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- ...in such case I recommended to use brms + projpred
- projpred avoids the overfit in model selection

# Use of reference models in model selection

- Background
- First example
- Bayesian and decision theoretical justification
- More examples

## Not a novel idea

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

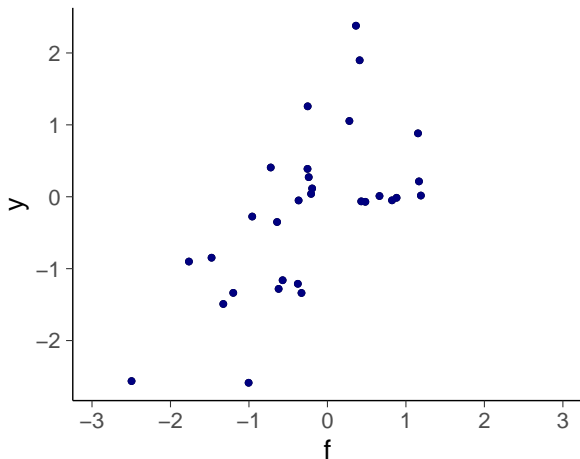


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  - one key part for practical computation
- Related approaches
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- Motivation in these
  - measurement cost in covariates
  - running cost of predictive model
  - easier explanation / learn from the model

## Example: Simulated regression

$$f \sim N(0, 1),$$
$$y | f \sim N(f, 1)$$

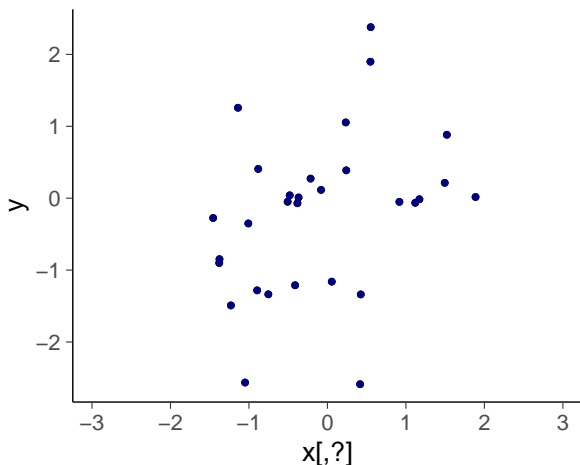


## Example: Simulated regression

$$\begin{array}{lll} f \sim \mathrm{N}(0, 1), & x_j | f \sim \mathrm{N}(\sqrt{\rho}f, 1 - \rho), & j = 1, \dots, 150, \\ y | f \sim \mathrm{N}(f, 1) & x_j | f \sim \mathrm{N}(0, 1), & j = 151, \dots, 500. \end{array}$$

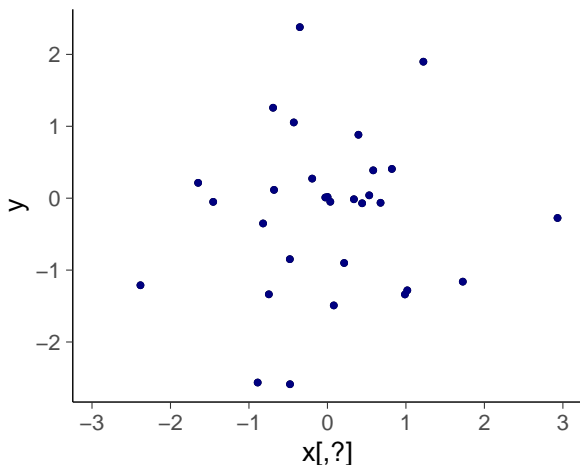
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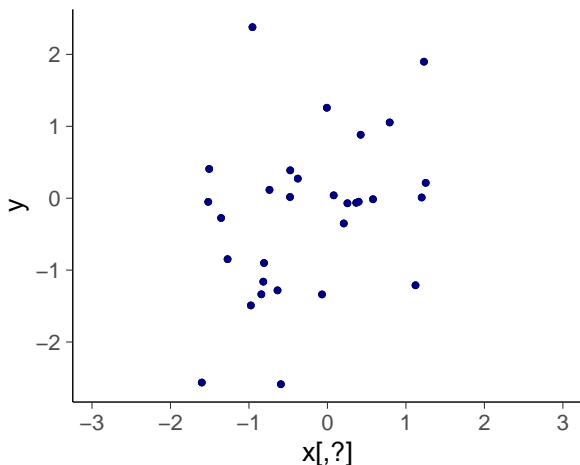
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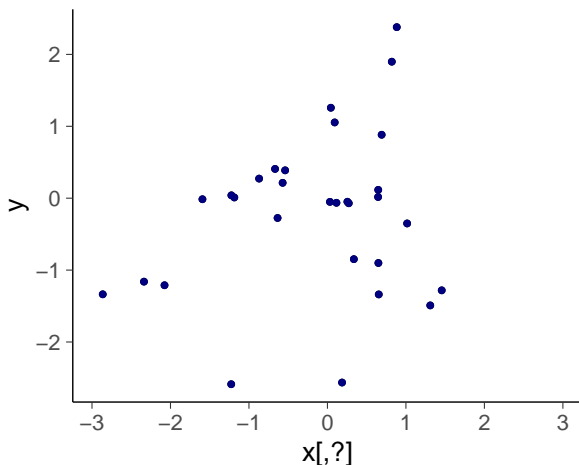
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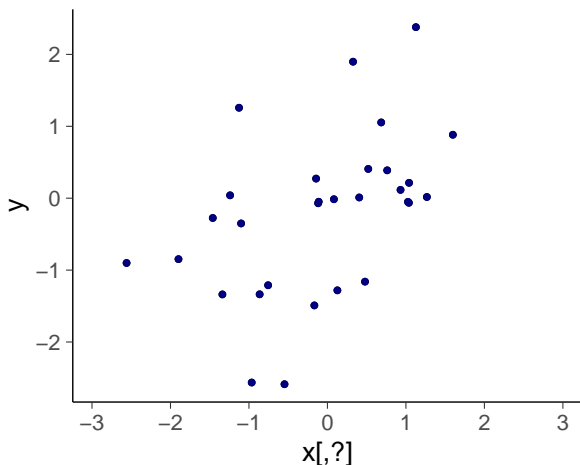
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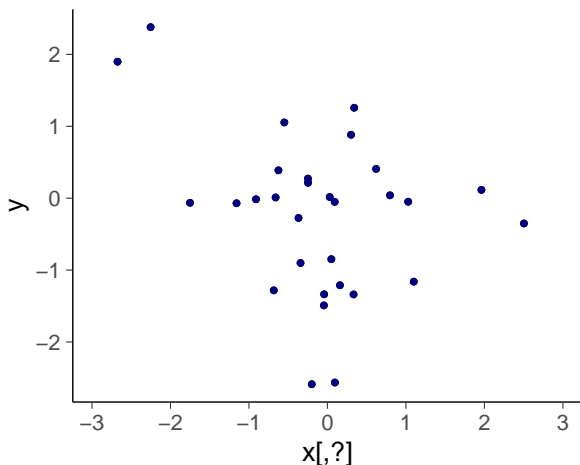
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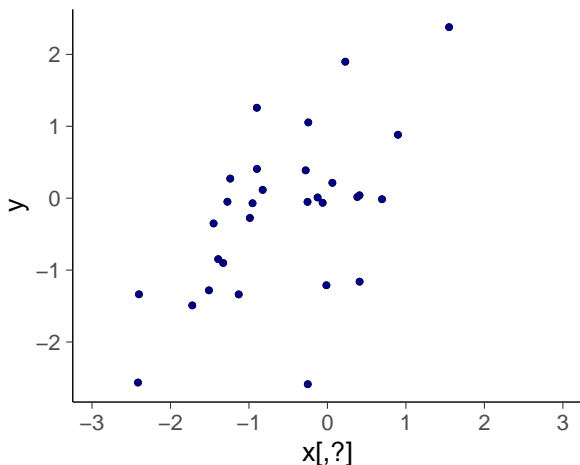
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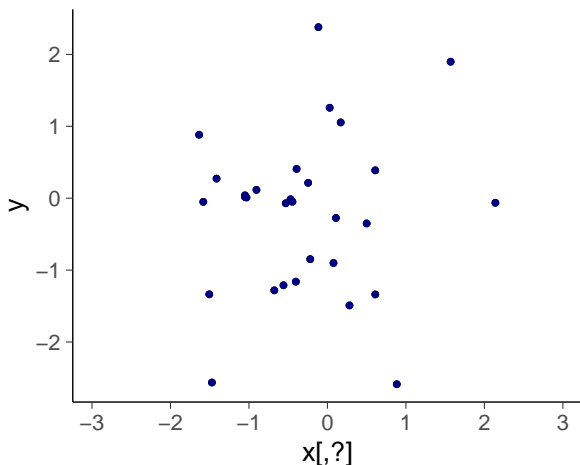
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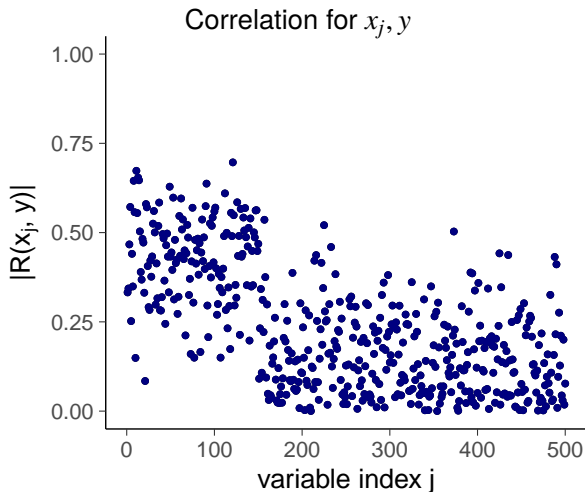
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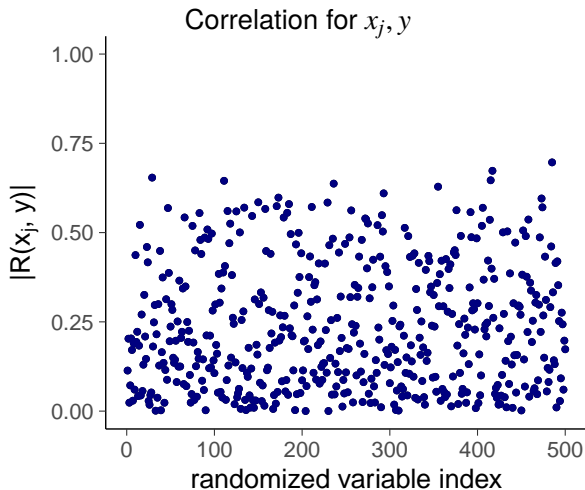
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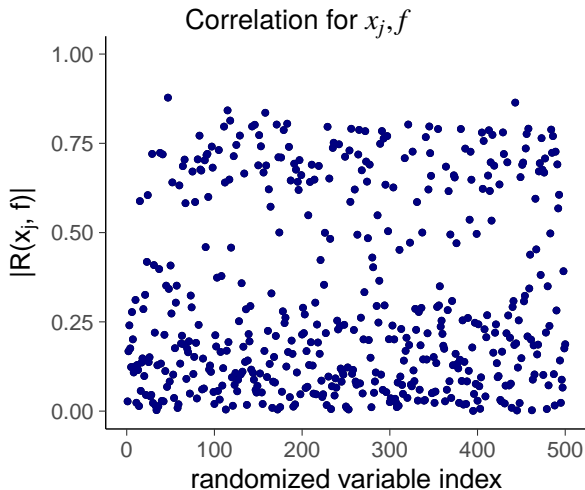
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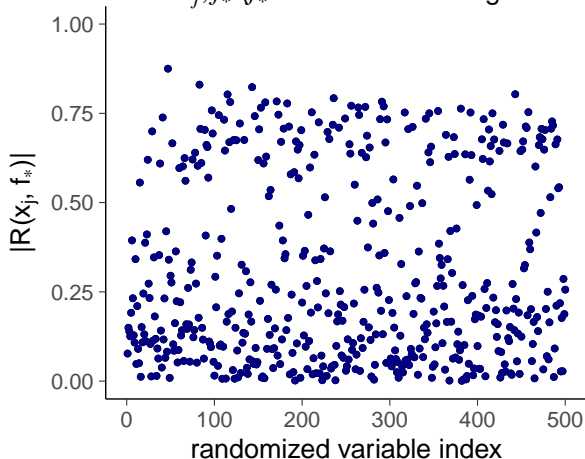
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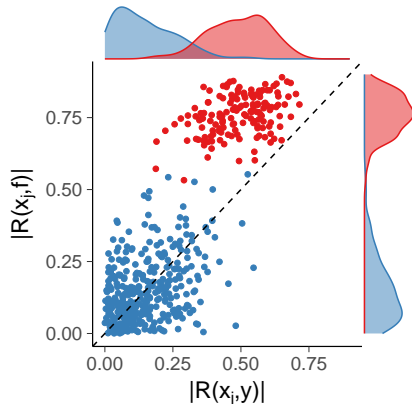
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Correlation for  $x_j, f_*$  ( $f_* = \text{PCA} + \text{linear regression}$ )



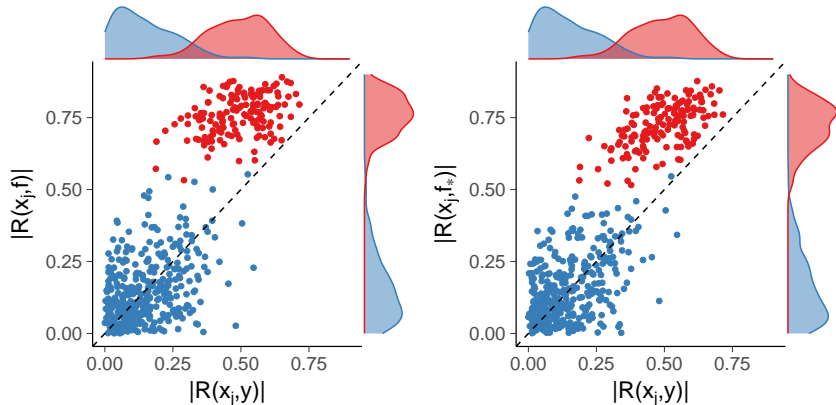
# Knowing the latent values would help



**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  $x_j$

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

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

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- Theory says to integrate over all the uncertainties
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  - $q(\theta)$  can have only point mass at some  $\theta_0$   
⇒ “Optimal point estimates”

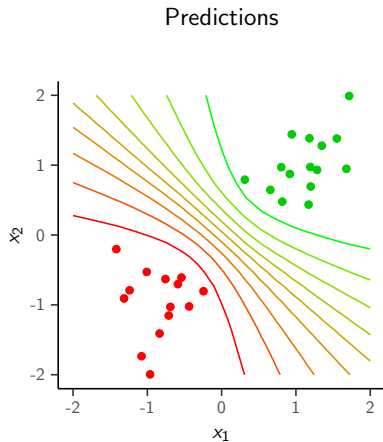
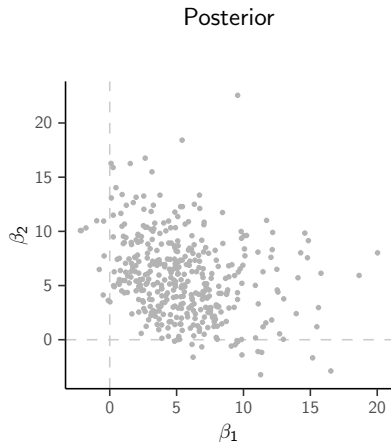
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⇒ “Which covariates can be discarded”
  - Much simpler model  
⇒ “Easier explanation”

# Logistic regression with two covariates

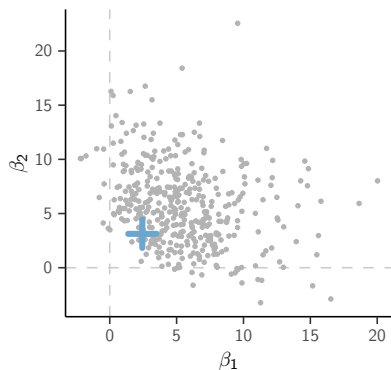


Full posterior for  $\beta_1$  and  $\beta_2$  and contours of predicted class probability

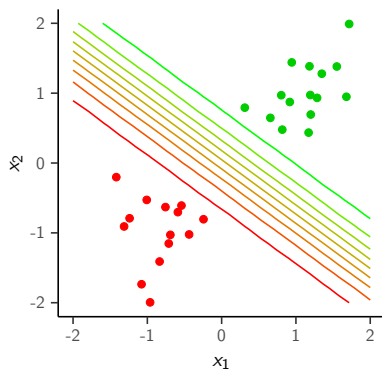


# Logistic regression with two covariates

Posterior

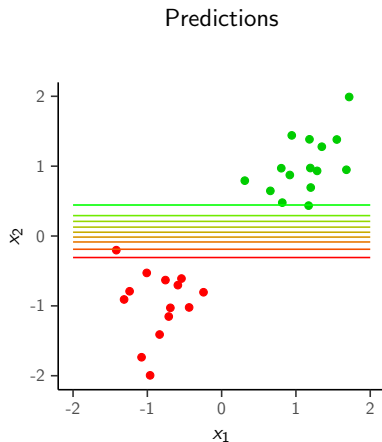
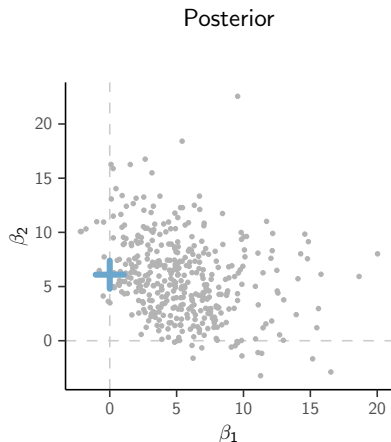


Predictions



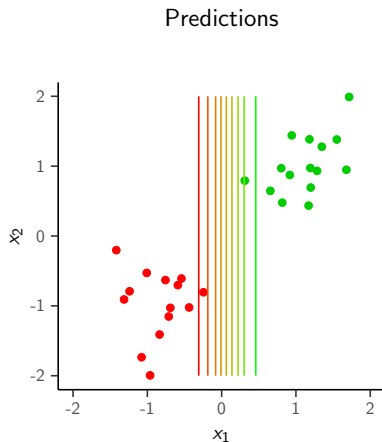
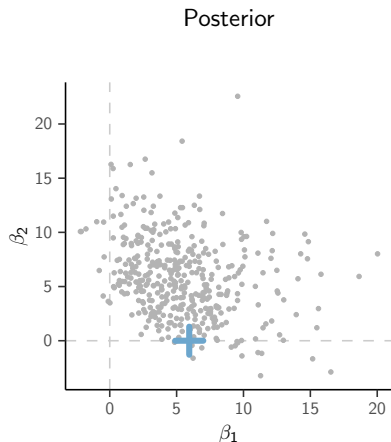
Projected point estimates for  $\beta_1$  and  $\beta_2$

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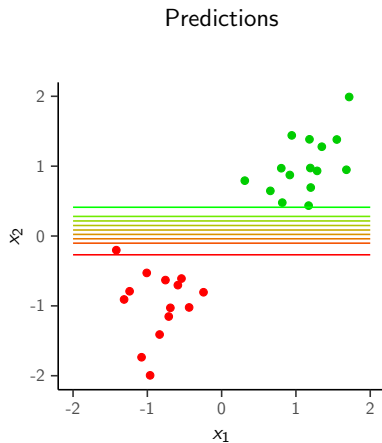
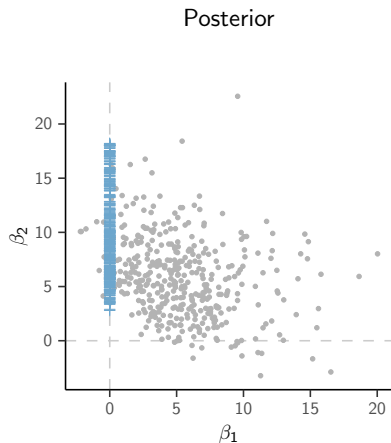
Projected point estimates, constraint  $\beta_1 = 0$

# Logistic regression with two covariates



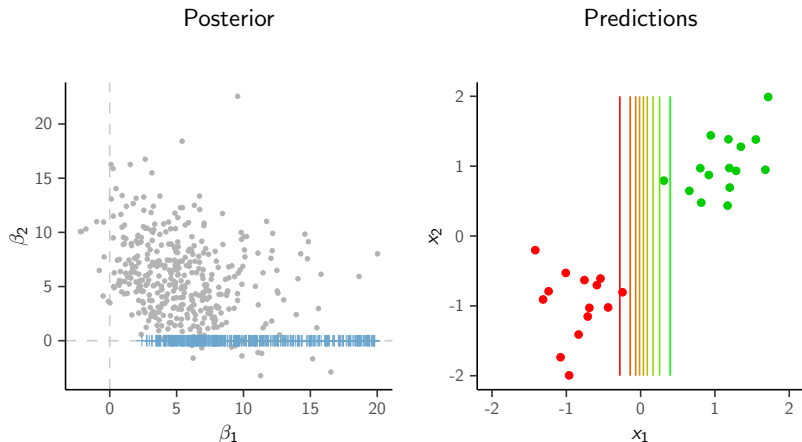
Projected point estimates, constraint  $\beta_2 = 0$

# Logistic regression with two covariates



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

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  - solves the problem of how to do the inference after the model selection

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  - Forward search
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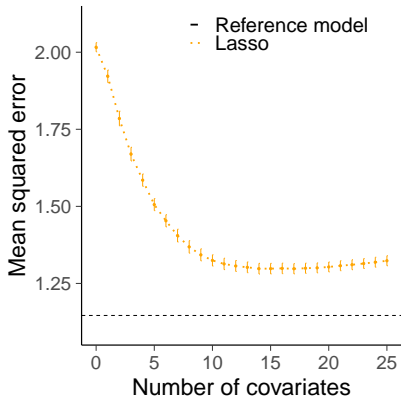
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  - $L_1$ -penalization (as in Lasso)
- Use cross-validation to select the appropriate model size
  - need to cross-validate over the search paths

# Projective selection vs. Lasso

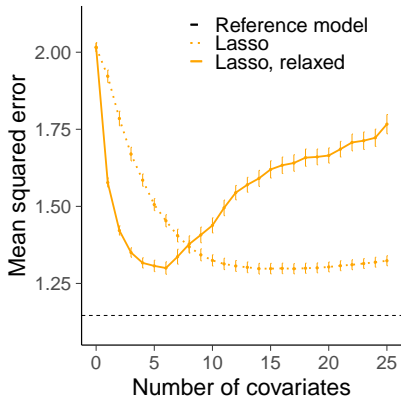
Same simulated regression data as before,

$$n = 50, p = 500, p_{\text{rel}} = 150, \rho = 0.5$$



# Projective selection vs. Lasso

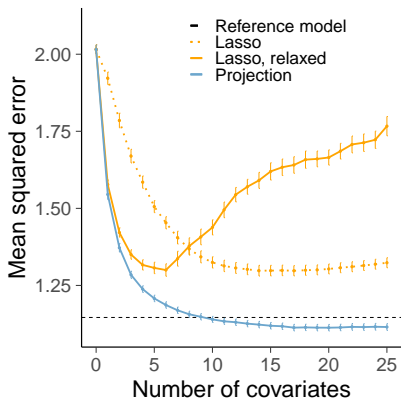
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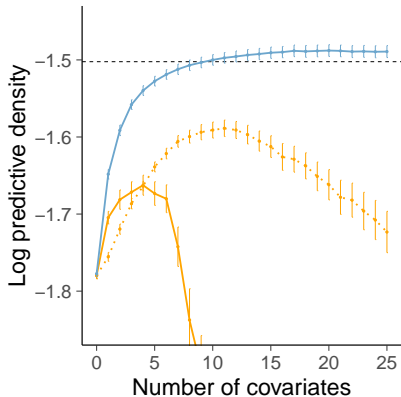
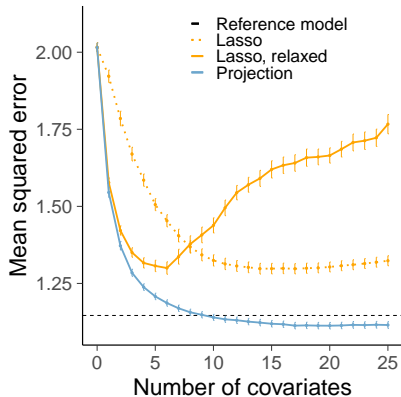




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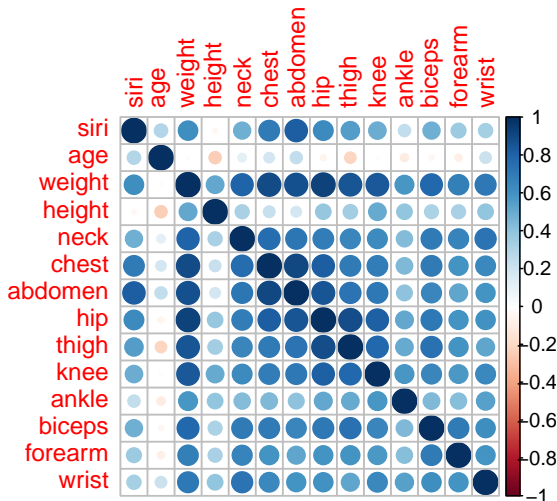


## Bodyfat: small $p$ example of projection predictive

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

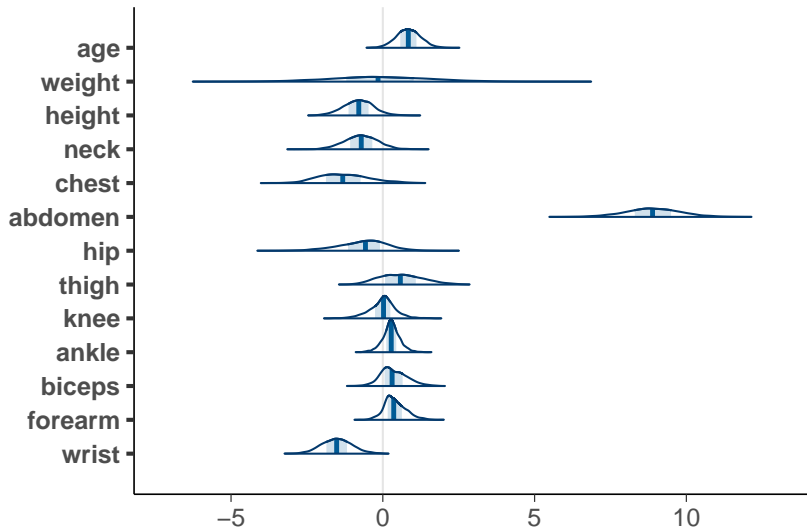
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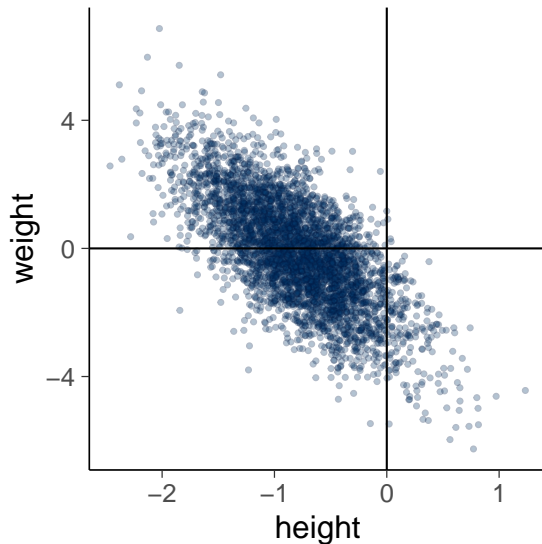
# Bodyfat

Marginal posteriors of coefficients



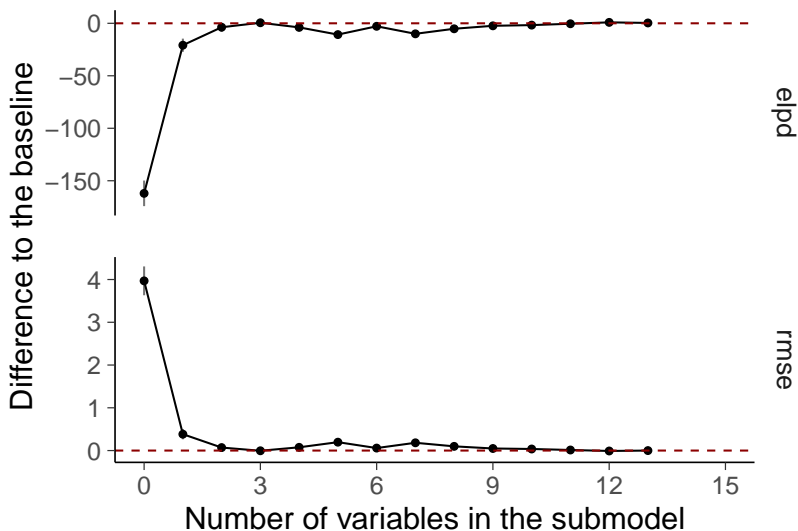
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Bivariate marginal of weight and height



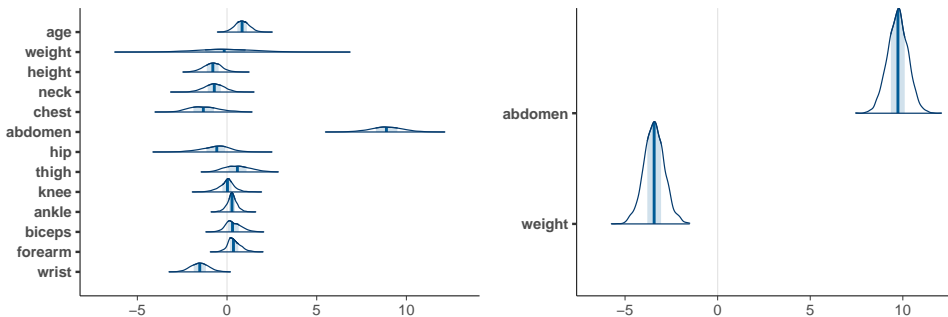
# Bodyfat

The predictive performance of the full and submodels



# Bodyfat

Marginals of the reference and projected posterior



## Predictive performance vs. selected variables

- The initial aim: find the minimal set of variables providing similar predictive performance as the reference model

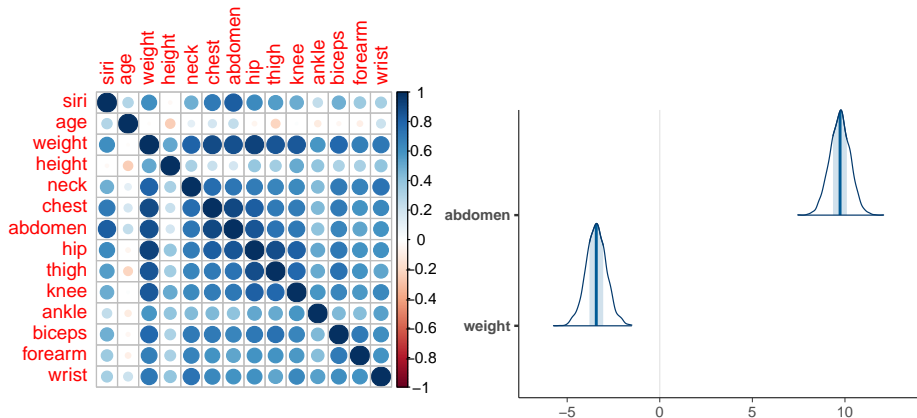


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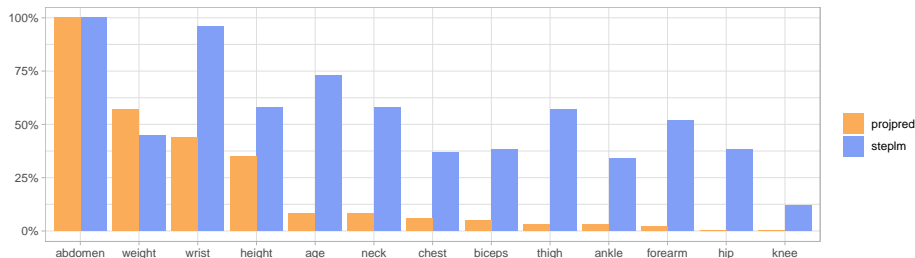
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- Some keep asking can it find the true variables
  - What do you mean by true variables?



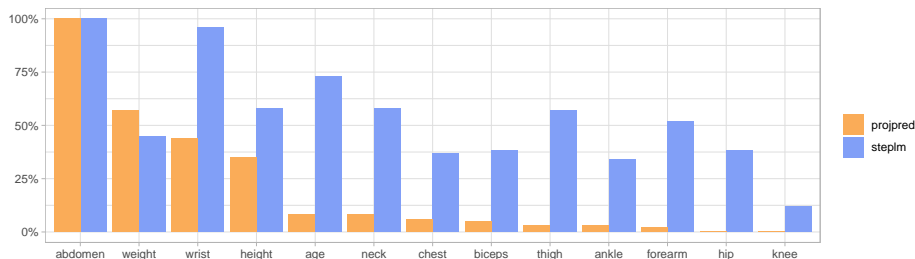
# Variability under data perturbation

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



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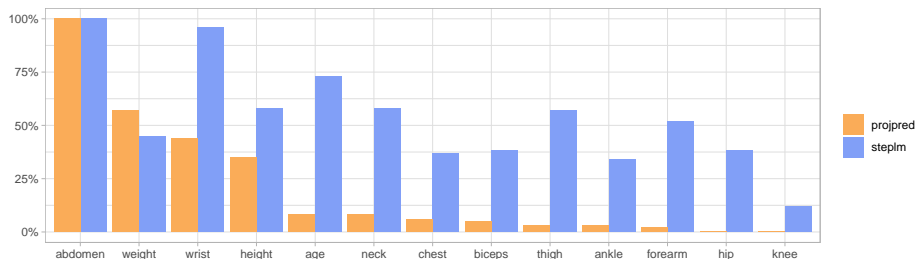
Comparing projection predictive variable selection (projpred) and stepwise maximum likelihood over bootstrapped datasets



M	projpred	Freq %	stepml	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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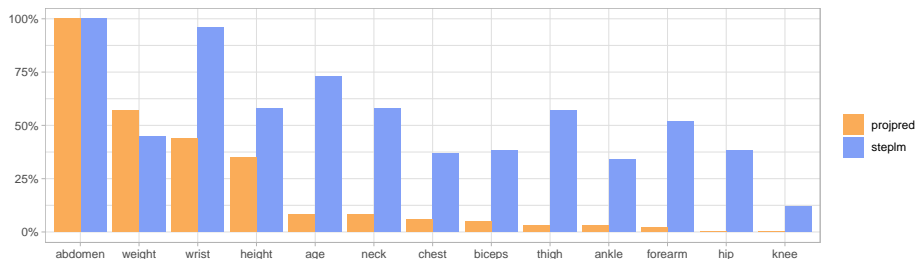
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- Reduced variability, but in case of noisy finite data, there will be some variability under data perturbation
- projpred uses
  - Bayesian inference for the reference
  - The reference model
  - Projection for submodel inference

# Variability under data perturbation

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



- Reduced variability, but in case of noisy finite data, there will be some variability under data perturbation
- projpred uses
  - Bayesian inference for the reference
  - The reference model
  - Projection for submodel inference

# 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

```
varsel <- cv_varsel(fit, method='L1', cv_method='kfold', K=5,  
                   validate_search=TRUE)
```