Floodgate: inference for model-free variable importance

Dempster's Colloquium 2021

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Zhang, L. and Janson, L., 2020. Floodgate: inference for model-free variable importance. arXiv preprint arXiv:2007.01283.

Collaborator

Lucas Janson

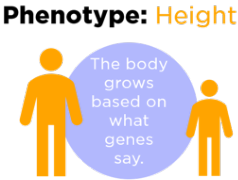
Overview

Problem setup

Setup: data (Y, X, Z) from some joint distribution.

- Y a outcome variable of interest (AKA response or dependent variable),
- X a explanatory variable of interest (AKA treatment, covariate, feature)
- $Z := (Z_1, \cdots, Z_p)$ a set of p further variables (AKA confounders, nuisance variables)

Examples:



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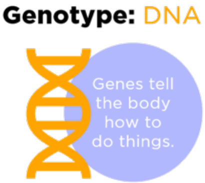

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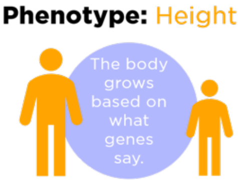

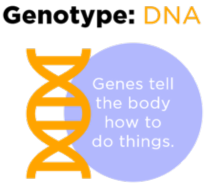

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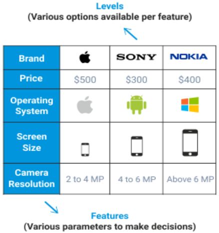

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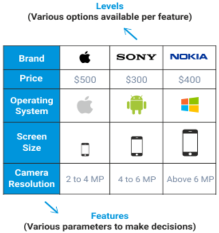

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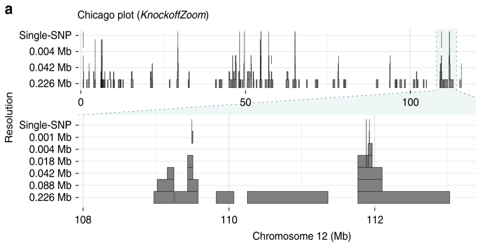
Is the variable X important or not?



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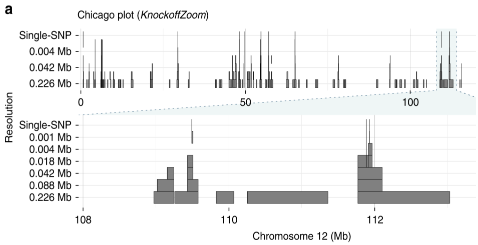

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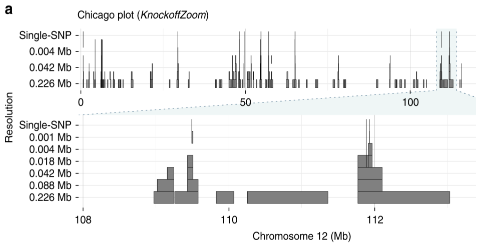

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How important is the variable X?

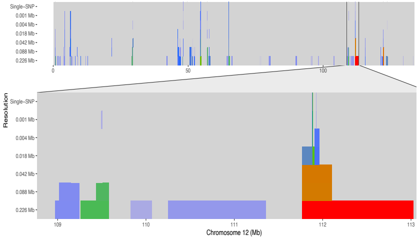

Figure: Infer the importance of a group of SNPs

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Related work

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- *Projection approaches:* Buja et al. (2015, 2019a,b), Rinaldo et al. (2019), Lee et al. (2016), Taylor et al. (2014), Berk et al. (2013), Buja and Brown (2014).
- *Semi-parametric approaches:* $\mathbb{E}\left[\mathrm{Cov}\left(Y, X \mid Z\right)\right]$; Robins et al. (2008, 2009); Li et al. (2011); Robins et al. (2017); Newey and Robins (2018), Shah and Peters (2018).
- *Random estimands:* Lei et al. (2018), Watson and Wright (2019), Rinaldo et al. (2019).
- *Same MOVI as us:* Saltelli et al. (2008), Williamson et al. (2017, 2020).

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Preview of our results

A1 : present a MOVI, the mMSE gap.

- ✓ Zero under the conditional independence $Y \perp\!\!\!\perp X \mid Z$.
- ✓ Strictly positive unless $\mathbb{E}[Y \mid X, Z]$ has no dependence on X at all.
- ✓ Direct predictive, causal and explanatory interpretations.

A2 : propose a method for inference for it: **floodgate**.

- ✓ Asymptotically-valid inference.
- ✓ Does not make any parametric/smoothness/sparsity assumptions about $Y \mid X, Z$ and built around any regression estimator.
- ✓ Width of confidence bounds proportional to the predictive performance.
- ✓ Assume $P_{X|Z}$ known, quantified robustness to misspecification and extension allowing known up to a parametric model.

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Our target MOVI: the mMSE gap

Definition (mMSE Gap)

The minimum mean squared error (mMSE) gap for variable X is defined as

$$\mathcal{I}^2 = \mathbb{E}\left[(Y - \mathbb{E}[Y \mid Z])^2\right] - \mathbb{E}\left[(Y - \mathbb{E}[Y \mid X, Z])^2\right].$$

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- **Variance decomposition**: $\mathcal{I}^2 = \mathrm{Var}(\mathbb{E}[Y \mid X, Z]) - \mathrm{Var}(\mathbb{E}[Y \mid Z])$.
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- Nonlinearity in the above functional.

Possible solution: assume we have a good estimator μ of $\mu^\star$?

How to do inference on $\mathcal{I}$?

True regression function $\mu^\star(x,z) := \mathbb{E}\left[Y \mid X = x, Z = z\right]$

$$\Rightarrow \quad \mathcal{I}^2 = \mathbb{E}\left[\mathrm{Var}(\mu^\star(X,Z) \mid Z)\right] = \mathbb{E}\left[\left(\mu^\star(X,Z) - \mathbb{E}\left[\mu^\star(X,Z) \mid Z\right]\right)^2\right]$$

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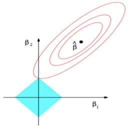
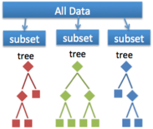
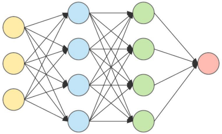
- Only known for limited class of estimators and data-generating distributions.
- Precludes most modern machine learning algorithms and methods that integrate hard-to-quantify domain knowledge.







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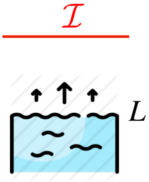

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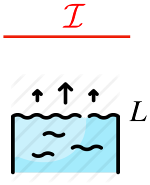

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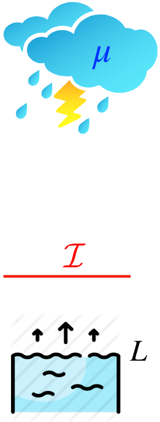

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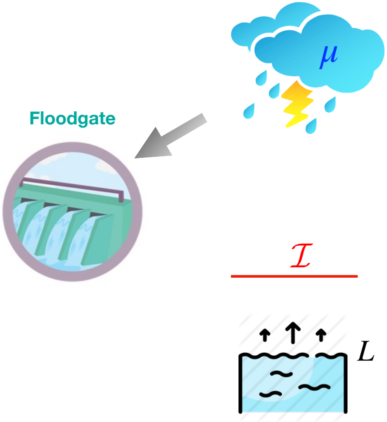

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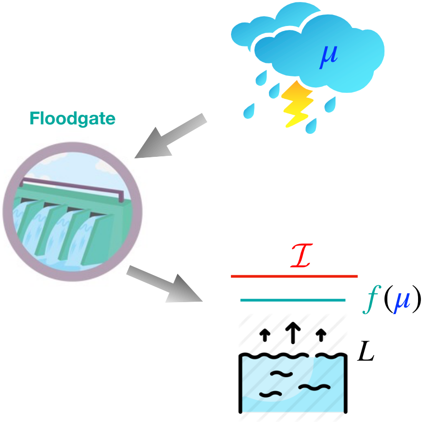

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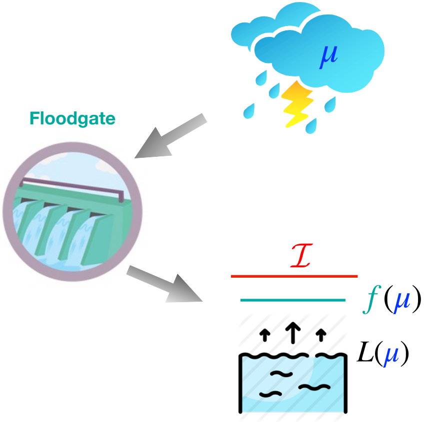

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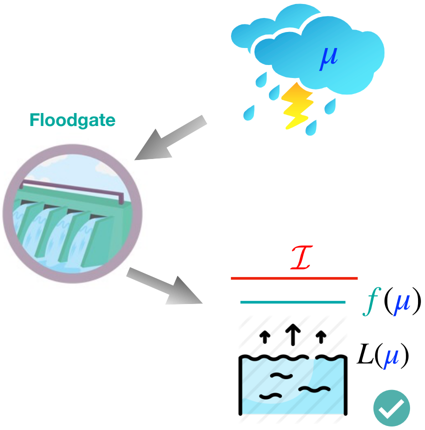

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Our choice of Floodgate functional

- Our choice:

$$f(\mu) := \frac{\mathbb{E}\left[\mathrm{Cov}(\mu^\star(X,Z), \mu(X,Z) \mid Z)\right]}{\sqrt{\mathbb{E}\left[\mathrm{Var}(\mu(X,Z) \mid Z)\right]}}$$

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Lemma (Zhang and Janson (2020))

For any μ such that $f(\mu)$ exists, we have $f(\mu) \leq \mathcal{I}$ and $f(\mu^\star) = \mathcal{I}$.

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$$f(\mu) = \frac{\mathbb{E}\left[Y\left(\mu(X,Z) - \mathbb{E}\left[\mu(X,Z) \mid Z\right]\right)\right]}{\sqrt{\mathbb{E}\left[\mathrm{Var}\left(\mu(X,Z) \mid Z\right)\right]}} = \frac{\text{a linear functional of } P_{(Y,X,Z)}}{\sqrt{\text{a linear functional of } P_Z}}$$

Inferential procedures

Input: $\mathcal{D} = \{(Y_i, X_i, Z_i)\}_{i=1}^n$; $\mathcal{D}'$; any regression algorithm $\mathcal{A}$; assume $P_{X|Z}$ known.

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2. Compute $\mathbb{E}\left[\mu(X, Z) \mid Z\right], \mathrm{Var}\left(\mu(X, Z) \mid Z\right)$.
3. Construct CLT-based LCB for $f(\mu)$: $L_n^\alpha(\mu)$ (with confidence level α) by Delta method.

$$\begin{pmatrix} \frac{1}{n}\sum_{i=1}^n Y_i\big(\mu(X_i, Z_i) - \mathbb{E}\left[\mu(X_i, Z_i) \mid Z_i\right]\big) \\ \frac{1}{n}\sum_{i=1}^n \mathrm{Var}\left(\mu(X_i, Z_i) \mid Z_i\right) \end{pmatrix} \xrightarrow{\text{asympt.}} \mathcal{N}\begin{pmatrix} \mathbb{E}\left[\mathrm{Cov}(\mu^\star(X, Z), \mu(X, Z) \mid Z)\right] \\ \mathbb{E}\left[\mathrm{Var}(\mu(X, Z) \mid Z)\right] \end{pmatrix}$$

Asymptotic validity

Theorem (Zhang and Janson (2020); informal)

Under mild moment conditions on Y and $\mu(X, Z)$, we have

$$\mathbb{P}\left(L_n^{\alpha}(\mu) \leq \mathcal{I}\right) \geq 1 - \alpha - O(n^{-1/2}).$$

- Point-wise result: the convergence rate result builds on recent Berry–Esseen type bounds for Delta method (Pinelis et al., 2016).

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- Constant in $O(n^{-1/2})$ has complicated dependence on μ and $P_{(Y,X,Z)}$.

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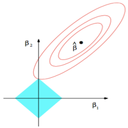
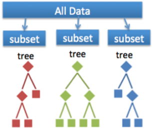
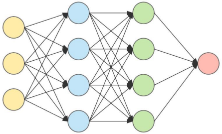
- Invariance of the floodgate procedure: e.g., $\mu(x, z) = ax + g(z)$, constant only depends on sign(a) and bivariate distribution of $\left(Y, \frac{X - \mathbb{E}[X \mid Z]}{\sqrt{\mathrm{Var}(X - \mathbb{E}[X \mid Z])}}\right)$.

Computation







- Allow the user to choose machine learning algorithms or integrate domain knowledge.

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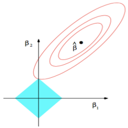

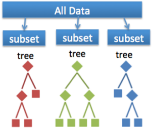

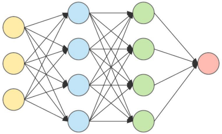

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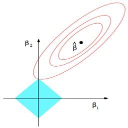

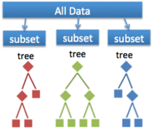

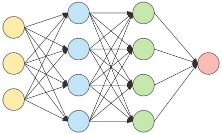

- Allow the user to choose machine learning algorithms or integrate domain knowledge.
- Only involve one time of model fitting.
- Under certain fitted models, can compute $\mathbb{E}\left[\mu(X,Z) \mid Z\right], \mathrm{Var}\left(\mu(X,Z) \mid Z\right)$ analytically, e.g., partial linear model with Gaussian design.

General computation

How to compute $\mathbb{E}\left[\mu(X,Z) \mid Z\right], \mathrm{Var}\left(\mu(X,Z) \mid Z\right)$ in a general way (e.g., μ is fitted based on random forest or neural networks)?

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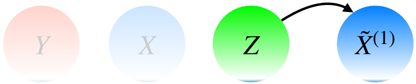

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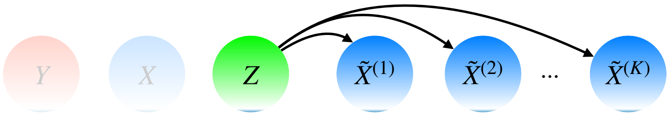

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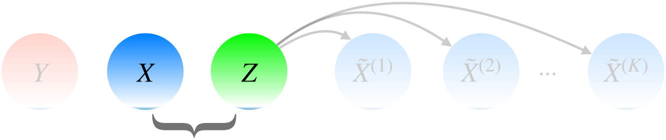

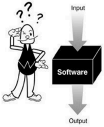

Black-box algorithm

$$\mu(X, Z)$$

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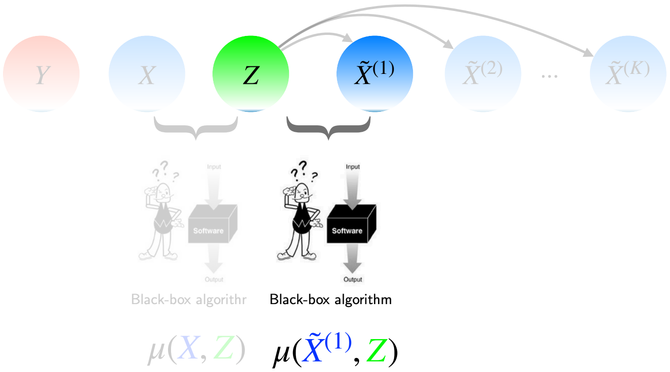

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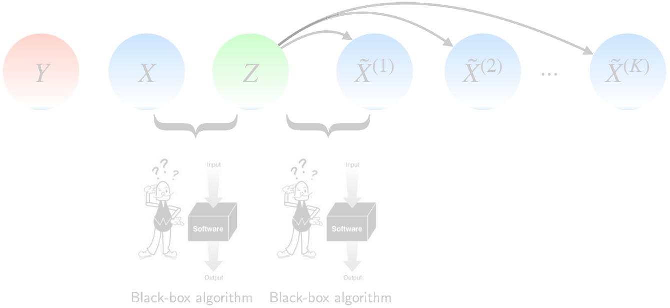

$\mu(X, Z)$ $\mu(\tilde{X}^{(1)}, Z)$

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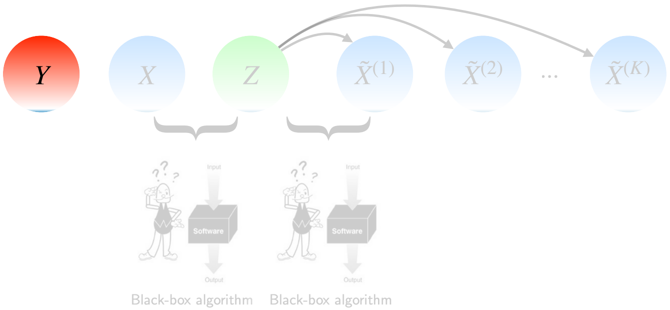

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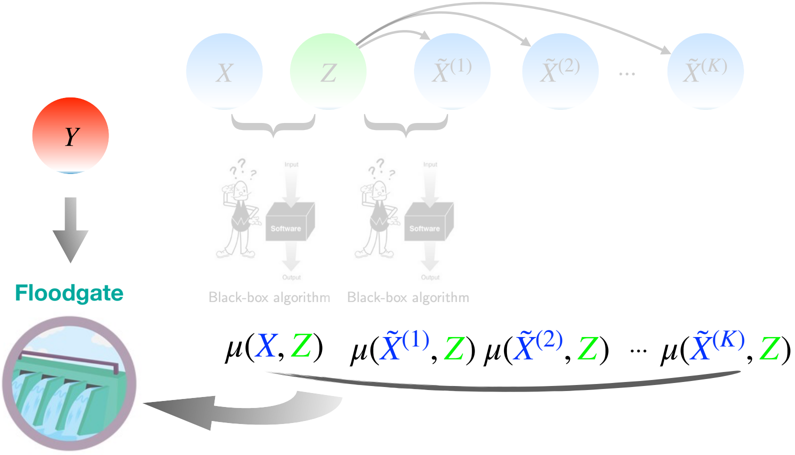

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- We know

$$\mathbb{E}\left[Y(\mu(X,Z) - \mu(\tilde{X},Z))\right] = \mathbb{E}\left[Y\left(\mu(X,Z) - \mathbb{E}\left[\mu(X,Z) \mid Z\right]\right)\right]$$

$$\frac{1}{2}\,\mathbb{E}\left[\left(\mu(X,Z) - \mu(\tilde{X},Z)\right)^2\right] = \mathbb{E}\left[\mathrm{Var}(\mu(X,Z) \mid Z)\right]$$

Upper confidence bound

Suppose there were no Z.

- $\mathcal{I}^2 = \mathrm{Var}\left(\mathbb{E}\left[Y \mid X\right]\right)$.
- $\mathrm{Var}\left(Y\right)$ is a trivial UCB, as $\mathcal{I}^2 \leq \mathrm{Var}\left(Y\right)$.

Theorem (Zhang and Janson (2020); informal)

Under our assumptions, any asymptotically-valid UCB$_\alpha$ will asymptotically be $\geq \mathrm{Var}\left(Y\right)$ with probability at least $1 - \alpha$.

Valid, nontrivial UCB **impossible** without structure on $Y \mid X$.

Intuition behind the UCB result

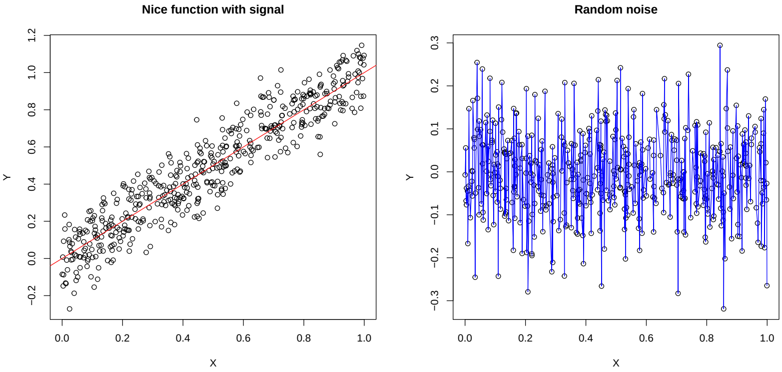

Figure: Left: $Y = X + \mathcal{N}(0, 0.1)$; Right: $Y \sim \mathcal{N}(0, 0.1)$.

Statistical accuracy

Statistical accuracy

Floodgate procedure is invariant with respect to a "equivalent" function class of μ,

$$S_\mu = \{c\mu(x, z) + g(z) : c > 0, g : \mathbb{R}^p \to \mathbb{R}\}.$$

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Under mild moment conditions on Y and noises, for μ_n with well-behaved moments,

$$\mathcal{I} - L_n^\alpha(\mu_n) = O_p\left(\inf_{\mu \in S_{\mu_n}} \mathbb{E}\left[(\mu(X,Z) - \mu^\star(X,Z))^2\right] + n^{-1/2}\right).$$

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Floodgate is **adaptive** to the accuracy of μ_n

(through the MSE of the best element of its equivalence class S_{μ_n})

Robustness

Suppose $P_{X|Z}$ unknown, we instead use its estimate $Q^{(n)}_{X|Z}$ to run floodgate.

Theorem (Zhang and Janson (2020); informal)

Under moment conditions on Y and noises, for μ_n with well-behaved moments under both the true distribution P and the specified one $Q^{(n)}$, then for floodgate with $Q^{(n)}_{X|Z}$ we have

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$$\Delta_n \leq c_1 \sqrt{\mathbb{E}\left[\chi^2\left(P_{X|Z} \,||\, Q^{(n)}_{X|Z}\right)\right]}$$

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Suppose $P_{X|Z}$ unknown, we instead use its estimate $Q^{(n)}_{X|Z}$ to run floodgate.

Theorem (Zhang and Janson (2020); informal)

Under moment conditions on Y and noises, for μ_n with well-behaved moments under both the true distribution P and the specified one $Q^{(n)}$, then for floodgate with $Q^{(n)}_{X|Z}$ we have

$$\mathbb{P}\left(L_n^{\alpha}(\mu_n) \leq \mathcal{I} + \Delta_n\right) \geq 1 - \alpha - O(n^{-1/2}),$$

where

$$\Delta_n \leq c_1 \sqrt{\mathbb{E}\left[\chi^2\left(P_{X|Z} \,||\, Q^{(n)}_{X|Z}\right)\right]} - c_2\, \mathbb{E}\left[(\bar{\mu}_n(X,Z) - \mu^{\star}(X,Z))^2\right]$$

where $\bar{\mu}_n$ is a particular representative of S_{μ_n} and $\chi^2(\cdot\,||\,\cdot)$ denotes the χ^2 divergence.

Robustness

Theorem (Zhang and Janson (2020); informal)

$$\mathbb{P}\left(L_n^{\alpha}(\mu_n) \leq \mathcal{I} + \Delta_n\right) \geq 1 - \alpha - O(n^{-1/2}),$$

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Note: by definition of $\bar{\mu}_n$, we have: $\mathcal{I} = 0 \quad \Rightarrow \mathbb{E}\left[(\bar{\mu}_n(X,Z) - \mu^\star(X,Z))^2\right] = 0$.

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Floodgate is robust if $P_{X|Z}$ well-estimated.

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Floodgate is robust if $P_{X|Z}$ well-estimated.

If $\mathcal{I} > 0$, floodgate is robust if $P_{X|Z}$ better-estimated than $\mathbb{E}[Y \mid X, Z]$.

Simulation setup

- $n = 1100$, $p = 1000$, and a sparsity of 30 unless stated otherwise.
- Linear: $X \sim \mathcal{N}(0, \Sigma)$, AR(1); $Y = X\beta + \mathcal{N}(0, 1)$, $||\beta||_0 = 30$, $|\beta_j| \in \{0, \frac{\text{amplitude}}{\sqrt{n}}\}$.
- Nonlinear: each component chosen from below; up to 3rd order interactions.

$$\sin(\pi x),\ \cos(\pi x),\ \sin(\pi x/2),\ \cos(\pi x)I(x > 0),\ x\sin(\pi x),\ x,\ |x|,\ x^2,\ x^3,\ e^x - 1.$$

- Number of replicates: 64.
- Default sample splitting proportion: 0.50.
- Four fitting algorithms: LASSO, Ridge, SAM, Random Forest.
- Number of null samples: $K = 500$.

Splitting proportion

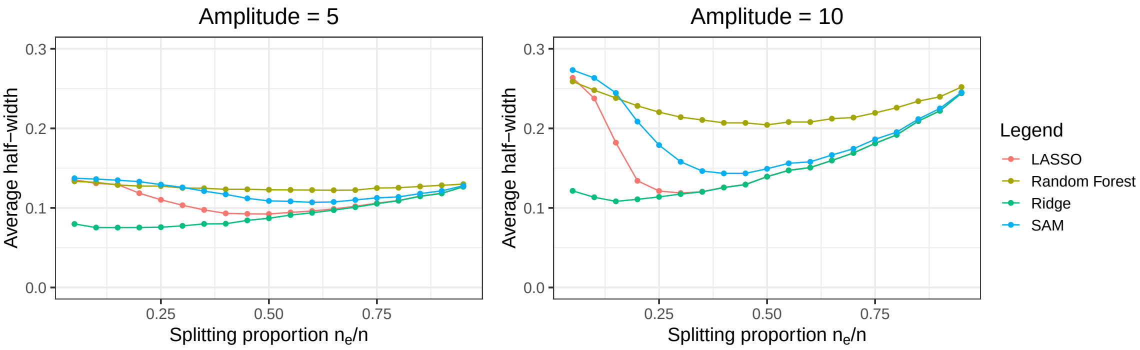

Figure: Linear setting.

Splitting proportion

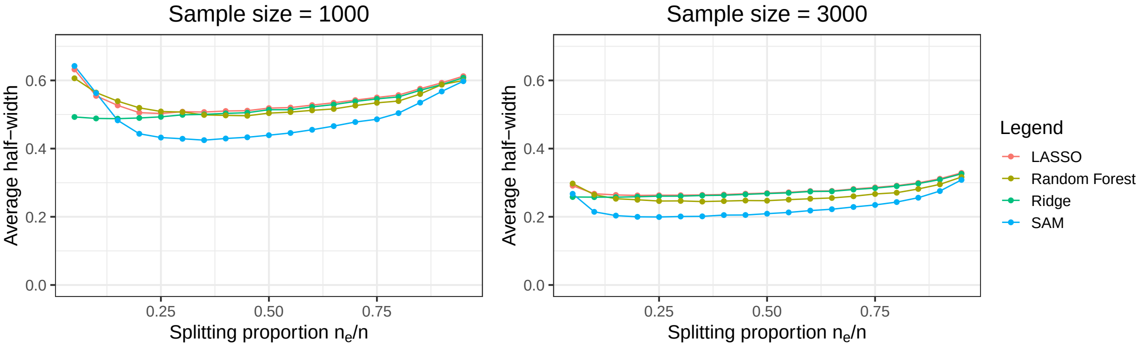

Figure: Nonlinear setting.

Covariate dimension

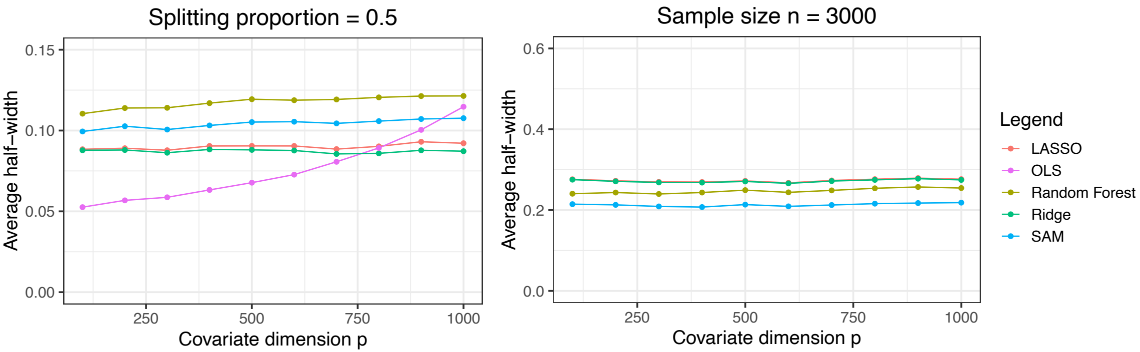

Figure: Left: Linear setting; Right: Nonlinear setting.

Robustness

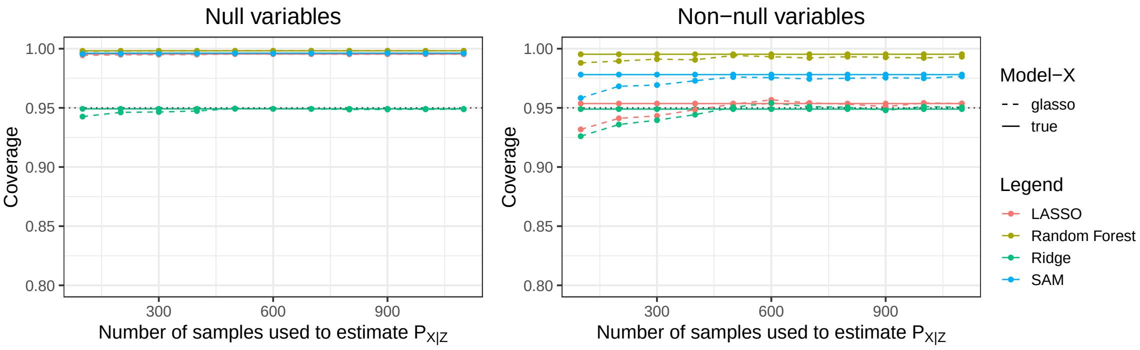

Figure: Linear setting.

Robustness

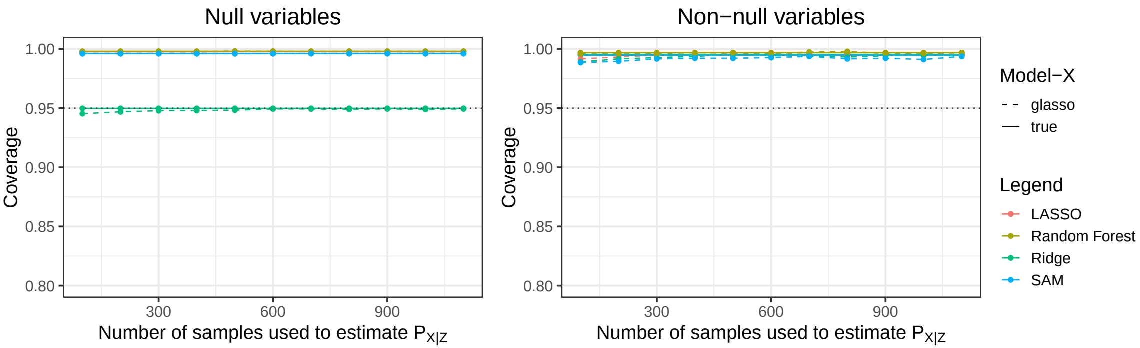

Figure: Nonlinear setting.

Genomic study of platelet count

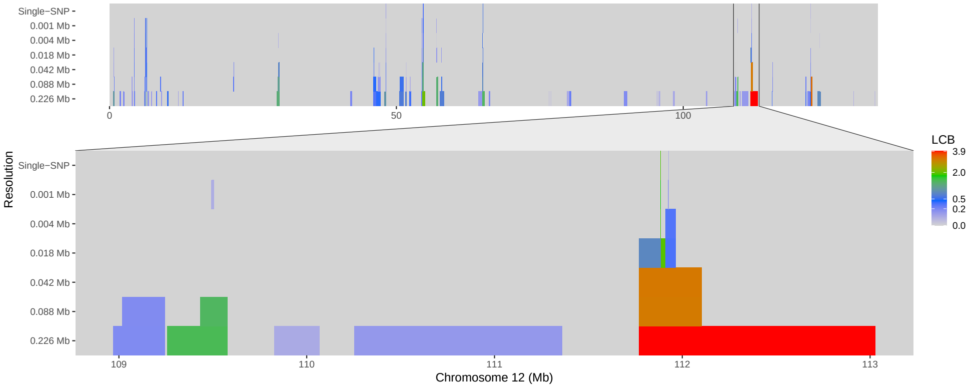

Figure: Colored Chicago plot (Sesia et al., 2020) with the color of each point representing the floodgate LCB for the importance of a group of SNPs on Chromosome 12 in the UK Biobank data at different resolutions (y-axis). Bottom plot shows a zoomed-in region of strong importance.

Extensions

Questions	Answers

Extensions

Questions	**Answers**
What if only know a model for $P_{X\|Z}$?	☑ Co-sufficient floodgate.

Extensions

Questions	Answers
What if only know a model for $P_{X\|Z}$?	☑ Co-sufficient floodgate.
Beyond the mMSE gap?	☑ Floodgate for MACM gap.

Extensions

Questions	**Answers**
What if only know a model for $P_{X\|Z}$?	☑ Co-sufficient floodgate.
Beyond the mMSE gap?	☑ Floodgate for MACM gap.
Inferring the MOVI w.r.t $\{X_j\}_{j \in \mathcal{G}}$?	☑ Easily extends.

Extensions

Questions	**Answers**
What if only know a model for $P_{X\|Z}$?	☑ Co-sufficient floodgate.
Beyond the mMSE gap?	☑ Floodgate for MACM gap.
Inferring the MOVI w.r.t $\{X_j\}_{j\in\mathcal{G}}$?	☑ Easily extends.
Transporting inference from $P_{(X,Z)}$ to $Q_{(X,Z)}$?	☑ Easily extends.

Extensions

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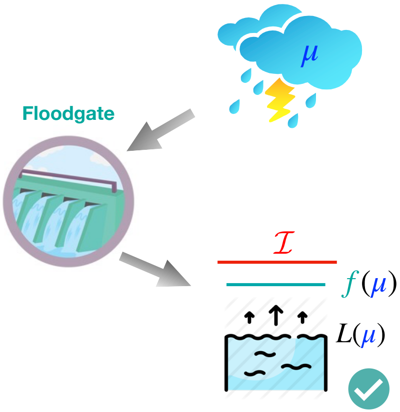
What if only know a model for $P_{X\|Z}$?	☑ Co-sufficient floodgate.
Beyond the mMSE gap?	☑ Floodgate for MACM gap.
Inferring the MOVI w.r.t $\{X_j\}_{j\in\mathcal{G}}$?	☑ Easily extends.
Transporting inference from $P_{(X,Z)}$ to $Q_{(X,Z)}$?	☑ Easily extends.
Adjusting for multiplicity and selection effects?	☑ Has answers.

Extensions

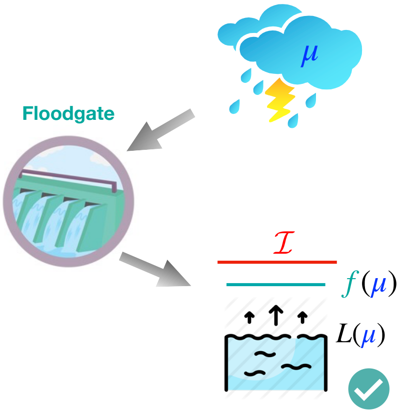
Questions	**Answers**
What if only know a model for $P_{X\|Z}$?	☑ Co-sufficient floodgate.
Beyond the mMSE gap?	☑ Floodgate for MACM gap.
Inferring the MOVI w.r.t $\{X_j\}_{j\in\mathcal{G}}$?	☑ Easily extends.
Transporting inference from $P_{(X,Z)}$ to $Q_{(X,Z)}$?	☑ Easily extends.
Adjusting for multiplicity and selection effects?	☑ Has answers.
Inferring the normalized mMSE gap $\frac{\mathcal{I}}{\sqrt{\mathrm{Var}(Y)}}$?	☑ Easily extends.

Summary



Floodgate: a new inferential approach for variable importance.

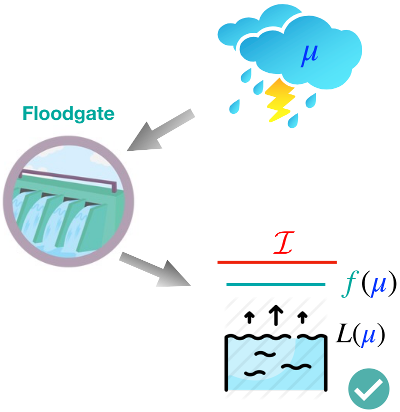
Summary



Floodgate: a new inferential approach for variable importance.

- Focus on an interpretable, sensitive and model-free MOVI: the mMSE gap.

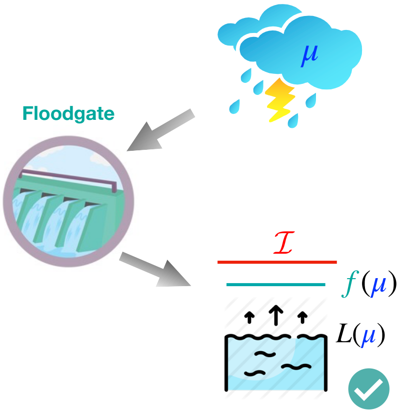
Summary



Floodgate: a new inferential approach for variable importance.

- Provide valid and robust LCBs for the mMSE gap.

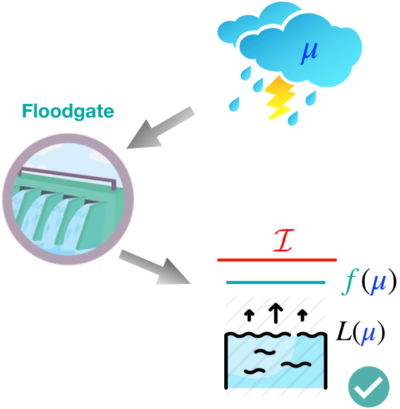
Summary



Floodgate: a new inferential approach for variable importance.

- Allow flexible regression algorithms, and is adaptive to the MSE.

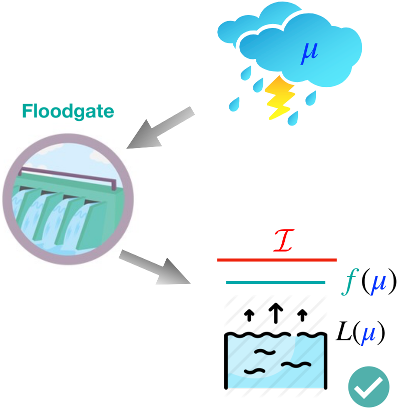
Discussion: beyond this paper



Floodgate: a new inferential approach for

____?

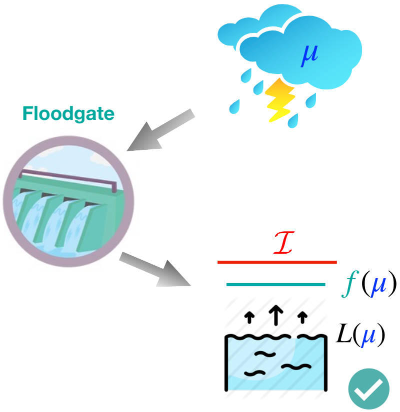
Discussion: beyond this paper



Floodgate: a new inferential approach for ________________________ ?

- How to characterize a class of feasible model-free targets?

Discussion: beyond this paper

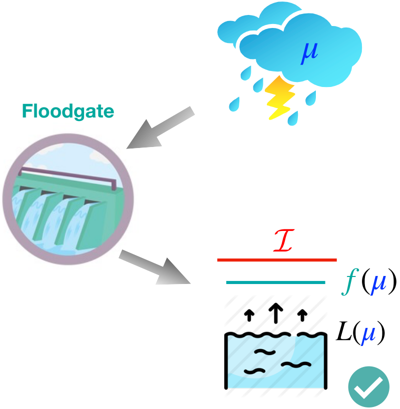


Floodgate: a new inferential approach for

________________________________?

- How to characterize a class of feasible model-free targets?
- How to construct floodgate functional f?

Discussion: beyond this paper



Floodgate: a new inferential approach for ________________?

- How to characterize a class of feasible model-free targets?
- How to construct floodgate functional f?
- How to obtain LCBs for $f(\cdot)$ under reasonable conditions?

Appendix

MACM gap

Definition (Mean absolute conditional mean gap)

The *mean absolute conditional mean (MACM) gap* for variable X is defined as

$$\mathcal{I}_{\ell_1} = \mathbb{E}\left[\left|\mathbb{E}\left[Y \mid Z\right] - \mathbb{E}\left[Y \mid X, Z\right]\right|\right]$$

whenever all the above expectations exist.

The subscript in $\mathcal{I}_{\ell_1}$ reflects its similarity to $\mathcal{I}^2 = \mathbb{E}\left[\left(\mathbb{E}\left[Y \mid Z\right] - \mathbb{E}\left[Y \mid X, Z\right]\right)^2\right]$ except with the square replaced by the absolute value (also known as the ℓ_1 norm).

Covariate dimension

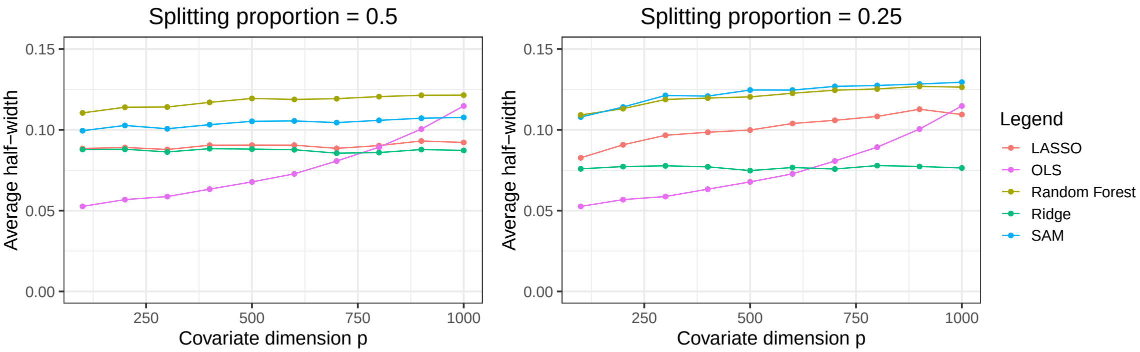


Figure: Linear setting.

Covariate dimension

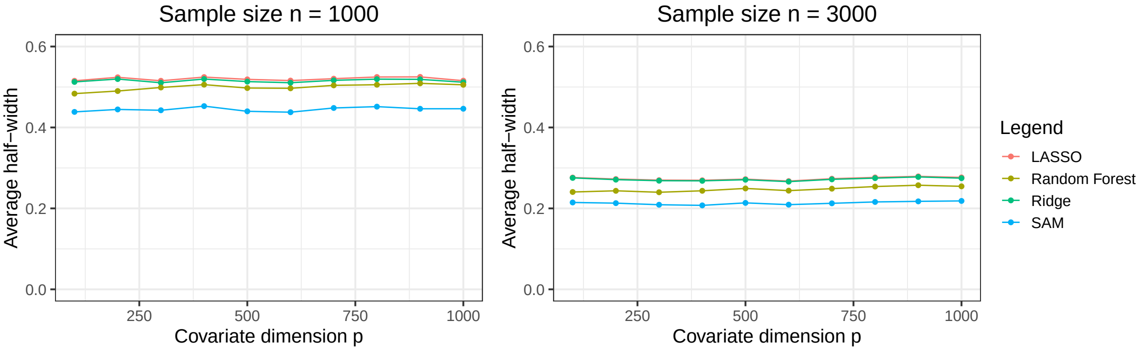


Figure: Nonlinear setting.

Sample size

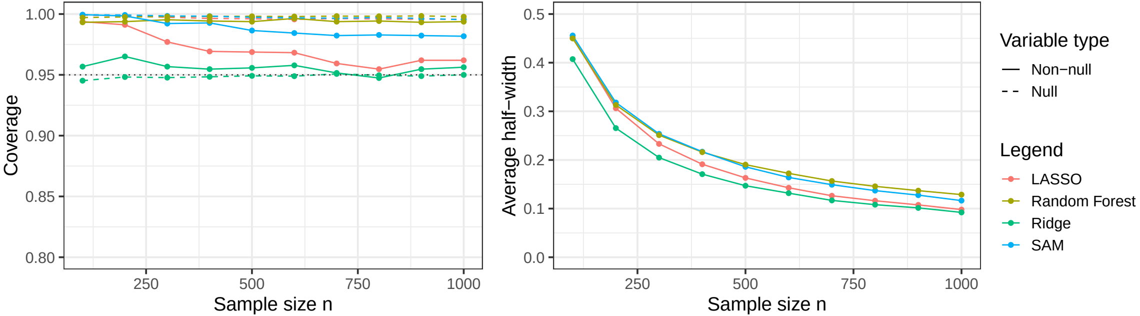


Figure: Linear setting.

Sample size

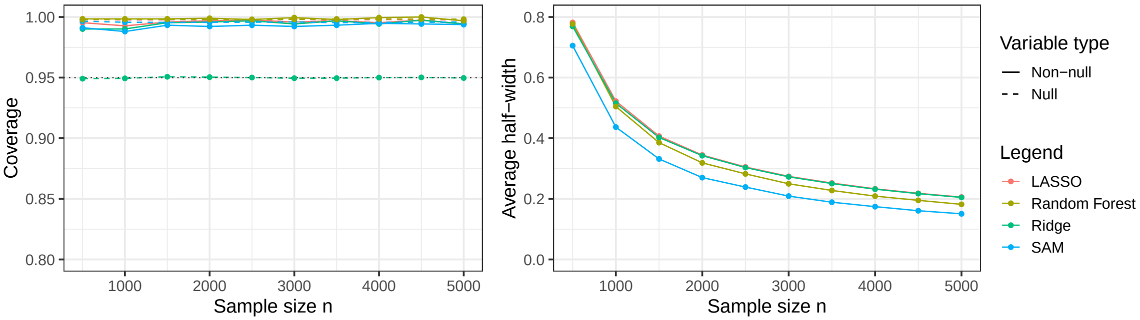


Figure: Nonlinear setting.

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