Debiased stochastic gradient descent to handle missing data in the linear regression case and its perspectives¹ Laboratoire Heudiasyc, UTC Compiègne

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Motivation: large-scale incomplete data

• Large-scaling: large *n* (number of observations), large *d* (dimension of the observations)

 \hookrightarrow Stochastic / online learning algorithms.

• Incompleteness for many reasons: delete observations with NA \rightarrow keep only 5% of the rows.

 \hookrightarrow Simple algorithmic solution?

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NA: Not Available							

SGD with missing values

2 Theoretical results

- Without missing values: rates
- Convergence of our algorithm
- Adaptation to estimated missing probabilities

3 Experiments

4 Perspectives

- Finite-sample setting
- More general loss function
- More general missing-data mechanisms

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Linear regression model

• $(X_{i:}, y_i)_{i \ge 1} \in \mathbb{R}^d \times \mathbb{R}$ i.i.d. observations

$$y_i = X_{i:}^T \beta^\star + \epsilon_i,$$

parametrized by $\beta^* \in \mathbb{R}^d$, with a noise term $\epsilon_i \in \mathbb{R}$.

- Loss function: $f_i(\beta) = (\langle X_{i:}, \beta \rangle y_i)^2 / 2.$
- True risk minimization:

$$eta^{\star} = rgmin_{eta \in \mathbb{R}^d} \left\{ R(eta) := \mathbb{E}_{(X_i:, y_i)} \left[f_i(eta)
ight]
ight\}$$

- Stochastic gradient method.
 - . At the heart of Machine Learning.
 - . Especially useful in high dimension.

Objective

Challenges

- Large-scaling: large number of observations, large d.
- Incomplete data: missing covariates, $(X_{i:})$'s partially known.
- Online-setting: the data come as it goes along.

How to adapt algorithms to the missing data case?

Optimization without missing values

Stochastic gradient descent

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• SGD: using unbiased estimates of $\nabla R(\beta_{k-1})$.

$$\beta_k = \beta_{k-1} - \alpha g_k(\beta_{k-1})$$

where α is the step-size and $g_k(\beta_{k-1}) = \nabla f_k(\beta_{k-1})$.

$$\mathbb{E}\left[g_k(\beta_{k-1})|\sigma(X_{1:},y_1,\ldots,X_{k-1:},y_{k-1})\right]=\nabla R(\beta_{k-1}),$$

• Averaged SGD: using the Polyak-Ruppert averaged iterates.

$$\bar{\beta}_k = \frac{1}{k+1} \sum_{i=0}^k \beta_i$$

 \checkmark It scales with large data

Optimization without missing values

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 \checkmark It scales with large data

2 challenges

- Obtaining unbiased stochastic gradients with missing data?
- Deriving rates of convergence?

Missing values setting Formalism

• Missing-data pattern (or mask) $D: D_{i:} \in \{0,1\}^d$, such that

$$\mathcal{D}_{ij} = \left\{egin{array}{cc} 0 & ext{if the } (i,j) ext{-entry is missing} \ 1 & ext{otherwise.} \end{array}
ight.$$

• Access to $X^{\mathrm{NA}}_{i:} \in (\mathbb{R} \cup \{\mathtt{NA}\})^d$ instead of $X_{i:}$

$$X_{i:}^{\mathrm{NA}} := X_{i:} \odot D_{i:} + \mathrm{NA}(1_d - D_{i:}),$$

 \odot element-wise product, $\mathbf{1}_d = (1 \dots 1)^T \in \mathbb{R}^d$, NA imes 0 = 0, NA imes 1 = NA.



 Heterogeneous Missing Completely At Random setting (MCAR) → Bernoulli mask

$$D = (\delta_{ij})_{1 \le i \le n, 1 \le j \le d}$$
 with $\delta_{ij} \sim \mathcal{B}(p_j)$,

with $1 - p_j$ the probability that the *j*-th covariate is missing.

 \checkmark different missing probability for each covariate



Heterogeneous case:

 $p_1 = 0.5, p_2 = 0.67, p_3 = 0.83, p_4 = 0.33, p_5 = 0.92.$

Homogeneous case: p = 0.65.

Existing works

Aim: estimate parameters of a linear regression.

- EM algorithm^a: maximization of the observed likelihood.
 - × strong assumption on the data distribution
 - X computationally costly, does not scale with large data.
 - × not simple to establish, no many implementations.
- Simple imputation: mean imputation, performing regression.



Dealing with missing values Existing works

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- Simple imputation: mean imputation, performing regression.
 - > bias in the estimates, correlation between the variables overestimated.
- (Multiple) imputation: mice^b
 - **X** not online, difficult to establish for Ridge regression.

^aDempster, Laird, and Rubin, "Maximum likelihood from incomplete data via the EM algorithm".

^bBuuren and Groothuis-Oudshoorn, "mice: Multivariate imputation by chained equations in R".

Naive imputation and debiasing

Naive imputation and debiasing

- Imputing naively by 0.
- Modifying usual algorithms to account for the imputation error.
- Dantzig selector².
- Lasso³.
- SGD⁴.

²Mathieu Rosenbaum, Alexandre B Tsybakov, et al. "Sparse recovery under matrix uncertainty". In: *The Annals of Statistics* 38.5 (2010), pp. 2620–2651.

³Po-Ling Loh and Martin J Wainwright. "High-dimensional regression with noisy and missing data: Provable guarantees with non-convexity". In: *Advances in Neural Information Processing Systems*. 2011, pp. 2726–2734.

⁴Anna Ma and Deanna Needell. "Stochastic Gradient Descent for Linear Systems with Missing Data". In: *arXiv preprint arXiv:1702.07098* (2017).

Our strategy inspired by Ma et Needell Online-streaming: for a new observation $(X_{k:}^{NA}, y_k)$

• Imputing the missing values by 0.

 $\tilde{X}_{k:} = X_{k:}^{\text{NA}} \odot D_{k:} = X_{k:} \odot D_{k:}$ imputed covariates

• Using a **debiased gradient** for the **averaged SGD**: Find $\tilde{g}_k(\beta_k)$ such that $\mathbb{E}[\tilde{g}_k(\beta_{k-1}) | \mathcal{F}_{k-1}] = \nabla R(\beta_{k-1})$

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•
$$\mathcal{F}_{k-1} = \sigma(X_{1:}, y_1, D_{1:} \dots, X_{k-1:}, y_{k-1}, D_{k-1:})$$

- $\cdot \nabla R(\beta_{k-1}) = \mathbb{E}_{(X_k; y_k)}[X_k: (X_k^T \beta_{k-1} y_k)]$
- . No access to $X_{k:}$, only to $ilde{X}_{k:}$.
- . Another source of randomness: $\mathbb{E} = \mathbb{E}_{(X_k, y_k), D_k} \stackrel{\text{indep}}{=} \mathbb{E}_{(X_k, y_k)} \mathbb{E}_{D_k}$
- . $\mathbb{E}_{D_{k:}}|\mathcal{F}_{k-1} \rightsquigarrow \mathbb{E}_{D_{k:}}|$
 - $\checkmark\,$ Mask at step k independent from the previous constructed iterate.

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• Using a **debiased gradient** for the **averaged SGD**: Find $\tilde{g}_k(\beta_k)$ such that $\mathbb{E}[\tilde{g}_k(\beta_{k-1}) | \mathcal{F}_{k-1}] = \nabla R(\beta_{k-1})$

$$\mathbb{E}_{D_{k:}}\left[\tilde{X}_{k:}\right] = \mathbb{E}_{D_{k:}}\left[\begin{pmatrix}\delta_{k1}X_{k1}\\\vdots\\\delta_{kd}X_{kd}\end{pmatrix}\right] = \begin{pmatrix}p_{1}X_{k1}\\\vdots\\p_{d}X_{kd}\end{pmatrix}$$

Thus

$$\mathbb{E}_{D_{k:}}\left[P^{-1}\tilde{X}_{k:}\right] := \begin{pmatrix}p_1^{-1} & & \\ & \ddots & \\ & & p_d^{-1}\end{pmatrix}\begin{pmatrix}p_1X_{k1}\\ \vdots\\ p_dX_{kd}\end{pmatrix} = X_{k:}$$

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One obtains

$$\tilde{g}_k(\beta_{k-1}) = P^{-1}\tilde{X}_{k:}\left(\tilde{X}_{k:}^T P^{-1}\beta_{k-1} - y_k\right) - (I-P)P^{-2} \operatorname{diag}\left(\tilde{X}_{k:}\tilde{X}_{k:}^T\right)\beta_{k-1}.$$

Averaged SGD for missing values

Debiasing the gradient

Algorithm 1 Averaged SGD for Heterogeneous Missing Data

Input: data
$$\tilde{X}, y, \alpha$$
 (step size)
Initialize $\beta_0 = 0_d$.
Set $P = \text{diag}((p_j)_{j \in \{1,...,d\}}) \in \mathbb{R}^{d \times d}$.
for $k = 1$ to n do
 $\tilde{g}_k(\beta_{k-1}) = P^{-1}\tilde{X}_{k:} \left(\tilde{X}_{k:}^T P^{-1}\beta_{k-1} - y_k\right) - (I - P)P^{-2}\text{diag}\left(\tilde{X}_{k:}\tilde{X}_{k:}^T\right)\beta_{k-1}$
 $\beta_k = \beta_{k-1} - \alpha \tilde{g}_k(\beta_{k-1})$
 $\bar{\beta}_k = \frac{1}{k+1} \sum_{i=0}^k \beta_i = \frac{k}{k+1} \bar{\beta}_{k-1} + \frac{1}{k+1} \beta_k$
end for

- $p = 1 \Rightarrow P^{-1} = I_d$ standard least squares stochastic algorithm.
- Computation cost for the gradient still weak.
- Trivially extended to ridge regularization (no change for the gradient): $\min_{\beta \in \mathbb{R}^d} R(\beta) + \lambda \|\beta\|^2, \lambda > 0$

SGD with NA: Take home message

- \checkmark We aim to estimate β^* with missing data.
- ✓ We consider an heterogeneous MCAR framework.
 - We provide an unbiased gradient oracle of the true risk.
- ✓ Only for Least Squares Regression.
- Requires independent points at each iteration: only for the first pass.
- Requires the knowledge of P.

Convergence?

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Optimization without missing values

• F is convex and L-smooth⁵ i.e. if F is twice differentiable,

 $\forall \beta \in \mathbb{R}^d, 0 \leq |\text{eigenvalues}(\nabla^2 F(\beta))| \leq L.$

X Convergence rate: $\mathcal{O}(k^{-1/2})$

- *F* is μ-strongly convex and *L*-smooth.
 X Convergence rate: O(μk⁻¹)
- *F* is convex and quadratic⁶.
 ✓ Convergence rate: *O*(*k*⁻¹)

⁵Arkadi Nemirovski et al. "Robust stochastic approximation approach to stochastic programming". In: *SIAM Journal on optimization* 19.4 (2009), pp. 1574–1609.

⁶Eric Moulines and Francis R Bach. "Non-asymptotic analysis of stochastic approximation algorithms for machine learning". In: *Advances in Neural Information Processing Systems*. 2011, pp. 451–459.

Technical lemmas

- Goal: establish a convergence rate.
- Assumptions on the data: $(X_{k:}, y_k) \in \mathbb{R}^d \times \mathbb{R}$ i.i.d., $\mathbb{E}[||X_{k:}||^2]$ and $\mathbb{E}[y_k^2]$ finite, $H := \mathbb{E}_{(X_{k:}, y_k)}[X_{k:}X_{k:}^T]$ invertible.

Lemma: noise induced by the imputation by 0 is structured

 $(\tilde{g}_k(\beta^{\star}))_k$ with β^{\star} is \mathcal{F}_k -measurable and $\forall k \geq 0$,

- $\mathbb{E}[\tilde{g}_k(\beta^\star) \mid \mathcal{F}_{k-1}] = 0$ a.s.
- $\mathbb{E}[\|\tilde{g}_k(\beta^*)\|^2 | \mathcal{F}_{k-1}]$ is a.s. finite.
- $\mathbb{E}[\tilde{g}_k(\beta^*)\tilde{g}_k(\beta^*)^T] \preccurlyeq C(\beta^*) = c(\beta^*)H.$

Lemma: $(\tilde{g}_k(\beta^*))_k$ are **a.s. co-coercive**

For any k,

- \tilde{g}_k is $L_{k,D}$ -Lipschitz
- there exists a random primitive function \tilde{f}_k which is a.s. convex

Convergence results

Theorem: convergence rate of $\mathcal{O}(k^{-1})$, streaming setting Assume that for any i, $||X_{i:}|| \leq \gamma$ almost surely for some $\gamma > 0$. For any constant step-size $\alpha \leq \frac{1}{2L}$, our algorithm ensures that, for any $k \geq 0$:

$$\mathbb{E}\left[R\left(\bar{\beta}_{k}\right)-R(\beta^{\star})\right] \leq \frac{2}{k} \left(\underbrace{\sqrt{c(\beta^{\star})d}}_{\text{variance term}} + \underbrace{\frac{\|\beta_{0}-\beta^{\star}\|}{\sqrt{\alpha}}}_{\text{bias term}}\right)^{2}$$

• $L := \sup_{k,D} \text{Lipschitz constants of } \tilde{g}_k$

• $p_m = \min_{j=1,...d} p_j$ minimal probability to be observed among the variables.

•
$$c(\beta^{\star}) = \underbrace{\frac{\operatorname{Var}(\epsilon_k)}{p_m^2}}_{\text{increasing with the missing values rate}} \operatorname{Var}(\frac{1}{p_m^2}) \gamma^2 \|\beta^{\star}\|^2$$

Theoretical results Comments

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- Optimal rate for least-squares regression.
- In the complete case: same bound as Bach and Moulines.
- Bound on the iterates for the ridge regression $(\beta \to R(\beta) + \lambda \|\beta\|^2$ is 2λ -strongly convex).

$$\mathbb{E}\left[\left\|\overline{\beta}_{k}-\beta^{\star}\right\|^{2}\right] \leq \frac{1}{\lambda k} \left(\sqrt{c(\beta^{\star})d}+\frac{\left\|\beta_{0}-\beta^{\star}\right\|}{\sqrt{\alpha}}\right)^{2}$$

Theoretical results What impact of missing values?

Fewer complete observations is better than more incomplete ones: is it better to access 200 incomplete observations (with a probability 50% of observing) or to have 100 complete observations?





Theoretical results What impact of missing values?

Fewer complete observations is better than more incomplete ones: is it better to access 200 incomplete observations (with a probability 50% of observing) or to have 100 complete observations?

- without missing observations: variance bound scales as $\mathcal{O}\left(\frac{\operatorname{Var}(\epsilon_k)d}{k}\right)$.
- with missing observations: $O\left(\frac{\operatorname{Var}(\epsilon_k)d}{kp_m^2} + \frac{C(X,\beta^*)}{kp_m^3}\right)$.
- variance bound larger by a factor p_m^{-1} for the estimator derived from k incomplete observations than for $k \times p_m$ complete observations.

The variance bound for 200 incomplete observations (with a probability 50% of observing) is twice as large as for 100 complete observations.

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What impact of missing values ?

We do better than discarding all observations which contain missing values:

$$X = \begin{pmatrix} X_1 & X_2 & X_3 & X_1 & X_2 & X_3 \\ 12 & 28 & 31 \\ NA & 23 & 89 \\ 32 & 6 & 24 \\ \vdots & \vdots & \vdots \\ NA & 3 & 7 \end{pmatrix} \qquad X = \begin{pmatrix} 12 & 28 & 31 \\ NA & 23 & 89 \\ 32 & 6 & 24 \\ \vdots & \vdots & \vdots \\ NA & 3 & 7 \end{pmatrix}$$

What impact of missing values ?

We do better than discarding all observations which contain missing values:

Example in the homogeneous case with p the proportion of being observed.

- keeping only the complete observations, any algorithm:
 - . number of complete observations $k_{co} \sim \mathcal{B}(k, p^d)$.
 - statistical lower bound: $\frac{\operatorname{Var}(\epsilon_k)d}{k_{res}}$.
 - . in expectation, lower bound on the risk larger than $\frac{\operatorname{Var}(\epsilon_k)d}{kn^d}$.
- keeping all the observations, averaged SGD: upper bound $O\left(\frac{\operatorname{Var}(\epsilon_k)d}{kp^2} + \frac{C(X,\beta^*)}{kp^3}\right)$.

Our strategy has an upper-bound p^{d-3} smaller than the lower bound of any algorithm relying only on the complete observations.

Result with estimated missing probabilities

Finite-sample setting: *n* is fixed

Algorithm and main result: requirement of $(p_j)_{j=1,...,d}$. \rightarrow estimator \bar{eta}_k

In practice: estimated missing probabilities $(\hat{p}_j)_{j=1,...,d}$ \rightarrow estimator $\bar{\hat{\beta}}_k$. (finite-sample setting: first half of the data to evaluate (\hat{p}_i) , second half to build $\bar{\hat{\beta}}_k$).

Result with estimated missing probabilities (simplified version) Under additional assumptions of **bounded iterates** and **strong**

convexity of the risk, Algorithm 1 ensures that, for any $k \ge 0$:

$$\mathbb{E}\left[R(\bar{\hat{\beta}}_k)-R(\bar{\beta}_k)\right]=\mathcal{O}(1/kp_m^6),$$

with $p_m = \min_{j \in \{1,\ldots,d\}} p_j$.

Convergence rates: Take home message

New results:

- ✓ Fast convergence rate because the noise is structured. Optimal w.r.t. k.
- ✓ Dependence with p: much better than deleting incomplete data, but not as good as pk complete observations
- ✓ Convergence with strong-convexity and estimated probabilities (preserved 1/k, degraded dependence in p)

Open questions:

What about empirical risk? [to be continued.]

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Experiments Synthetic data: setting

- $X_{i:} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \Sigma)$, where Σ with uniform random eigenvectors and decreasing eigenvalues, $\epsilon_i \sim \mathcal{N}(0, 1)$
- $y_i = X_{i:}\beta + \epsilon_i$, for β fixed
- d = 10, 30% missing values.
- AvSGD averaged iterates with a constant step size $\alpha = \frac{1}{2L}^{a}$.
- SGD^b with iterates $\beta_{k+1} = \beta_k \alpha_k \tilde{g}_{i_k}(\beta_k)$, and decreasing step size $\alpha_k = \frac{1}{\sqrt{k+1}}$.
- SGD_cst^b with a constant step size $\alpha = \frac{1}{2L}^{a}$

^aL is considered to be known.

 $^b{\rm Ma}$ and Needell, "Stochastic Gradient Descent for Linear Systems with Missing Data".

Synthetic data: convergence rate

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Figure: Empirical excess risk $(R_n(\beta_k) - R_n(\beta^*))$.

- Multiple passes (left): saturation.
- One pass (right): saturation for SGD_cst, $\mathcal{O}(n^{-1/2})$ for SGD, $\mathcal{O}(n^{-1})$ for AvSGD.

Real dataset: Superconductivity, prediction task

- Goal: predict the critical temperature of each superconductor. **Complete** dataset: 81 guantitatives features, 21263 superconductors.
- Introduction of 30% of heterogeneous MCAR missing values, probabilities of being observed vary between 0.7 and 1.
- Dataset divided into training and test set, with no missing values in the test set.
- Prediction of the critical temperature: $\hat{y}_{n+1} = X_{n+1}^T \hat{\beta}$ with the coefficient

 - . $\hat{\beta} = \beta_n^{\text{AvSGD}}$ by applying **AvSGD** on the training set. . $\hat{\beta} = \beta_n^{\text{EM}}$ by applying the EM algorithm on the training set.
 - $\hat{\beta} = \bar{\beta}_{n}^{\text{AvSGD}}$ by imputing the missing data naively by the mean in the training set, and applying the averaged SGD without missing data (Mean+AvSGD)

Real dataset: Superconductivity, prediction task



Figure: Prediction error $\|\hat{y} - y\|^2 / \|y\|^2$ boxplots.

- EM out of range (due to large number of covariates).
- AvSGD performs well, very close to the one obtained from the complete dataset (AvSGD complete) with or without_regularization.

Take home message

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New results:

 $\checkmark\,$ SGD for dealing with heterogeneous MCAR data with a least squares loss.

Open questions:

- Dealing with more general loss function. [to be continued.]
- More complex missing-data patterns such as MAR and MNAR. [to be continued.]

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Context:

- Finite-sample setting: n is fixed
- Minimizing the empirical risk:

$$\beta_{\star}^{n} = \arg\min_{\beta \in \mathbb{R}^{d}} \left\{ R_{n}(\beta) := \frac{1}{n} \sum_{i=1}^{n} f_{i}(\beta) \right\}$$

Point to discuss:

- True risk in the finite sample setting?
- Unbiased gradients for the empirical risk?
- Interest of the empirical risk in presence of missing data?

Remark 1: convergence rate for the true risk when *n* is fixed

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✓ Same convergence rate holds.

But only for one epoch (= use only once each data). Otherwise: $D_k \not\cong \beta_{k-1} \rightarrow$ bias in the gradient.

Remark 2: no unbiased gradients for the empirical risk?

How to choose the k-th obstervation ?

- \checkmark k uniformly at random \Rightarrow we use a data several times.
- × k not chosen uniformly at random \Rightarrow sampling not uniform and bias in the gradient.

Remark 2: no unbiased gradients for the empirical risk?

How to choose the k-th obstervation ?

- \checkmark k uniformly at random \Rightarrow we use a data several times.
- × k not chosen uniformly at random \Rightarrow sampling not uniform and bias in the gradient.

Idea? Interesting paper on without-replacement sampling^a

- Draw a new permutation on $\{1, \ldots, n\}$ uniformly at random and process the individual in that order.
- Results on the convergence rate preserved for SGD.
- To be adapted for the averaged SGD with NA.

^aShamir, "Without-replacement sampling for stochastic gradient methods".

Remark 3: is the empirical risk natural with missing values?

• Without NA: interest of the empirical risk is known exactly \Rightarrow we can minimize it with precision.

• Without NA: empirical risk not observed.

✓ Gradient debiased for least-squares loss.Open question: What for the logistic loss?

$$f_i(\beta) = \frac{1}{n} \sum_i \log(1 + \exp(-y_i X_i^T \beta)), y_i \in \{1, -1\}$$

Gradient: $\nabla f_i(\beta) = \frac{-y_i X_i}{1 + \exp(y_i X_i^T \beta)}$

- Debiasing the gradient?
- Deriving the theoretical results?

- Gradient: $\nabla f_k(\beta) = \frac{-y_k X_k}{1 + \exp(y_k X_k^T \beta)}$.
- Iteration k: $\beta_k = \beta_{k-1} \alpha \tilde{g}_k(\beta)$.

PB for debiasing: compute $\mathbb{E}\left[\frac{u}{1+\exp(u)}\right]$, when *u* is Gaussian. Ideas:

- \checkmark Partially debiasing (only the numerator),
- $\checkmark\,$ Approximating the gradient and debiasing this approximation.
- \rightarrow Only debiasing the numerator: $\tilde{g}_k(\beta) = \frac{-y_k X_k}{\rho(1 + \exp(y_k X_k^T \beta))}$

 \rightarrow Debiasing the approximation of the gradient:

$$\frac{-y_k X_k}{1+\exp(y_k X_k^T \beta)} \approx \frac{-y_k X_k}{2} + \frac{X_k^T \beta X_k}{4}$$

- Hessian: $H_k(\beta) = \frac{\exp(y_k X_k^T \beta)}{1 + \exp(y_k X_k^T \beta)} X_k^T X_k.$
- Iteration k of Bach and Moulines: $\beta_k = \beta_{k-1} - \alpha (\nabla f_k(\bar{\beta}_{k-1}) + H_k(\bar{\beta}_{k-1})(\beta_{k-1} - \bar{\beta}_{k-1}))$

 \rightarrow Use the partially debiasing of the gradient and debiasing the quadratic part $X_k^T X_k$ of the Hessian.

 \rightarrow Debiasing the approximation of the gradient and debiasing the upper-bound of the Hessian $H_k(\beta) \leq \frac{1}{4}X_k^T X_k$

Open question 3: other missing-data mechanisms

✓ Heterogeneous MCAR data:

$$D = \left(\delta_{ij}
ight)_{1 \leq i \leq n, 1 \leq j \leq d} \quad ext{with} \quad \delta_{ij} \sim \mathcal{B}(p_j).$$

Open question: What for the MAR or MNAR data? We can not debiase the gradient using

$$\mathbb{E}_{D_k,X_k,y_k} \neq \mathbb{E}_{D_k}\mathbb{E}_{X_k,y_k}$$

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- MCAR: $D_k \perp X_k, y_k$
- MAR: $D_k \perp X_k^{\text{mis}} | X_k^{\text{obs}}, y_k$
- MNAR: other cases.

Open question 3: other missing-data mechanisms



Figure: 1 pass, assuming MAR data

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Thanks !

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Missing values setting

Mechanism assumption

- Why data is missing?
- Missing-data mechanism⁷: $\mathcal{L}(D|X)$
- Example: Income & Age, with missing values on Income.
- MCAR: the missing-data pattern is independent of the data.
- MAR: the missing-data pattern depends on the observed values.
- **MNAR**: the missing-data pattern depends on the missing values (and potentially on the observed values too).

Algorithms Step-size

Algorithm true for $\alpha \leq \frac{1}{2L} \rightarrow$ we can overestimate *L* (but not underestimate) We take $\alpha = \frac{1}{2L}$, where *L* is chosen:

- oracle value: we proved $L \leq \frac{1}{p_m^2} \max_k \|X_{k:}\|^2$ a.s.
- estimated value: $\hat{L}_n^{\text{NA}} = \frac{1}{\hat{p}_m^2} \max_{1 \le k \le n} \frac{\|\tilde{X}_{k:}\|^2 d}{\sum_j D_{kj}}$, with $\hat{p}_m = \min_{1 \le j \le d} \hat{p}_j$, and $\hat{p}_j = \frac{\sum_k D_{kj}}{n}$. ($\|\tilde{X}_{k:}\|^2$ divided by the proportion of the NA in the row).

Algorithm

Polynomial features

d = 2. Accounting for the effects of X_{k1}^2 , X_{k2}^2 , $X_{k1}X_{k2}$.

- augmented design matrix: $(X_{:1}|X_{:2}|X_{:1}X_{:2}|X_{:2}^2|X_{:2}^2)^T$.
- Debiased gradient: $U^{\odot 1} \odot \tilde{X}_{k:} \tilde{X}_{k:}^T \beta_k \operatorname{diag}(U)^{\odot 1} \odot \tilde{X}_{k:} y_k$

$$U = \begin{pmatrix} p_1 & p_1p_2 & p_1p_2 & p_1 & p_1p_2 \\ p_1p_2 & p_2 & p_1p_2 & p_1p_2 & p_2 \\ p_1p_2 & p_1p_2 & p_1p_2 & p_1p_2 & p_1p_2 \\ p_1 & p_1p_2 & p_1p_2 & p_1 & p_1p_2 \\ p_1p_2 & p_2 & p_1p_2 & p_1p_2 & p_2 \end{pmatrix},$$

 $U^{\odot-1}$: formed of the inverse coefficients of U.

Algorithm

Polynomial features

d = 2. Accounting for the effects of X_{k1}^2 , X_{k2}^2 , $X_{k1}X_{k2}$.



Figure: Empirical excess risk $(R_n(\beta_k) - R_n(\beta^*))$ given *n* for synthetic data $(n = 10^5, d = 10)$ when the model accounts mixed effects.

Algorithm

Polynomial features

For real data (Superconductivity dataset) 3 algorithms to compare :

- the averaged SGD on complete data (blue)
- the proposed debiased averaged SGD (orange)
- the averaged SGD run on imputed-by-0 data without any debiasing (green)



Figure: Empirical excess risk $(R_n(\beta_k) - R_n(\beta^*))$ given *n* for the superconductivity dataset (n = 21263) (containing 81 initial features) and d = 3403 with polynomial features of degree 2.

Synthetic data: homogeneous vs heterogeneous



Figure: Empirical excess risk $R_n(\beta_k) - R_n(\beta^*)$, $n = 10^5$.

- Missing values introduced with different missingness probabilities.
- Taking into account the heterogeneity in the algorithm (plain line): good rate of convergence for **AvSGD**.
- Ignoring the heterogeneity (dashed line): stagnation far from the optimum in termes of empirical risk.

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Real dataset: Traumabase, model estimation

- Goal: model the level of platelet upon arrival at the hospital from the clinical data of 15785 patients.
- Explanatory variables selected by doctors: seven quantitative (missing) variables.
- Model estimation: do the effect of the variables on the platelet make sense ?
- Similar results than EM algorithm but effects of HR and Δ .Hemo are not in agreement with the doctors opinion.

Variable	Effect	NA %
Lactate	_	16%
Δ .Hemo	+	16%
VE	_	9%
RBC	_	8%
SI	_	2%
HR	+	1%
Age	_	0%

Real dataset, Superconductivity, prediction task Comparison to **two-step heuristics** (no theoretical guarantees):

- the covariates imputed
 - mean (naive)
 - IterativeImputer (estimates each feature from all the others)
- linear regression (LR) performed on the competed dataset



Missing data setting

Missing-data patterns dependent

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In our setting: independent missing-data patterns

 $D_{.j} \perp D_{.j'}, j \neq j'$

Dependent missing-data patterns $\tilde{g}_k(\beta) := (W \odot (\tilde{X}_k; \tilde{X}_k^T))\beta - y_k P^{-1} \tilde{X}_k;$ with $W \in \mathbb{R}^{d \times d}$, and $W_{ij} := 1/\mathbb{E}[\delta_{ki}\delta_{kj}]$ for $1 \le i, j \le d$

Key assumption for fast rate?

•
$$\nabla R(\beta_{k-1}) = \mathbb{E}_{(X_{k:},y_k)}[X_{k:}(X_{k:}^T\beta_{k-1}-y_k)] = H(\beta_{k-1}-\beta^*).$$

• We do:
$$\beta_k = \beta_{k-1} - \alpha \tilde{g}_k(\beta_{k-1})$$
.

 What is the noise induced by using the unbiased stochastic gradient *g̃_k*?

$$\nabla R(\beta_{k-1}) - \tilde{g}_k(\beta_{k-1}) = \underbrace{(H - X_k; X_k^T)(\beta_{k-1} - \beta^\star)}_{\text{multiplicative noise}} - \underbrace{X_k; \epsilon_k}_{\text{additive noise}} =: \zeta_k$$

• Assumption on the additive noise?

$$\beta_{k} = \beta_{k-1} - \alpha H(\beta_{k} - \beta^{\star}) + \alpha \zeta_{k}$$
$$H(\beta_{k} - \beta^{\star}) = \beta_{k-1} - \beta_{k} + \alpha \zeta_{k}$$
$$(\bar{\beta}_{k} - \beta^{\star}) = H^{-1} \frac{(\beta_{0} - \beta^{\star})}{\alpha n} + H^{-1} \sum_{k=1}^{n} \frac{\zeta_{k}}{n}$$

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