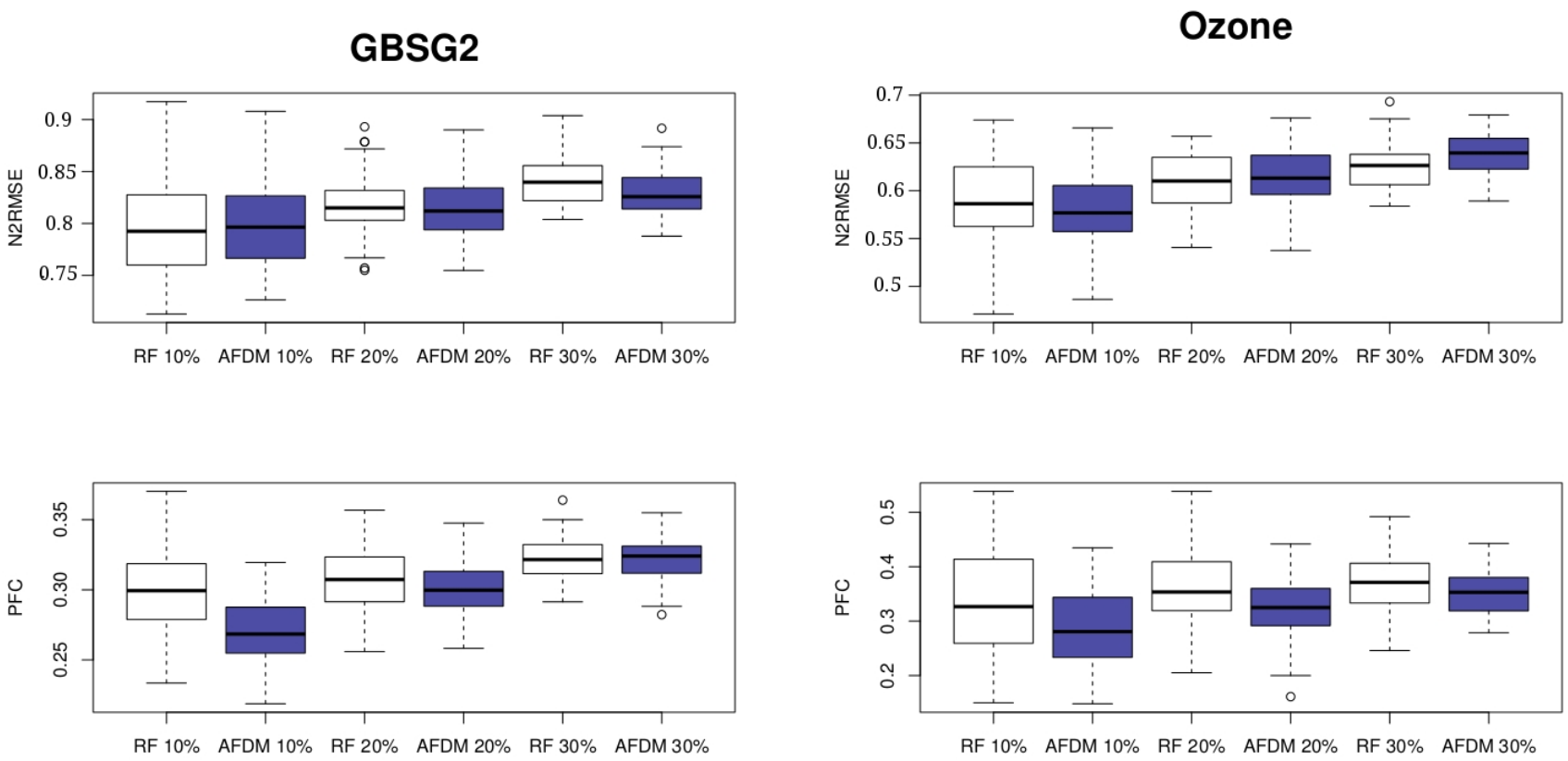
- Relationships between variables
- Number of categories
- percentage of missing values (10%,20%,30%)

Criteria:

- for continuous data: RMSE
- for categorical data: proportion of falsely classified entries

Comparison on real data sets

Imputations obtained with random forest & FAMD algorithm



Summary

Imputations with PC methods are good:

- for strong linear relationships
- for categorical variables
- especially for rare categories (weights of MCA)

$\Rightarrow$ Number of components S?? Cross-Validation (GCV)

Imputations with RF are good:

- for strong non-linear relationships between continuous variables
- when there are interactions

$\Rightarrow$ No tunning parameters?

Rq: categorical data improve the imputation on continuous data and continuous data improve the imputation on categorical data

Summary

Imputations with PC methods are good:

- for strong linear relationships
- for categorical variables
- especially for rare categories (weights of MCA)

$\Rightarrow$ Number of components S?? Cross-Validation (GCV)

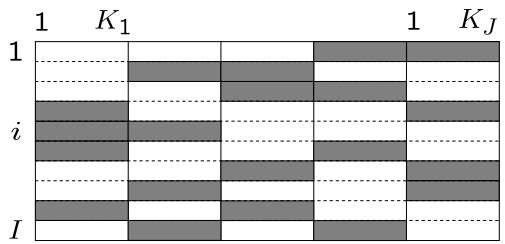
Imputations with RF are good:

- for strong non-linear relationships between continuous variables (cutting continuous variables into categories)
- when there are interactions (creating interactions)

$\Rightarrow$ No tunning parameters?

Rq: categorical data improve the imputation on continuous data and continuous data improve the imputation on categorical data

Multi-blocks data set



- Sensory analysis: products described by people and by physico-chemical measurements

  (each judge can't taste more than 8 products: Planned missing products per judge, experimental design: BIB)

- Biology. DNA/RNA (samples without expression data)

Continuous / categorical / contingency sets of variables

$\Rightarrow$ Missing rows per subtable
$\Rightarrow$ Regularized iterative Multiple Factor Analysis (Husson & Josse, 2013)

Mixed imputation in practice

```
> library(missMDA)
> res.ncp <- estim_ncpFAMD(ozo)
> res.famd <-imputeFAMD(ozo, ncp = 2)
> res.famd$completeObs

> library(missForest)
> res.rf <- missForest(ozo)
> res.rf$ximp
```

Categorical imputation in practice

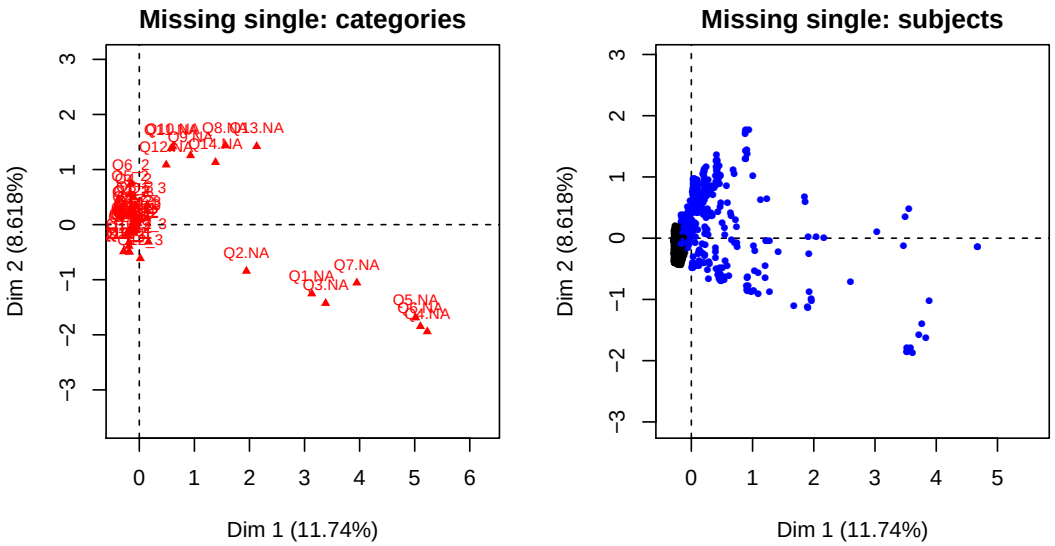
- 1232 respondents, 14 questions, 35 categories, 9% of missing values concerning 42% of respondents

In missMDA (Youtube)

```
data(vnf)
summary(vnf)
MCA(vnf)

#1) select the number of components
nb <- estim_ncpMCA(vnf, ncp.max = 5) #Time-consuming, nb = 4

#2) Impute the indicator matrix
res.impute <- imputeMCA(vnf, ncp = 4)
res.impute$tab.disj
res.impute$comp
summary(res.impute$comp)

# MCA on the incomplete data vnf
res.mca <- MCA(vnf, tab.disj = res.impute$tab.disj)
plot(res.mca, invisible=c("var"))
plot(res.mca,invisible=c("ind"),autoLab="yes", selectMod="cos2 5", cex  = 0.6)
```

Categorical imputation in practice

- 1232 respondents, 14 questions, 35 categories, 9% of missing values concerning 42% of respondents



Categorical imputation in practice

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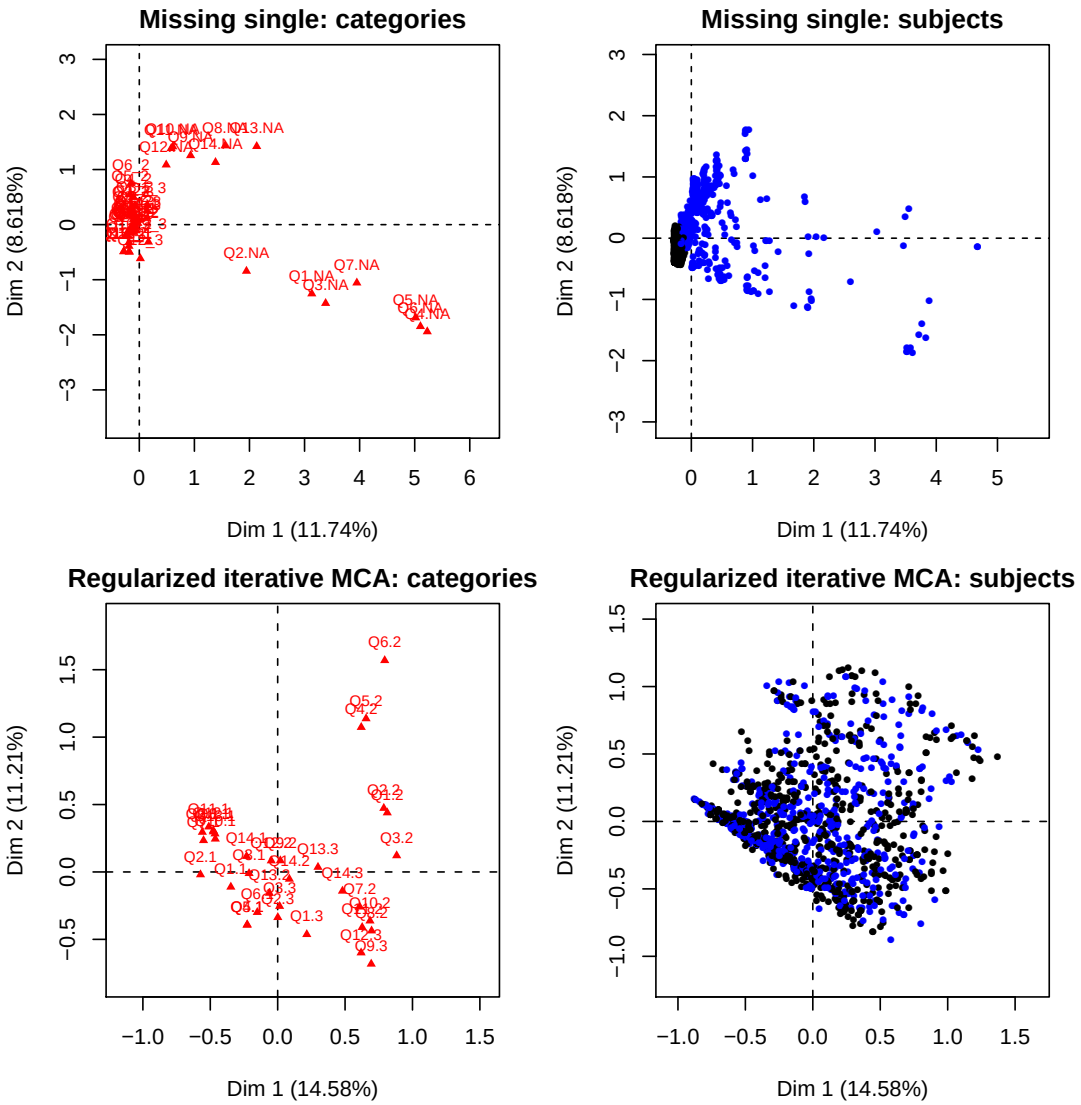


Journal impact factors

journalmetrics.com provides 27000 journals/ 15 years of metrics.

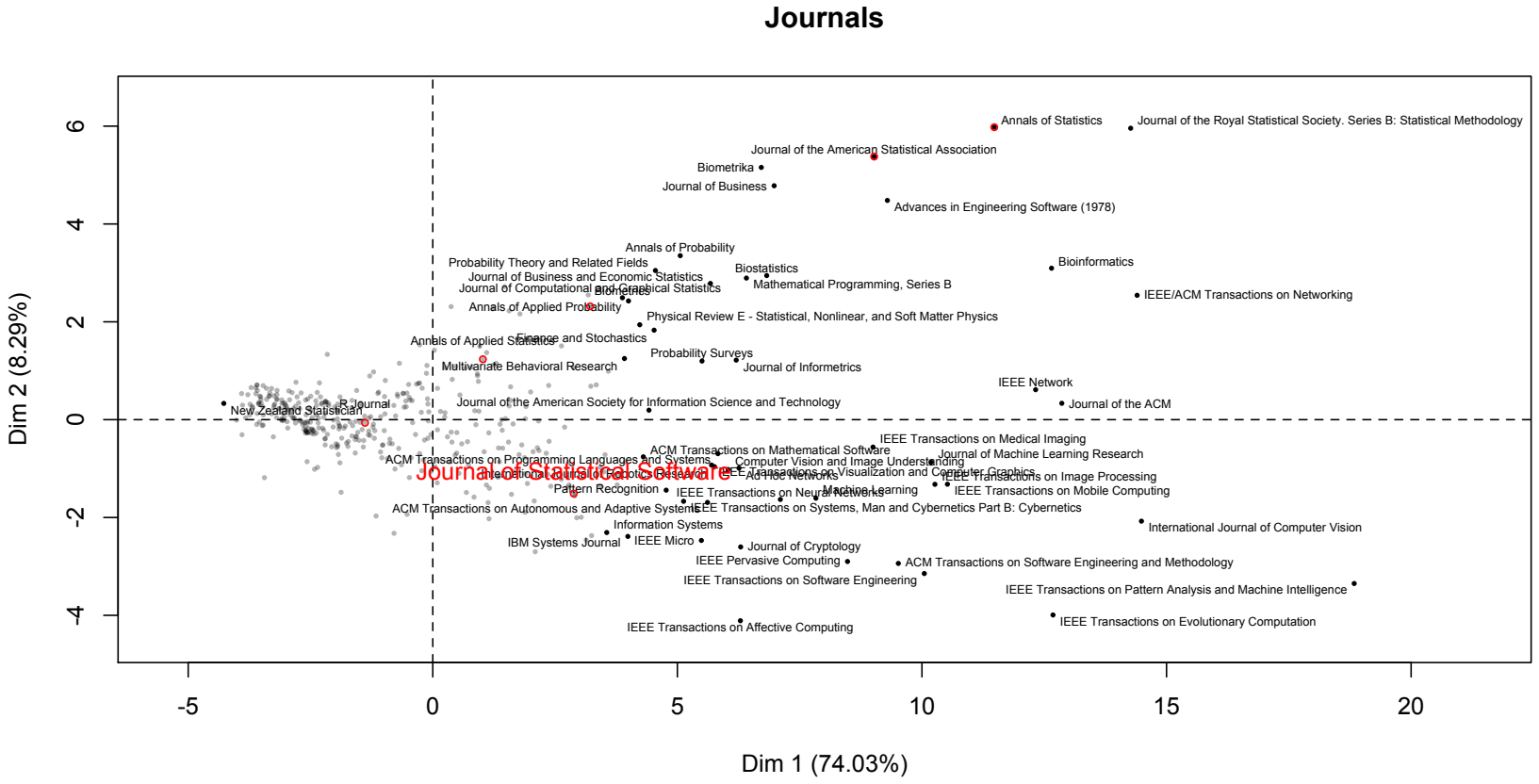
443 journals (Computer Science, Statistics, Probability and Mathematics). 45 metrics, some may be NA, 15 years by 3 types of measures:

- IPP - Impact Per Publication (like the ISI impact factor but for 3 (rather than 2) years.
- SNIP - Source Normalized Impact Per Paper: Tries to weight by the number of citations per subject field to adjust for different citation cultures.
- SJR - SCImago Journal Rank: Tries to capture average prestige per publication.

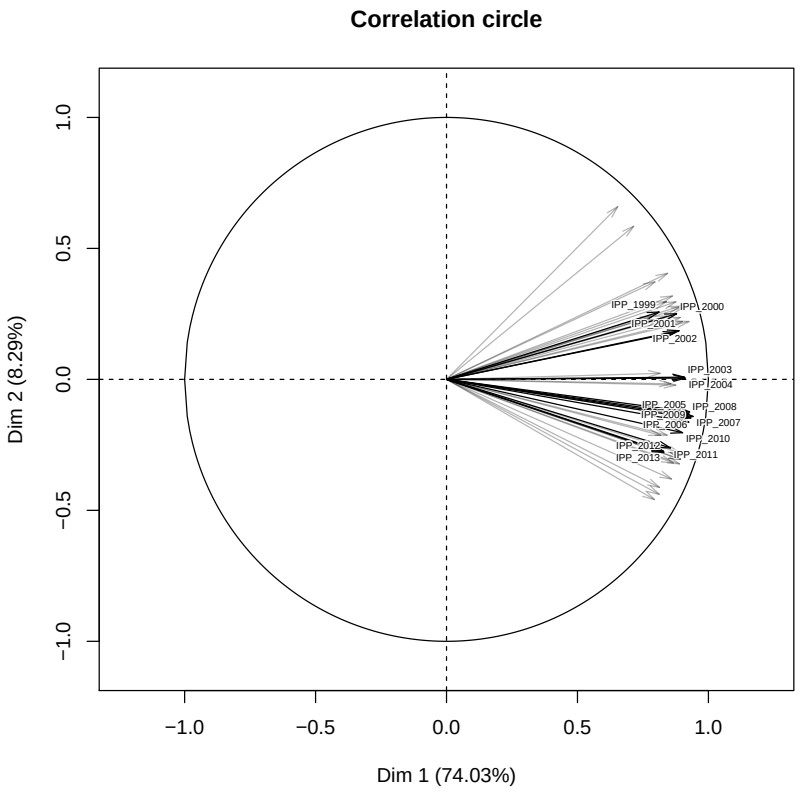
Multi-table imputation in practice

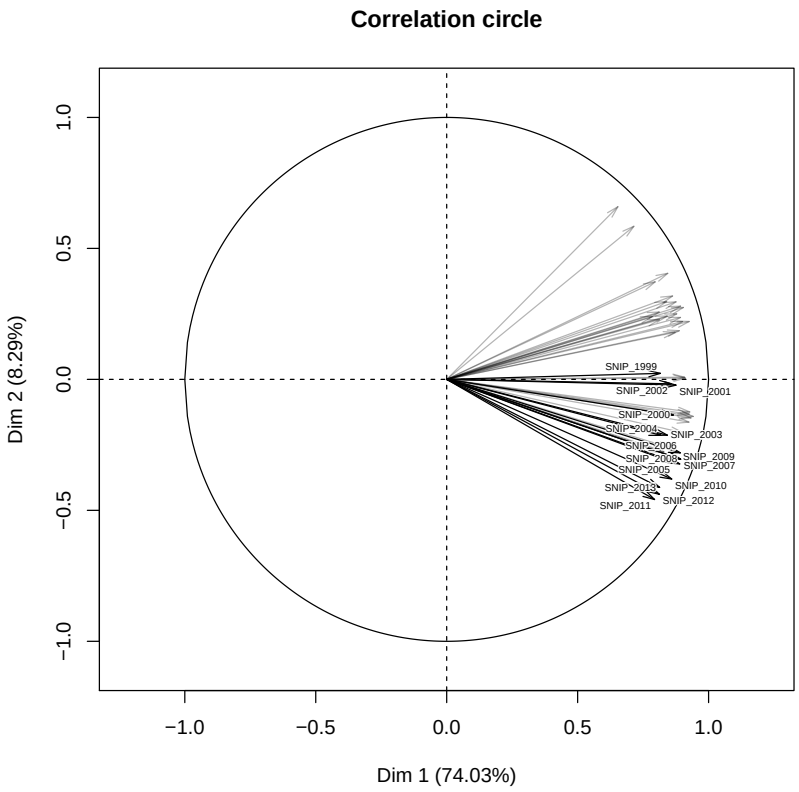
```
> library(denoiseR)
> library(missMDA)
> data(impactfactor)
> year=NULL; for (i in 1: 15) year= c(year, seq(i,45,15))
> res.imp <- imputeMFA(impactfactor,  group = rep(3, 15),  type = rep("s", 15))

##
> res.mfa  <-MFA(res.imp$completeObs, group=rep(3,15),  type=rep("s",15),
name.group=paste("year", 1999:2013,sep="_"),graph=F)

plot(res.mfa, choix = "ind", select = "contrib 15", habillage = "group", cex =
points(res.mfa$ind$coord[c("Journal of Statistical Software",
"Journal of the American Statistical Association", "Annals of Statistics"),
1:2], col=2, cex=0.6)
text(res.mfa$ind$coord[c("Journal of Statistical Software"), 1],
res.mfa$ind$coord[c("Journal of Statistical Software"), 2],cex=1,
labels=c("Journal of Statistical Software"),pos=3, col=2)

plot.MFA(res.mfa,choix="var", cex=0.5,shadow=TRUE, autoLab = "yes")

plot(res.mfa, select="IEEE/ACM Transactions on Networking",
partial="all",
habillage="group",unselect=0.9,chrono=TRUE)
```

MFA with missing values

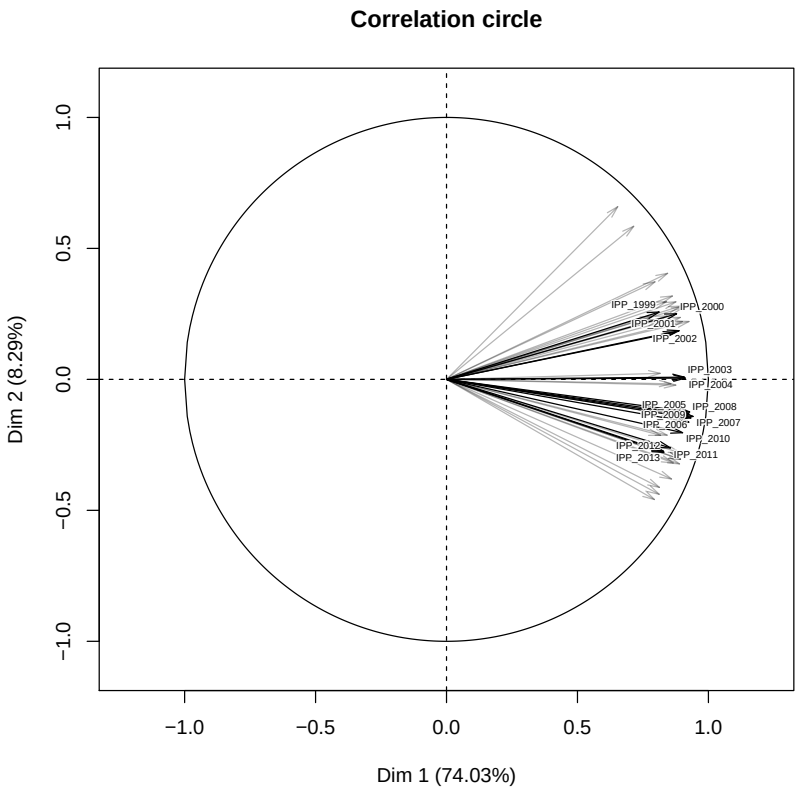


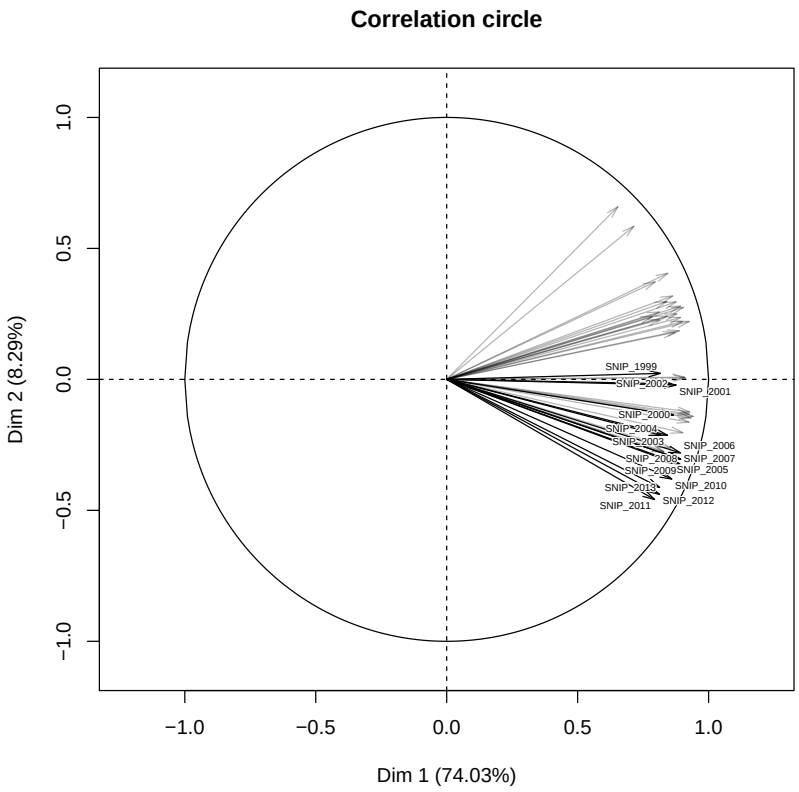
MFA with missing values





MFA with missing values

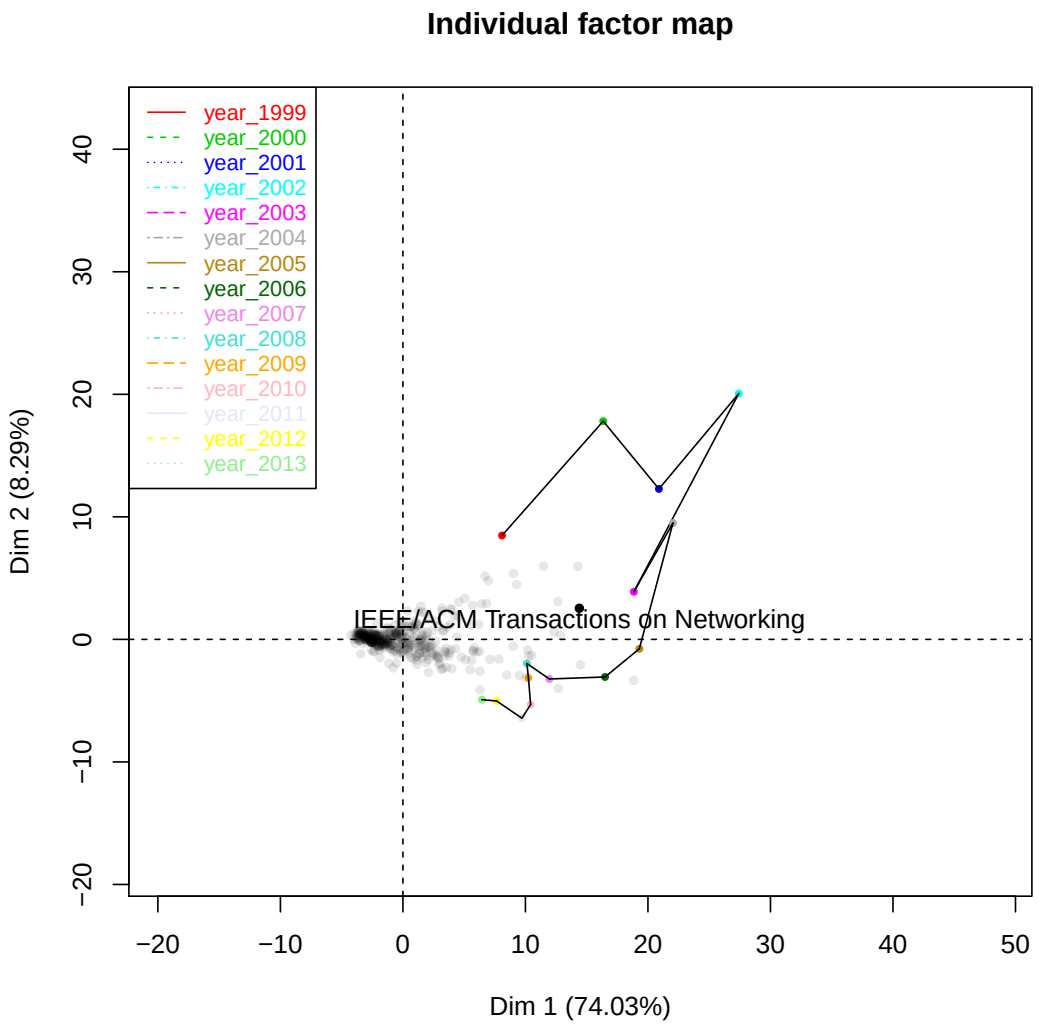




MFA with missing values

Rows: 47000 journals / Groups: 15 years of data/ Variables: 3 scores each year. Many missing...

ACM Transactions on Networking trajectory.pdf



Outline

1. Introduction
2. Single imputation with PCA
3. SI Practice
4. Single imputation for mixed variables
5. Multiple imputation for continuous data
6. Multiple imputation for categorical data
7. Conclusion
8. Distribution

Ozone data set

	maxO3	T9	T12	T15	Ne9	Ne12	Ne15	Vx9	Vx12	Vx15	maxO3v
0601	NA	15.6	18.5	18.4	4	4	8	NA	-1.7101	-0.6946	84
0602	82	17	18.4	17.7	5	5	7	NA	NA	NA	87
0603	92	NA	17.6	19.5	2	5	4	2.9544	1.8794	0.5209	82
0604	114	16.2	NA	NA	1	1	0	NA	NA	NA	92
0605	94	17.4	20.5	NA	8	8	7	-0.5	NA	-4.3301	114
0606	80	17.7	NA	18.3	NA	NA	NA	-5.6382	-5	-6	94
0607	NA	16.8	15.6	14.9	7	8	8	-4.3301	-1.8794	-3.7588	80
0610	79	14.9	17.5	18.9	5	5	4	0	-1.0419	-1.3892	NA
0611	101	NA	19.6	21.4	2	4	4	-0.766	NA	-2.2981	79
0612	NA	18.3	21.9	22.9	5	6	8	1.2856	-2.2981	-3.9392	101
0613	101	17.3	19.3	20.2	NA	NA	NA	-1.5	-1.5	-0.8682	NA
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
0919	NA	14.8	16.3	15.9	7	7	7	-4.3301	-6.0622	-5.1962	42
0920	71	15.5	18	17.4	7	7	6	-3.9392	-3.0642	0	NA
0921	96	NA	NA	NA	3	3	3	NA	NA	NA	71
0922	98	NA	NA	NA	2	2	2	4	5	4.3301	96
0923	92	14.7	17.6	18.2	1	4	6	5.1962	5.1423	3.5	98
0924	NA	13.3	17.7	17.7	NA	NA	NA	-0.9397	-0.766	-0.5	92
0925	84	13.3	17.7	17.8	3	5	6	0	-1	-1.2856	NA
0927	NA	16.2	20.8	22.1	6	5	5	-0.6946	-2	-1.3681	71
0928	99	16.9	23	22.6	NA	4	7	1.5	0.8682	0.8682	NA
0929	NA	16.9	19.8	22.1	6	5	3	-4	-3.7588	-4	99
0930	70	15.7	18.6	20.7	NA	NA	NA	0	-1.0419	-4	NA

http://www.airbreizh.asso.fr/

Aim: regression with missing values

Recap

- Pattern and missing values mechanism (desc. stats + expert)
- MAR: ignore missing values mechanism for inference

$\Rightarrow$ Estimate parameters θ -method stat from incomplete data

1) **Maximum likelihood**: Expectation Maximization

Recap

- Pattern and missing values mechanism (desc. stats + expert)
- MAR: ignore missing values mechanism for inference

$\Rightarrow$ Estimate parameters θ -method stat from incomplete data

1) **Maximum likelihood**: Expectation Maximization

2) **Single imputation**

- Mean: NO!!
- Joint model with Gaussian distribution $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$ (estim parameters - impute from the predictive) - package `Amelia`, `mice`

Recap

- Pattern and missing values mechanism (desc. stats + expert)
- MAR: ignore missing values mechanism for inference

$\Rightarrow$ Estimate parameters θ -method stat from incomplete data

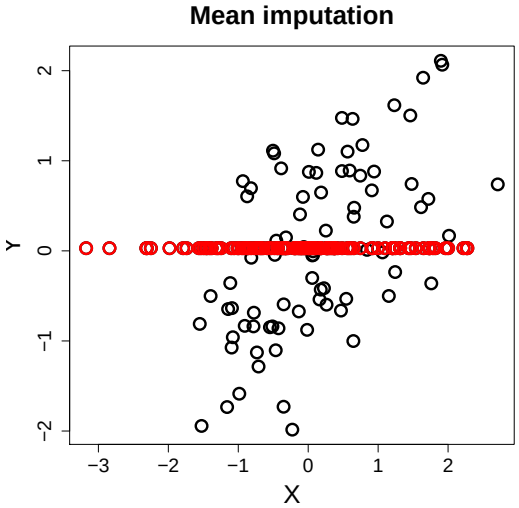
1) **Maximum likelihood**: Expectation Maximization
2) **Single imputation**
   - Mean: NO!!
   - Joint model with Gaussian distribution $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$ (estim parameters - impute from the predictive) - package `Amelia`, `mice`
   - Joint model with PCA $x_{ij} = \sum_{s=1}^{S} \sqrt{\tilde{\lambda}_s} \tilde{u}_{is} \tilde{v}_{js} + \varepsilon_{ij}$ (Iterative PCA) `missMDA` (Youtube) - PCA with missing `FactoMineR`
   - Conditional model with Forest packages `missForest`
     $\Rightarrow$ Properties depends on the methods properties

Complete ozone

```
         maxO3     T9    T12    T15   Ne9  Ne12  Ne15    Vx9   Vx12   Vx15  maxO3v
20010601  87.000 15.600 18.500 20.471 4.000 4.000 8.000  0.695 -1.710 -0.695  84.000
20010602  82.000 18.505 20.870 21.799 5.000 5.000 7.000 -4.330 -4.000 -3.000  87.000
20010603  92.000 15.300 17.600 19.500 2.000 3.984 3.812  2.954  1.951  0.521  82.000
20010604 114.000 16.200 19.700 24.693 1.000 1.000 0.000  2.044  0.347 -0.174  92.000
20010605  94.000 18.968 20.500 20.400 5.294 5.272 5.056 -0.500 -2.954 -4.330 114.000
20010606  80.000 17.700 19.800 18.300 6.000 7.020 7.000 -5.638 -5.000 -6.000  94.000
20010607  79.000 16.800 15.600 14.900 7.000 8.000 6.556 -4.330 -1.879 -3.759  80.000
20010610  79.000 14.900 17.500 18.900 5.000 5.000 5.016  0.000 -1.042 -1.389  99.000
20010611 101.000 16.100 19.600 21.400 2.000 4.691 4.000 -0.766 -1.026 -2.298  79.000
20010612 106.000 18.300 22.494 22.900 5.000 4.627 4.495  1.286 -2.298 -3.939 101.000
20010613 101.000 17.300 19.300 20.200 7.000 7.000 3.000 -1.500 -1.500 -0.868 106.000
.....

20010915  69.000 17.100 17.700 17.500 6.000 7.000 8.000 -5.196 -2.736 -1.042  71.000
20010916  71.000 15.400 18.091 16.600 4.000 5.000 5.000 -3.830  0.000  1.389  69.000
20010917  60.000 15.283 18.565 19.556 4.000 5.000 4.000  0.000  3.214  0.000  71.000
20010918  42.000 14.091 14.300 14.900 8.000 7.000 7.000 -2.500 -3.214 -2.500  60.000
20010919  65.000 14.800 16.425 15.900 7.000 7.982 7.000 -4.341 -6.062 -5.196  42.000
20010920  71.000 15.500 18.000 17.400 7.000 7.000 6.000 -3.939 -3.064  0.000  65.000
20010924  76.000 13.300 17.700 17.700 5.631 5.883 5.453 -0.940 -0.766 -0.500  65.139
20010925  75.573 13.300 18.434 17.800 3.000 5.000 5.001  0.000 -1.000 -1.286  76.000
20010927  77.000 16.200 20.800 20.499 5.368 5.495 5.177 -0.695 -2.000 -1.473  71.000
20010928  99.000 18.074 22.169 23.651 3.531 3.610 3.561  1.500  0.868  0.868  93.135
20010929  83.000 19.855 22.663 23.847 5.374 5.000 3.000 -4.000 -3.759 -4.000  99.000
20010930  70.000 15.700 18.600 20.700 7.000 6.405 7.000 -2.584 -1.042 -4.000  83.000
```

```
> library(missMDA)
> res.comp <- imputePCA(ozo[, 1:11])
> res.comp$comp
```

Single imputation methods: Danger!



$\mu_y = 0$	0.01
$\sigma_y = 1$	0.5
$\rho = 0.6$	0.30
$CI\mu_y 95\%$	

Confidence interval for a mean

Let $Y = (Y_1, \ldots, Y_n)'$ be i.i.d. independent Gaussian random with expectation μ_y and variance $\sigma_y^2 > 0$.

- The empirical mean $\bar{Y} = n^{-1} \sum_{i=1}^{n} Y_i$
- $\bar{Y} \sim \mathcal{N}(\mu_y, \sigma_y^2/n)$
- A confidence interval for μ

$$\mathbb{P}\left(\bar{Y} - \frac{\sigma_y}{\sqrt{n}} z_{1-\alpha/2} \leq \mu \leq \bar{Y} + \frac{\sigma_y}{\sqrt{n}} z_{1-\alpha/2}\right) = 1 - \alpha$$

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Variance unknown:

$$\frac{\sqrt{n}}{\widehat{\sigma_y}} \left(\bar{Y} - \mu_y\right) \sim T(n-1)$$

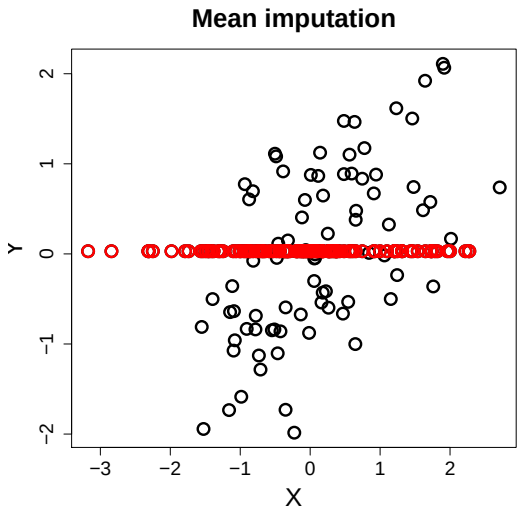
$$\left[\bar{y} - \frac{\widehat{\sigma}_y}{\sqrt{n}} t_{1-\alpha/2}(n-1) \ , \ \bar{y} + \frac{\hat{\sigma}_y}{\sqrt{n}} t_{1-\alpha/2}(n-1)\right]$$

Simulation

- Generate bivariate Gaussian data ($\mu_y = 0, \sigma_y = 1, \rho = 0.6$)
- Put missing values on y
- Imput missing entries
- Compute the confidence interval of μ_y - count if the true value $\mu_y = 0$ is in the confidence interval
- Repeat the steps 10000 times
- Give the coverage

Single imputation methods

$$\left[\bar{y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}; \bar{Y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}\right]$$

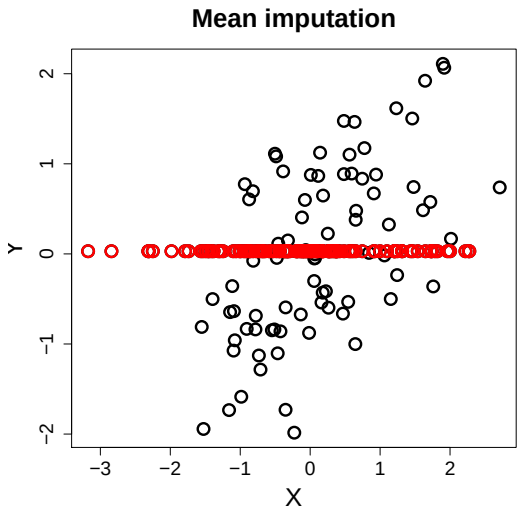


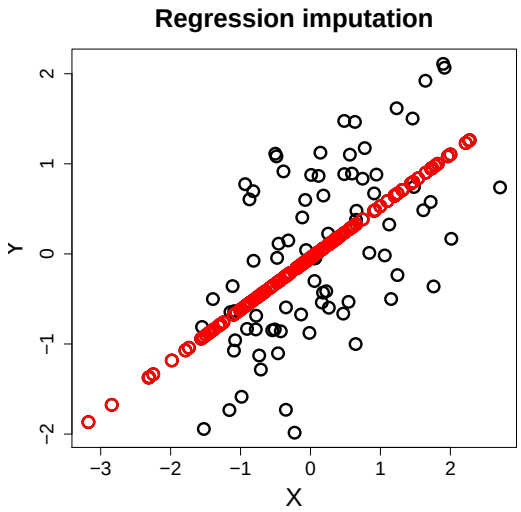
$\mu_y = 0$	0.01
$\sigma_y = 1$	0.5
$\rho = 0.6$	0.30
$CI\mu_y 95\%$	39.4

The idea of imputation is both seductive and dangerous *(Dempster and Rubin, 1983)*

Single imputation methods

$$\left[\bar{y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}; \bar{Y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}\right]$$



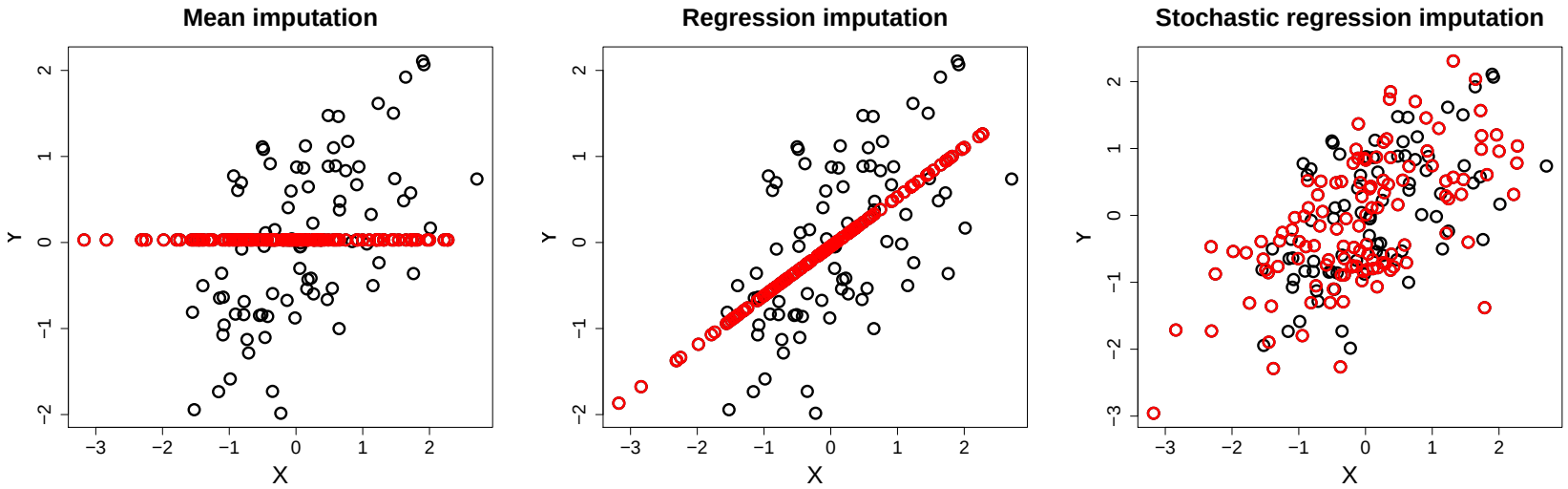


$\mu_y = 0$	0.01	0.01
$\sigma_y = 1$	0.5	0.72
$\rho = 0.6$	0.30	0.78
$CI\mu_y 95\%$	39.4	61.6

The idea of imputation is both seductive and dangerous *(Dempster and Rubin, 1983)*

Single imputation methods

$$\left[\bar{y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}; \bar{Y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}\right]$$

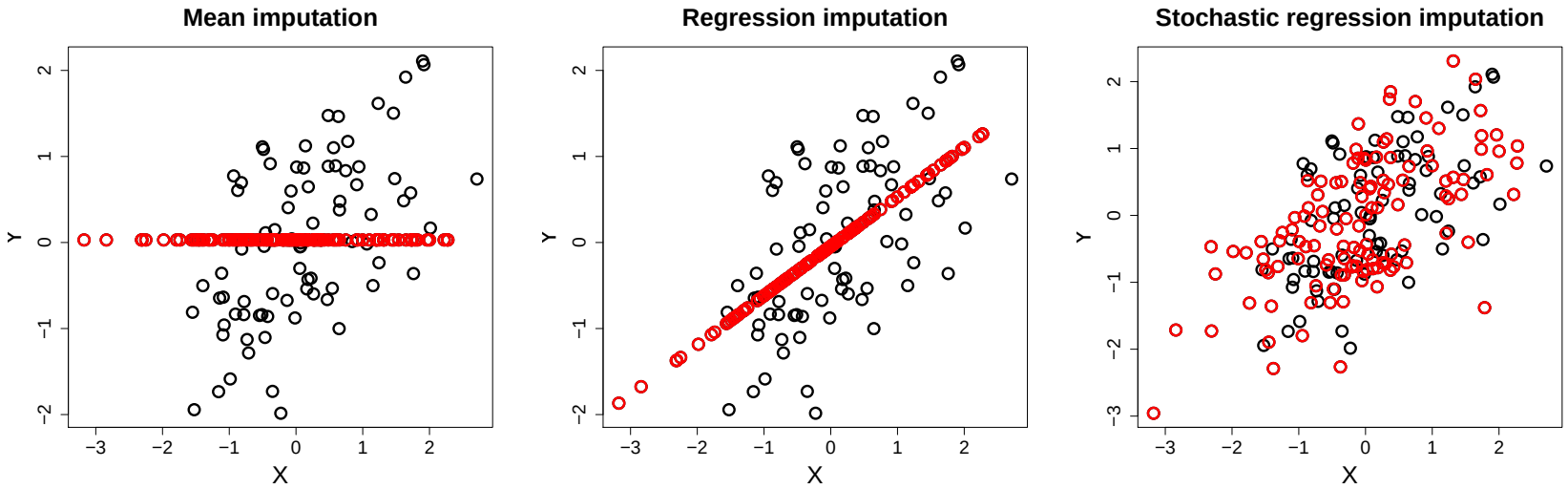


$\mu_y = 0$	0.01	0.01	0.01
$\sigma_y = 1$	0.5	0.72	0.99
$\rho = 0.6$	0.30	0.78	0.59
$CI\mu_y 95\%$	39.4	61.6	70.8

The idea of imputation is both seductive and dangerous *(Dempster and Rubin, 1983)*

Single imputation methods

$$\left[\bar{y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}; \bar{Y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}\right]$$



	Mean imputation	Regression imputation	Stochastic regression imputation
$\mu_y = 0$	0.01	0.01	0.01
$\sigma_y = 1$	0.5	0.72	0.99
$\rho = 0.6$	0.30	0.78	0.59
$CI\mu_y 95\%$	39.4	61.6	70.8

The idea of imputation is both seductive and dangerous *(Dempster and Rubin, 1983)*

$\Rightarrow$ Standard errors of the parameters ($\hat{\sigma}_{\hat{\mu}_y}$) calculated from the imputed data set are underestimated

Underestimation of variance

Classical confidence interval for μ_y $\left[\bar{y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}; \bar{Y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}\right]$

Asymptotic variance with missing values (Little & Rubin, p140):

$$\frac{\hat{\sigma}_y^2}{n_{obs}}\left(1 - \hat{\rho}^2\frac{n - n_{obs}}{n_{obs}}\right) = \frac{\hat{\sigma}_y^2}{n}\left(1 + \frac{n - n_{obs}}{n_{obs}}(1 - \hat{\rho}^2)\right)$$

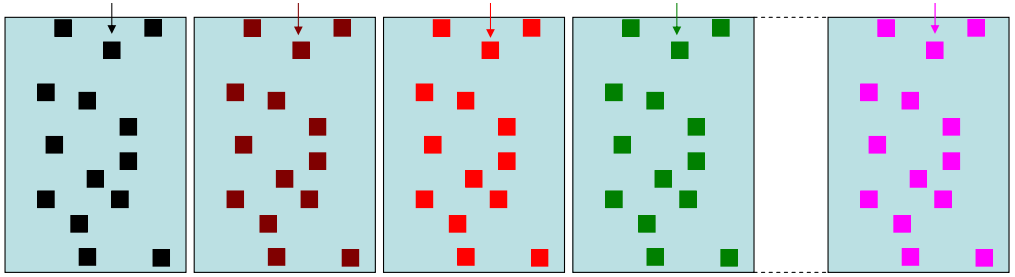
$\Rightarrow$ When the $\rho = 1$, we trust the prediction and the coverage given by stochastic regression is OK.

$\Rightarrow$ Coverage of single imputation is too low: need to take into account the uncertainty associated to the predictions.

Multiple imputation (Rubin, 1987)

Single imputation: underestimation of standard errors
$\Rightarrow$ a single value can't reflect the uncertainty of prediction

1. Generate M plausible values for each missing value



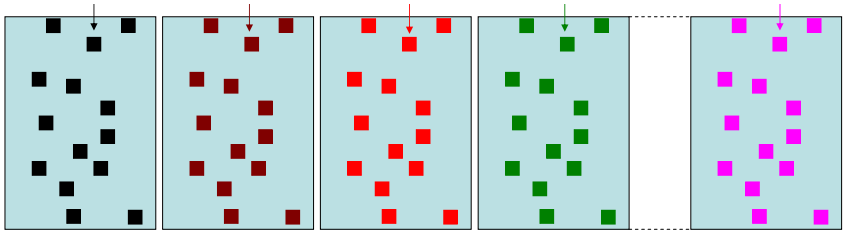
2. Perform the analysis on each imputed data set: $\hat{\theta}_m, \widehat{Var}\left(\hat{\theta}_m\right)$
3. Combine the results: $\hat{\theta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\theta}_m$
$$T = \frac{1}{M}\sum_{m=1}^{M}\widehat{Var}\left(\hat{\theta}_m\right) + \left(1+\frac{1}{M}\right)\frac{1}{M-1}\sum_{m=1}^{M}\left(\hat{\theta}_m - \hat{\theta}\right)^2$$

$\Rightarrow$ Aim: provide estimation of the parameters and of their variability (taken into account the variability due to missing values)

Multiple imputation

Single imputation: a single value can't reflect the uncertainty of prediction $\Rightarrow$ underestimate the standard errors

1. Generating M imputed data sets



2. Performing the analysis on each imputed data set
3. Combining: variance = within + between imputation variance

$$\hat{\beta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\beta}_m$$
$$T = \frac{1}{M}\sum_m \widehat{Var}\left(\hat{\beta}_m\right) + \left(1+\frac{1}{M}\right)\frac{1}{M-1}\sum_m\left(\hat{\beta}_m - \hat{\beta}\right)^2$$

Multiple imputation: bivariate case

1. Generating M imputed data sets

   First idea: several stochastic regression
   for $m = 1, ..., M$, draw y_i from the predictive $\mathcal{N}(x_i\hat{\beta}, \hat{\sigma}^2)$

2. Performing the analysis on each imputed data set
3. Combining: variance = within + between imputation variance

	$M = 1$	$M = 50$
$\mu_y = 0$	0.01	0.01
$\sigma_y = 1$	0.99	0.99
$\rho = 0.6$	0.59	0.59
$CI\mu_y 95\%$	70.8	81.8

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$CI\mu_y 95\%$	70.8	81.8

$\Rightarrow$ Variability of the parameters is missing: "improper" imputation
$\Rightarrow$ Prediction variance = estimation variance plus noise

Regression: variance of prediction

$$y_{n+1} = x'_{n+1}\beta + \varepsilon_{n+1}$$
$$\hat{y}_{n+1} = x'_{n+1}\hat{\beta}$$
$$\hat{\beta} = (X'X)^{-1}X'Y$$

$$\begin{aligned} V[\hat{y}_{n+1} - y_{n+1}] &= V[x'_{n+1}(\hat{\beta} - \beta) - \varepsilon_{n+1}] \\ &= x'_{n+1}V(\hat{\beta} - \beta)x_{n+1} + \sigma^2] \\ &= \hat{\sigma}^2\left(x'_{n+1}(X'X)^{-1}x_{n+1} + 1\right) \end{aligned}$$

CI for the prediction

$$\left[x'_{n+1}\hat{\beta} + -t_{n-p}(1-\alpha/2)\hat{\sigma}\sqrt{(x'_{n+1}(X'X)^{-1}x_{n+1} + 1)}\right]$$

Multiple imputation continuous data: bivariate case

$\Rightarrow$ Proper multiple imputation with $y_i = x_i\beta + \varepsilon_i$

1. Variability of the parameters, M plausible: $(\hat{\beta})^1, ..., (\hat{\beta})^M$

   $\Rightarrow$ Bootstrap
   $\Rightarrow$ Posterior distribution: Data Augmentation (Tanner & Wong, 1987)

2. Noise: for $m = 1, ..., M$, missing values y_i^m are imputed by drawing from the predictive distribution $\mathcal{N}(x_i\hat{\beta}^m, (\hat{\sigma}^2)^m)$

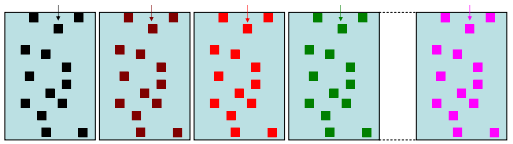
	Improper	Proper
$CI\mu_y 95\%$	0.818	0.935

Multiple imputation

$\Rightarrow$ Aim: provide estimation of the parameters and of their variability (taken into account the variability due to missing values)

Single imputation: a single value can't reflect the uncertainty of prediction $\Rightarrow$ underestimate the standard errors

1. Generating M imputed data sets: variance of prediction



2. Performing the analysis on each imputed data set
3. Combining: variance = within + between imputation variance

$$\hat{\beta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\beta}_m$$

$$T = \frac{1}{M}\sum \widehat{Var}\left(\hat{\beta}_m\right) + \left(1+\frac{1}{M}\right)\frac{1}{M-1}\sum\left(\hat{\beta}_m - \hat{\beta}\right)^2$$

Multiple imputation

$\Rightarrow$ Aim: provide estimation of the parameters and of their variability (taken into account the variability due to missing values)

Single imputation: a single value can't reflect the uncertainty of prediction $\Rightarrow$ underestimate the standard errors

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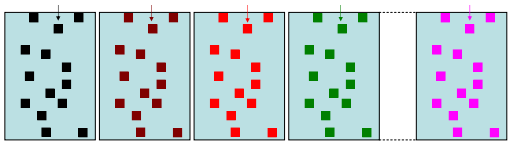


   1) Variance of estimation of the parameters + 2) Noise
2. Performing the analysis on each imputed data set
3. Combining: variance = within + between imputation variance

$$\hat{\beta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\beta}_m$$

$$T = \frac{1}{M}\sum \widehat{Var}\left(\hat{\beta}_m\right) + \left(1+\frac{1}{M}\right)\frac{1}{M-1}\sum\left(\hat{\beta}_m - \hat{\beta}\right)^2$$

Joint modeling

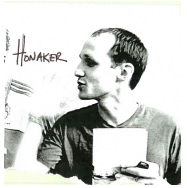
$\Rightarrow$ Hypothesis $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$

Algorithm Expectation Maximization Bootstrap:

1. Bootstrap rows: $X^1, \ldots, X^M$
   EM algorithm: $(\hat{\mu}^1, \hat{\Sigma}^1), \ldots, (\hat{\mu}^M, \hat{\Sigma}^M)$
2. Imputation: x_{ij}^m drawn from $\mathcal{N}\left(\hat{\mu}^m, \hat{\Sigma}^m\right)$

Easy to parallelized. Implemented in `Amelia` (website)

Amelia Earhart



James Honaker

Gary King

Matt Blackwell

Fully conditional modeling

⇒ Hypothesis: one model/variable

1. Initial imputation: mean imputation
2. For a variable j

   2.2 Imputation of the missing values in variable j with a model of X_j on the other X_{-j}: stochastic regression x_{ij} from $\mathcal{N}\left((x_{i,-j})'\hat{\beta}^{-j}, \hat{\sigma}^{-j}\right)$
3. Cycling through variables

⇒ Iteratively refine the imputation.
⇒ With continuous variables and a regression/variable: $\mathcal{N}(\mu, \Sigma)$

Implemented in `mice` (website) and Python

"*There is no clear-cut method for determining whether the MICE algorithm has converged*"

Stef van Buuren

Fully conditional modeling

$\Rightarrow$ Hypothesis: one model/variable

1. Initial imputation: mean imputation
2. For a variable j
   - 2.1 $(\hat{\beta}^{-j}, \hat{\sigma}^{-j})$ drawn from a Bootstrap: $(\hat{\beta}^{-j}, \hat{\sigma}^{-j})^1, ..., (\hat{\beta}^{-j}, \hat{\sigma}^{-j})^M$
   - 2.2 Imputation of the missing values in variable j with a model of X_j on the other X_{-j}: stochastic regression x_{ij} from $\mathcal{N}\left((x_{i,-j})'\hat{\beta}^{-j}, \hat{\sigma}^{-j}\right)$
3. Cycling through variables

Get M imputed data

$\Rightarrow$ Iteratively refine the imputation.

$\Rightarrow$ With continuous variables and a regression/variable: $\mathcal{N}(\mu, \Sigma)$

Implemented in `mice` (website) and Python

"*There is no clear-cut method for determining whether the MICE algorithm has converged*"

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Joint / Conditional modeling

⇒ Both seen imputed values are drawn from a Joint distribution (even if joint does not exist)
⇒ Conditional modeling takes the lead?

- Flexible: one model/variable. Easy to deal with interactions and variables of different nature (binary, ordinal, categorical...)
- Many statistical models are conditional models!
- Tailor to your data
- Appears to work quite well in practice

⇒ Drawbacks: one model/variable... tedious...

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- Appears to work quite well in practice

$\Rightarrow$ Drawbacks: one model/variable... tedious...

$\Rightarrow$ What to do with high correlation or when $n < p$?

- JM shrinks the covariance $\Sigma + k\mathbb{I}$ (selection of k?)
- CM: ridge regression or predictors selection/variable $\Rightarrow$ a lot of tuning ... not so easy ...

Multiple imputation with Bootstrap/Bayesian PCA

$$x_{ij} = \mu_{ij} + \varepsilon_{ij} = \sum_{s=1}^{S} \sqrt{\tilde{\lambda}_s} \tilde{u}_{is} \tilde{v}_{js} + \varepsilon_{ij} \ , \ \varepsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$$

1. Variability of the parameters, M plausible: $(\hat{\mu}_{ij})^1, ..., (\hat{\mu}_{ij})^M$ Bootstrap - Iterative PCA
2. Noise: for $m = 1, ..., M$, missing values x_{ij}^m drawn $\mathcal{N}(\hat{\mu}_{ij}^m, \hat{\sigma}^2)$

Implemented in `missMDA` (website)

François Husson

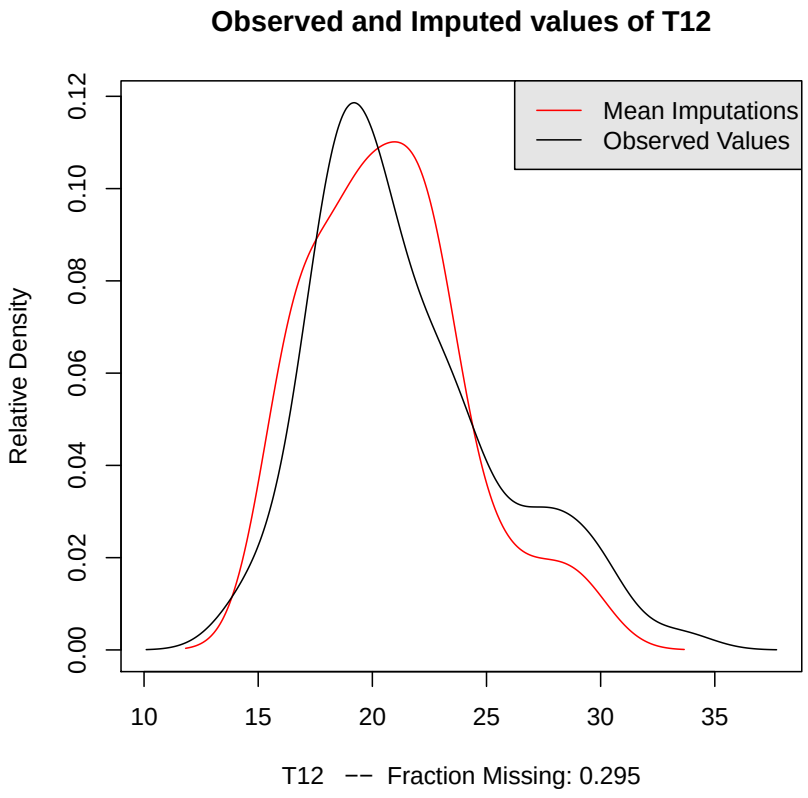
Multiple imputation in practice

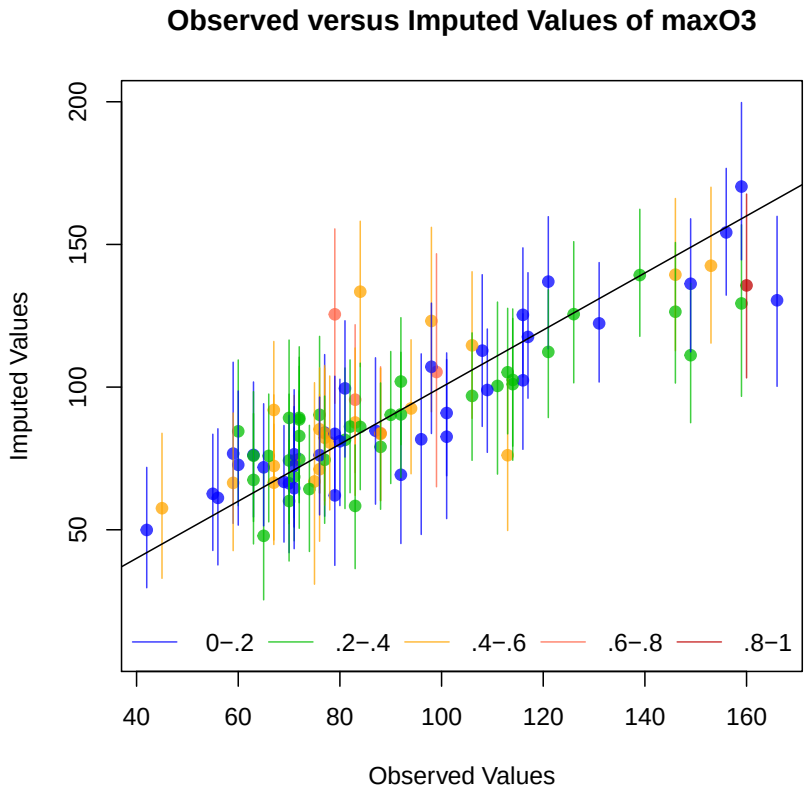
⇒ Step 1: Generate M imputed data sets

```
> library(Amelia)
> res.amelia <- amelia(don, m = 100)

> library(mice)
> res.mice <- mice(don, m = 100, defaultMethod = "norm.boot")

> library(missMDA)
>  res.MIPCA <- MIPCA(don, ncp = 2, nboot  = 100)
> res.MIPCA$res.MI
```

Multiple imputation in practice

⇒ Step 2: visualization



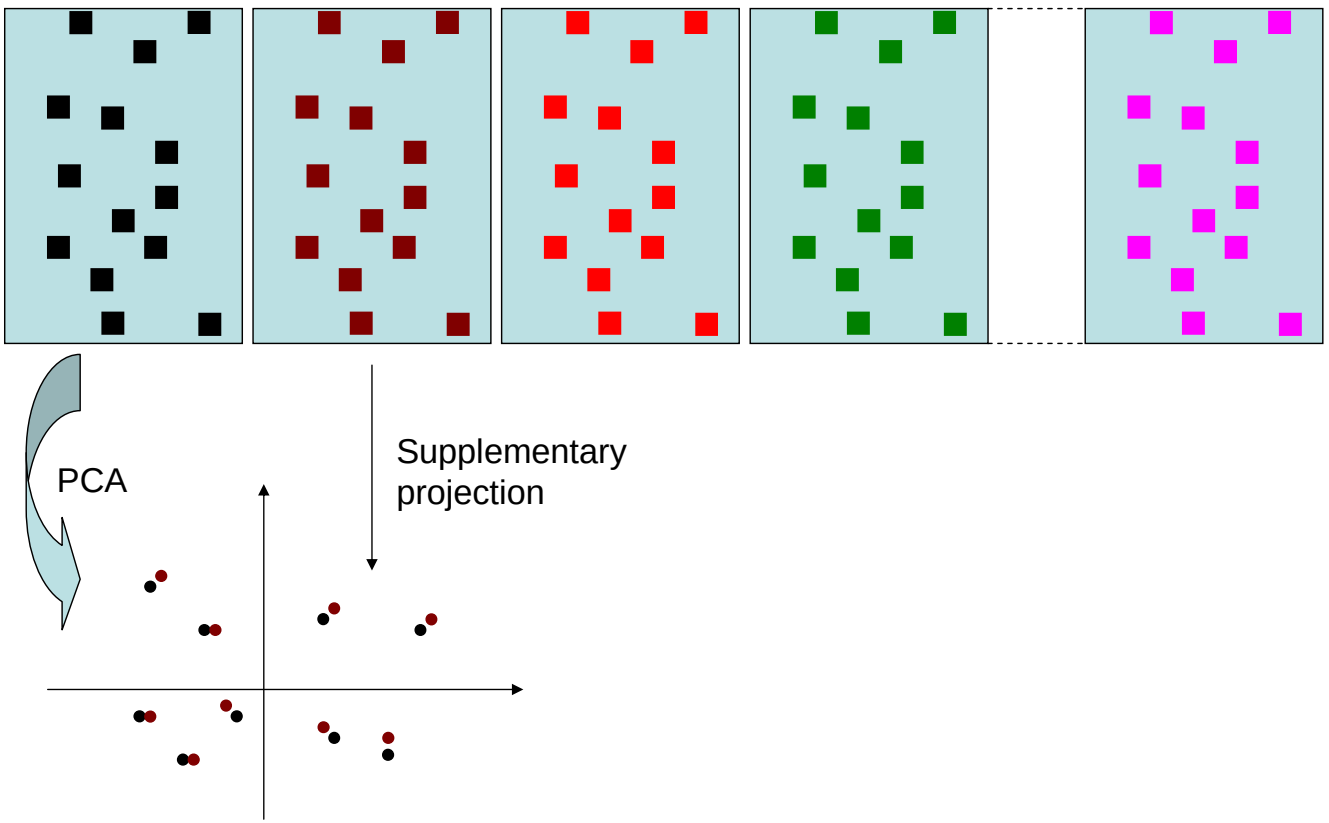



```
# library(Amelia)
> res.amelia <- amelia(don, m = 100)
> compare.density(res.amelia, var = "T12")
> overimpute(res.amelia, var = "maxO3")

# library(missMDA)
res.over<-Overimpute(res.MIPCA)
```

Multiple imputation in practice

⇒ Step 2: visualization

⇒ Individuals position (and variables) with other predictions



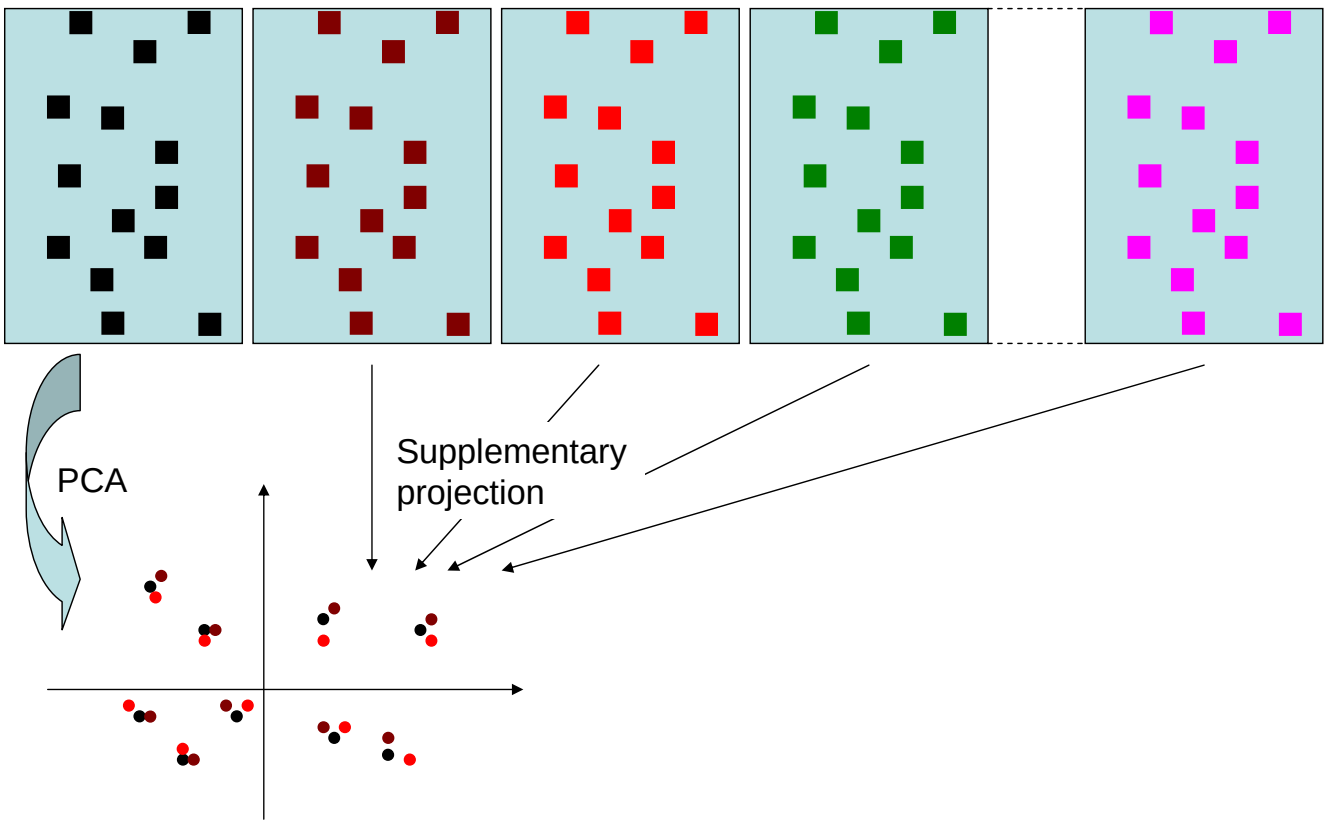
Regularized iterative PCA

⇒ reference configuration

Multiple imputation in practice

⇒ Step 2: visualization

⇒ Individuals position (and variables) with other predictions



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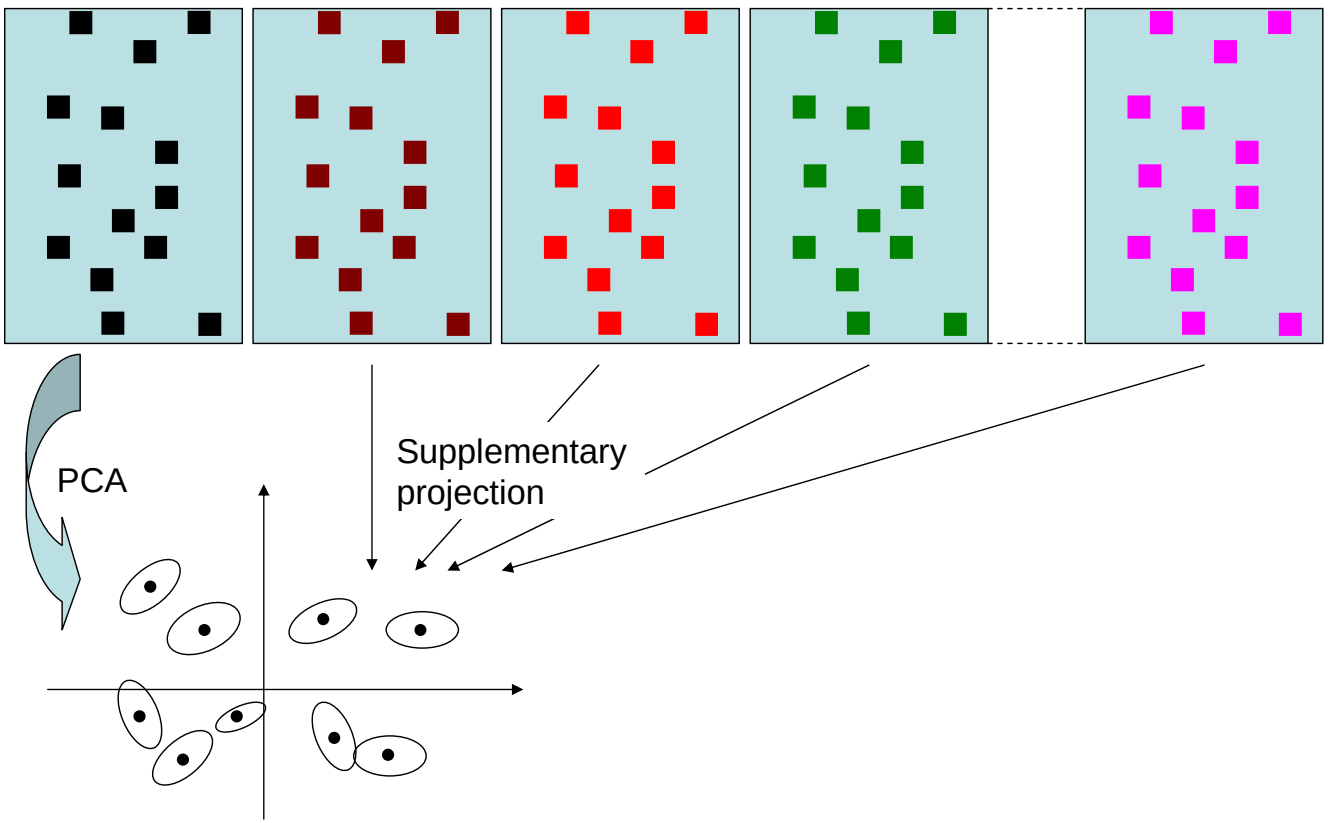
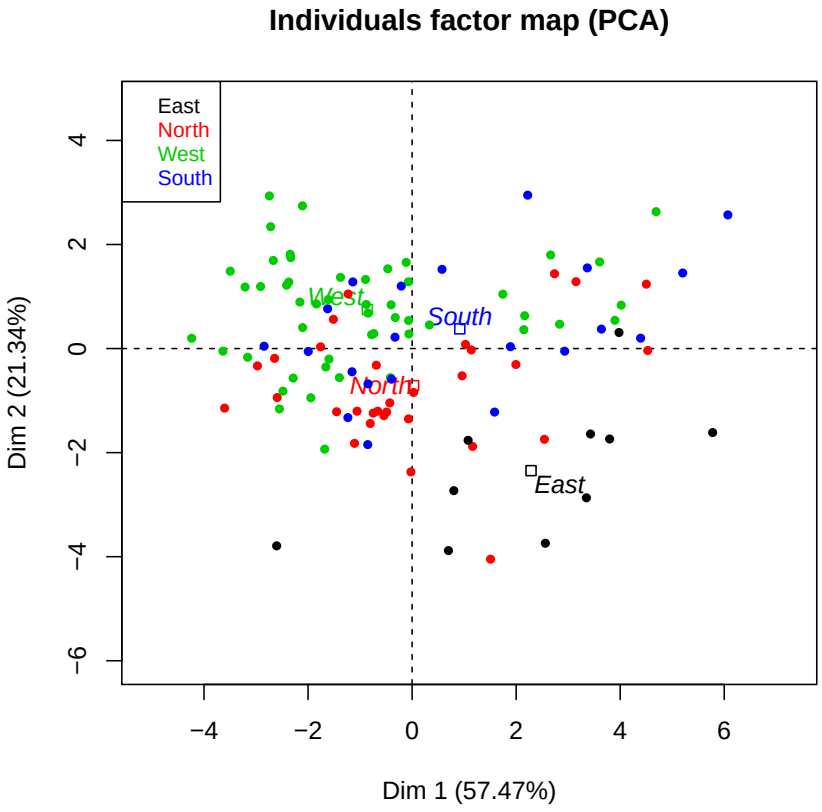
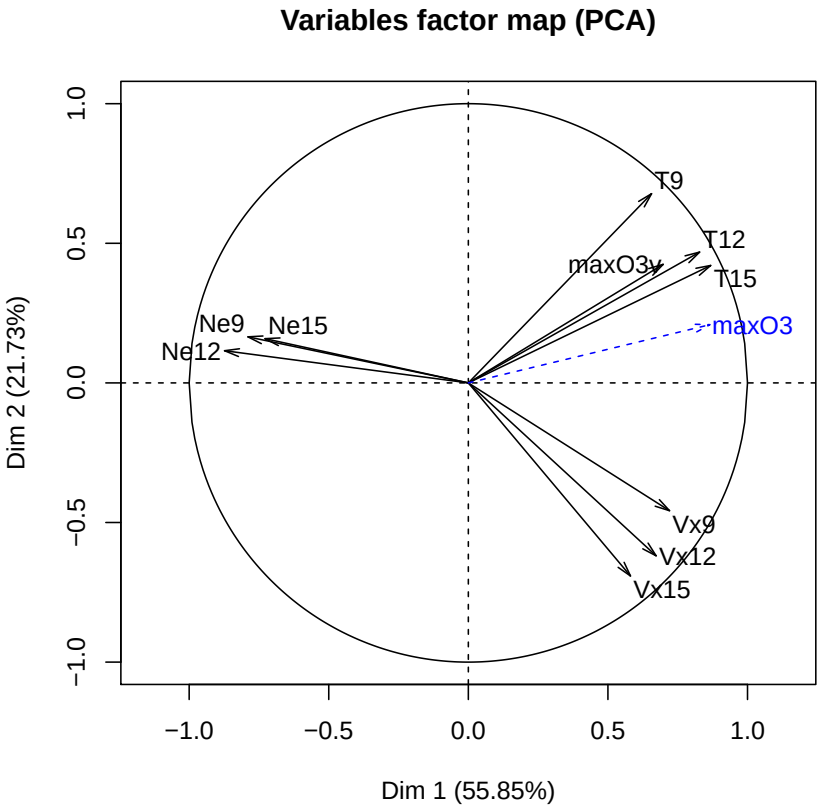


Regularized iterative PCA

⇒ reference configuration

PCA representation



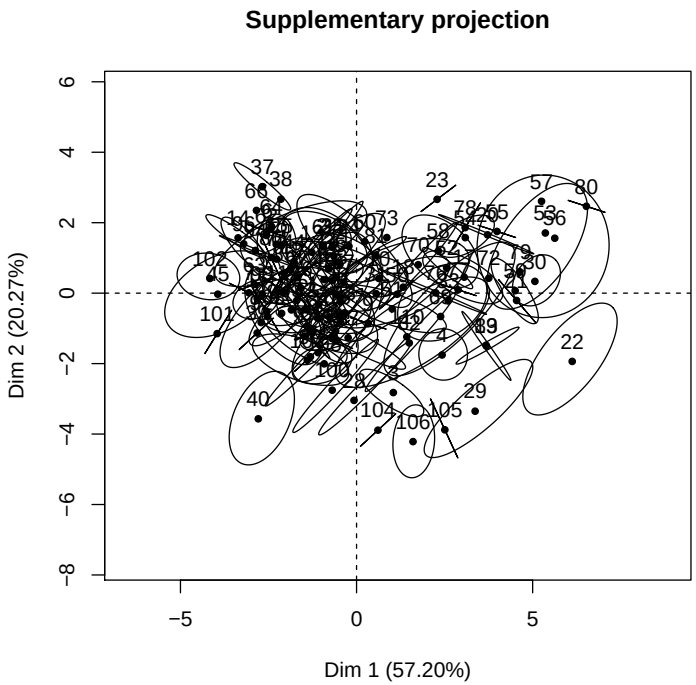


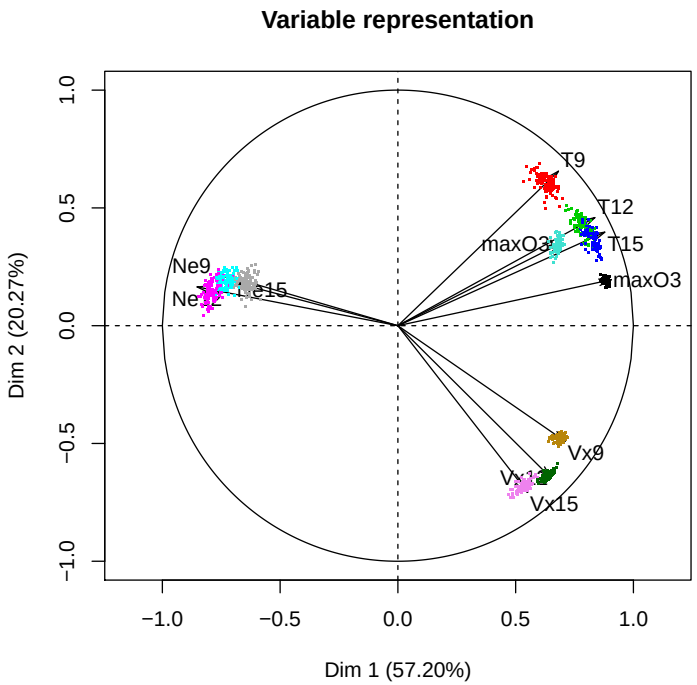

```
> imp <- cbind.data.frame(res.comp$completeObs, ozo[, 12])
> res.pca <- PCA(imp,quanti.sup = 1, quali.sup = 12)
> plot(res.pca, hab =12, lab = "quali"); plot(res.pca, choix = "var")
> res.pca$ind$coord #scores (principal components)
```

Multiple imputation in practice

⇒ Step 2: visualization

```
> res.MIPCA <- MIPCA(don, ncp = 2)
> plot(res.MIPCA, choice = "ind.supp"); plot(res.MIPCA, choice = "var")
```





⇒ Percentage of NA?

Multiple imputation in practice

⇒ Step 3. Regression on each table and pool the results

$$\hat{\beta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\beta}_m$$

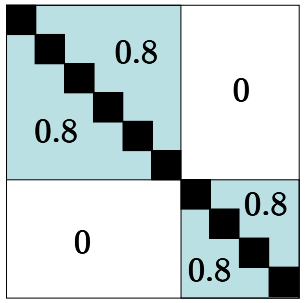
$$T = \frac{1}{M}\sum_m \widehat{Var}\left(\hat{\beta}_m\right) + \left(1+\frac{1}{M}\right)\frac{1}{M-1}\sum_m\left(\hat{\beta}_m - \hat{\beta}\right)^2$$

```
> library(mice)
> res.mice <- mice(don, m = 100)
> imp.micerf <- mice(don, m = 100, defaultMethod = "rf")
> lm.mice.out <- with(res.mice, lm(maxO3 ~ T9+T12+T15+Ne9+...+Vx15+maxO3v))
> pool.mice <- pool(lm.mice.out)
> summary(pool.mice)
```

```
              est    se     t    df Pr(>|t|)  lo 95 hi 95 nmis  fmi lambda
(Intercept) 19.31 16.30  1.18 50.48     0.24 -13.43 52.05   NA 0.46   0.44
T9          -0.88  2.25 -0.39 26.43     0.70  -5.50  3.75   37 0.71   0.69
T12          3.29  2.38  1.38 27.54     0.18  -1.59  8.18   33 0.70   0.68
....
Vx15         0.23  1.33  0.17 39.00     0.87  -2.47  2.93   21 0.57   0.55
maxO3v       0.36  0.10  3.65 46.03     0.00   0.16  0.56   12 0.50   0.48
```

Simulations

- 1000 simulations
  - data set drawn from $\mathcal{N}_p(\mu, \Sigma)$ with a two-block structure, varying n (30 or 200), p (6 or 60) and ρ (0.3 or 0.9)



  - 10% or 30% of missing values using a MCAR mechanism
  - multiple imputation using $M = 20$ imputed data
- Quantities of interest: $\theta_1 = \mathbb{E}[Y], \theta_2 = \beta_1, \theta_3 = \rho$
- Criteria
  - bias
  - CI width, coverage

Results for the expectation

	parameters				confidence interval width			coverage		
	n	p	ρ	%	*Amelia*	*MICE*	*BayesMIPCA*	*Amelia*	*MICE*	*BayesMIPCA*
1	30	6	0.3	0.1	0.803	0.805	0.781	0.955	0.953	0.950
2	30	6	0.3	0.3		1.010	0.898		0.971	0.949
3	30	6	0.9	0.1	0.763	0.759	0.756	0.952	0.95	0.949
4	30	6	0.9	0.3		0.818	0.783		0.965	0.953
5	30	60	0.3	0.1			0.775			0.955
6	30	60	0.3	0.3			0.864			0.952
7	30	60	0.9	0.1			0.742			0.953
8	30	60	0.9	0.3			0.759			0.954
9	200	6	0.3	0.1	0.291	0.294	0.292	0.947	0.947	0.946
10	200	6	0.3	0.3	0.328	0.334	0.325	0.954	0.959	0.952
11	200	6	0.9	0.1	0.281	0.281	0.281	0.953	0.95	0.952
12	200	6	0.9	0.3	0.288	0.289	0.288	0.948	0.951	0.951
13	200	60	0.3	0.1		0.304	0.289		0.957	0.945
14	200	60	0.3	0.3		0.384	0.313		0.981	0.958
15	200	60	0.9	0.1		0.282	0.279		0.951	0.948
16	200	60	0.9	0.3		0.296	0.283		0.958	0.952

Joint, conditional and PCA

$\Rightarrow$ Good estimates of the parameters and their variance from an incomplete data (coverage close to 0.95)
The variability due to missing values is well taken into account

`Amelia` & `mice` have difficulties with large correlations or $n < p$
`missMDA` does not but requires a tuning parameter: number of dim.

`Amelia` & `missMDA` are based on linear relationships
`mice` is more flexible (one model per variable)

MI based on PCA works in a large range of configuration, $n < p$, $n > p$
strong or weak relationships, low or high percentage of missing values

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3. SI Practice
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6. Multiple imputation for categorical data
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Multiple imputation for categorical data

$\Rightarrow$ Joint modeling:

- Log-linear model (Schafer, 1997): pb many levels R package cat
- Transform categorical into dummies and use $X_{i.} \sim \mathcal{N}(\mu, \Sigma)$
- Latent class models (Vermunt J.K, 2014) - nonparametric Bayesian (Dunson, 2015), Dirichlet process mixture of products of multinomial distributions, dpmpm (Y. Si & J. P. Reiter, 2014) - R package mi, (Gelman *et al.*)

$\Rightarrow$ Conditional model: logistic, multinomial logit, random forests R package (`mice`)

Multiple imputation for categorical data

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⇒ Conditional model: logistic, multinomial logit, random forests R package (`mice`)

⇒ MI with MCA provides valid inferences

- reduce the dimensionality
- applied on data of various dimensions (many categories)
- especially for rare categories

Multiple imputation with MCA

1. Variability of the parameters: M sets $(U_{n\times S}, \Lambda_{S\times S}, V^{\top}_{m\times S})$ using a non-parametric bootstrap

$\hat{X}_1$

1	0	...	1	0	0
1	0	...	1	0	0
1	0	...			
			0.01	0.80	0.19
			0	0	1
0.25	0.75				
0	1		0	0	1

$\hat{X}_2$

1	0	...	1	0	0
1	0	...	1	0	0
1	0	...			
			0.60	0.2	0.20
			0	0	1
0.26	0.74				
0	1		0	0	1

...

$\hat{X}_M$

1	0	...	1	0
1	0	...	1	0
1	0	...		
			0.11	0.74
			0	0
0.20	0.80			
0	1		0	0

2. Categories drawn from multinomial disribution using the values in $\left(\hat{X}_m\right)_{1\leq m\leq M}$

y	...	Attack
y	...	Attack
y	...	
		Suicide
	...	Accident
n		
n	...	S

y	...	Attack
y	...	Attack
y	...	
		Attack
	...	Accident
n		
n	...	B

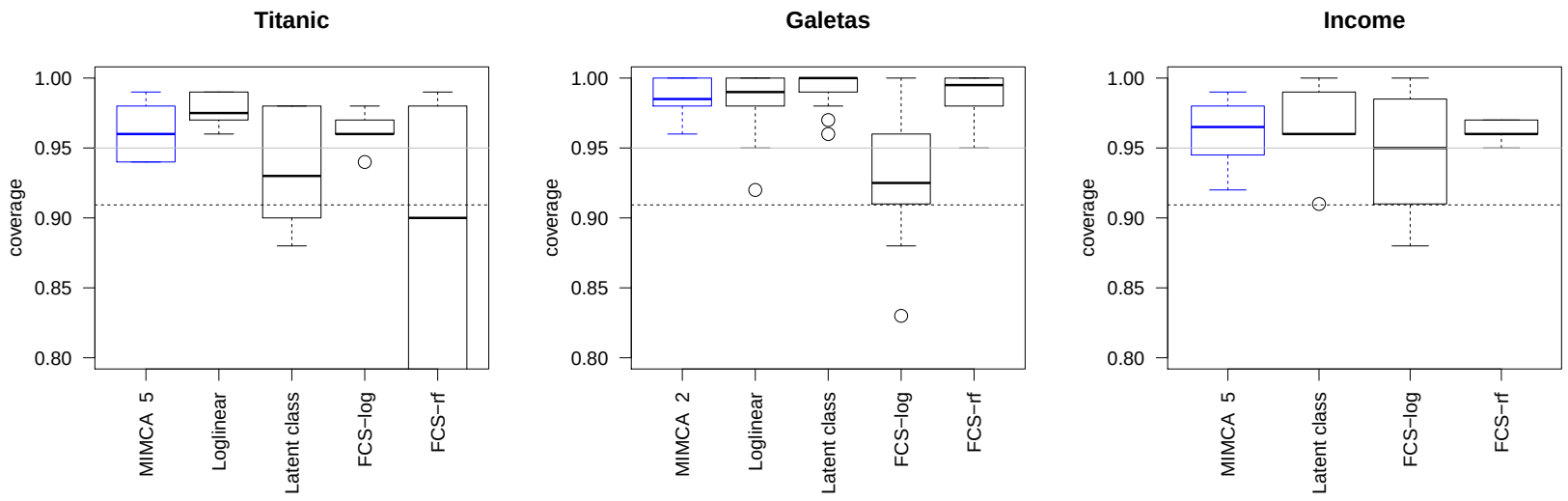
...

y	...	Attack
y	...	Attack
y	...	
		Suicide
	...	Accident
n		
n	...	Suicide

Simulations

- Quantities of interest: $\theta =$ parameters of a logistic model
- 200 simulations from real data sets
  - the real data set is considered as a population
  - drawn one sample from the data set
  - generate 20% of missing values
  - multiple imputation using $M = 5$ imputed data
- Criteria
  - bias
  - CI width, coverage

Results - Inference



	Titanic	Galetas	Income
Number of variables	4	4	14
Number of categories	≤ 4	≤ 11	≤ 9

Results - Time second

	Titanic	Galetas	Income
MIMCA	2.750	8.972	**58.729**
Loglinear	0.740	4.597	NA
Non-parametric latent class	10.854	17.414	143.652
Cond logistic	4.781	38.016	881.188
Cond forests	265.771	112.987	6329.514

	Titanic	Galetas	Income
Number of individuals	2201	1192	6876
Number of variables	4	4	14
Number of categories	≤ 4	≤ 11	≤ 9

Audigier, V., Husson, F. & Josse, J. (2016). MIMCA: Multiple imputation for categorical variables with multiple correspondence analysis. *Statistics & Computing*.

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To conclude

Take home message:

- "***The idea of imputation is both seductive and dangerous***. *It is seductive because it can lull the user into the pleasurable state of believing that the data are complete after all, and it is dangerous because it lumps together situations where the problem is sufficiently minor that it can be legitimately handled in this way and situations where standard estimators applied to the real and imputed data have substantial biases.*" (Dempster and Rubin, 1983)
- Single imputation aims to complete a dataset as best as possible (prediction)
- Multiple imputation aims to perform other statistical methods after and to estimate parameters and their variability taking into account the missing values uncertainty
- Single imputation can be appropriate for point estimates

To conclude

Take home message:

- Principal component methods powerful to impute large data sets of different dimensions with continuous, categorical variables: reduce the dimensionality and take into account the similarities between rows and relationship between variables.

  Provides correct inferences for analysis model based on relationships between pairs of variables

  Requires to choose the number of dimensions S

- Handling missing values in PCA, MCA, FAMD, Multiple Factor Analysis (MFA), Correspondence analysis for contingency tables
- Preprocessing before clustering
- Package R missMDA (youtube, website, blog)

Challenges

$\Rightarrow$ MI theory:

- Imputation model as complex as the analysis model (interaction)
- Good theory for regression parameters: others?
- MI theory with new asymptotic small n, large p ?

  $\Rightarrow$ Still an active area of research
  $\Rightarrow$ Imputation/Multiple imputation for prediction.

$\Rightarrow$ Some practical issues:

- Imputation not in agreement (X and X^2): missing passive
- Imputation out of range?
- Problems of logical bounds (> 0)
- Multiple imputation is an appealing method .... but ... with big data?

Ressources

⇒ Softwares:

- van Buuren webpage:
  http://www.stefvanbuuren.nl/mi/Software.html
- R task View: Official Statistics & Survey Methodology

⇒ Books:

- van Buuren (2018, online!). *Flexible Imputation of Missing Data*. Chapman & Hall/CRC
- Carpenter & Kenward (2013). *Multiple Imputation and its Application*. Wiley
- Kim & Shao (2013). Statistical Methods for handling Incomplete Data, Chapman & Hall/CRC.
- G. Molenberghs, G. Fitzmaurice, M.G. Kenward, A. Tsiatis & G. Verbeke (nov 2014). *Handbook of Missing Data*. Chapman & Hall/CRC

⇒ J.L. Schafer & J.W. Graham, 2002. Missing Data: Our View of the State of the Art. *Psychological Methods*, **7** 147-177

Contributors on the topic of multiple imputation

- J. Honaker - G. King - M. Blackwell (Harvard): `Amelia`
- S. van Buuren (Utrecht): `mice`
- F. Husson (Rennes)- J. Josse: `missMDA`
- A. Gelman - J. Hill - Y. Su (Colombia): `mi`
- J. Reiter (Duke): `NPBayesImpute` Non-Parametric Bayesian Multiple Imputation for Categorical Data
- J. Bartlett - J. Carpenter - M. Kenward (UCL): `smcfcs` Substantive model compatible FCS multiple imputation
- H. Goldstein (Bristol) : `realcom` for multi-level data
- J.K. Vermunt (Tilburg): `poLCA` latent class models
- ...

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8 hospital databases

Combining data from different institutional databases promises many advantages in personalizing medical care (large n, more chance for finding patients like me)

$\Rightarrow$ NIH requires sharing of data from funded projects

8 hospital databases

Combining data from different institutional databases promises many advantages in personalizing medical care (large n, more chance for finding patients like me)

$\Rightarrow$ NIH requires sharing of data from funded projects

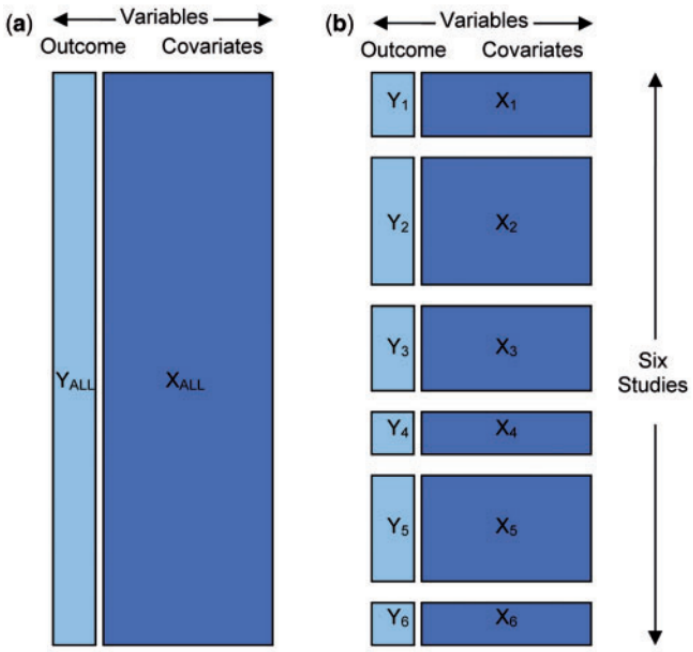
$\Rightarrow$ The problem: high barriers to aggregation of medical data

- lack of standardization of ontologies
- privacy concerns
- proprietary attitude towards data, reluctance to cede control
- complexity/size of aggregated data, updates problems

Solution: distributed computation

⇒ Data aggregation is not always necessary

⇒ NIH splits the storage of aggregated data across several centers

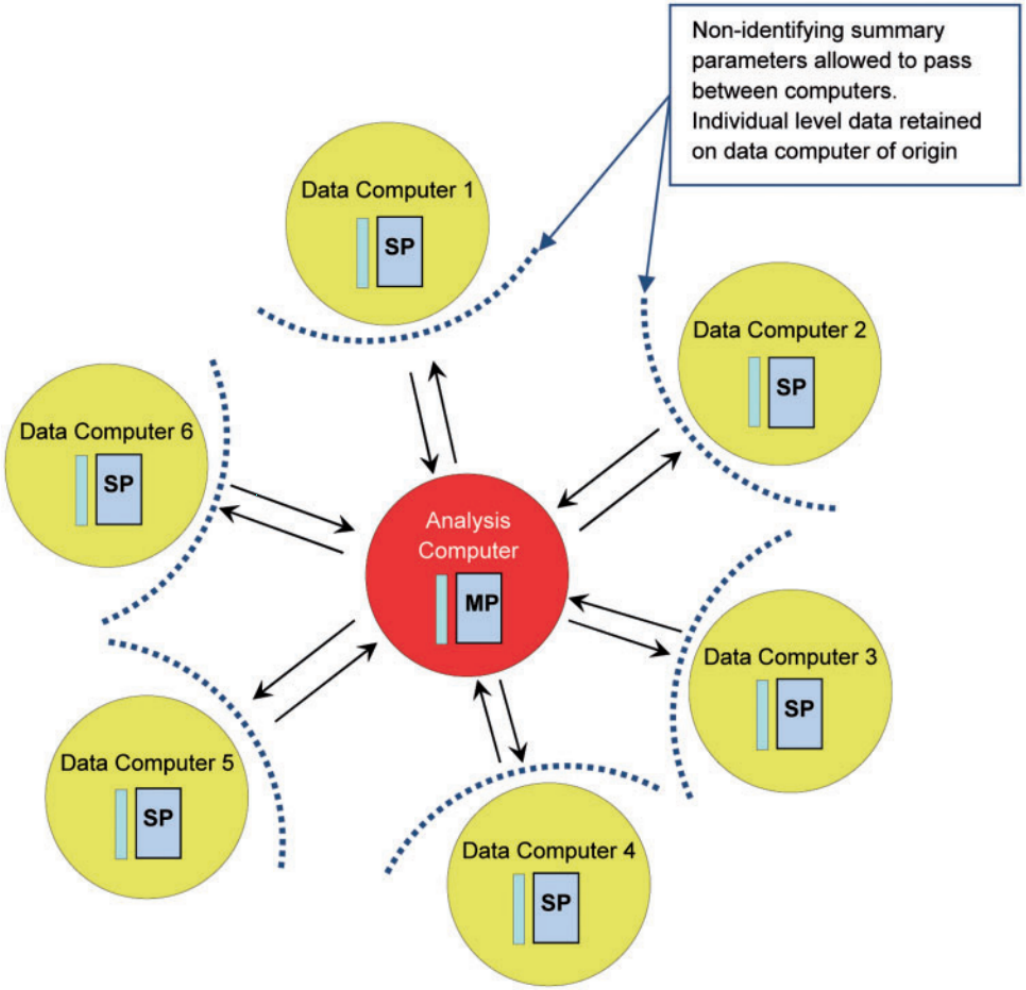


⇒ Data can stay at site

⇒ Computations can be distributed (share burden)

⇒ Hospitals only share intermediate results instead of the raw data

Topology: master-workers (Wolfson, et. al (2010))



$\Rightarrow$ Ex: Each site share the sum of age $\tilde{X}_i$ and the number of patients n_i. The master computes $\bar{X} = \sum n_i \tilde{X}_i / \sum n_i$

Solution: distributed computation

$\Rightarrow$ Many models fitting can be implemented:

- Maximizing a likelihood. Intermediate computations break up into sums of quantities computed on local data at sites. Log-likelihood, score function and Fisher information can partition into sums. (OK for logistic regression)
- Singular Value Decomposition. Iterative algorithms available for SVD using quantities computed on local data at sites.
- And more.

Implemented in the R package discomp (Narasimhan et. al., 2017)

Singular value decomposition

SVD: $X_{n\times p} : U_{n\times s} D_{s\times s} V'_{p\times s}$

Power method to get the first direction:

Data: $\boldsymbol{X} \in \mathcal{R}^{n\times p}$
Result: $u \in \mathcal{R}^n$, $v \in \mathcal{R}^p$, and $d > 0$
$u \leftarrow (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \ldots, \frac{1}{\sqrt{n}})$;
repeat
  $v \leftarrow \boldsymbol{X}^\top u$;
  $v \leftarrow v/\|v\|$;
  $u \leftarrow \boldsymbol{X} v$;
  $d \leftarrow \|u\|$;
  $u \leftarrow u/\|u\|$;
until *convergence*;

Other dims: "deflation", same procedure in the residuals $(X - udv')$

$\Rightarrow$ Involves inner products and sums: distributed

Privacy preserving rank k SVD

Data: each worker has private data $\boldsymbol{X}_i \in \mathcal{R}^{n_i \times p}$
Result: $V \in \mathcal{R}^{p \times k}$, and $d_1 \geq \ldots d_k \geq 0$
$V \leftarrow 0$, $d \leftarrow 0$ **foreach** *worker site* j **do**
  $U^{[j]} = 0$;
  transmit n_j to master;
end
for $i \leftarrow 1$ **to** k **do**
  foreach *worker site* j **do** $u^{[j]} \leftarrow (1, 1, \ldots, 1)$ of length n_j;
  $\|u\| \leftarrow \sqrt{\sum_j n_j}$;
  transmit $\|u\|, V$, and D to workers;
  repeat
    foreach *worker site* j **do**
      $u^{[j]} \leftarrow u^{[j]} / \|u\|$;
      calculate $v^{[j]} \leftarrow (\boldsymbol{X}^{[j]} - U^{[j]} D V^\top)^\top u^{[j]}$;
      transmit $v^{[j]}$ to master;
    end
    $v \leftarrow \sum_j v^{[j]}$;
    $v \leftarrow v / \|v\|$;
    transmit v to workers;
    foreach *worker site* j **do**
      calculate $u^{[j]} \leftarrow \boldsymbol{X}^{[j]} v$;
      transmit $\|u^{[j]}\|$ to master;
    end
    $\|u\| \leftarrow \sum_j \|u^{[j]}\|$;
    transmit $\|u\|$ to workers;
    $d_i \leftarrow \|u\|$;
  until *convergence*;
  $V \leftarrow \texttt{cbind}(V, v)$;
  foreach *worker site* j **do** $U^{[j]} \leftarrow \texttt{cbind}(U^{[j]}, u^{[j]})$;
end

Expectation - Maximization (Dempster *et al.*, 1977)

Need the modification of the estimation process (not always easy!)

Rationale to get ML estimates on the observed values max L_{obs} through max of L_{comp} of $X = (X_{obs}, X_{miss})$. Augment the data to simplify the problem

E step (conditional expectation):

$$Q(\theta, \theta^{\ell}) = \int \ln(f(X|\theta)) f(X_{miss}|X_{obs}, \theta^{\ell}) dX_{miss}$$

M step (maximization):

$$\theta^{\ell+1} = \text{argmax}_{\theta} Q(\theta, \theta^{\ell})$$

Result: when $\theta^{\ell+1}$ max $Q(\theta, \theta^{\ell})$ then $L(X_{obs}, \theta^{\ell+1}) \geq L(X_{obs}, \theta^{\ell})$

Maximum likelihood approach

Hypothesis $\mathbf{x}_{i.} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$\Rightarrow$ Point estimates with EM:

```
> library(norm)
> pre <- prelim.norm(as.matrix(don))
> thetahat <- em.norm(pre)
> getparam.norm(pre,thetahat)
```

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$\Rightarrow$ Variances:

- Supplemented EM (Meng, 1991)
- Bootstrap approach:
  - Bootstrap rows: $\mathbf{X}^1, \ldots, \mathbf{X}^B$
  - EM algorithm: $(\hat{\boldsymbol{\mu}}^1, \hat{\boldsymbol{\Sigma}}^1), \ldots, (\hat{\boldsymbol{\mu}}^B, \hat{\boldsymbol{\Sigma}}^B)$

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Issue: develop a specific method for each statistical method

Joint modeling

$\Rightarrow$ Hypothesis $\mathbf{x}_{i.} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Bivariate case with missing values on Y (stochastic regression):

- Estimate β and σ
- Draw from the predictive $y_i \sim \mathcal{N}\left(x_i\hat{\beta}, \hat{\sigma}^2\right)$

Extension to the multivariate case:

- Estimate $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ from an incomplete dataset with EM
- Draw from $\mathcal{N}\left(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}\right)$

```
> pre <- prelim.norm(as.matrix(don))
> thetahat <- em.norm(pre)
> rngseed(123)
> imp <- imp.norm(pre,thetahat,don)
```

Conditional modeling

$\Rightarrow$ A model per variable

Example with regression:

1. Initial imputation: mean imputation
2. Fit a stochastic regression $\mathbf{X}_j^{obs}$ on the other variables $\mathbf{X}_{-j}^{obs}$
   Predict $\mathbf{X}_j^{miss}$ using the trained regression on $\mathbf{X}_{-j}^{miss}$
3. Cycling through variables

```
> library(mice)
> res.cm <- mice(don, m=1)
```

Conditional modeling

$\Rightarrow$ A model per variable

Example with regression:

1. Initial imputation: mean imputation
2. Fit a stochastic regression $\mathbf{X}_j^{obs}$ on the other variables $\mathbf{X}_{-j}^{obs}$
   Predict $\mathbf{X}_j^{miss}$ using the trained regression on $\mathbf{X}_{-j}^{miss}$
3. Cycling through variables

$\Rightarrow$ With continuous variables and a regression/variable: $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$\Rightarrow$ Flexibility: different models for each variable

```
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```

Bayesian PCA (Josse *et al.*, 2013) complete case

Model: $x_{ij} = \sum_{s=1}^{S} \tilde{x}_{ij}^{(s)} + \varepsilon_{ij}$, $\varepsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$

Prior: $\tilde{x}_{ij}^{(s)} \sim \mathcal{N}(0, \tau_s^2)$

Posterior: $\left(\tilde{x}_{ij}^{(s)} | x_{ij}^{(s)}\right) = \mathcal{N}(\Phi_s x_{ij}^{(s)}, \sigma^2 \Phi_s)$ with $\Phi_s = \dfrac{\tau_s^2}{\tau_s^2 + \sigma^2}$

Empirical Bayes: max the likelihood of $\left(x_{ij}^{(s)}\right) \sim \mathcal{N}(0, \tau_s^2 + \sigma^2)$ as a function of τ_s^2 to obtain: $\hat{\tau_s}^2 = (\lambda_s - \hat{\sigma}^2)$

$$\hat{\Phi}_s = \frac{\lambda_s - \hat{\sigma}^2}{\lambda_s} = \frac{\text{signal variance}}{\text{total variance}}$$

Bayesian PCA (Josse *et al.*, 2013) complete case

Point estimate: expectation of the posterior distribution

$$\hat{x}_{ij}^{\text{rPCA}} = \sum_{s=1}^{S} \left(\frac{\lambda_s - \hat{\sigma}^2}{\lambda_s} \right) \sqrt{\lambda_s} u_{is} v_{js} = \sum_{s=1}^{S} \left(\sqrt{\lambda_s} - \frac{\hat{\sigma}^2}{\sqrt{\lambda_s}} \right) u_{is} v_{js}$$

$$\hat{x}_{ij}^{\text{PCA}} = \sum_{s=1}^{S} \sqrt{\lambda_s} u_{is} v_{js}$$

$\Rightarrow$ Regularized version of the Max. Likelihood

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$\Rightarrow$ Regularized version of the Max. Likelihood

$$Y = \mathbf{X}\beta + \varepsilon,\ \varepsilon \sim \mathcal{N}(0, \sigma^2)$$
$$\beta \sim \mathcal{N}(0,\ \tau^2)$$
$$\hat{\beta}^{\text{MAP}} = (\mathbf{X}'\mathbf{X} + \kappa)^{-1}\mathbf{X}'Y, \text{ with } \kappa = \sigma^2/\tau^2$$

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$\Rightarrow$ Other priors: other regularizations (Todeschini *et al*, 2013)