Chapter 7

- 7.1 Measures of predictive accuracy
- 7.2 Information criteria and cross-validation
  - Instead of 7.2, read:
    Vehtari, A., Gelman, A., Gabry, J. (2017). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. Statistics and Computing. 27(5):1413–1432. arXiv preprint.
- 7.3 Model comparison based on predictive performance
- 7.4 Model comparison using Bayes factors
- 7.5 Continuous model expansion / sensitivity analysis
- 7.5 Example (may be skipped)

Model assesment, selection and inference after selection

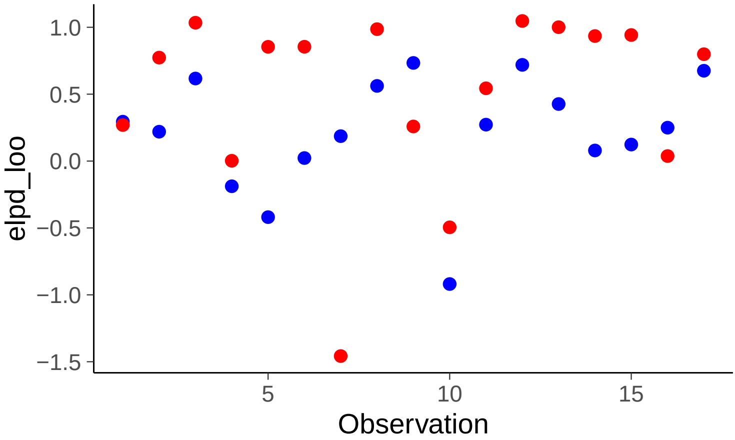
- Extra material at https://avehtari.github.io/modelselection/
  - Videos, Slides, Notebooks, References
  - The most relevant for the course is the first part of the talk “Model assessment, comparison and selection at Master class in Bayesian statistics, CIRM, Marseille”

Model comparison

- "A popular hypothesis has it that primates with larger brains produce more energetic milk, so that brains can grow quickly" (from Statistical Rethinking)
    - Model 1: formula = kcal.per.g $\sim$ neocortex
    - Model 2: formula = kcal.per.g $\sim$ neocortex + log(mass)

mc-stan.org/loo/articles/loo2-example.html

Pointwise comparison LOO models: Model 1



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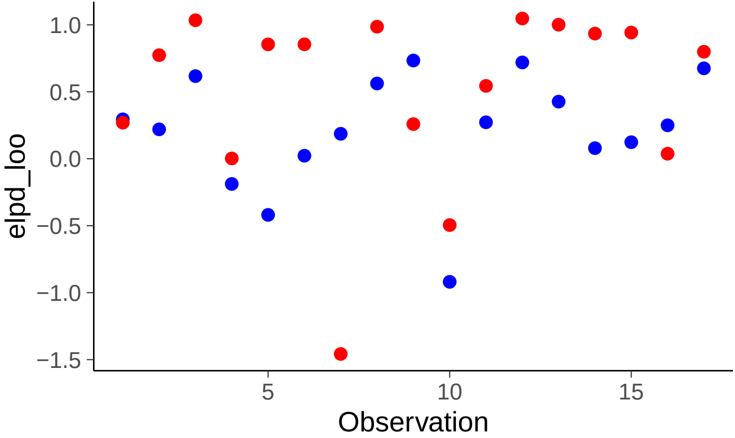

Model 1 elpd_loo $\approx$ 3.7, SE=1.8
Model 2 elpd_loo $\approx$ 8.4, SE=2.8

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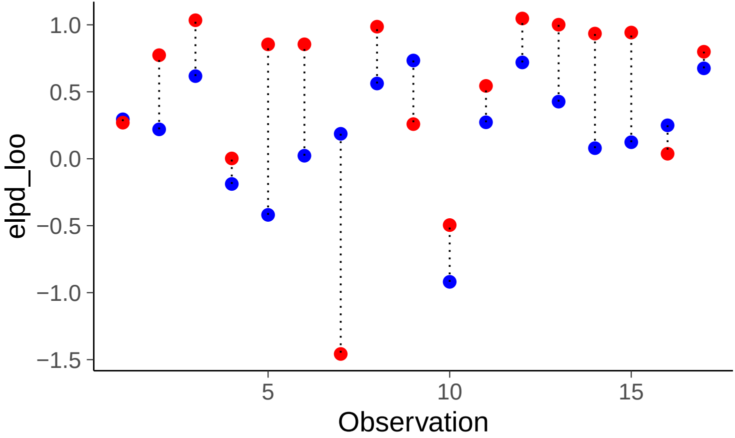

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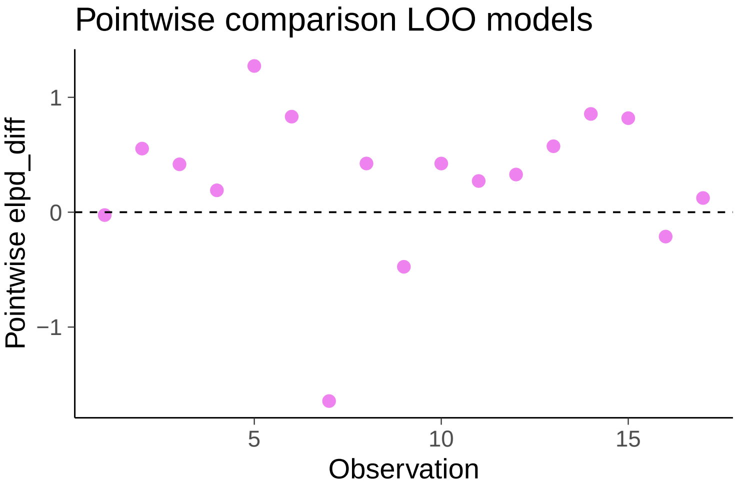
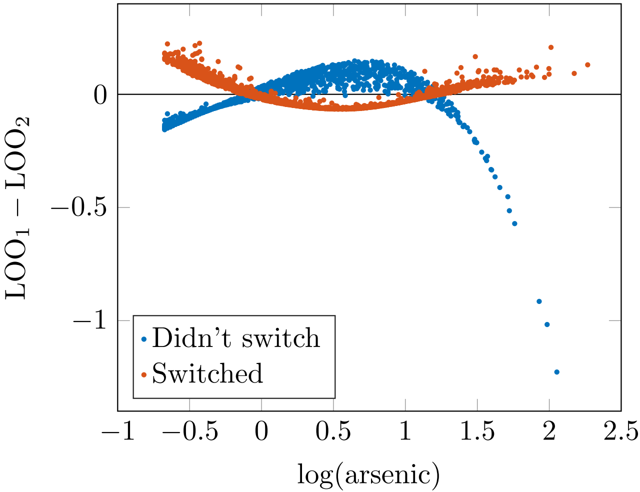



```
Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
      4.7       2.7
```

Arsenic well example – Model comparison

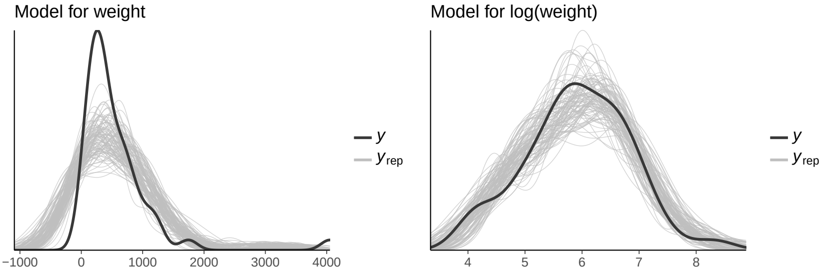


An estimated difference in $\mathrm{elpd}_{\mathrm{loo}}$ of 16.4 with SE of 4.4.

see Vehtari, Gelman & Gabry (2017a)

Sometimes cross-validation is not needed

- Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2019): Regression and Other Stories, Chapter 11.

- BDA3, Chapter 6
- Gabry, Simpson, Vehtari, Betancourt, Gelman (2018). Visualization in Bayesian workflow. JRSS A, preprint arXiv:1709.01449
- mc-stan.org/bayesplot/articles/graphical-ppcs.html
- betanalpha.github.io/assets/case_studies/principled_bayesian_workflow.html

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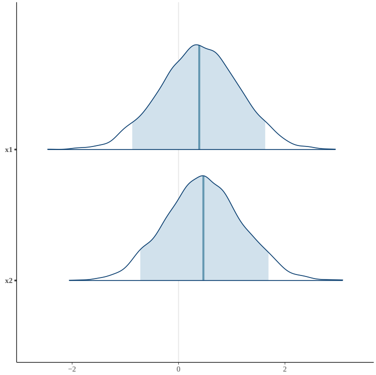
- In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly
  avehtari.github.io/modelselection/betablockers.html

Sometimes predictive model comparison can be useful



Marginal posterior intervals

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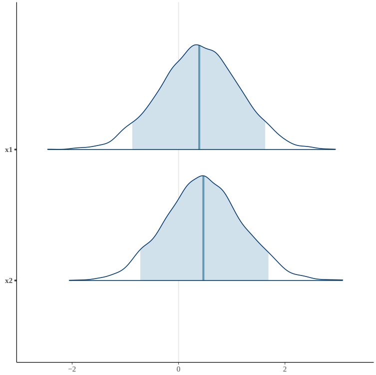

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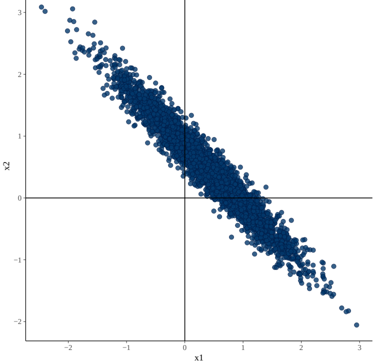

Joint posterior density

rstanarm + bayesplot

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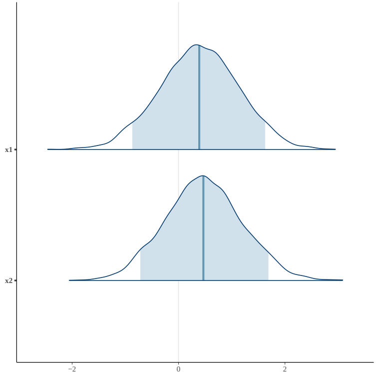

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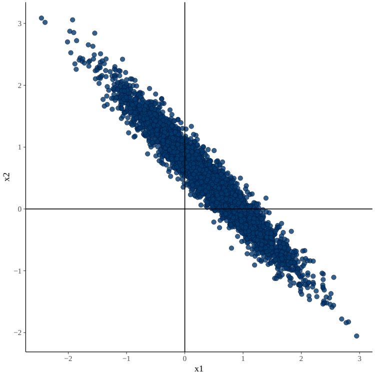

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see also Collinear demo

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- Continuous expansion including all models?
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- If needed integrate over the model space = model averaging
- Bayesian stacking may work better than BMA
  - Yao, Vehtari, Simpson, & Gelman (2018)

Cross-validation and model selection

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  - selection process leads to overfitting
- Overfitting in selection process is not unique for cross-validation

Selection induced bias and overfitting

- Selection induced bias in cross-validation
  - same data is used to assess the performance and make the selection
  - the selected model fits more to the data
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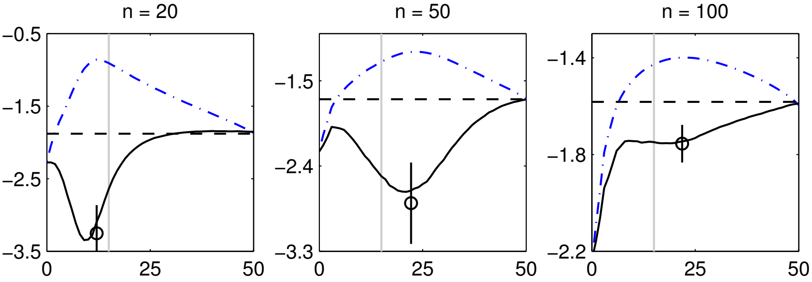
- Bigger problem if there is a large number of models as in covariate selection

Selection induced bias in variable selection



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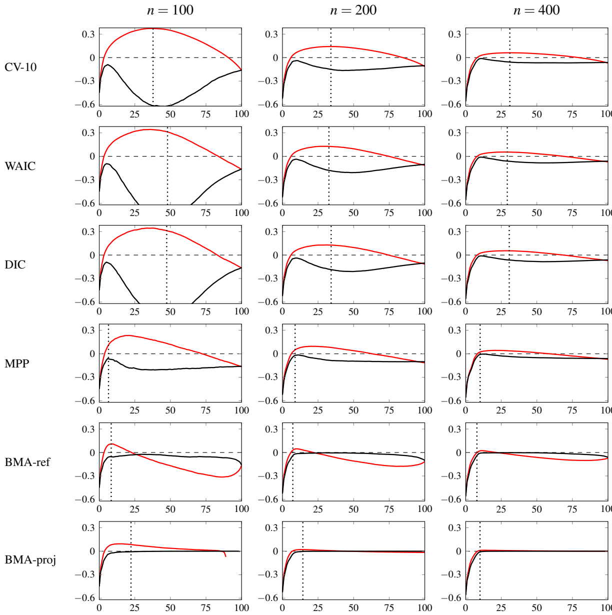

Piironen & Vehtari (2017)

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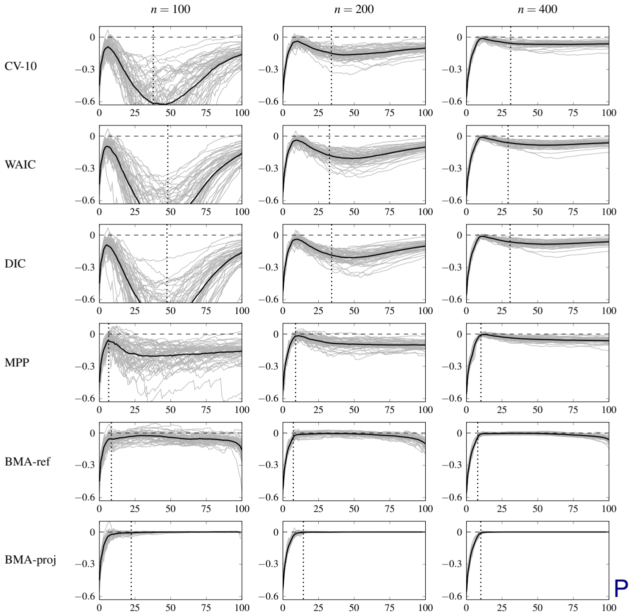

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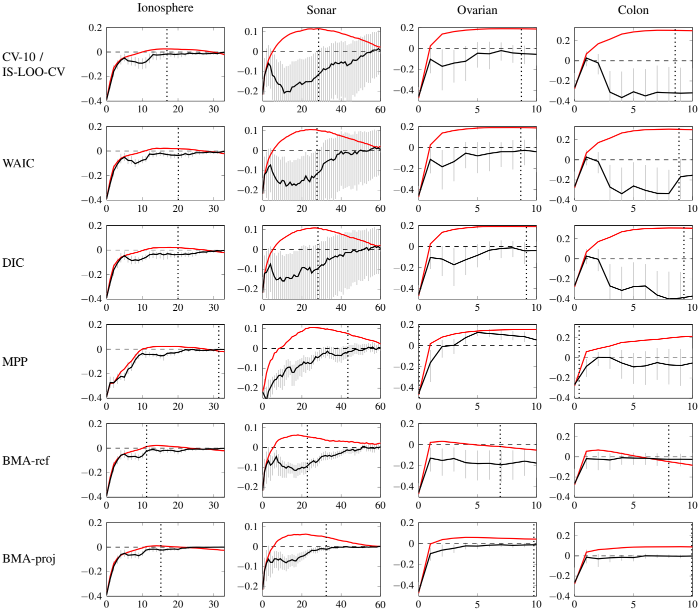

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Take-home messages

- It's good to think predictions of observables, because observables are the only ones we can observe
- Cross-validation can simulate predicting and observing new data
- Cross-validation is good if you don't trust your model
- Different variants of cross-validation are useful in different scenarios
- Cross-validation has high variance, and **if** you trust your model you can beat cross-validation in accuracy

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Rich model vs feature selection?

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  - Include all available prior information
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  - No need for feature selection
- Variable selection can be useful if
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  - improve explainability
- Two options for variable selection
  - Find a minimal subset of features that yield a good predictive model
  - Identify all features that have predictive information

Why shrinkage priors alone do not solve the variable selection problem

- A common strategy:
  - Fit model with a shrinkage prior
  - Select variables based on marginal posteriors (of the regression coefficients)

Why shrinkage priors alone do not solve the variable selection problem

- A common strategy:
  - Fit model with a shrinkage prior
  - Select variables based on marginal posteriors (of the regression coefficients)
- Problems
  - Marginal posteriors are difficult with correlated features
  - How to do post-selection inference correctly?

Example

Consider data

$$
\begin{aligned}
f &\sim \mathrm{N}(0,1), \\
y \mid f &\sim \mathrm{N}(f,1) \\
x_j \mid f &\sim \mathrm{N}(\sqrt{\rho} f,\ 1-\rho), && j = 1,\ldots,25\,, \\
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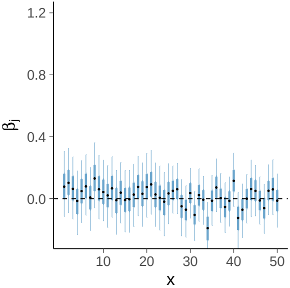
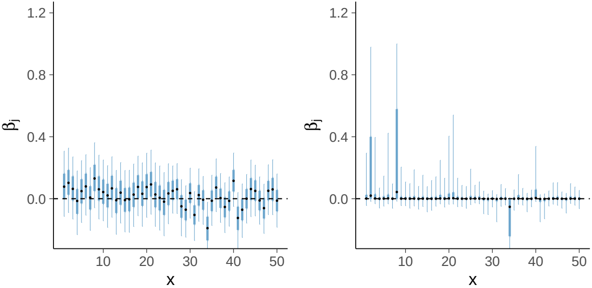
Generate one data set $\{x^{(i)}, y^{(i)}\}_{i=1}^{n}$ with $n = 50$ and $\rho = 0.8$ and assess the feature relevances

Example



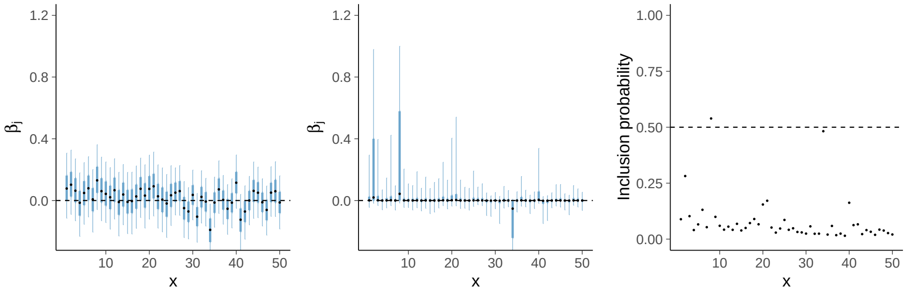
A) Gaussian prior, posterior median with 50% and 90% intervals

Example



A) Gaussian prior, posterior median with 50% and 90% intervals
B) Horseshoe prior, same things

Example



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C) Spike-and-slab prior, posterior inclusion probabilities

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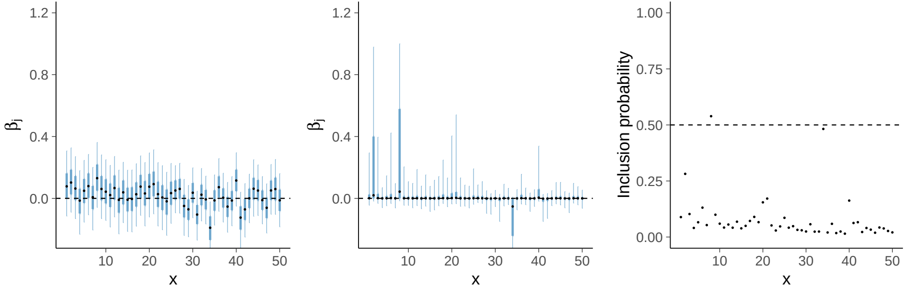

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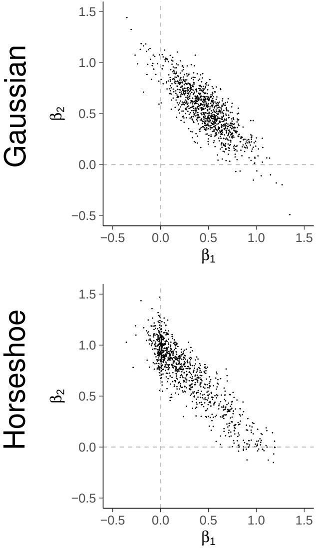
Half of the features relevant, but all marginals substantially overlapping with zero

What happens?



$p_{\text{rel}} = 2$

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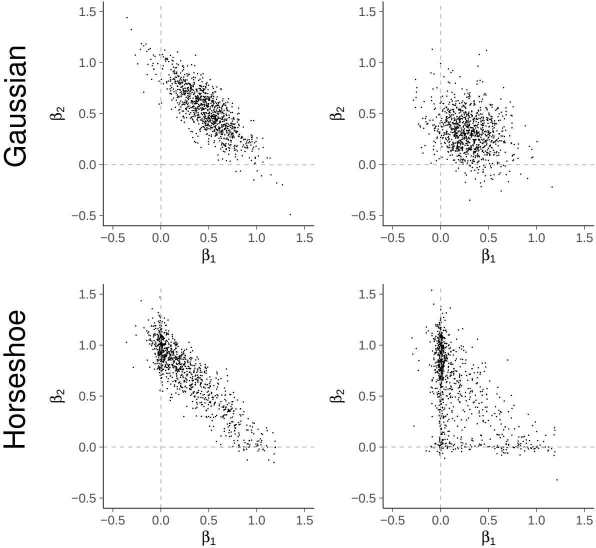
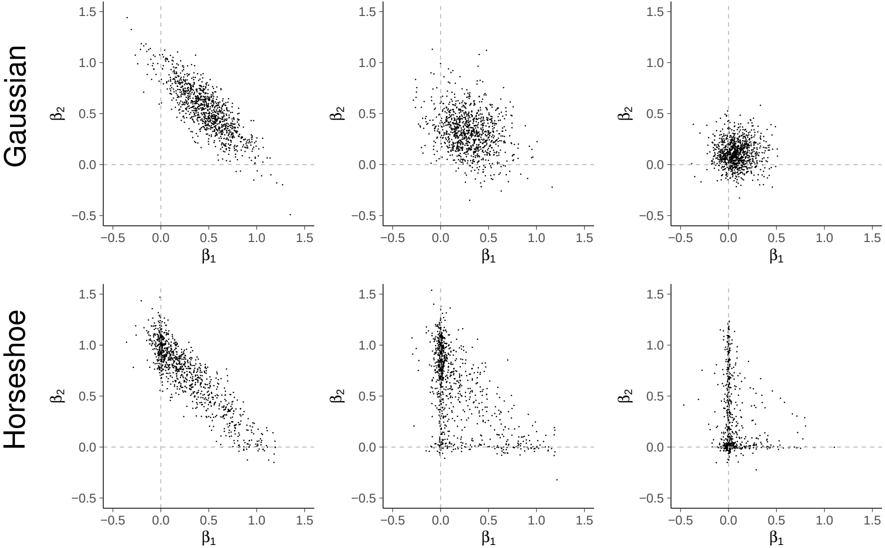


$p_{\text{rel}} = 2$ $\qquad$ $p_{\text{rel}} = 5$

What happens?



$p_{\text{rel}} = 2$ $p_{\text{rel}} = 5$ $p_{\text{rel}} = 25$

Focus on predictive performance

- Two stage approach
  - Construct a best predictive model you can
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  - Construct a best predictive model you can
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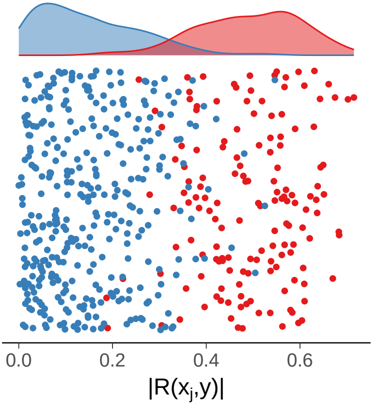
    $\Rightarrow$ *projection*
- Instead of looking at the marginals, find the minimal subset of features which have (almost) the same predictive performance as the reference model

Reference model improves variable selection

Same data generating mechanism, but
$n = 30$, $p = 500$, $p_{\text{rel}} = 150$, $\rho = 0.5$.



irrelevant x_j, relevant x_j

Sample correlation with y

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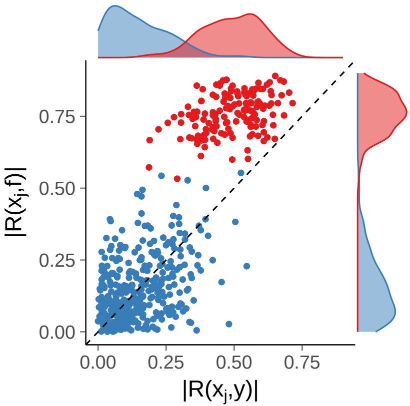

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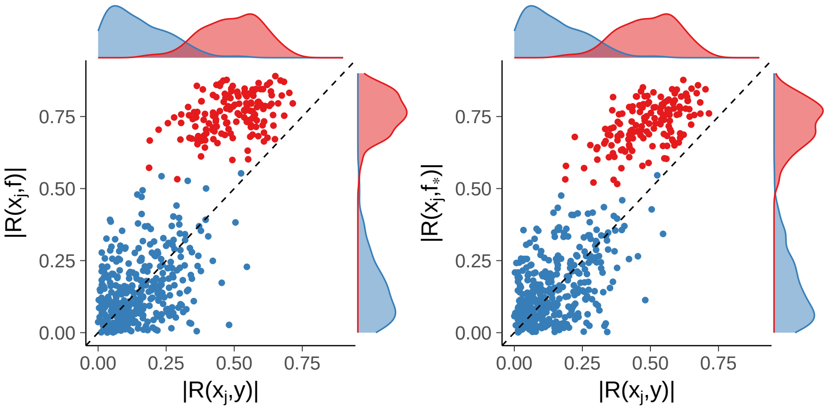
A) Sample correlation with y vs. sample correlation with f

Reference model improves variable selection



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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 supervised principal components

(Iterative) Supervised Principal Components

- Dimension reduction for high dimensional small data with highly correlating features
  - dimension reduction helps to speed up later computation without discarding much information
  - supervised means that features correlating with the target are favored in construcing the principal components
- Piironen and Vehtari (2018). Iterative supervised principal components. 21st AISTATS, PMLR 84:106-114. Online.

Predictive projection, idea

- Model simplification technique

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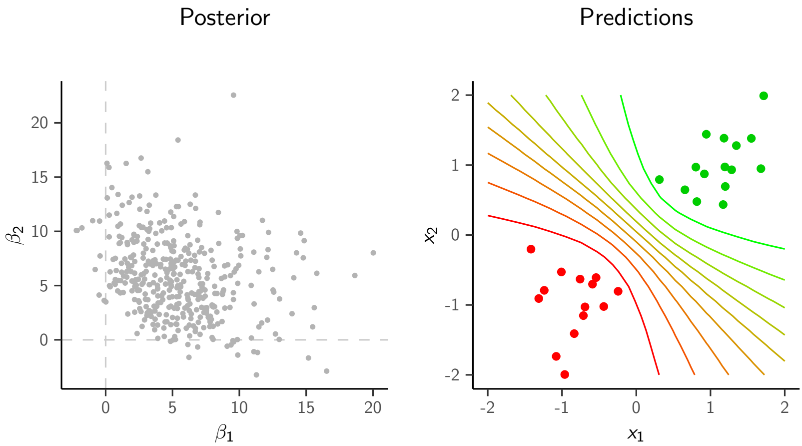
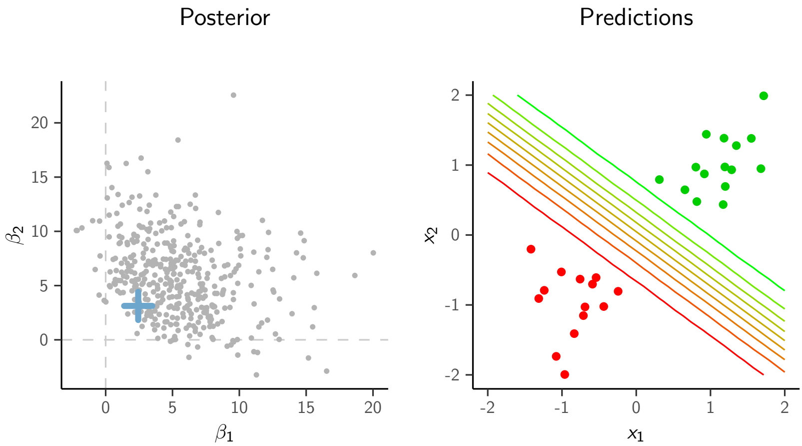
- The decision theoretic idea of conditioning the smaller model inference on the full model can be tracked to Lindley (1968)
  - draw by draw projection introduced by Goutis & Robert (1998), and Dupuis & Robert (2003)
  - see also many related references in a review by Vehtari & Ojanen (2012)

Logistic regression with two features



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

Logistic regression with two features



Projected point estimates for β_1 and β_2

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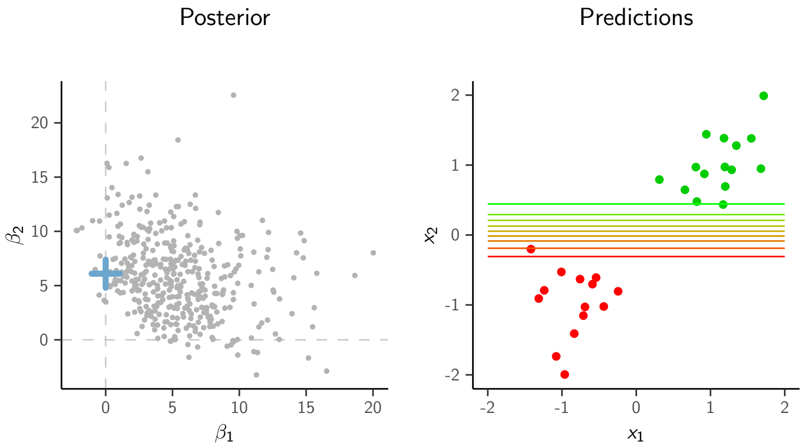
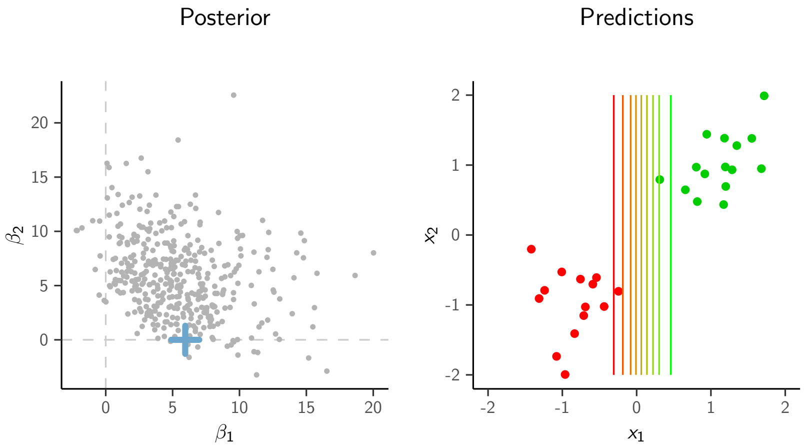


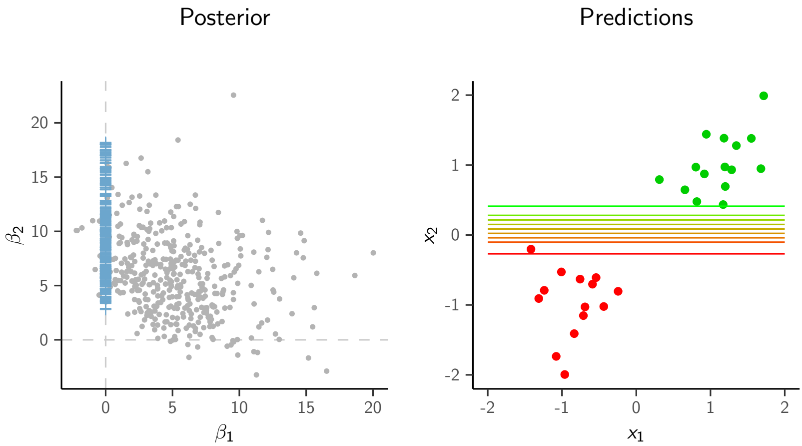
Projected point estimates, constraint $\beta_1 = 0$

Logistic regression with two features



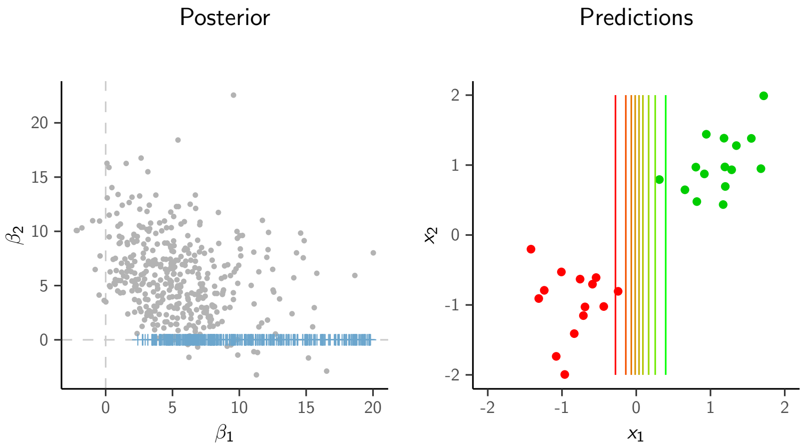
Projected point estimates, constraint $\beta_2 = 0$

Logistic regression with two features



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

Logistic regression with two features



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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

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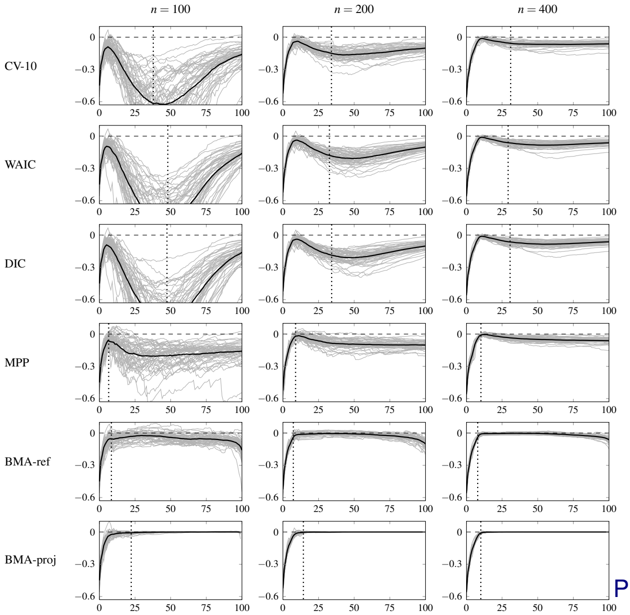
Selection induced bias in variable selection



Piironen & Vehtari (2017)

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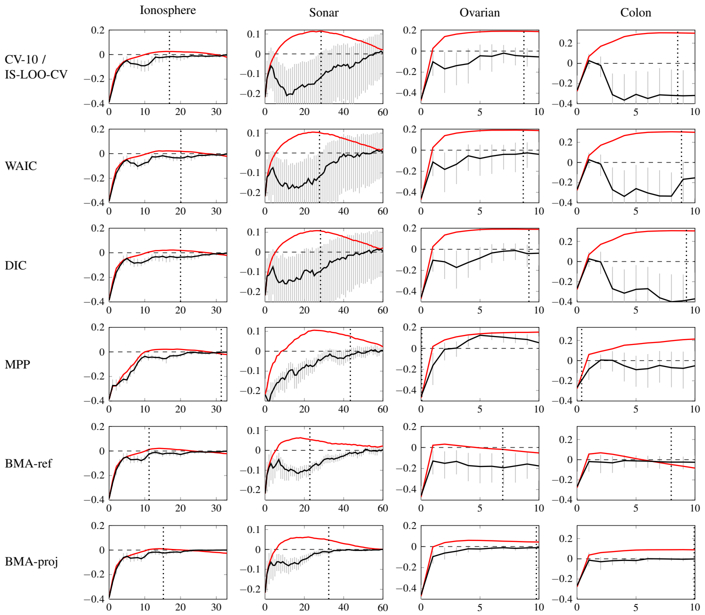

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Bodyfat: small p example of projection predictive

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

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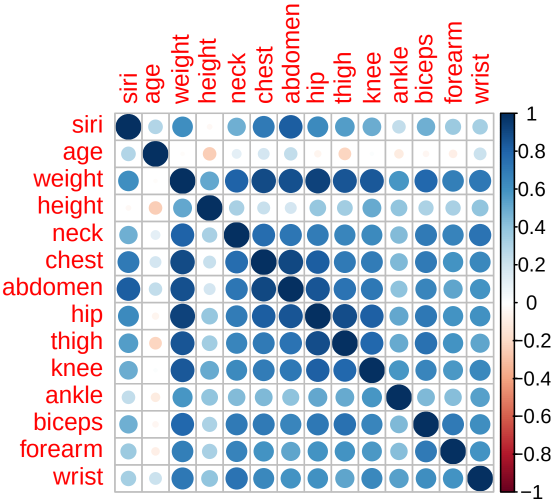
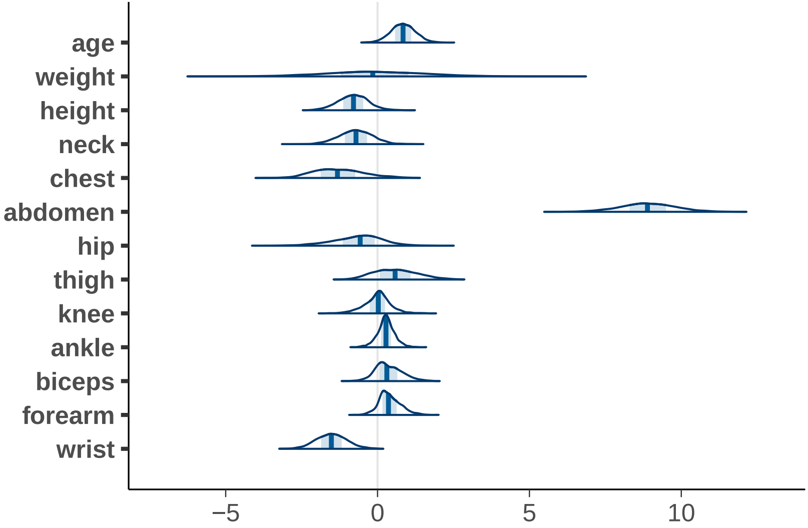


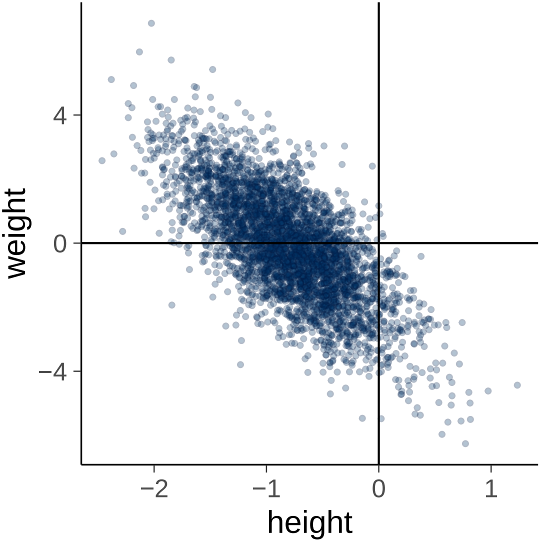
Bodyfat

Marginal posteriors of coefficients



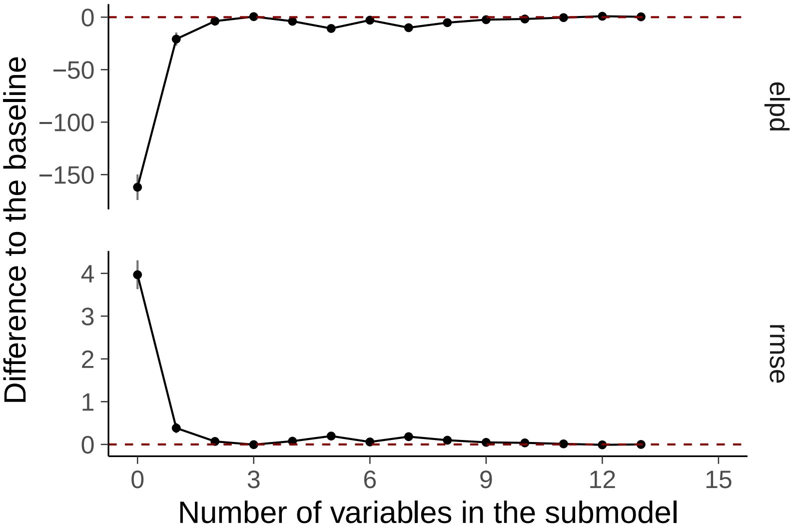
Bodyfat

Bivariate marginal of weight and height



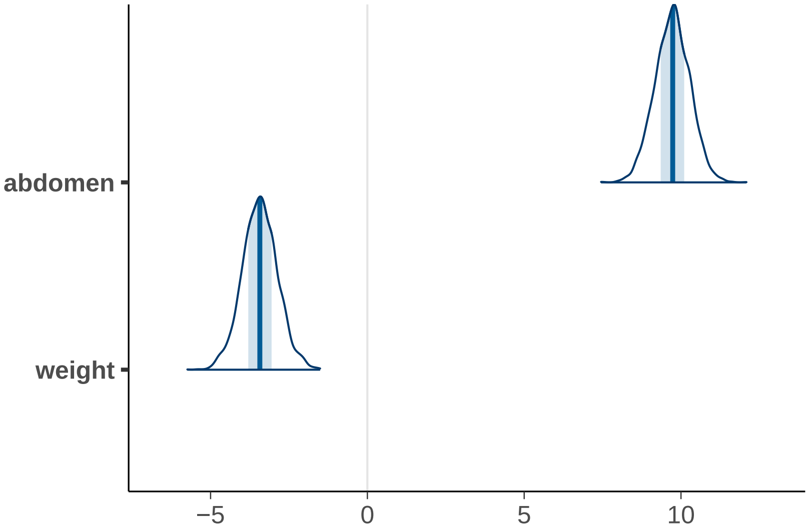
Bodyfat

The predictive performance of the full and submodels



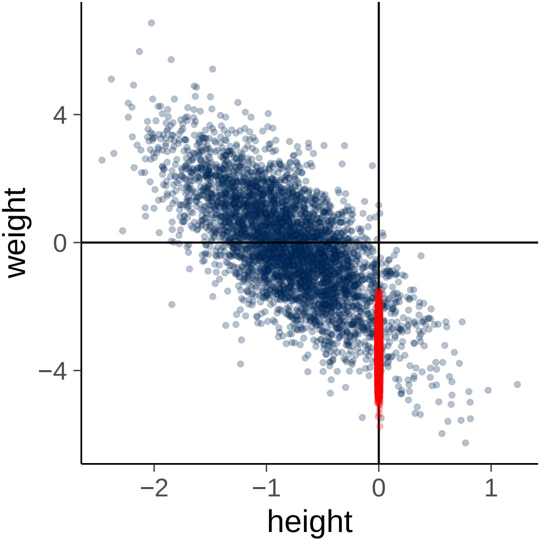
Bodyfat

Marginals of projected posterior



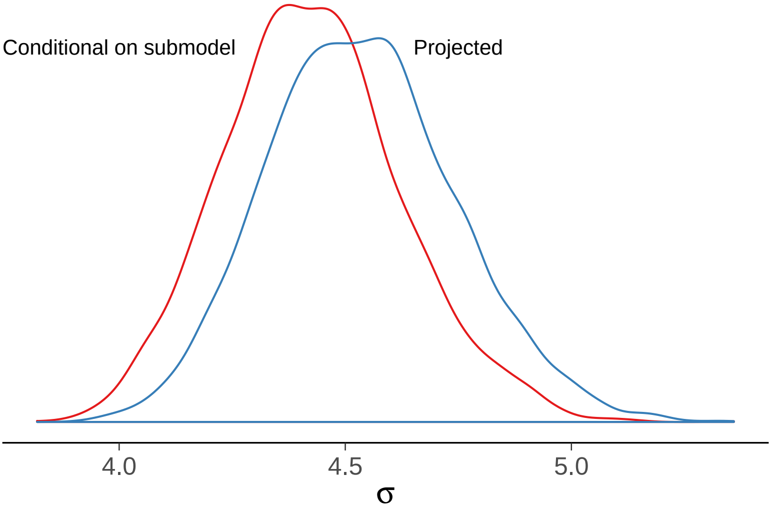
Bodyfat

Projected posterior is not just the conditional of joint



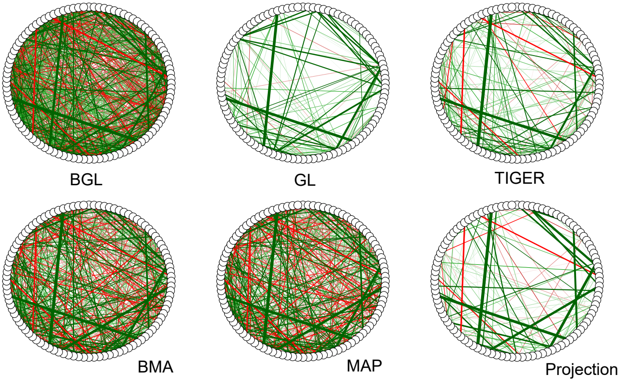
Bodyfat

Projected posterior is different than posterior conditioned only on selected features



Projection of Gaussian graphical models

- Williams, Piironen, Vehtari, Rast (2018). Bayesian estimation of Gaussian graphical models with projection predictive selection. arXiv:1801.05725



CEU genetic network. BGL: Bayesian glasso; GL: glasso; TIGER: tuning insensitive graph estimation and regression; BMA: Bayesian model averaging; MAP: Maximum a posteriori; Projection: projection predictive selection.

More results

- More results projpred vs. Lasso and elastic net:
  Piironen, Paasiniemi, Vehtari (2018). Projective Inference in High-dimensional Problems: Prediction and Feature Selection. arXiv:1810.02406
- More results projpred vs. marginal posterior probabilities:
  Piironen and Vehtari (2017). Comparison of Bayesian predictive methods for model selection. Statistics and Computing, 27(3):711-735. doi:10.1007/s11222-016-9649-y.
- projpred for Gaussian graphical models:
  Williams, Piironen, Vehtari, Rast (2018). Bayesian estimation of Gaussian graphical models with projection predictive selection. arXiv:1801.05725
- More results for Bayes SPC:
  Piironen and Vehtari (2018). Iterative supervised principal components. 21st AISTATS, PMLR 84:106-114. Online.
- Several case studies for small to moderate dimensional ($p = 4 \dots 100$) small data:
  Vehtari (2018). Model assesment, selection and inference after selection. https://avehtari.github.io/modelselection/

Take-home messages (part 2)

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- R-package `projpred` in CRAN and github
  https://github.com/stan-dev/projpred
  (easy to use, e.g. with RStan, RStanARM, brms)

References

References and more at avehtari.github.io/masterclass/ and avehtari.github.io/modelselection//

- Model selection tutorial at StanCon 2018 Asilomar
  - more about projection predictive variable selection
- Regularized horseshoe talk at StanCon 2018 Asilomar
- Several case studies
- References with links to open access pdfs