MSc Data Science for Business

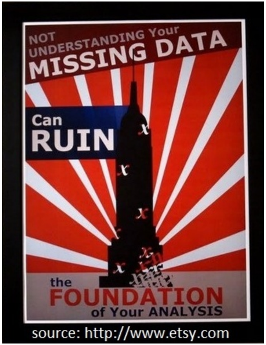
Introduction to Machine Learning

Map 534

Julie Josse

Dealing with missing values

J. Josse



Previous lecture: dimensionality reduction and clustering

Today: Missing values

- PCA with missing values
- Matrix completion
- Inference with missing values
- Categorical/mixed data

Outline

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

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

....

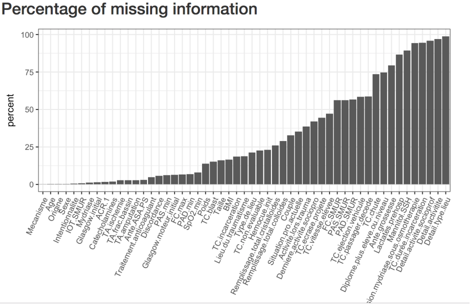
	SpO2	Temperature	Lactates	Hb	Glasgow	Transfusion	....
1	97	35.6	<NA>	12.7	12	yes	
2	100	36.5	4.8	11.1	15	no	
3	100	36	3.9	11.4	3	no	
4	100	36.7	1.66	13	15	yes	
6	100	36	NM	14.4	15	no	
7	100	36.6	NM	14.3	15	yes	
9	100	37.5	13	15.9	15	yes	
10	100	36.9	NM	13.7	15	no	
11	100	36.6	1.2	14.2	14	no	

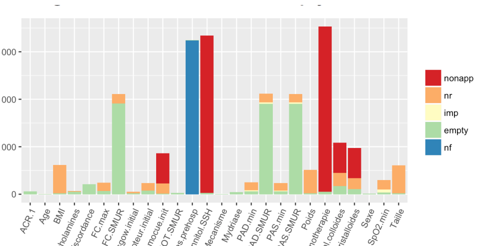
....

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

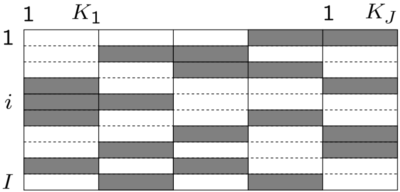
$\Rightarrow$ Logistic regressions/Random Forests with missing

Public Assistance - Paris Hospitals





Multi-blocks data set

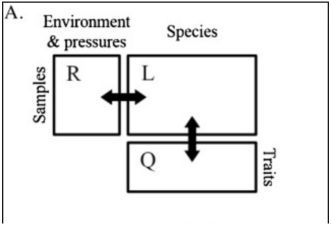


L'OREAL: 100 000 women in different countries - 300 variables

- 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)

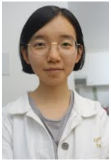


⇒ Aims: Assess the effect of time on species abundances
Monitor the population and assess wetlands conservation policies.
⇒ 70% of missing values in contingency tables

On going works

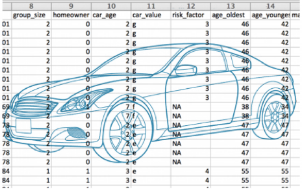
- François Husson (Agrocampus)
- Genevieve Robin (PhD student), B. Narasimhan (Stanford): distributed matrix completion for multilevel medical data
- Genevieve Robin (PhD student), R. Tibshirani (Stanford): imputation of contingency tables with side information
- Wei Jiang (PhD student): glm with missing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






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

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



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 %

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

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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$X = (X_{miss}, X_{obs})$. 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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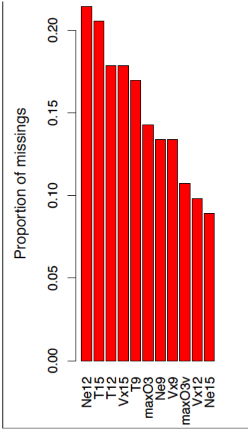
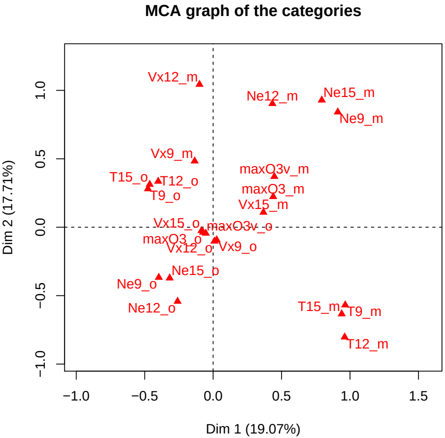
- MNAR: probability depends on the value itself $f(M|X_{obs}, X_{miss}; \phi) = f(M|X_{miss}; \phi)$
  $\Rightarrow$ Ex, Age Income.

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

Visualization - Multiple Correspondence Analysis





Implemented in VIM, naniar (Matthias Templ, Nick Tierney) - FactoMineR (YouTube): visu pattern, mechanism
To get hint on the missing values pattern)

Recommended methods

$\Rightarrow$ Modify the estimation process to deal with missing values.
Maximum likelihood: EM algorithm to obtain point estimates + Supplemented EM (Meng & Rubin, 1991) or Louis for their variability

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

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

Ex: Logistic regression with missing values SAEM algorithm

```
library(devtools)
install_github("wjiang94/misaem")
```

One specific algorithm for each statistical method...

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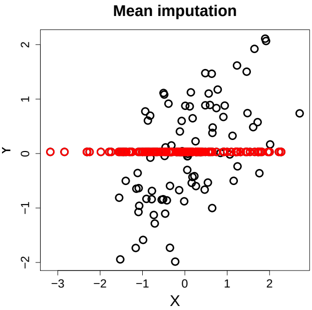
One specific algorithm for each statistical method...

⇒ Imputation (multiple) to get a completed data set on which you can perform any statistical method (Rubin, 1976)

Dealing with missing values

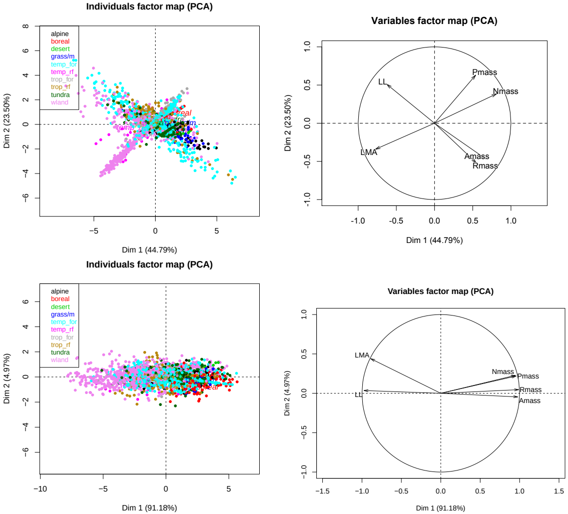
$\Rightarrow$ Imputation to get a completed data set



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

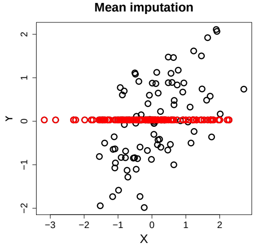
$\hat{\mu}_y = 0.01$
$\hat{\sigma}_y = 0.5$
$\hat{\rho} = 0.30$

Dealing with missing values



Wright IJ, et al. (2004). The worldwide leaf economics spectrum. *Nature*,
69 000 species - LMA (leaf mass per area), LL (leaf lifespan), Amass (photosynthetic assimilation), Nmass (leaf nitrogen), Pmass (leaf phosphorus), Rmass (dark respiration rate)

Imputation methods

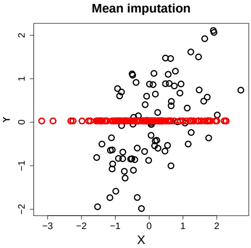


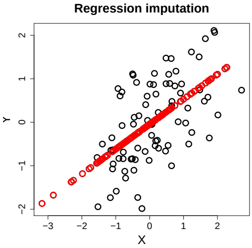
$\mu_y = 0$
$\sigma_y = 1$
$\rho = 0.6$

0.01
0.5
0.30

Imputation methods

- 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.

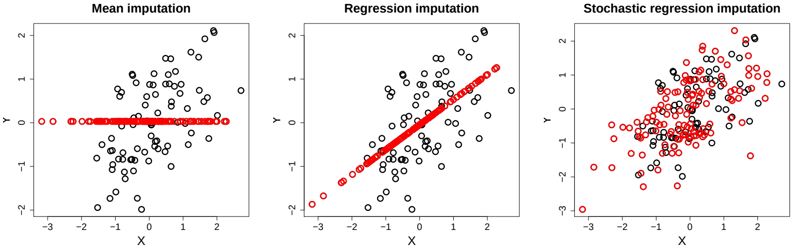




$\mu_y = 0$	0.01	0.01
$\sigma_y = 1$	0.5	0.72
$\rho = 0.6$	0.30	0.78

Imputation methods

- 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



$\mu_y = 0$	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 assuming a joint modeling with gaussian distribution

based on Gaussian assumption: $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$

• Bivariate with missing on $x_{.1}$ (stochastic reg): estimate β and σ
- impute from the predictive $x_{i1} \sim \mathcal{N}\left(x_{i2}\hat{\beta}, \hat{\sigma}^2\right)$
• Extension to multivariate case: estimate μ and Σ from an incomplete data with EM - impute by drawing from $\mathcal{N}\left(\hat{\mu}, \hat{\Sigma}\right)$
equivalence conditional expectation and regression (Ex + lecture notes: complement Schur)

packages `Amelia`, `mice` (conditional)

```
> 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 `VIM`, `yaImpute`, `impute`, etc)
- random forest (package `missForest`)

⇒ Stef van Buuren webpage (mice)
⇒ R miss-tatic Task View
⇒ Statistical Science issue (2018)

⇒ Imputation by PCA

Outline

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 $\Rightarrow$ Do not distort the distances between individuals

PCA (complete)

Find the subspace that best represents the data

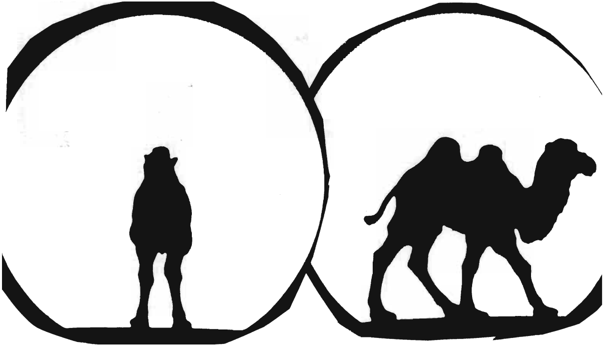


Figure: Camel or dromedary? source J.P. Fénelon

$\Rightarrow$ Best approximation with projection
$\Rightarrow$ Best representation of the variability $\Rightarrow$ Do not distort the distances between individuals

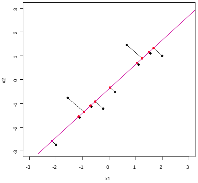
PCA reconstruction

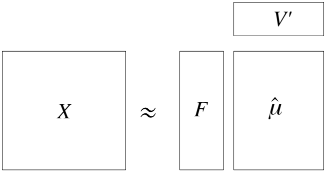
X

-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
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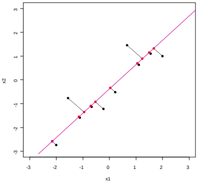

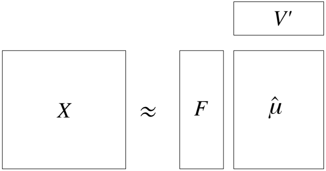

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SVD X: $\hat{\mu}^{\mathrm{PCA}} = U_{n\times S} \Lambda^{\frac{1}{2}}_{S\times S} V'_{p\times S}$ $\quad F = U\Lambda^{\frac{1}{2}}$ PC - scores

$= F_{n\times S} V'_{p\times S}$ $\quad V$ 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

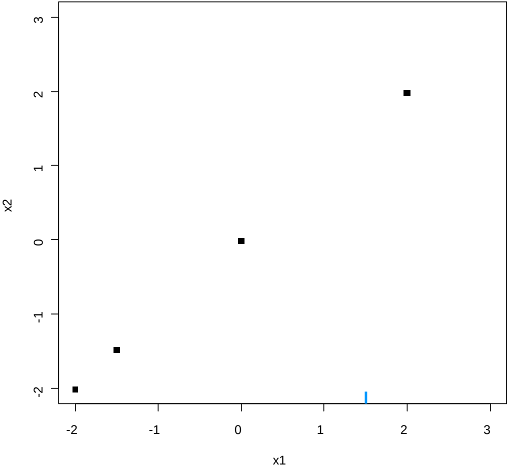
$$\text{argmin}_{\mu} \left\{ \| W_{n \times p} * (X - \mu) \|_2^2 : \text{rank}\,(\mu) \leq S \right\}$$

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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1.5	**NA**
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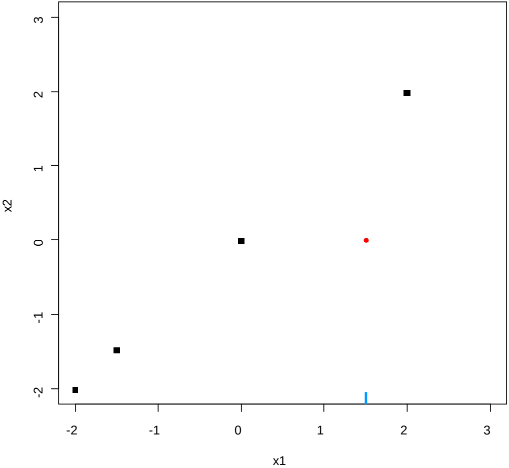

Initialization $\ell = 0$: X^0 (mean imputation)

Iterative PCA

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0.0	-0.01
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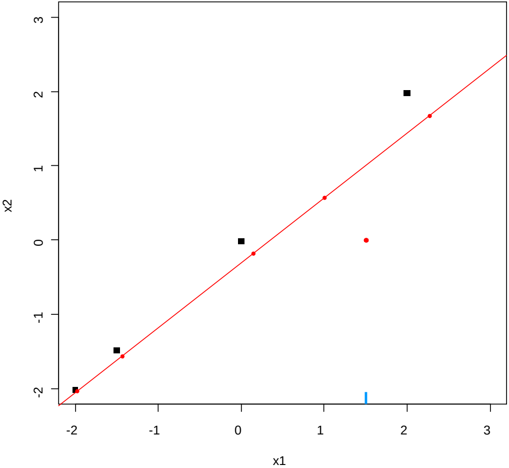
0.0	-0.01
1.5	**0.00**
2.0	1.98

$\widehat{x1}$	$\widehat{x2}$
-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 $\rightarrow (U^\ell, \Lambda^\ell, V^\ell)$;

Iterative PCA

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.00**
2.0	1.98

$\widehat{x1}$	$\widehat{x2}$
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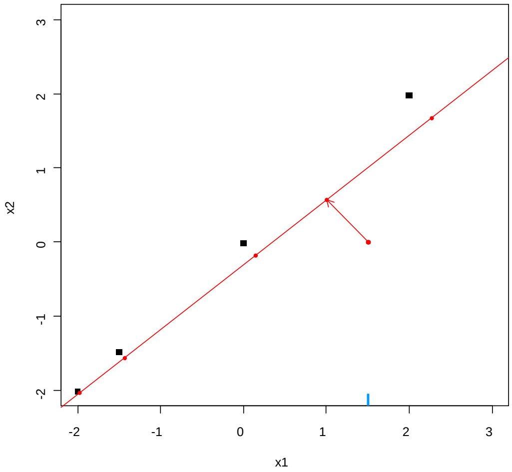
0.15	-0.18
1.00	**0.57**
2.27	1.67



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

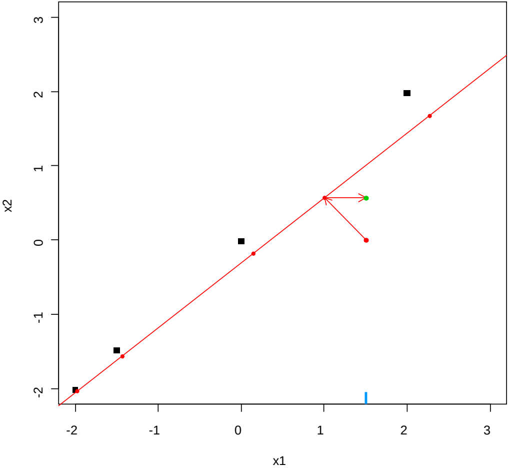
Iterative PCA

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.00**
2.0	1.98

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.57**
2.0	1.98



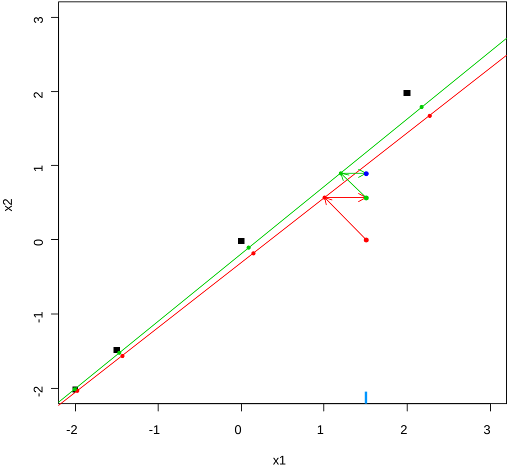
The new imputed dataset is $\hat{X}^{\ell} = W * X + (\mathbf{1} - W) * \hat{\mu}^{\ell}$

Iterative PCA

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.57**
2.0	1.98

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.57**
2.0	1.98



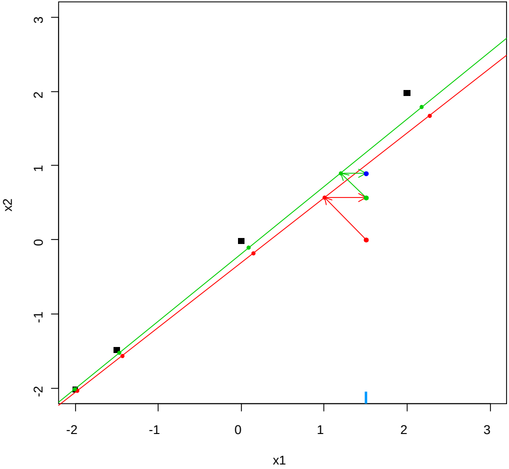
Iterative PCA

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.57**
2.0	1.98

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.90**
2.0	1.98



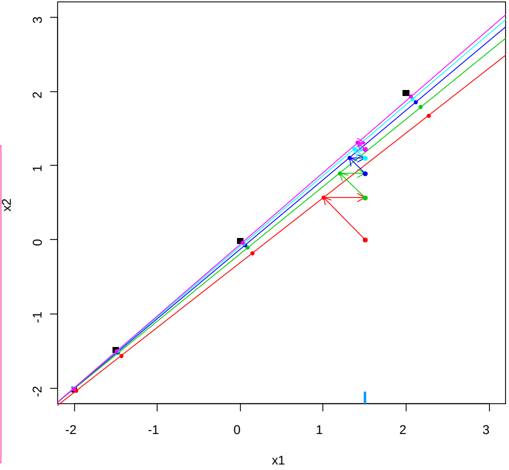
Iterative PCA

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

x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.00**
2.0	1.98

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

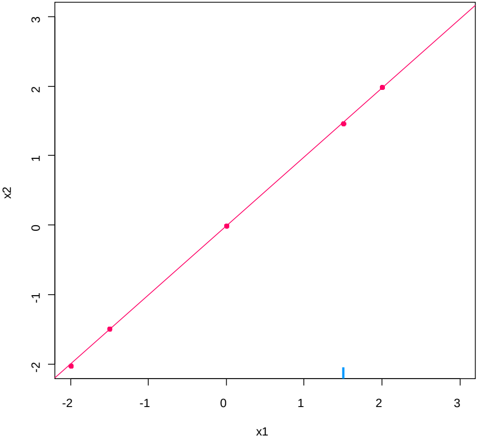
x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**0.57**
2.0	1.98



Steps are repeated until convergence

Iterative PCA

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



x1	x2
-2.0	-2.01
-1.5	-1.48
0.0	-0.01
1.5	**1.46**
2.0	1.98

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

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

$\Rightarrow$ $\hat{\mu}$ from incomplete data: EM algo $X = \mu + \varepsilon, \; \varepsilon_{ij} \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$
with μ of low rank , $x_{ij} = \sum_{s=1}^{S} \sqrt{\tilde{\lambda}_s} \tilde{u}_{is} \tilde{v}_{js} + \varepsilon_{ij}$
$\Rightarrow$ Completed data: good imputation (matrix completion, Netflix)

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

$\Rightarrow$ $\hat{\mu}$ from incomplete data: EM algo $X = \mu + \varepsilon$, $\varepsilon_{ij} \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$
with μ of low rank , $x_{ij} = \sum_{s=1}^{S} \sqrt{\tilde{\lambda}_s} \tilde{u}_{is} \tilde{v}_{js} + \varepsilon_{ij}$

$\Rightarrow$ Completed data: good imputation (matrix completion, Netflix)

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

Selecting S? Generalized cross-validation (J. & Husson, 2012)

Soft thresholding iterative SVD

$\Rightarrow$ Overfitting issues of iterative PCA: many parameters ($U_{n\times S}$, $V_{S\times p}$)/observed values (S large - many NA); noisy data

$\Rightarrow$ Regularized versions. Init - estimation - imputation steps:

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

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

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

SoftImpute for large matrices. T. Hastie, R. Mazumber, 2015, Matrix Completion and Low-Rank SVD via Fast Alternating Least Squares. *JMLR*

Implemented in `softImpute`

Regularized iterative PCA

$\Rightarrow$ 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

⇒ Results of PCA obtained from an incomplete data set: graph of observations and correlation circle. Missing values are skipped $||W * (X - \mu)||^2$

⇒ Very good quality of imputation. Using similarities between individuals and relationship between variables. Popular in machine learning 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)

⇒ Different noise regime

- low noise: iterative PCA (tuning S: cross-validation, GCV)
- moderate: iterative regularized PCA (tuning σ, S)
- high noise (SNR low, S large): soft thresholding (tuning λ, σ)
  Implemented in R packages `denoiseR` (Josse, Wager, Sardy)

The imputed data set should be analysed with caution with other methods

Incomplete ozone

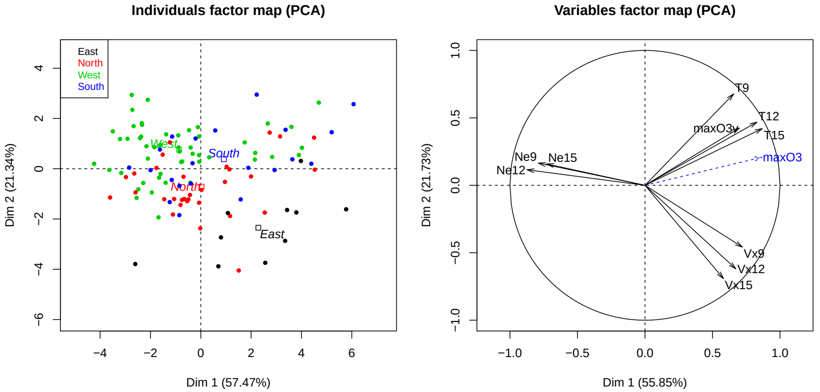
	O3	T9	T12	T15	Ne9	Ne12	Ne15	Vx9	Vx12	Vx15	O3v
0601	87	15.6	18.5	18.4	4	4	8	NA	-1.7101	-0.6946	84
0602	82	NA	18.4	17.7	5	5	7	NA	NA	NA	87
0603	92	NA	17.6	19.5	2	5	4	2.9544	1.8794	0.5209	82
0604	114	16.2	NA	NA	1	1	0	NA	NA	NA	92
0605	94	17.4	20.5	NA	8	8	7	-0.5	NA	-4.3301	114
0606	80	17.7	NA	18.3	NA	NA	NA	-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
```

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)
```

Random Forests versus PCA

	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

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)

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

	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

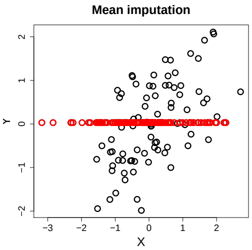
$\Rightarrow$ with Random Forests $\Rightarrow$ with PCA

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

$\Rightarrow$ Non linear relationship well handled by forests

Outline

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

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

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

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

Variance unknown:

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

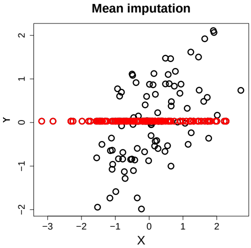
$$\left[\bar{y} - \frac{\widehat{\sigma}_y}{\sqrt{n}} t_{1-\alpha/2}(n-1) \ , \ \bar{y} + \frac{\hat{\sigma}_y}{\sqrt{n}} t_{1-\alpha/2}(n-1)\right]$$

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

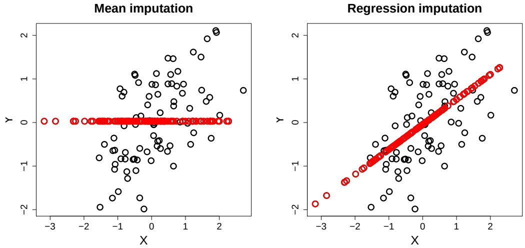
$$\left[\bar{y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}; \bar{Y} - qt_{n-1}\frac{\hat{\sigma}_y}{\sqrt{n}}\right]$$



$\mu_y = 0$	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)*

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

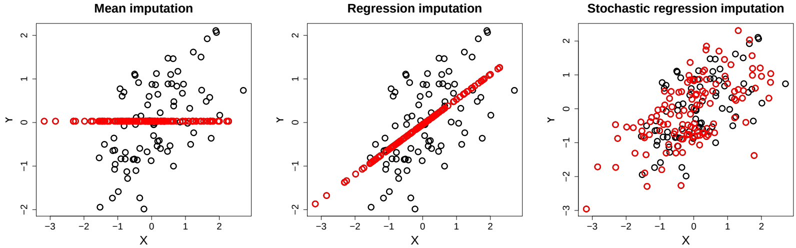


$\mu_y = 0$	0.01	0.01
$\sigma_y = 1$	0.5	0.72
$\rho = 0.6$	0.30	0.78
$CI\mu_y 95\%$	39.4	61.6

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

Single imputation methods

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



	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)*

Single imputation methods

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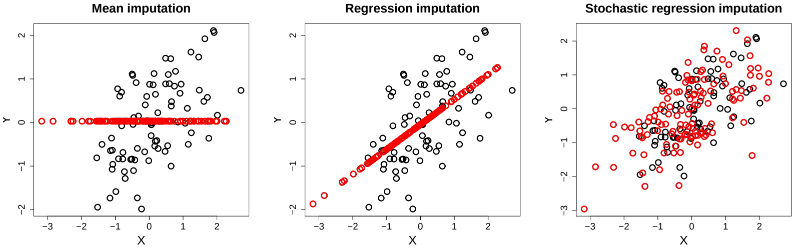

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The idea of imputation is both seductive and dangerous *(Dempster and Rubin, 1983)*

$\Rightarrow$ Standard errors of the parameters ($\hat{\sigma}_{\hat{\mu}_y}$) calculated from the

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):

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

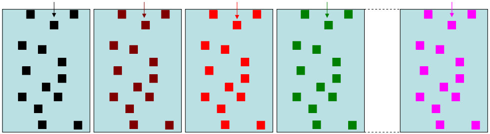
$\Rightarrow$ When the $\rho = 1$, we trust the prediction and the coverage given by stochastic regression is OK.

$\Rightarrow$ 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: $\hat{\theta}_m, \widehat{Var}\left(\hat{\theta}_m\right)$

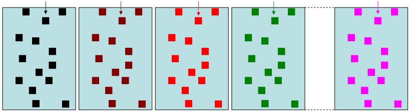
3. Combine the results: $\hat{\theta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\theta}_m$
$$T = \frac{1}{M}\sum_{m=1}^{M}\widehat{Var}\left(\hat{\theta}_m\right) + \left(1+\frac{1}{M}\right)\frac{1}{M-1}\sum_{m=1}^{M}\left(\hat{\theta}_m - \hat{\theta}\right)^2$$

$\Rightarrow$ 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 ⇒ 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)

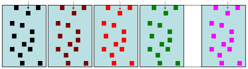
2. Noise: for $m = 1, ..., M$, missing values y_i^m are imputed by drawing from the predictive distribution $\mathcal{N}(x_i\hat{\beta}^m, (\hat{\sigma}^2)^m)$

	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

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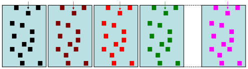
1. Generating M imputed data sets: variance of prediction



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

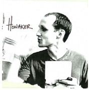
$\Rightarrow$ Hypothesis $x_{i.} \sim \mathcal{N}(\mu, \Sigma)$

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*

Fully conditional modeling

⇒ 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

⇒ 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

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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- Many statistical models are conditional models!
- Tailor to your data
- Appears to work quite well in practice

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

⇒ 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 ⇒ a lot of tuning ... not so easy ...

Multiple imputation with Bootstrap 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: $(\hat{\mu}_{ij})^1, ..., (\hat{\mu}_{ij})^M$
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

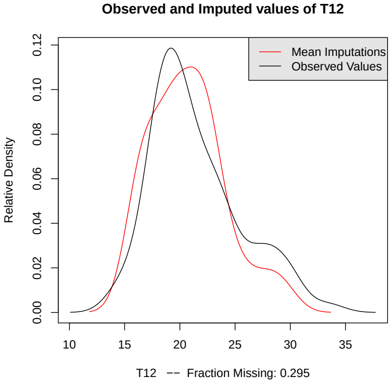
Multiple imputation in practice

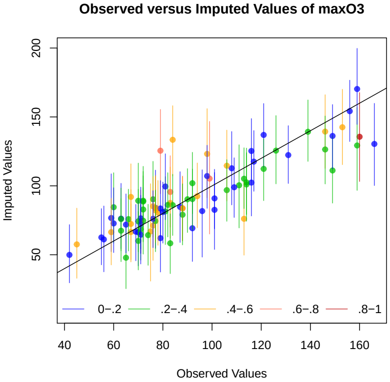
⇒ Step 1: Generate M imputed data sets

```
> 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



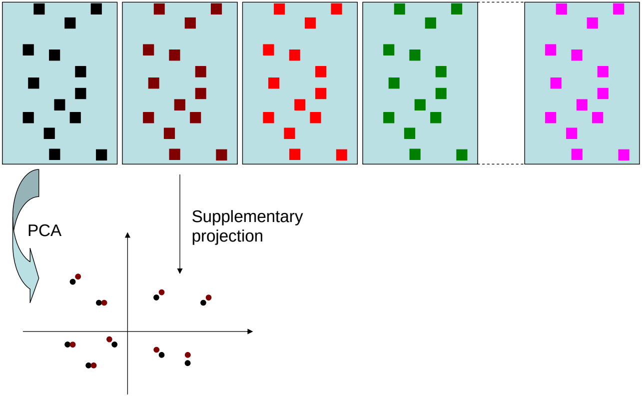



```
# library(Amelia)
> res.amelia <- amelia(don, m = 100)
> compare.density(res.amelia, var = "T12")
> overimpute(res.amelia, var = "maxO3")

# library(missMDA)
```

Multiple imputation in practice

⇒ Step 2: visualization

⇒ Individuals position (and variables) with other predictions

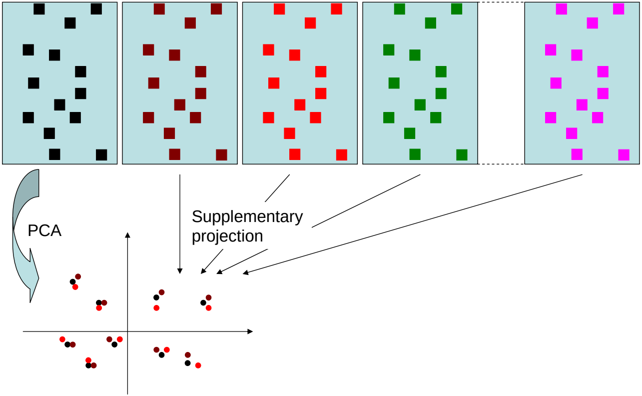


Regularized iterative PCA
⇒ reference configuration

Multiple imputation in practice

⇒ Step 2: visualization

⇒ Individuals position (and variables) with other predictions



Regularized iterative PCA

⇒ reference configuration

Multiple imputation in practice

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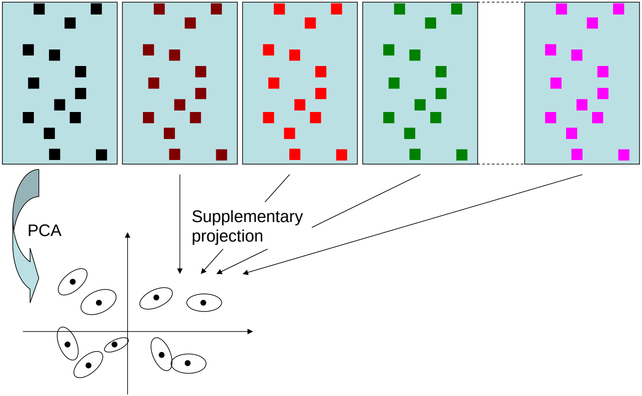
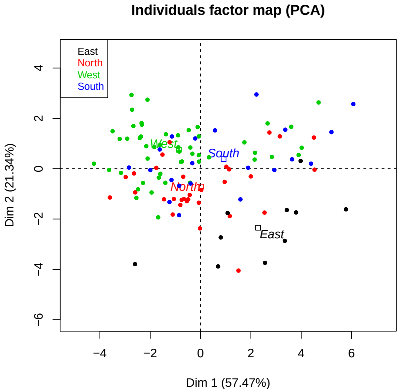
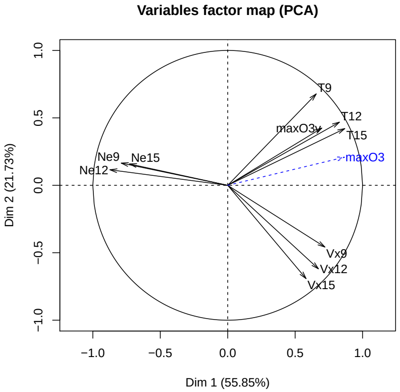


Regularized iterative PCA

⇒ reference configuration

PCA representation



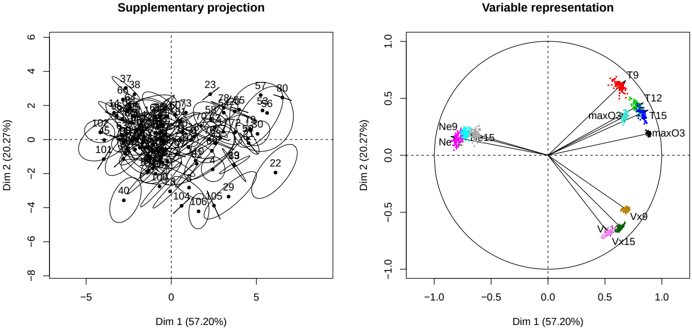



```
> imp <- cbind.data.frame(res.comp$completeObs, ozo[, 12])
> res.pca <- PCA(imp,quanti.sup = 1, quali.sup = 12)
> plot(res.pca, hab =12, lab = "quali"); plot(res.pca, choix = "var")
> res.pca$ind$coord #scores (principal components)
```

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

$\Rightarrow$ 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
```

Outline

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

$$X = \left|\begin{array}{c|c|c} y & \dots & attack \\ y & \dots & attack \\ y & \dots & attack \\ n & \dots & suicide \\ & & \\ & & \\ n & \dots & accident \\ n & \dots & suicide \end{array}\right| \quad A = \left|\begin{array}{cc|c|ccc} 1 & 0 & \dots & 1 & 0 & 0 \\ 1 & 0 & \dots & 1 & 0 & 0 \\ 1 & 0 & \dots & 1 & 0 & 0 \\ 0 & 1 & \dots & 0 & 1 & 0 \\ & & & & & \\ & & & & & \\ 0 & 1 & \dots & 0 & 0 & 1 \\ 0 & 1 & \dots & 0 & 1 & 0 \end{array}\right| \quad D_p = \begin{pmatrix} p_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & p_J \end{pmatrix}$$

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

	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
```

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   (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
```

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   (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)*

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   (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`

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

```
library(missMDA); MIMCA()
```

Multiple imputation for categorical data

⇒ Joint modeling:

- Log-linear model (Schafer, 1997) (cat): pb many levels
- Latent class models (Vermunt, 2014) - nonparametric Bayesian (Si & Reiter, 2014, Murray & Reiter, 2016) (MixedDataImpute, NPBayesImpute, NestedCategBayesImpute)

⇒ Conditional model: logistic, multinomial logit, forests (mice)

⇒ MIMCA provides valid inference (ex. logistic reg with missing) applied to data of various size (many levels, rare levels)

Time (seconds)	Titanic	Galetas	Income
rows-variables-levels	(2000 - 4 - 4)	(1000 - 4 -11)	(6000 - 14 - 9)
MIMCA	2.750	8.972	**58.729**
Loglinear	0.740	4.597	NA
Nonparametric bayes	10.854	17.414	143.652
Cond logistic	4.781	38.016	881.188
Cond forests	265.771	112.987	6329.514

Outline

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 for single & multiple imputation of quanti & categorical data (rare categories): dimensionality reduction and capture similarities between obs and variables. (be careful some implementations do not handle well categorical data)
  $\Rightarrow$ Correct inferences for analysis model based on relationships between pairs of variables
  $\Rightarrow$ SVD can be distributed! Master - Slave, privacy preserving
  $\Rightarrow$ 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 one (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.
  - $\Rightarrow$ Variable selection

$\Rightarrow$ 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 appealing .... but ... with large data?

Ressources implementation

Package missMDA:
http://factominer.free.fr/missMDA/index.html

Youtube: https://www.youtube.com/watch?v=OOM8_FH6_8o&list=PLnZgp6epRBbQzxFnQrcxg09kRt-PA66T_playlist

Article JSS:
https://www.jstatsoft.org/article/view/v070i01