Evaluation of Machine Learning Models for Non-Standard Data Structures

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Background

This presentation is based on the following paper:

Hornung, R., Nalenz, N., Schneider, L., Bender, A., Bothmann, L., Dumpert, F., Bischl, B., Augustin, A., Boulesteix, A.-L., 2023.
Evaluating machine learning models in non-standard settings: An overview and new findings.
arXiv:2310.15108. Statistical Science (to appear).

Background

- Machine learning (**ML**) applications in **official statistics** frequently deal with **complex data structures** most of which violate the standard i.i.d. assumption.

- Such data structures include spatial and clustered data, as well as data under concept drift.

- The presence of these complex structures **can introduce bias** in generalization error (**GE**) **estimates** derived from **ordinary resampling** methods like cross-validation.

- **Tailored resampling** techniques are **necessary** for each data structure to obtain (largely) unbiased GE estimates.

Background

- A **shared aspect** of these specialized procedures is that they **ensure** that the **test data** relate to the **training data** in the **same way** that the **future data** relate to the data used for constructing the ML model.

- I will give an **overview** of such methods for the following **selection of complex data structures**: clustered data, spatial data, unequal sampling probabilities, concept drift, and hierarchically structured outcomes.

- This overview **synthesizes** insights from the **existing literature** and **our simulation studies**.

Clustered data

- In official statistics clustered data are frequently encountered, where **observations are grouped** based on structural relationships (e.g., individuals within a household).
- **When** the observations are **randomly assigned** to the training and test datasets, members of the **same cluster** appear **in both**.
- As a result, the **ML models within** the **resampling** tend to work **better on** the **test data** sets **than** on observations from **independent clusters**.
- **If** the **aim** of the prediction is to **predict** the outcome of observations from **new clusters**, this can lead to **underestimation** of the GE.

Clustered data

- **Empirical studies** have consistently shown **severe** GE **underestimation when** clusters involve **repeated measurements** of the **same entities**.
- **Our simulations** suggest that this **underestimation** tends to be **modest for** clusters constituted of **distinct entities**. **However**, the presence of **cluster-constant covariates** can exacerbate this effect.
- The **recommended** solution is **cluster-level resampling**, ensuring that training and test datasets comprise entirely **separate clusters**, thus avoiding any overlap.

Spatial data

- Spatial data, common in official statistics, inherently exhibit **spatial correlation**—observations **near** each other tend to be **more similar** than those farther apart.

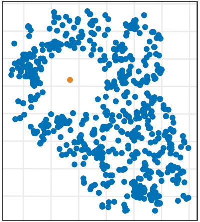
- It is **well known** from the literature that spatial correlation **must be taken into account** when **estimating the GE** to avoid underestimation.

- **Spatial cross-validation** methods are used here. These methods provide **adjustable parameters** to **fine-tune** the **separation** between training and test data.

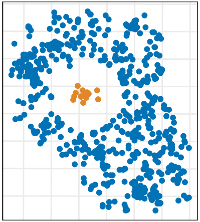
- The **selection** and **customization** of these methods **depends strongly on the application**, especially the **proximity** of the **new data** relative to the existing data.

Spatial data: Popular variants of spatial CV

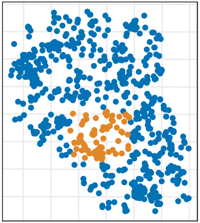
Leave−one−out CV
(w/ buffer)



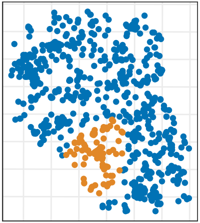
Leave−one−disc−out CV
(w/ buffer)



Leave−one−block−out CV with
geometric blocks (w/o buffer)



Leave−one−block−out CV with
clustered blocks (w/o buffer)



Unequal sampling probabilities

- In official statistics, the observations often have **unequal sampling probabilities**, e.g., to represent minorities adequately.
- The **resulting samples** are **not representative** of the population to which the ML model is to be applied.
- **Neglecting** this leads to **biased GE estimates**.
- This bias can be **corrected using** the **Horvitz-Thompson** theorem, **inversely weighting errors** by sampling probabilities.
- Our simulations indicate that the **bias** of conventional GE estimation **varies by ML method**. Yet, **Horvitz-Thompson**-based correction **consistently** ensured **unbiased** GE estimates.

Concept drift

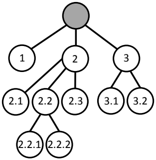
- Concept drift refers to **changes in the distribution** of data **over time**, **affecting predictive performance** in official statistics, where models are applied over long periods and concepts evolve.

- Accurately accounting for concept drift is **critical** in **GE estimation** to avoid **bias**.

- Our simulation results indicate that **largely unbiased** GE estimates can be obtained by using the **most recent observations as test data** ("out-of-sample validation").

- They also underscore the importance of **frequent model updating** and ensuring the **test dataset** is **not very small**.

Hierarchically structured outcomes



- Many official statistics **classification systems** are hierarchically structured, notably **tree-structured**.
- Despite the availability of **various evaluation metrics** for hierarchical predictions, **resampling** method **recommendations** are **lacking**.
- **Hypothesizing** that **stratified** cross-validation has **lower bias** and **variance** for hierarchical outcomes, we compared it with ordinary cross-validation in a simulation study.
- **Ordinary** cross-validation **slightly underestimated performance**, whereas **stratified** cross-validation showed **no bias** except for very small datasets; the **variances** of the estimates **did not differ** between the two approaches.

Figure from Hornung et al. (2023)

Summary of GE estimation for complex data structures

- **Clustered data:** Implement **cluster-level resampling** to prevent cluster overlap between training and test data.
- **Spatial data:** Apply **spatial cross-validation** techniques, ensuring the prediction goal drives the selection and customization of these methods.
- **Unequal sampling probabilities:** **Adjust** GE estimates **using** the **Horvitz-Thompson** theorem for bias correction.
- **Concept drift:** Apply out-of-sample validation by using the **most recent data** for **testing**; avoid very small test datasets.
- **Hierarchically structured outcomes:** Use **stratified cross-validation** to estimate performance, which avoids the slight bias associated with ordinary cross-validation.

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