Using reference models in variable selection

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Abstract

Variable selection, or more generally, model reduction is an important aspect of the statistical workflow aiming to provide insights from data. In this paper, we discuss and demonstrate the benefits of using a reference model in variable selection. A reference model acts as a noise-filter on the target variable by modeling its data generating mechanism. As a result, using the reference model predictions in the model selection procedure reduces the variability and improves stability leading to improved model selection performance. Assuming that a Bayesian reference model describes the true distribution of future data well, the theoretically preferred usage of the reference model is to project its predictive distribution to a reduced model leading to projection predictive variable selection approach. Alternatively, reference models may also be used in an ad-hoc manner in combination with common variable selection methods. In several numerical experiments, we investigate the performance of the projective prediction approach as well as alternative variable selection methods with and without reference models. Our results indicate that the use of reference models generally translates into better and more stable variable selection. Additionally, we demonstrate that the projection predictive approach shows superior performance as compared to alternative variable selection methods independently of whether or not they use reference models.

1 Introduction

In statistical applications, one of the main steps in the modelling workflow is variable selection, which is a special case of model reduction. Variable selection (also known as feature or covariate selection) may have multiple goals. First, if the variables themselves are of interest, we can use variable selection to infer which variables contain predictive information about the target. Second, as simpler models come with the advantages of reduced measurement costs and improved interpretability, we may be interested in finding the minimal subset of variables which still provides good predictive performance (or good balance between simplicity and predictive performance). When the predictive capability is guiding the selection, the true data generation mechanism of future data can be approximated either by using the observed data directly or alternatively by using predictions from a reference model (Vehtari and Ojanen, 2012).

In data-based approaches, such as Lasso selection (Tibshirani, 1996) or stepwise backward/forward regression (Venables and Ripley, 2013; Harrell, 2015), the observed empirical data distribution is utilised as a proxy of future data usually in combination with cross-validation or information criteria to provide estimates for out-of-sample predictive performance. In contrast, reference model based methods approximate the future data generation mechanism using the predictive distribution of a reference model, which can be, for example, a full-encompassing model including all variables. The main assumption under any reference model approach is that we operate in an M-complete framework (Bernardo and Smith, 2009; Vehtari and Ojanen, 2012), that is, we have constructed a model which reflects our beliefs about the future data in the best possible way and which has passed model checking and criticism (see, e.g. Gelman et al., 2013; Gabry et al., 2019). The reference model approach has been used in Bayesian statistics at least since the seminal work of Lindley (1968). For more historical references, see Vehtari and Ojanen (2012) and Piironen and Vehtari (2017a), and for most recent methodological developments see Piironen et al. (2020).

Reference models have been also used in non-Bayesian contexts, in which Harrell (2015) describes them as full models that can be thought of as a ”gold standard” (for a given application). For example, Faraggi et al. (2001) deal with the necessity of identifying interpretable risk groups in the context of survival data using neural networks, which typically perform very well in terms of prediction, but whose variables are difficult to
be understood in terms of relevance. Paul et al. (2008), using the term preconditioning, explore approximating models fitting Lasso or stepwise regression against consistent estimates \( \hat{y} \) of a reference model instead of the observed responses \( y \). Whatever the terminology or applied statistical framework, reference models offer a powerful approach to improving variable selection as we will demonstrate in the present paper.

This paper is structured as follows. In Section 2, we review the concept of the reference model, its benefits with examples and how it can be used as a filter on data in a simple way. In Section 3 and Section 4, we show the benefits of a reference model approaches for minimal and complete variable selection, respectively, before we end with a conclusion in Section 5.

## 2 Reference models in variable selection

In this section, we will provide an initial motivation and intuition for the use of reference models to improve variable selection methods. We will start with a case study that is repeatedly used throughout the paper to illustrate the benefits of reference models before we dive deeper into the theoretical reasons why reference models help in variable selection.

### 2.1 Body fat example: Part 1

To motivate the further discussion and experiments, we start by a simple variable selection example using body fat data by Johnson (1996). We compare the projective prediction approach \((\text{projpred}, \text{Piironen et al. (2020)})\) which uses a reference model, and classic stepwise backward regression \((\text{steplm})\). The experiments are implemented in \(R\) (R Core Team, 2018).

The target variable of interest is the amount of body fat, which is obtained by a complex and expensive procedure consisting in immersing a person in a water tank and carrying out different measurements and computations. Additionally, we have information about 13 variables which are anthropometric measurements (e.g., height, weight and circumference of different body parts). The variables are highly correlated which causes additional challenge in the variable selection. In total, we have 251 observations. The goal is to find the model which is able to predict the amount of body fat well while requiring the least amount of measurements for a new person.

Heinze et al. (2018) report results using steplm with a significance level of 0.157 with AIC selection (Akaike, 1974), fixing abdomen and height to be always included in the model. For better comparison we do not fix any of the variables. The steplm approach is carried out combining the \texttt{step}\ and \texttt{lm} functions in \(R\).

For the selection via projpred, the Bayesian reference model includes all the variables using a regularised horseshoe prior (Piironen and Vehtari, 2017b) on the variable coefficients. Submodels are explored using forward search (the results are not sensitive to whether forward or backward search is used), and the predictive utility is the expected log-predictive density (elpd) estimated using approximate leave-one-out cross-validation via Pareto-smoothed importance-sampling (PSIS-LOO-CV; Vehtari et al., 2017). We select the smallest submodel with an elpd score similar to the reference model when taking into account the uncertainty in estimating the predictive model performance. See Appendix A for brief review of projection predictive approach, and papers by Piironen and Vehtari (2017a) and Piironen et al. (2020) for more details. The complete projpred approach is implemented in the \texttt{projpred} \(R\) package (Piironen et al., 2019).

The inclusion frequencies of each variable in the final model given 100 bootstrap samples are shown in Figure 1. In case of projpred there are two variables, ‘abdomen’ and ‘weight’, which have inclusion frequencies above 50% (‘abdomen’ is the only one included always), the third most frequently included is ‘wrist’ at 44%, and the fourth one is ‘height’ at 35%. The steplm approach has seven variables with inclusion frequencies above 50%. Such a higher variability and lower stability of steplm can be observed also in the bootstrap model selection frequencies reported in Table 1. For example, the first five selected models have a cumulative frequency of 76% with projpred, but only of 14% with steplm. In addition, the sizes of the selected models with projpred are much smaller than the ones selected with steplm.
Figure 1: Body fat example: Bootstrap inclusion frequencies calculated from 100 bootstrap samples. The projpred approach has less variability on which variables are selected.

| 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., age, height, hip, neck, thigh, wrist              | 2      |
| 5 | abdom., weight, wrist | 8     | abdom., age, height, hip, neck, 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      |

Table 1: Body fat example: Bootstrap model selection frequencies from 100 bootstrap samples. The projpred approach has less variability on which variable combinations are selected.

The first two rows of Table 2 show the predictive performances, in terms of cross-validated root mean square error (RMSE), of the full model and the selected models using projpred or steplm. There is no significant difference in predictive performance of the selected models by different approaches even if there is clear difference in the number of selected variables. This can be explained by high correlation between the variables and different combinations can provide similar predictive accuracy.

We repeat the experiment with a modified data set by adding 84 unrelated noisy variables, resulting in 100 variables in total. The last two rows of Table 2 show the cross-validated RMSE, the size of the selected model and the number of selected noisy variables using projpred or steplm. The results show that projpred has similar predictive performance and the same number of selected variables as with the original data, whereas the stepwise regression has worse predictive performance and the number of selected variables is much higher and include a large number of irrelevant variables.

Both projpred and steplm compare a large number of models using either forward or backward search, which can lead to selection induced overfitting, but even with 100 variables, projpred is able to select a submodel with similar performance as the full model. In this example, the two compared methods also differ in other aspects than the usage of a reference model, such as that projpred uses Bayesian inference and steplm uses maximum likelihood estimation. However, as we show in the present paper, one of the primary difference with respect to quality of the variable selection is indeed whether or not a reference model is applied.

### 2.2 Benefits and costs of using a reference model

A properly designed reference model is able to filter parts of the noise present in the data, and hence to provide an improved and more stable selection process. This holds even if the reference model does not perfectly resemble the true data generating process. Moreover, our analyses indicate that the substantial reduction of variance attributable to noise is usually more important than small potential bias due to model misspecification. We argue that, regardless of how the reference model is set up and used in the inference procedure, it can be
Table 2: Body fat example: Predictive performances with original data (first two rows) and with extra noisy variables (last two rows) estimated with 10-fold cross-validation. Abbreviations: RMSE = root mean squared error; Full = full model; Sel = selected submodel; # Sel = total number of selected variables; # Sel noisy = number of selected noisy variables. 10-CV avg = average over the 10 folds in cross-validation. 10-CV sd = standard deviation over the 10 folds in cross-validation.

always seen as acting as a filter on the observed data. Furthermore, regardless of what specific model selection method is used, a reference model can be used instead of raw data during the selection process to improve the stability and selection performance. Our results indicate that the core reason why the reference model based methods perform well is the reference model itself, rather than the specific way of using it. In general, the less data we have and the more complex the estimated models are, the higher is the benefit of using a reference models as the basis for variable selection.

If one of the models to be compared is the full model, which can be used as a reference model, there is no additional cost of using a reference model as it was estimated as part of the analysis anyway. Sometimes including all the available variables in an elaborate model can be computationally demanding. In such a case, even simpler screening or dimensionality reduction techniques, as for example the supervised principal components (Bair et al., 2006; Piironen and Vehtari, 2018) can produce useful reference models.

2.3 Why the reference model helps

A good predictive model is able to filter part of the noise present in the data. The noise is the main source of the instability in the selection and tends to obscure the relevance of the variables in relation to the target variable of interest. We demonstrate it with the following simple explanatory example taken from Piironen et al. (2020). The data generation mechanism is

\[
\begin{align*}
    f & \sim N(0, 1) \\
    Y \mid f & \sim N(f, 1) \\
    X_j \mid f & \overset{iid}{\sim} N(\sqrt{\rho} f, 1 - \rho) \quad j = 1, \ldots, k \\
    X_j \mid f & \overset{iid}{\sim} N(0, 1) \quad j = k + 1, \ldots, p,
\end{align*}
\]

where \( f \) is the latent variable of interest of which \( Y \) is a noisy observation. The first \( k \) variables are strongly related to the target variable \( Y \) and correlated among themselves. Precisely, \( \rho \) is the correlation among any pair of the first \( k \) variables, whereas \( \sqrt{\rho} \) and \( \sqrt{\rho}/2 \) are the level of correlation between any relevant variable and, respectively, \( f \) and \( Y \). If we had an infinite amount of observations, the sample correlation would be equal to the true correlation between \( X_j \) and \( Y \). However, even in this ideal asymptotic regime, this correlation would still remain a biased indicator of the true relevance of each variable (represented by the correlation between \( X_j \) and \( f \)) due to the intrinsic noisy nature of \( Y \).

When using a reference model, we first obtain predictions for \( f \) using all the variables \( \{X_j\}_{j=1}^p \), taking into account that we have only observed the noisy representation \( Y \) of \( f \). If our model is good, we are able to describe \( f \) better than \( Y \) itself can, which improves the accuracy in the estimation of the relevance of the variables. Figure 2 illustrates this process in the form of a scatter plot of (absolute) correlations of the variables with \( Y \) against the corresponding correlations with the predictions of a reference model (in this case the posterior predictive means of model (7); see Section 4.3). Looking at the marginal distributions, we see that using a reference model to filter out noise in the data, the two groups of variables (relevant and non-relevant) can be distinguished much better than when the correlation is computed using the observed noisy data directly.
In the body fat example above, our two simultaneous goals were to obtain good predictive performance and to select a smaller number of variables. When the goal is to select a minimal subset of variables, which have similar predictive performance as the full model, we call it minimal subset variable selection. This minimal subset might exclude variables which have some predictive information about the target but, given the minimal subset, these variables are not able to provide such additional information that would improve predictive performance in a substantial manner. The usual reason for this is that the relevant variables which are not in the minimal subset are highly correlated with variables already in the minimal subset. We will return to a problem of finding all the variables with some predictive power in Section 4.

3 Simulation study 1

Using the data generating mechanism (1), we simulate data sets of different sizes with a relatively large number of variables \( p = 70 \), with \( k = 20 \) of them being predictive. We compare the minimal subset variable selection performance of the projection predictive approach (which uses a reference model and it is referred to as projpred), a Bayesian stepwise forward selection with and without a reference model, and maximum likelihood stepwise forward selection with and without a reference model (steplm). The following is a summary of the implementation of the compared methods:

- **projpred**: the projective prediction approach is used. The reference model is a Bayesian linear regression model using the first five supervised principal components (Piironen and Vehtari, 2018) as predictors and the full posterior predictive distribution as the basis of the projection. The search heuristic is forward search and the predictive performance is estimated via 10-fold cross-validation. The selection continues until the predictive performance is close to the predictive performance of the reference model. See more details in Appendix A.

- **Bayesian stepwise selection (without a reference model)**: at each step, the fitted model is a Bayesian linear regression using the regularised horseshoe prior and the variable included is the one with the highest Bayesian \( p \)-value defined as \( \min\{P(\theta \leq 0 \mid D), P(\theta > 0 \mid D)\} \), where \( D \) stays for the observed data. The selection continues if the reduced model has an elpd score higher (i.e., better) than the current model.

- **Bayesian stepwise selection (with a reference model)**: the reference model is the same as for projpred, but only point predictions (posterior predictive means) \( \hat{y} \) are used to replace the target variable \( y \). The same Bayesian \( p \)-value selection strategy as in the data based Bayesian stepwise selection is used.

- **steplm (without a reference model)**: stepwise selection using AIC as in the body fat example.
Figure 3: Simulation study 1: Root mean square error (RMSE) against false discovery rate in the minimal subset variable selection with one standard deviation error bars. The projpred approach has the smallest RMSE and false discovery ratio.

Figure 4: Simulation study 1: Entropy score in the minimal subset variable selection. The projpred approach has much smaller entropy score than the other approaches.

- **steplm (with a reference model)**: the reference model is the same as for projpred, but only point predictions (posterior predictive means) \( \hat{y} \) are used to replace the target variable \( y \). The same AIC selection strategy as in the data based steplm is used.

In Figure 3, the predictive performance is shown for different values of \( n \) and \( \rho \) in terms of RMSE and the false discovery rate (FDR, the ratio of the number of non-relevant selected variables over the number of selected variables) of the selected submodel, averaged after 100 data simulations. We see that projpred has superior FDR and the smallest RMSE. Using a reference model improves steplm significantly, but the minimal subset variable selection stays unreliable. Stepwise Bayesian linear regression is better than steplm when comparing both methods with and without a reference model, respectively. However, the minimal subset variable selection of the Bayesian linear regression is still less reliable than projpred.

When the variable selection is repeated with different simulated data sets, there is some variability in the selected variables. We measure the stability of variable selection by computing the entropy of the observed distribution of the included variables over different models. The smallest entropy would be obtained if the approach always selected the same set of variables, and the largest entropy would be observed if the approach would always select different sets of variables. Therefore, lower entropy corresponds to a more stable selection. Highly correlated predictive variables may happen to be selected alternately, thus making stability estimation of the selection a non-trivial task. Entropy can not distinguish the interchangeability due to correlation from instability. Thus, such a measure should be considered as a relative, and not as an absolute, measure of stability. Figure 4 shows the entropy scores for the different compared methods. The use of a reference model improves the stability of steplm in variable selection slightly, while it makes little difference for the Bayesian linear regression. The projpred approach turns out to be far more stable than all other methods. This is likely due to projpred being based on better decision theoretical formulation which 1) takes into account the full predictive distribution and not just point estimate and 2) projects the reference model posterior to the submodel instead of using a simple refit of submodels.
Noisy features selected | RMSE
---|---
20 | 40 | 60 | 4 | 6 | 8

Approach | data | ref

Figure 5: Body fat example: Stepwise backward selection with and without using a reference model. The x-axis denotes the number of selected irrelevant variables on the left and the out-of-sample RMSE on the right-hand side based on 100 bootstrap samples. The reference approach reduces the number of noisy variables selected and the out-of-sample RMSE.

Table 3: Body fat example: Means and standard deviations (between brackets) of the results shown in Figure 5.

| Method                      | RMSE  | Selected noisy |
|-----------------------------|-------|----------------|
| Stepwise selection          | 6.9 (0.7) | 48 (7) |
| Reference model + Stepwise selection | 4.7 (0.5) | 25 (7) |

3.2 Body fat example: Part 2

Here we repeat the selection of Section 2.1 via stepwise backward regression. In this case, the overall number of variables (original plus noisy) is 100, as it was in the last part of Section 2.1. We compare results with and without using a simple reference model approach outlined in (7) with steplm. Figure 5 shows the number of irrelevant variables included in the final model and the out-of-sample root mean square error (RMSE). Results are based on 100 bootstrap samples on the whole dataset, and the predictive performance is tested on the observations excluded at each bootstrap sample. We observe that the reference model reduces the number of irrelevant variables included in the final model. This leads to less overfitting and thus to improved out-of-sample predictive performance in terms of RMSE. The reference model approach applied to the stepwise backward regression achieves outstanding improvements considering its simplicity, yet it does not reach the goodness of the much more sophisticated projective prediction approach (see results of Section 2.1).

4 Complete variable selection

An alternative to minimal subset variable selection is complete variable selection in which the goal is to find all relevant variables that have some predictive information about the target. In complete variable selection, it is possible that there are theoretically relevant variables, but given finite noisy data we are not able to infer their relevance. The projection predictive approach was originally designed for the minimal subset variable selection but we will test a simple iterative variant for the complete variable selection case in this Section. In addition, we analyse the benefits of the reference model approach in combination with three other methods which have been specifically designed for complete variable selection. As the criteria of selection performance, we evaluate the average false discovery rate and the average sensitivity (i.e., the ratio of the number of relevant selected variables over the total number of relevant variables). We also provide a comparison of the stability of the selection by means of a stability measure proposed by Nogueira et al. (2017), which goes from 0 to 1 and a higher value means a more stable selection.

4.1 Iterative projections

We modify the projection predictive approach for complete variable selection by using it iteratively. Applying the straightforward implementation of projpred, we are able to select a minimal subset of variables, which yield to a model with a predictive performance comparable to the full model's predictive performance. The iterative projection repeats the projpred selection for different iterations, at each time excluding the variables selected in the previous iterations from the search. At each iteration the selected submodel size corresponds to
the one having a predictive performance close enough to the baseline model, which in this iterative version is the submodel with the highest predictive score explored at the current iteration. This translates in the following stopping rule at each iteration:

$$\min\{i \in \{0, \ldots, p\} : P(\text{elpd}_i - \text{elpd}_{\text{best}} > 0) \geq \alpha\}$$

where $i$ indexes the submodel size and “best” stands for the best predictive explored submodel at the considered iteration. The algorithm terminates when the empty model (only intercept) satisfies the stopping rule (see Algorithm 1). The choice of the hyperparameter $\alpha$ is non-trivial, and we have observed sensitivity of the selection to such a choice, mainly when using cross-validation with a small number of observations or not very predictive variables. In our experiments we chose the default value used in the projpred R-package, that is, $\alpha = 0.16$.

**Result:** $R := \{\text{selected variables}\}$

$F := \{\text{set of variables}\}$

Fit reference model:

while $F \neq \{\emptyset\}$ do

projection.HeuristicSearch();

projection.elpdEstimate();

$S = \min\{\text{sub} : P(\text{elpd}_{\text{sub}} - \text{elpd}_{\text{base}} > 0) \geq \alpha\}$;

if $S = \{\emptyset\}$ then

break;

else

$R = R \cup S$;

$F = F \setminus S$;

end

end

Algorithm 1: Automated iterative projections

In the experiments shown in the next sections, we include an additional iterative method which we refer to as ‘iterative lasso’. It consists of the same iterative algorithm as iterative projpred expect for not using any reference model, but the lasso method for variable selection, instead. That is, it uses the observed target values instead of predictions of the reference model. The comparison with iterative lasso can help to disentangle the effects of the iterative procedure and the usage of a reference model in complete feature selection.

### 4.2 Alternative complete variable selection methods

We consider three alternative complete selection methods: the control of the local false discovery rate (Efron, 2008, 2012), the empirical Bayes median (Johnstone and Silverman, 2004), and the selection by posterior credible intervals.

The control of the local false discovery rate consists of testing the $z$-values $\{z_j\}_{j=1}^p$ of a normal mean problem (explained in Section 4.3) on whether they belong to the theoretical null distribution $f_0$ (i.e., the null hypothesis $H_0$ meaning no relevance) against the alternative hypothesis distribution $f_1$. In our case $f_0$ corresponds to the standard normal distribution (see expression (6)). The quantity of interest is the local false discovery rate ($\text{loc.fdr}$) defined as:

$$\text{loc.fdr}(z) = P(H_0 | z) = \frac{f_0(z)\pi_0}{f(z)},$$

where $\pi_0$ is the prior probability of $H_0$ and $f(z) = \pi_0 f_0(z) + (1 - \pi_0)f_1(z)$ is the marginal distribution of the $z$-values. The latter is estimated using splines with 7 degrees of freedom. We select variables with local false discovery rate below 0.2, which is suggested by Efron (2012) as it corresponds to a Bayes factor larger than 36 (assuming $\pi_0 \geq 0.9$). The results of the comparison are not sensitive to the specific value. To estimate $\pi_0$ from the data, we use the default setting provided by the R-package locfdr (Efron et al., 2015).
The empirical Bayes median approach consists of fitting a Bayesian model with a prior composed by a mixture of a delta spike in zero and a heavy-tailed distribution. We use the implementation in the R-package EbayesThresh (Silverman et al., 2017). As suggested by Johnstone and Silverman (2004), we use a Laplace distribution resulting in a thresholding property, that is, there exists a threshold value such that all the data under that threshold have posterior median equal to zero. Therefore the selection is done by selecting only those parameters whose posterior median is different from zero. The hyperparameter of the Laplace distribution and the mixing weight of the prior are estimated by marginal maximum likelihood.

The selection by 90% posterior credible intervals is done using the regularised horseshoe prior (Piironen and Vehtari, 2017b) and selecting those variables whose posterior distribution does not include zero in the interval between the 5% and the 95% quantiles.

All of these methods provide a complete selection approach and we compare their performance with and without using a reference model. That is, in the data condition, we apply the method on the original data while, in the reference model condition, we replace it by their mean predictions \( \hat{y} \) based on the reference model.

4.3 Simulation study 2

The iterative projection applies straightforwardly to data, whereas to investigate the performance of the three alternative complete selection approaches, we are going to use simulations based on the normal means problem. The normal means problem consists of estimating the (usually sparse) vector of means of a vector of normally distributed observations. The dimensionality of the vector of means is denoted by \( p \) and \( \{z_j\}_{j=1}^p \) is the vector of observations of the random variables \( \{Z_j\}_{j=1}^p \). The task is to estimate the latent variables \( \{\theta_j\}_{j=1}^p \) of the following model:

\[
Z_j|\theta_j, \sigma^2 \sim N(\theta_j, \sigma^2), \quad j = 1, \ldots, p. \tag{4}
\]

This is equivalent to a linear regression where the design matrix is the identity matrix with the number of observations.

In our experiments, we retrieve the normal means problem from the sample correlations between the target variables using the Fisher \( z \)-transformation function \( \tanh^{-1}(\cdot) \) as \( T_F(\cdot) \). Assuming each pair \((Y, X_j)\) to be bivariate normally distributed, the corresponding transformed correlations are approximately normally distributed with known variance:

\[
T_F(r_j) \overset{ind}{\sim} N \left( T_F(\rho_j), \frac{1}{n-3} \right), \quad j = 1, \ldots, p. \tag{5}
\]

Therefore, rescaling the quantities \( T_F(r_j) \) by \( \sqrt{n-3} \) and denoting the results as \( z_j \), we have the formulation (4) of the normal means problem, this time with unit variance:

\[
Z_j|\theta_j \overset{ind}{\sim} N(\theta_j, 1), \quad j = 1, \ldots, p. \tag{6}
\]

In this case, the quantities of interest \( \theta_j \) are equal to \( \sqrt{n-3} T_F(\rho_j) \).

In our simulations, we use different levels of correlation \( \rho \in \{0, 0.3, 0.5\} \) and numbers of observations \( n \in \{50, 70, 100\} \). The total number of variables \( p \) and the number of relevant variables \( k \) are fixed to \( p = 1000 \) and \( k = 100 \), respectively. In general, the lower \( \rho \) and \( n \), the more challenging the variable selection is. For this example, Piironen et al. (2020) proposed to use a reference model which a Bayesian linear regression
using the first five supervised principal components (SPC) as variables and imposing an hierarchical prior on their coefficients:

\[
Y_i | \beta, \sigma^2, u_i \sim N(u_i^T \beta, \sigma^2) \quad i = 1, \ldots, n \\
\beta_j \sim N(0, \tau^2) \quad j = 1, \ldots, 5 \\
\tau \sim t_4(0, s_{\text{max}}) \\
\sigma \sim t_4(0, 10) .
\]

In the above, \(u_{ij}\) represents the \(j\)-th SPC evaluated at observation \(i\), and \(s_{\text{max}}\) denotes the sample standard deviation of the largest SPC. The SPCs are computed using the R-package dimreduce (https://github.com/jpiironen/dimreduce) setting the screening threshold parameter at 0.6\(s_{\text{max}}\). In our experiments, the results are not sensitive to the specific choice of the screening threshold, yet a more principled approach would be to use cross-validation to select the threshold as done by Piironen et al. (2020).

Figure 6 shows the average sensitivity on the vertical axis and the average false discovery rate on the horizontal axis based on 100 data simulations for the different combinations of \(n\) and \(\rho\). The best selection performance is on the top-left corner of each plot, as it implies the lowest false discovery rate and the highest sensitivity. We see that regardless of the applied selection method, the use of a reference model improves the selection performance, as it reduces the false discovery rate (shifting to the left) or increases the sensitivity (shifting upwards). In accordance with what can be expected, the larger data set size \((n)\) and the higher the true correlations \((\rho)\), the easier the selection is. Thus, for easier selection scenarios, the benefits of the reference model are smaller since the raw data already provide enough information to identify the relevant variables. The iterative projpred has good false discovery rate in all cases, and the sensitivity is good except when the number of observations and the correlation level are small. It performs better than the iterative lasso selection in any of the simulated scenarios. Tuning \(\alpha\) might lead to improved selection, yet the main source of poor
Figure 8: Body fat example with noisy variables: Complete variable selection sensitivity against false discovery rate based on 100 bootstrap samples with one standard deviation error bars. The improvement from using the reference approach is small (except that the projpred is much better than lasso).

Figure 9: Body fat example with noisy variables: Complete variable selection stability estimates with 0.95 confidence intervals based on 100 bootstrap samples. The improvement from using the reference approach is small (except that the projpred is much better than lasso).

performance could well be the miscalibration of the uncertainty of the predictive utility score for misspecified models with cross-validation (Bengio and Grandvalet, 2004).

Figure 7 shows the estimates of the stability measure proposed by Nogueira et al. (2017) with 0.95 confidence intervals based on 100 simulations. Such a measure takes into account the variability of the subset of the selected variables at each simulation (originally at each bootstrap sample), modelling the selection of each variable as a Bernoulli process. Further details are available in Nogueira et al. (2017). The reference model helps in improving the stability of the selection: again, the benefits are bigger when the problem is more difficult (small \( n \) and \( \rho \)). In addition, we observe less uncertainty in the stability estimates for the reference approach (i.e., smaller width of the 95% intervals), which can be still connected to the overall stability of the procedure. As in Figure 6, the iterative projection does not perform well in the hardest scenarios.

4.4 Body fat example: Part 3

We conclude our complete selection experiments using the body fat dataset one more time. As earlier we add noisy uncorrelated variables to the original data to get a total of 100 variables. Since we do not have a ground truth available with regard the original variables of the data, we assume it is reasonable to consider all of them relevant, at least to some degree. The artificially added variables are naturally irrelevant by construction. We compute correlations between each variable and the target variable, that is the amount of fat, and transform them by Fisher-Z-transformation. The original assumption in order for (5) to hold is that the variables are jointly normally distributed. In our experience the normal approximation in (5) is still reasonable, but after rescaling by \( \sqrt{n - 3} \) we do not fix the variance to be one, and instead estimate it from the data. We compare the iterative projection, the control of the local false discovery rate (loc.fdr), the empirical Bayes median (EB.med) and the selection by posterior credible intervals at level 90% (ci.90). In order to vary the difficulty of the selection, we bootstrap subsamples of different sizes, going from \( n = 50 \) up to \( n = 251 \) (i.e., the full size of the data). For each condition, results are averaged over 100 bootstrap samples of the respective size.

Figure 8 shows the sensitivity against the false discovery rate. In almost all of the bootstrapped subsamples,
the reference model improves the selection both in terms of sensitivity and false discovery rate. When $n = 50$, we observe worse false discovery rates, yet by a lower amount compared to the gain in sensitivity. Again, we observe that the benefits are more evident as the selection becomes more challenging (i.e., lower number of observations). The great performance of projpred in minimal subset selection is not carried over for the complete variable selection with iterative projpred (even changing the reference model with a full encompassing linear regression with regularised horseshoe prior), and the methods specifically designed for the complete variable selection perform better. However we still observe a better selection with respect to iterative lasso in any of the examined scenarios, mainly in terms of false discovery rate. Figure 9 shows the stability results using the measure by Nogueira et al. (2017). The benefits of the reference model are here marginal with only small improvements.

In this example, we have used the reference model defined as a linear regression over some supervised principal components, because it is natural for a large number of correlating variables, and has fairly good predictive performance plus it is computationally efficient. We do not argue that this is always the best choice and more sophisticated models can lead to even better results. Here the purpose of the experiments were to motivate the use of reference models in general, and as we needed to average results over a lot of repetitions per simulation condition, we preferred such a comparably simple and computationally fast reference model.

5 Conclusion

In this paper, we demonstrated the benefits of using a reference model to improve variable selection, or more generally, model reduction. We have motivated and explained the general benefits of a reference model regardless of the method it is applied in combination with. Specifically, we have seen how the reference model acts as an approximation of the data generation mechanism through its predictive distribution. Such approximation is generally less noisy than the sample estimation available purely from the observed data, leading to the main benefits of the reference model approach. In our comparisons, we have analysed the effect of a reference model in the form of a filter on the observed target values on top of different widely used variable selection methods. Overall, using a reference model leads to more accurate and stable selection results independently of the specific selection method. These benefits apply to a large family of different methods all involving a reference model in one way or the other. Some of these approaches have been present in the literature for some time (e.g., see references in Vehtari and Ojanen, 2012; Piironen et al., 2020) but often without a clear explanation of why they are actually favourable and how they connect to other related approaches. We hope that the present paper can fill some of these gaps by providing a unifying framework and understanding of reference models.

We argue that, whenever it is possible to construct a reasonable reference model, it should be employed on top of the preferred selection procedure or as an integral part of more complex methods, for example, the projective prediction approach (Piironen et al., 2020). Note that one of the main challenges in many real world application will consist in devising a sensible reference model itself and assessing its predictive performance. To build good predictive reference models, which are specifically tuned to the data and problem at hand, we recommend them to be developed using a robust Bayesian modelling workflow, for instance, as outlined by Gelman et al. (2013) and Gabry et al. (2019).

Another main result of this paper is that the projective prediction approach shows superior performance in minimal subset variable selection compared to alternative methods whether or not these methods make use of a reference model. That is, while the reference model is certainly one important aspect the projective prediction approach, it is not the only reason for its superior performance. Rather, by incorporating the full uncertainty of the posterior predictive distribution into the variable selection procedure (instead of just using point estimates) and using principled cross-validation method, projective predictions combine several desirable variables into a single procedure (Piironen et al., 2020). In summary, we would strongly recommend using projective predictions for minimal subset variable selection if possible and feasible. However, if this is not an option in a given situation, we would in any case recommend using a reference model on top of the chosen variable selection method.
The projective prediction approach was not designed for the complete variable selection. We tested a simple iterative version of projpred, with mixed results and the methods specifically designed for complete variable selection (especially loc.fdr) performed better in our experiments. It is left for future research to develop a better projective prediction approach for complete variable selection problems.

All Bayesian models in this paper have been implemented in the probabilistic programming language Stan (Carpenter et al., 2017) and fit via dynamic Hamiltonian Monte Carlo (Hoffman and Gelman, 2014; Betancourt, 2017), through the R-packages rstan (Stan Development Team, 2019) and rstanarm (Goodrich et al., 2019). Graphics elaborations have been done using ggplot2 (Wickham, 2016) and the tidyverse framework (Wickham et al., 2019). The code to run all the experiments is available on GitHub (https://github.com/fpavone/ref-approach-paper).

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Appendix

Appendix A: Projective Predictions

The projective prediction (projpred) approach was developed and is thoroughly described by Piironen et al. (2020). In this appendix, we provide a high level description of the method so that readers do not need to study paper by Piironen et al. (2020) in detail to understand the main ideas behind projpred.

The parameter distribution of a given candidate submodel is denoted by $\pi$ and the induced predictive distribution by $q_{\pi}(\tilde{y})$. We would like to choose $\pi$ so that $q_{\pi}(\tilde{y})$ maximises some predictive performance utility, for example, the expected log-predictive density (elpd) defined as:

$$
elpd[q_{\pi}] = \int \log q_{\pi}(\tilde{y}) p_{\pi}(\tilde{y}) d\tilde{y},$$

where $p_{\pi}(\tilde{y})$ denotes the (usually unknown) true generating mechanism of future data $\tilde{y}$. If we refer to the posterior predictive distribution of a reference model with $p(\tilde{y}|D)$, where $D$ stands for the data on which we conditioned on, we can approximate (8) using $p(\tilde{y}|D)$ instead of the true data generation mechanism $p_{\pi}(\tilde{y})$. The maximisation of the elpd using the reference model’s predictive distribution is equivalent to the minimisation of the Kullback-Leibler (KL) divergence from the reference model’s predictive distribution to the submodel’s predictive distribution:

$$
\max_{\pi} \int \log q_{\pi}(\tilde{y}) p_{\pi}(\tilde{y}|D) d\tilde{y} \quad \iff \quad \min_{\pi} \text{KL}[p(\tilde{y}|D) \parallel q_{\pi}(\tilde{y})]
$$

The term on the right-hand side of Equation (9) describes what is referred to as the projection of the predictive distribution, which is the general idea behind the projection predictive approach (see Piironen et al., 2020). We now summarise the workflow of the projection predictive approach in the particular case of the draw-by-draw projection (original formulation by Dupuis and Robert, 2003), following Piironen et al. (2020). Suppose we have observed $n$ statistical units with target values $\{y_i\}_{i=1}^n$ and a set of observed variables for which we want to obtain a minimally relevant subset. Then, the main steps are the following:

1. Devise and fit a reference model. Let $\{\theta_s^*\}_{s=1}^S$ be the set of $S$ draws from the reference model’s posterior.

2. Rank the variables according to their relevance using some heuristics and consider as candidate submodels only those which preserve this order, starting from including only the highest ranked variable. The submodels are then naturally identified by their model size. This step is not strictly necessary but reduces the number of submodels to considered in the following steps and thus reduces computation time.
3. For each submodel \( \pi \) selected in Step 2, project each of the reference model’s posterior draws \( \theta^*_s \) as follows:

\[
\theta^*_\perp = \arg\min_{\theta^s \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \text{KL} [p(\tilde{y}_i | \theta^s) \| q_{\pi}(\tilde{y}_i | \theta^s)],
\]

where \( p(\tilde{y}_i | \theta^s) \) stands for the predictive distribution of the reference model with parameters fixed at \( \theta^s \) and conditioning on all the variable values related to the statistical unit (identified by the subscript \( i \)), whereas \( q_{\pi}(\tilde{y}_i | \theta^s) \) is the predictive distribution of the submodel. The projected draws \( \theta^*_\perp \) then present the projected posterior for the submodel.

4. For each submodel (size), test the predictive performance for a chosen predictive utility score, for example, via cross-validation. Fast cross-validation can be performed using approximate leave-one-out cross-validation via Pareto-smoothed importance-sampling (PSIS-LOO-CV; Vehtari et al., 2017).

5. Choose the smallest submodel (size) that is sufficiently close to the reference model’s predictive utility score. The results in this paper were not sensitive to the specific choice of how “sufficiently close” is defined, and we used the same definition as Piironen et al. (2020).

In general, Expression (10) is not an easy optimisation problem. However, in the special case of the submodels being generalised linear models with a likelihood coming from the exponential family, (10) reduces to a maximum likelihood estimation problem, which can be easily solved (Dupuis and Robert, 2003). For further details on the projective prediction workflow and implementation see the paper by Piironen et al. (2020).