Distributed multilevel matrix completion for medical databases

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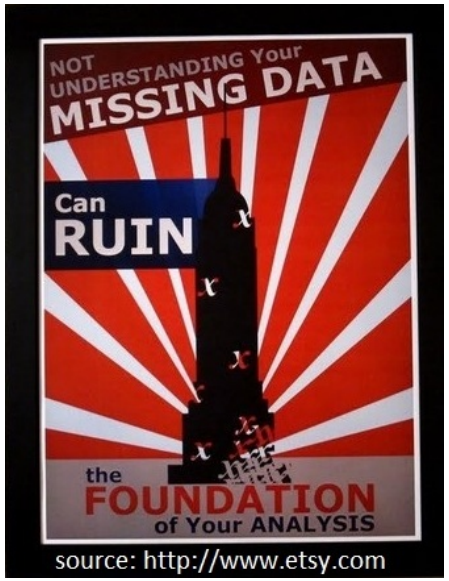

January 15, 2018

Overview

Outline

Collaborators

Imputation of mixed data with multilevel SVD
Distributed computation

Genevieve Robin, François Husson, Balasubramanian Narasimhan

Polytechnique, Agrocampus, Stanford (stat/biomedical)



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 with categorical/continuous values

Public Assistance - Paris Hospitals

Traumabase: 15000 patients/ 250 variables/ 6 hospitals

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

$\Rightarrow$ (Logistic) regressions with missing categorical/continuous values

Public Assistance - Paris Hospitals

⇒ 6 hospitals: multilevel structure (patients within hospital)

Hopital effect: lack of standardization

⇒ Missing values

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1            Beaujon        Fall    54    m    85     NR    NR 180 110
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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
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9               HEGP   White weapon 16    m    98   1.92 26.58 118  54
...................

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```

1) Handling missing values in multilevel data

Public Assistance - Paris Hospitals

⇒ 6 hospitals: multilevel structure (patients within hospital)

Hopital effect: lack of standardization

2) Data not aggregated but which stay on each site

⇒ Missing values

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```

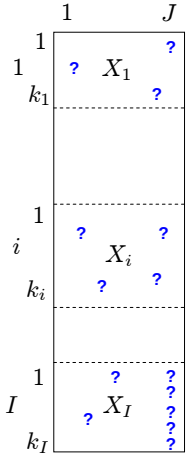
1) Handling missing values in multilevel data

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.

$\Rightarrow$ Still an issue with "big data"
Data integration: data from different sources



Multilevel structure: sporadically - systematic missing values (one variable missing in one hospital)

Solutions to handle missing values

Litterature: Schaefer (2002); Little & Rubin (2002); Gelman & Meng (2004); Kim & Shao (2013); Carpenter & Kenward (2013); van Buuren (2015)

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

$\Rightarrow$ Imputation (multiple) to get a completed data set on which you can perform any statistical method (Rubin, 1976)
Famous imputation based on SVD (PCA) - quantitative

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Famous imputation based on SVD (PCA) - quantitative

Extension to imputation with multilevel SVD

Outline

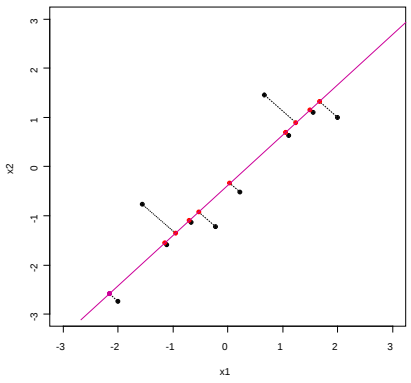
PCA reconstruction

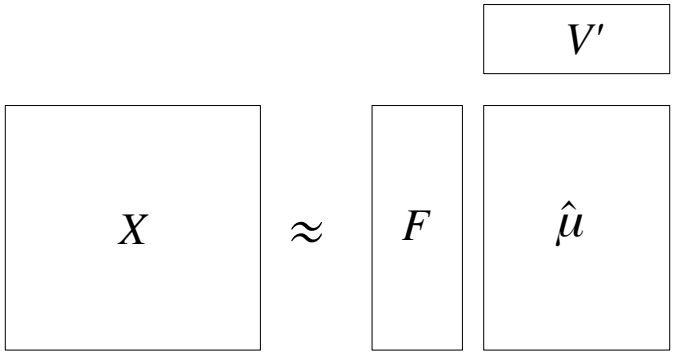
X

-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 $k < p$ $\|A\|_2^2 = \mathrm{tr}(AA^\top)$:

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

SVD X: $\hat{\mu}^{\mathrm{PCA}} = U_{n\times k} D_{k\times k} V'_{p\times k}$ $\quad F = UD$ PC - scores

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

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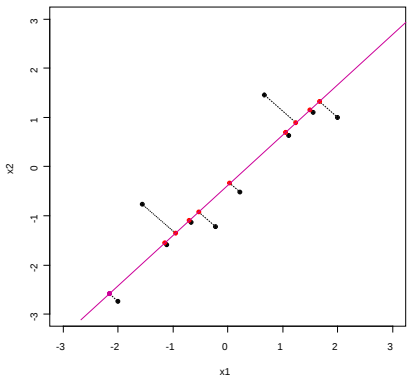

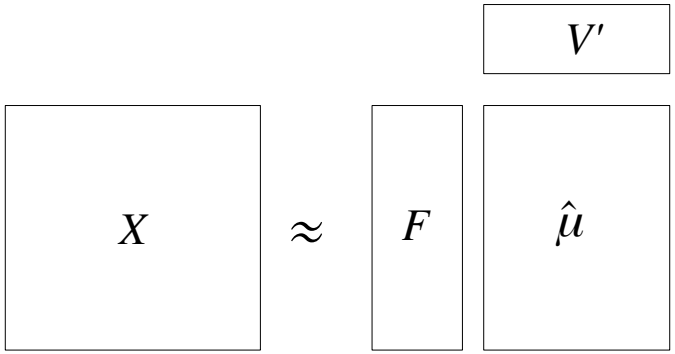

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Missing values in PCA

$\Rightarrow$ PCA: least squares

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

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

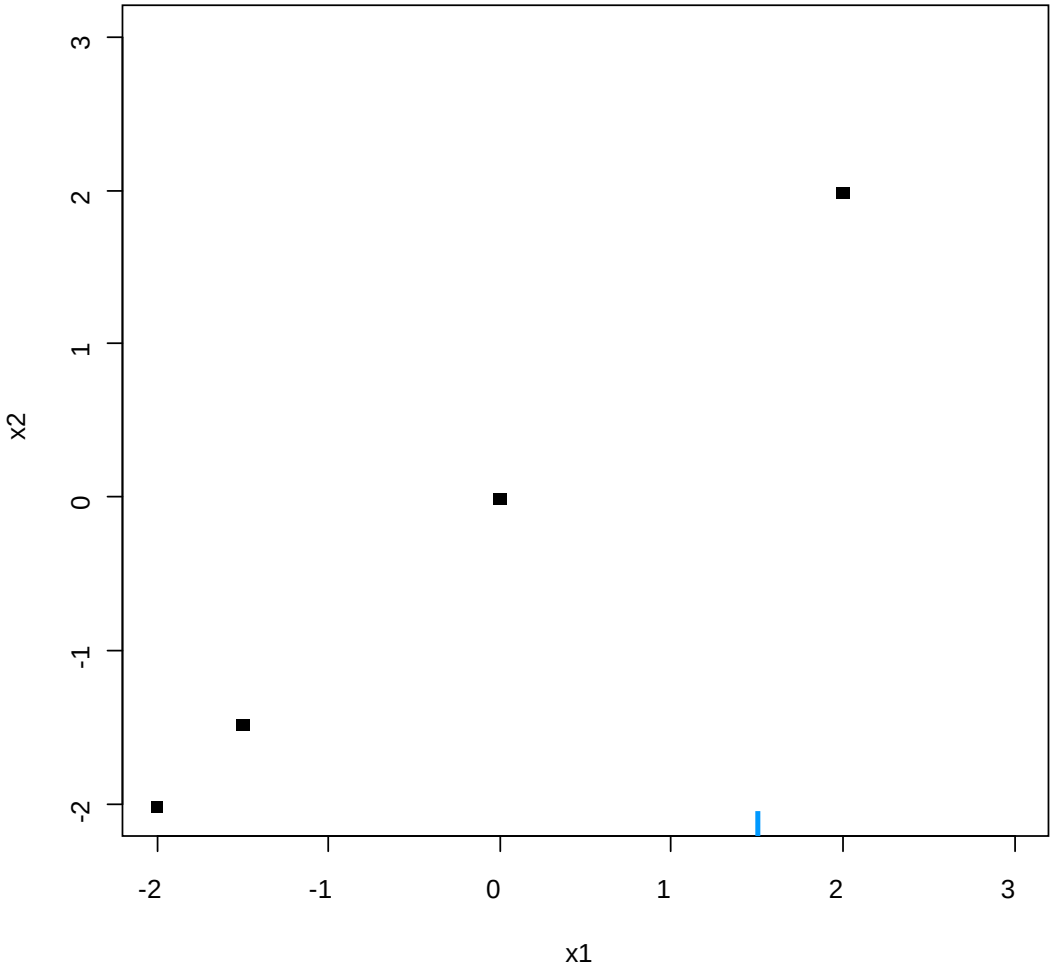
$$\text{argmin}_{\mu} \left\{ \|W_{n\times p} \odot (X - \mu)\|_2^2 : \text{rank}\,(\mu) \leq k \right\}$$

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

Many algorithms:
Gabriel & Zamir, 1979: weighted alternating least squares (without explicit imputation)
Kiers, 1997: iterative PCA (with imputation)

Iterative PCA

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



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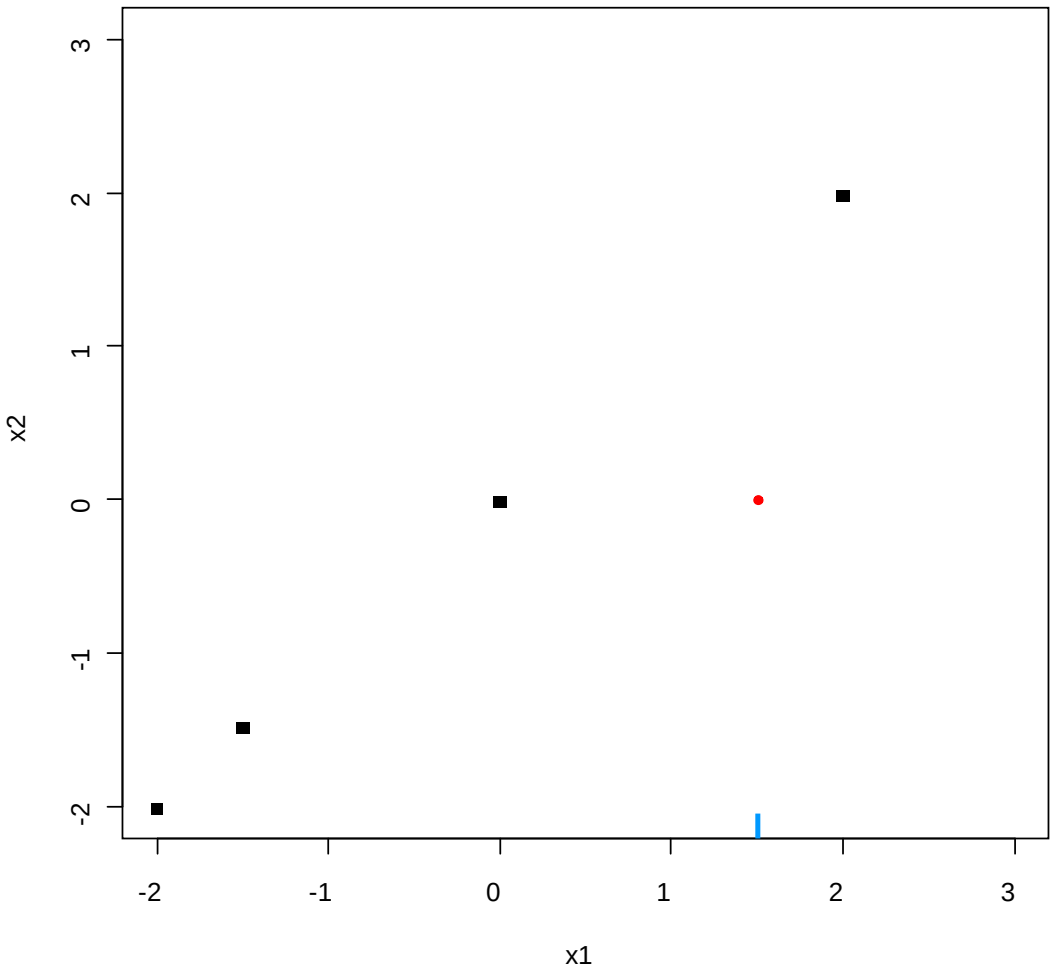

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-1.44	-1.56
0.15	-0.18
1.00	0.57
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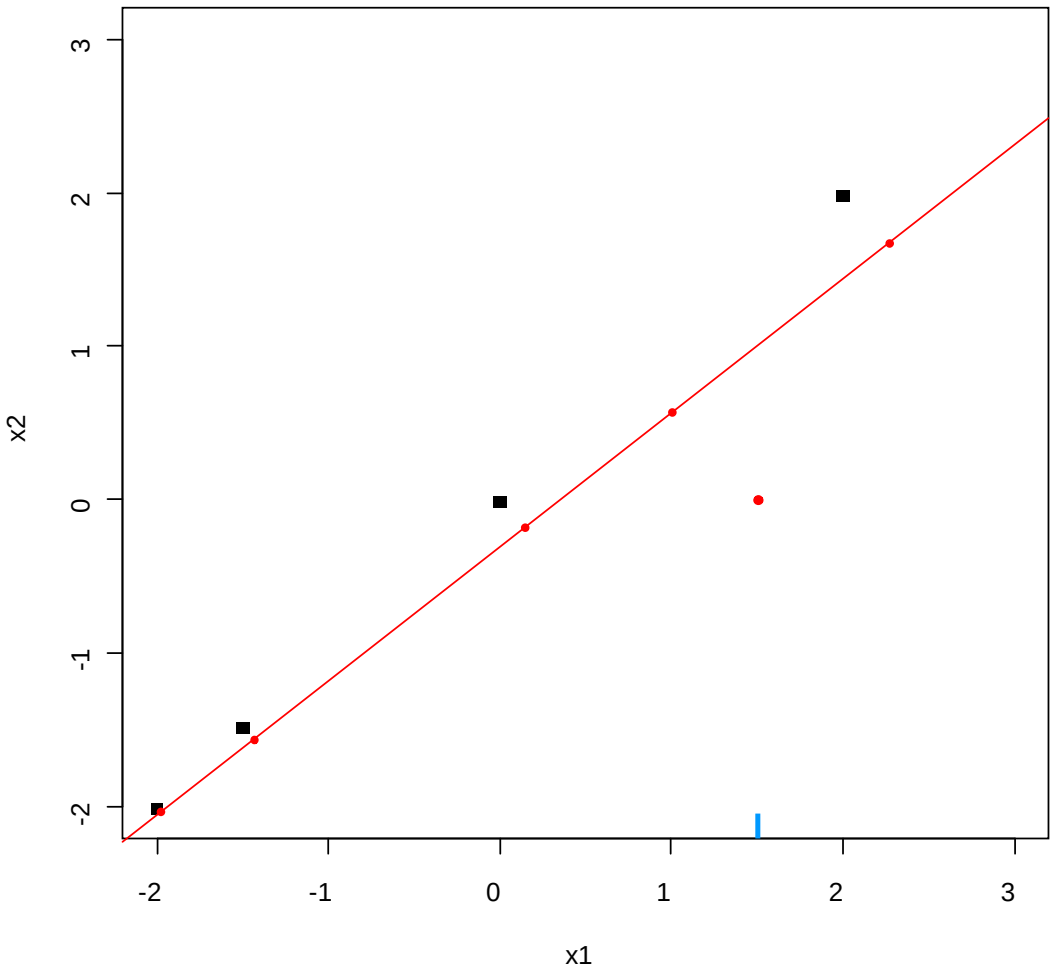

PCA on the completed data set $\rightarrow (U^{\ell}, \Lambda^{\ell}, D^{\ell})$;

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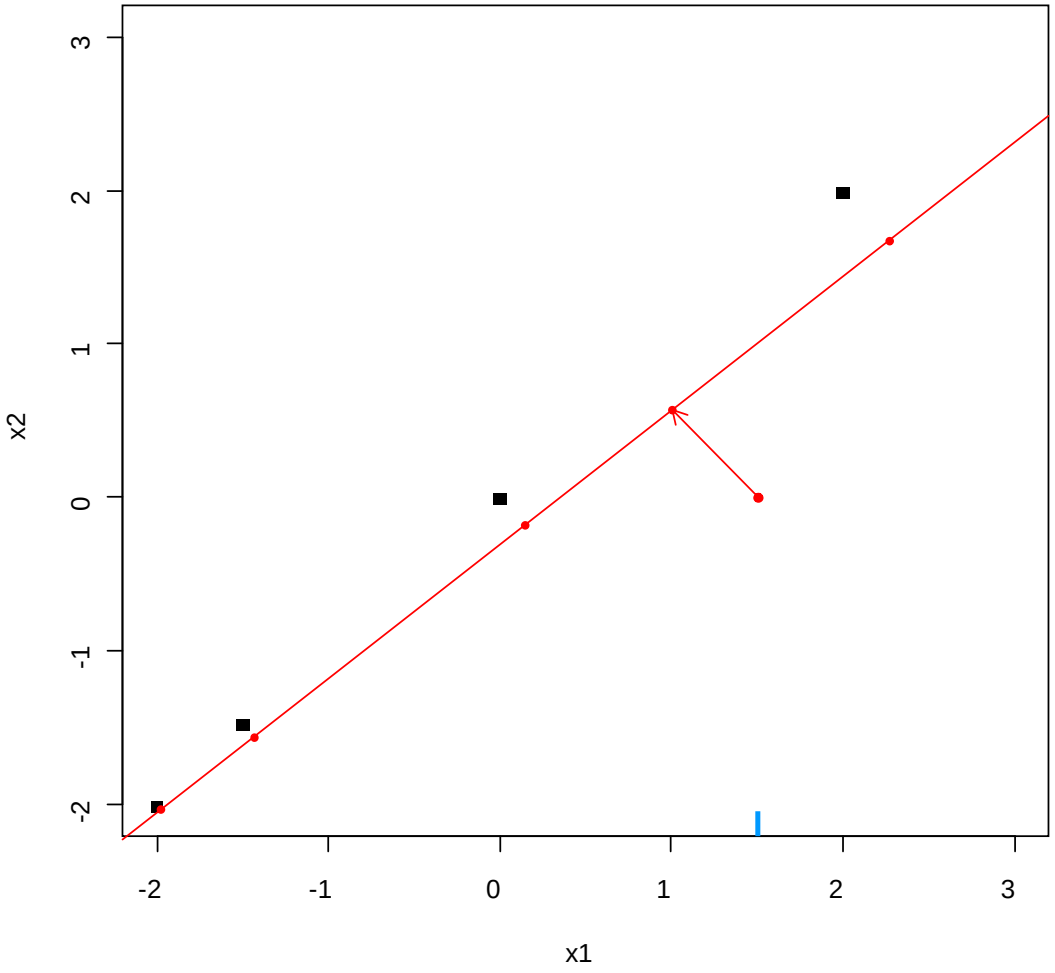

Missing values imputed with the fitted matrix $\hat{\mu}^{\ell} = U^{\ell} D^{\ell} V^{\ell\prime}$

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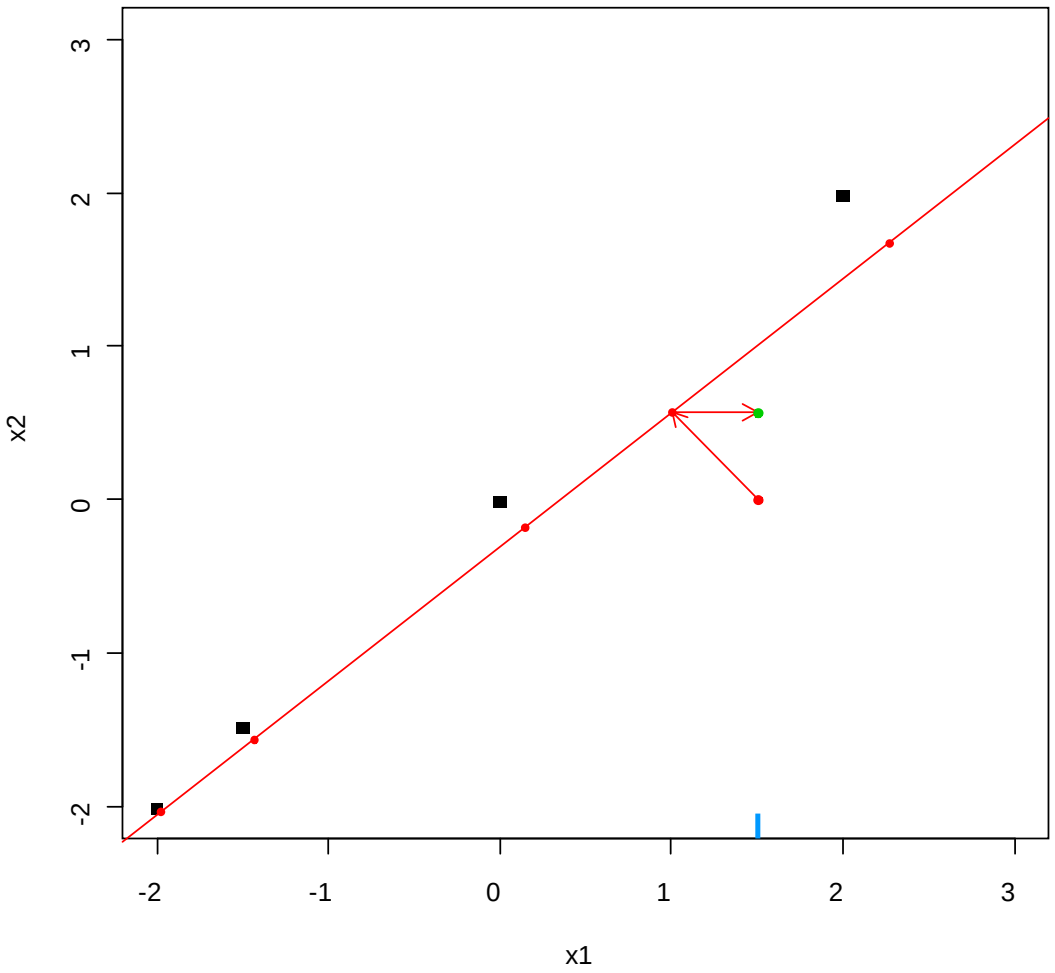

The new imputed dataset is $\hat{X}^\ell = W \odot X + (\mathbf{1} - W) \odot \hat{\mu}^\ell$

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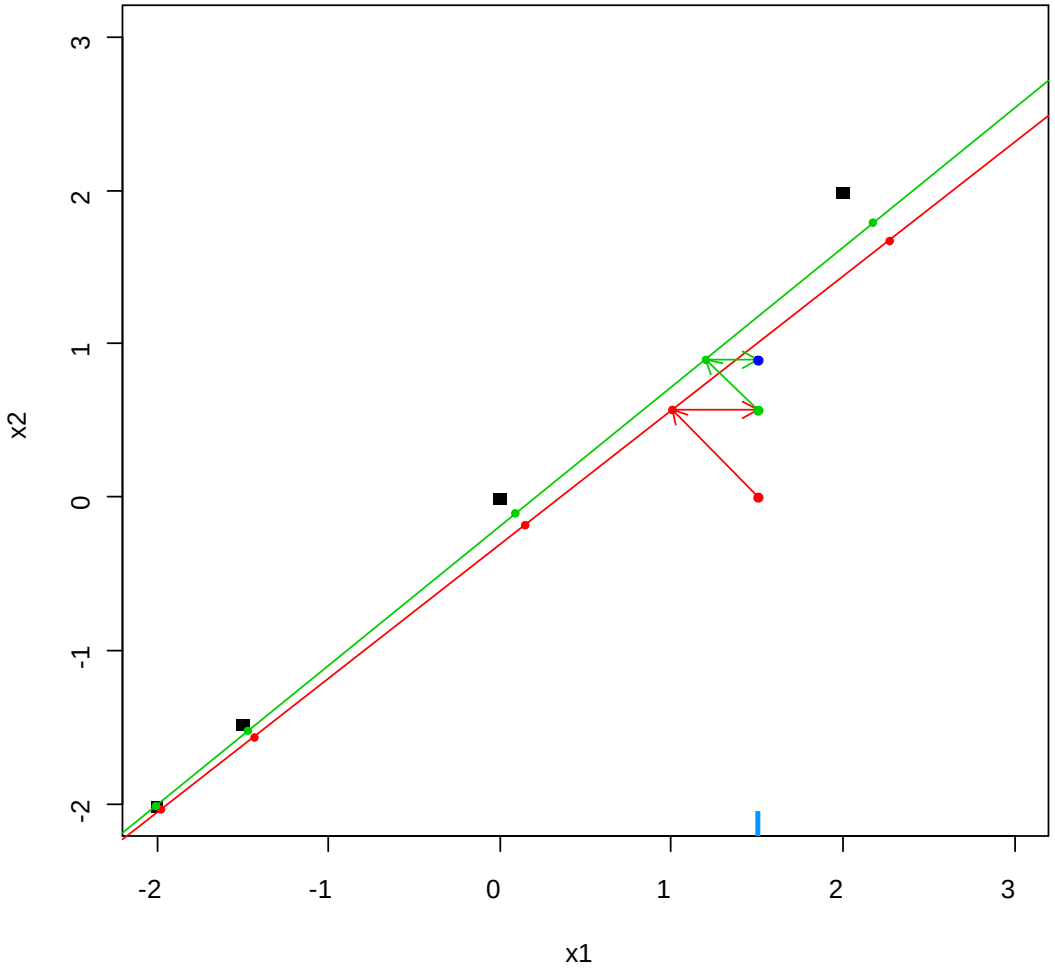

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$\hat{x}1$	$\hat{x}2$
-2.00	-2.01
-1.47	-1.52
0.09	-0.11
1.20	**0.90**
2.18	1.78

x1	x2
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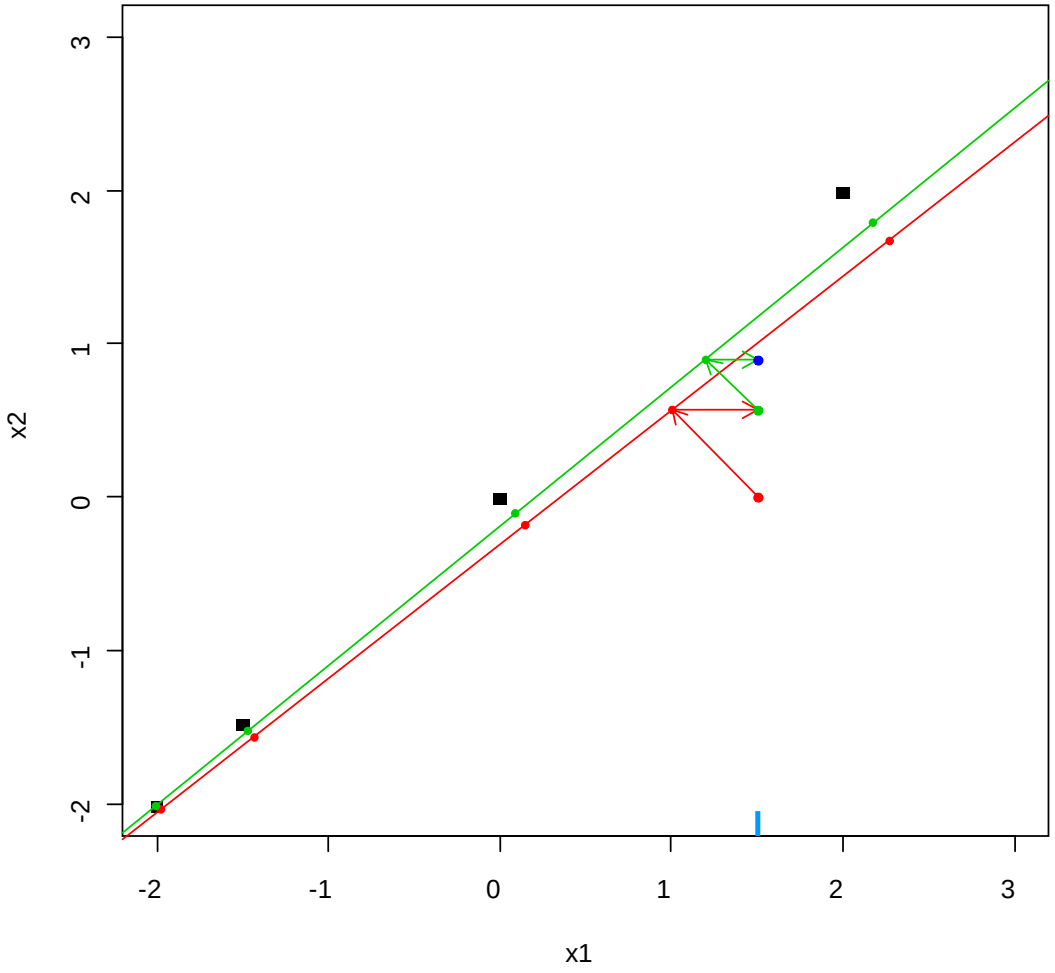

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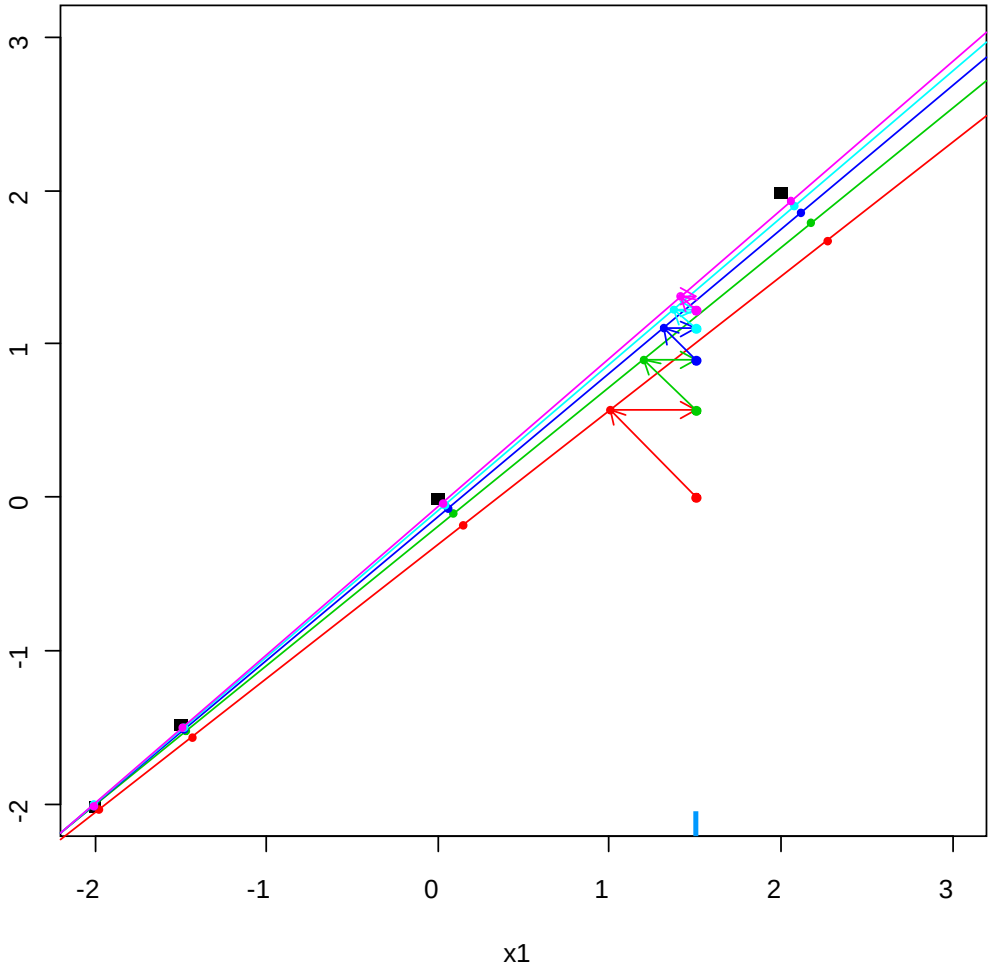

Steps are repeated until convergence

Iterative PCA

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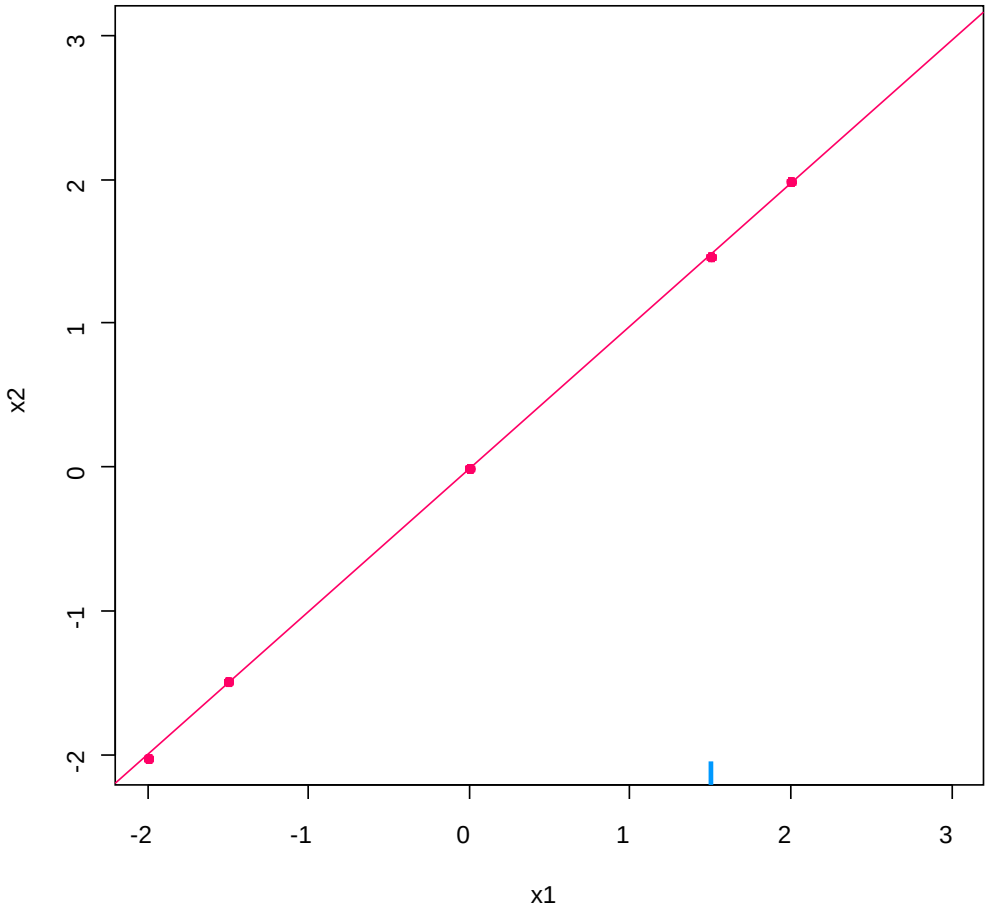

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PCA on the completed data set $\rightarrow (U^\ell, D^\ell, V^\ell)$

Missing values imputed with the fitted matrix $\hat{\mu}^\ell = U^\ell D^\ell V^{\ell\prime}$

Iterative PCA

1. initialization $\ell = 0$: X^0 (mean imputation)
2. step ℓ:
   (a) PCA on the completed data $\rightarrow (U^\ell, D^\ell, V^\ell)$; k dim kept
   (b) $(\hat{\mu}^\ell)^k = U^\ell D^\ell V^{\ell\prime}$ $\qquad X^\ell = W \odot X + (1 - W) \odot \hat{\mu}^\ell$
3. steps of estimation and imputation are repeated

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$\Rightarrow$ $\hat{\mu}$ from incomplete data: EM algo: $X = FV' + \varepsilon$
$X = \mu + \varepsilon,\ \varepsilon_{ij} \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ with μ of low rank

$\Rightarrow$ Completed data: good imputation (matrix completion, Netflix)
(Udell & Townsend Nice Latent Variable Models Have Log-Rank, 2017)

Selecting k? Generalized cross-validation (Josse & Husson, 2012)

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Regularized iterative SVD

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

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

Imputation by $\hat{\mu}^{\text{PCA}} = \sum_{q=1}^{k} d_q u_q v_q^{'}$ is replaced by

$(\hat{\mu})_\lambda = \sum_{q=1}^{n} (d_q - \lambda)_+ u_q v_q^{'}$ $\text{argmin}_\mu \left\{ \|W \odot (X - \mu)\|_2^2 + \lambda \|\mu\|_* \right\}$

$\hat{\mu} = \sum_{q=1}^{k} \left(d_l - \frac{\hat{\sigma}^2}{d_q} \right) u_q v_q'$

Hastie et.al. (2015), Verbank, J. & Husson (2013); Gavish & Donoho (2014), J. & Wager (2015), J. & Sardy (2014)

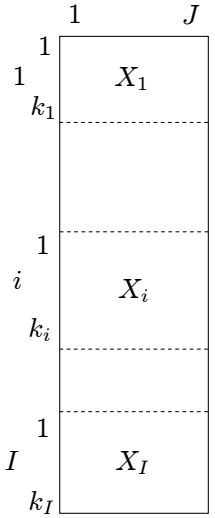
$\Rightarrow$ Iterative SVD algorithms good to impute data
$\Rightarrow$ Model makes sense: data = structure of rank k + noise

Outline

Multilevel component analysis

Ex: inhabitants nested within countries $X \in \mathbb{R}^{K \times J}$

- similarities between countries? level 1
- similarities between inhabitants within each country? level 2
- relationship between variables at each level



$$x_{ijk_i} = x_{.j.} + (x_{ij.} - x_{.j.}) \quad + \quad (x_{ijk_i} - x_{ij.})$$
$$\text{Between} \quad + \quad \text{Within}$$

Analysis of variance: split the sum of squares for each variable j

$$\sum_{i=1}^{I}\sum_{k=1}^{k_i}(x_{ijk_i})^2 = \sum_{i=1}^{I} k_i(x_{.j.})^2 + \sum_{i=1}^{I} k_i(x_{ij.} - x_{.j.})^2 + \sum_{i=1}^{I}\sum_{k=1}^{k_i}(x_{ijk_i} - x_{ij.})^2$$

Multilevel PCA MLPCA

$\Rightarrow$ Model for the between and within part $i = 1, ..., I$ groups, J var

$$X_{i_{(k_i \times J)}} = 1_{k_i} m' + 1_{k_i} F_i^{b'} V^{b'} + F_i^w V^{w'} + E_i$$

- F_i^b $(Q_b \times 1)$ between component scores of group i
- V^b $(J \times Q_b)$ between loading matrix
- F_i^w $(k_i \times Q_w)$ within component scores of group i
- V_w $(J \times Q_w)$ within loading matrix. Constant across groups

Fitted by solving the least squares (Timmerman, 2006)

$$\text{argmin}\, F(m, F_i^b, V^b, F_i^w, V^w) = \sum_{i=1}^{I} \left\| X_i - 1_{k_i} m' - 1_{k_i} F_i^{b'} V^{b'} - F_i^w V^{w'} \right\|^2$$

$\sum_{i=1}^{I} k_i F_i^b = 0_{Q_b}$ and $1'_{k_i} F_i^w = 0_{Q_w}$, $\forall i$ for identifiability.

MLPCA - quantitative data

$i = 1, ..., I$ groups, J var, k_i nb obs in group i
$\Rightarrow$ Estimation: minimize the RSS

$$\text{argmin}\, F() = \sum_{i=1}^{I} \left\| X_i - 1_{k_i} m' - 1_{k_i} F_i^{b'} V^{b'} - F_i^w V^{w'} \right\|^2,$$

$\sum_{i=1}^{I} k_i F_i^b = 0_{Q_b}$ and $1'_{k_i} F_i^w = 0_{Q_w}$, $\forall i$ for identifiability.

$(\hat{F}^b, \hat{V}^b)$: Weigthed PCA on the between part: SVD on WX_m; X_m $(I \times J)$ the means of the variables per group, W $(I \times I)$ $w_{ii} = \sqrt{k_i}$

$(\hat{F}^w, \hat{V}^w)$ PCA on the within part: SVD on the centered data per group X^w $(K \times J)$, $K = \sum_i k_i$

$\Rightarrow$ With missing values: Weighted Least Squares
$\Rightarrow$ Iterative imputation algorithm (imputation - estimation)

Iterative MLPCA

2. iteration ℓ: *estimation of the between structure*
   - SVD $WX_m^\ell = PDQ'$; Q_b eigenvectors are kept:
     $\hat{F}_i^b = [W^{-1}P_{Q_b}]_i$, $\hat{F}^b$ concatenation by row of $[\mathbf{1}_{k_i}\hat{F}_i^b]$
     $\hat{V}^b = Q_{Q_b}D_{Q_b}$, $(J \times Q_b)$
   - the between hat matrix is computed: $(\hat{X}^b)^\ell = \hat{F}^b\hat{V}^{b'}$
3. iteration ℓ: *imputation of the missing values with the fitted values*
   - $\hat{X}^\ell = \mathbf{1}_K\hat{m}^{(\ell-1)'} + (\hat{X}^b)^\ell + (\hat{X}^w)^{(\ell-1)}$. The newly imputed dataset is
     $X^\ell = W \odot X + (\mathbf{1}_K \times \mathbf{1}'_J - W) \odot \hat{X}^\ell$
   - $\hat{m}^\ell$ is computed on X^ℓ
4. iteration ℓ: *estimation of the within structure*
   - SVD $(X^w)^\ell = PDQ'$; Q_w eigenvectors are kept:
     $F^w = P_{Qw}$ $(K \times Q_w)$
     $V^w = Q_{Qw}D_{Qw}$ $(J \times Q_w)$
   - the within hat matrix is computed $(\hat{X}^w)^\ell = \hat{F}^w\hat{V}^{w'}$
5. iteration ℓ: *imputation of the missing values with the fitted values*
   - $X^{\ell+1} = M \odot X + (\mathbf{1}_K \times \mathbf{1}'_J - M) \odot \left(\mathbf{1}_K\hat{m}^{(\ell)'} + (\hat{X}^b)^\ell + (\hat{X}^w)^\ell\right)$
   - $\hat{m}^{\ell+1}$ is computed on $X^{\ell+1}$

Regularized iterative MLSCA

Estimation SVD - Imputation $\hat{X} = \mathbf{1}_K \hat{m}' + \hat{F}^b \hat{V}^{b'} + \hat{F}^w \hat{V}^{w'}$

$\hat{V}^b = Q_{Q_b} D_{Q_b} = Q_{Q_b} \mathrm{diag}\,(d_1, ..., d_{Q_b})$, as:

$$Q_{Q_b} \mathrm{diag}\left(d_1 - \frac{\hat{\sigma}_b^2}{d_1}, ..., d_{Q_b} - \frac{\hat{\sigma}_b^2}{d_{Q_b}} \right), \ \hat{\sigma}_b^2 = \frac{1}{J - Q_b} \sum_{q=Q_b+1}^{J} d_q$$

$$\hat{V}^w = Q_{Q_w} \mathrm{diag}\left(d_1 - \frac{\hat{\sigma}_w^2}{d_1}, ..., d_{Q_w} - \frac{\hat{\sigma}_w^2}{d_{Q_w}} \right)$$

Multiple Correspondence Analysis (MCA)

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

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

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

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

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

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

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"*

Multilevel MCA

$\Rightarrow$ Start with the matrix of dummy variables A and define a between and a within part
$\Rightarrow$ Then, MCA is applied on each part

Between: Apply MCA on the matrix with the mean of A per group i (proportion of obs taking each category in group i) (proportion of some disease in a particular hospital). $\hat{A}^b = F^b V^{b'} D_p^{1/2} + 1_n p'$

Within part Apply MCA on the data where the between part has been swept out (SVD is applied to $\frac{1}{np}\left(A - \hat{A}^b\right) D_p^{-1/2}$)
$\hat{A}^w = (np) F^w V^{w'} D_p^{1/2}$.

$$\hat{A} = \hat{A}^b + \hat{A}^w$$

Regularized iterative Multilevel MCA

	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	...

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)

	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	...

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)
- Iterate until convergence
  1. estimation: Multilevel MCA on the completed data $\rightarrow$ $\hat{F}^b, \hat{V}^b, \hat{F}^w, \hat{V}^w$

	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	...

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)
- Iterate until convergence
  1. estimation: Multilevel MCA on the completed data $\rightarrow$ $\hat{F}^b, \hat{V}^b, \hat{F}^w, \hat{V}^w$
  2. imputation with the fitted matrix $\hat{A} = \hat{A}^b + \hat{A}^w$

	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	...

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)
- Iterate until convergence
  1. estimation: Multilevel MCA on the completed data $\rightarrow$ $\hat{F}^b, \hat{V}^b, \hat{F}^w, \hat{V}^w$
  2. imputation with the fitted matrix $\hat{A} = \hat{A}^b + \hat{A}^w$
  3. 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	...

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)
- Iterate until convergence
  1. estimation: Multilevel MCA on the completed data $\rightarrow$ $\hat{F}^b, \hat{V}^b, \hat{F}^w, \hat{V}^w$
  2. imputation with the fitted matrix $\hat{A} = \hat{A}^b + \hat{A}^w$
  3. 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

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)
- Iterate until convergence
  1. estimation: Multilevel MCA on the completed data $\rightarrow$ $\hat{F}^b, \hat{V}^b, \hat{F}^w, \hat{V}^w$
  2. imputation with the fitted matrix $\hat{A} = \hat{A}^b + \hat{A}^w$
  3. 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 impute categories: majority or draw

Regularized iterative Multilevel MCA

- Initialization: imputation of the indicator matrix (proportions)
- Iterate until convergence
  1. estimation: Multilevel MCA on the completed data $\rightarrow$ $\hat{F}^b, \hat{V}^b, \hat{F}^w, \hat{V}^w$
  2. imputation with the fitted matrix $\hat{A} = \hat{A}^b + \hat{A}^w$
  3. 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 impute categories: majority or draw

Public Assistance - Paris Hospitals

Traumabase: 15000 patients/ 250 variables/ 6 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	

.....

Imputed Paris Hospitals data

Traumabase: 15000 patients/ 250 variables/ 6 hospitals

```
               Center       Accident   Age Sex Weight Height   BMI BP SBP
1            Beaujon        Fall         54    m 85.00   1.84 27.04  83  13
2              Lille        Other        33    m 80.00   1.80 24.69  33  98
3  Pitie Salpetriere        Gun          26    m 81.78   1.85 24.33  34  98
4            Beaujon        AVP moto     63    m 80.00   1.80 24.69  48 125
6  Pitie Salpetriere        AVP bicycle  33    m 75.00   1.83 24.53   6 122
7  Pitie Salpetriere        AVP pedestri 30    m 81.89   1.82 25.24   9 102
9               HEGP        White weapon 16    m 98.00   1.92 26.58  21  90
10            Toulon        White weapon 20    m 81.68   1.82 25.05  27 109
11           Bicetre        Fall         61    m 84.00   1.70 29.07  47   8
   SpO2 Temperature Lactates Hb Glasgow............
1    46          61   289.07 33      14
2     2          72   464.00 16      14
3     2          65   416.00 19       7
4     2          74   130.00 36       6
6     2          65   285.91 50       6
7     2          73   244.99 49       6
9     2          83   196.00 65       6
10    2          76   262.44 43       6
11    2          73    84.00 48       5
```

Design

The simulated data:

- $X_{i_{(k_i \times J)}} = 1_{k_i} m' + 1_{k_i} F_i^{b'} V^{b'} + F_i^w V^{w'} + E_i$, with $E_{ijk_i} \sim \mathcal{N}(0, \sigma)$
- 5 groups, 10 variables, $Q_b = 2$, $Q_w = 2$

Many scenarios are considered:

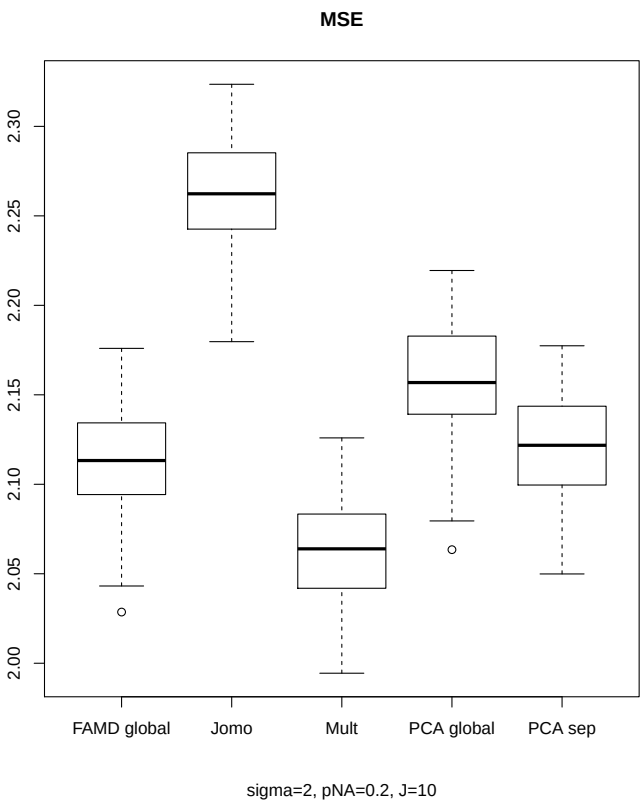
- number of measurement occasions: 10-20, 70-100
- level of noise: low, strong
- percentage of missing values: 10%, 25%, 40%
- missing values mechanism: MCAR, 2 MAR situations

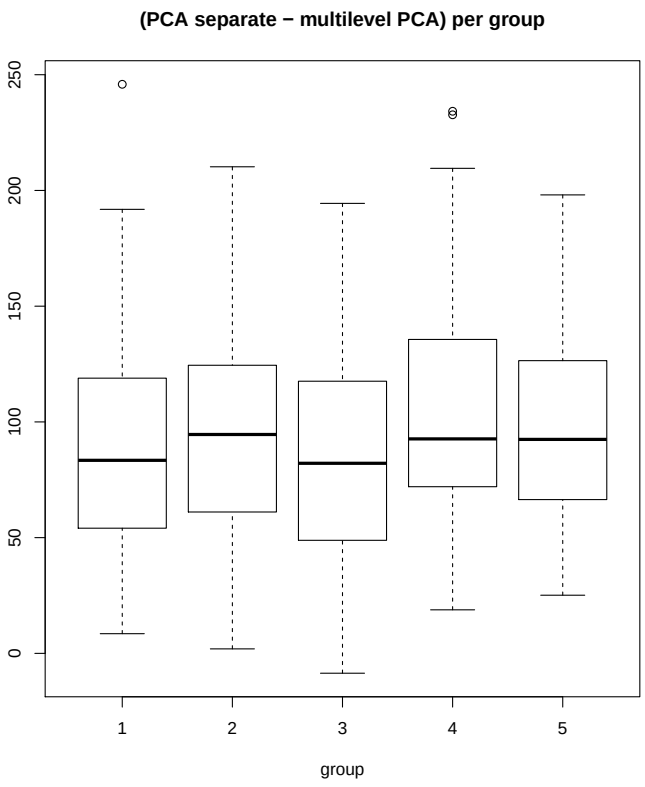
$\Rightarrow$ Prediction error: $\frac{1}{KJ} \sum (x_{ijk_i} - \hat{x_{ijk_i}})^2$

Results

Competitors:

- Conditional model with random effect regression (mice)
- Random forests (bühlmann, 2012) (not designed)
- Global PCA - Separate PCA
- Global mixed PCA (with hospital)





Results

	$J = 10$	$J = 30$	$5cat$	$5cat$
Global PCA	0.09	0.3		
mice	11	282		
Multilevel SVD	1.5	1.2	2	7
Global mixed PCA	0.4	0.7	1	4
Random forest	59	200	27	246

Table: Time in seconds for a dataset with 20% NA, $I = 5$ $k_i = 200$

- PCA mixed as Random Forest
- mice (random effect model): difficulties with large dimensions
- Separate PCA: pb with many missing values
- Multilevel SVD = global SVD when no group effect
- Imputation properties depends on the method (linear)
- Other methods do not handle categorical variables

Outline

6 hospital databases

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

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

6 hospital databases

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

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

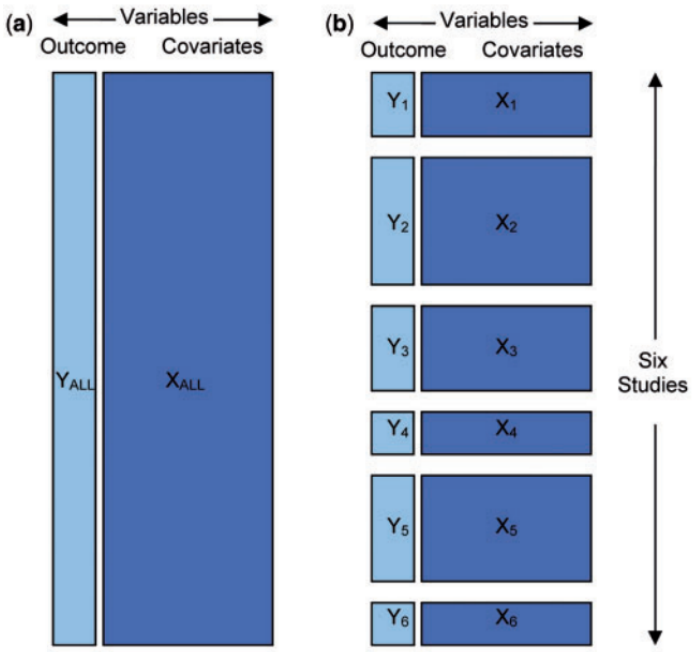
$\Rightarrow$ The problem: high barriers to aggregation of medical data

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

Solution: distributed computation

⇒ Data aggregation is not always necessary

⇒ NIH splits the storage of aggregated data across several centers

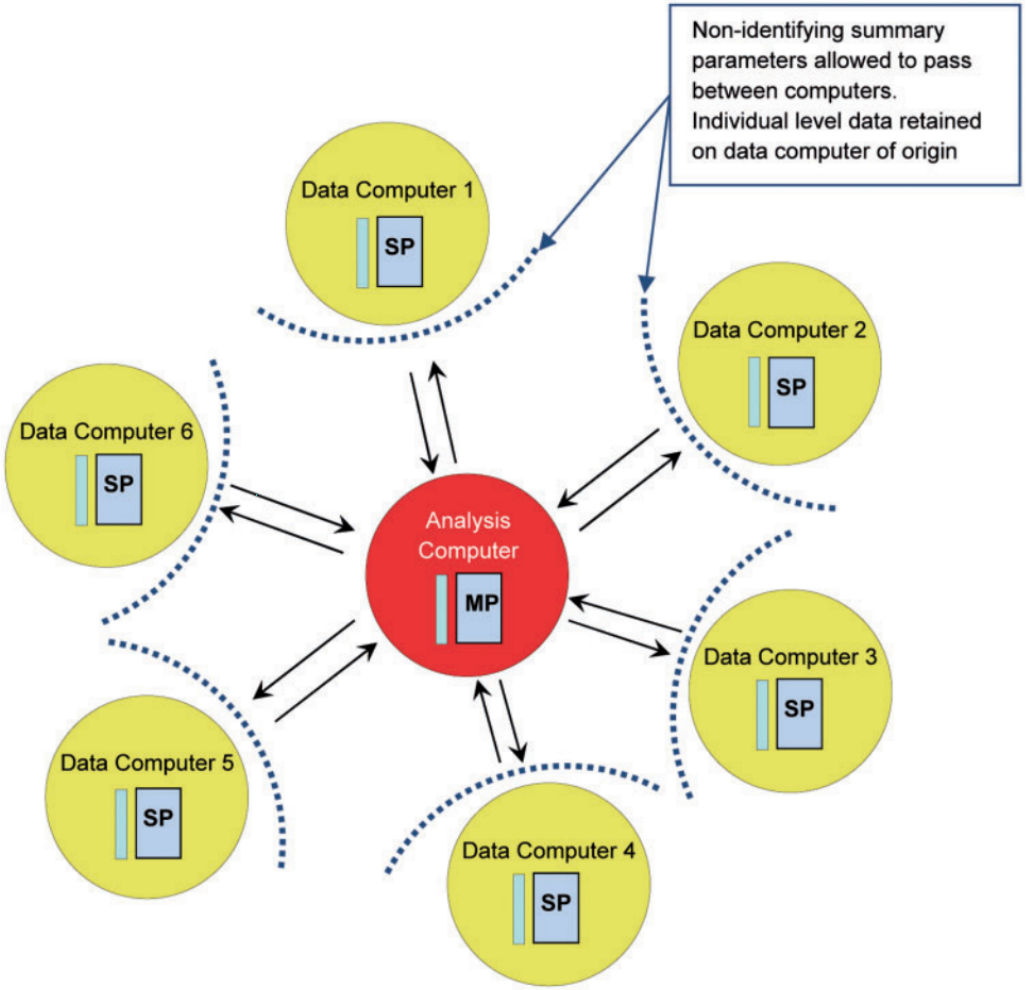


⇒ Data can stay at site

⇒ Computations can be distributed (share burden)

⇒ Hospitals only share intermediate results instead of the raw data

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



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

Solution: distributed computation

⇒ Many models fitting can be implemented:

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

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

Singular value decomposition

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

Power method to get the first direction:

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

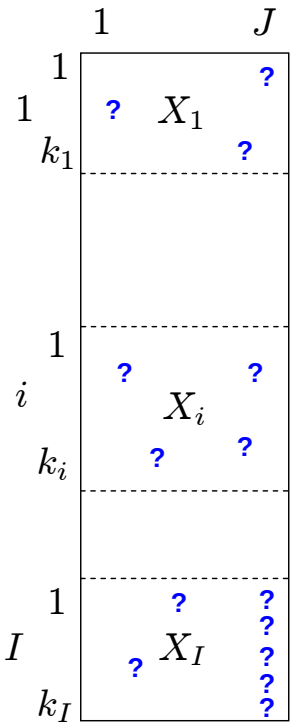
Other dims: "deflation", same procedure in the residuals $(X - udv')$

$\Rightarrow$ Involves inner products and sums: distributed

Privacy preserving rank k SVD

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

Multilevel imputation



⇒ Impute multilevel data with Multilevel SVD
⇒ Distributed multilevel imputation
⇒ Impute the data of one hospital using the data of the others
⇒ Incentive to encourage the hospitals to participate in the project
⇒ Apply other statistical methods on the imputed data (logistic regression)

Take home message - On going work

Multilevel PCA powerful for single imputation of continuous & categorical multilevel data: reduce the dimensionality - capture the similarities between rows and relationship between variables at both levels.

Method without missing values

$\Rightarrow$ Computationaly fast - distributed - Implemented R package missMDA

- Numbers of components Q_b and Q_w ?

- Inference after imputation. Underestimation of the variance with single imputation

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cross-validation?

• Inference after imputation. Underestimation of the variance with single imputation
Multiple imputation: bootstrap + drawn from the predictive distribution
$\mathcal{N}\left(\mathbf{1}_K \hat{m}' + \hat{F}^b \hat{B}^{b'} + \hat{F}^w \hat{B}^{w'}, \hat{\sigma}^2\right)$

Research activities

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

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