Debiasing Averaged Stochastic Gradient Descent to handle missing values Séminaire Parisien de Statistiques

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### Motivation: Large-scale incomplete data

- Large-scaling: large *n* (number of observations), large *d* (dimension of the observations).
   ↔ Stochastic / online learning algorithms
- Incompleteness for many reasons Delete observations with NA → keep only 5% of the rows.:(
   ↔ Simpler algorithmic solutions?

#### Traumabase: 15000 patients/ 250 var/ 15 hospitals

	Center	Age	Sex	Weight	Height	Heart rate	Lactates	
	Beaujon	54	m	85	NA	NA	NA	
	Lille	33	m	80	1.8	180	4.8	
	Pitie	26	m	NA	NA	NA	3.9	
Not	Available							
NOL	Available.							

NA:

### Outline

#### SGD with missing data

#### 2 Convergence results

- Without missing values: rates and proofs
- Convergence of Algorithm 1
- Rates for empirical risk? Beyond one pass?
- Adaptation to estimated missing probabilities

#### 3 Experiments

### Setting

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

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

parametrized by  $\beta^{\star} \in \mathbb{R}^d$ , 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:

$$\beta^{\star} = \arg\min_{\beta \in \mathbb{R}^{d}} \left\{ \mathbb{R}(\beta) := \mathbb{E}_{(X_{i:}, y_{i})} \left[ f_{i}(\beta) \right] \right\}$$

- Stochastic gradient method.
  - . At the heart of Machine Learning.
  - . Very well suited for large d and n.

### Objective - missing data

- Problem:  $(X_{i:})$ 's partially known
  - 1. What should we estimate?
- True risk minimization:

$$\beta^{\star} = \arg\min_{\beta \in \mathbb{R}^{d}} \left\{ R(\beta) := \mathbb{E}_{(X_{i:}, y_{i})} \left[ f_{i}(\beta) \right] \right\}$$

2. How to adapt algorithms to the missing data case?

### Optimization without missing values

Stochastic gradient descent

Stochastic gradient descent (SGD): using unbiased estimates of ∇F(β<sub>k-1</sub>).

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

where  $\alpha$  is the step-size and  $\mathbb{E}[g_k(\beta_{k-1})|\mathcal{F}_{k-1}] = \nabla F(\beta_{k-1}),$  $\mathcal{F}_{k-1} = \sigma(X_{1:}, y_1, \dots, X_{k-1:}, y_{k-1})$  the filtration.

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

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

$$\overline{\beta}_{k} = \frac{1}{k+1} \sum_{i=0}^{k} \beta_{i}$$
It scales with large data.

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#### 2 questions

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

#### Missing values setting Formalism

j= 1 .- 8.

• 
$$D_{i:}^{l} \in \{0,1\}^{d}$$
 binary mask, such that

$$D_{ij} = \begin{cases} 0 & \text{if the } (i,j)\text{-entry is missing} \\ 1 & \text{otherwise.} \end{cases}$$

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

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

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

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

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

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

#### Dealing with missing values Existing work<sup>4</sup>

 Expectation Maximization algorithm<sup>1</sup> (maximization of the observed likelihood)

 $\times$  parametric assumptions: Gaussian assumption for the covariates, no solution available for large dimension  $\mathbb{Z}$ .

Matrix completion (predicting NA before applying usual algorithms)
 X it can lead to bias and underestimation of the variance of the estimate<sup>2</sup>.

 Imputing naively by 0 and modifying the usual algorithms to account for the imputation error: in particular, a modified SGD<sup>3</sup>.

<sup>1</sup>Arthur P Dempster, Nan M Laird, and Donald B Rubin. "Maximum likelihood from incomplete data via the EM algorithm". In: *Journal of the Royal Statistical Society: Series B (Methodological)* 39.1 (1977), pp. 1–22.

<sup>2</sup>Roderick JA Little and Donald B Rubin. *Statistical analysis with missing data*. Vol. 793. John Wiley & Sons, 2019.

<sup>3</sup>Anna Ma and Deanna Needell. "Stochastic Gradient Descent for Linear Systems with Missing Data". In: *arXiv preprint arXiv:1702.07098* (2017).

<sup>4</sup>Imke Mayer et al. "R-miss-tastic: a unified platform for missing values methods and workflows". In: *arXiv preprint arXiv:1908.04822* (2019).

Our strategy inspired by Ma et Needell Online-streaming: for a new observation  $(X_{i:}^{NA}, y_i)$ • Imputing the missing values by 0.  $\tilde{X}_{i:} = X_{i:}^{NA} \odot D_{i:} = X_{i:} \odot D_{i:}$  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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• 
$$\mathcal{F}_{k-1} = \sigma(X_{1:}, y_1, D_{1:}, \dots, X_{k-1:}, y_{k-1}, D_{k-1:})$$

- .  $\nabla R(\beta_{k-1}) = \mathbb{E}_{(X_{k:}, y_k)}[X_{k:}(X_{k:}^T \beta_{k-1} y_k)]$
- . No access to  $X_{k:}$ , only to  $ilde{X}_{k:}$ .
- . Another source of randomness:  $\mathbb{E} = \mathbb{E}_{(X_{k:}, y_k), D_{k:}} \stackrel{\text{indep}}{=} \mathbb{E}_{(X_{k:}, y_k)} \mathbb{E}_{D_{k:}}$
- .  $\mathbb{E}_{D_{k:}}|\mathcal{F}_{k-1} \rightsquigarrow \mathbb{E}_{D_{k:}}|$ 
  - ✓ 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  $\mathbb{E}\left[\tilde{g}_k(\beta_{k-1}) \mid \mathcal{F}_{k-1}\right] = \nabla R(\beta_{k-1})$ 

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

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

ra

Thus

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

• Imputing the missing values by **0**.

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

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

One obtains

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

$$\nabla F(\beta) = (x^{T}\beta \gamma) x$$
  
 $queduetie in X$ 
 $B = \gamma X$ 

### 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  $\beta_*$  with missing data.
  - We consider a **heterogeneous** MCAR framework
- $\checkmark$  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

convergence rates and proof techniques

- If F is convex and L-smooth.<sup>5</sup>  $\checkmark$  Convergence rate:  $\mathcal{O}(k^{-1/2})$
- If F is convex and L-smooth,  $\mu$ -strongly convex.
  - × Convergence rate:  $\mathcal{O}((\mu k)^{-1})$ , with  $\mu$  known.
- If F is convex and quadratic, e.g., for least-squares regression<sup>6</sup>.
  ✓ Convergence rate: O(k<sup>-1</sup>)
  ? Why do we get a faster rate for quadratic functions?
  ? What does it require?

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

<sup>&</sup>lt;sup>6</sup>Francis Bach and Eric Moulines. "Non-strongly-convex smooth stochastic approximation with convergence rate O (1/n)". In: *Advances in neural information processing systems*. 2013, pp. 773–781.

Faster rates for Least Squares regression  
• Typical proof for convex:  

$$\begin{aligned} & \left\| \begin{array}{c} & \\ B_{k-1} \\ \end{array} \right\|_{\mu}^{2} \\ & \left\| \begin{array}{c} B_{k-1} \\ \end{array} \right\|_{\mu}^{2} \\ & \left\| \begin{array}$$

#### Faster rates for Least Squares regression

•

• Typical proof for quadratic:

$$\frac{P_{J}}{\alpha} = \frac{B_{n}}{\beta_{n}} - \alpha \nabla F(B_{n,1}) + \alpha \varepsilon$$

$$\alpha H(B_{d} - B_{x}) = B_{n,1} - B_{n} + \alpha \varepsilon$$

$$\left(\overline{B_{n}} - B_{x}\right) = H \frac{B_{o} - B_{x}}{\alpha n} + \frac{A}{n} \frac{\sum_{i=1}^{n} (H^{2}\varepsilon_{i})}{\sum_{i=1}^{n} (H^{2}\varepsilon_{i})}$$

$$E = H H^{2}\varepsilon_{i} = tr(H^{2}\varepsilon_{i})$$
is bounded

### Summary



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- 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  $\beta^\star$  is  $\mathcal{F}_k$ -measurable and  $\forall k \ge 0$ ,

- $\mathbb{E}[\tilde{g}_k(\beta^\star) \mid \mathcal{F}_{k-1}] = 0$  a.s.
- $\mathbb{E}[\|\tilde{g}_k(\beta^{\star})\|^2 | \mathcal{F}_{k-1}]$  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  $\alpha \leq \frac{1}{2L}$ , ensures that, for any  $k \geq 0$ :



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

•  $c(\beta^{\star}) = \underbrace{\frac{\operatorname{Var}(\epsilon_k)}{p_m^2}}_{\text{increasing with the missing values rate}} \operatorname{multiplicative noise (induced by naive imputation)}_{p_m^3} \gamma^2 \|\beta^{\star}\|^2$ 

#### Theoretical results Comments

- Optimal rate for least-squares regression.
- In the complete case: same bound as Bach and Moulines.
- Bound on the iterates for the ridge regression (β → R(β) + λ||β||<sup>2</sup> is 2λ-strongly convex).

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



k p<sup>2</sup>

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?







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?

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

**Open Questions:** Lower bound!

**Possible Approach** Gaussian assumptions on the data distribution: use the distribution of the full data knowing observed data.

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:  $\frac{\operatorname{Var}(\epsilon_k)d}{k_{co}}$ .
- . in expectation, lower bound on the risk larger than  $\frac{\operatorname{Var}(\epsilon_k)d}{kp^d}$
- 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.

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Finite-sample setting

#### **Open Question: rates for ERM?**

- Empirical risk:  $\beta_{\star}^{n} = \arg \min_{\beta \in \mathbb{R}^{d}} \{R_{n}(\beta) := \frac{1}{n} \sum_{i=1}^{n} f_{i}(\beta)\}$ How to choose the *k*-th obstervation?
  - $\checkmark$  k uniformly at random  $\Rightarrow$  we use a data several times.
  - X k not chosen uniformly at random  $\Rightarrow$  sampling not uniform and bias in the gradient.

<sup>7</sup>Ohad Shamir. "Without-Replacement Sampling for Stochastic Gradient Methods". In: *Proceedings of the 30th International Conference on Neural Information Processing Systems*. NIPS'16. Barcelona, Spain: Curran Associates Inc., 2016, pp. 46–54. ISBN: 9781510838819.

#### Theoretical results Finite-sample setting

#### **Open Question: rates for ERM?**

- Empirical risk:  $\beta_{\star}^{n} = \arg \min_{\beta \in \mathbb{R}^{d}} \left\{ R_{n}(\beta) := \frac{1}{n} \sum_{i=1}^{n} f_{i}(\beta) \right\}$ How to choose the *k*-th obstervation?
  - $\checkmark$  k uniformly at random  $\Rightarrow$  we use a data several times.
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Implications:

- No unbiased gradients for the empirical risk so far.
- Keep in mind: empirical risk is in any case not observed.

**Possible Approach**: similar to wo replacement sampling for ERM.<sup>7</sup>

<sup>&</sup>lt;sup>7</sup>Shamir, "Without-Replacement Sampling for Stochastic Gradient Methods".

Comparison with related work

Comparison with Ma et Needell<sup>8</sup>:

- $\mu$ -strongly convex problem
- no averaged iterates
- $\Rightarrow$  convergence rate of  $\mathcal{O}(\frac{\log n}{\mu n})$ .
  - $\checkmark$   $\mu$  generally out of reach.
  - X only homogeneous MCAR data.
  - X main theorem mathematically invalid (empirical risk).

<sup>&</sup>lt;sup>8</sup>Ma and Needell, "Stochastic Gradient Descent for Linear Systems with Missing Data".

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Finite-sample setting: *n* is fixed

- Algorithm and main result: requirement of  $(p_j)_{j=1,...,d}$ .  $\rightarrow$  estimator  $\bar{\beta}_k$
- In practice: estimated missing probabilities (p̂<sub>j</sub>)<sub>j=1,...,d</sub>
   → estimator β̂<sub>k</sub>. (finite-sample setting: first half of the data to
   evaluate (p̂<sub>j</sub>), second half to build β̂<sub>k</sub>).

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  $k \ge 0$ :

$$\mathbb{E}\left[R(ar{eta}_k)-R(ar{eta}_k)
ight]=\mathcal{O}(1/kp_m^6),$$

$$\hat{\beta}_{j} \geq \frac{P_{j}}{\epsilon}$$

- n Pm

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

#### Proof Sketch

### Open questions

#### OQ: Tighter convergence rate with estimated probabilities:

- Without strong convexity
- Better dependence w.r.t. *p*.

Approach: Proof related to *stability* approaches.

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OQ: Tighter convergence rate with estimated probabilities:

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Approach: Proof related to *stability* approaches.

OQ: working in a distributed or federated framework

- Each participant has its own missing value probability
- Each participant has its own objective function.

Approach: Federated Learning algorithms. Estimation of probabilities based on a global prior + local estimation.

### 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 erasing incomplete data, but not as good as pk complete observations
- ✓ Convergence with strong-convexity and estimated probabilities (preserved  $k^{-1}$ , degraded dependence in p)

#### Partial answers & open questions:

- Matching lower bound?
- ERM, Beyond one pass? impossible to minimize ER to arbitrary precision, but a guarantee for the first pass seems possible.
- Better dependence in p for estimated probabilities case?
- Distributed & multi-agent frameworks are crucial.
- In practice?

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#### Synthetic data: convergence rate



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.

### Experiments





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.

### Conclusion

- ✓ A new algorithm with a fast rate to perform SGD with missing data.
- Python implementation of regularized regression with missing values for large scale data.
- More details in the paper<sup>9</sup>!

Many perspectives:

- Dealing with more general loss function.
- More complex missing-data patterns such as MAR and MNAR.
- Lower bounds
- Distributed case
- Bounds on the empirical risk, tighter bound for estimated p.

<sup>&</sup>lt;sup>9</sup>A. S. et al. "Debiasing Stochastic Gradient Descent to handle missing values". In: *Advances in Neural Information Processing System* (2020).