Consistency between ML and classical approaches for covariate identification

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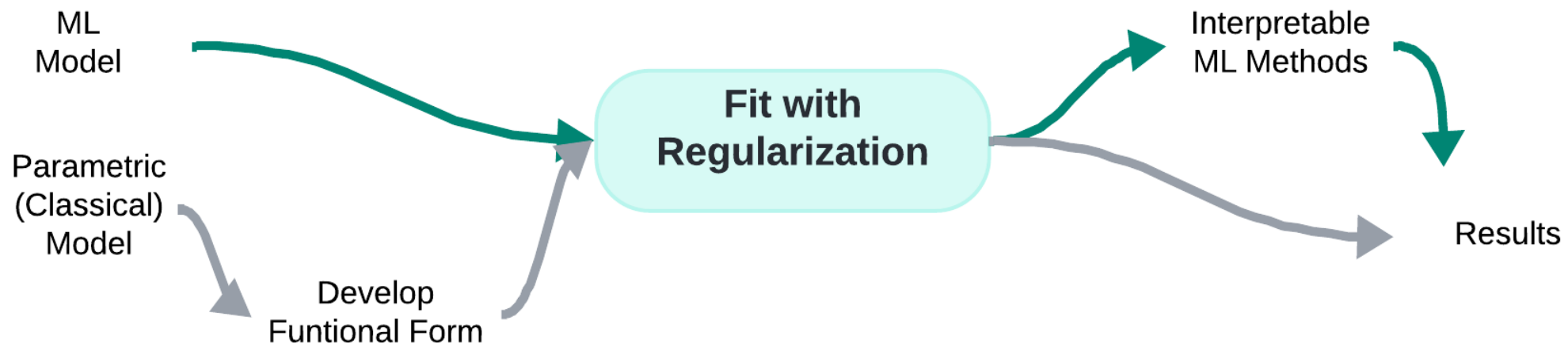
METRUM
RESEARCH GROUP

ASCPT 2024 ANNUAL MEETING

BIG IDEA

- Machine Learning ideas (e.g. regularization) applied to other models is a powerful combination

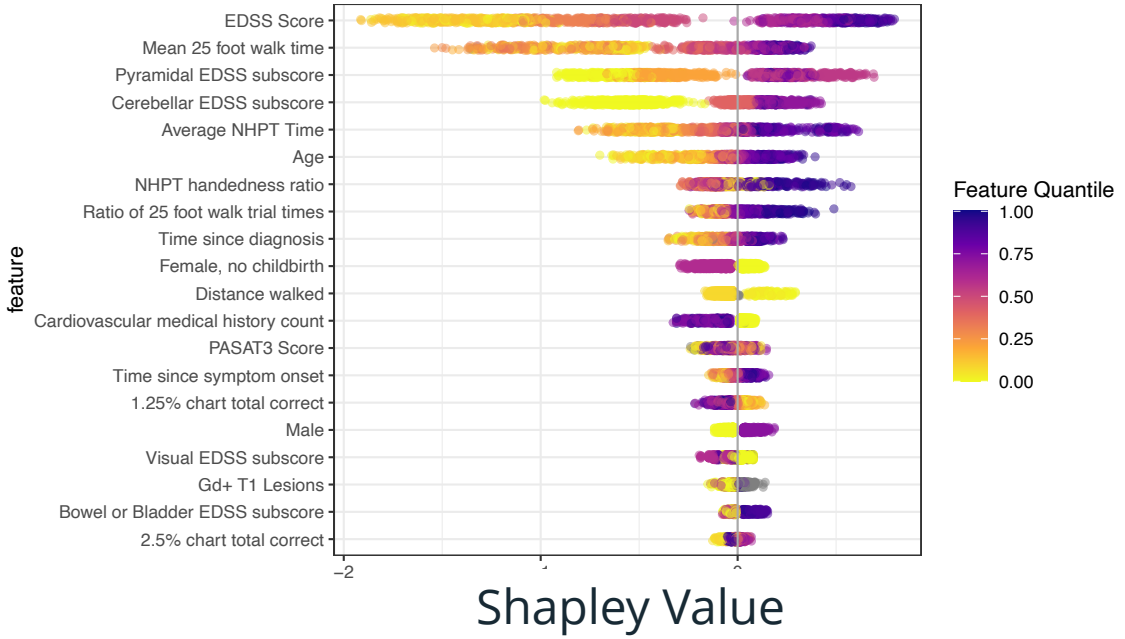


ML WORKFLOW: REGULARIZATION *AND* INTERPRETABLE AI

- Assemble data and choose model structure
- Tune (regularizing) hyperparameters for complex data
  - Large number of covariates
  - Complex relationships (nonlinear, interactions)
  - Non-standard data types (-omics)
- Interpret model fit
  - Shapley values
  - Variable importance
  - Predictions

SHAPLEY VALUES FOR COVARIATE INTERPRETATION

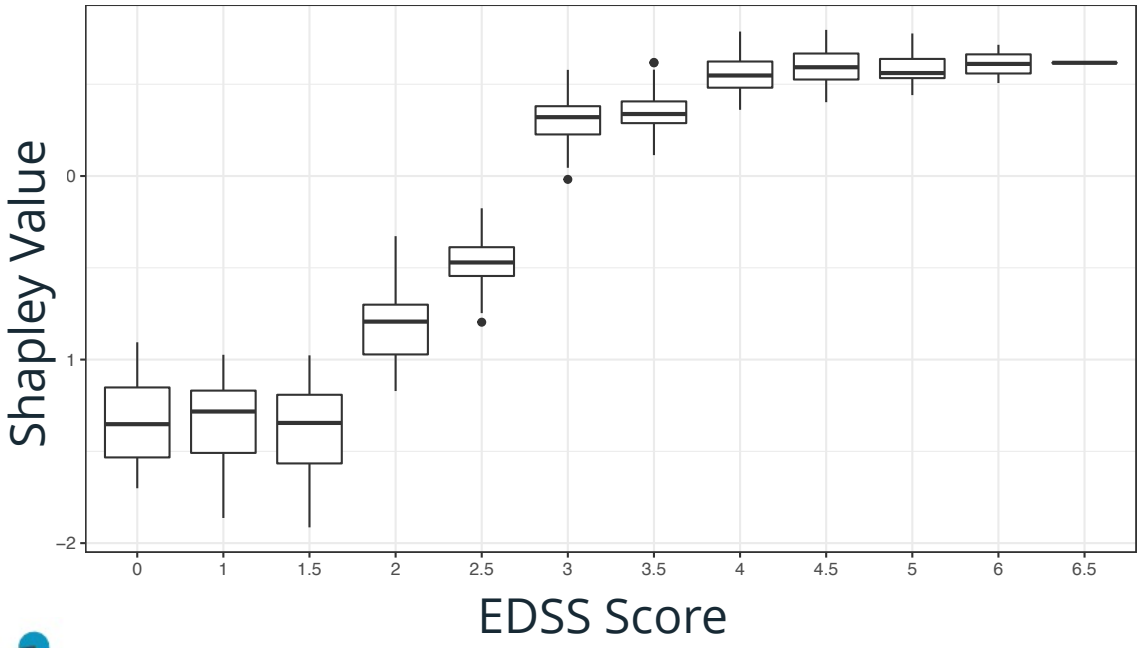
- Idea: Value of players (features) drafted onto sports team (model)
- Characterize:
  - magnitude
  - variability
  - shape
- Example: Predicting changes in subtype of Multiple Sclerosis

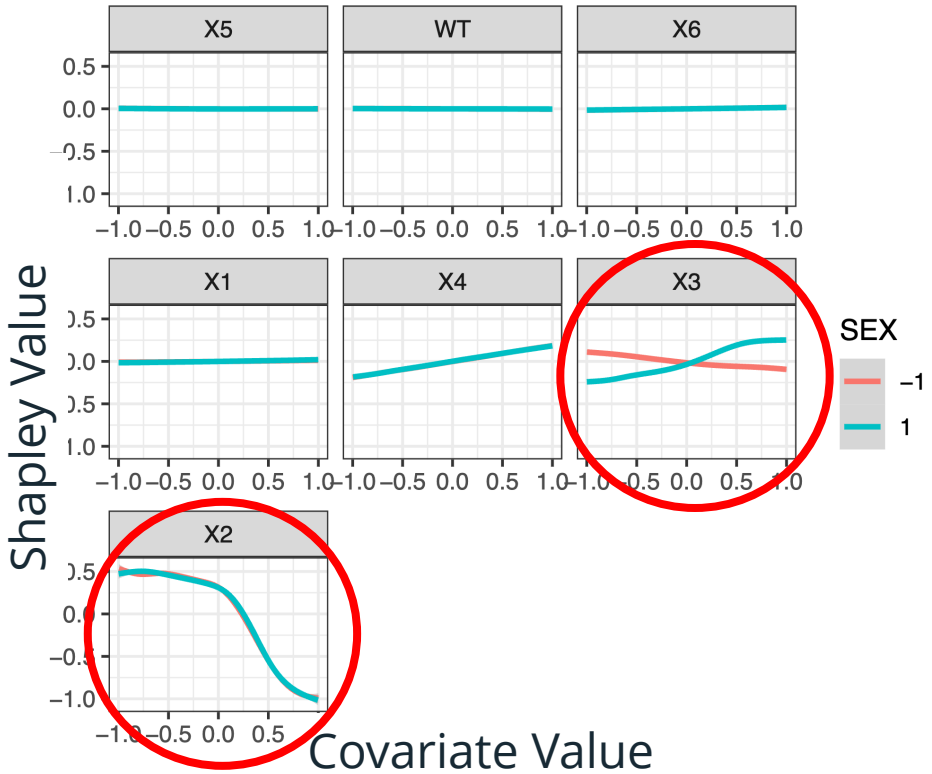


Wiens et. al. American Conference on Pharmacometrics 2022

SHAPLEY VALUES: COVARIATE RELATIONSHIPS

Non-linearity and Interactions





Wiens et. al. American Conference on Pharmacometrics 2022

Wiens, M; Husband, H; Reilly, B; Callisto, S. American Conference on Pharmacometrics 2023

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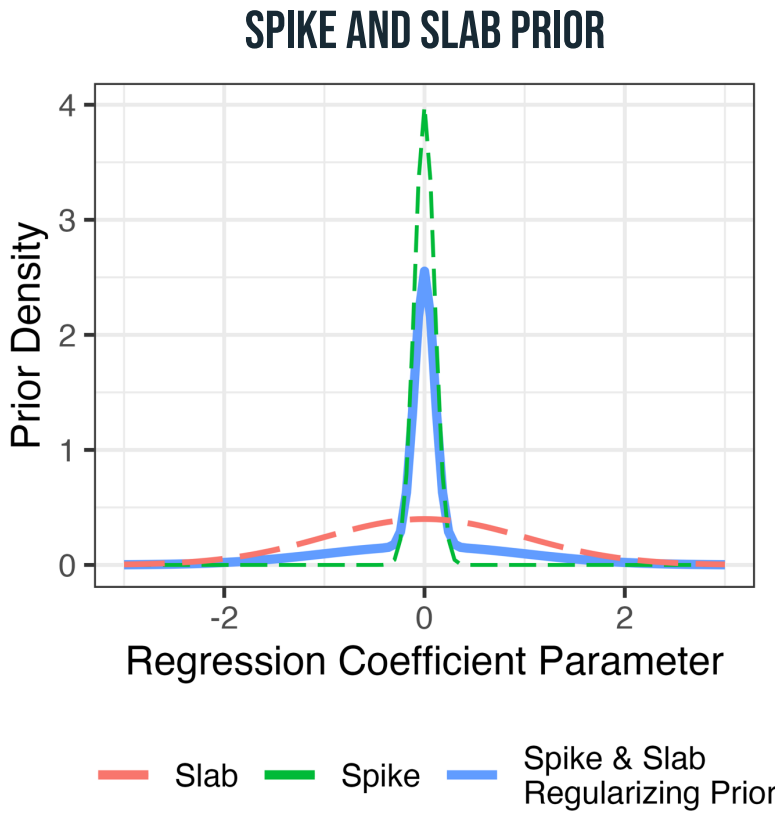
REGULARIZATION IN PARAMETRIC MODELS

What if we don't think we can estimate or need an ML model, but have lots of covariates?

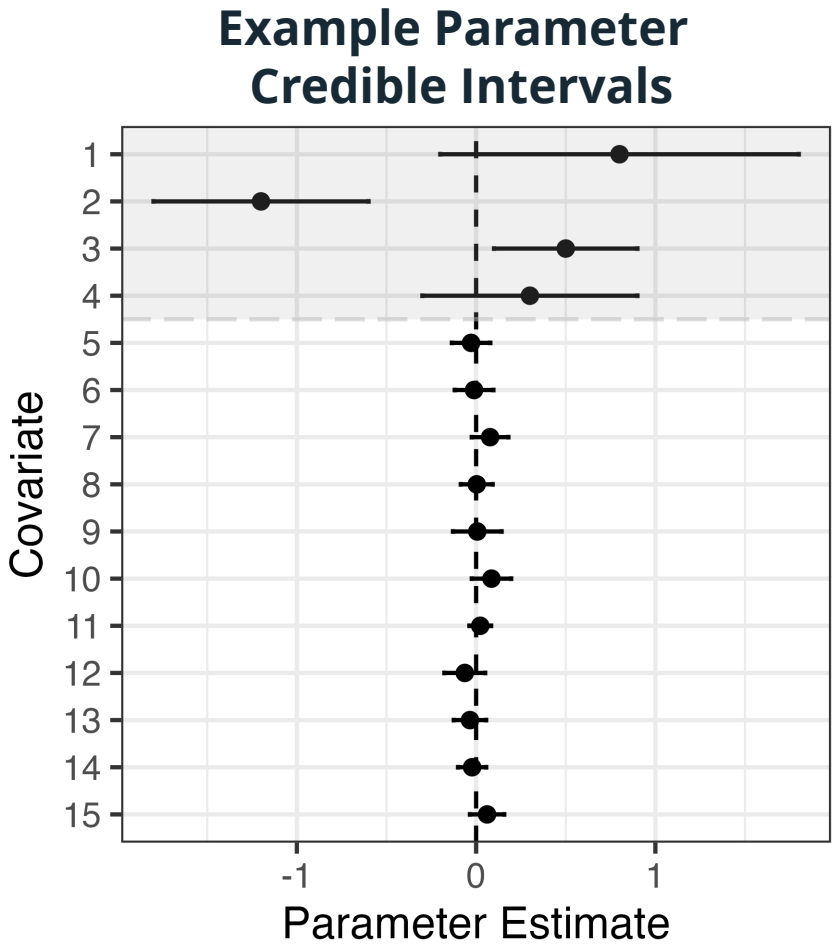
- Regularization for Bayesian Models
  - Shrink irrelevant effects to 0
  - Using informative priors
  - Priors are linked to real-world assumptions
- *Spike-and-Slab* or *Horseshoe* in exposure-response
- Straightforward implementation in Stan/brms



Garica, R and Rogers, J. Boston Pharmaceutical Symposium 2023

SPARSITY-INDUCING PRIORS FOR VARIABLE SELECTION: RESULTS

- Clear differences between important covariates and irrelevant covariates
- No need for correlation heuristics
  - Beware of confounding if using a lot of covariates
- Probabilistic inferences about variable selection from the model



CONCLUSIONS

- Shapley Values for interpreting ML models
  - More than just finding important covariates
  - Can be applied to complicated parametric models
- Opportunities and applications for regularizing parametric models
- Value in incorporating pieces of ML into other analyses
  - Bayesian non-parametrics
  - Probability weights in causal inference