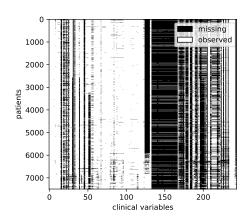
# Going beyond the fear of emptyness to gain consistency

Alexis Ayme, Claire Boyer, Aymeric Dieuleveut, Julie Josse, Marine Le Morvan, **Erwan Scornet**, Gael Varoquaux

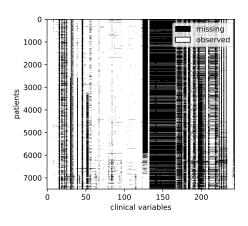




Traumabase clinical records.

#### Sources of missingness:

- Survey nonresponse.
- Sensor failure.
- Changing data gathering procedure.
- Database join.



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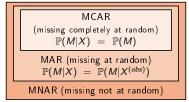
Traumabase clinical records.

An  $n \times p$  matrix, each entry is missing with probability 0.01

- $p = 5 \implies \approx 95\%$  of rows kept;
- $p = 300 \implies \approx 5\%$  of rows kept.

# Missing data and linear models

- Classic literature focuses on estimation and imputation (Rubin 76) via
  - Likelihood based methods under MAR.
  - Multiple imputation under MAR.



#### Linear model

$$Y = X^T \beta^* + \text{noise}$$

- $Y \in \mathbb{R}$  (regression) outcome is always observed
- $X \in \mathbb{R}^d$  contains missing values!
- $\triangleright \beta^*$  model parameter

#### 1. Estimation:

- ightharpoonup provide an estimate of  $\beta^*$
- → Inference, and prediction with complete data.

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#### 2 Prediction:

► We want to predict Y for a new X with missing entries

Warning: A good estimate of  $\beta^*$  does not lead to a prediction of Y

$$X = (\text{na}, 5, \text{na}, -6)$$
  $X^{\top} \beta^* = ??$ 

## Formalizing the problem

► **Assumption** - The response *Y* is a function of the (unavailable) complete data plus some noise:

$$Y = f^*(X) + \varepsilon, \quad X \in \mathbb{R}^d, Y \in \mathbb{R}.$$

Optimization problem:

$$\min_{f:(\mathbb{R}\cup\{\mathbb{N}A\})^d\mapsto\mathbb{R}}\mathcal{R}(f):=\mathbb{E}\left[\left(Y-f(\widetilde{X})\right)^2\right]$$

A Bayes predictor is a minimizer of the risk. It is given by:

$$\widetilde{f}^{\star}(\widetilde{X}) := \mathbb{E}\left[Y|X_{obs(M)},M\right] = \mathbb{E}\left[f(X)|X_{obs(M)},M\right]$$

where  $M \in \{0,1\}^d$  is the missingness indicator.

- lacktriangle The Bayes rate  $\mathcal{R}^\star$  is the risk of the Bayes predictor:  $\mathcal{R}^\star = \mathcal{R}(\tilde{f}^\star)$ .
- **A** Bayes optimal function f achieves the Bayes rate, i.e,  $\mathcal{R}(f) = \mathcal{R}^{\star}$ .

## Supervised learning with missing values

$$\widetilde{X} = X \odot (1 - M) + \text{NA} \odot M$$
. New feature space is  $\widetilde{\mathbb{R}}^d = (\mathbb{R} \cup \{\text{NA}\})^d$ .

$$Y = \begin{pmatrix} 4.6 \\ 7.9 \\ 8.3 \\ 4.6 \end{pmatrix} \tilde{X} = \begin{pmatrix} 9.1 & \text{NA} & 1 \\ 2.1 & \text{NA} & 3 \\ \text{NA} & 9.6 & 2 \\ \text{NA} & 5.5 & 6 \end{pmatrix} X = \begin{pmatrix} 9.1 & 8.5 & 1 \\ 2.1 & 3.5 & 3 \\ 6.7 & 9.6 & 2 \\ 4.2 & 5.5 & 6 \end{pmatrix} M = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

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## Finding the Bayes predictor.

$$f^* \in \underset{f \colon \widetilde{\mathbb{R}}^d \to \mathbb{R}}{\operatorname{argmin}} \mathbb{E}\left[\left(Y - f(\tilde{X})\right)^2\right].$$

$$f^*(\tilde{X}) = \sum_{m \in \{0,1\}^d} \mathbb{E}\left[Y | X_{obs(m)}, M = m\right] \mathbb{1}_{M=m}$$

 $\Rightarrow$  One model per pattern (2<sup>d</sup>) (Rubin, 1984, generalized propensity score)

## Bayes predictor.

$$f^{\star}(\tilde{X}) = \sum_{m \in \{0,1\}^d} \mathbb{E}\left[Y|X_{obs(m)}, M = m\right] \mathbb{1}_{M=m}$$

- Difficulty due to the half nature of the input space
- ► Worst case: 2<sup>d</sup> models to learn

#### Two common strategies:

- Impute-then-regress strategies impute the data then learn on the imputed data set
  - Computationally efficient but possibly inconsistent
- ► Pattern-by-pattern strategies use a different predictor for each missing pattern
  - Consistent by design but intractable in most situations

Summary 8 / 42

#### 1. Impute-then-regress procedures with consistent predictors

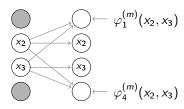
- 2. Linear regression with missing values
- 3. Linear regression: A pattern-by-pattern approach
- 4. Linear regression: Impute-then-regress procedures via zero-imputation
- Random features models: a way to study the success of naive imputation

## Impute-then-Regress procedures

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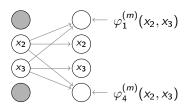
$$g \circ \Phi$$
, where  $\Phi \in \mathcal{F}^I$ ,  $g : \mathbb{R}^d \mapsto \mathbb{R}$ .



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Can Impute-then-Regress procedures be Bayes optimal?

Given an imputation function  $\Phi$ , we define  $g_{\Phi}^{\star}$  the minimizer of the population risk on imputed data as

$$g_\Phi^\star \in \operatorname*{argmin}_{g:\mathbb{R}^d \mapsto \mathbb{R}} \quad \mathbb{E}\left[\left(Y - g \circ \Phi(\widetilde{X})\right)^2
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## Theorem (Le Morvan et al., 2021)

Assume that X admits a density, the response Y is generated as  $Y = f^*(X) + \varepsilon$  and  $\Phi \in \mathcal{F}^I_\infty$  ( $C^\infty$  imputation functions). Then,

- for all missing data mechanisms,
- and for almost all imputation functions,

 $g_{\Phi}^{\star} \circ \Phi$  is Bayes optimal.

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- for all missing data mechanisms,
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$$g_{\Phi}^{\star} \circ \Phi$$
 is Bayes optimal.

For almost all imputation functions, and all missing data mechanisms, a universally consistent algorithm trained on the imputed data is a consistent procedure.

## Which imputation function should one choose?



## Which imputation function should one choose?



Question

Are there continuous Impute-then-Regress decompositions of Bayes predictors?

From now on, we suppose  $f^*$  (Byes predictor with complete data) is smooth and consider the conditional expectation  $\Phi^{CI}$ .

# Learning on conditionally imputed data

Question

What can we say about the optimal predictor on the conditionally imputed data:  $g_{\Phi^{Cl}}^{\star} \circ \Phi^{Cl}$ ?

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What can we say about the optimal predictor on the conditionally imputed data:  $g_{\Phi^{Cl}}^{\star} \circ \Phi^{Cl}$ ?

## Theorem (Le Morvan et al., 2021)

Suppose that  $f^* \circ \Phi^{Cl}$  is not Bayes optimal, and that the probability of observing all variables is strictly positive, i.e., P(M=0,X=x)>0, for all x. Then there is no continuous function g such that  $g \circ \Phi^{Cl}$  is Bayes optimal.

- In the above setting,  $g_{\Phi^{Cl}}^*$  is not continuous. Thus, imputing via conditional expectation leads to a difficult learning problem.
- ► Almost all imputations lead to consistent estimators but some ease the training of the supervised learning algorithm.

## Bayes predictor.

$$f^{\star}(\tilde{X}) = \sum_{m \in \{0,1\}^d} \mathbb{E}\left[Y|X_{obs(m)}, M = m\right] \mathbb{1}_{M=m}$$

#### Two common strategies:

- Impute-then-regress strategies impute the data then learn on the imputed data set
  - Computationally efficient but possibly inconsistent
  - Consistent if used with a non-parametric learning algorithm (forests, tree boosting, nearest neighbor...)
- Pattern-by-pattern strategies use a different predictor for each missing pattern
  - Consistent by design but intractable in most situations

Summary 14 / 42

1. Impute-then-regress procedures with consistent predictors

2. Linear regression with missing values

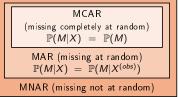
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Kandom features models: a way to study the success of naive imputation

#### Our aim

Predict on new data, which may contain missing entries.



#### Linear model

$$Y = X^T \beta^* + \text{noise}$$

- $Y \in \mathbb{R}$  (regression) outcome is always observed
- $X \in \mathbb{R}^d$  contains missing values!
- $\triangleright \beta^*$  model parameter

Let

$$Y=X_1+X_2+\varepsilon,$$

where  $X_2 = \exp(X_1) + \varepsilon_1$ . Now, assume that only  $X_1$  is observed. Then, the model can be rewritten as

$$Y = X_1 + \exp(X_1) + \varepsilon + \varepsilon_1,$$

where  $f(X_1) = X_1 + \exp(X_1)$  is the Bayes predictor.

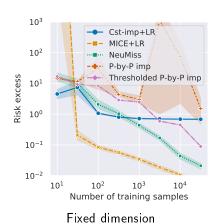
Here, the submodel for which only  $X_1$  is observed is not linear.

- ⇒ There exists a large variety of submodels for a same linear model.
- $\Rightarrow$  Submodel natures depend on the structure of X and on the missing-value mechanism.

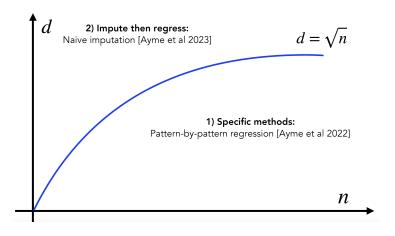
# Handling missing values in linear models for prediction 1/42

#### 2 possible approaches

- ► Patter-by-pattern methods
- ► Impute-then-regress procedures



10<sup>2</sup> 0-imp+SGD opti-imp+Ridge MICE+Ridge  $10^{1}$ Pat-by-Pat NeuMiss **Risk excess** 10<sup>0</sup>  $10^{-1}$  $d = \sqrt{n}$ d = n $10^{-2}$ 10<sup>1</sup>  $10^{2}$  $10^{3}$ Number of features d Fixed sample size



Summary 19/42

1. Impute-then-regress procedures with consistent predictors

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3. Linear regression: A pattern-by-pattern approach

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5. Random features models: a way to study the success of naive imputation

# Specific methods: formalization

▶ Dataset  $\mathcal{D}_n = \{(Z_i, Y_i), i \in [n]\}$  where

$$Z_i = (X_{obs(M_i)}, M_i).$$

New test point  $Z = (X_{obs(M)}, M)$  (with unknown target Y).

## Goal in prediction

Find a linear function  $\hat{f}$  that minimizes the risk

$$R_{\mathsf{miss}}(\widehat{f}) = \mathbb{E}\left[\left(\widehat{f}(Z) - Y\right)^2\right].$$

Consider either

$$ightharpoonup X \sim \mathcal{N}\left(\mu, \Sigma
ight)$$

Gaussian (G)

or,

$$lacksquare$$
  $X|(M=m) \sim \mathcal{N}(\mu^m, \Sigma^m)$  Gaussian pattern mixture model (GPMM)

Decompose the Bayes predictor

$$f^{\star}(Z) = \sum_{m \in \mathcal{M}} f_m^{\star}(X_{obs(m)}) \mathbb{1}_{M=m},$$

with  $f_m^*$  the Bayes predictor conditionally on the event (M = m).

## Proposition

[Le Morvan et al 2020]

If [(MCAR or MAR) and G] or GPMM then, for all  $m \in \mathcal{M}$ ,

$$f_m^*$$
 is linear

## A missing-distribution-free upper bound

Predictor  $\widehat{f}(Z) = \sum_{m \in \mathcal{M}} \widehat{f}_m(X_{obs(m)}) \mathbb{1}_{M=m}$  (pattern-by-pattern OLS) where  $\widehat{f}_m$  is a modified least-square regression rule trained on

$$\mathcal{D}_m = \left\{ (X_{i,obs(m)}, Y_i), M_i = m \right\}.$$

Theorem (simplified) [Le Morvan et al. 2020] [Ayme, Boyer, Dieuleveut, S. 2022]

If [(MCAR or MAR) and G] or GPMM then

$$\mathbb{E}\left[\left(\widehat{f}(Z) - f^{\star}(Z)\right)^{2}\right] \lesssim \log(n)2^{d} \frac{d}{n}$$

where the constant depends on the level of noise.

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where the constant depends on the level of noise.

- ▶ This result does not depend on the distribution of missing patterns.
- Number of parameters is  $p := d2^d$ . This result suffers from the curse of dimensionality even with small d.

# A missing pattern distribution adaptive bound

Idea: Regression only on high frequency missing patterns

$$\widehat{f}(Z) = \sum_{m} \widehat{f}_m(X_{obs(m)}) \mathbb{1}_{M=m} \mathbb{1}_{|\mathcal{D}_m| \geqslant d}.$$

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#### Theorem [Ayme, Boyer, Dieuleveut, S. 2022]

$$\mathbb{E}\left[\left(\widehat{f}(Z) - f^{\star}(Z)\right)^{2}\right] \lesssim \log(n)\mathcal{E}_{p}\left(d/n\right),$$

with  $\mathcal{E}_p(d/n) := \sum_m \min(p_m, d/n)$ .

- ► Valid for MCAR, MAR and MNAR settings.
- Adaptive to missing data distribution via  $\mathcal{E}_p(d/n) \leqslant \operatorname{Card}(\mathcal{M})(d/n)$ .

#### Examples

- 1. Uniform distribution:  $\mathcal{E}_p\left(\frac{d}{n}\right) = 2^d d/n$
- 2. Bernoulli distribution:  $M_i \sim \mathcal{B}(\varepsilon)$  with  $\varepsilon \leqslant d/n$ :  $\mathcal{E}_p\left(\frac{d}{n}\right) = d^2/n$

A lower bound

Let  $\mathcal{P}_p$  be a class of data distributions  $\left\{ \begin{array}{l} X | (M=m) \sim \mathcal{N}(\mu^m, \Sigma^m) \\ \text{Linear model} \\ \mathbb{P}[M=m] = p_m \end{array} \right.$ 

$$\underbrace{\min_{\mathsf{error}}^{\mathsf{Minimax}}(\rho) = \underbrace{\min_{\tilde{f}} \quad \max_{\mathbb{P} \in \mathcal{P}_{\rho}} \quad \mathbb{E}_{\mathbb{P}}\left[(\tilde{f}(Z) - f^{\star}(Z))^{2}\right] }_{\mathsf{Best algo}}$$

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#### Theorem

[Ayme, Boyer, Dieuleveut, S. 2022]

$$\sigma^{2} \mathcal{E}_{p} \left( \frac{1}{n} \right) \lesssim \underset{\text{error}}{\text{Minimax}} (p) \leqslant \mathbb{E} \left[ \left( \widehat{f}(Z) - f^{*}(Z) \right)^{2} \right] \lesssim \log(n) \mathcal{E}_{p} \left( \frac{d}{n} \right)$$

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$$\underbrace{\mathsf{Worst case on a class}}_{\mathcal{P}_p \text{ of problems}}$$

#### Theorem

[Ayme, Boyer, Dieuleveut, S. 2022]

$$\sigma^2 \mathcal{E}_p \left( \frac{1}{n} \right) \lesssim \frac{\mathsf{Minimax}}{\mathsf{error}} (p) \leqslant \mathbb{E} \left[ \left( \widehat{f}(Z) - f^*(Z) \right)^2 \right] \lesssim \log(n) \mathcal{E}_p \left( \frac{d}{n} \right)$$

#### Examples

- Uniform distribution
- ▶ Bernoulli distribution  $M_j \sim \mathcal{B}(\varepsilon)$  with  $\varepsilon \leqslant d/n$

$$\mathcal{E}_p\left(\frac{1}{n}\right) = 2^d/n$$
  $\mathcal{E}_p\left(\frac{d}{n}\right) = 2^d d/n$ 

$$\mathcal{E}_{p}\left(\frac{1}{n}\right) = d/n$$
  $\mathcal{E}_{p}\left(\frac{d}{n}\right) = d^{2}/n$ 

### Take-home messages

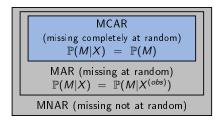
- For data regimes where n is large, several problems can be learned, even for MNAR.
- The procedure can be modified to adapt to the distribution of missing patterns.
- The dimension is an issue, even under the classical assumptions (MAR)

- 1. Impute-then-regress procedures with consistent predictors
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### Impute-then-regress?

- ► Impute-then-regress method
  - 1. Impute the missing values by 0 to get  $X_{imp}$  (e.g., via df.fillna(0))
  - 2. Perform a SGD regression

- Impute-then-regress method
  - 1. Impute the missing values by 0 to get  $X_{imp}$  (e.g., via df.fillna(0))
  - 2. Perform a SGD regression
- Focus on MCAR values:  $M_1, \ldots, M_d \sim \mathcal{B}(\rho)$  $\rho = \text{probability to be observed}$



impute by 0 = doesn't exploit observed values?

### Risk decomposition

- $ightharpoonup R^* = \text{optimal risk without missing data}$
- $ightharpoonup R_{
  m miss}^{\star} = {
  m optimal} \; {
  m risk} \; {
  m with} \; {
  m missing} \; {
  m data}$

$$\Delta_{\mathrm{miss}} := \mathit{R}^{\star}_{\mathrm{miss}} - \mathit{R}^{\star} \qquad \qquad \text{(missing data error)}$$

- $ightharpoonup R_{\rm imp}( heta) = {
  m the \ risk \ of} \ f_{ heta}(X_{
  m obs},M) = heta^ op X_{
  m imp}$
- $lacktriangleright R_{
  m imp}( heta_{
  m imp}^\star) =$  optimal risk of linear prediction after imputation by 0

$$\Delta_{\mathrm{imp/miss}} := R_{\mathrm{imp}}(\theta_{\mathrm{imp}}^{\star}) - R_{\mathrm{miss}}^{\star} \qquad \qquad \text{(imputation error)}$$

Risk decomposition:

$$R_{
m miss}(f_{ heta}) = R^{\star} + \underbrace{\Delta_{
m miss} + \Delta_{
m imp/miss}}_{
m missing data and imputation error} + \underbrace{R_{
m miss}(f_{ heta}) - R_{
m imp}(\theta_{
m imp}^{\star})}_{
m estimation/optimization error}$$

### Toy example: how imputed inputs disturb learning

- ► Complete model
  - $Y = X_1$
  - $\qquad \qquad X = (X_1, \ldots, X_1)$
  - $ightharpoonup R^* = 0$
  - $ightharpoonup M_1,\ldots,M_d\sim \mathcal{B}(1/2)$

- ► Complete model
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  - $X = (X_1, ..., X_1)$
  - $R^* = 0$
  - $ightharpoonup M_1, \ldots, M_d \sim \mathcal{B}(1/2)$
- $\blacktriangleright$  With imputed inputs and  $\theta_1 = (1, 0, \dots, 0)^{\top}$ 
  - $X_{imn}^{\top}\theta_1 = X_1M_1$
- lacktriangle With imputed inputs and  $\theta_2 = 2(1/d, 1/d, \dots, 1/d)^{\top}$ 
  - $begin{array}{c} begin{array}{c} X_{\mathsf{imp}}^{\top} \theta_2 = \frac{2}{d} X_1 \sum_i M_i \end{array}$

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  - $begin{array}{c} begin{array}{c} X_{\mathsf{imp}}^{\top} \theta_2 = \frac{2}{d} X_1 \sum_i M_i \end{array}$

correlation  $\Rightarrow$  low imputation/missing values error ?

## Learning w/ imputed-by-0 data = ridge reg?

Ridge-regularized risk with complete data

$$R_{\lambda}(\theta) = R(\theta) + \lambda \|\theta\|_{2}^{2}$$

Standard in high-dimension settings

#### Theorem

[Ayme, Boyer, Dieuleveut, S. 2023]

Under the MCAR Bernoulli model of probability  $\rho$  of observation and  $Var(X_j) = 1 \ \forall j$ ,

$$R_{\mathsf{imp}}(\theta) = R(\rho\theta) + \rho(1-\rho)\|\theta\|_2^2$$

#### Consequences

- 1.  $\Delta_{\rm miss} + \Delta_{\rm imp/miss} = {\rm ridge}$  bias for  $\lambda = \frac{1-\rho}{\rho}$
- 2.  $\theta_{imp}^{\star}$  on a small ball around 0 (implicit regularization)
- Imputed MCAR missing values seem to be at the same price of ridge regularization

### Learning with low-rank and imputed-by-0 data

**Low-rank data**: covariance matrix  $\Sigma = [XX^T]$  is

$$\Sigma = \sum_{j=1}^{r} \lambda_j v_j v_j^{\top},$$

with  $\lambda_1 = \cdots = \lambda_r$  and  $r \ll d$ .

Bias on low-rank data:

$$\Delta_{
m miss} + \Delta_{
m imp/miss} \lesssim rac{1-
ho}{
ho}rac{r}{d}\mathbb{E}[Y^2]$$

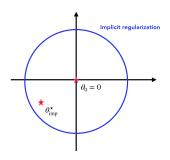
correlation ⇒ low imputation/missing values error !

### Learning with imputed-by-0 data via SGD

Averaged SGD iterates:

$$\left\{ \begin{array}{ll} \theta_{\mathsf{imp},t} &= \left[I - \gamma X_{\mathsf{imp},t} X_{\mathsf{imp},t}^{\top}\right] \theta_{\mathsf{imp},t-1} + \gamma Y_{t} X_{\mathsf{imp},t} \\ \bar{\theta}_{\mathsf{imp},n} &= \frac{1}{n+1} \sum_{t=1}^{n} \theta_{\mathsf{imp},t} \end{array} \right.$$

- ► Why use SGD?
  - 1. Streaming online (one pass only)
  - 2. Minimizes directly the generalization risk *R*
  - 3. Friendly assumptions
  - 4. Leverage the implicit regularization of naive imputations choosing  $\theta_{\text{imp.0}} = 0$  and  $\gamma = 1/d\sqrt{n}$ .



### Learning with imputed-by-0 data via SGD

#### Theorem

[Ayme, Boyer, Dieuleveut, S. 2023]

Under classical assumptions for SGD,

$$\mathbb{E}\left[R_{\mathsf{imp}}(\bar{\theta}_{\mathsf{imp},n})\right] - R^\star \leqslant \Delta_{\mathrm{miss}} + \Delta_{\mathrm{imp/miss}} + \frac{d}{\sqrt{n}} \|\theta_{\mathsf{imp}}^\star\|_2^2 + \frac{\mathsf{noise \ variance}}{\sqrt{n}}$$

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Example: low-rank setting

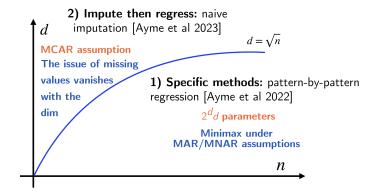
$$\mathbb{E}\left[R_{\mathsf{imp}}(\bar{\theta}_{\mathsf{imp},n})\right] - R^\star \lesssim \left(\frac{1}{\rho\sqrt{n}} + \frac{1-\rho}{d}\right)\frac{r}{d}\mathbb{E}Y^2 + \frac{\mathsf{noise \ variance}}{\sqrt{n}}$$

▶ Imputation bias vanishes for  $d \gg \sqrt{n}$ 

### Naive imputation implicitly regularizes HD linear models

MCAR inputs (observation rate=ρ) Performing standard linear regression on imputed-by-0 data Adding a ridge regularization w/ parameter  $\lambda = \frac{1-\text{observation rate}}{\text{observation rate}}$ 

► All in all



Summary 35 / 42

1 Impute then regress procedures with consistent predictors

2. Linear regression with missing values

3. Linear regression: A pattern-by-pattern approach

4. Linear regression: Impute-then-regress procedures via zero-imputation

5. Random features models: a way to study the success of naive imputation

### Toy example of Random features

Latent observations (hidden)  $Z \in \mathbb{R}^p$  with p = 4:

$$Z = (age, weight, height, hair color)$$

- ► Target:  $Y = \beta^{\top} Z + \text{noise}$
- ▶ We take **randomly** *d* features of *Z* to obtain *X*:
  - ightharpoonup Low dimension d=2:

$$X = (age, height)$$

uncorrelated regime

ightharpoonup High dimension d=10:

$$X = (age, height, height, age, weight, hair color, weight, age, height)$$

correlated regime

### First random features models

#### Gaussian random features:

- Input:  $X_{i,j} = Z_i^\top W_j$ Latent variables  $Z_1, \dots, Z_n \overset{i.i.d.}{\sim} \mathcal{N}(0, I_p)$ Random weights  $W_1, \dots, W_d \overset{i.i.d.}{\sim} \mathcal{U}(\mathbb{S}^{p-1})$
- Output:  $Y_i = Z_i^{\top} \beta^* + \text{noise of variance } \sigma^2$

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Input:  $X_{i,j} = Z_i^\top W_j$ Latent variables  $Z_1, \dots, Z_n \overset{i.i.d.}{\sim} \mathcal{N}(0, I_p)$ Random weights  $W_1, \dots, W_d \overset{i.i.d.}{\sim} \mathcal{U}(\mathbb{S}^{p-1})$ 

• Output:  $Y_i = Z_i^{\top} \beta^* + \text{noise of variance } \sigma^2$ 

#### Key quantities:

- $ightharpoonup R^*(d) = \text{optimal risk without missing data}$
- $ightharpoonup R_{
  m miss}^{\star}(d)=$  optimal risk with missing data

$$\Delta_{\mathrm{miss}}(d) := [R_{\mathrm{miss}}^{\star}(d) - R^{\star}(d)]$$

 $ightharpoonup R^\star_{\mathrm{imp}}(d) = \mathsf{optimal}$  risk of linear prediction after imputation by 0

$$\Delta_{\mathrm{imp/miss}}(d) := \left[ R_{\mathrm{imp}}^{\star}(d) - R_{\mathrm{miss}}^{\star}(d) \right]$$

$$R_{\mathrm{miss}}(f_{\bar{\theta}}) = R^{\star}(d) + \underbrace{\Delta_{\mathrm{miss}}(d) + \Delta_{\mathrm{imp/miss}}(d)}_{\text{missing data and imputation error}} + \underbrace{\left[ R_{\mathrm{miss}}(f_{\bar{\theta}}) - R_{\mathrm{imp}}^{\star}(d) \right]}_{\text{estimation/optimization error}}$$

#### Theorem

[Ayme, Boyer, Dieuleveut, Scornet 2024]

Under MCAR assumptions,

Optimal risk without missing data

$$[R^{\star}(d)] = \begin{cases} \sigma^2 + \frac{p-d}{p} \|\beta^{\star}\|_2^2, & \text{when } d$$

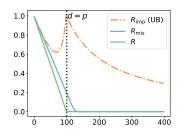
Error due to missing data

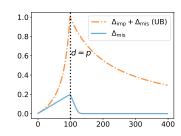
$$\left\{ \begin{array}{l} \Delta_{\mathrm{miss}}(d) = (1-\rho)\frac{d}{p}\|\beta^\star\|_2^2 & \text{when } d$$

Error due to linear prediction on imputed data

$$\begin{cases} \Delta_{\mathrm{imp/miss}}(d) \leqslant \frac{\rho(d-1)}{p - \rho(d-1) - 2} \Delta_{\mathrm{miss}}(d) & \text{when } d$$

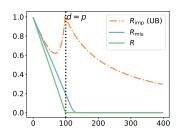
### The story of naive imputation and missing values

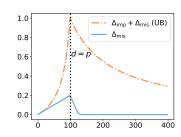




- ► Low dimensions (uncorrelated regime):
  - Missing values error represents  $1-\rho$  of the explained variance without missing values: missing features are lost
  - ► Error due to imputation is negligible: imputation is optimal

### The story of naive imputation and missing values





- Low dimensions (uncorrelated regime):
  - Missing values error represents  $1-\rho$  of the explained variance without missing values: missing features are lost
  - ► Error due to imputation is negligible: imputation is optimal
- ► High dimensions (correlated regime):
  - Error due to missing values error decreases exponentially fast: missing features can be retrieve from the others
  - ► Extension of the low rank setting for the imputation bias: correlation ⇒ low imputation bias

 $\lim_{d} \Delta_{\text{imp/miss}}(d) + \Delta_{\text{miss}}(d) = 0$  **still holds**, for instance when

- ► General random features:
  - Non-linear inputs:  $X_{i,j} = \psi(Z_i, W_j)$
  - Non-linear output:  $Y = f^*(Z) + \varepsilon$  with  $f^*$  continuous

Ex: Random Fourier features (RFF)

$$W_j = (A_j, B_j) \sim \mathcal{N}(0, I) \otimes \mathcal{U}([0, 2\pi])$$
  
$$X_{i,j} = \cos(A_j^\top Z_i + B_j)$$

► Non-MCAR missing values:

Ex: Logistic model on the latent covariate:

$$\mathbb{P}(M_j = 1|Z) = \frac{1}{1 + e^{w'_{0j} + w'_j^{\top} Z}}$$

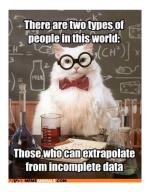
Conclusion 41/42

Bayes predictor  $f^{\star}(\tilde{X}) = \sum_{m \in \{0,1\}^d} \mathbb{E}\left[Y | X_{obs(m)}, M = m\right] \mathbb{1}_{M=m}$ .

#### Two common strategies:

- Impute-then-regress strategies impute the data then learn on the imputed data set
  - Computationally efficient but possibly inconsistent
  - Consistent if used with a non-parametric learning algorithm
  - Linear models Zero imputation is inconsistent but converges in high-dimensional settings (rate of  $\sqrt{d/n}$ )
- Pattern-by-pattern strategies use a different predictor for each missing pattern
  - Consistent by design but intractable in most situations
  - Linear models Rate of consistency of  $d^2/n$  for independent Bernoulli missing indicators **but**  $2^d/n$  in general (not improvable)

Conclusion 42 / 42

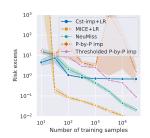


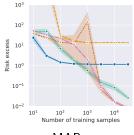
# Thank you!

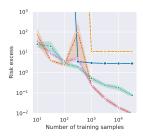
- Near-optimal rate of consistency for linear models with missing values. A. Ayme, C. Boyer, A. Dieuleveut, E. Scornet. ICML 2022.
- Naive imputation implicitly regularizes high-dimensional linear models. A. Ayme, C. Boyer, A. Dieuleveut, E. Scornet. ICML 2023.
- Random features models: a way to study the success of naive imputation.

  A. Ayme, C. Boyer, A. Dieuleveut, E. Scornet. ICML 2024.

### Numerical XP for prediction







WCAR		
Unbiased	Rate	
No	Fast	
Yes	Fast	
Yes	Fast	
Yes	Slow	
Yes	Slow	
	Unbiased No Yes Yes Yes Yes	

MCAD

MAR		
Unbiased	Rate	
No	Fast	
No	Fast	
Yes	Slow	
Yes	Slow	
Yes	Fast	

MNAR	
Unbiased	Rate
No	Fast
No	Fast
Yes	Slow
Yes	Slow
Yes	Fast