Sobol-CPI: a Doubly Robust Conditional Permutation Importance Statistic

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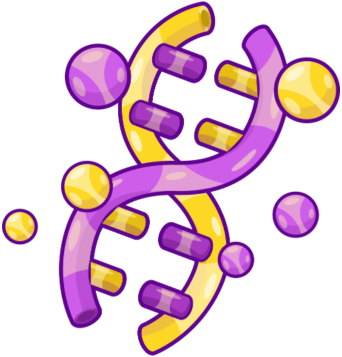
Motivation: Intrinsic Variable Importance

How can we define / learn the importance of each covariate X^j with respect to an outcome y?



X

y

Try to study their relationship using a ML model:

$$\widehat{m} \in \underset{f \in \mathscr{F}}{\operatorname{argmin}} \widehat{\mathbb{E}} \left[\mathscr{L}(f(X), y) \right]. \quad (1)$$

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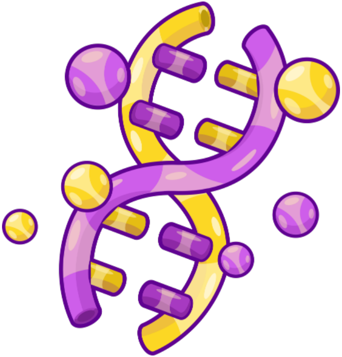

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Problematic: Model misspecification

Goals for a VI measure:

- statistically valid
- model-agnostic
- computationally feasible

Main challenges:

- non-linearity
- high-dimensionality
- correlation

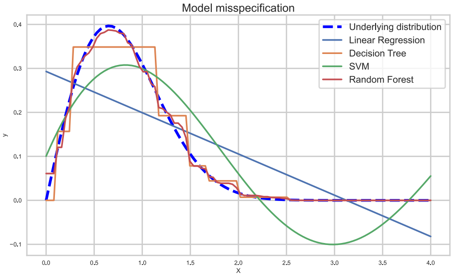

Figure 1: Interpreting the underlying distribution with simple models may be misleading. We need a **model-agnostic** measure.

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Standard approaches

- The importance of j, $\psi(j, P_0)$, is usually obtained by:

Predictability **using** the covariate j	**vs**	Predictability **without** the covariate j

- Approaches to measure the predictability without j (Covert et al. (2021) JMLR):
  - **Removal-based:** Refit a model $\widehat{m}_{-j}$ to regress y given X^{-j}.
  - **Permutation-based:** Modify X^j and predict with $\widehat{m}$.

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Goal: the Generalized Total Sobol Index

$$\psi_{\mathrm{TSI}}(j, P_0) = \mathbb{E}\left[\mathscr{L}(y, m_{-j}(X^{-j})) - \mathscr{L}(y, m(X))\right]$$

(Williamson et al. (2021) Biometrics, Williamson et al. (2021) JASA, Bénard et al. (2022) Biometrika, Verdinelli et al. (2023) Statistical Science).

Literature review: General model-agnostic framework

- **Leave One Covariate Out(LOCO)**:

$$\widehat{\psi}_{\mathrm{LOCO}}(j, P_0) = \frac{1}{n_{\mathrm{test}}} \sum_{i=1}^{n_{\mathrm{test}}} \mathscr{L}(y_i, \widehat{m}_{-j}(x_i^{-j})) - \mathscr{L}(y_i, \widehat{m}(x_i)). \qquad (2)$$

  - ✓ It estimates an interpretable quantity ($\psi_{\mathrm{TSI}}(j, P_0)$).
  - ✓ Type-I error control (Williamson et al. (2021) JASA).
  - × In practice: unstable and computational intensive.

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- **Permutation Feature Importance(PFI)**:

$$\widehat{\psi}_{\mathrm{PFI}}(j, P_0) = \frac{1}{n_{\mathrm{test}}} \sum_{i=1}^{n_{\mathrm{test}}} \mathscr{L}(y_i, \widehat{m}(x_i^{(j)})) - \mathscr{L}(y_i, \widehat{m}(x_i)). \tag{3}$$

where the j-th covariate is permuted.

- ✓ Fast (no need to retrain $\widehat{m}$).
- × Extrapolation bias (Chamma et al. (2023) NeurIPS).
- × Not interesting theoretically (Bénard et al (2022) Biometrika).
- Instead of breaking the relationship of X^j with X^{-j} and y, we only need to break it with y!

Literature review: General model-agnostic framework

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where the j-th covariate is permuted.

- **Conditional Permutation Importance(CPI)**:

$$\widehat{\psi}_{\mathrm{CPI}}(j, P_0) = \frac{1}{n_{\mathrm{test}}} \sum_{i=1}^{n_{\mathrm{test}}} \mathscr{L}\left(y_i, \widehat{m}(\widetilde{x}_i'^{(j)})\right) - \mathscr{L}\left(y_i, \widehat{m}(x_i)\right), \tag{4}$$

where the j-th covariate is *conditionally* permuted.

  - ✓ Works well in practice(Chamma et al. (2023) NeurIPS).
  - × Not an interesting theoretical quantity.

Improving variable selection: double robustness of CPI

- To detect a null covariate $j \in \mathscr{H}_0$, it is sufficient to either have a good estimate of $\widehat{m}$ or a good conditional sampler:
  - If $\widehat{m} \approx m \in \mathscr{F}_{-j} := \{f, f(u) = f(v) \text{ for } u_{-j} = v_{-j}\}$, then $m(\widetilde{X}'^{(j)}) = m(X)$ and

$$\mathbb{E}\left[\mathscr{L}(y, m(\widetilde{X}'^{(j)}))|\mathscr{D}_{\text{train}}\right] - \mathbb{E}\left[\mathscr{L}(y, m(X))|\mathscr{D}_{\text{train}}\right] \approx 0.$$

  - If $\widetilde{X}'^{(j)} \approx \widetilde{X}^{(j)}$, then $\widetilde{X}^{(j)} \overset{\text{i.i.d.}}{\sim} X$ and $\widetilde{X}^{(j)j} \perp\!\!\!\perp y | X^{-j}$ so

$$\mathbb{E}\left[\mathscr{L}(y, \widehat{m}(\widetilde{X}^{(j)}))|\mathscr{D}_{\text{train}}\right] - \mathbb{E}\left[\mathscr{L}(y, \widehat{m}(X))|\mathscr{D}_{\text{train}}\right] \approx 0.$$

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Proposition 1

Assuming $y = X\beta + \varepsilon$ with X Gaussian, then

$$\mathbb{E}[\widehat{\psi}_{\text{LOCO}}(j, P_0)] = \psi_{\text{TSI}}(j, P_0) + O(1/\boldsymbol{n}_{\text{train}}),$$
$$\mathbb{E}[\widehat{\psi}_{\text{CPI}}(j, P_0)] = \psi_{\text{TSI}}(j, P_0) + O(1/\boldsymbol{n}_{\text{train}}^2).$$

Sobol-CPI: a new Total Sobol Index estimate

- **Goal:** $\psi_{\mathrm{TSI}}(j, P_0) = \mathbb{E}\left[\mathscr{L}(y, m_{-j}(X^{-j})) - \mathscr{L}(y, m(X))\right]$.
- We can use the Tower's property:

$$m_{-j}(X^{-j}) = \mathbb{E}\left[y \mid X^{-j}\right] \tag{5}$$

$$= \mathbb{E}\left[\mathbb{E}[y \mid X] \mid X^{-j}\right] \tag{6}$$

$$= \mathbb{E}\left[m(X) \mid X^{-j}\right] \tag{7}$$

$$= \mathbb{E}\left[m(\widetilde{X}^{(j)}) \mid X^{-j}\right]. \tag{8}$$

Sobol-CPI: a new Total Sobol Index estimate

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- $m_{-j}(X^{-j}) = \mathbb{E}\left[m(\widetilde{X}^{(j)}) \mid X^{-j}\right]$.
- Generate n_{cal} conditionally independent samples/ observation.
- **Sobol-CPI**:

$$\widehat{\psi}_{\mathrm{Sobol-CPI}}(j, P_0) = \frac{1}{n_{\mathrm{test}}} \sum_{i=1}^{n_{\mathrm{test}}} \mathscr{L}\left(y_i, \frac{1}{n_{\mathrm{cal}}} \sum_{l=1}^{n_{\mathrm{cal}}} \widehat{m}(\widetilde{x}_{i,l}'^{(j)})\right) - \mathscr{L}\left(y_i, \widehat{m}(x_i)\right). \tag{5}$$

✓ It is **nonparametric efficient**, **fast**, and **stable**.

✓ It links removal with permutation approaches (**explainable**).

✓ It provides **type-I error** control!

Sobol-CPI: a new Total Sobol Index estimate

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- ✓ It is **nonparametric efficient**, **fast**, and **stable**.
- ✓ It links removal with permutation approaches (**explainable**).
- ✓ It provides **type-I error** control!
- If $\mathscr{L} = \ell^2$, fixing n_{cal}, then
  $\widehat{\psi}_{\mathrm{Sobol-CPI}}(j,P_0) \xrightarrow{n_{\mathrm{train}}, n_{\mathrm{test}} \to \infty} (1 + 1/n_{\mathrm{cal}})\psi_{\mathrm{TSI}}(j,P_0)$.

Double robustness in practice

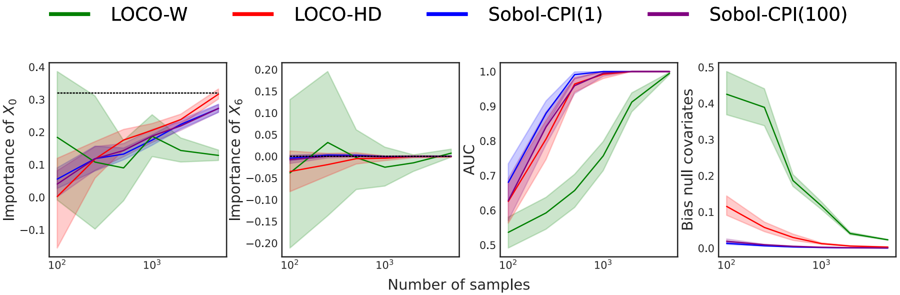

Figure 2: **Double robustness with complex learners:** $\widehat{m}$ a Superlearner and $y = X_0 X_1 \mathbb{I}_{X_2>0} + 2X_3X_4\mathbb{I}_{X_2<0}$, with $X \sim \mathcal{N}(\mu, \Sigma)$, where $\Sigma_{i,j} = 0.6^{|i-j|}$, $p = 50$, and $\mu = \mathbf{0}$.

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Conclusion

- ✓ Sobol-CPI provides a **general** and **consistent** VIM.
- ✓ A simple, valid, and fast conditional sampler exists.
- ✓ It is **fast**: it remains a permutation-based approach!
- ✓ It leverages CPI's **double robustness**:
  To detect j null, a good $\widehat{m}$ or a good conditional sampler suffices.
- ✓ It can be also applied to causality: Paillard et al. (2025) ICML.

Conclusion

Methods	**LOCO**	**PFI**	**CPI**	**Sobol-CPI**
Fast	✗	✓	✓	✓
No extrapolation	✓	✗	✓	✓
Interpretable	✓	✗	✗	✓
Double Robustness	✗	✗	✓	✓
Type-I error control	✓	✗	✗	✓

Thank You, Questions?

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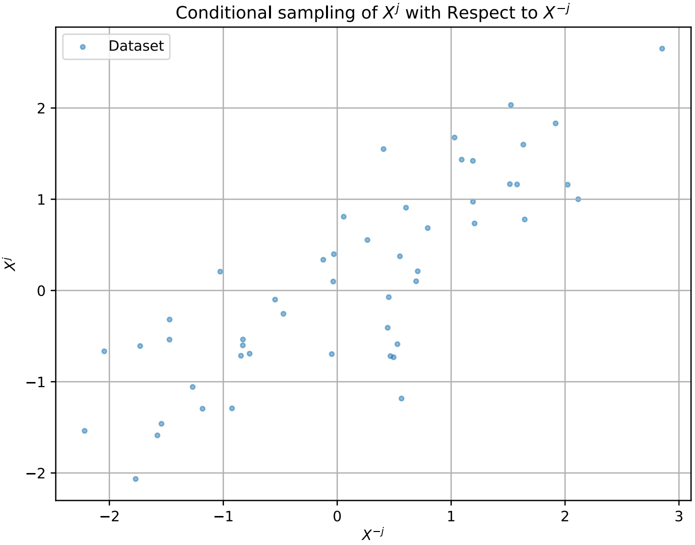

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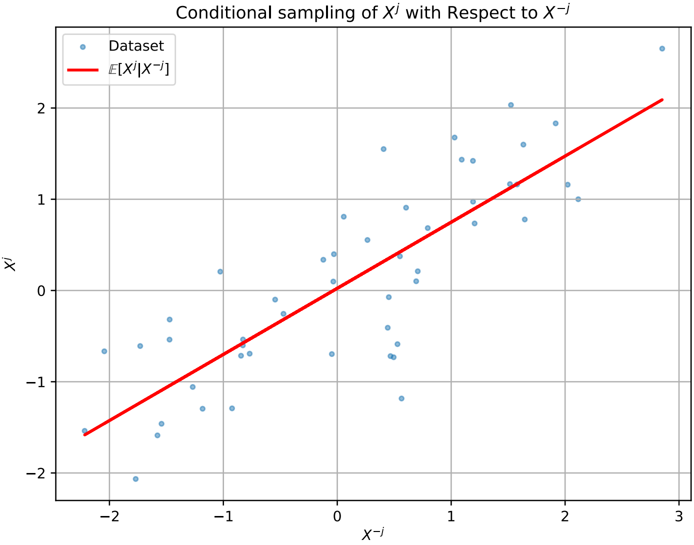

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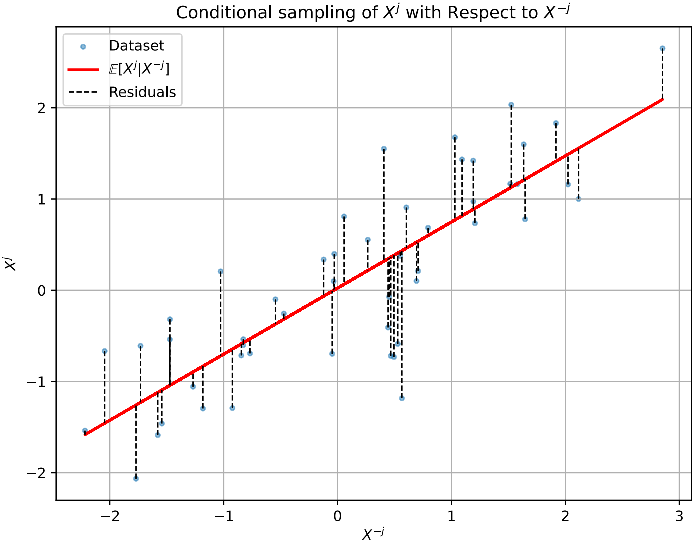

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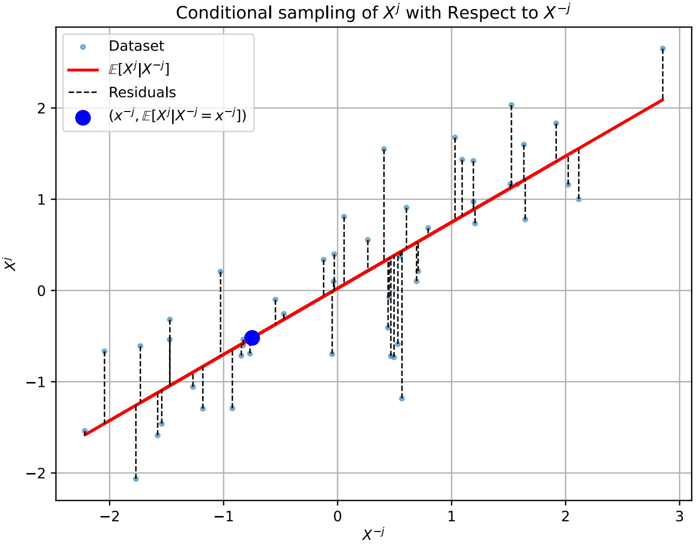

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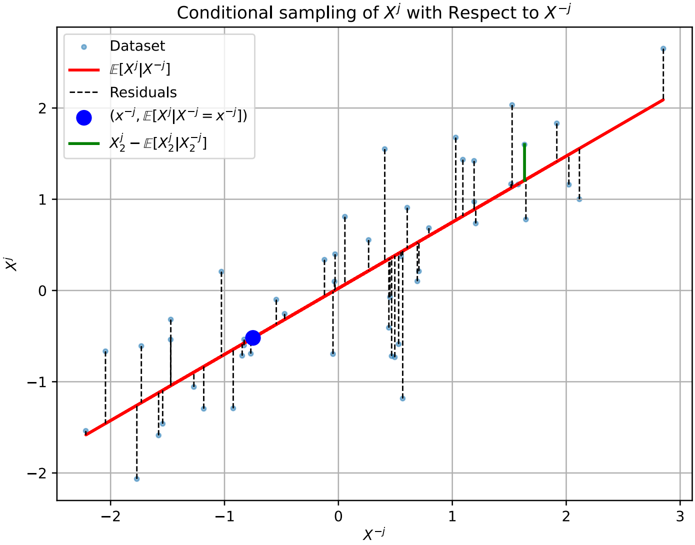

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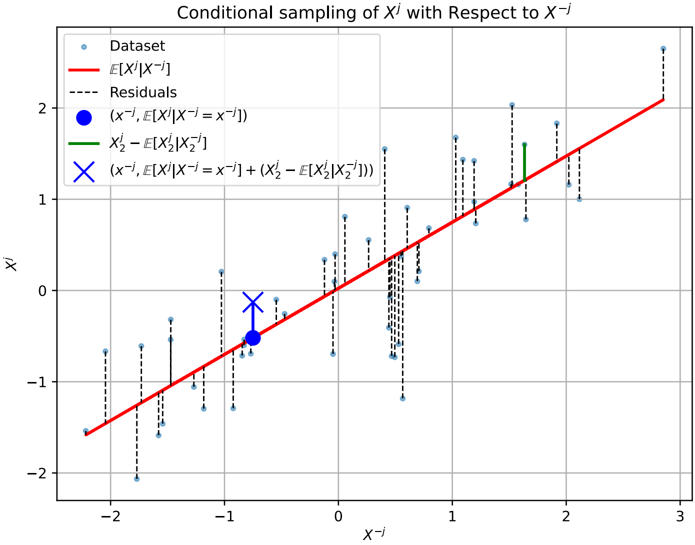

Validity of the conditional sampling

- In practice, we need to train a regressor $\widehat{\nu}_{-j}$ of X^j on X^{-j}. Then, for an x, we predict $\widehat{\nu}_{-j}(x^{-j})$ and add a permuted residual $(x'^j - \widehat{\nu}_{-j}(x'^j))$.

Assumption 1

$X^j = \nu_{-j}(X^{-j}) + \varepsilon$ with $\varepsilon \perp\!\!\!\perp X^{-j}$.

Lemma 2 (Internship contribution)

Under Assumption 1 and assuming the consistency of $\widehat{\nu}_{-j}$, the conditional step of the CPI, presented in Chamma et al.(2023) NeurIPS, is valid.

Double robustness using complex models

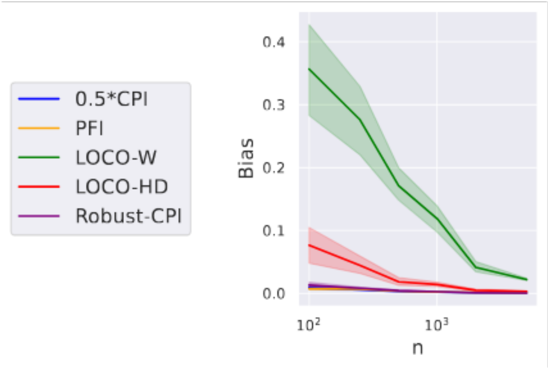

Figure 3: Bias on estimating ψ_{TSI} for null covariates with $y = X_1 X_2 \mathbb{1}_{X_3>0} + 2X_4 X_5 \mathbb{1}_{X_3<0}$, $p = 50$ and $\rho = 0.6$ using super-learner.

Effect of n-cal

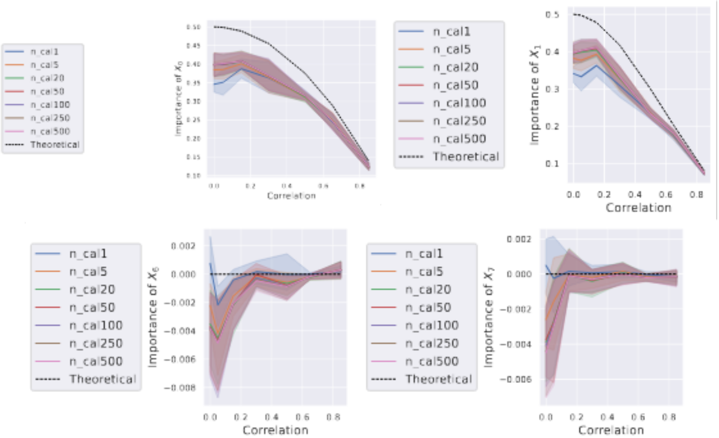

Figure 4: Bias of different Robust-CPI(n_{cal}) on estimating ψ_{TSI} for X_1, X_2 on the top and X_6, X_7 on the bottom, with $y = X_1X_2\mathbb{1}_{X_3>0} + 2X_4X_5\mathbb{1}_{X_3<0}$, $p = 50$ and $n = 5000$ using super-learner.

Effect of n-cal

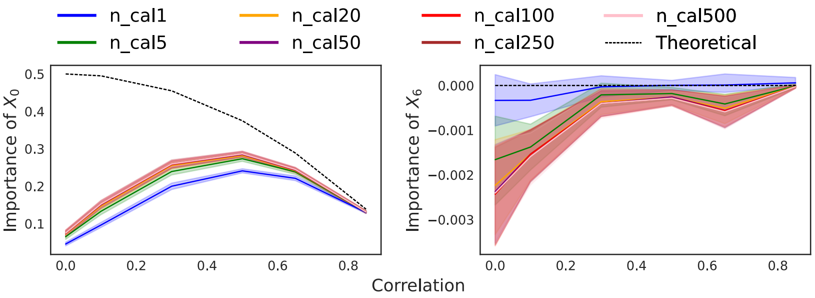

Figure 5: **Calibration set size effect as a trade-off between Variable Importance and Variable Selection:** Total Sobol Index estimation in a nonlinear setting. The first figure represents an important covariate (X_0), while the second represents a non-important covariate (X_6). We observe that with a larger n_{cal}, the importance estimation of the non-null covariate is slightly improved, enhancing variable importance. However, for the null covariate, there is a slightly greater bias, making variable selection less accurate.