

SUPPLEMENTARY MATERIAL

High Dimensional Imputation for the Social Sciences: A Comparison of State-of-the-Art Methods

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ARTICLE HISTORY

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1. Software and other computational details

The code to run the simulation was written in the R statistical programming language (version 4.0.3). All experiments were run using a 2.6 GHz Intel Xeon(R) Gold 6126 processor, 523.78 GB of Memory. The operating system was Windows Server 2012 R2. Computations were run in parallel across 30 cores. Parallel computing was implemented using the R package *parallel* and to ensure replicability of the findings seeds were set using the method by ? implemented in the R package *rlecuyer*. Code to run the studies can be found at <https://github.com/EdoardoCostantini/imputeHD-comp>. In the following, each step of the simulation procedure is described in details for both experiments.

2. Convergence check details

Convergence of the imputation models was assessed in a preprocessing step. Before running the actual simulation studies, 10 datasets were generated according to each experimental set up. Missing values in each dataset were imputed by running 5 parallel imputation chains for each Multiple Imputation method. Convergence was checked by plotting the mean of the imputed values for each variable in each stream, against the iteration number. In each parallel run, all the MI algorithms run for 250 iterations. The imputation algorithms were considered to have converged after 50 iterations, after which 10 imputed data sets were store and used for the subsequent standard complete-data analysis and pooling. The only exception was blasso, which required approximately 2000 iterations for convergence.

3. Ridge penalty cross-validation details

The ridge penalty used in the bridge algorithm was fixed across iterations . The value used in the simulation was determined by means of cross-validation in a pre-processing phase. The grid of possible values for the ridge penalty was $10^{-1}, 10^{-2}, \dots, 10^{-8}$. For

each of 100 data repetitions, bridge imputation was performed with each of the different penalty parameters and used to obtain 10 differently imputed datasets. For each data replication, the Fraction of Missing Information (FMI) (?) associated with each parameter in the analysis models of interest (see next section for details) was computed and then averaged across repetitions. The mean of these average parameter FMIs was used as a composite measure of FMI associated with each ridge penalty value. Finally, the penalty value with the smallest composite FMI was selected.

4. Additional Figures

4.0.1. Experiment 1

Figures 1 and 2 report the Percentage Relative Bias and Confidence Interval Coverage, respectively, for each parameter estimate in the saturated model described above. In the figures, single horizontal lines, representing the PRB (or CIC) of a parameter estimate for a single variable, combine to form larger horizontal bars giving an aggregate account of how each method performed across multiple variables with missing values.

4.0.1.1. Means. Focusing first on the item means (top rows), all methods achieved a bias that is smaller than the 10% threshold for all item means, in all conditions. The largest PRB is within 10 percentage points from 0 for all methods. Looking at relative performances, in all conditions, MI-OP provided negligible bias, and IURR and MI-PCA resulted in the smallest estimation bias among the other methods.

In the conditions with low proportion of missing values (condition 1 and 2), only the tree-based MI methods, missForest, and CC showed CIC significantly different from nominal coverage rates. In the conditions with high proportion of missing values (condition 3 and 4), all methods showed some signs of either under-coverage or over-coverage of the true values, with CICs outside of the interval (.94, .96). The only exceptions to the trend were MI-OP, MI-PCA, and Bridge which showed non-significant deviations from nominal coverage for almost all estimates.

4.0.1.2. Variances. Moving to the item variances (central rows), IURR, blasso, and the tree-based methods resulted in the lowest biases across all conditions, even in the high-dim-high-pm condition (condition 4). These low biases were mostly paired with low deviations from nominal coverage, except for the high-dim-high-pm condition (condition 4) where IURR and the tree-based methods resulted in extreme under-coverage of the true item variances ($CIC < .9$). Apart from MI-OP, Blasso was the method with best coverage in this final condition.

Directly using regularized regression within the imputation models (DURR) showed poor performance with regard to the item variances: in all conditions but the first, it led to large (negative) bias, with a PRB as large as 10% in the last condition, accompanied by clear signs of CI under-coverage. Bridge was the only MI method showing larger bias than DURR, in all the high-dimensional conditions (2 and 4): imputing the data with Bridge led to all item variance estimates showing a bias larger than 20% the size of the true value.

MI-PCA also showed poor performance with a noticeable positive bias in all conditions that became extreme in high-dim-high-pm condition (condition 4), where the PRBs exceeded 20%. This poor performance was reflected in extreme confidence in-

terval under-coverage of the true item variances in the final experimental condition.

Single data imputation with missForest and complete case analysis led to substantial negative bias and CI under-coverage for all item variances, even in condition 1.

4.0.1.3. Covariances. Finally, the third row in Figure 1 shows the estimation bias for the 15 covariances between the 6 items with missing values. As covariances depend on two variables, recovering the correct estimates after imputation is more difficult than with means and variances. This explains the generally worse performance reported in the figure.

Indirect Use of Regularized Regression (IURR) performed noticeably better than most other methods, with negligible negative bias and acceptable coverage for all covariances in conditions 1, 2 and 3, but it struggled with a large negative bias and extreme under-coverage for the majority of the 15 covariances in the high-dim-high-pm condition (condition 4).

MI-PCA showed negligible negative bias of the covariance estimates in all conditions, performing as well as MI-OP in all but the last condition, where it still maintained acceptably low values of PRB ($|PRB| < 10\%$). Furthermore, MI-PCA showed virtually no deviation from nominal coverage, with a CIC pattern similar to that of MI-OP, in all but the last condition, where it manifested only mild *over*-coverage of the items covariances.

All other methods, including DURR, showed absolute PRBs larger than the 10% threshold in all but the first condition, with mild to extreme signs of under-coverage. Bridge displayed acceptably low biases and coverage in the low dimensional conditions, and extremely large biases and low CI coverage in all the high dimensional conditions. Single data approaches, like missForest and CC, showed extreme bias and under-coverage of covariances between items with missing values, even in condition 1.

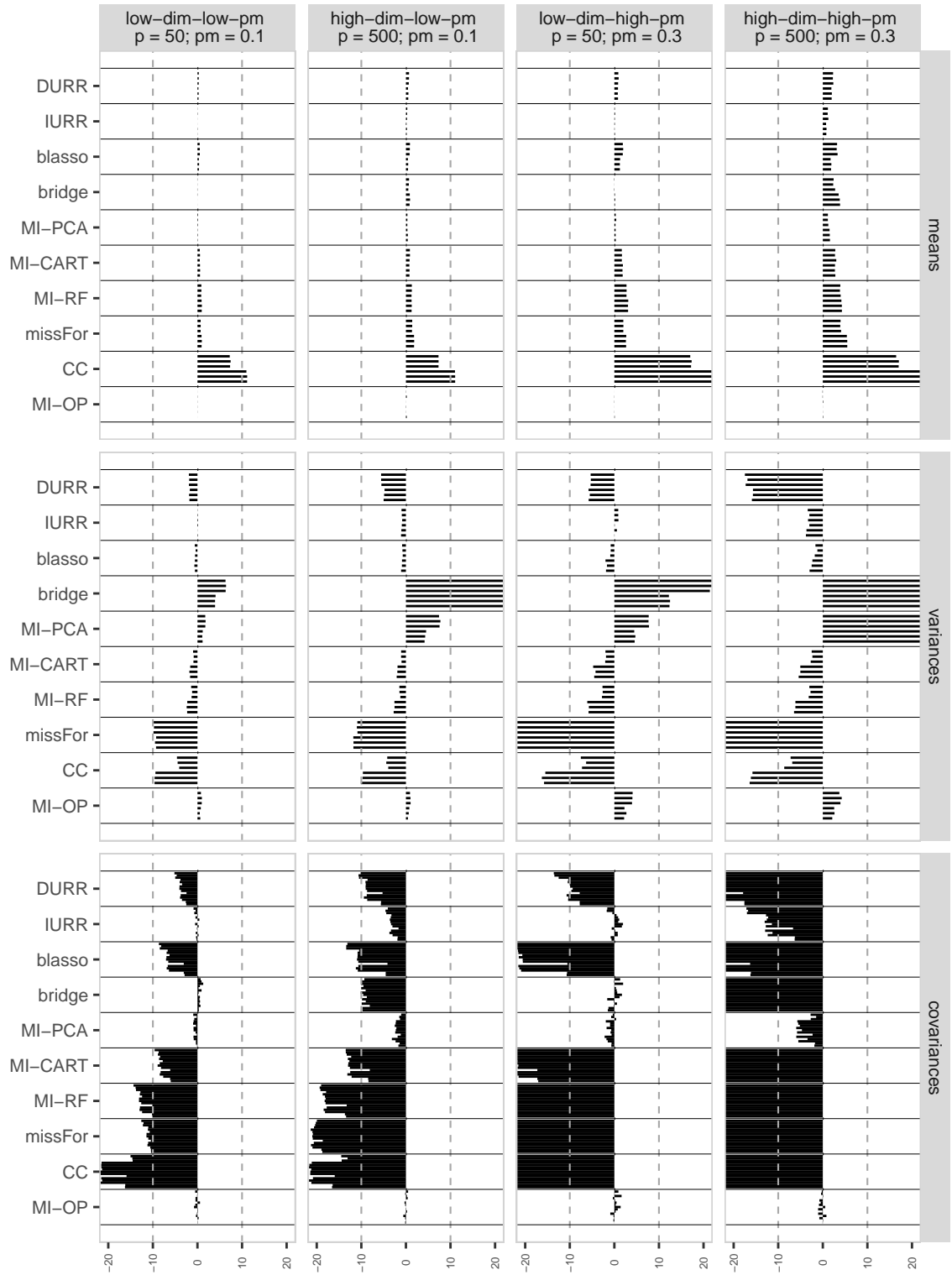


Figure 1. Percent Relative Bias (PRB) for item means, variances, and covariances. For every method, single horizontal lines, representing the PRB of a parameter estimate on a single variable (or pair of variables), combine to form larger horizontal bars giving an aggregate account of how each method performed across multiple variables with missing values.

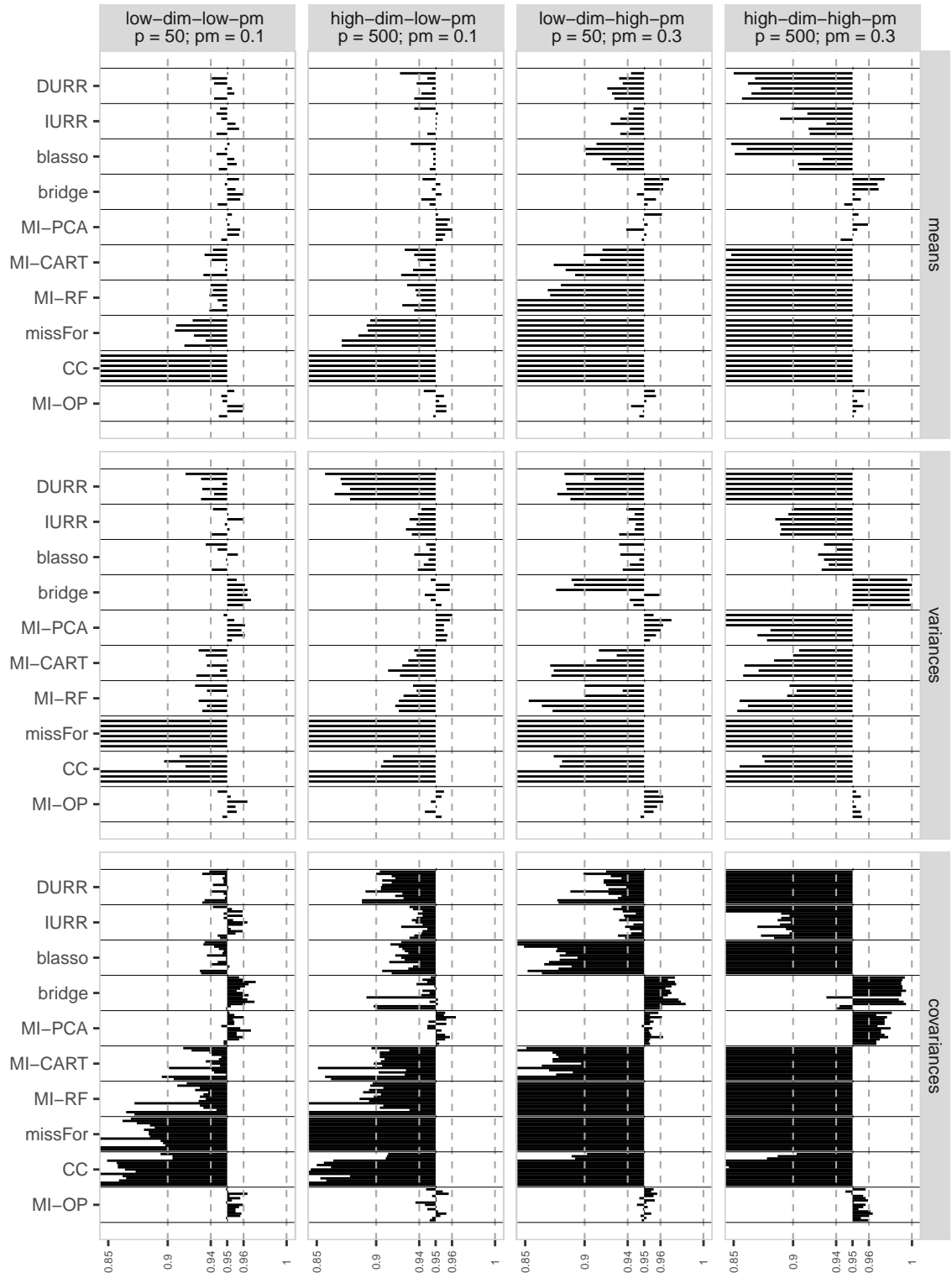


Figure 2. Confidence Interval Coverage (CIC) for item means, variances, and covariances. For every method, single horizontal lines, representing the CIC of a parameter estimate on a single variable (or pair of variables), combine to form larger horizontal bars giving an aggregate account of how each method performed across multiple variables with missing values.

4.0.2. Experiment 2

Figures ?? and ?? report the PRB and CIC of the estimated means, variances, and covariances of the 10 items with missing values in the first four conditions of Experiment 2, the ones characterized by high factor loadings (strong latent structure). Figures 5 and 6 in appendix reports the same values for the low factor loading conditions.

4.0.2.1. Means. All methods provided unbiased estimates of the item means with PRBs that were almost 0 for all items. As the proportion of missing cases increased (conditions 3 and 4) there was a slight increase in PRB values for all methods except IURR, bridge, and MI-PCA. However, only Complete Case analysis led to unacceptable bias in these scenarios. DURR, IURR and MI-PCA also showed little to no deviations from nominal coverage in all conditions, while blasso, MI-CART, MI-RF, and bridge led to significant under-coverage when the proportion of missing cases was high (conditions 3 and 4). missForest also led to extreme under-coverage of the true values.

4.0.2.2. Variances. All MI methods, except Bridge, resulted in acceptable bias levels for item variances estimates in all conditions, but the least biased estimates were obtained by MI-OP, IURR and MI-PCA. CIC decreased as the proportion of missing cases increased (from condition 1 and 2 to conditions 3 and 4). For high pm , only IURR and MI-PCA maintained CICs mostly within the range .94-.96, while blasso and the MI tree-based methods led to mild to extreme under-coverage (CIC \downarrow 90%).

The large positive bias (and low CIC) for the item variances that afflicted MI-PCA in the multivariate-normal set up (figures 1 and 2) is not present in figures ?? and ?. However, that pattern reappeared when the latent structure was weak, as can be seen in Figure 5 and 6 in the Appendix (conditions 5 to 8, factor loadings between .5 and .8). Single data approaches, missForest and CC, showed again extreme (negative) bias and CI under-coverage in almost all conditions.

4.0.2.3. Covariances. For all the conditions with high factor loadings in experiment 2, IURR and DURR showed acceptable covariance biases ($|\text{PRB}| < 10\%$). However, they led to large negative bias in all the conditions with low factor loadings (see 5 and 6 in the Appendix) The other methods followed the same pattern as in experiment 1: the MI-PCA approach resulted in the lowest bias and deviation from nominal coverage for the covariances of the observed items; all other methods led to large negative biases and mild-to-extreme under-coverage for all the covariances, in all conditions.

4.0.2.4. Factor Loadings. Figure 8 shows the PRB values for all the factor loadings estimated by the Confirmatory Factor Analysis described above. Most MI-Methods provided acceptably low bias for these estimates in all conditions except the one with both large proportion of missing values and high dimensional input data matrix (condition 4 and 8).

MI-OP, IURR, and MI-PCA outperformed all other methods and produced virtually unbiased estimates of the factor loadings in all conditions. In particular, MI-PCA outperformed IURR when factor loadings were low (panel b, conditions 5 to 8), maintaining inconsequential biases even when data were high-dimensional and the proportion of missing values was high.

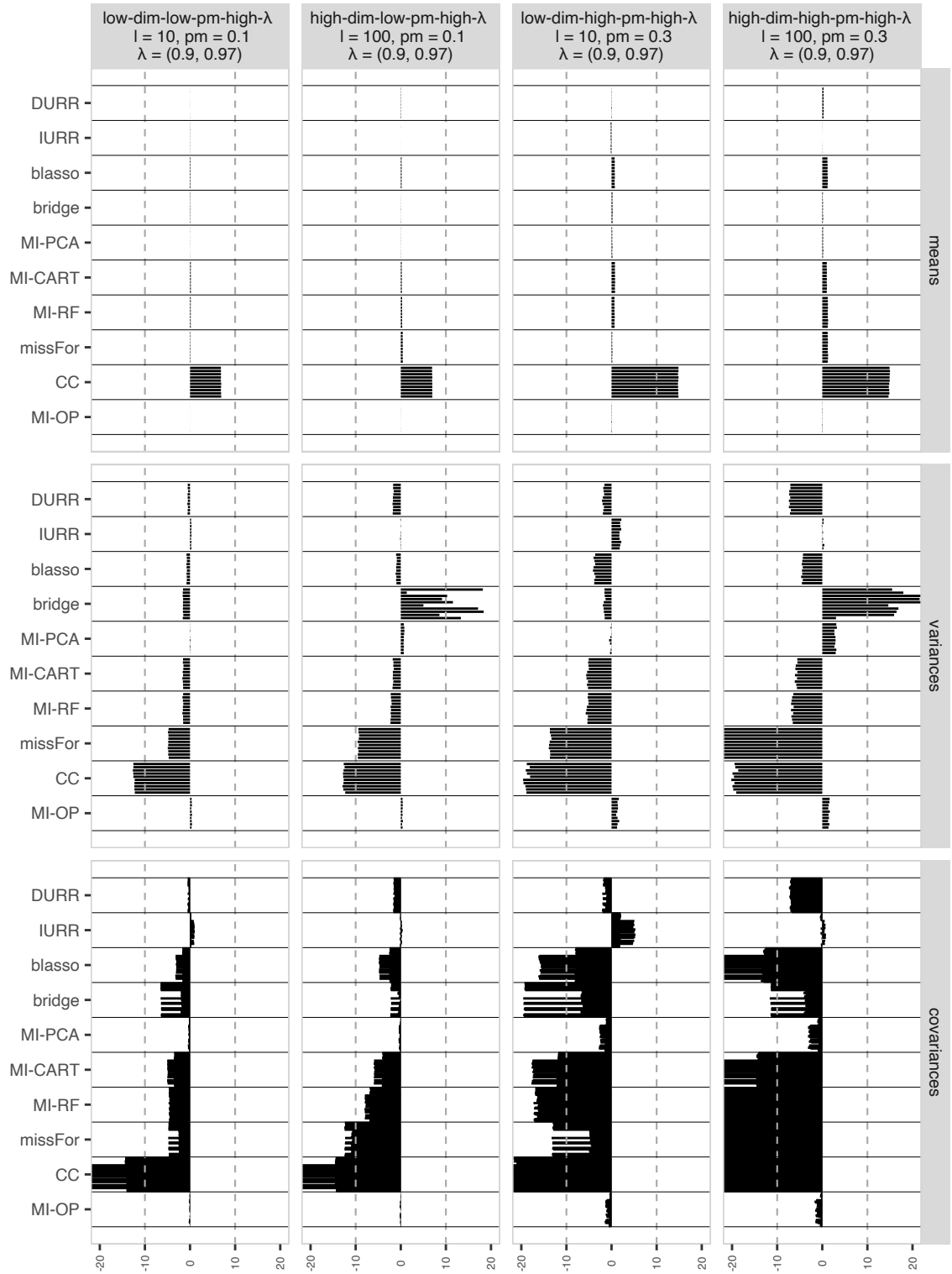


Figure 3. PRBs for the means, variances and covariances (PRB) for condition 1 to 4. For every method, single horizontal lines, representing the PRB of a parameter estimate on a single variable (or pair of variables), combine to form larger horizontal bars giving an aggregate account of how each method performed across multiple variables with missing values.

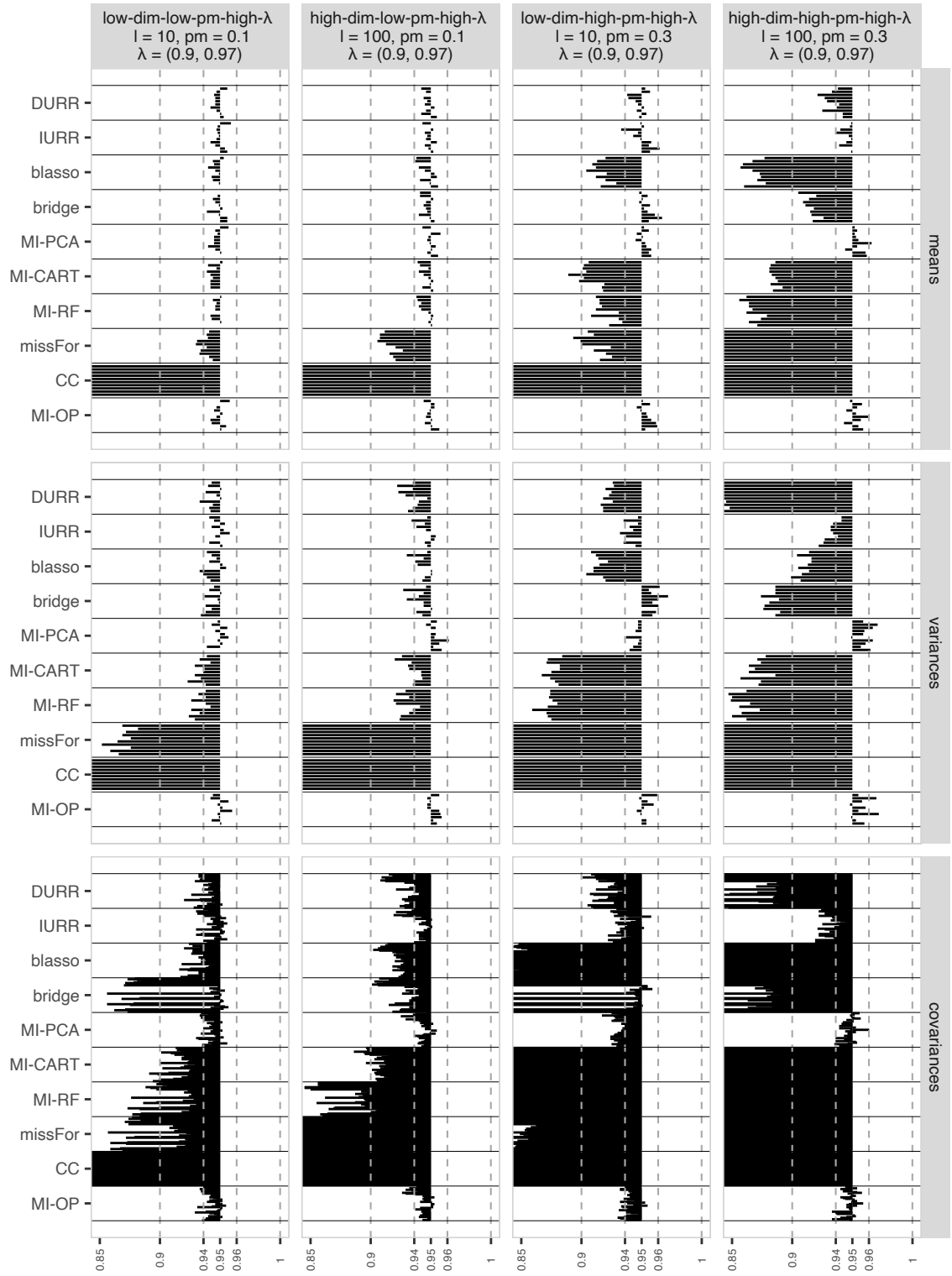


Figure 4. CIC for the means, variances, and covariances for condition 1 to 4. For every method, single horizontal lines, representing the CIC of a parameter estimate on a single variable (or pair of variables), combine to form larger horizontal bars giving an aggregate account of how each method performed across multiple variables with missing values.

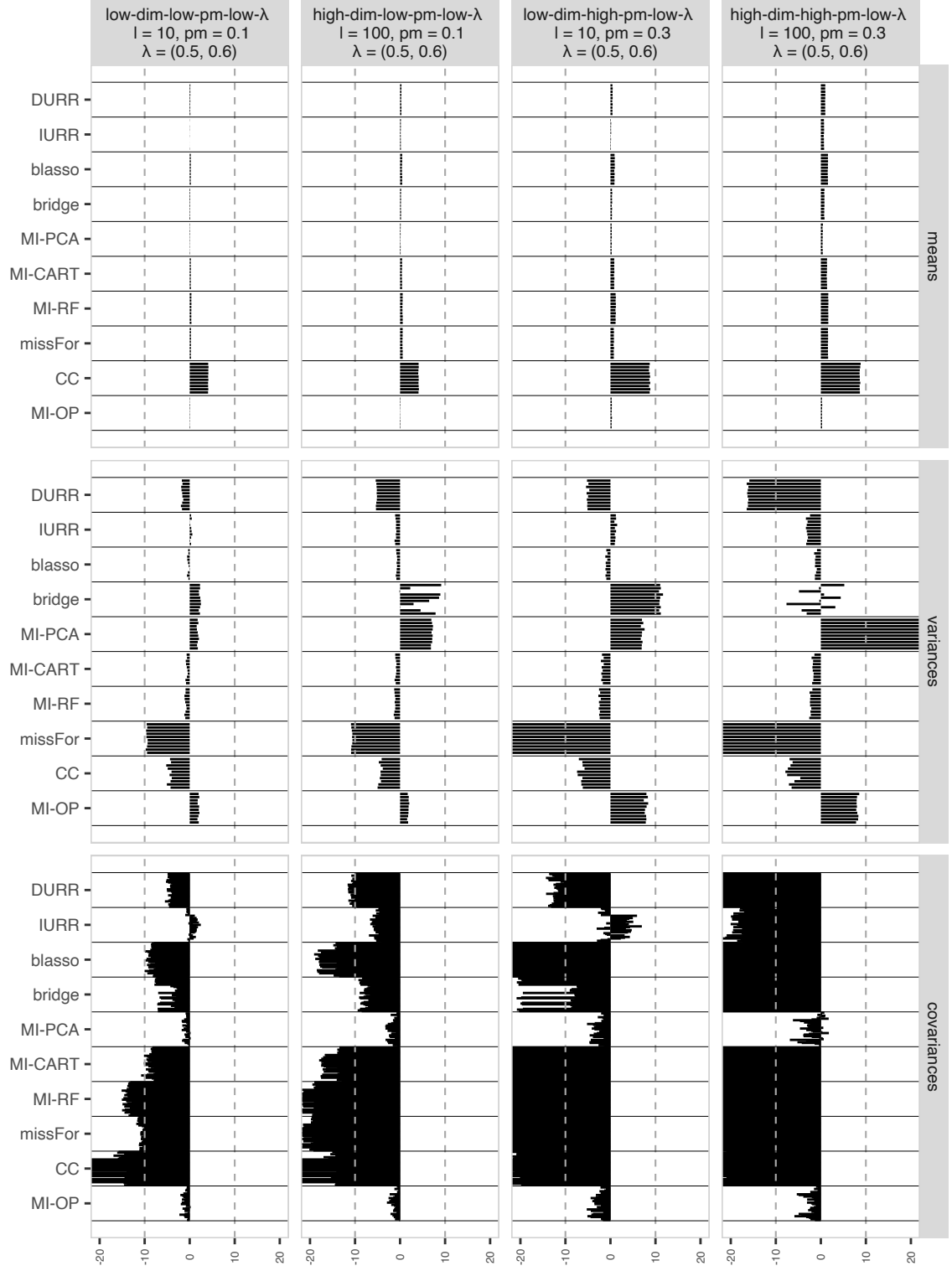


Figure 5. Bias estimation for the means (SB), variances and covariances (PRB) for condition 5 to 8.

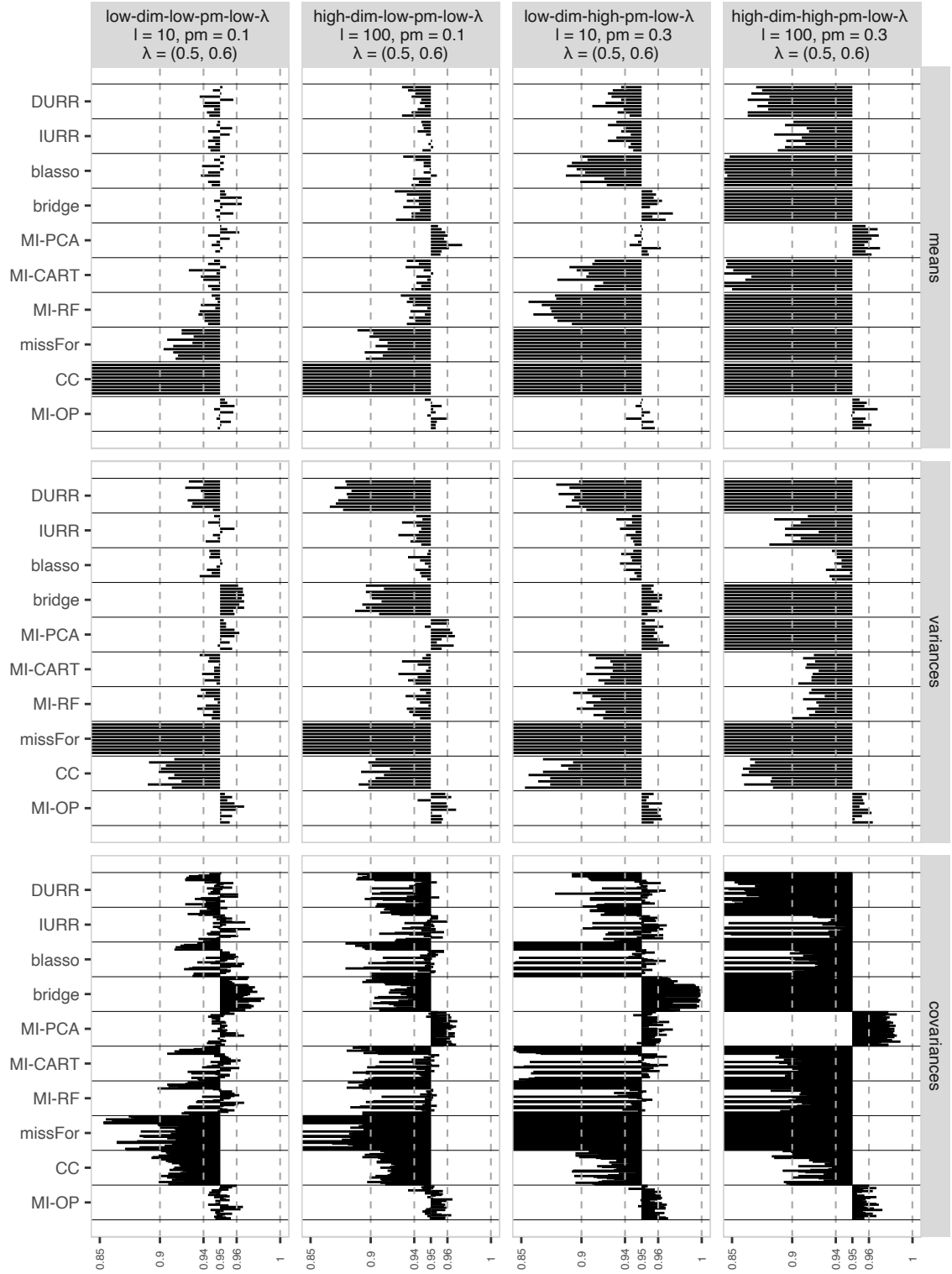


Figure 6. Confidence Interval Coverage (CIC) for the means, variances, and covariances for condition 5 to 8.

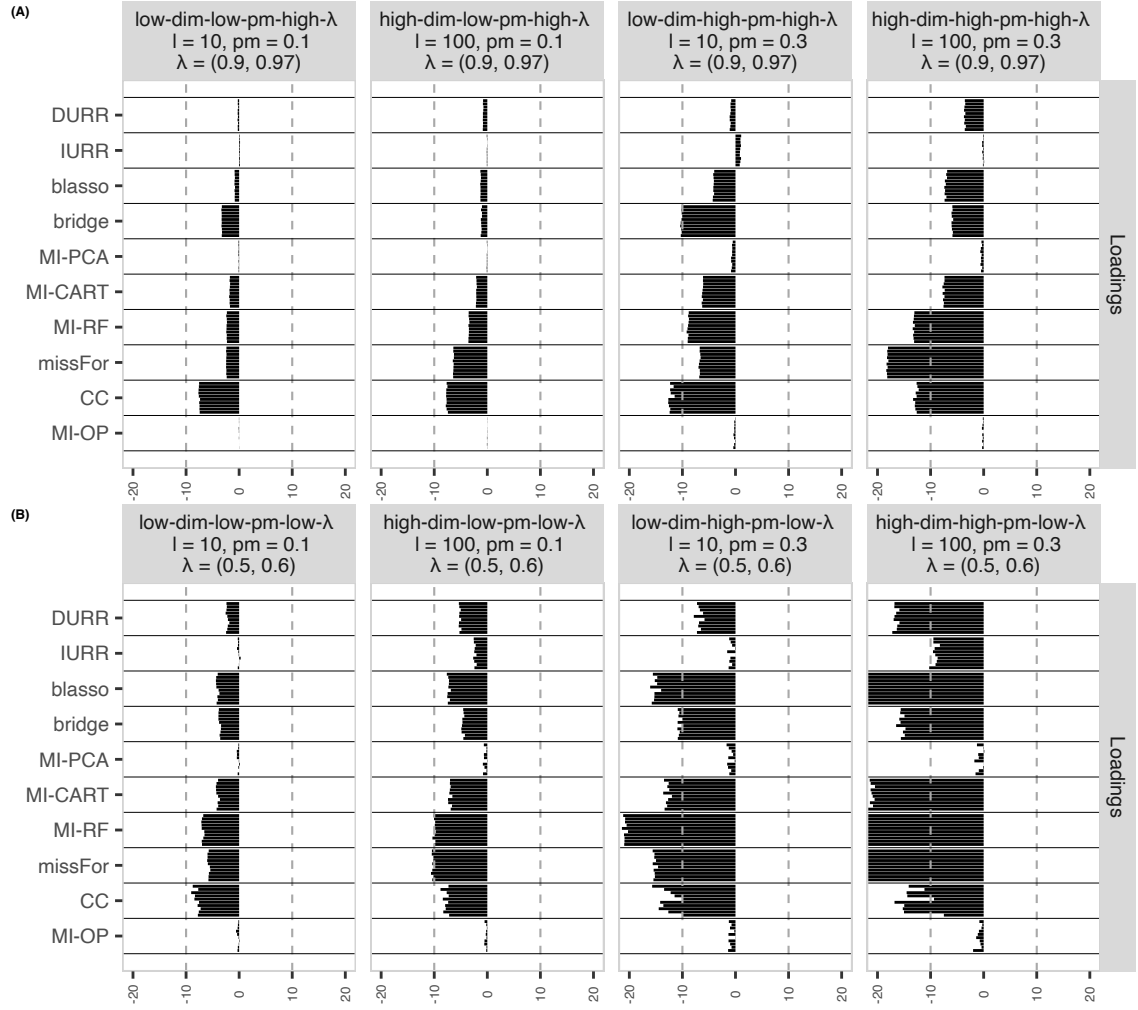


Figure 7. Percent Relative Bias (PRB) for the factor loadings in conditions 1 to 4 (panel A) and conditions 5 to 8 (panel B). Within each panel, for every method, single horizontal lines report the PRB of the factor loading estimation for each item with missing values.

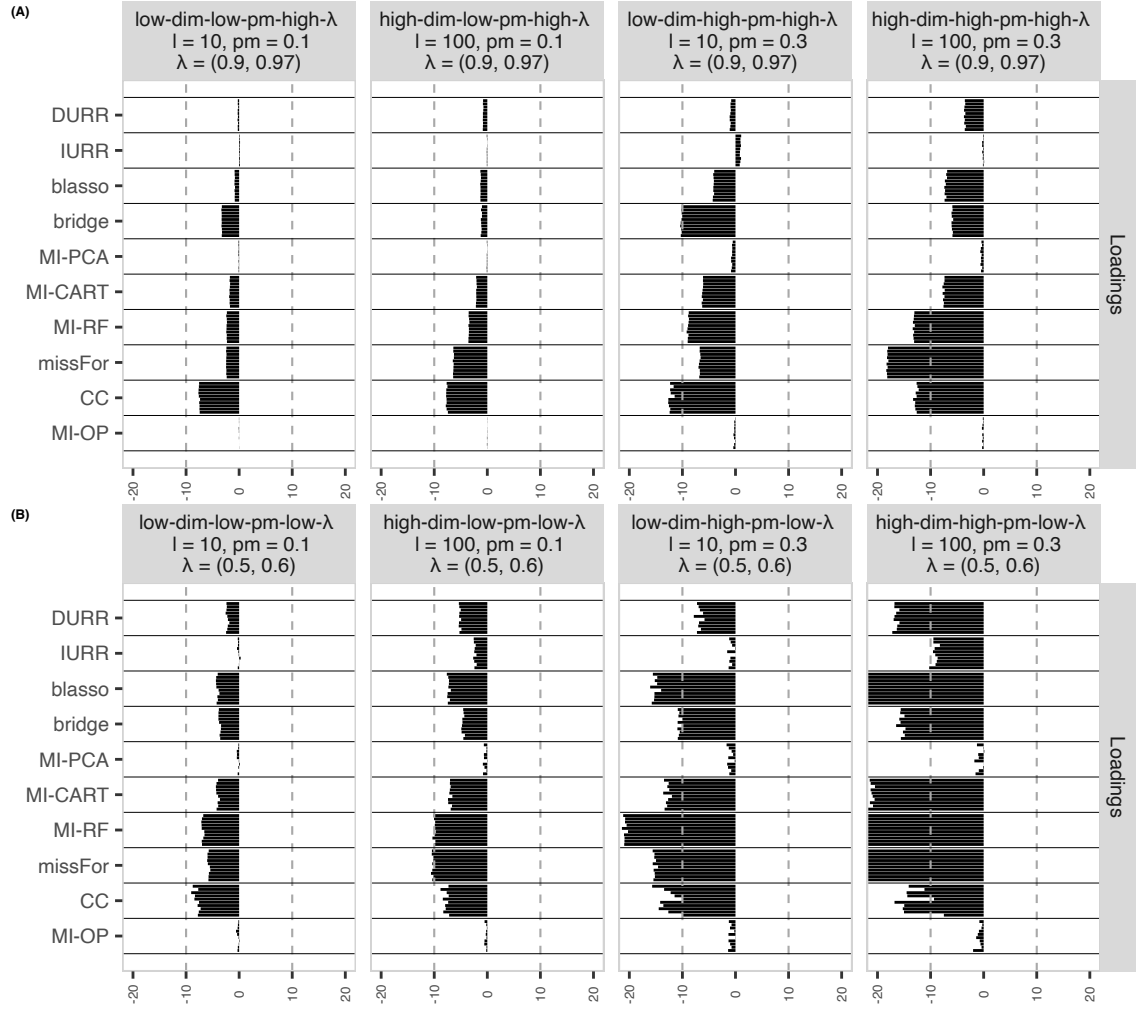


Figure 8. Percent Relative Bias (PRB) for the factor loadings in conditions 1 to 4 (panel A) and conditions 5 to 8 (panel B). Within each panel, for every method, single horizontal lines report the PRB of the factor loading estimation for each item with missing values.

4.0.3. Resampling Study

Supplements to resampling study

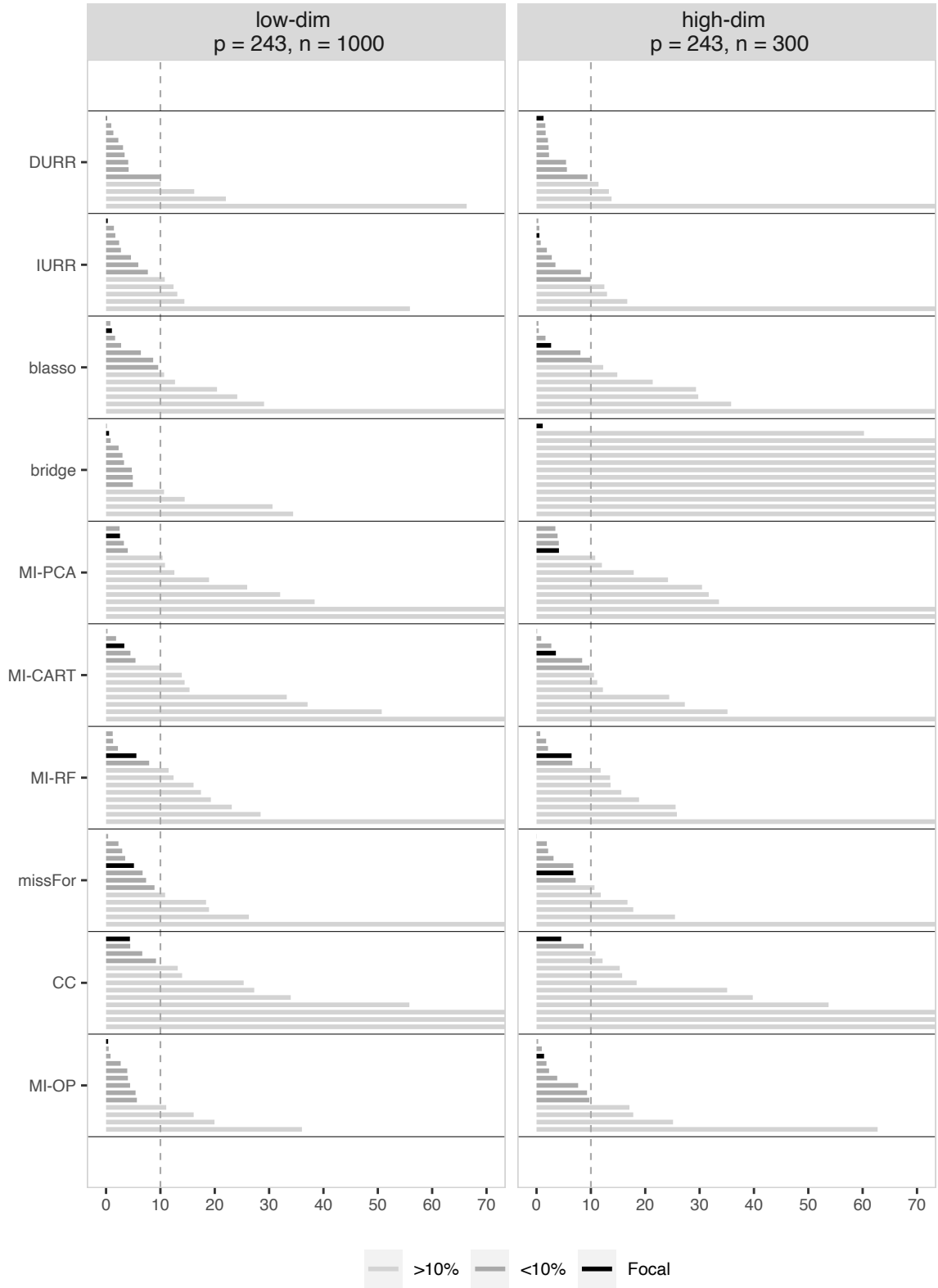


Figure 9. PRBs for all the model parameters in model 1. The order of the bars is based on the absolute value of the PRBs. The values for the intercept, the focal regression coefficient, and the regression coefficient with which most methods struggle (Largest Bias) are highlighted

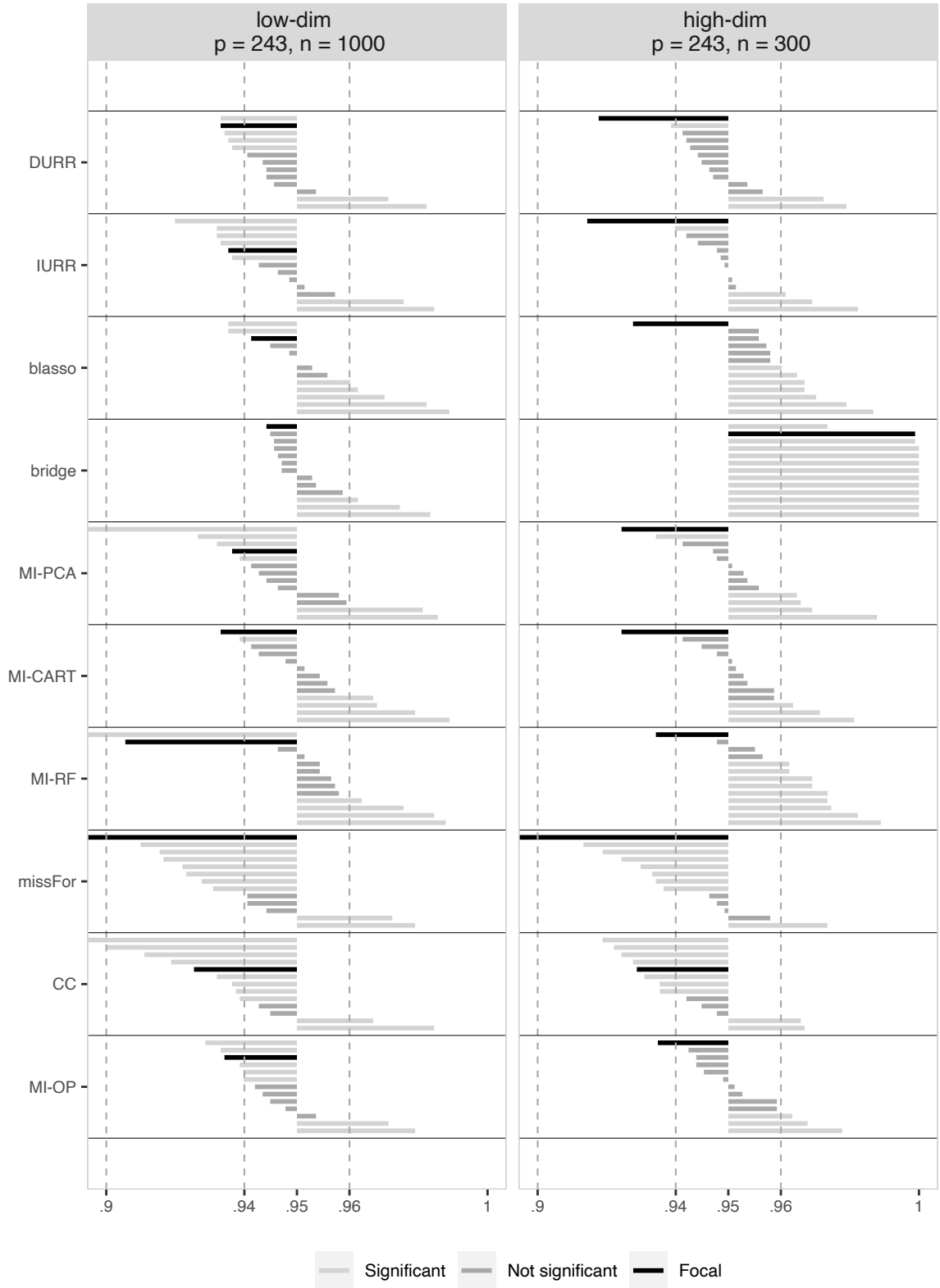


Figure 10. CIC for all model parameter in model 1. Bars are sorted in by ascending value. The values for the intercept, the focal regression coefficient, and the regression coefficient with which most methods struggle (Largest Bias) are highlighted

4.1. Experiment 3: Resampling study

Figure 11 reports the absolute values of the PRBs for every parameter in Model 2, ordered by size, under each of the different imputation methods.

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Figure 12 reports the CIC for each parameter estimate in model 2. When using MI-OP, CICs showed a deviation from nominal coverage for only two parameters, with a slight tendency toward over-coverage.

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All MI methods led to significant under-coverage of the true parameter values with CIC smaller than the threshold value 0.94. Although coverage of the true values was not particularly good for any of the methods selected, the Gold Standard confidence intervals were also under-covering the true value of β_1 in Model 1. This was likely due to the right-skewed nature of the distribution of the dependent variable (euthanasia acceptance). Most MI imputation methods achieved coverages similar to that of the Gold Standard method, and more importantly their relative difference, compared to the GS coverages, was in line with what can be seen for β_1 in Model 2.

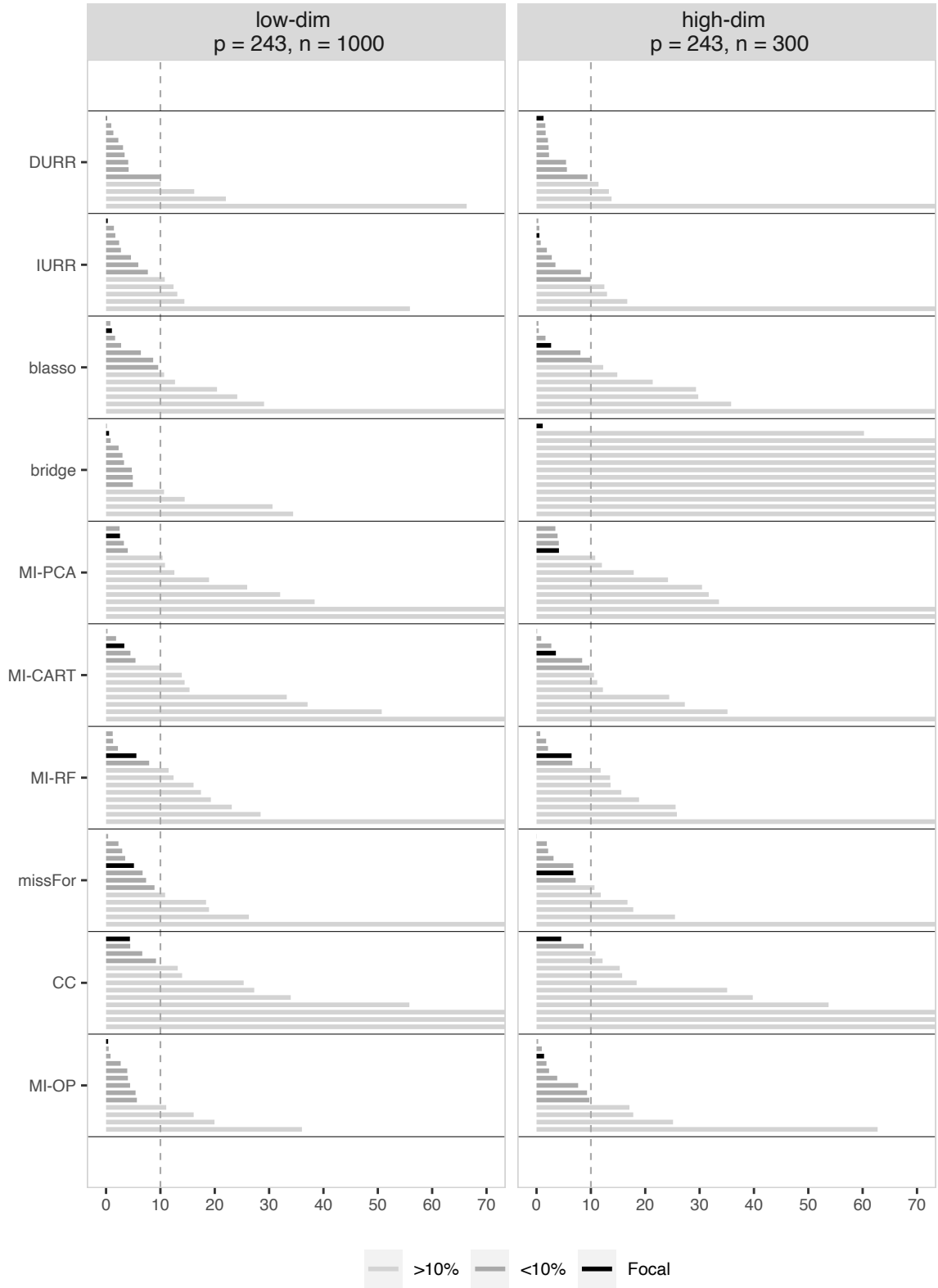


Figure 11. PRBs for all the model parameters in model 1. The order of the bars is based on the absolute value of the PRBs. The values for the intercept, the focal regression coefficient, and the regression coefficient with which most methods struggle (Largest Bias) are highlighted

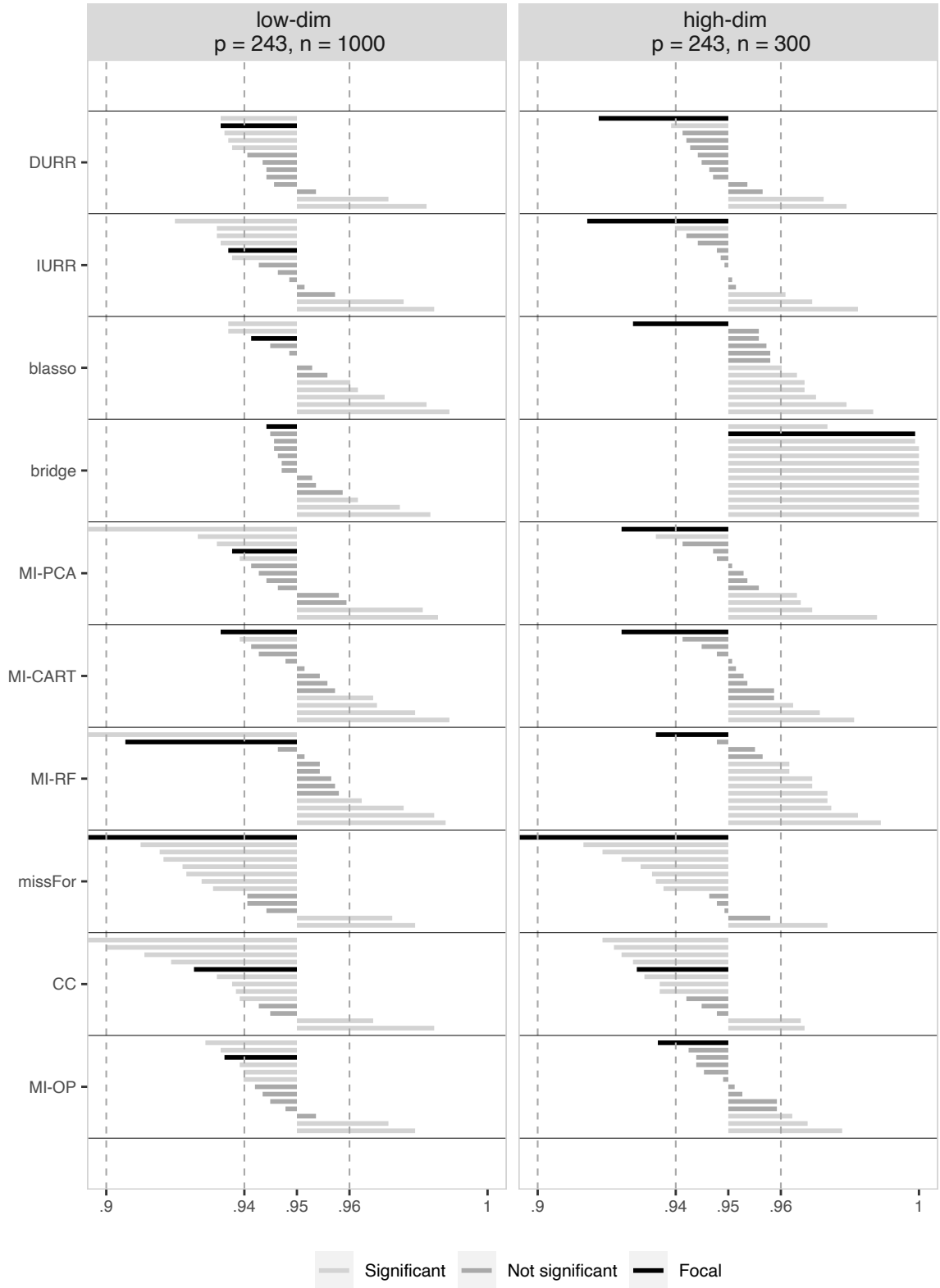


Figure 12. CIC for all model parameter in model 1. Bars are sorted in by ascending value. The values for the intercept, the focal regression coefficient, and the regression coefficient with which most methods struggle (Largest Bias) are highlighted