



OTTAWA 2023

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mcmml
Munich Center for Machine Learning



CPS 82 – Statistical Methodology I

A general framework for reporting methods in regression analysis

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Interpretable ML

“Determining trust in individual predictions is an important problem when [models are] used for decision making.”

– Ribeiro (2016)

Medicine

“The reign of the p-value is over: what alternative analyses could we employ to fill the power vacuum?”

– Halsey (2019)

“Science is undergoing a crisis that has been referred to, since the early 21st century, as a crisis of confidence and a crisis of replication.”

– Frias-Navarro (2020)

Sociology

“In disciplines with high theoretical diversity, such as sociology, [standard literature searches often do not suffice] to fully exploit the entire body of relevant work.”

– Roelfs (2013)

Econometricrics

“Although the literature on how to implement and interpret interactions is vast, there remains confusion and disconsensus among researchers about how to interpret a main effect in the presence of moderation.”

– Busenbark (2022)

Interpretable ML

- *Individual conditional expectation plots*
- *Marginal plots*
- *Partial dependence plots*

Medicine

- *Predicted change in probability*
- *Average treatment effect*

*proposals for
interpretable and comparable
effect size measures and
visualization techniques*

Sociology

- *Average predictive comparisons*
- *Unit change*

Econometricrics

- *Marginal effects*
- *Adjusted predictions*

The framework's setting I

- The proposed framework applies to any (thus far parametric, i.e. finite dimensional parameter space Θ) models where the conditional expectation of the target variable can be written as

$$\mathbb{E}[Y|X] = g_{\theta}(X)$$

where the function $g_{\theta} : \mathbb{R}^p \rightarrow \mathbb{R}$, $p \in \mathbb{N}$, is at least once partially differentiable w.r.t. each metric element of $X \forall \theta \in \Theta$.

- Here, we consider the function g_{θ} to be indexed by $\theta \in \Theta$ in the sense of the following mapping

$$g : \Theta \rightarrow \mathcal{M}(\mathbb{R}^p), \quad \theta \mapsto g_{\theta}$$

with $\mathcal{M}(\mathbb{R}^p) := \{f : \mathbb{R}^p \rightarrow \mathbb{R} \mid f \text{ is } (\mathcal{B}(\mathbb{R}^p), \mathcal{B}(\mathbb{R}))\text{-measurable}\}$, $p \in \mathbb{N}$.

The framework's setting II

- Given this, we propose to utilize probability measures to derive appropriately weighted means of functions of g_θ over areas of interest.
- Specifically, for some function $h : \mathbb{R}^d \rightarrow \mathbb{R}$, $d \in \mathbb{N}_{>0}$, and set $D \subseteq \mathbb{R}^{\tilde{d}}$, $d \geq \tilde{d} \in \mathbb{N}_{>0}$, we consider probability measures μ that satisfy the following requirements:
 - (M1) μ is a probability measure on $(\mathbb{R}^{\tilde{d}}, \mathcal{B}(\mathbb{R}^{\tilde{d}}))$.
 - (M2) $\text{supp}(\mu) \subseteq D$, if required as a result of μ being normalized w.r.t. D .
 - (M3) $\int_{\mathbb{R}^{\tilde{d}}} |h(x)| d\mu(x) < \infty$, if $\tilde{d} = d$, or $\forall x_a \in \mathbb{R}^{d-\tilde{d}} : \int_{\mathbb{R}^{\tilde{d}}} |h(x_a, x_b)| d\mu(x_b) < \infty$, if $\tilde{d} < d$.

Methodological challenges

- Surprisingly: finding a coherent notation and setting that are formally correct, especially for categorical regressors/features.
- Solutions for models containing interaction terms.
- Formalizing existing methods, such as *marginal effects & adjusted predictions* and *average predictive comparisons* to allow for proving that they are a special case of the current framework.

Quantities in the framework

- **generalized marginal effects** - change of conditional expectation, averaged over a certain set of regressor/feature values.
- **individualized expectation** - conditional expectation, averaged over a certain set of regressor/feature values.
- **individualized predictive distribution** - distribution of the target variable with a specific individualized expectation set as expected value.

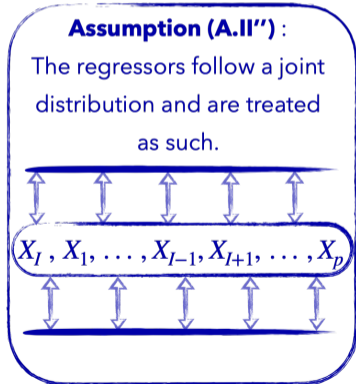
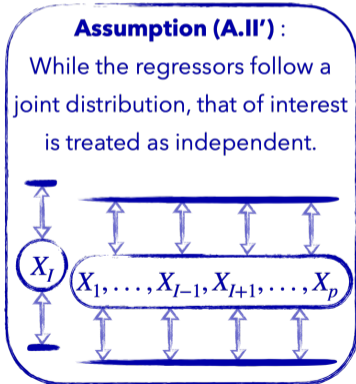
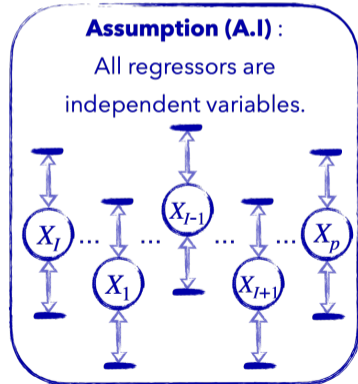
Advantages compared to existing effect size estimates and visualizations

1. For each definition, the user can individually determine probability measures that represent the situationally appropriate averaging over the inputs.
→ Quantities may be seen as *tool kits* that can be specified to derive effects/expectations etc. over areas of interest.
2. After specification, one gets functions of the parameter vector θ for each quantity.
→ This allows us to provide a consistent method of calculating point estimates and well-interpretable uncertainty regions.

Assumptions

In our framework, a regressor/feature whose effect on the target variable is of interest (X_I) has to be chosen for each quantity.

To aide in the choices of probability measures, we have identified the following "assumptions":



Choices of probability measures

One of the main contributions of the proposed framework is its flexibility to be tailored to most research settings, so there are no universally best choices of probability measure.

Still, here are some examples that will often be reasonably applicable:

- The distribution given by the **relative frequency** in a given data set.
- The (discrete) **Uniform distribution** - for metric regressors this choice additionally has nice computational properties.
- The distribution of characteristics in the population as **determined by previous studies**.

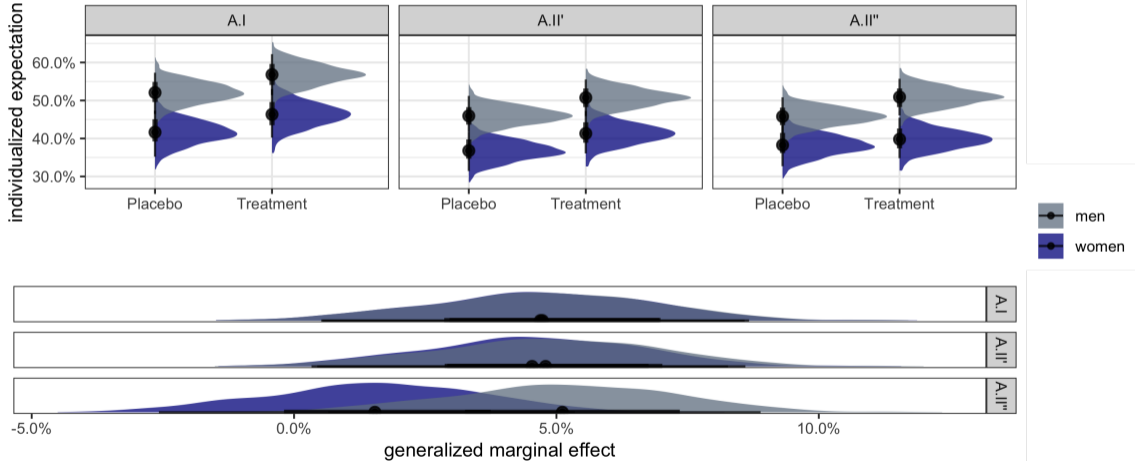
⇒ Each combination of assumption and marginal probability measure choice leads to a different interpretation of the resulting quantity!

Uncertainty modelling

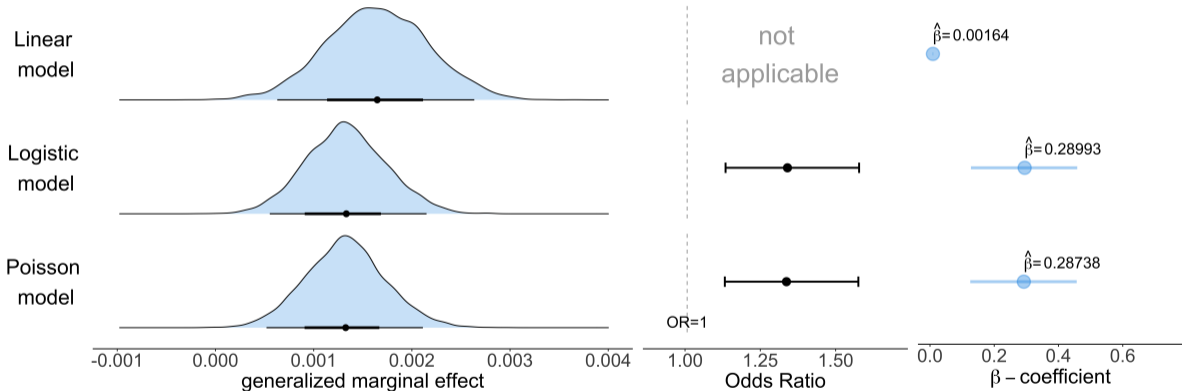
- We take a Bayesian approach to quantifying uncertainty – but all methods can still be applied to the results of both Bayesian and frequentist analyses!
- Specifically, this is achieved by treating θ as a random variable with distribution equal to
 - the posterior distribution given by a Bayesian analysis
 - $N(\hat{\theta}, \Sigma_{\hat{\theta}})$ for the frequentist point estimate $\hat{\theta}$ and covariance matrix $\Sigma_{\hat{\theta}}$

and then deriving a point estimate (e.g. *median*) and credible set (e.g. *equal-tailed interval*) directly for the random variable defined by $q \circ \theta$, for any considered quantity q .

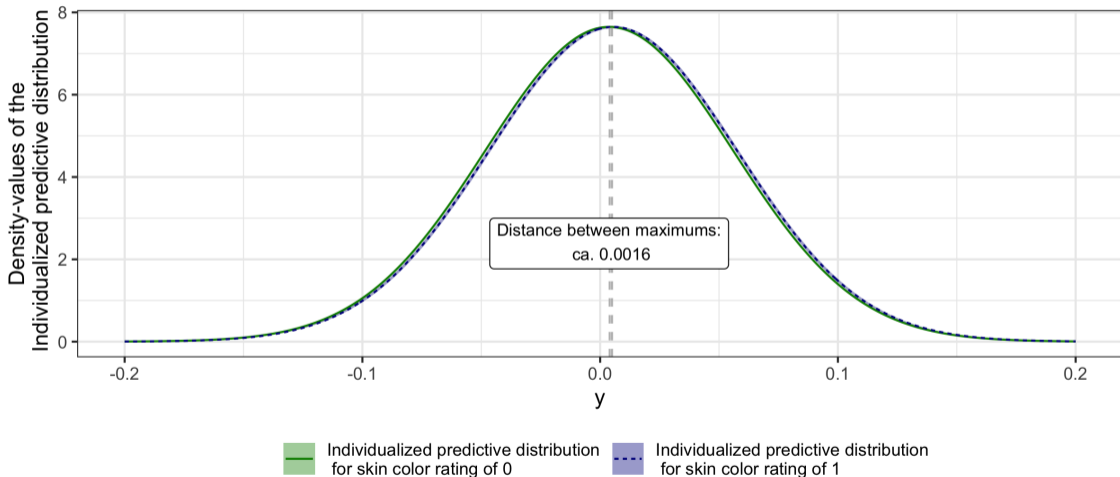
Example: Evidence-based decision making



Example: Multi-Analyst Studies



Example: Visualization through individualized predictive distribution



Outlook

- We are currently working on extending the framework to non- and semi-parametric settings.
- The developed framework can only be meaningful if it is communicated and recommended to practitioners on a large scale. To this end, both user-friendly implementation and tutorial papers aimed at various disciplines are important tools.
- Time-to-event modelling (survival analysis) is an interesting example of settings where the conditional expectation of the target variable is not always readily available – we continue to investigate how said expectation may still be derived in these settings so that they may be incorporated into our framework.

References



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Thank you
for your attention!

