Targeted learning under shape constraints

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Motivation

The road map of causal learning tells us to incorporate all the knowledge that we have into the statistical model for the distribution of the data

In many real applications, subject matter knowledge is available regarding the shape of the underlying conditional density and regression functions

Examples of biologically motivated shapes are

- risk of disease is not decreasing with age (given other covariates)
- The risk of disease should be a monotone function of age (given other covariates)
- The number of comorbidities increases the risk of disease
- the effect of a biomarker on the risk of disease is an unimodal function (given other covariates)

Target and nuisance parameters

Consider a real-valued target parameter $\psi : \mathcal{P} \to \mathbb{R}$

$$\psi(\mathrm{P}_{Q,G}) = \nu(Q)$$

for some functional $\nu : \mathcal{Q} \to \mathbb{R}$ such that G and 'all other parts' of Q are nuisance parameters.

Shape constraints on a function-valued target parameter have been considered by many, e.g., Groeneboom and Jongbloed [2014], Westling and Carone [2020], Wu and Westling [2022].

Today, we will mostly discuss imposing shape-constraints on nuisance parameters.

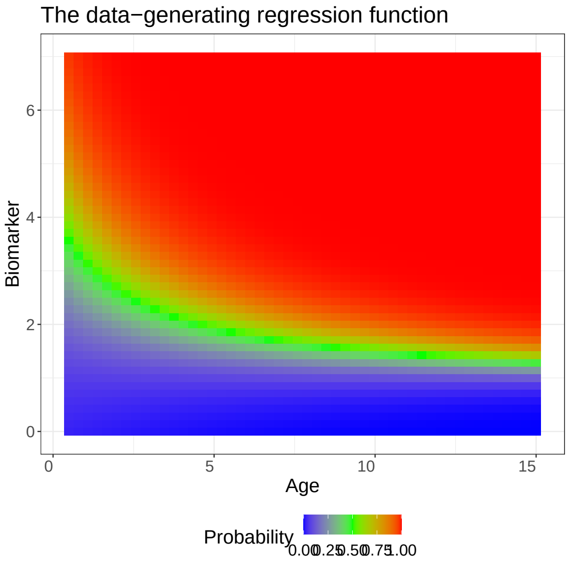
Working hypotheses

- Shape constraints can be incorporated into machine learning for nuisance parameters
- Biologically motivated shape constraints may lead to improved estimators

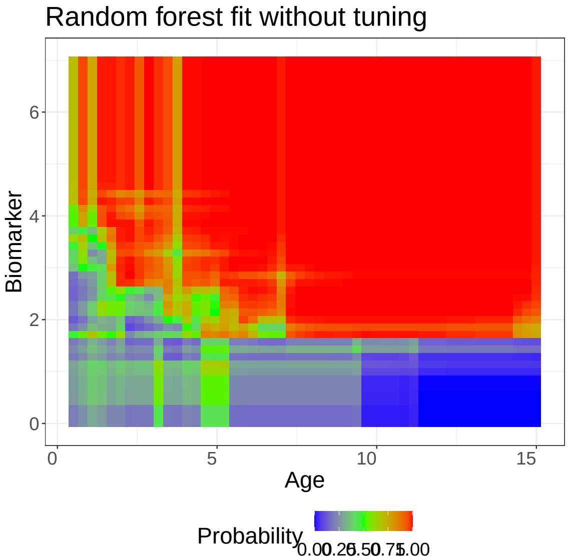
Goal for the workshop

- Discuss some initial hypotheses and ideas
- Help us move in the right research direction

Multivariate shape constraints



Machine learning (from the shelf)



Shape constraints

Examples

- Monotonicity
- Unimodality
- Convexity
- Log-concave density

Tools to incorporate shape constraints into machine learning

- Model specification/architecture
- Internal parameter tuning
- External penalty/loss function
- Smoothing applied to the fitted object
- Log-concave sampling
- what else?

Information bounds

Conjecture 1

Some shape constraints will not restrict the tangent space, and hence imposing such shape constraints does not change the information bound for the statistical estimation problem.

- Which shape constraints satisfy this when imposed on G and/or Q?
- Can we still improve a targeted minimum loss estimator (TMLE) by imposing such shape constraints on the nuisance parameters?

Conjecture 2

Constructing a TMLE under a shape constrained model will typically result in a sub-model that is not contained in the shape constrained model (c.f., van der Vaart [1989]).

Conjecture 3

Imposing shape constraints can improve the convergence rates of machine learning [e.g., Fang et al., 2021].

(Un)necessary restrictions on nuisance parameters?

Undersmoothing

It has been shown that undersmoothing of the estimators of the nuisance parameters is needed when they are 'plugged-in' to estimate a low-dimensional target parameter [e.g., Goldstein and Khasminskii, 1996, Hjort and Walker, 2001, van der Laan et al., 2022].

Could shape constraints induce unnecessary/unfortunate smoothing?

Biologically reasonable nuisance parameter estimators?

Should we pay attention to whether nuisance parameters are estimated by biologically meaningful estimators?

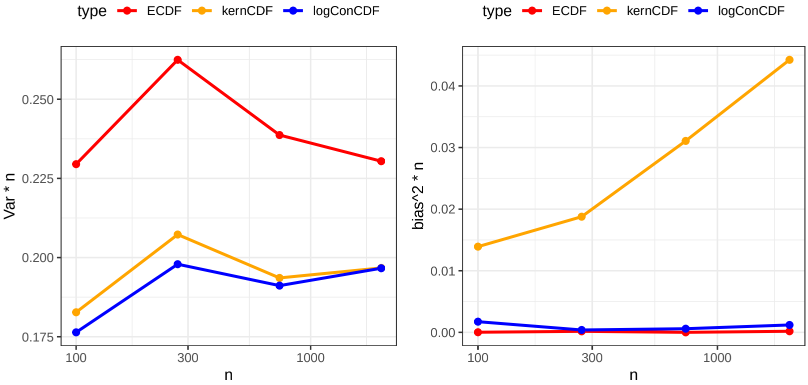
Should we accept a biologically unreasonable estimator of a nuisance parameter as long as it provides a good estimator of the target parameter?

Estimating a cumulative distribution function

ECDF Empirical cumulative distribution function

kernCDF Estimator based on smoothed kernel density estimator

logConCDF Estimator based on log-concave density estimator [Dümbgen and Rufibach, 2009, Rufibach and Duembgen, 2023]



Challenges for future research

- Should we distinguish between learning Q vs G parts of a causal model/information loss model?
- How do we translate "marginal" smoothness constraints into constraints on a multivariate function?
- In longitudinal settings, need to discuss shape-constraints on the history (filtration): an older value of a variable (such as A1c in diabetes) should have a lower effect than a newer value of the same variable.

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