Statistical inference with missing values

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12 Dec. 2019 Spotkania Entuzjastów R @ Wydzial MiNI PW

Missing values

When we attempt to explore data as a source of knowledge, **missing** values lies in the process of obtaining, recording, and preparing the data.

- Unanswered questions in a survey
- loss of data
- machines that fail

"We should be suspicious of any dataset (large or small) which appears perfect." — David J. Hand



Paris Hospitals - TraumaBase dataset

$20\,000$ severely traumatised patients $+\,250$ measurements

		Center	Accident	Age	Sex	Weight	Height	BM:	I 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

	Sp02	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	NA	14.4	15	no
7	100	36.6	NA	14.3	15	yes
9	100	37.5	13	15.9	15	yes
10	100	36.9	NA	13.7	15	no
11	100	36.6	1.2	14.2	14	no

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- ⇒ Predict the Glasgow score, whether to start a blood transfusion, etc...
- ⇒ Linear regression /Logistic regression /Random Forests with missing covariates

Missing values problematic

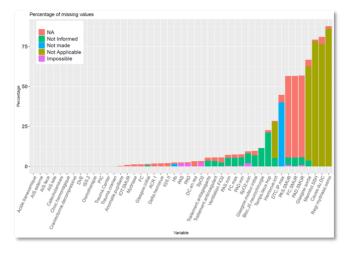
List-wise deletion (default 1m function in R)

 \Rightarrow loss of information

Missing values problematic

List-wise deletion (default 1m function in R)

⇒ loss of information



 \Rightarrow less than 10% remained

Single imputation

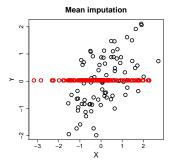
- $(x_i, y_i) \sim \mathcal{N}(\mu, \Sigma)$ i.i.d.
- 70% missing entries on y randomly

Date completion by the mean of observed values in $y \Rightarrow$ Estimate parameters:

Single imputation

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Date completion by the mean of observed values in $y \Rightarrow$ Estimate parameters:



$$\mu_y = 0$$

$$\sigma_y = 1$$

$$\rho = 0.6$$

$$\hat{\mu}_y = 0.01$$

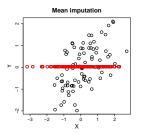
$$\hat{\sigma}_y = 0.5$$

$$\hat{\rho} = 0.30$$

⇒ Biased estimates

Imputation methods

Mean imputation

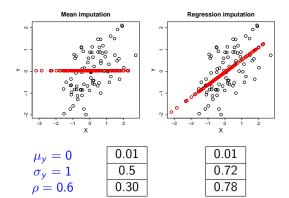


$$\mu_y = 0
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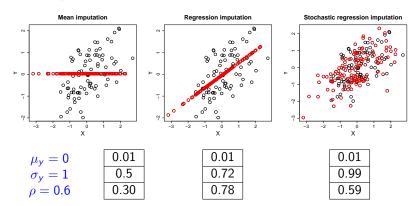
Imputation methods

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- Impute by regression: impute $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ \Rightarrow variance underestimated and correlation overestimated.



Imputation methods

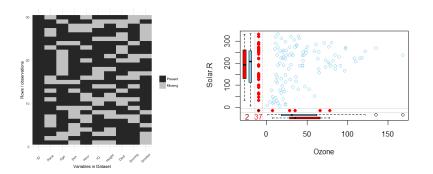
- Mean imputation
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- Impute by stochastic regression: impute $\hat{y}_i \sim \mathcal{N}\left(x_i\hat{\beta}, \hat{\sigma}^2\right)$ \Rightarrow preserve distribution



Missing pattern and mechanism

Dealing with missing values depends on:

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



R packages: VIM, naniar (Matthias Templ, Nick Tierney) FactoMineR (YouTube):

References on more imputation methods

• based on multivariate Gaussian assumption: $x_i \sim \mathcal{N}\left(\mu, \Sigma\right)$ estimate μ and Σ from an incomplete data with EM \rightarrow impute by drawing from $\mathcal{N}\left(\hat{\mu}, \hat{\Sigma}\right)$

R packages: Amelia, mice

k-nearest neighbor
 R packages: VIM, yaImpute, impute

PCA or MCA

R package: missMDA

random forest

R package: missForest

- \Rightarrow R-miss-tastic (Josse et al.): Methods and references for managing missing data
- ⇒ Flexible imputation of missing data (Stef van Buuren)

Modify the estimation process to deal with missing values.

Maximum observed likelihood: EM algorithm to obtain point estimates

Modify the estimation process to deal with missing values. **Maximum observed likelihood:** EM algorithm to obtain point estimates Eample: Hypothesis $x_i \sim \mathcal{N}(\mu, \Sigma)$, point estimates with EM

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- \Rightarrow One specific algorithm for each statistical method.
- ⇒ Not many implementations even for simple models.

Package misaem: logistic regression with missing values (Jiang et al., 2018)

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Specialized focus on: Model selection with missing covariates, e.g. Measurements $\stackrel{\text{Predict}}{\longrightarrow}$ Platelet

joint work with Malgorzata Bogdan, Julie Josse, Blazej Miasojedow, Veronika Rockova

Model selection in high-dimension

Linear regression model: $y = X\beta + \varepsilon$,

- $y = (y_i)$: vector of response of length n
- $X = (X_{ij})$: a standardized design matrix of dimension $n \times p$
- $\beta = (\beta_j)$: regression coefficient of length p
- $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n)$

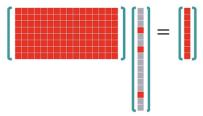
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Assumptions:

- high-dimension: p large (including $p \ge n$)
- β is sparse with k < n nonzero coefficients



I_1 penalization methods

LASSO (Tibshirani, 1996)

$$\hat{\beta}_{LASSO} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \frac{1}{2} \|y - X\beta\|^2 + \lambda \|\beta\|_1,$$

detects important variables with high probability but includes many false positives.

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$$\hat{\beta}_{SLOPE} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \frac{1}{2} \|y - X\beta\|^2 + \sigma \sum_{i=1}^p \lambda_i |\beta|_{(j)},$$

where
$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$$
 and $|\beta|_{(1)} \geq |\beta|_{(2)} \geq \cdots \geq |\beta|_{(p)}$.

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To control **False Discovery Rate (FDR)** at level q: $\lambda_{BH}(j) = \phi^{-1}(1 - q_i), \quad q_i = \frac{jq}{2n}, \quad X^T X = I,$ ther

$$FDR = \mathbb{E}\left[\frac{\#\mathsf{False rejections}}{\#\mathsf{Rejections}}\right] \le q$$

Bayesian SLOPE

Problem: λ for SLOPE leading to FDR control are typically large. SLOPE often returns an inconsistent estimation.

 \Rightarrow improve?

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$$\Rightarrow$$
 improve?

SLOPE estimate = MAP of a Bayesian regression with SLOPE prior.

$$\hat{\beta}_{SLOPE} = \operatorname{argmax}_{\beta} p(y \mid X, \beta, \sigma^{2}; \lambda) \propto p(y \mid X, \beta) p(\beta \mid \sigma^{2}; \lambda)$$

where the SLOPE prior:

$$\mathrm{p}(\beta \mid \sigma^2; \lambda) \propto \prod_{j=1}^p \exp\left(-rac{1}{\sigma} \lambda_j |\beta|_{(j)}\right)$$

Adaptive Bayesian SLOPE

We propose an adaptive version of Bayesian SLOPE (ABSLOPE), with the prior for β as

$$\mathrm{p}(\beta \mid \gamma, c, \sigma^2; \lambda) \propto c^{\sum_{j=1}^p \mathbb{I}(\gamma_j = 1)} \prod_j \exp\left\{ -\frac{\mathsf{w}_j}{|\beta_j|} \frac{1}{\sigma} \lambda_{r(\mathbf{W}\beta, j)} \right\},$$

Interpretation of the model:

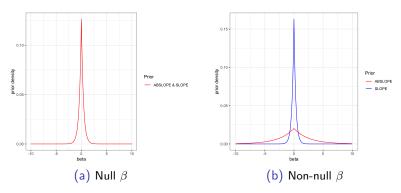
- β_j is large enough \Rightarrow true signal; $0 \Rightarrow$ noise.
- $\gamma_j \in \{0,1\}$ signal indicator. $\gamma_j | \theta \sim Bernoulli(\theta)$ and θ the sparsity.
- $c \in [0,1]$: the inverse of average signal magnitude.
- $W = \text{diag}(w_1, w_2, \dots, w_p)$ and its diagonal element:

$$w_j = c\gamma_j + (1-\gamma_j) = egin{cases} c, & \gamma_j = 1 \ 1, & \gamma_j = 0 \end{cases}.$$

Adaptive Bayesian SLOPE

Advantage of introducing W:

- when $\gamma_j = 0$, $w_j = 1$, i.e., the null variables are treated with the regular SLOPE penalty
- when $\gamma_j = 1$, $w_j = c < 1$, i.e, **smaller penalty** $\lambda_{r(W\beta,j)}$ for true predictors than the regular SLOPE one



Rysunek: comparison of SLOPE prior and ABSLOPE prior

Model selection with missing values

Decomposition: $X = (X_{\text{obs}}, X_{\text{mis}})$

Pattern: matrix M with $M_{ij} = \begin{cases} 1, & \text{if } X_{ij} \text{ is observed} \\ 0, & \text{otherwise} \end{cases}$

Assumption 1: Missing mechanism - Missing at random (MAR)

 $p(M \mid X_{\rm obs}, X_{\rm mis}) = p(M \mid X_{\rm obs}) \implies \text{ignorable missing patterns}$ e.g. People at older age didn't tell his income at larger probability.

Assumption 2: Distribution of covariates

$$X_i \sim_{\mathrm{i.i.d.}} \mathcal{N}_p(\mu, \Sigma), \quad i = 1, \cdots, n.$$

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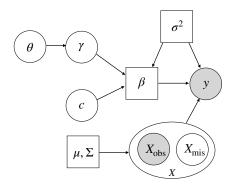
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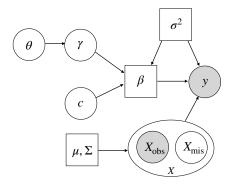
Problem: With NA, only a few methods are available to select a model, and their performances are limited. For example,

- (Claeskens and Consentino, 2008) adapts AIC to missing values ⇒ Impossible to deal with high dimensional analysis.
- (Loh and Wainwright, 2012) LASSO with NA
 - \Rightarrow Non-convex optimization; requires to know bound of $\|\beta\|_1$
 - \Rightarrow difficult in practice

ABSLOPE with missingness: Summary



ABSLOPE with missingness: Summary



$$\begin{aligned} \ell_{\text{comp}} &= \log p(y, X, \gamma, c; \ \beta, \theta, \sigma^2) + \textit{pen}(\beta) \\ &= \log \left\{ p(X; \ \mu, \Sigma) \, p(y \mid X; \ \beta, \sigma^2) \, p(\gamma; \ \theta) \, p(c) \right\} + \textit{pen}(\beta) \end{aligned}$$

Objective: Maximize $\ell_{\text{obs}} = \iiint \ell_{\text{comp}} dX_{\text{mis}} dc d\theta d\gamma$.

EM algorithm

• E step: evaluate

$$Q^t = \mathbb{E}(\ell_{\text{comp}}) \quad \text{wrt} \quad p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^t, \sigma^t, \mu^t, \Sigma^t).$$

M step: update

$$\beta^t, \sigma^t, \mu^t, \Sigma^t = \operatorname{argmax} Q^t$$

Problem: The function Q is not tractable. \Rightarrow

1 Monte Carlo EM ? (Wei and Tanner 1990)

EM algorithm

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Problem: The function Q is not tractable. \Rightarrow

- Monte Carlo EM ? Expensive to generate a large number of samples.
- 2 Stochastic Approximation EM (book, Lavielle 2014)
 - One sample in each iteration;

Adapted SAEM algorithm

- E step:
 - $Q^t = \mathbb{E}(\ell_{\text{comp}}) \quad \text{wrt} \quad p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^t, \sigma^t, \mu^t, \Sigma^t).$
 - Simulation: draw one sample $(X_{\mathrm{mis}}^t, \gamma^t, c^t, \theta^t)$ from

$$p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^{t-1}, \sigma^{t-1}, \mu^{t-1}, \Sigma^{t-1});$$
 [Gibbs sampling]

Stochastic approximation: update function Q with

$$Q^t = Q^{t-1} + \eta_t \left(\ell_{\text{comp}} \Big|_{X_{\text{mis}}^t, \gamma^t, c^t, \theta^t} - Q^{t-1} \right).$$

Adapted SAEM algorithm

- *E step:*
 - $Q^t = \mathbb{E}(\ell_{\text{comp}})$ wrt $p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^t, \sigma^t, \mu^t, \Sigma^t)$.
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ight).$$

• *M step*: β^{t+1} , σ^{t+1} , μ^{t+1} , Σ^{t+1} = argmax Q^{t+1} . [Proximal gradient descent, Shrinkage of covariance]

Details of initialization, generating samples and optimization are in the draft (arXiv:1909.06631)

Install package:

```
library(devtools)
install_github("wjiang94/ABSLOPE")
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lambda = create_lambda_bhq(ncol(X),fdr=0.10)
list.res = ABSLOPE(X, y, lambda)
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A fast and simplified algorithm (Rcpp):

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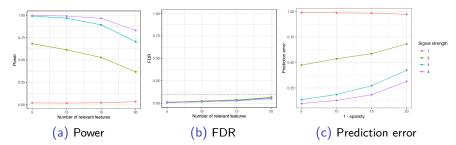
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Values:

```
list.res$beta
list.res$gamma
```

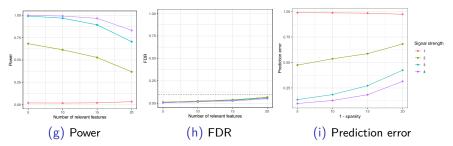
Simulation study (200 rep. \Rightarrow average)

n=p=100, no correlation and 10% missingness

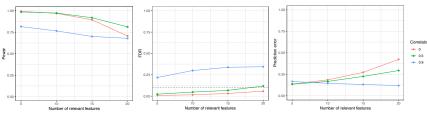


Simulation study (200 rep. \Rightarrow average)

n=p=100, no correlation and 10% missingness



n=p=100, with 10% missingness and strong signal



(j) Power

(k) FDR

(I) Prediction error

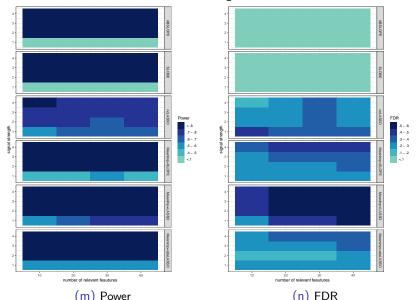
Method comparison

- ABSLOPE and SLOBE
- ncLASSO: non convex LASSO (Loh and Wainwright, 2012)
 - **MeanImp** + **SLOPE**: Mean imputation followed by SLOPE with known σ
- MeanImp + LASSO: Mean imputation followed by LASSO, with λ tuned by cross validation
- MeanImp + adaLASSO: Mean imputation followed by adaptive LASSO (Zou, 2006)

In the SLOPE type methods, $\lambda={\sf BH}$ sequence which controls the FDR at level ${\bf 0.1}$

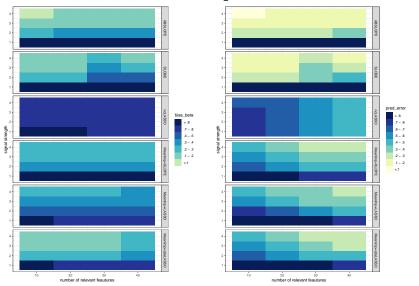
Method comparison (200 rep. \Rightarrow average)

 500×500 dataset, 10% missingness, with correlation



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 500×500 dataset, 10% missingness, with correlation



(a) Bias of β

(b) Prediction error

Computational cost

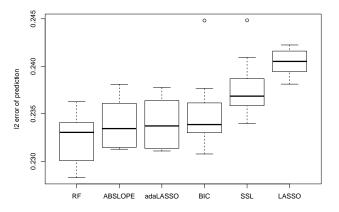
Execution time (seconds)	n :	= p = 1	00	n=p=500			
for one simulation	min	mean	max	min	mean	max	
ABSLOPE	12.83	14.33	20.98	646.53	696.09	975.73	
SLOBE	0.31	0.34	0.66	14.23	15.07	29.52	
ncLASSO	16.38	20.89	51.35	91.90	100.71	171.00	
MeanImp + SLOPE	0.01	0.02	0.09	0.24	0.28	0.53	
MeanImp + LASSO	0.10	0.14	0.32	1.75	1.85	3.06	

[Fast implementation: Parallel computing + Rcpp (C++)]

More on the real data...

TraumaBase: Measurements $\stackrel{\mathsf{Predict}}{\longrightarrow}$ Platelet

Cross-validation: random splits to training and test sets \times 10



- Comparable to random forest
- Interpretable model selection and estimation results

Conclusion & Future research

Conclusion:

- ABSLOPE penalizes larger coefficients more stringently to control FDR, meanwhile it applies a weighting matrix to improve the estimation;
- Modeling in a Bayesian framework gives detailed structure of predictors as sparsity and signal strength;
- Simulation study shows that ABSLOPE is competitive to other methods in terms of power, FDR and prediction error.

Future research:

- Consider categorical or mixed data
- Deal with other missing mechanisms
- Application on genetic dataset

Thank you! Dziękuję







