Outline

- Variable selection with projpred
- Bayesian software for Python users

Variable selection

- The process of identifying the most relevant variables in a model from a larger set of predictors.
- We assume variables contribute unevenly to the outcome.
  - We may want to identify the most "important" ones.
  - Sometimes we also want to rank them.

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- We can always include all available variables in a model
- Theory says this is a good idea, in particular if we use predictively consistent priors
- However, sometimes we need to reduce the number of variables
  - measurement cost in covariates
  - running cost of predictive model
  - easier explanation / learn from the model

The problem with variable selection

- The number of potential models is 2^p, where p is the number of variables
- Evaluating all models can be computationally infeasible even for moderate p
- The proccess is prone to overfitting

How to overcome the problem?

- We recommend to use a technique called projection predictive inference
- It can be easily done with `brms` + `projpred`

Variable selection with projpred

- The main advantage is that it reduces overfitting
- Other advantages are:
  - Automatic model building and fitting process.
  - Reduced number of models we need to fit.
  - Reduced time it takes to fit each model.

Main concepts

- Reference model:
- Search strategy:
- Projection:

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- Reference model:
  - A model that includes all available variables and describes the data well.
- Search strategy:
  - A method for searching through the model space.
- Projection:
  - A way to estimate the posterior distribution of a model given a reference model.

Using a reference model is not a novel idea

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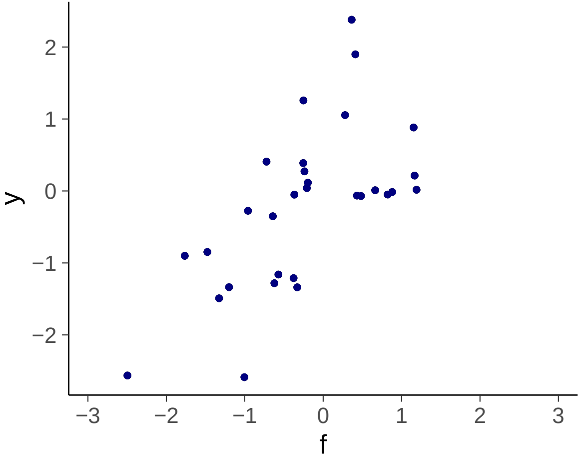
  - one key part for practical computation
- Related approaches
  - gold standard, preconditioning, teacher and student, distilling, . . .

Example: Simulated regression

$$\begin{aligned} f &\sim \mathrm{N}(0,1), \\ y \mid f &\sim \mathrm{N}(f,1) \end{aligned}$$



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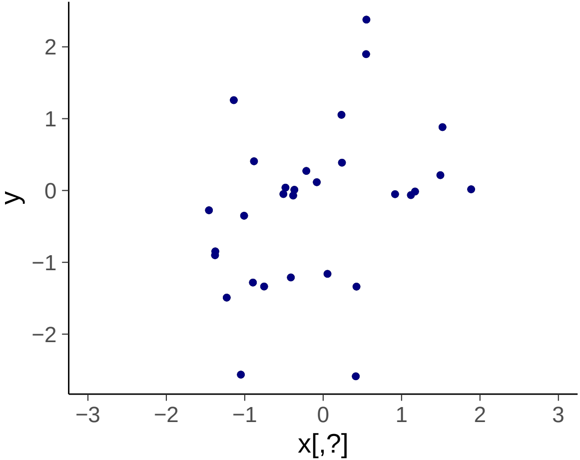

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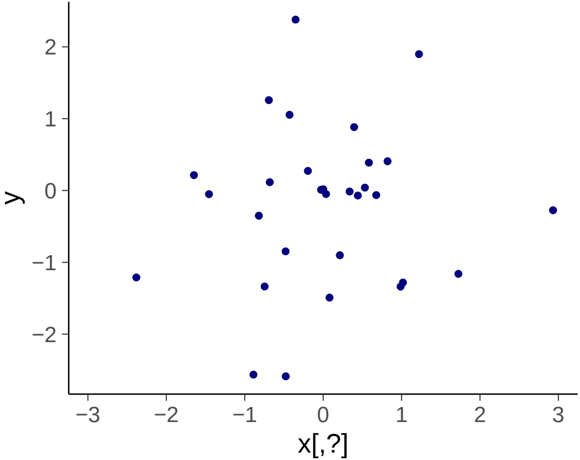

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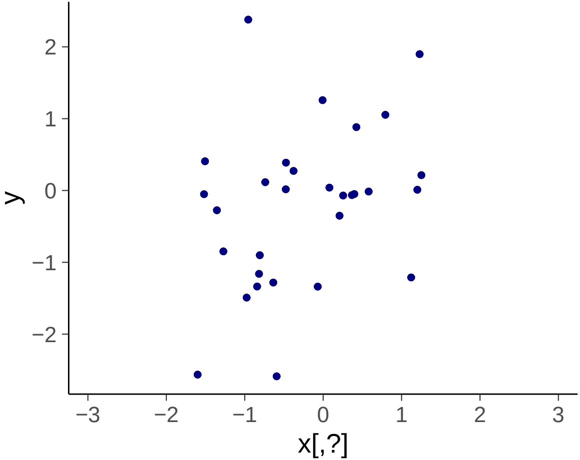

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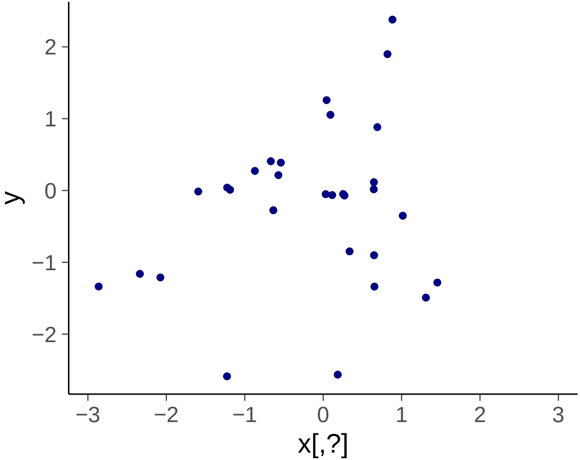

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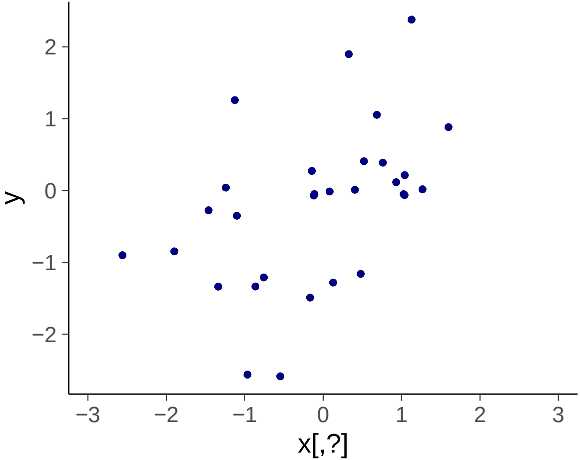

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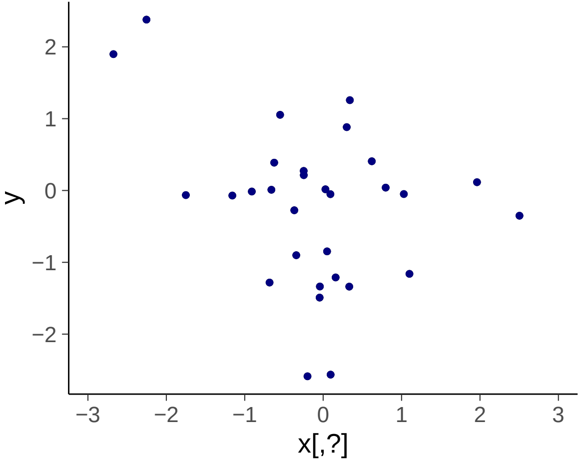

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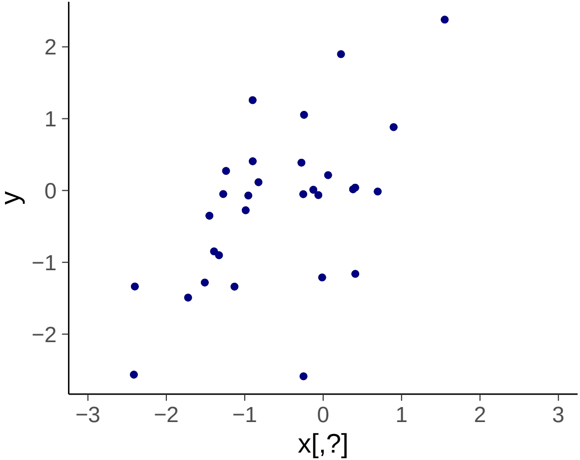

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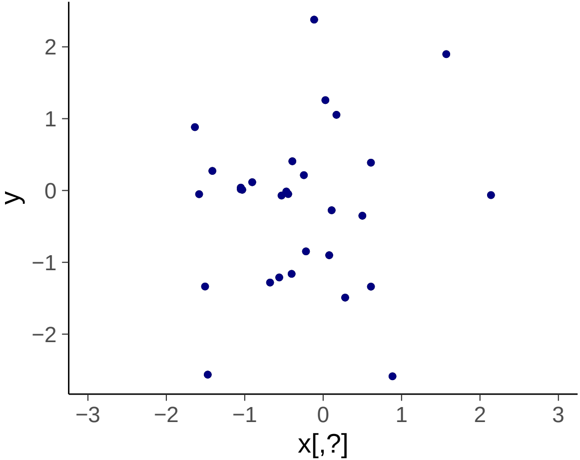

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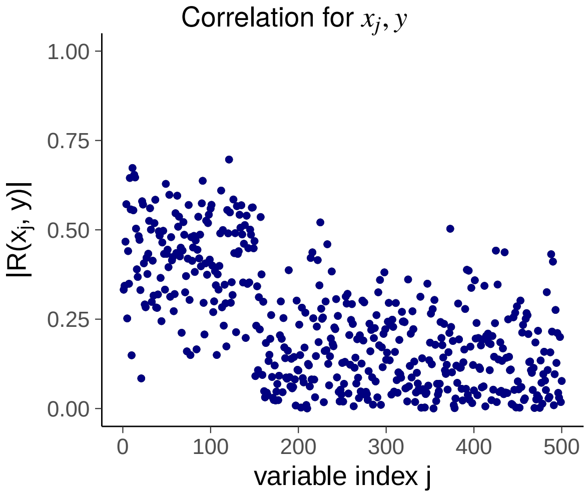

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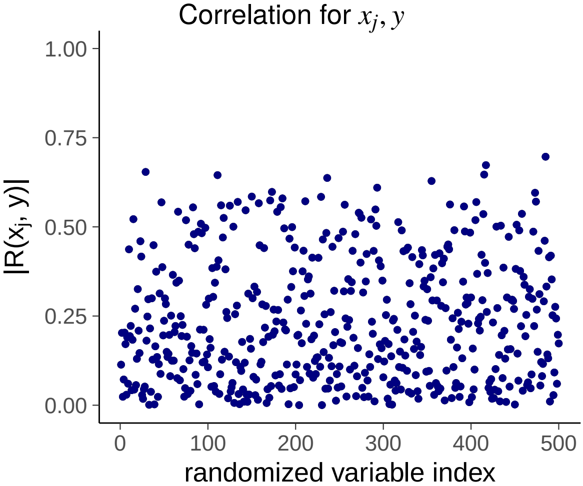

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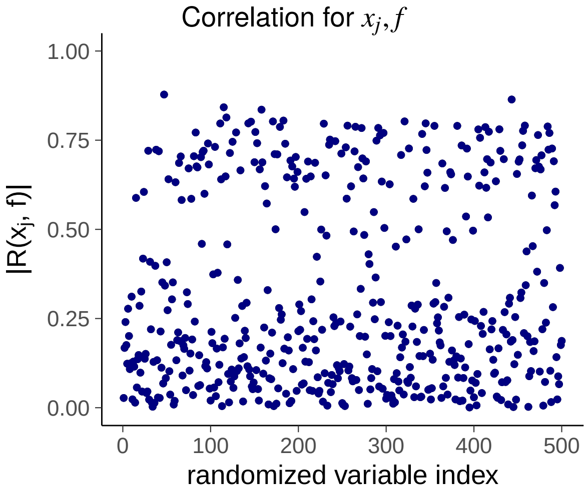

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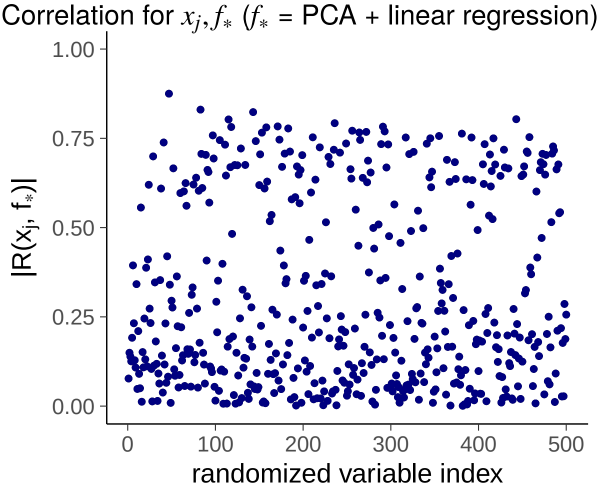
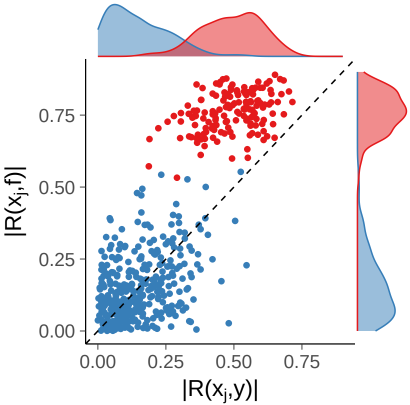


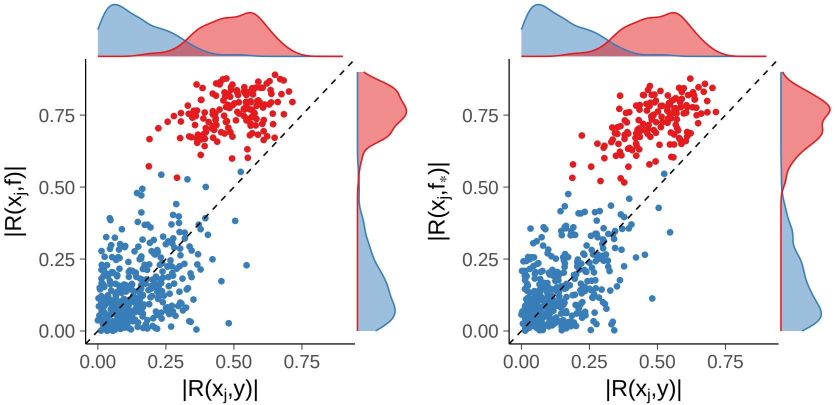
Knowing the latent values would help



irrelevant x_j, relevant x_j

A) Sample correlation with y vs. sample correlation with f

Estimating the latent values with a reference model helps



irrelevant x_j, relevant x_j

A) Sample correlation with y vs. sample correlation with f

B) Sample correlation with y vs. sample correlation with f_*

$f_* =$ linear regression fit with 3 principal components

Bayesian justification

- Theory says to integrate over all the uncertainties
  - build a rich model
  - make model checking etc.
  - this model can be the reference model

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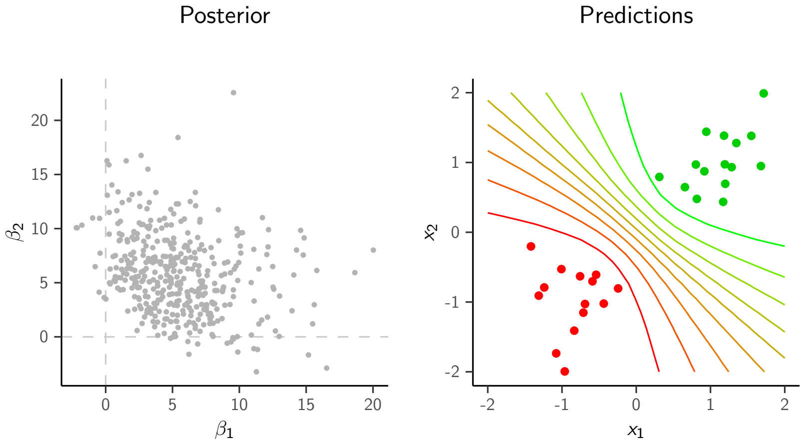
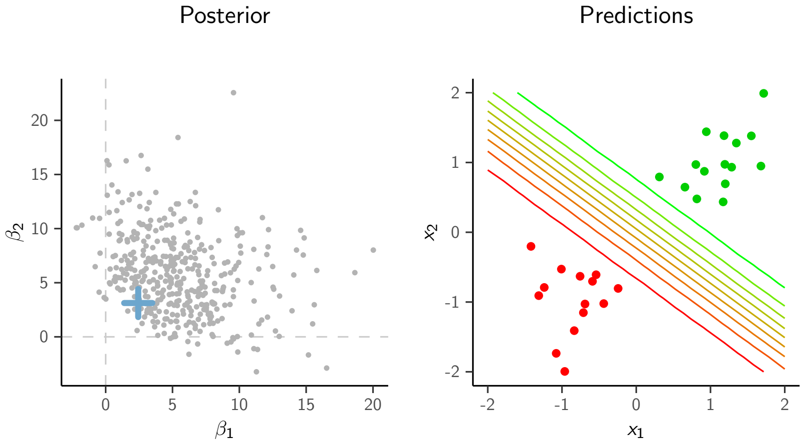
  - Some covariates must have exactly zero regression coefficient $\Rightarrow$ "Which covariates can be discarded"
  - Much simpler model $\Rightarrow$ "Easier explanation"

Logistic regression with two covariates



Full posterior for β_1 and β_2 and contours of predicted class probability

Logistic regression with two covariates



Projected point estimates for β_1 and β_2

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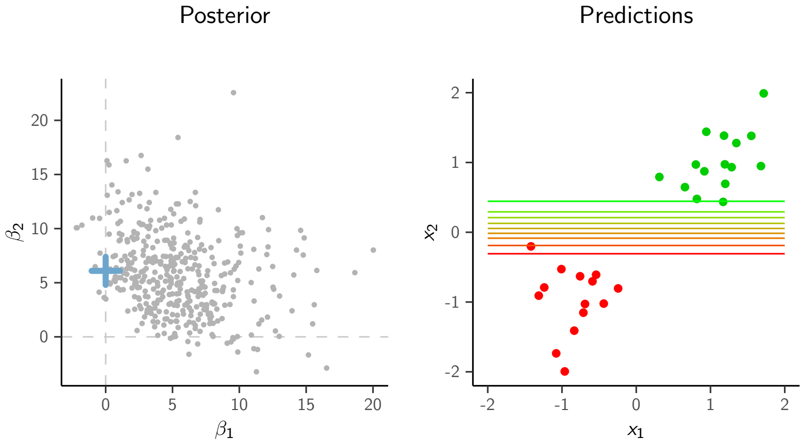

Projected point estimates, constraint $\beta_1 = 0$

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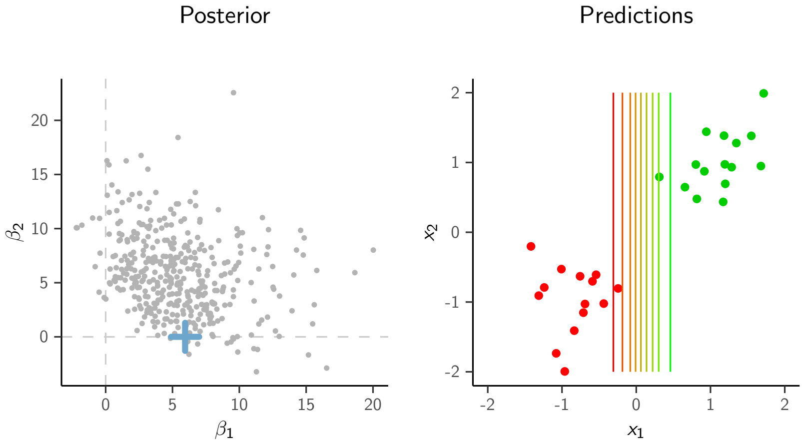

Projected point estimates, constraint $\beta_2 = 0$

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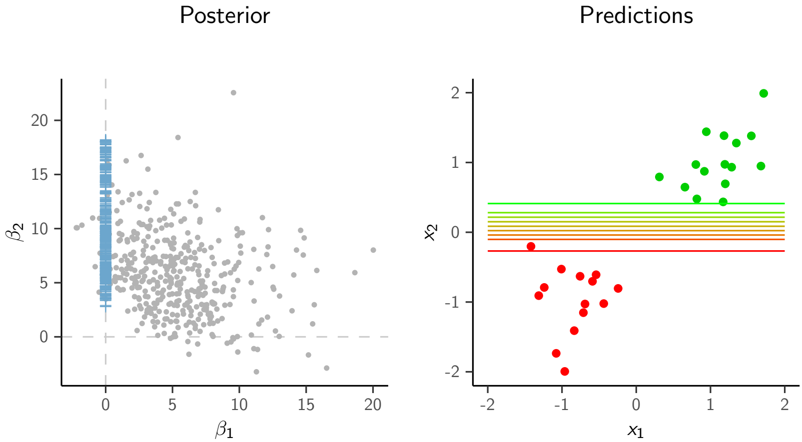

Draw-by-draw projection, constraint $\beta_1 = 0$

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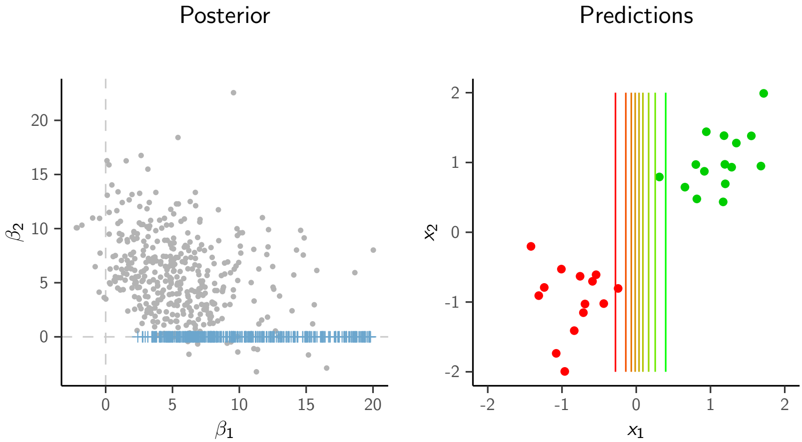

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  - even if we constrain some coefficients to be 0, the predictive inference is conditoned on the information related features contributed to the reference model
  - solves the problem of how to do the inference after the model selection

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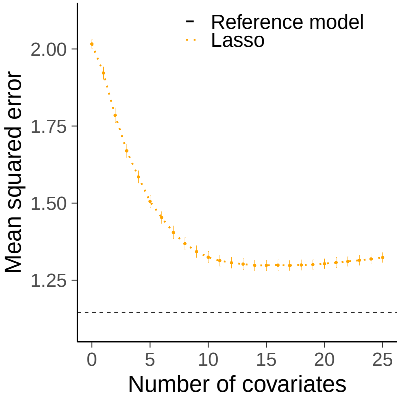
- For a given model size, choose feature combination with minimal projective loss
- Use cross-validation to select the appropriate model size
  - In some cases like, $p >> n$, we need to cross-validate over the search paths

Projective selection vs. Lasso

Same simulated regression data as before,
$n = 50$, $p = 500$, $p_{\text{rel}} = 150$, $\rho = 0.5$



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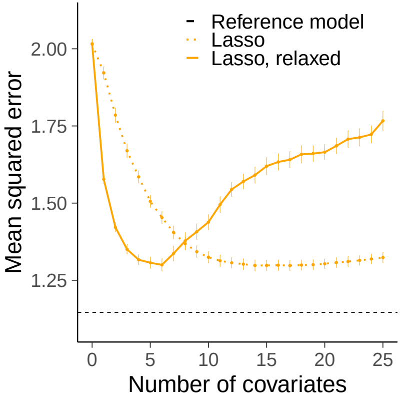

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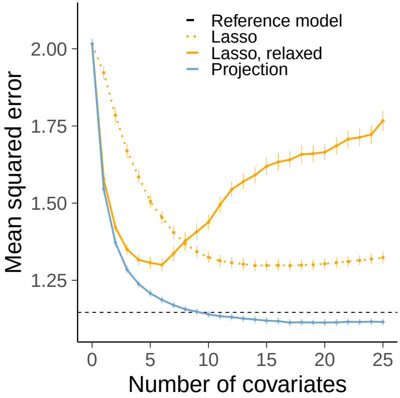

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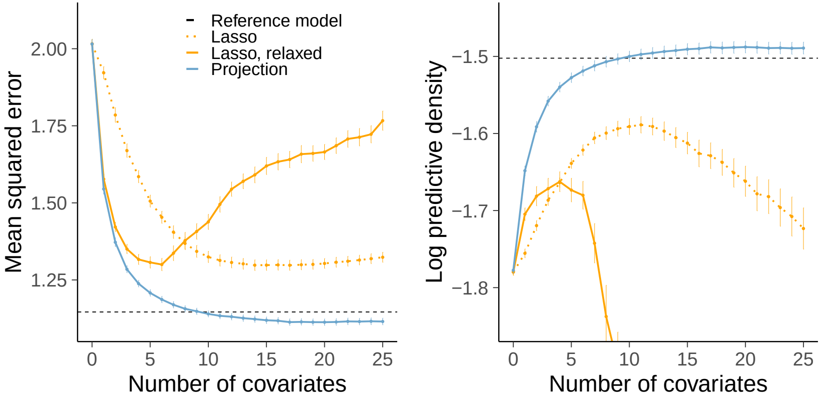

Bodyfat: small p example of projection predictive

Predict bodyfat percentage. The reference value is obtained by immersing person in water. $n = 251$.

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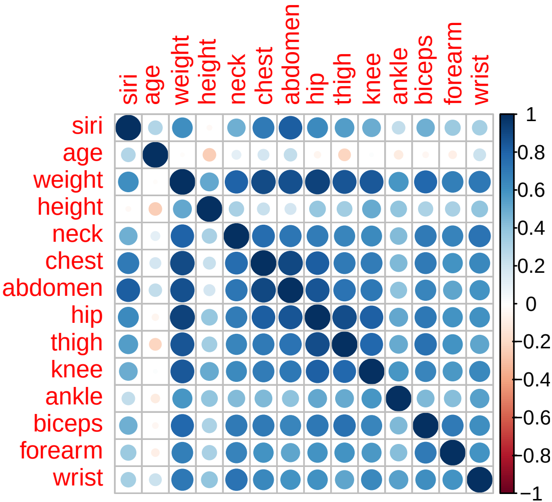
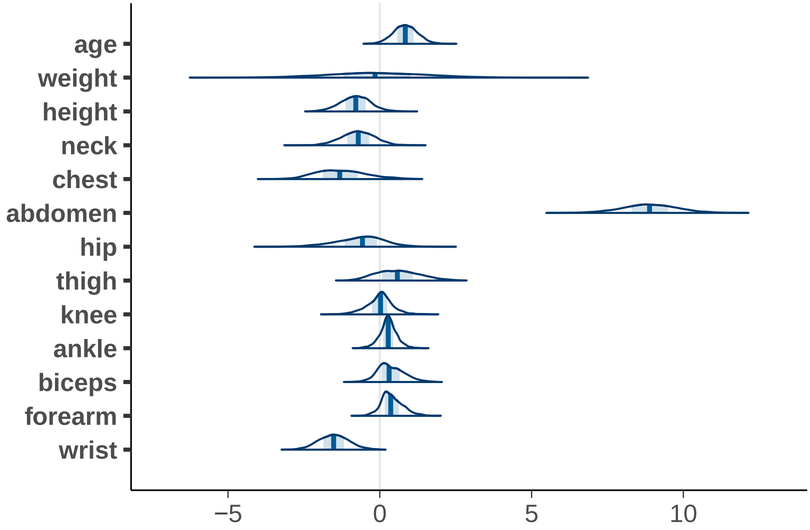


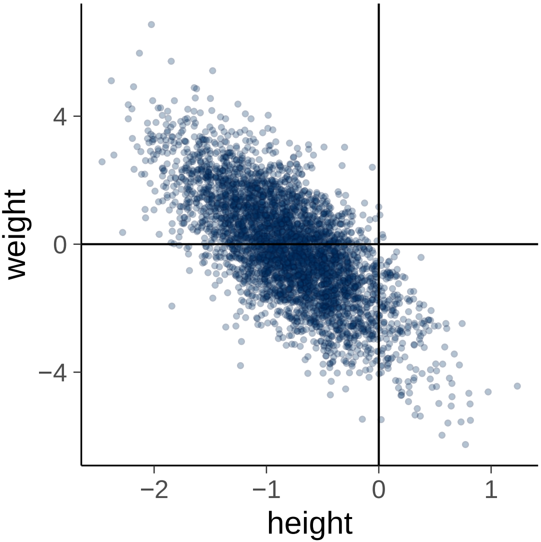
Bodyfat

Marginal posteriors of coefficients



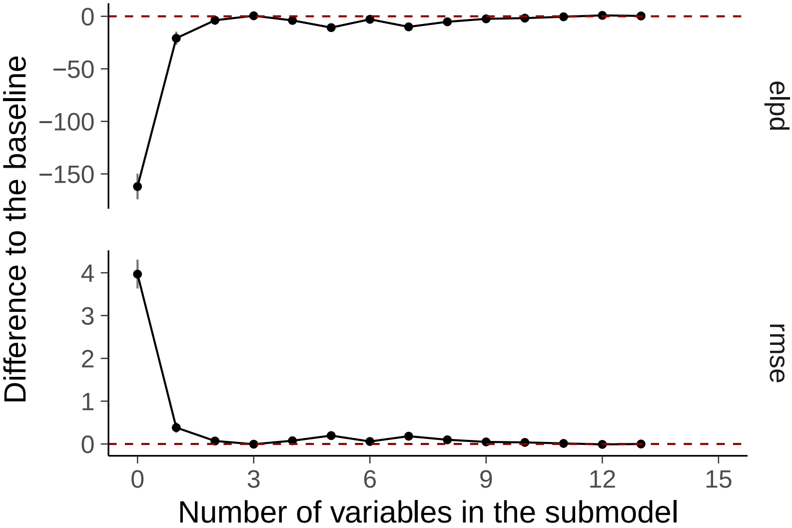
Bodyfat

Bivariate marginal of weight and height



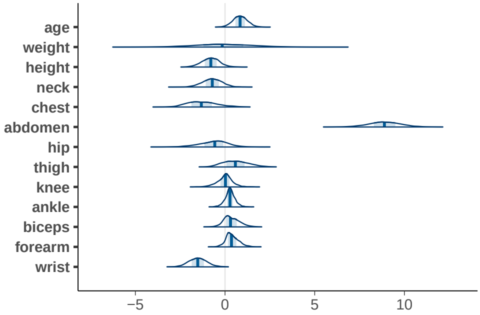
Bodyfat

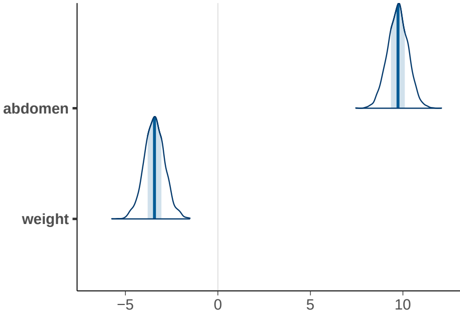
The predictive performance of the full and submodels



Bodyfat

Marginals of the reference and projected posterior





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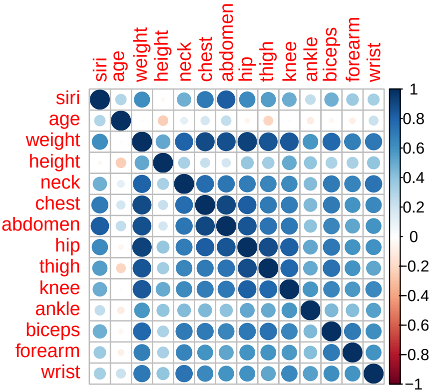
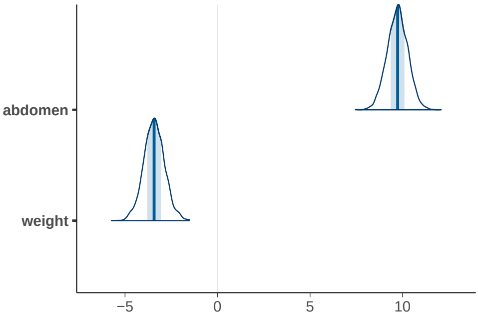
Predictive performance vs. selected variables

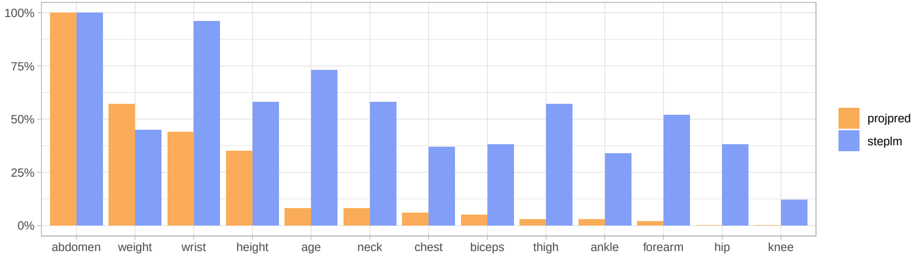
- The initial aim: find the minimal set of variables providing similar predictive performance as the reference model
- Some keep asking can it find the true variables
  - What do you mean by true variables?





Variability under data perturbation

Comparing projection predictive variable selection (projpred) and stepwise maximum likelihood over bootstrapped datasets



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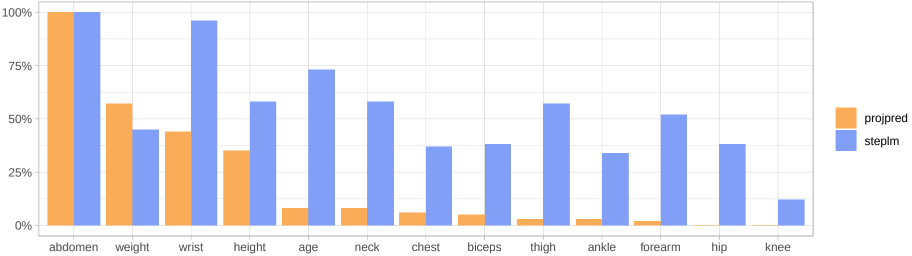

M	projpred	Freq %	steplm	Freq %
1	abdom., weight	39	abdom., age, forearm, height, hip, neck, thigh, wrist	4
2	abdom., wrist	10	abdom., age, chest, forearm, height, neck, thigh, wrist	4
3	abdom., height	10	abdom., forearm, height, neck, wrist	2
4	abdom., height, wrist	9	abdom., forearm, neck, weight, wrist	2
5	abdom., weight, wrist	8	abdom., age, height, hip, thigh, wrist	2
6	abdom., chest, height, wrist	2	abdom., age, height, hip, neck, thigh, wrist	2
7	abdom., biceps, weight, wrist	2	abdom., age, ankle, forearm, height, hip, neck, thigh, wrist	2
8	abdom., height, weight, wrist	2	abdom., age, biceps, chest, height, neck, wrist	2
9	abdom., age, wrist	2	abdom., age, biceps, chest, forearm, height, neck, thigh, wrist	2
10	abdom., age, height, neck, thigh, wrist	2	abdom., age, ankle, biceps, weight, wrist	2

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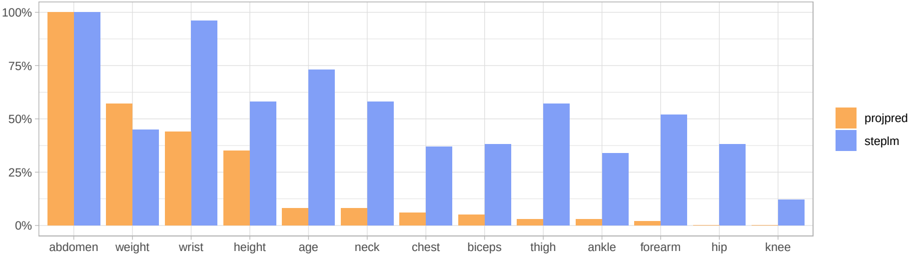

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Variability under data perturbation

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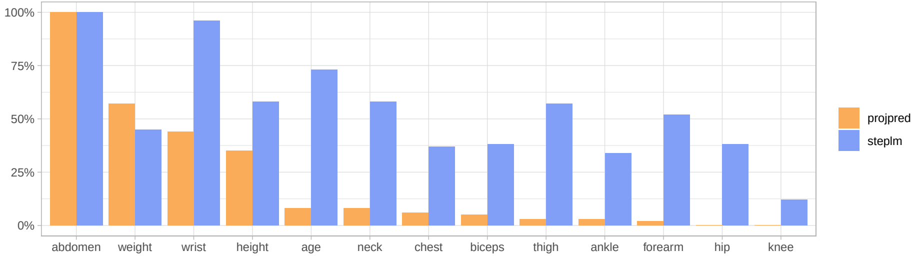

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- projpred uses
  - Bayesian inference for the reference
  - The reference model
  - Projection for submodel inference

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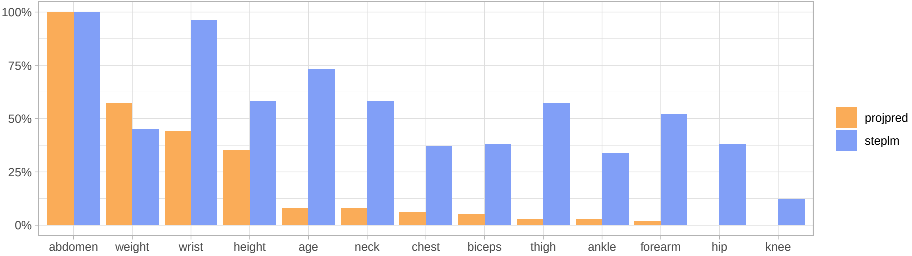

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Multilevel regression and GAMMs

- `projpred` supports also hierarchical models in `brms`
  Catalina, Bürkner, and Vehtari (2022). Projection predictive inference for generalized linear and additive multilevel models. *Proceedings of the 24th International Conference on Artificial Intelligence and Statistics (AISTATS), PMLR* 151:4446–4461.
  https://proceedings.mlr.press/v151/catalina22a.html

Scaling

- So far the biggest number of variables we've tested is 22K
  - 96s for creating a reference model
  - 14s for projection predictive variable selection

Intro paper and brms and rstanarm + projpred examples

- McLatchie, Rögnvaldsson, Weber, and Aki Vehtari (2024). Advances in projection predictive inference. *Statistical Science*. https://arxiv.org/abs/2306.15581
- https://mc-stan.org/projpred/articles/projpred.html
- https://users.aalto.fi/~ave/casestudies.html
- Fast and often sufficient if $n \gg p$

```
varsel <- cv_varsel(fit, method='forward', cv_method='loo',
                    validate_search=FALSE)
```

- Slower but needed if not $n \gg p$

```
varsel <- cv_varsel(fit, method='forward', cv_method='kfold', K=10,
                    validate_search=TRUE)
```

- If p is very big use subsampling loo

```
# nloo should be a positive integer smaller than the number of observa
varsel <- cv_varsel(fit, cv_method='loo',
                    validate_search=TRUE, nloo=50)
```

Bayesian Python packages

- Probabilistic programming languages
  - Stan (via CmdStanPy)
  - PyMC
  - NumPyro
  - ...
- Workflow packages
  - ArviZ, MCMC diagnostics, model checking, model comparison, plotting, prior-sensitivity...
  - Bambi, BAyesian Model-Building Interface
  - Kulprit, projective inference

Download Jupyter Notebook with examples.