Predictive uncertainty quantification with missing covariates

On the hardness of distribution-free group conditional coverage

Margaux Zaffran

December 16, 2024

International Conference on Statistics and Data Science

Julie Josse

PreMeDICaL

Inria

Yaniv Romano

Technion – Israel Institute of Technology

Aymeric Dieuleveut

CMAP

École Polytechnique

↪ Aymeric will present methodological results tomorrow at 9am in room Fregate!

Distribution-free predictive uncertainty quantification

Quantifying predictive uncertainty

- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables
- n training samples $\left(X^{(k)}, Y^{(k)}\right)_{k=1}^{n}$
- Goal: predict an unseen point $Y^{(n+1)}$ at $X^{(n+1)}$ with **confidence**
- How? Given a miscoverage level $\alpha \in [0, 1]$, build a predictive set $\mathcal{C}_\alpha$ such that:

$$\mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}\right)\right\} \geq 1 - \alpha, \qquad \text{(validity)}$$

  and $\mathcal{C}_\alpha$ should be as small as possible, in order to be informative.

- *Construction* of the predictive intervals should be
  - agnostic to the learning model[1]
  - agnostic to the data distribution
- *Validity* should be ensured
  - in finite samples
  - for all data distribution and underlying learnt model

[1] The underlying model can be any probabilistic model tailored for the application task at hand.

Distribution-free marginal validity is achievable

Conformal prediction (Vovk et al., 2005; Papadopoulos et al., 2002; Lei et al., 2018) builds an estimated predictive set $\widehat{C}_\alpha$ based on n data points.

Conformal prediction achieves marginal validity (Vovk et al., 2005)

$\widehat{C}_\alpha$ outputted by conformal prediction is such that for any distribution $\mathcal{D}$ on $(\mathcal{X}, \mathcal{Y})$, it holds:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right)\right) \geq 1 - \alpha.$$

✗ Marginal coverage: $\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right) \cancel{|X^{(n+1)} = x}\right) \geq 1 - \alpha.$

Definition of distribution-free features conditional validity

$\widehat{C}_\alpha$ = estimated predictive set based on n data points.

Distribution-free X-conditional validity

$\widehat{C}_\alpha$ achieves distribution-free X-conditional validity if for any distribution $\mathcal{D}$, it holds:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right) | X^{(n+1)}\right) \overset{a.s.}{\geq} 1-\alpha.$$

Limits of distribution-free conditional predictive uncertainty quantification

Informative conditional coverage as such is impossible

Impossibility results (Vovk, 2012; Lei and Wasserman, 2014)[2]

If $\widehat{C}_\alpha$ is distribution-free X-conditionally valid, then, for any $\mathcal{D}$, for $\mathcal{D}_X$–almost all $\mathcal{D}_X$–**non-atoms** $\mathbf{x} \in \mathcal{X}$, it holds:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n)}}\left\{\text{mes}\left(\widehat{C}_\alpha(x)\right) = \infty\right\} \geq 1 - \alpha.$$

- Asymptotic (with the sample size) conditional coverage
  $\hookrightarrow$ Romano et al. (2019); Kivaranovic et al. (2020); Chernozhukov et al. (2021); Sesia and Romano (2021); Izbicki et al. (2022)
- Approximate conditional coverage
  $\hookrightarrow$ Romano et al. (2020); Guan (2022); Jung et al. (2023); Gibbs et al. (2023)
  Target $\mathbb{P}(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right) | X^{(n+1)} \in \mathcal{R}(x)) \geq 1 - \alpha$

[2] An analogous statement is also available for the classification framework.
Non exhaustive references.

Definition of distribution-free group conditional validity ($\mathcal{G}$CV)

$\widehat{C}_\alpha$ = estimated predictive set based on n data points.

$\mathcal{G}$ a set of "groups" (i.e., define G a random variable taking its values in $\mathcal{G}$).

Distribution-free $\mathcal{G}$-conditional validity ($\mathcal{G}$CV)

$\widehat{C}_\alpha$ achieves distribution-free $\mathcal{G}$-conditional validity if for any distribution $\mathcal{D}$ on $(\mathcal{X}, \mathcal{G}, \mathcal{Y})$, it holds that:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}, G^{(n+1)}\right) | G^{(n+1)}\right) \overset{a.s.}{\geq} 1 - \alpha.$$

General $\mathcal{G}$CV hardness result **(Z., Josse, Romano and Dieuleveut, 2024)**[3]

If any $\widehat{C}_\alpha$ is distribution-free $\mathcal{G}$-conditionally valid then **for any distribution** $\mathcal{D}$, for any group $g \in \mathcal{G}$ such that $\mathcal{D}_G(g) > 0$, it holds:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(\mathrm{mes}\left(\widehat{C}_\alpha\left(X^{(n+1)}, g\right)\right) = \infty\right) \geq 1 - \alpha - \Delta_{g,n}$$
$$\geq 1 - \alpha - \mathcal{D}_G(g)\sqrt{n+1}.$$

Irreducible term: consider $\widehat{C}_\alpha$ outputting $\mathcal{Y}$ with probability $1-\alpha$ and $\emptyset$ otherwise.

$\Delta_{g,n}$ term: smaller than $\mathcal{D}_G(g)\sqrt{n+1}$

$\hookrightarrow$ gets negligible (making the lower bound nearly $1-\alpha$) **only** for low probability groups compared to n.

[3] An analogous statement is also available for the classification framework.

Restricting the link between G and (X or Y) does not allow informative $\mathcal{G}$CV

$G \perp\!\!\!\perp X$ hardness result **(Z., Josse, Romano and Dieuleveut, 2024)**

If any $\widehat{C}_\alpha$ is $\mathcal{G}$CV under $G \perp\!\!\!\perp X$, then for any distribution $\mathcal{D}$ such that $G \perp\!\!\!\perp X$, for any group g such that $\mathcal{D}_G(g) > 0$, it holds:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(\text{mes}\left(\widehat{C}_\alpha\left(X^{(n+1)}, g\right)\right) = \infty\right) \geq 1-\alpha-\Delta_{g,n} \geq 1-\alpha-\mathcal{D}_G(g)\sqrt{n+1}.$$

$Y \perp\!\!\!\perp G \mid X$ hardness result **(Z., Josse, Romano and Dieuleveut, 2024)**

If any $\widehat{C}_\alpha$ is MCV under $Y \perp\!\!\!\perp G \mid X$, then for any distribution $\mathcal{D}$ such that $Y \perp\!\!\!\perp G \mid X$, for any mask m such that $\frac{1}{\sqrt{2}} \geq \mathcal{D}_G(g) > 0$, it holds:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(\text{mes}\left(\widehat{C}_\alpha\left(X^{(n+1)}, g\right)\right) = \infty\right) \geq 1-\alpha-\Delta_{g,n} \geq 1-\alpha-2\mathcal{D}_G(g)\sqrt{n+1}.$$

$\Rightarrow$ need to restrict both the link between G and X, as well as between G and Y.

Analogous statements are also available for the classification framework.

Application to learning with missing covariates

Missing values are ubiquitous and challenging

Data: $\left(X^{(k)}, M^{(k)}, Y^{(k)}\right)_{k=1}^{n}$

Y	X_1	X_2	X_3
22	5	6	3
19	6	8	NA
19	5	3	6
7	NA	9	NA
13	4	9	0
20	NA	NA	1
9	8	NA	4

Mask $M =$

$(M_1$	M_2	$M_3)$
0	0	0
0	0	1
0	0	0
1	0	1
0	0	0
1	1	0
0	1	0

$\hookrightarrow$ 2^d potential masks.

$\hookrightarrow$ M can depend on X or Y (depending on the missing mechanism[4]).

$\Rightarrow$ Statistical and computational challenges.

[4] Three mechanisms connecting X and M from Rubin (1976), *Inference and missing data*, Biometrika

Supervised learning with missing values: impute-then-predict

Impute-then-predict procedures are widely used.

1. Replace NA using an imputation function (e.g. the mean), noted ϕ.

$$\begin{array}{c} x^{(1)} \\ x^{(2)} \\ x^{(3)} \\ x^{(4)} \end{array} \begin{bmatrix} -1 & -10 & 6 & 0 \\ 4 & \texttt{NA} & -2 & 2 \\ 5 & 1 & 2 & \texttt{NA} \\ 0 & \texttt{NA} & \texttt{NA} & 1 \end{bmatrix} \xrightarrow{\phi} \begin{array}{c} u^{(1)} \\ u^{(2)} \\ u^{(3)} \\ u^{(4)} \end{array} \begin{bmatrix} -1 & -10 & 6 & 0 \\ 4 & -4.5 & -2 & 2 \\ 5 & 1 & 2 & 1 \\ 0 & -4.5 & 3 & 1 \end{bmatrix}$$

2. Train your algorithm (Random Forest, Neural Nets, etc.) on the imputed data: $\left\{ \underbrace{\phi\left(X^{(k)}_{\mathrm{obs}(M^{(k)})}, M^{(k)}\right)}_{U^{(k)}=\text{imputed } X^{(k)}}, Y^{(k)} \right\}_{k=1}^{n}$.

$\hookrightarrow$ we consider an impute-then-predict pipeline in this work.

Goals of predictive uncertainty quantification with missing values

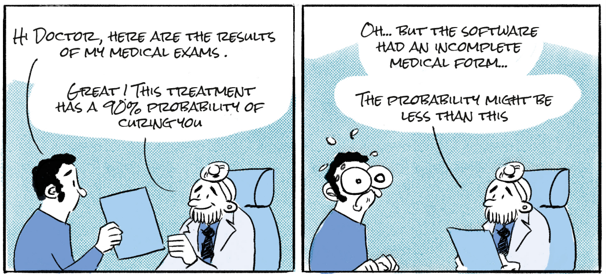
Goal: predict $Y^{(n+1)}$ with **confidence** $1-\alpha$, i.e. build the smallest $\mathcal{C}_\alpha$ such that:

1. Marginal Validity (MV)

$$\mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}, M^{(n+1)}\right)\right\} \geq 1-\alpha. \qquad \text{(MV)}$$

2. Mask-Conditional-Validity (MCV)

$$\mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}, M^{(n+1)}\right) | M^{(n+1)}\right\} \overset{a.s.}{\geq} 1-\alpha. \qquad \text{(MCV)}$$



Illustrations @theoremlinger

Validities of predictive uncertainty quantification with missing values

Goal: predict $Y^{(n+1)}$ with **confidence** $1-\alpha$, i.e. build the smallest $\mathcal{C}_\alpha$ such that:

1. Marginal Validity (MV)

$$\mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}, M^{(n+1)}\right)\right\} \geq 1-\alpha. \quad \text{(MV)}$$

2. Mask-Conditional-Validity (MCV)

$$\mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}, M^{(n+1)}\right) | M^{(n+1)}\right\} \overset{a.s.}{\geq} 1-\alpha. \quad \text{(MCV)}$$

	Exisiting approaches	New approach (Z., Josse, Romano and Dieuleveut, 2024)
(MV)	✓ (Z., Dieuleveut, Josse, and Romano, 2023)	✓
(MCV)	✗	✓ under $M \perp\!\!\!\perp (X, Y)$

Thanks for listening and feel free to reach out to us!

Tomorrow at 9am in room Fregate: methodological results by Aymeric!

References i

Chernozhukov, V., Wüthrich, K., and Zhu, Y. (2021). Distributional conformal prediction. *Proceedings of the National Academy of Sciences*, 118(48).

Gibbs, I., Cherian, J. J., and Candès, E. J. (2023). Conformal prediction with conditional guarantees. arXiv: 2305.12616.

Guan, L. (2022). Localized conformal prediction: a generalized inference framework for conformal prediction. *Biometrika*, 110(1).

Izbicki, R., Shimizu, G., and Stern, R. B. (2022). CD-split and HPD-split: Efficient conformal regions in high dimensions. *Journal of Machine Learning Research*, 23(87).

Jung, C., Noarov, G., Ramalingam, R., and Roth, A. (2023). Batch multivalid conformal prediction. In *International Conference on Learning Representations*.

Kivaranovic, D., Johnson, K. D., and Leeb, H. (2020). Adaptive, Distribution-Free Prediction Intervals for Deep Networks. In *International Conference on Artificial Intelligence and Statistics*. PMLR.

Lei, J., G'Sell, M., Rinaldo, A., Tibshirani, R. J., and Wasserman, L. (2018). Distribution-Free Predictive Inference for Regression. *Journal of the American Statistical Association*.

Lei, J. and Wasserman, L. (2014). Distribution-free prediction bands for non-parametric regression. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 76(1).

Papadopoulos, H., Proedrou, K., Vovk, V., and Gammerman, A. (2002). Inductive Confidence Machines for Regression. In *Machine Learning: ECML*. Springer.

Romano, Y., Barber, R. F., Sabatti, C., and Candès, E. (2020). With Malice Toward None: Assessing Uncertainty via Equalized Coverage. *Harvard Data Science Review*, 2(2).

Romano, Y., Patterson, E., and Candès, E. (2019). Conformalized Quantile Regression. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Rubin, D. B. (1976). Inference and missing data. *Biometrika*, 63(3).

Sesia, M. and Romano, Y. (2021). Conformal prediction using conditional histograms. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Vovk, V. (2012). Conditional Validity of Inductive Conformal Predictors. In *Asian Conference on Machine Learning*. PMLR.

References iv

Vovk, V., Gammerman, A., and Shafer, G. (2005). *Algorithmic Learning in a Random World*. Springer US.

Zaffran, M., Dieuleveut, A., Josse, J., and Romano, Y. (2023). Conformal prediction with missing values. In *Proceedings of the 40th International Conference on Machine Learning*. PMLR.

Zaffran, M., Josse, J., Romano, Y., and Dieuleveut, A. (2024). Predictive uncertainty quantification with missing covariates. *arXiv:2405.15641*.