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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- 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.

Useing a reference model is not a novel idea

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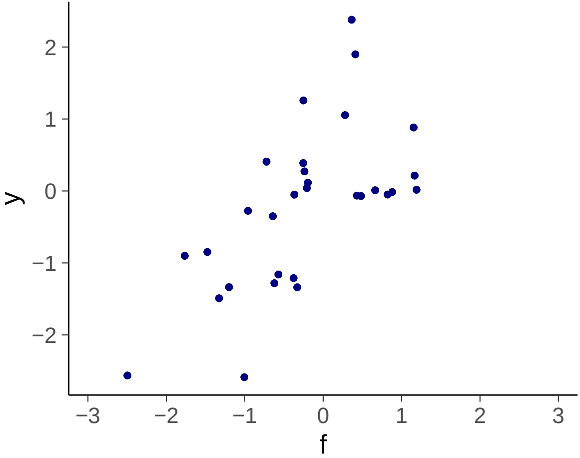
  - one key part for practical computation
- Related approaches
  - gold standard, preconditioning, teacher and student, distilling, . . .

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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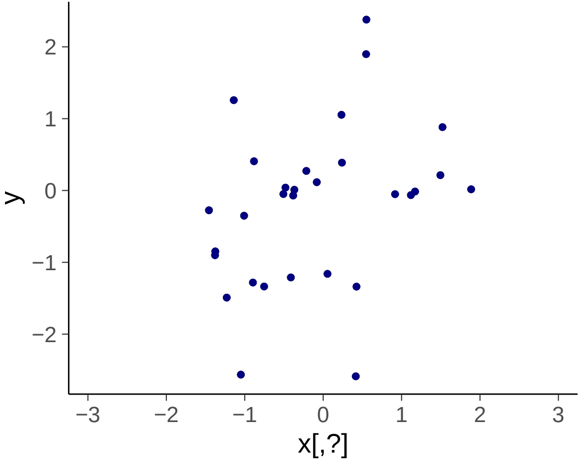

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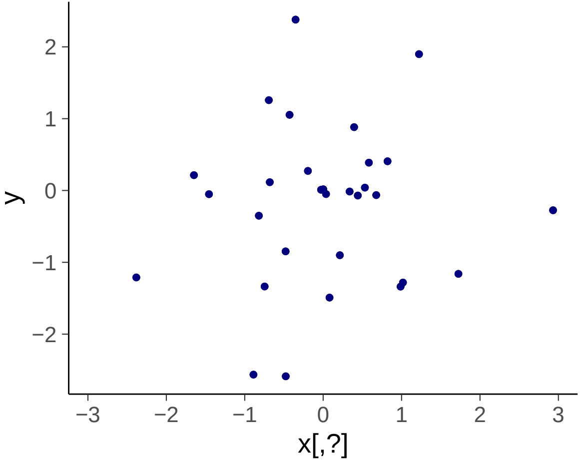

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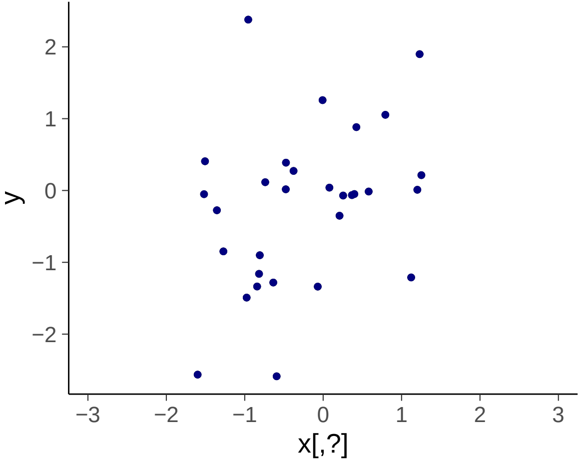

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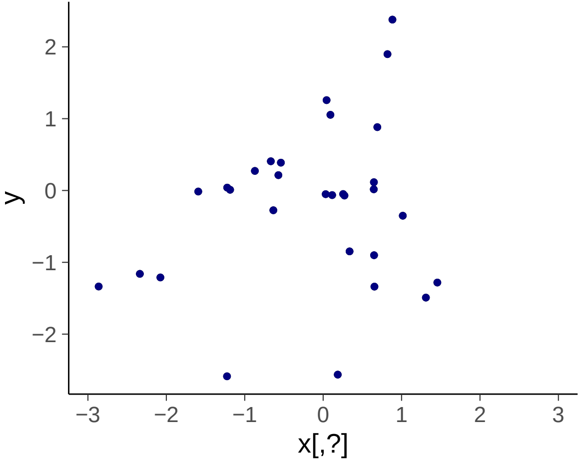

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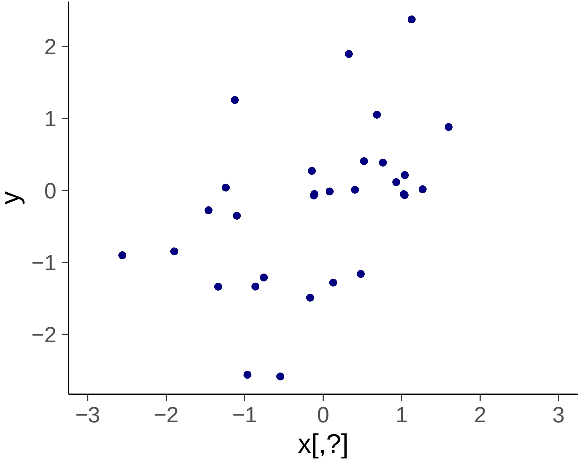

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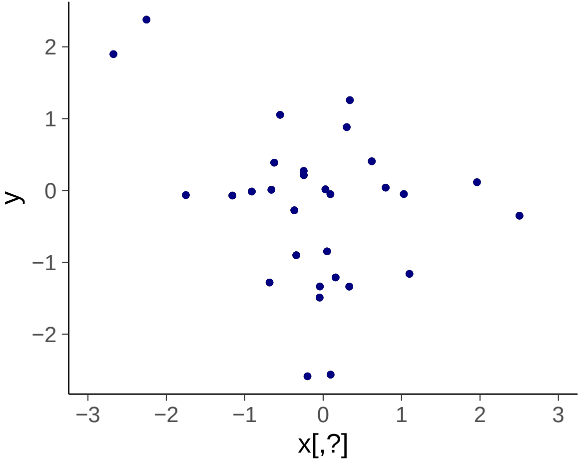

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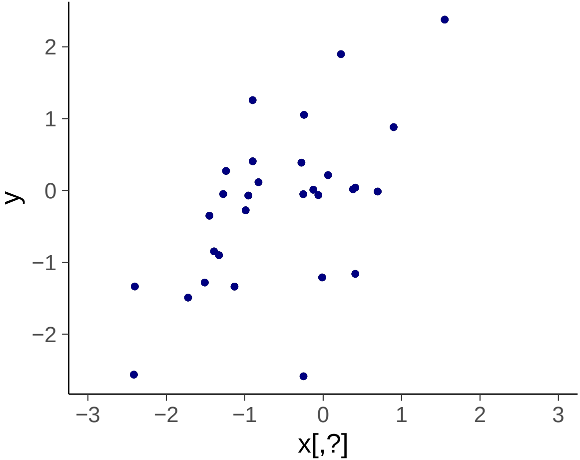

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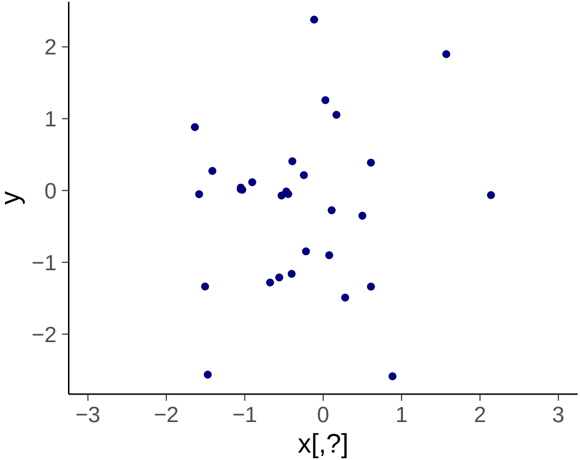

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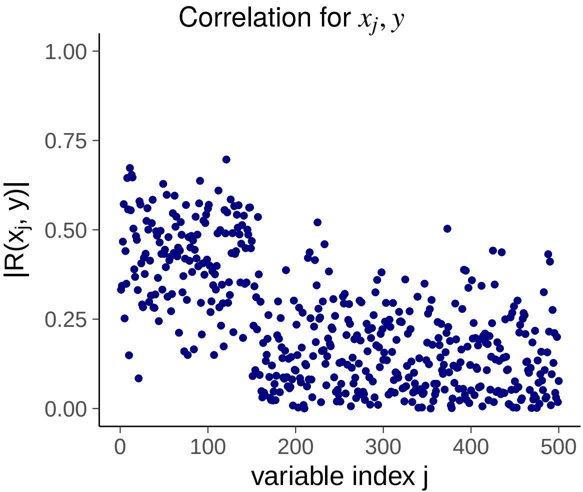

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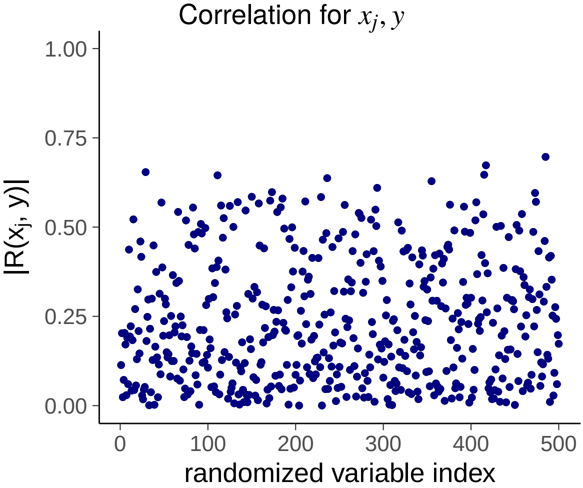

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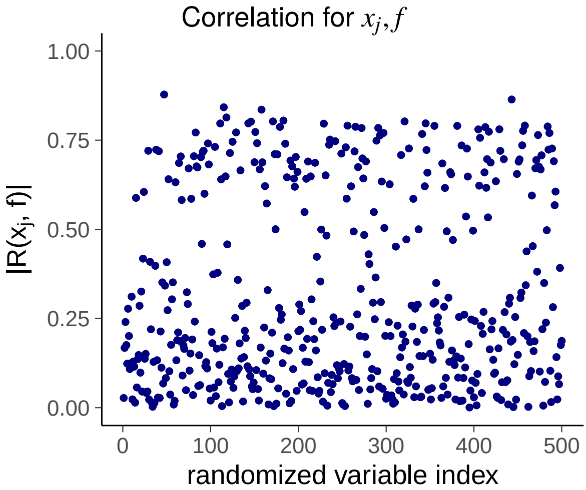

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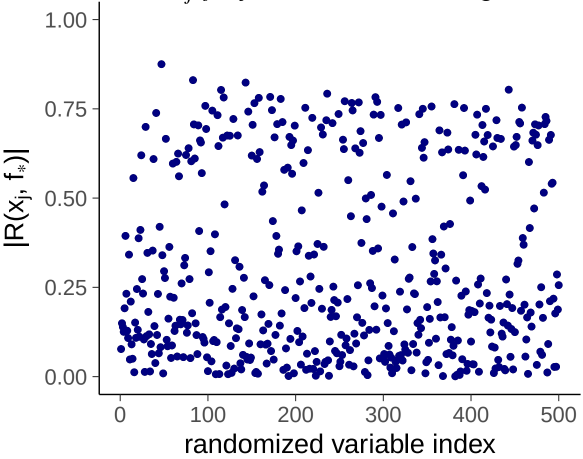
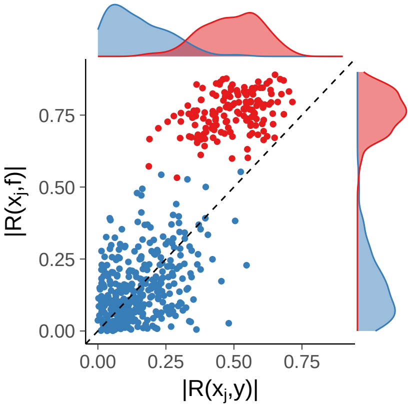
Correlation for x_j, f_* (f_* = PCA + linear regression)



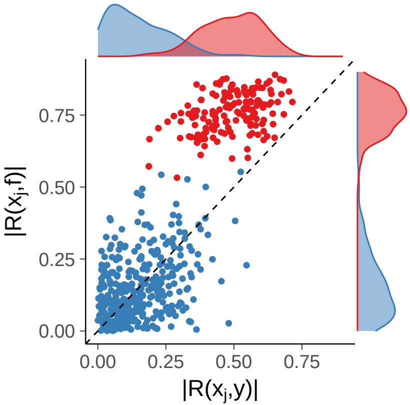
Knowing the latent values would help



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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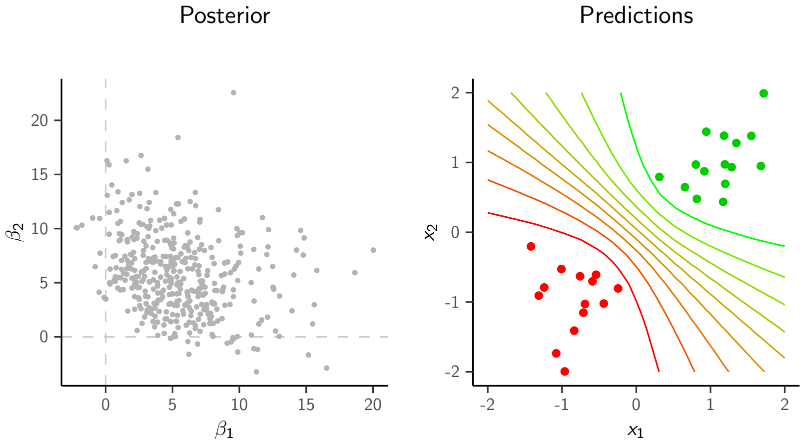
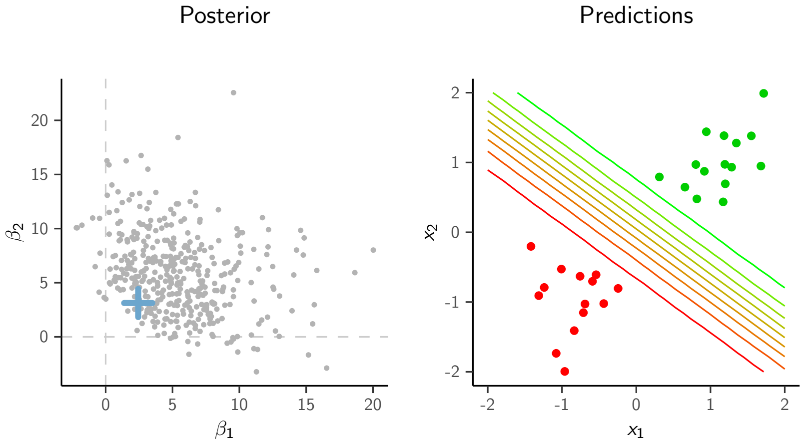
  - $q(\theta)$ can have only point mass at some θ_0 $\Rightarrow$ "Optimal point estimates"
  - Some covariates must have exactly zero regression coefficient $\Rightarrow$ "Which covariates can be discarded"
  - Much simpler model $\Rightarrow$ "Easier explanation"

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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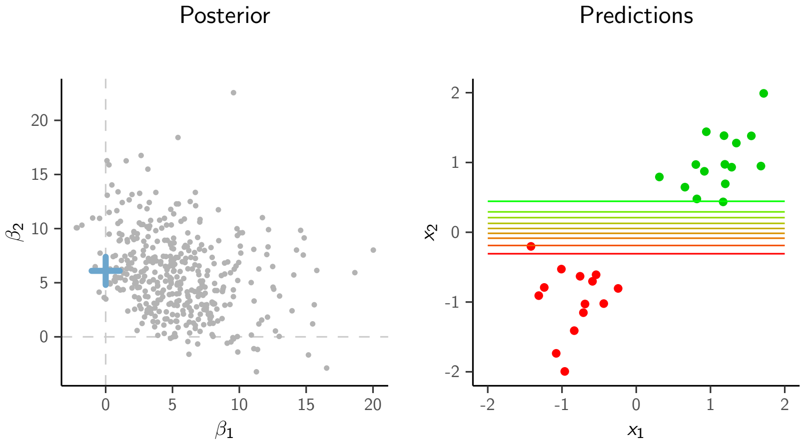

Projected point estimates, constraint $\beta_1 = 0$

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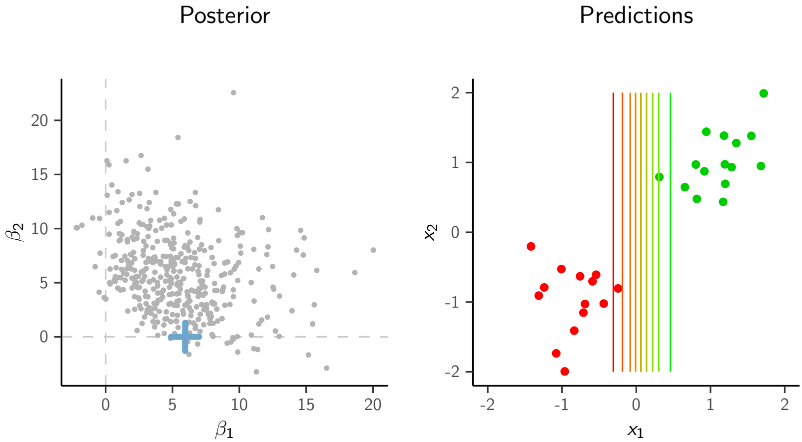

Projected point estimates, constraint $\beta_2 = 0$

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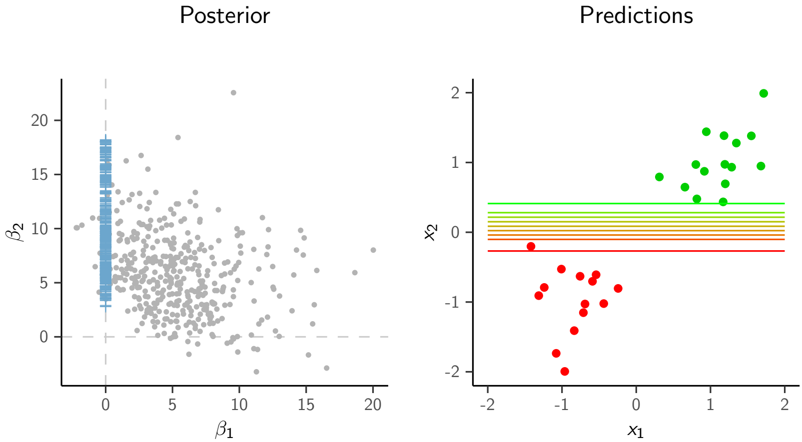

Draw-by-draw projection, constraint $\beta_1 = 0$

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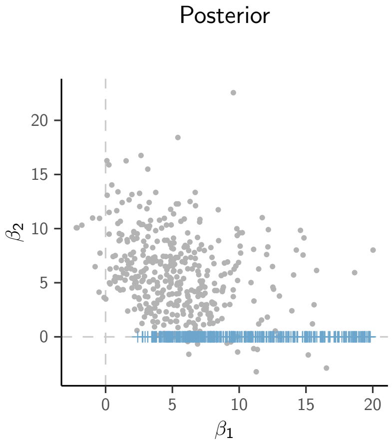

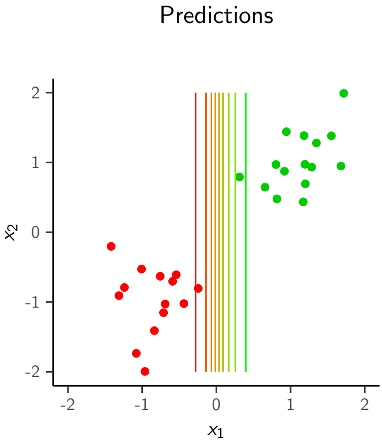

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  - even if we constrain some coefficients to be 0, the predictive inference is conditoned on the information related features contributed to the reference model
  - solves the problem of how to do the inference after the model selection

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  - Monte Carlo search
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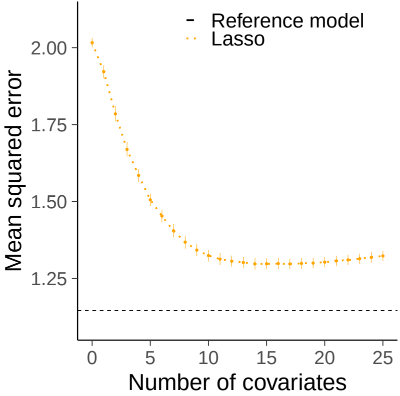
  - L_1-penalization (as in Lasso)
- For a given model size, choose feature combination with minimal projective loss
- Use cross-validation to select the appropriate model size
  - In some cases like, $p >> n$, we need to cross-validate over the search paths

Projective selection vs. Lasso

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



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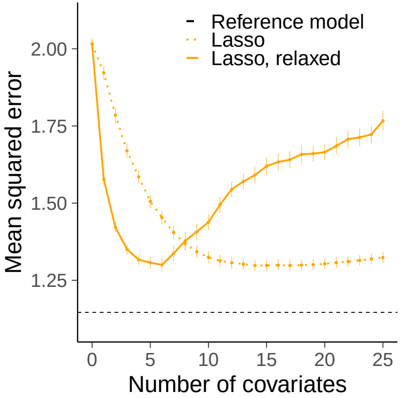

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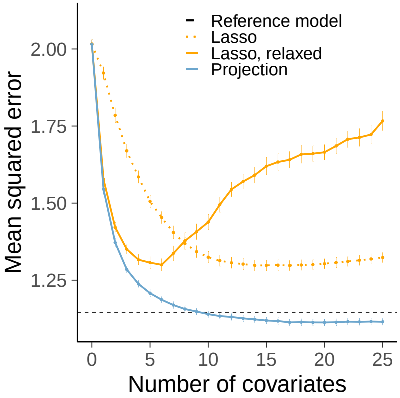

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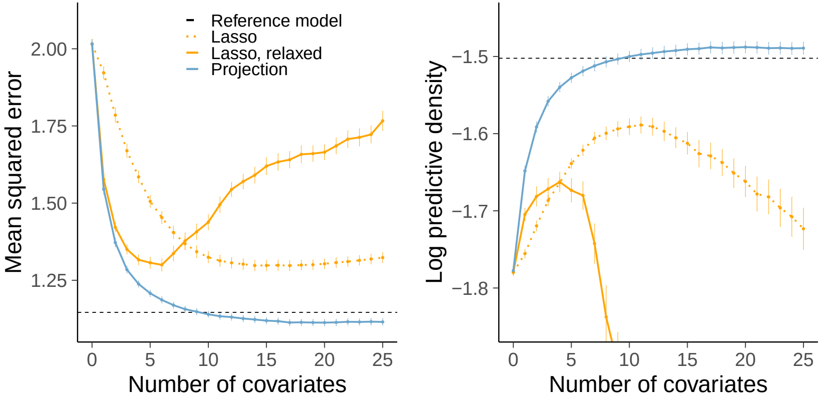

Bodyfat: small p example of projection predictive

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

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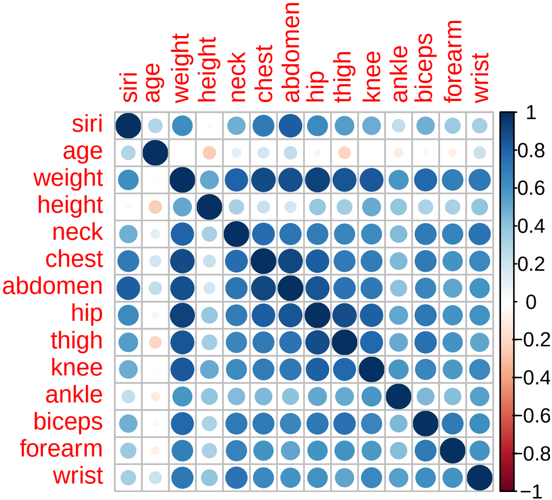
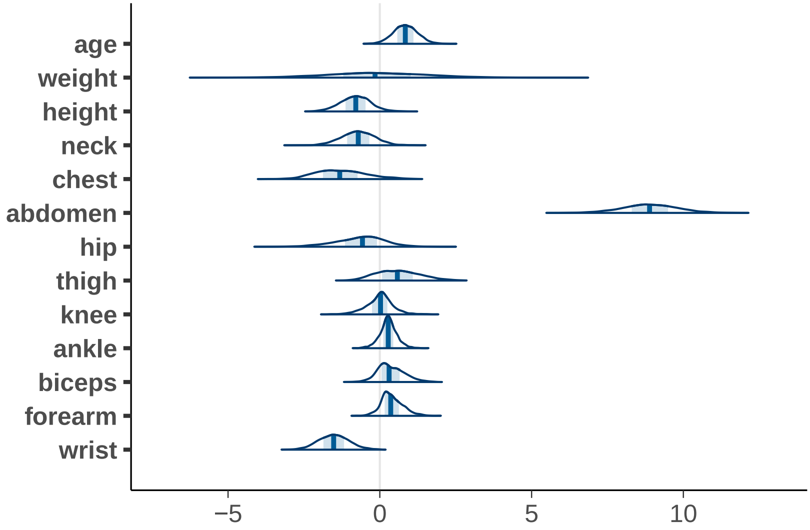


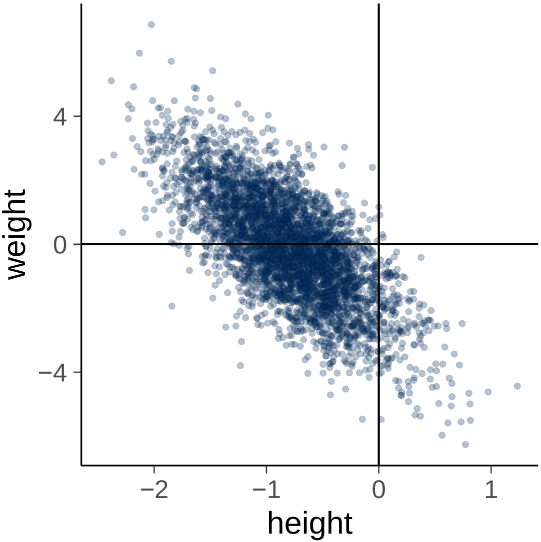
Bodyfat

Marginal posteriors of coefficients



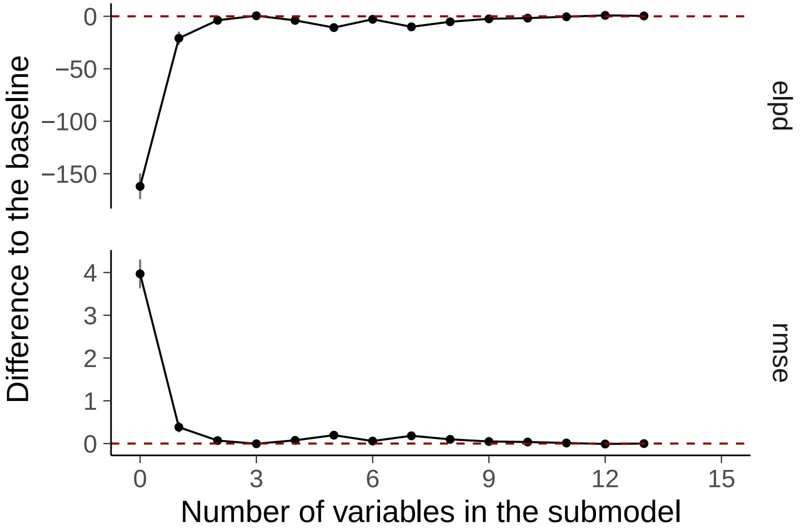
Bodyfat

Bivariate marginal of weight and height



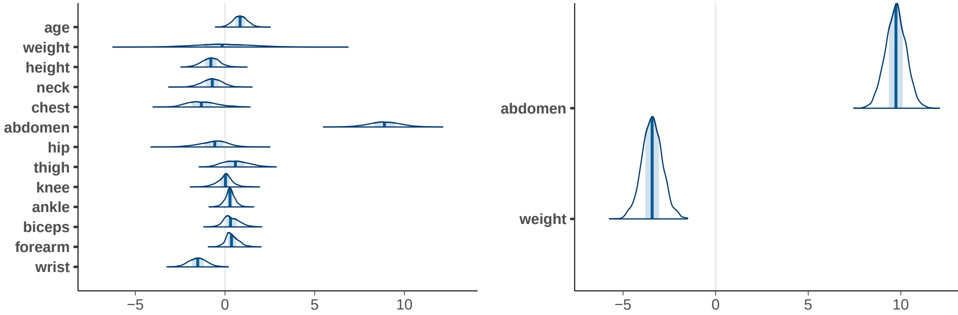
Bodyfat

The predictive performance of the full and submodels



Bodyfat

Marginals of the reference and projected posterior



Predictive performance vs. selected variables

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Predictive performance vs. selected variables

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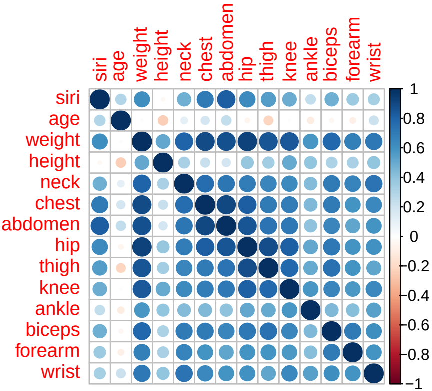
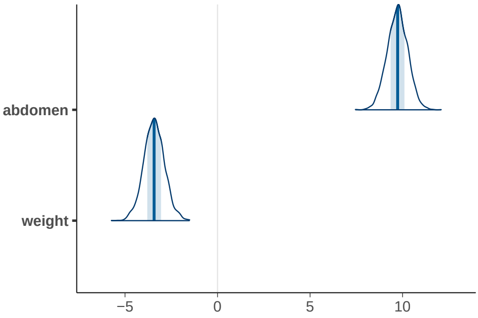
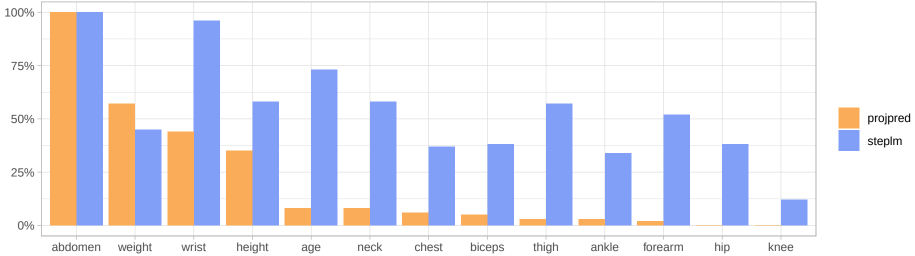
- Some keep asking can it find the true variables
  - What do you mean by true variables?





Variability under data perturbation

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



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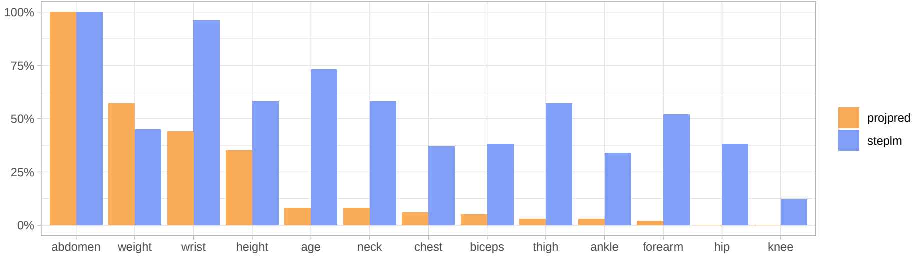

M	projpred	Freq %	steplm	Freq %
1	abdom., weight	39	abdom., age, forearm, height, hip, neck, thigh, wrist	4
2	abdom., wrist	10	abdom., age, chest, forearm, height, neck, thigh, wrist	4
3	abdom., height	10	abdom., forearm, height, neck, wrist	2
4	abdom., height, wrist	9	abdom., forearm, neck, weight, 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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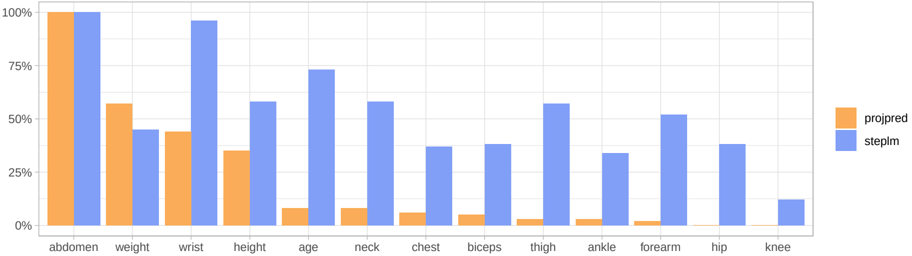
Comparing projection predictive variable selection (projpred) and stepwise maximum likelihood over bootstrapped datasets



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Variability under data perturbation

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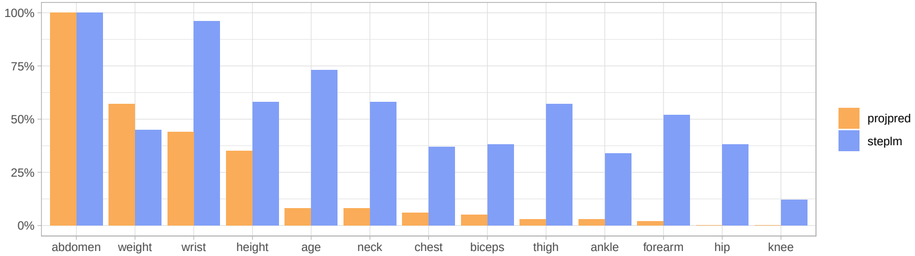

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  - Bayesian inference for the reference
  - The reference model
  - Projection for submodel inference

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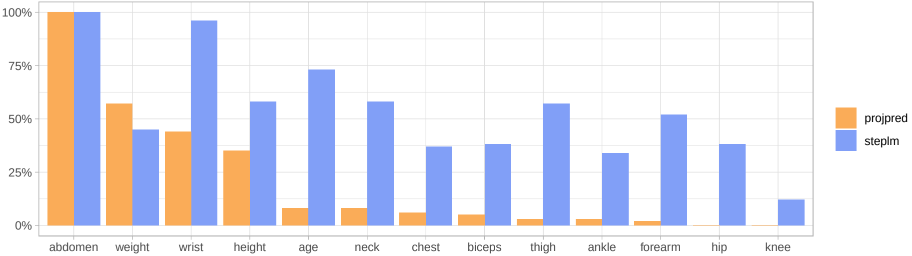

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Multilevel regression and GAMMs

- `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 (still under development)