Variable Selection Methods Comparison

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Background

- Variable selection methods help to optimize models in high-dimensional settings where we need to select predictors that balance fitness and complexity.
- The presence of weak predictors is a problem that plagues traditional variable selection methods.

Statistical Methods to be Studied

Step-wise forward method

- Starts with the empty model, and iteratively adds the variables that best improve the model fit. That is often done by sequentially adding predictors with the largest reduction in AIC. For linear models,

$$AIC = n \log \left(\sum_{i=1}^{n} (y_i - \widehat{y}_i)^2 / n \right) + 2p.$$

Automated LASSO regression

- Estimates model parameters by optimizing a penalized loss function:

$$\min_{\beta} \frac{1}{2n} \sum_{i=1}^{n} (y_i - \boldsymbol{x}_i \boldsymbol{\beta})^2 + \lambda \sum_{k=1}^{p} |\beta_k|.$$

Objectives

(1) Evaluate the effectiveness of both methods in identifying weak and strong predictors.

(2) Examine how the absence of “weak” predictors affects parameter estimations.

Types of Signals

- Strong signals

$$S_{strong} = \{j : |\beta_j| > c\sqrt{\log(p)/n} \text{ for some } c > 0,\ 1 \leq j \leq p\}$$

- Weak-but-correlated (WBC) signals

$$S_{WBC} = \{j : 0 < |\beta_j| \leq c\sqrt{\log(p)/n} \text{ and } \mathrm{corr}(X_j, X_j') \neq 0 \\ \text{for some } j' \in S_1,\ 1 \leq j \leq p\}$$

- Weak-and-independent (WAI) signals

$$S_{WAI} = \{j : 0 < |\beta_j| \leq c\sqrt{\log(p)/n} \text{ and } \mathrm{corr}(X_j, X_j') = 0 \\ \text{for all } j' \in S_1,\ 1 \leq j \leq p\}$$

- Null signals: $S_{null} = \{j : \beta_j = 0,\ 1 \leq j \leq p\}$

Types of Signals

Thus, p predictors can be partitioned as

$$\{1, \cdots, p\} = S_{strong} \cup S_{WBC} \cup S_{WAI} \cup S_{null}.$$

- We assume that $|S_{strong}| = p_S$, $|S_{WBC}| = p_{WBC}$, $|S_{WAI}| = p_{WAI}$.
- The number of true predictors $p_S + p_{WBC} + p_{WAI}$ should be less than n.

Data Generation

- Normality assumption

$$\mathbf{y} \sim N(\mathbf{X}\beta, \sigma^2\mathbf{I})$$

- For $j \in S_{strong}$, $\beta_j = 20$; For $j \in S_{WBC} \cup S_{WAI}$, $\beta_j = 0.5$.
- We choose $c = 20$ so that $0.5 \leq c\sqrt{\log p/n} < 20$ for all scenarios to be investigated.
- For the error term, we set $\sigma = 8$.

Data Generation - Design Matrix

- We assume

$$\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- All predictors are standardized. Then we have $\boldsymbol{\mu} = \mathbf{0}$ and $\Sigma_{i,i} = 1$ for all i.
- We set $p_{WBC} \geq p_{strong}$. For each strong predictor (except one of them), we set $[p_{WBC}/p_{strong}]$ WBC predictors to be correlated with it. Each WBC predictor is set to be correlated with one and only one strong predictor.
- All other elements of $\boldsymbol{\Sigma}$ are 0.

We use the `MASS::mvrnorm` function to generate data following a multivariate normal distribution.

Data Generation - Simulation Code

```
corr_matrix = matrix(rep(0, len = p^2), nrow = p)
corr_num = pwbc %/% ps
for (i in 1:(ps - 1)) {
  for (j in (ps + 1 + (i - 1)*corr_num):(ps + i*corr_num))
    corr_matrix[i, j] = corr
    corr_matrix[j, i] = corr
  }
}
for (j in (ps + 1 + (ps - 1)*corr_num):(ps + pwbc)) {
    corr_matrix[ps, j] = corr
    corr_matrix[j, ps] = corr
}
diag(corr_matrix) = 1
X = MASS::mvrnorm(n, mu = rep(0, p), Sigma = corr_matrix)
beta = c(rep(20, ps), rep(0.5, pwbc + pwai),
         rep(0, p - ps - pwbc - pwai))
Y = X %*% beta + rnorm(n, mean = 0, sd = 8)
```

Investigation Settings and Scenarios

Fixed

- Number of parameters: $p = 100$
- Ratio of true and null signals: $2 : 3$
- Correlation between strong and WBC: $corr = 0.4$

Unfixed

- Number of observations:
  $n = 100$ (high dimensional)$, 500, 2000$
- Ratio of strong, WBC, and WAI signals:
  $p_{strong} : p_{WBC} : p_{WAI} = 1 : 4 : 5$ and $3 : 3 : 4$

Evaluation Metrics

Define true predictors as positive and null predictors as negative

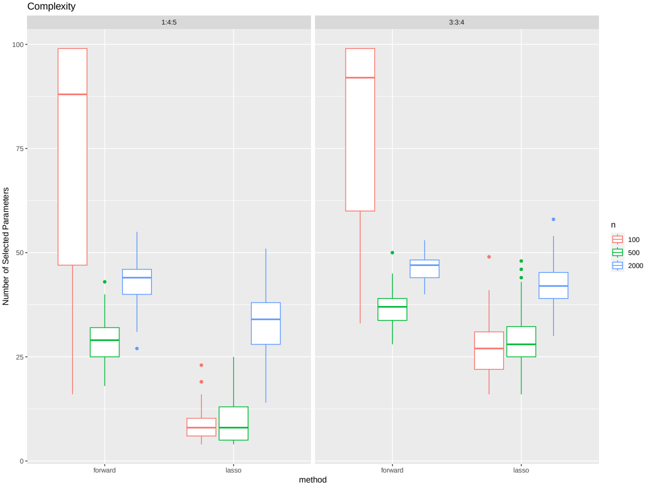
Signal Identification

- **Complexity:** Number of Selected Parameters
- **Sensitivity:** $\frac{TP}{TP+FN}$
- **Specificity:** $\frac{TN}{TN+FP}$
- **F1-score:** $\frac{2 \cdot \text{sensitivity} \cdot \text{precision}}{\text{sensitivity}+\text{precision}}$
- **Accuracy:** $\frac{TP+TN}{TP+TN+FP+FN}$

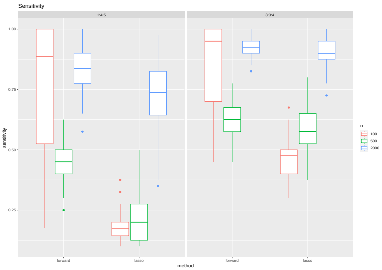
Parameter Estimation

- **RMSE:** $\sqrt{\frac{1}{p}\sum_{i=1}^{p}(\hat{\beta}_i - \beta_i)^2}$
- **Variance:** $\sqrt{\frac{1}{p}\sum_{i=1}^{p}(\hat{\beta}_i - \bar{\beta}_i)^2}$

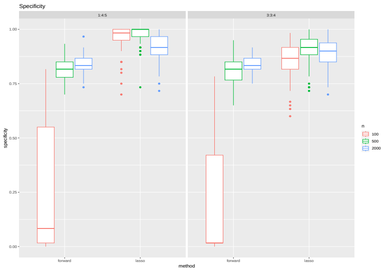
Signal Identification Performance - I



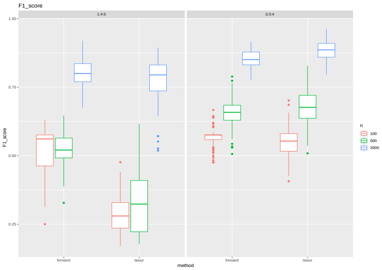
Signal Identification Performance - II



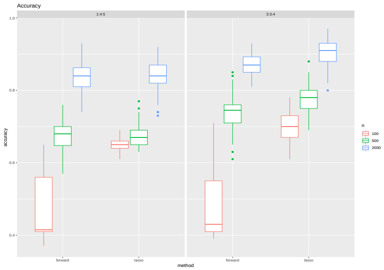
(a) Sensitivity



(b) Specificity

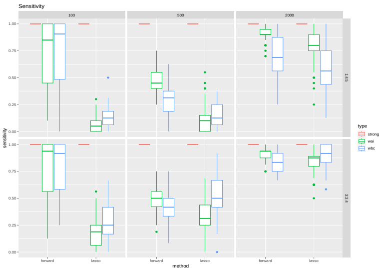


(c) F1-Score

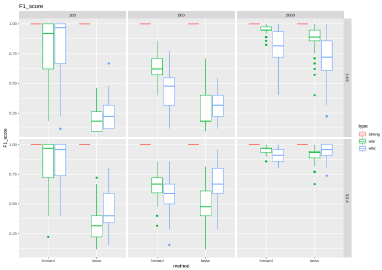


(d) Accuracy

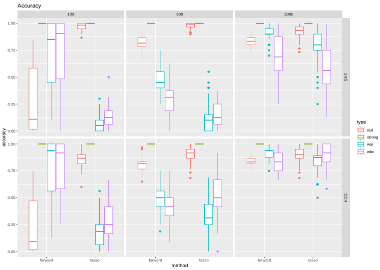
Signal Identification Performance - II



(e) Sensitivity by Signal

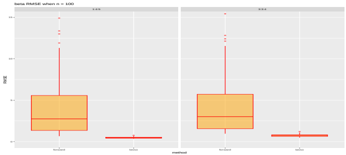


(f) F1-Score by Signal

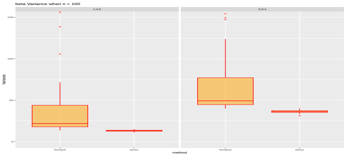


(g) Accuracy by Signal

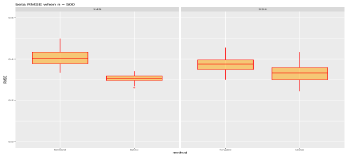
Signal Identification Performance - III



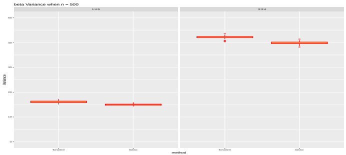
(a) RMSE n=100



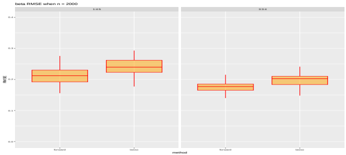
(b) Variance n=100



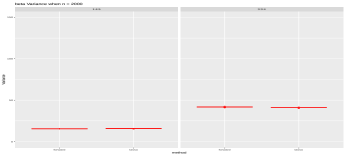
(c) RMSE n=500



(d) Variance n=500



(e) RMSE n=2000



(f) Variance n=2000

Predictors Identification Conclusions

High Dimensional Scenario(n=100)

- Forward selection tends to select lots of predictors and Lasso tends to select few
- Forward selection tends to be assertive and better at identifying weak signals, with extremely high sensitivity, low specificity
- Lasso tend to be conservative and better at identifying null signals, with extremely high specificity, low sensitivity
- Both identify strong predictors perfectly

Predictors Identification Conclusions

High Dimensional Scenario(n=100)

- Forward selection performs better than Lasso on F1-score but worse on overall accuracy
- Both models seem to be too radical in predictor identification
- Lasso performs better on parameter estimation than forward selection

Predictors Identification Conclusions

Normal Scenario(n=500, 2000)

- Forward selection tends to select more predictors than Lasso, but both get closer to actual number as n increases
- Lasso is better at identifying null predictors than forward selection, but poorer at identifying other weak predictors (under-screening). Both models nicely identify strong predictors.
- Identification differences of all metrics are narrowed down with n increasing

Predictors Identification Conclusions

Normal Scenario(n=500, 2000)

- When there are more strong predictors, weak-but-correlated predictors become easier to be identified, especially for Lasso. However, parameter estimation also becomes more unstable
- Lasso performs better on parameter estimation than forward when n is not large, and conversely as n increases

Missing Weak Predictors Analysis

- How missing "weak" predictors impacts the parameter estimations
- Definition: missing weak predictors = true weak predictors but estimated as null

Missing Weak Predictors Analysis

- How to evaluate parameter estimations: RMSE
- Most missing: simulations that have the least non-null estimations
- Least missing: simulations that have the most non-null estimations
- Middle: in between

Missing Weak Predictors Analysis - Result: n=100

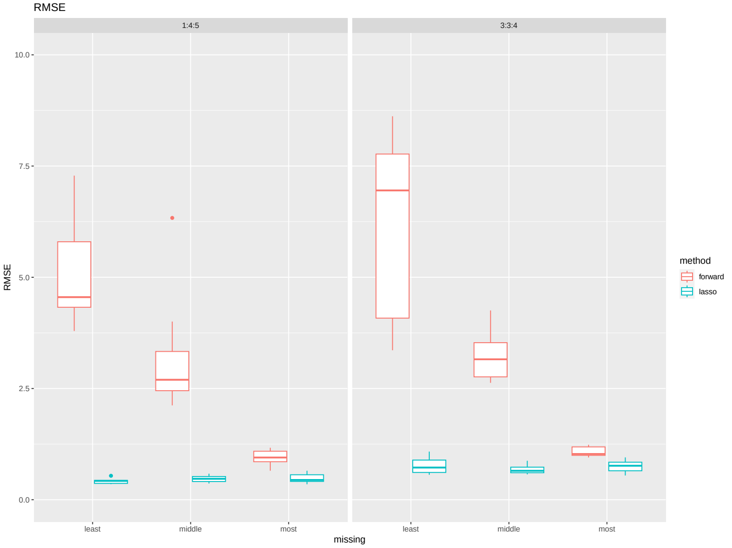


Figure 2: RMSE when n=100

Missing Weak Predictors Analysis - Result: n=500

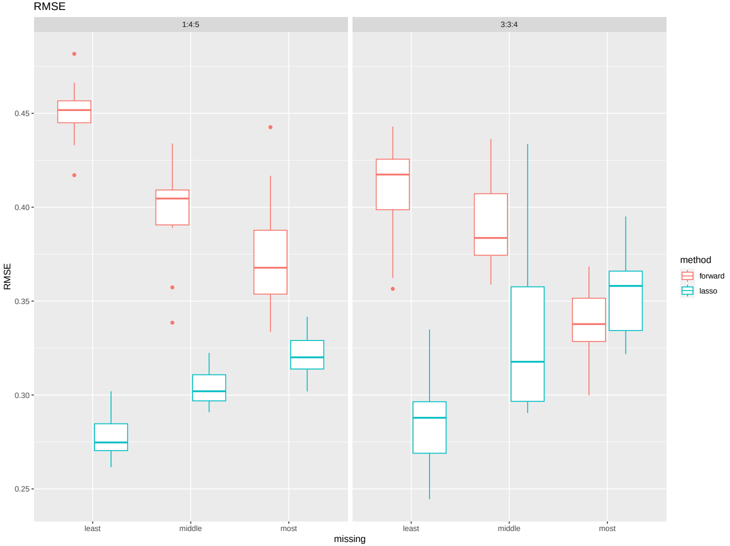


Figure 3: RMSE when n=500

Missing Weak Predictors Analysis - Result: n=2000

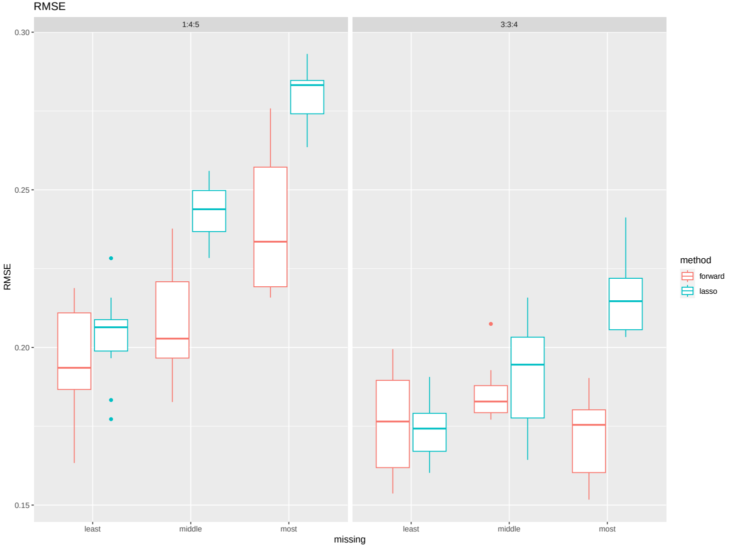


Figure 4: RMSE when n=2000

Missing Weak Predictors Analysis

- No apparent patterns between different ratios
- In high-dimensional scenarios, Lasso performs much better than forward selection according to RMSE, no matter how much missing.
- When n is large enough, RMSE of both methods become small.
- When $n = 500$, Lasso is slightly better than forward selection, however, when $n = 2000$, just the reverse.
- In Lasso, RMSE seems to increase if the missing amount increases, but in forward selection, RMSE decreases when missing amount increases.

Discussions

- There is much freedom when designing the simulations.
- In our algorithm, we have 5 parameters. n, p, ratio, c, corr
- More parameters can be adjusted.

Limitations and Future Work

- Limitation: We reproduced high-dimensional scenarios, but we still don't know the solution.
- Future Work: We may adjust other parameters to investigate further.

Reference

1. Li Y, Hong HG, Ahmed SE, Li Y. Weak signals in high-dimensional regression: Detection, estimation and prediction. Appl Stochastic Models Bus Ind. 2018;1–16. https://doi.org/10.1002/asmb.2340

Q&A

- Thanks for listening!
- Any questions?