Handling Missing data with Principal Component Analysis

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Seminar on Applied Statistics

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  - Certain variables might have missingness or even only be sporadically observed if their collection was not enforced.

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- Split-questionnaires: to reduce respondent burden, only subsets of questions are asked to individuals

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  - Data: 24-hour recall, self-reported measurement of daily fat intake. Missing data: true fat intake

Sometimes we make up missing data

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- Causal inference: we only observe the outcome under the assigned treatment – what would the outcome be had the subject been assigned to another treatment?
  - One can argue that "potential outcomes" under other treatments are made up missing data as their values never existed, although they could have existed

Data Example: Paris Hospitals

Traumabase (Paris Hospitals): 15000 patients/ 250 variables/ 11 hospitals.

	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	

....

- Predict whether to start a blood transfusion, to administer fresh frozen plasma, etc.
- Study the effect of a treatment on survival.

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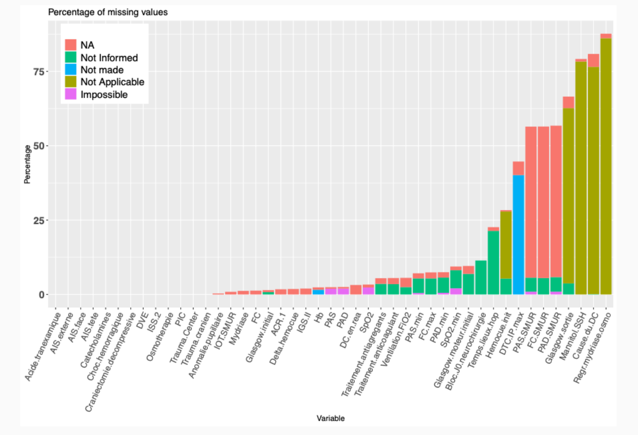

- Missing: Not Recorded, Not Made, Note Applicable, etc.
- Multilevel data/ data integration: systematic missing variable in on hospital

Data Example: Ozone dataset

	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/

Impacts of the missingness

- Loss of non-relevant and/or non-explanatory information
    - Null impact
- Loss of relevant and/or explanatory information
    - Impact depending of proportion of missing values
    - Possible bias in the estimation of the precision and the accuracy

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3. Design method that handle missing values.

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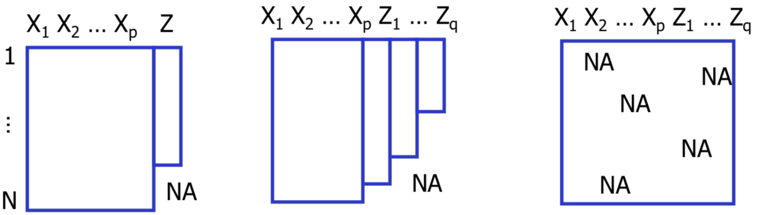
Pattern of missing data:



Univariate Monotone General (non-monotone)

Missing data mechanisms

Let $X = (X_{obs}, X_{miss})$ a complete data model. Assume $X = (X_1, \ldots, X_p)$. Let $M = (M_{ik})$, $1 \leq i \leq p$, $1 \leq k \leq n$ where

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- **MNAR:** the probability of being missing varies for reasons that are unknown to us. For example, in public opinion research occurs if those with weaker opinions respond less often. MNAR is the most complex case.

Missing data mechanisms: example

Age	Income (Inc)	M_{Age}	M_{Inc}
24	1500	1	1
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29	4200	1	1
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- If the observations are MNAR, the missingness of the Income depends on the Income itself and may depend on the Age. A possible interpretation is that very rich or poor people are less likely to give their incomes.

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  - MAR vs MNAR?: not possible based on your observed data – MNAR mechanisms depend on data that are not observed
  - The data analyst must adopt an assumption about the mechanism without being able to verify it
- Inference under MNAR is more realistic but more complicated. Most approaches for inference with missing data assume MAR.

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Maximum Likelihood estimation:

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

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If the data are **MAR** (or **MCAR**),

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Ignorable missing values

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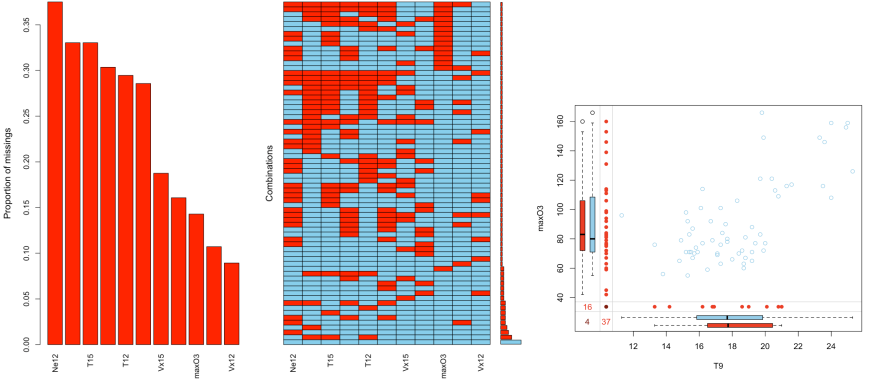
MAR is the minimal property to access the likelihood of missing data.

Contents

Visualization

- It is crucial to perform some descriptive statistics (how many missing? how many variables, individuals with missing?) and try to inspect and vizualize the pattern of missing entries and get hints on the mechanism that generated the missingness.



R package: VIM (M. Templ), naniar (N. Tierney), FactoMineR (Husson *et al.*).

Methods for handling missing values

1. Simple methods:

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Complete-Case Analysis

Idea: discard observations with missingness, run intended analysis with remaining data.

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Gender	Age	Income	...
F	25	60,000	...
M	?	?	...
?	51	?	...
F	?	150,300	
...	...	...	...

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    - Example: suppose we are interested in estimating the median income of the some population. We send out an email asking a questionnaire to be completed, amongst which participants are asked to say how much they earn. But only a proportion of the target sample return the questionnaire, and so we have missing incomes for the remaining people. If those that returned an answer to the income question have systematically higher or lower incomes than those who did not return an answer, the median income of the complete cases will be biased.

Mean Imputation

Impute mean of observed values:

Age	*Income*
25	60,000
?	?
51	?
?	150,300
$\vdots$	$\vdots$

$\Longrightarrow$

Age	*Income*
25	60,000
$\hat{\mu}^1_{Age}$	$\hat{\mu}^1_{Income}$
51	$\hat{\mu}^1_{Income}$
$\hat{\mu}^1_{Age}$	150,300
$\vdots$	$\vdots$

Mean Imputation

- Consider n couples $(X_1, Y_1), \ldots, (X_n, Y_n)$ where $X_i \sim \mathcal{N}(\mu_X, \sigma_X^2)$ and $Y_i \sim \mathcal{N}(\mu_Y, \sigma_Y^2)$.
- 70% of missing entries completely at random on Y.
- Simulated data: $n = 300$, $\mu_X = \mu_Y = 0$, $\sigma_X = \sigma_Y = 1$, $\rho_{XY} = 0.7$.

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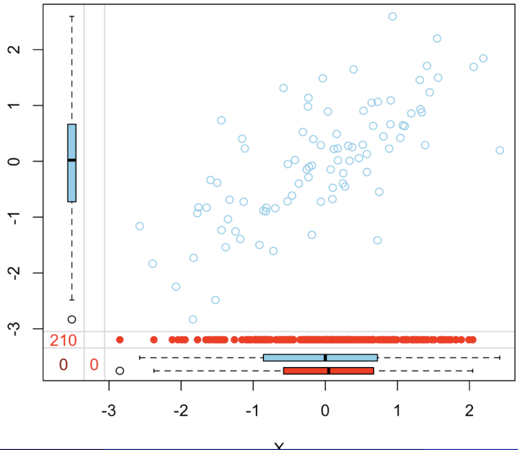

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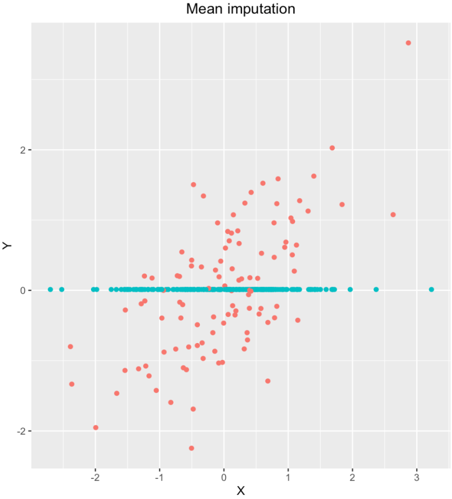

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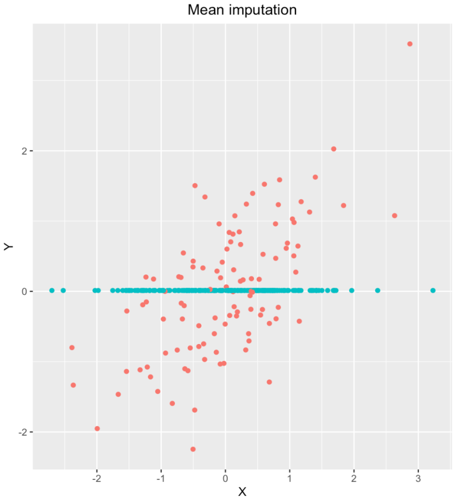

- preserve the mean of the imputed variable,

$$\mu_Y = 0 \qquad \hat{\mu}_Y = 0.02$$
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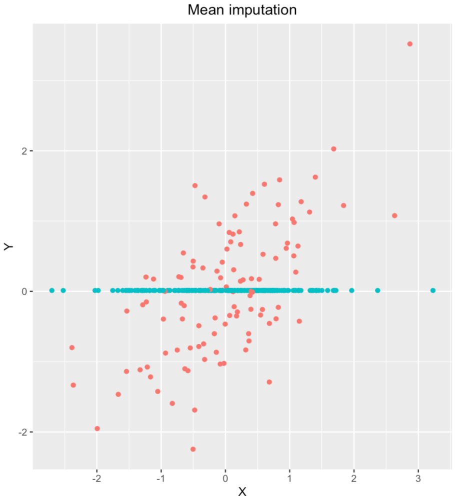

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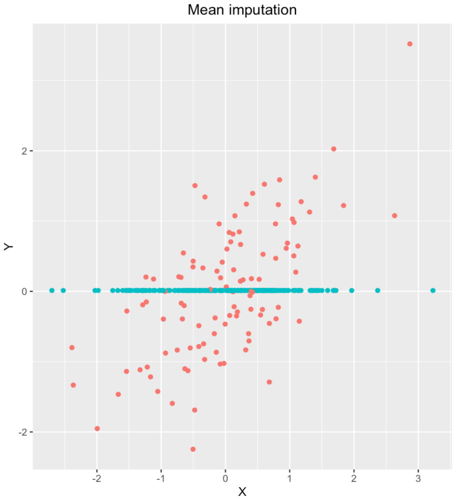

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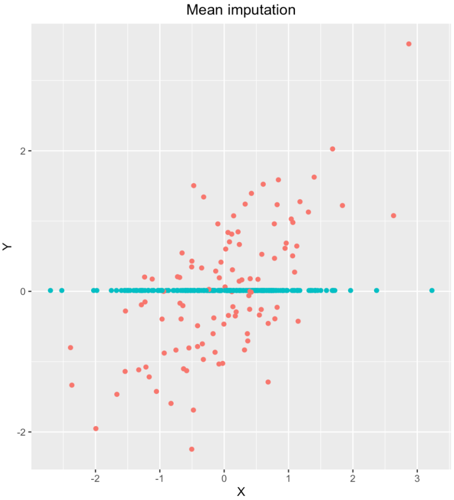

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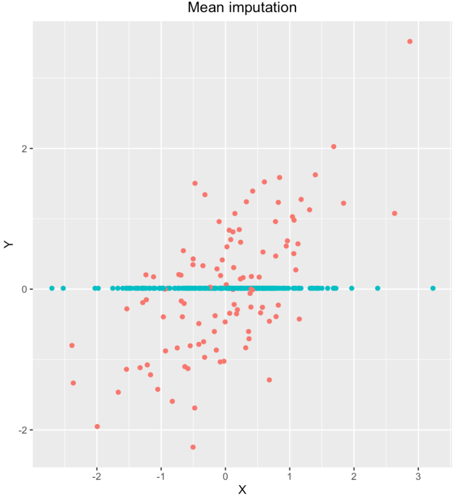

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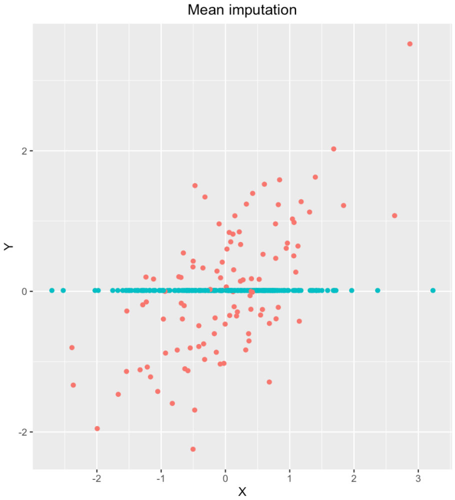

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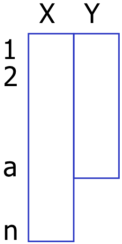
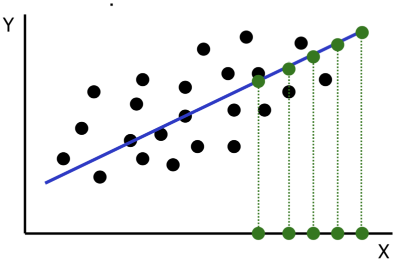
- Validity depends on model used for imputation

Regression Imputation

- Example: simple linear regression





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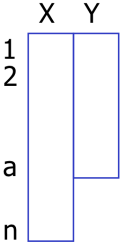

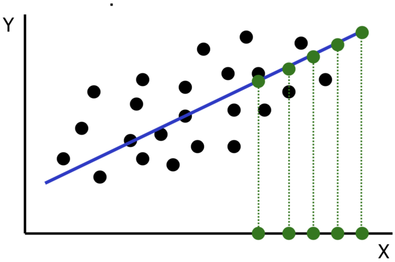

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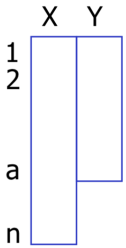

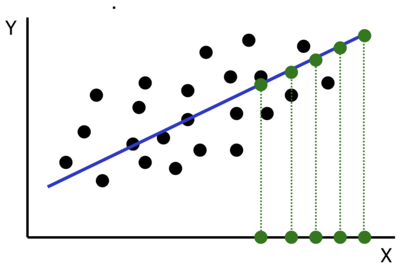

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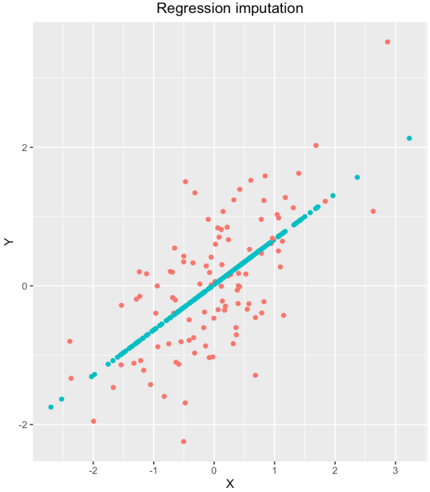

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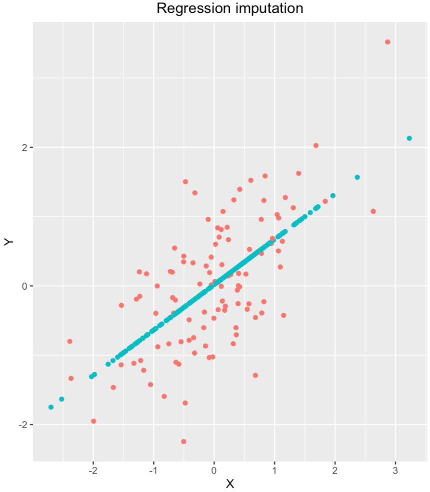

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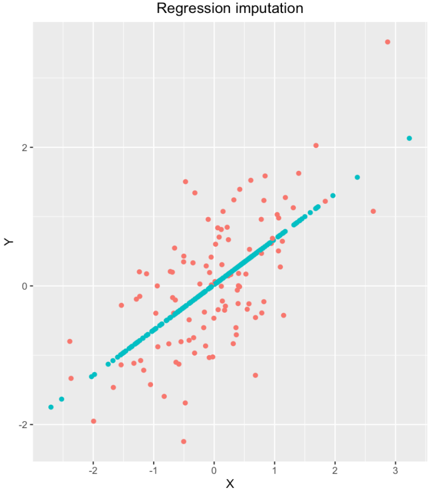

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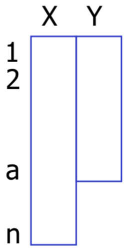
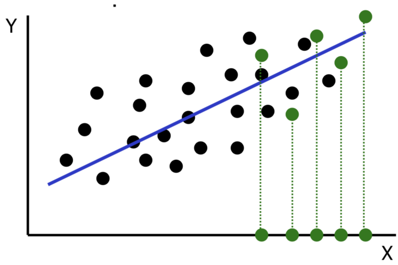
Stochastic Regression Imputation

- Estimate the coefficients β_0, β_1 and the variance σ^2, then impute from the predictive $Y_i \sim \mathcal{N}(\hat{\beta}_0 + \hat{\beta}_1 x_i, \hat{\sigma}^2)$





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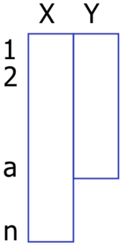

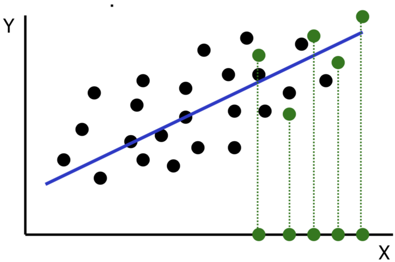

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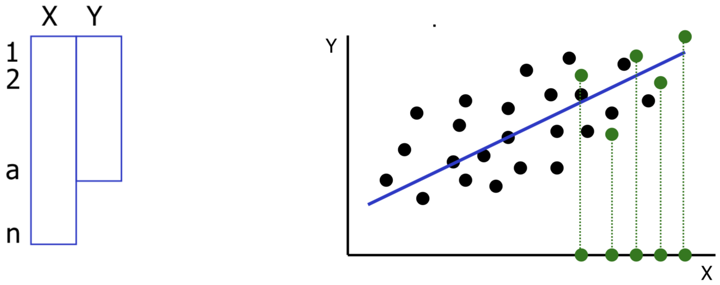

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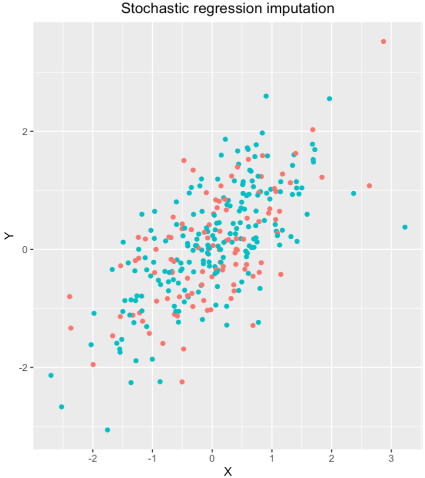
Regression Imputation



- Stochastic regression imputation preserve distribution

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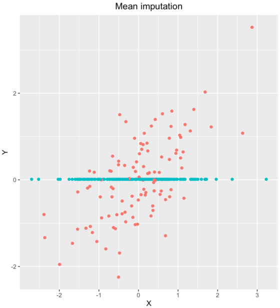
Single Imputation with means and regression: summary



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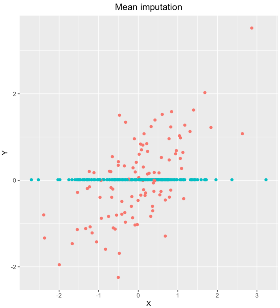

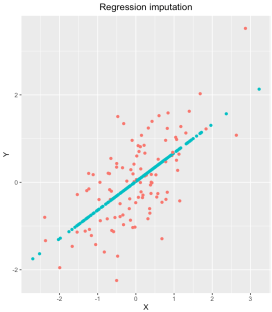

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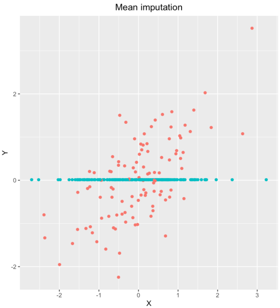

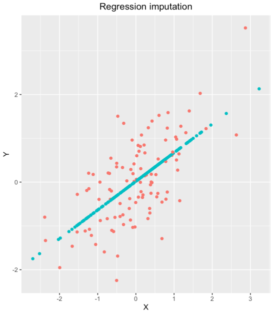

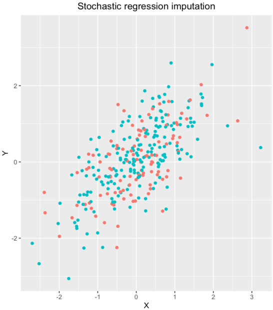

	Mean imputation	Regression imputation	Stochastic regression imputation
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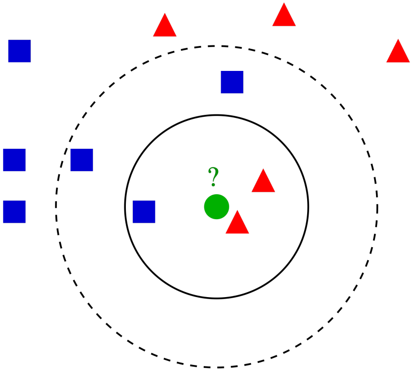
Imputation with K-Nearest Neighbors

- **Idea**: The missing value is replaced by an observed value of an individual having similar characteristics.
  - similar characteristics $\Leftrightarrow$ "nearest neighbor"
    - determine an appropriate distance function on one or multiple auxiliary variables



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ID	Height	Age	Weight
1	5	45	77
2	5.11	26	47
3	5.6	30	55
4	5.9	34	59
5	4.8	40	72
6	5.8	36	60
7	5.3	19	40
8	5.8	28	60
9	5.5	23	45
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11	5.5	38	?

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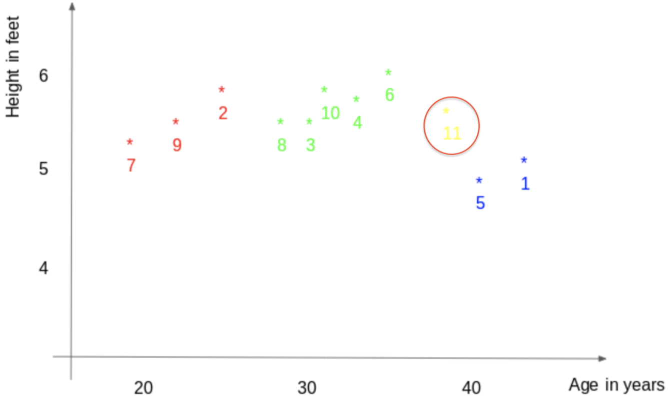
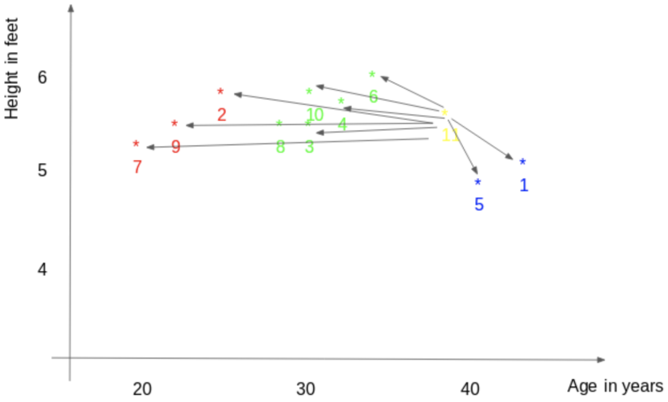


KNN: example

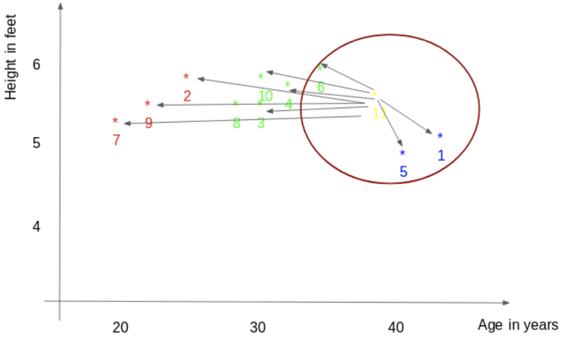
Step 1: Calculate the distance.

- Euclidean distance: $d(x, y) = \sqrt{\sum_{j=1}^{p} (x_j - y_j)^2}$ for two vectors $x = (x_1, \ldots, x_p)$ and $y = (y_1, \ldots, y_p)$.



KNN: example

Step 2 & 3: Determine the k nearest neighbors (k closes points) based on the distance and compute the predicted value for $ID11$.
If we choose $k = 3$: $ID11 = (77 + 72 + 60)3 = 69.66$.



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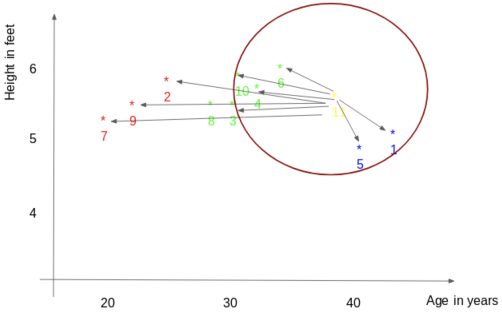

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- As this quantity cannot be computed explicitly in general cases, the EM algorithm finds the MLE by iteratively maximizing the expected complete-data log-likelihood. Denote the complete-data log-likelihood as

$$L_{comp}(\theta; X) = \log f(X_{obs}, X_{miss}; \theta).$$

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- **M step (maximization):** Determine $\theta^{(t+1)}$ by maximizing the function Q

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta, \theta^{(t)}).$$

Convergence criterion: $|\hat{\theta}^{(t)} - \hat{\theta}^{(t-1)}| \leq \epsilon$.

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Implementation in **R**: package norm

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- Best approximation of the data with projection.
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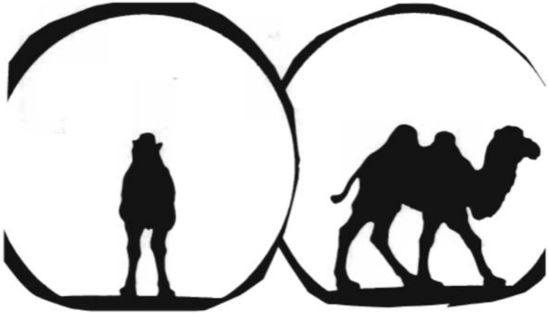

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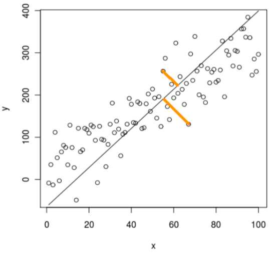
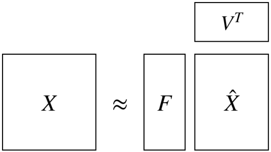
PCA reconstruction





- Minimizes distance between observations and their projections.
- Approximate the matrix $X_{n \times p}$ with a low rank matrix $S < p$ in the least square sense ($\| \cdot \|$ the Frobenius norm: $\|X\|_2^2 = tr(XX^T)$):

$$\operatorname{argmin}_Q \left\{ \|X_{n \times p} - Q_{n \times p}\|_2^2 : rank(Q) \leq S \right\}.$$

- The PCA solution (Eckart & Young, 1936) is the truncated singular value decomposition (SVD) of X at the order S:

$$\hat{X} = U_{n \times S} \Lambda_{S \times S}^{1/2} V_{S \times p}^T = F_{n \times S} V_{S \times p}^T.$$

$F = U\Lambda^{1/2}$: PC scores; V: principal axes - loadings.

PCA with missing values

- PCA complete: least squares criterion

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Algorithms: weighted alternating least squares (Gabriel and Zamir, 1979); iterative PCA (Kiers, 1997). See Josse and Husson[1], 2012 for more references.

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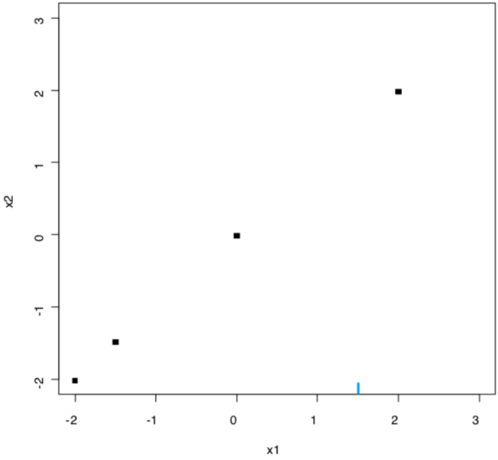
   (b) compute the fitted matrix $(\hat{X}_{ij}^{S})^{(t)} = U^{(t)} {\Lambda^{(t)}}^{1/2} {V^{(t)}}^{T}$ and define the new imputed data as $X^{(t)} = W \odot X + (\mathbf{1}_{n\times p} - W) \odot (\hat{X}_{ij}^{S})^{(t)}$, where $\mathbf{1}_{n\times p}$ is a matrix filled with ones. The observed values are the same and the missing ones are replaced by the fitted values.
3. Repeat steps (2a) and (2b) until the change in the imputed matrix smaller than a given threshold, for instance $\sum_{ij} \left(\hat{X}_{ij}^{(t)} - \hat{X}_{ij}^{(t-1)}\right)^2 \leq \epsilon$.

Selection of the number of dimensions S: Cross-Validation.

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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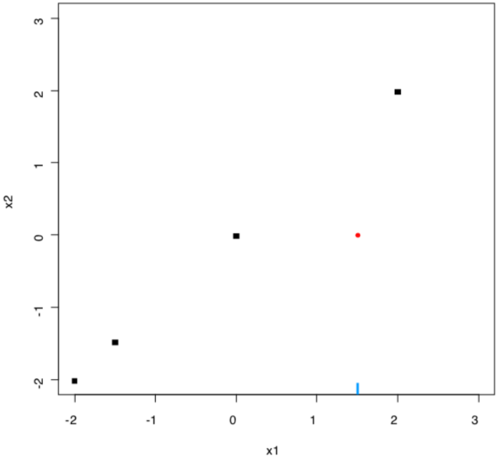


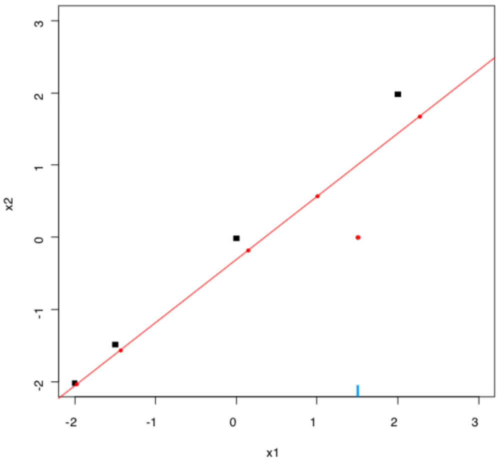
Initialization $t = 0$: $X^{(0)}$ (mean imputation)

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



PCA on the completed dataset: $(U^{(t)}, \Lambda^{(t)}, V^{(t)})$

Iterative PCA

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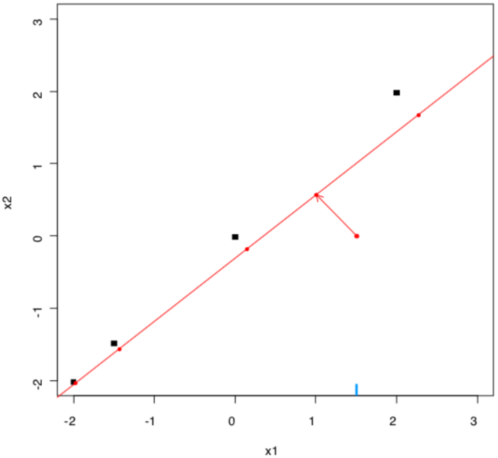

Missing values imputed with the fitted matrix $\hat{X}^{(t)} = U^{(t)} {\Lambda^{(t)}}^{1/2} {V^{(t)}}^{T}$

Iterative PCA

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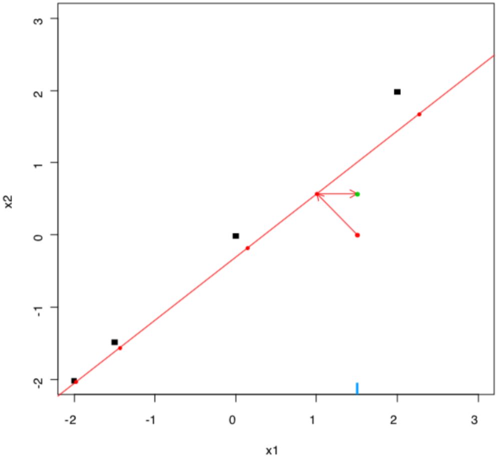

The new imputed dataset is $X^{(t)} = W \odot X + (\mathbf{1}_{n\times p} - W) \odot \hat{X}^{(t)}$

Iterative PCA

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-1.5	-1.48
0.0	-0.01
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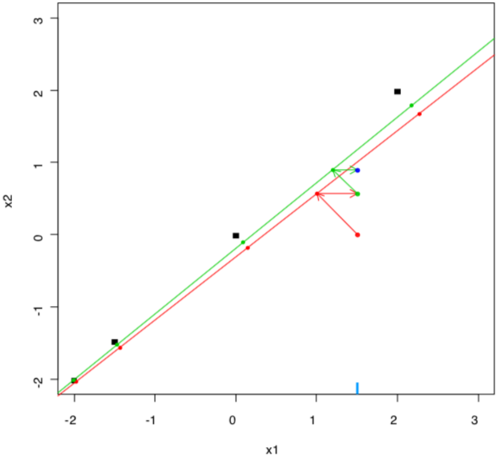

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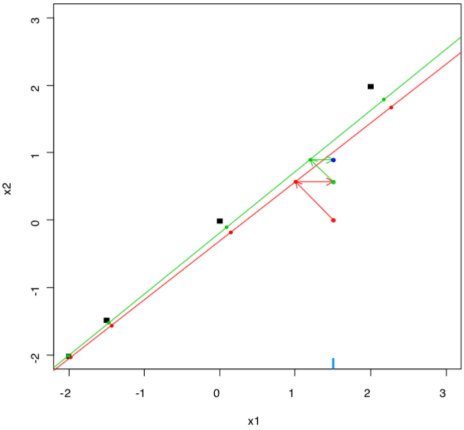
0.0	-0.01
1.5	**0.57**
2.0	1.98

$\widehat{x1}$	$\widehat{x2}$
-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



PCA on the completed dataset: $(U^{(t+1)}, \Lambda^{(t+1)}, V^{(t+1)})$

Missing values imputed with the fitted matrix $\hat{X}^{(t+1)} = U^{(t+1)} {\Lambda^{(t+1)}}^{1/2} {V^{(t+1)}}^{T}$

Iterative PCA

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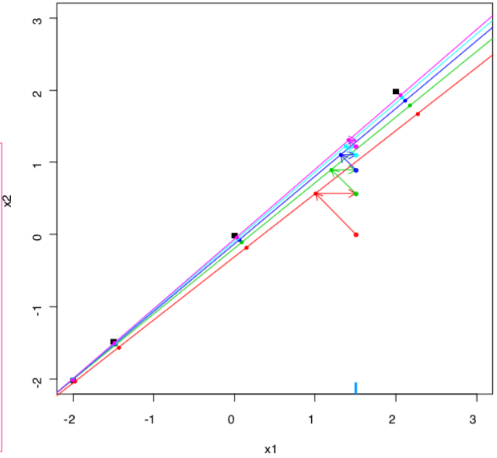

Steps are repeated until convergence

Selection of S: Cross-Validation

- Review of of six methods of cross-validation in PCA: Bro *et al.*[2](2008).

[2] Bro, R., Kjeldahl, K., Smilde, A.K., Kiers. Cross-validation of component model: a critical look at current methods. Analytical and Bioanalytical Chemistry 390, 1241–1251.

Selection of S: Cross-Validation

- Review of of six methods of cross-validation in PCA: Bro *et al.*[2](2008).
- Criterion using the mean square error of prediction (MSEP):

$$MSEP(S) = \frac{1}{np} \sum_{i=1}^{n} \sum_{j=1}^{p} \left(X_{ij} - (\hat{X}_{ij}^{S})^{-ij} \right)^2.$$

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Estimate $(\hat{X}^{S})^{-ij}$ for fixed S and each $(i,j) \Rightarrow$ computational burden.

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- In a regression, denote a linear fitting method as $\hat{y} = Py$ with y a response vector and P a smoothing matrix. Craven & Whaba (1979) have shown

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

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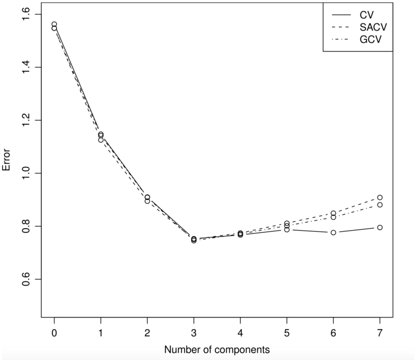
- Write PCA as $\hat{X}^S = PX$, we get

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

[2] Bro, R., Kjeldahl, K., Smilde, A.K., Kiers. Cross-validation of component model: a critical look at current methods. Analytical and Bioanalytical Chemistry 390, 1241–1251.

Cross-validation approximations



MSEP for cross-validation:

$$CV(S) = \frac{1}{np}\sum_{i=1}^{n}\sum_{j=1}^{p}\left(X_{ij} - (\hat{X}_{ij}^{S})^{-ij}\right)^2$$

Smoothing approximation of cross-validation (SACV) and Generalized CV (Josse & Husson[3], 2012):

$$SACV(S) = \frac{1}{np}\sum_{i=1}^{n}\sum_{j=1}^{p}\left(\frac{X_{ij} - \hat{X}_{ij}^{S}}{1 - P_{ij,ij}}\right)^2$$

$$GCV(S) = \frac{1}{np}\frac{\sum_{i=1}^{n}\sum_{j=1}^{p}\left(X_{ij} - \hat{X}_{ij}^{S}\right)^2}{(1 - tr(P)/np)^2}$$

R package: missMDA

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

Overfitting

Overfitting occurs when:

- Many parameters are estimated with respect to the number of observed values (the number of dimensions S and of missing values are important).
- Data are very noisy.

$\Rightarrow$ Trust to much the relationship between variables.

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Solution: Shrinkage methods.

Regularized iterative PCA[4]

The imputation step:

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

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

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

with σ^2 estimated by

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

R package: missMDA (F. Husson, J. Josse).

[3] J Josse, J Pagès, and F Husson. Gestion des données manquantes en analyse en composantes principales. Journal de la Société Française de Statistique, 150:28–51, 2009.

Soft thresholding SVD

We replace the imputation step $\hat{X}_{ij} = \sum_{s=1}^{S} \sqrt{\lambda_s} u_{is} v_{js}$ by a "shrunk" imputation step

$$\hat{X}_{ij}^{Soft} = \sum_{s=1}^{p} (\sqrt{\lambda_s} - \lambda)_+ u_{is} v_{js},$$

where $\hat{X}^{Soft}$ is the closed form solution to

$$\underset{Q}{\operatorname{argmin}} \left\{ \| W \odot (X - Q) \|_2^2 + \lambda \| Q \|_\star \right\},$$

where the nuclear norm $\|Q\|_\star$ is the sum of the singular values of Q.

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R package: softImpute (T. Hastie *et al.*, 2015, Matrix Completion and Low-Rank SVD via Fast Alternating Least Squares. JMLR)

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Selection of λ:

- Josse & Sardy, Adaptive shrinkage of singular values, Stat Comput, 2015.
- Josse & Wager, Bootstrap-Based Regularization for Low-Rank Matrix Estimation, JMLR, 2016.
- Gavish & Donoho, Optimal Shrinkage of Singular Values, 2016.

Implementation in R: package denoiseR (Josse, Wage, Sardy, denoiseR: A Package for Low Rank Matrix Estimation, 2018).

Single imputation with PCA: summary

- Impute large datasets of different dimensions with continuous, categorial variables:
  - reduce the dimensionality,
  - takes into account the similarities between individuals and the relationships between variables.
- Imputations with PCA are good for strong linear relationships.
- Tunning parameter: number of components S.

Contents

Why multiple imputation?

"Imputing one value for a missing datum cannot be correct in general, because we don't know what value to impute with certainty (if we did, it wouldn't be missing)." (Donald B. Rubin)

Single imputation cannot take into account the variability of the missing values prediction
$\Rightarrow$ underestimation of the variability
$\Rightarrow$ confidence intervals and tests that are not valid even if the imputation model is correct.

Solution: Multiple imputation.

Single imputation: confidence interval for mean

CI 95% for μ_Y:

$$\left[\bar{y} - t_{n-1}^{0.025} \times \frac{\hat{\sigma}_Y}{\sqrt{n}}\,;\, \bar{y} - t_{n-1}^{0.025} \times \frac{\hat{\sigma}_Y}{\sqrt{n}}\right]$$

Compute the coverage of the confidence interval for μ_Y.

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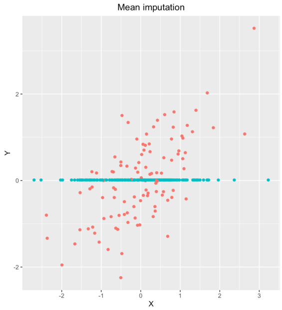

$\mu_Y = 0$ $\quad \hat{\mu}_Y = 0.02$

$\sigma_Y = 1$ $\quad \hat{\sigma}_Y = 0.58$

$\rho = 0.7$ $\quad \hat{\rho} = 0.43$

CI 95% $\quad$ 42.9%

Single imputation: confidence interval for mean

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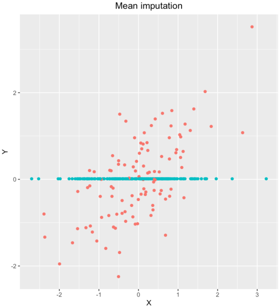

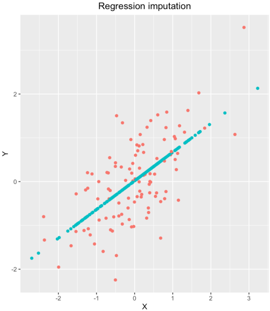

	Mean imputation	Regression imputation
$\mu_Y = 0$	$\hat{\mu}_Y = 0.02$	$\hat{\mu}_Y = 0.04$
$\sigma_Y = 1$	$\hat{\sigma}_Y = 0.58$	$\hat{\sigma}_Y = 0.81$
$\rho = 0.7$	$\hat{\rho} = 0.43$	$\hat{\rho} = 0.86$
CI 95%	42.9%	66.4%

Single imputation: confidence interval for mean

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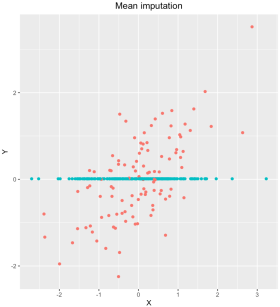
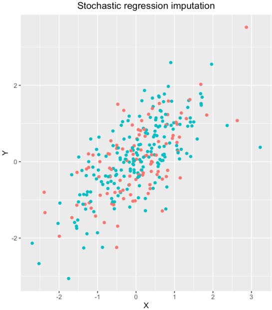
$$\left[\bar{y} - t_{n-1}^{0.025} \times \frac{\hat{\sigma}_Y}{\sqrt{n}} \; ; \; \bar{y} - t_{n-1}^{0.025} \times \frac{\hat{\sigma}_Y}{\sqrt{n}}\right]$$

Compute the coverage of the confidence interval for μ_Y.





	Mean imputation	Regression imputation	Stochastic regression imputation
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Single imputation: confidence interval for mean

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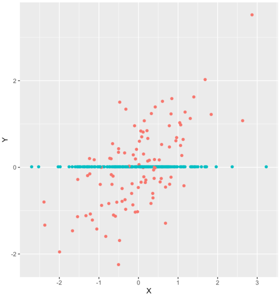
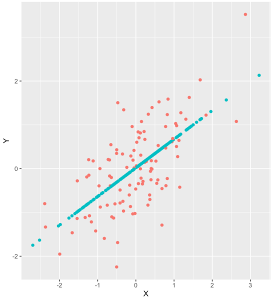
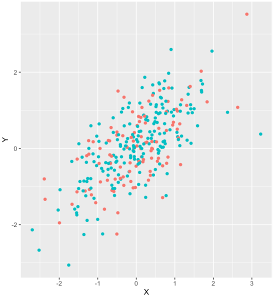
Mean imputation



Regression imputation



Stochastic regression imputation



	Mean imputation	Regression imputation	Stochastic regression imputation
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$\Rightarrow$ Standard errors calculated from the imputed data are underestimated

Multiple imputation

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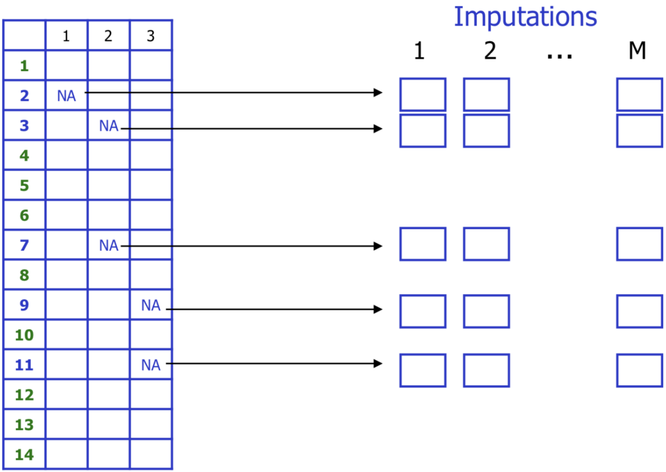
  - to preserve the important relations between the variables
- The goals is not
  - to predict the missing values with the greatest precision
  - to describe the data in the best possible way

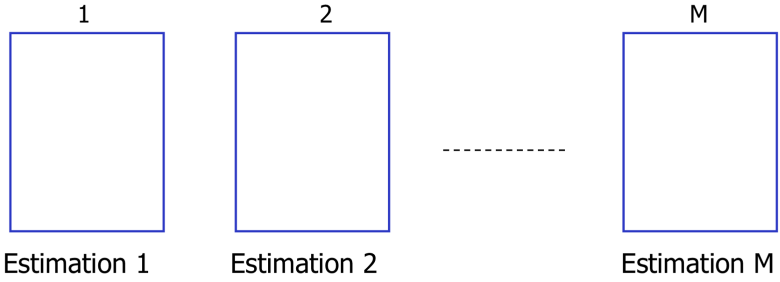
Multiple imputation: Step 1

- Generate $M > 1$ plausible for each missing value (*i.e.* M completed datasets).



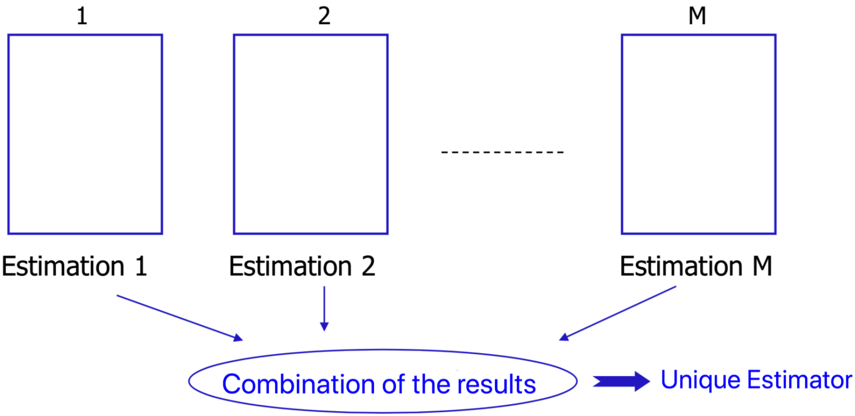
Multiple imputation: Step 2

- Perform independently the analysis on each imputed dataset: $\hat{\theta}_m$, $\widehat{\mathbb{V}ar}(\hat{\theta}_m)$.



Multiple imputation: Step 3

- Combine the results (Rubin's rules).



Multiple imputation: Step 3

- Combine the results (Rubin's rules).

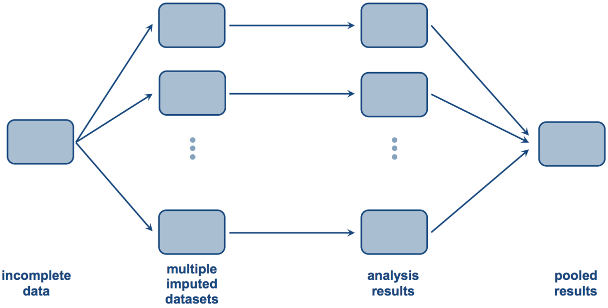
$$\hat{\theta} = \frac{1}{M} \sum_{m=1}^{M} \hat{\theta}_m,$$

$$\widehat{\mathbb{V}ar}(\hat{\theta}) = \frac{1}{M} \sum_{m=1}^{M} \widehat{\mathbb{V}ar}(\hat{\theta}_m) + \left(1 + \frac{1}{M}\right) \frac{1}{M-1} \sum_{m=1}^{M} \left(\hat{\theta}_m - \hat{\theta}\right)^2 .$$

Variance $=$ Within $+$ Between imputation variance

$\Rightarrow$ variability of missing values taken into account.

Multiple imputation: Summary



Three steps:

1. **Imputation:** impute multiple times to get multiple completed datasets.
2. **Analysis:** analyse each of the datasets.
3. **Pooling:** combine results, taking into account additional uncertainty.

R packages for missing data imputation

- Imputations with Random Forests (RF): missForest (Daniel J. Stekhoven).
  ⇒ Good for non-linear relationships between continuous variables and when there are interactions.
- Imputations for Categorical data/Mixed/Multi-Blocks/MultiLevel: Multiple Correspondence Analysis (MCA)/ Regularized iterative MCA. R package: missMDA (Husson & Josse).
- Time Series imputation: imputeTS package (Steffen Moritz).

R packages for missing data imputation

- See Missing values taskview[5] (Julie Josse, Nicholas Tierney, Nathalie Vialaneix).
  - Single imputation:
    - *k-nearest neighbors:* DMwR, impute, VIM, wNNSel (for imputation in large dimensional datasets)
    - *regression based imputations:* VIM (linear regression based imputation in the function `regressionImp`), imputation
    - *Based on random forest:* missForest
    - *PCA/Singular Value Decomposition/matrix completion:* missMDA, softImpute
  - Multiple imputation: Amelia, mice, missMDA, miceMNAR
  - Specific application fields: visit Missing values taskview for further information.

[5] https://cran.r-project.org/web/views/MissingData.html

Contents

References

This talk relies mainly on the following sources:

Julie Josse. Course at École de recherche à Aussois 2018. http://juliejosse.com/

Marie Davidian. Course at NC State University, spring 2017. https://www4.stat.ncsu.edu/~davidian/st790/index.html

Stef van Buuren. Flexible Imputation of Missing Data, 2nd edition. Chapman & HallCRC, 2018. https://stefvanbuuren.name/fimd/

J. Josse and F. Husson. *Selecting the number of components in principal component analysis using cross-validation approximations*. Computational Statistics and Data Analysis, 56 (2012) 1869–1879.