1. Baseline

RMSE = 0.93
RMSPE = 0.43
r = 0.96
R^2 = 0.92
CCC = 0.96

2. Scaled

RMSE = 13.90
RMSPE = 4.72
r = 0.96
R^2 = -16.8
CCC = 0.36

3. Outlier Focused

RMSE = 54.06
RMSPE = 13.27
r = 0.41
R^2 = -268.15
CCC = 0.05

4. Clustered

RMSE = 3.84
RMSPE = 4.64
r = 0.91
R^2 = -0.36
CCC = 0.73

Block A

RMSE = 3.77
RMSPE = 1.45
r = 0.46
R^2 = -10.44
CCC = 0.17

Block B

RMSE = 3.91
RMSPE = 6.34
r = 0.26
R^2 = -12.96
CCC = 0.08

Observations

Predicted Values

Ground Truth and Prediction Probability

ID	Original Labels		Inverted Labels	
	Ground Truth	Prediction Probability	Ground Truth	Prediction Probability
1	**(+)**	0.99	(-)	0.01
2	(-)	0.70	**(+)**	0.30
3	**(+)**	0.38	(-)	0.62
4	**(+)**	0.33	(-)	0.67
5	**(+)**	0.26	(-)	0.74
6	(-)	0.16	**(+)**	0.84
7	(-)	0.15	**(+)**	0.85
8	(-)	0.14	**(+)**	0.86
9	(-)	0.12	**(+)**	0.88
10	(-)	0.07	**(+)**	0.93

Confusion Matrixes

Predictions

	(+)	(-)	
(+)	TP	FN	→ Recall or Sensitivity $\frac{TP}{TP + FN}$
(-)	FP	TN	→ Specificity $\frac{FP}{FP + TN}$

Precision $\frac{TP}{TP + FP}$

Original Labels @0.50

Predictions

	(+)	(-)
(+)	1	3
(-)	1	5

Accuracy@0.50 = 0.600
Precision@0.50 = 0.500
Recall@0.50 = 0.250
MCC@0.50 = 0.100
PR AUC = 0.767
ROC AUC = 0.875

Inverted Labels @0.50

Predictions

	(+)	(-)
(+)	5	1
(-)	3	1

Accuracy@0.50 = 0.600
Precision@0.50 = **0.625**
Recall@0.50 = **0.833**
MCC@0.50 = 0.100
PR AUC = **0.941**
ROC AUC = 0.875

Receiver Operating Characteristic Curve

True Positive Rate vs False Positive Rate

Legend: ROC — ROC (Inversed label) — Random Guess

Precision-Recall (PR) Curve

Precision vs Recall

@0.25
@0.25
@0.50
@0.50

PR AUC of the Original Labels = 0.76
PR AUC of the Inverted Labels = 0.94

Legend: PR (Original labels) — PR (Inversed labels)

Receiver Operating Characteristics (ROC) Curve

Sensitivity (Recall) vs 1 - Specificity

Precision@0.25 = 0.80
Recall@0.25 = 1.00
MCC@0.25 = 0.82

Precision@0.25 = 0.66
Recall@0.25 = 1.00
MCC@0.25 = 0.41

Precision@0.50 = 0.63
Recall@0.50 = 0.83
MCC@0.50 = 0.10

Precision@0.50 = 0.50
Recall@0.50 = 0.25
MCC@0.50 = 0.10

ROC AUC of the Original Labels = 0.88
ROC AUC of the Inverted Labels = 0.88

Legend: ROC (Original labels) — ROC (Inversed labels) — Random Guess

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Block A

r =	0.33
R^2 =	-0.71
RMSE =	1.46

Block B

r =	0.25
R^2 =	-1.10
RMSE =	1.52

	(+)	(-)
(+)	4	0
(-)	1	5

	(+)	(-)
(+)	6	0
(-)	3	1

	Original Labels		Inverted Labels	
ID	Ground Truth	Prediction Probability	Ground Truth	Prediction Probability
1	(+)	0.99	(-)	0.01
2	(-)	0.70	(+)	0.30
3	(+)	0.38	(-)	0.62
4	(+)	0.33	(-)	0.67
5	(+)	0.26	(-)	0.74
6	(-)	0.16	(+)	0.84
7	(-)	0.15	(+)	0.85
8	(-)	0.14	(+)	0.86
9	(-)	0.12	(+)	0.88
10	(-)	0.07	(+)	0.93

Matthews Correlation Coefficient (MCC) Curve

MCC (Original labels)
MCC (Inversed labels)

Precision@0.25 = 0.80
Recall@0.25 = 1.00
MCC@0.25 = 0.82

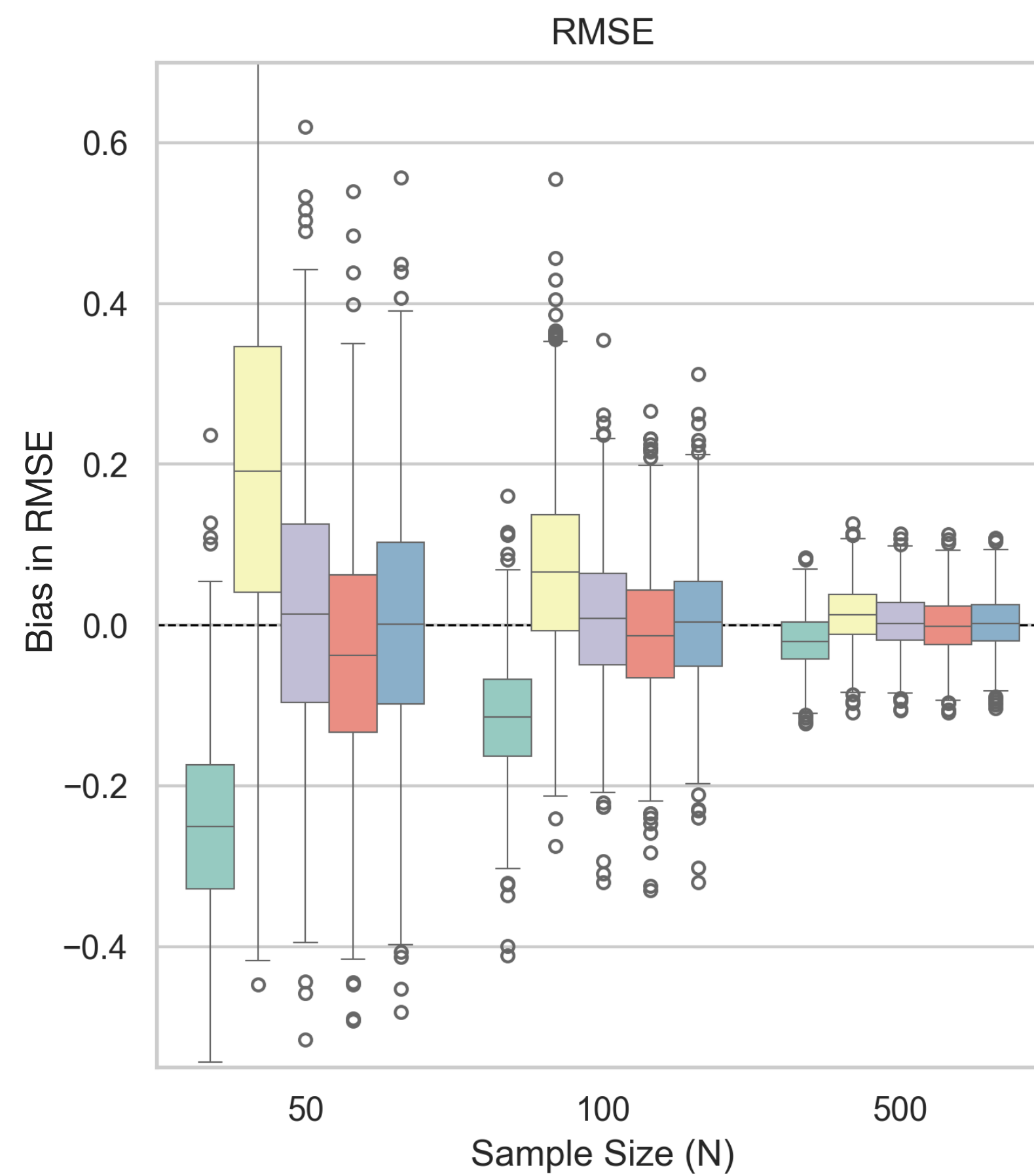Precision@0.75 = 1.00
Recall@0.75 = 0.83
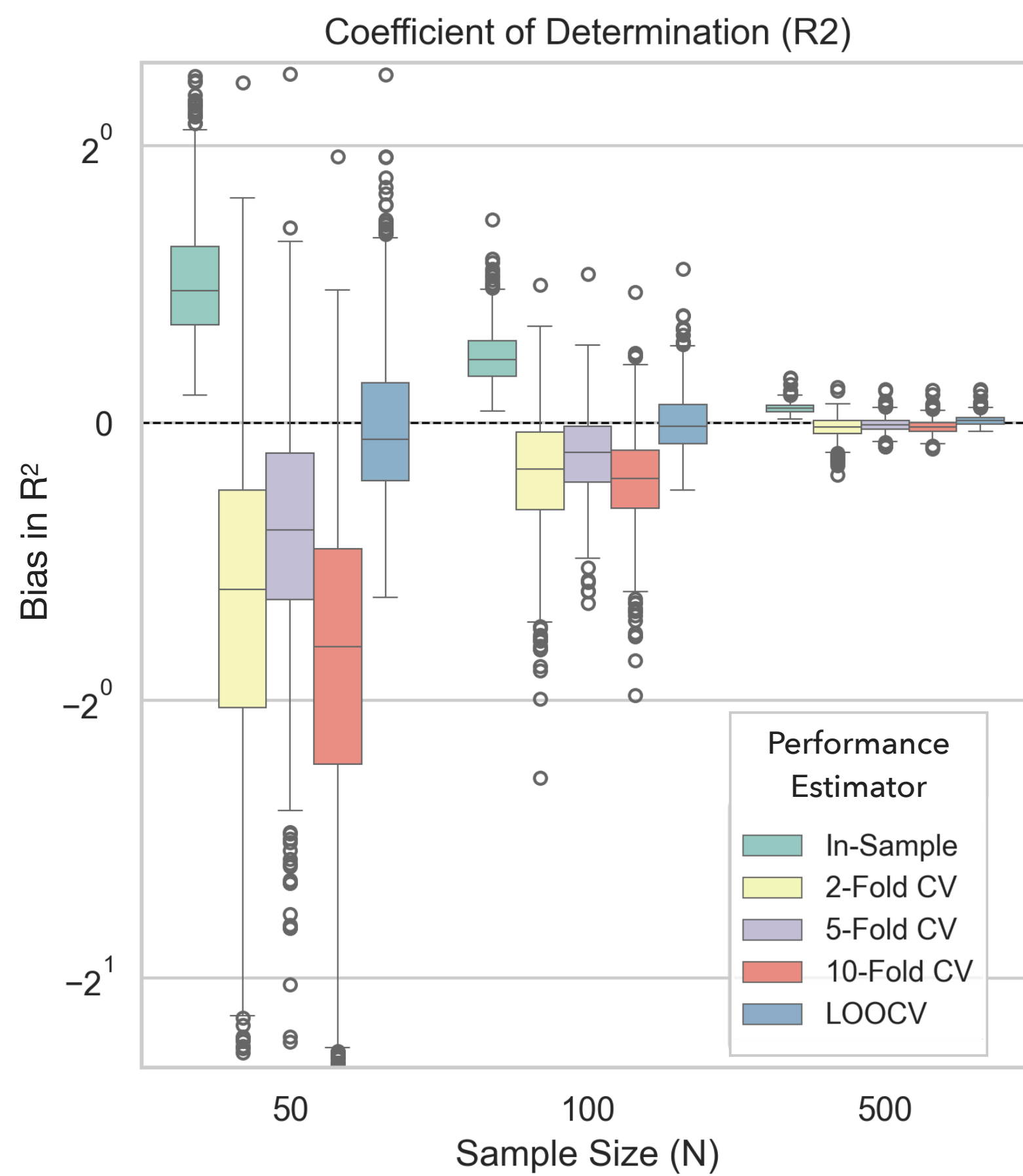MCC@0.75 = 0.82

Confidence Threshold

MCC
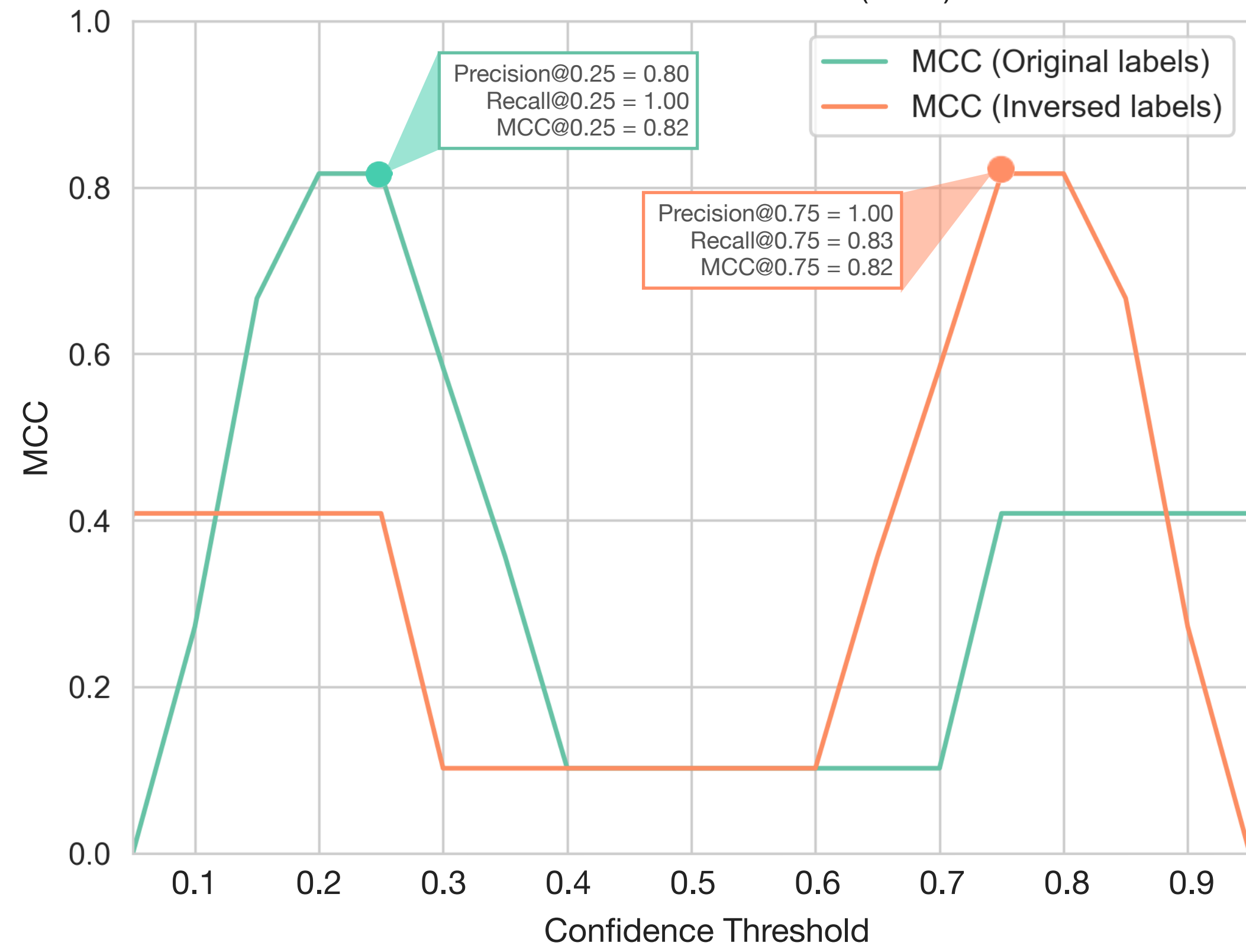
Confusion Matrix at the Optimum Threshold

Original Labels @0.25

		Predictions	
		(+)	(-)
Ground Truth	(+)	4	0
	(-)	1	5

Inverted Labels @0.75

		Predictions	
		(+)	(-)
Ground Truth	(+)	5	1
	(-)	0	4
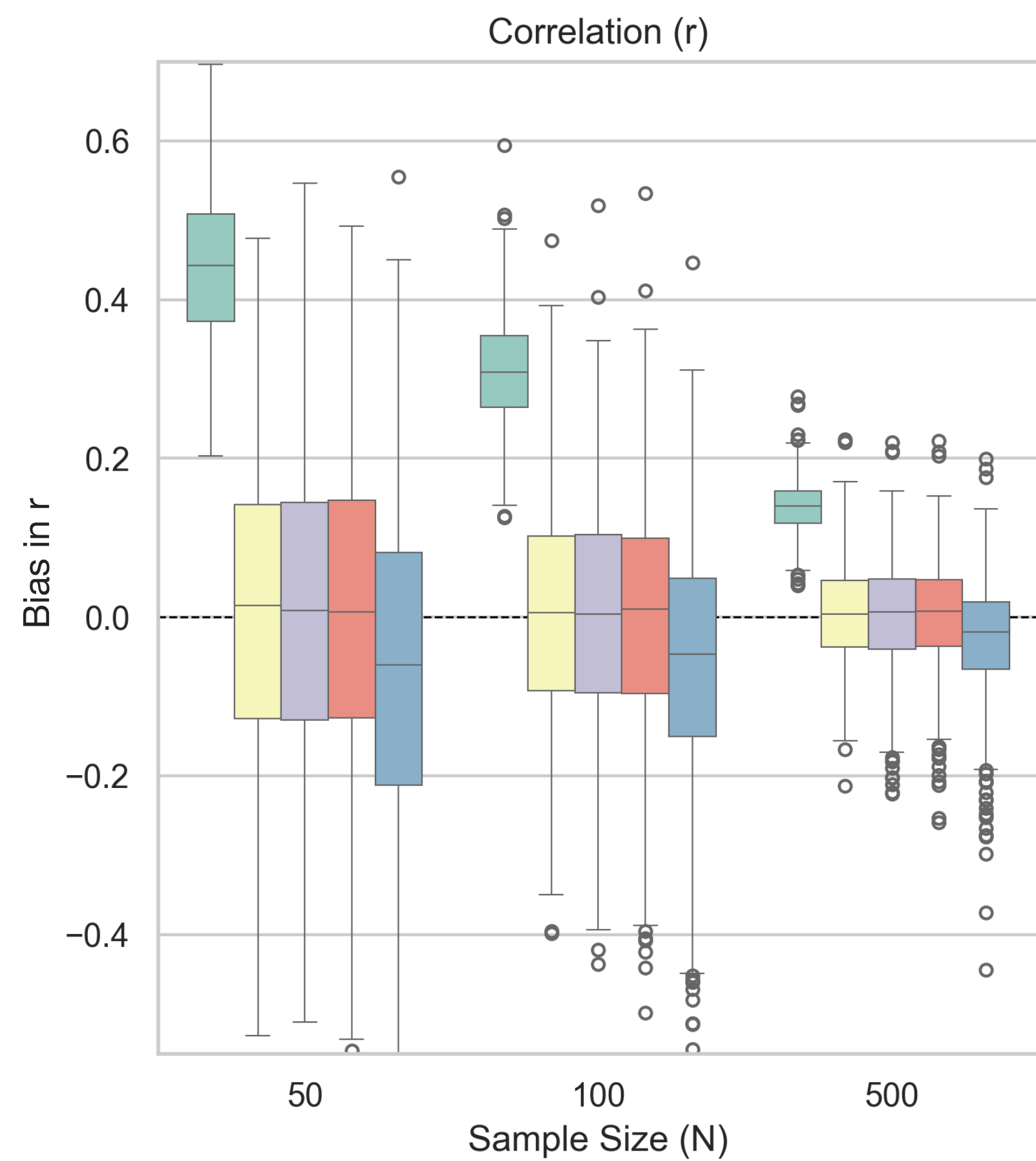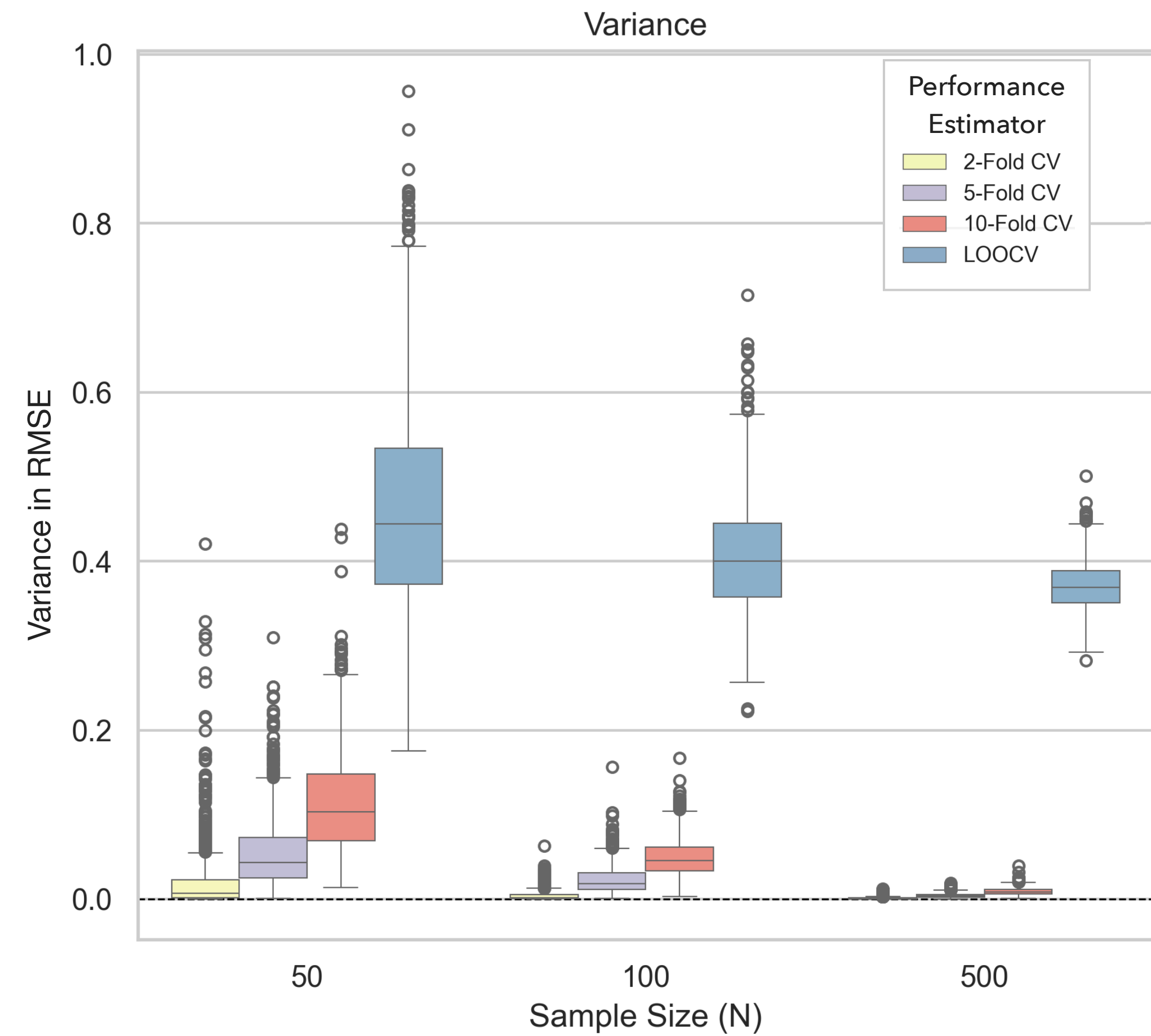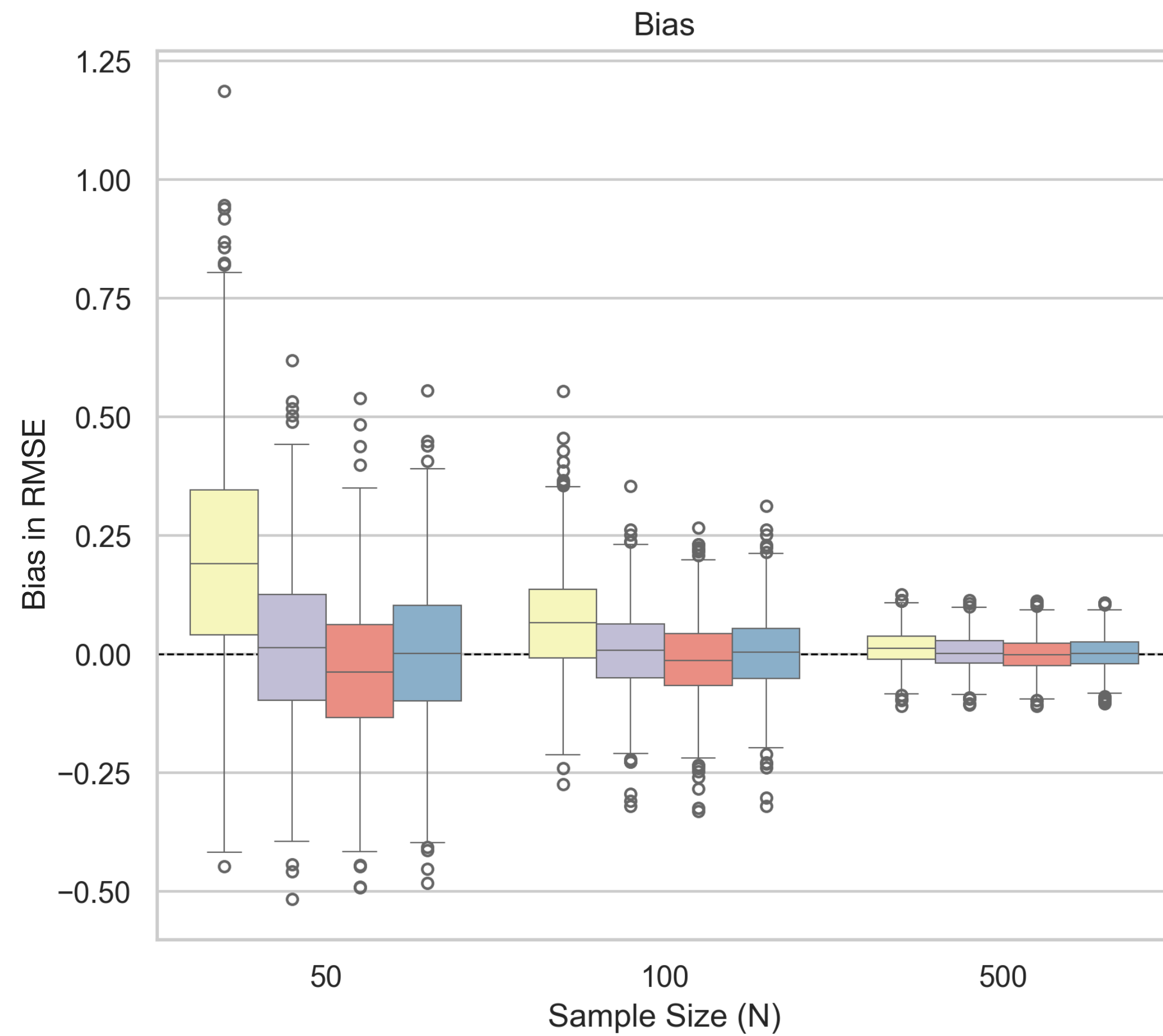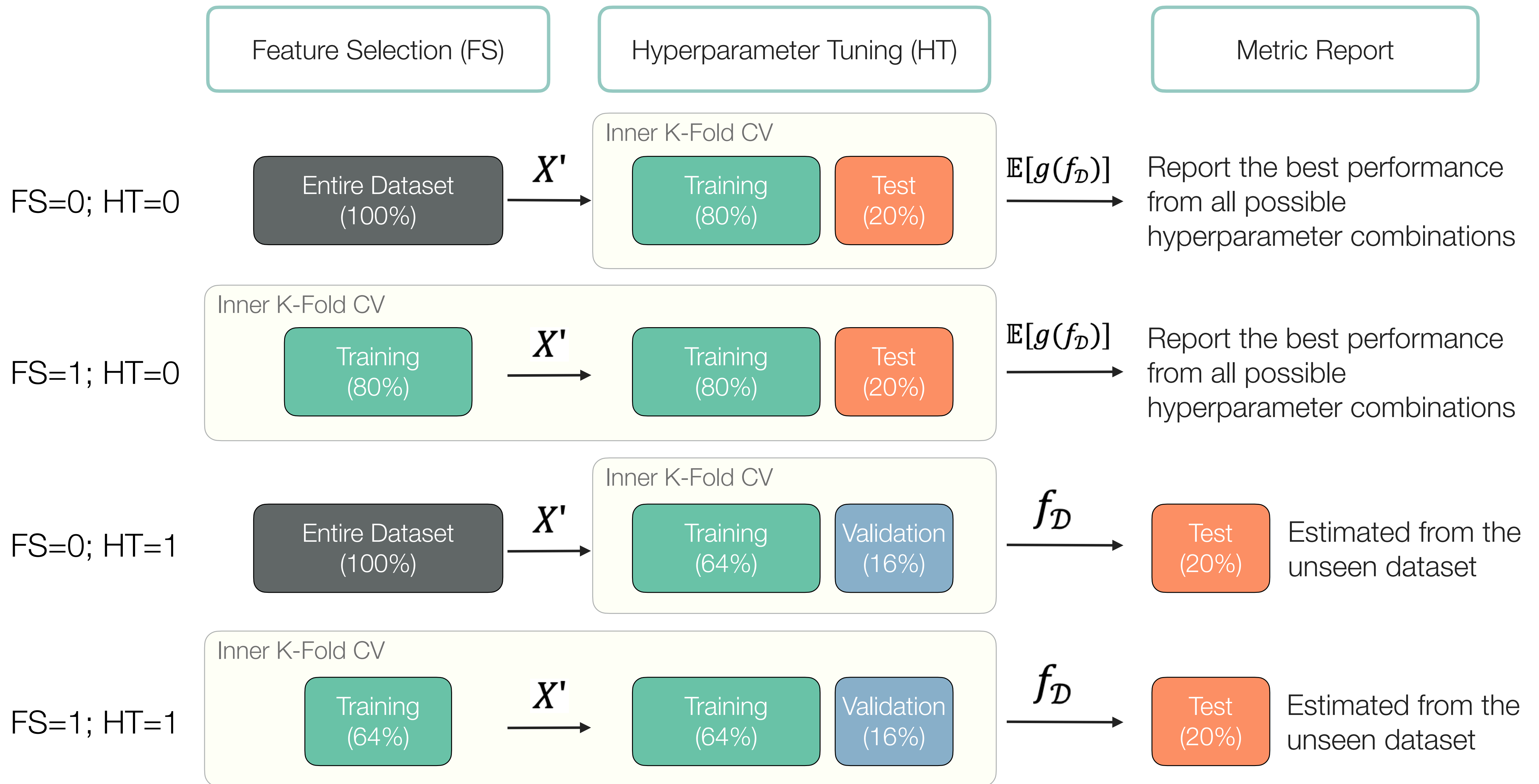
Correlation (r)

Coefficient of Determination (R2)

RMSE

Bias

Variance

FS=0; HT=0

Feature Selection (FS)
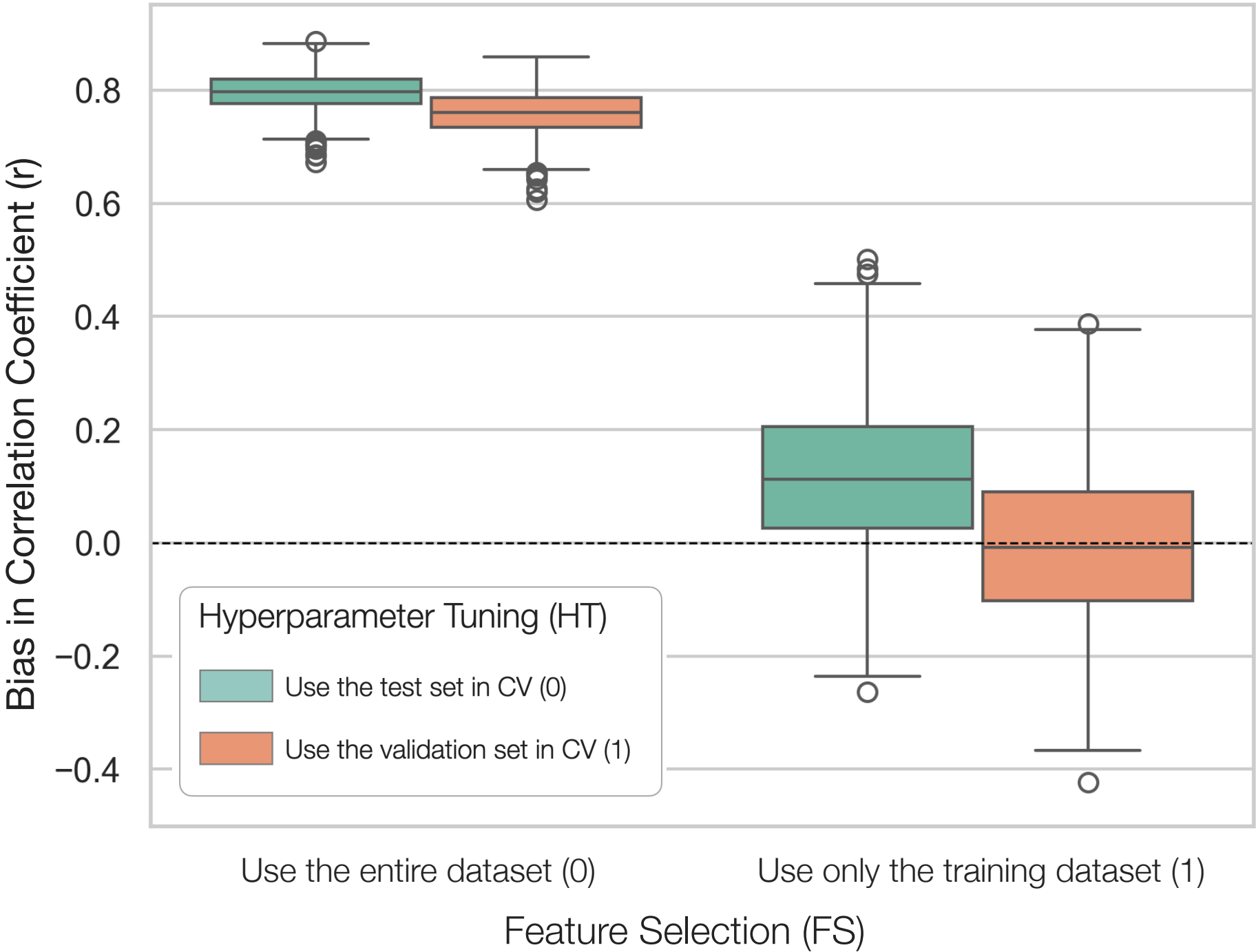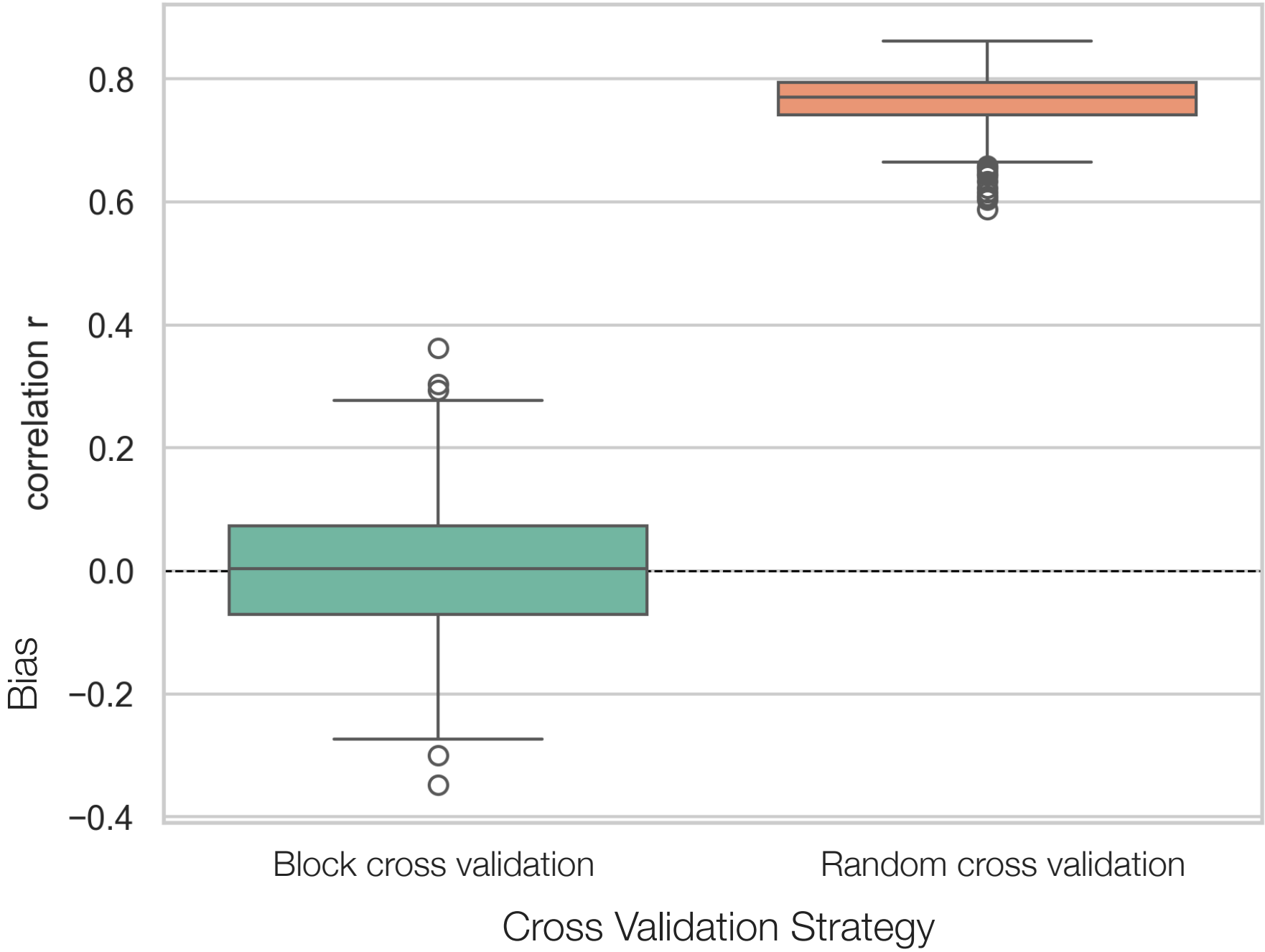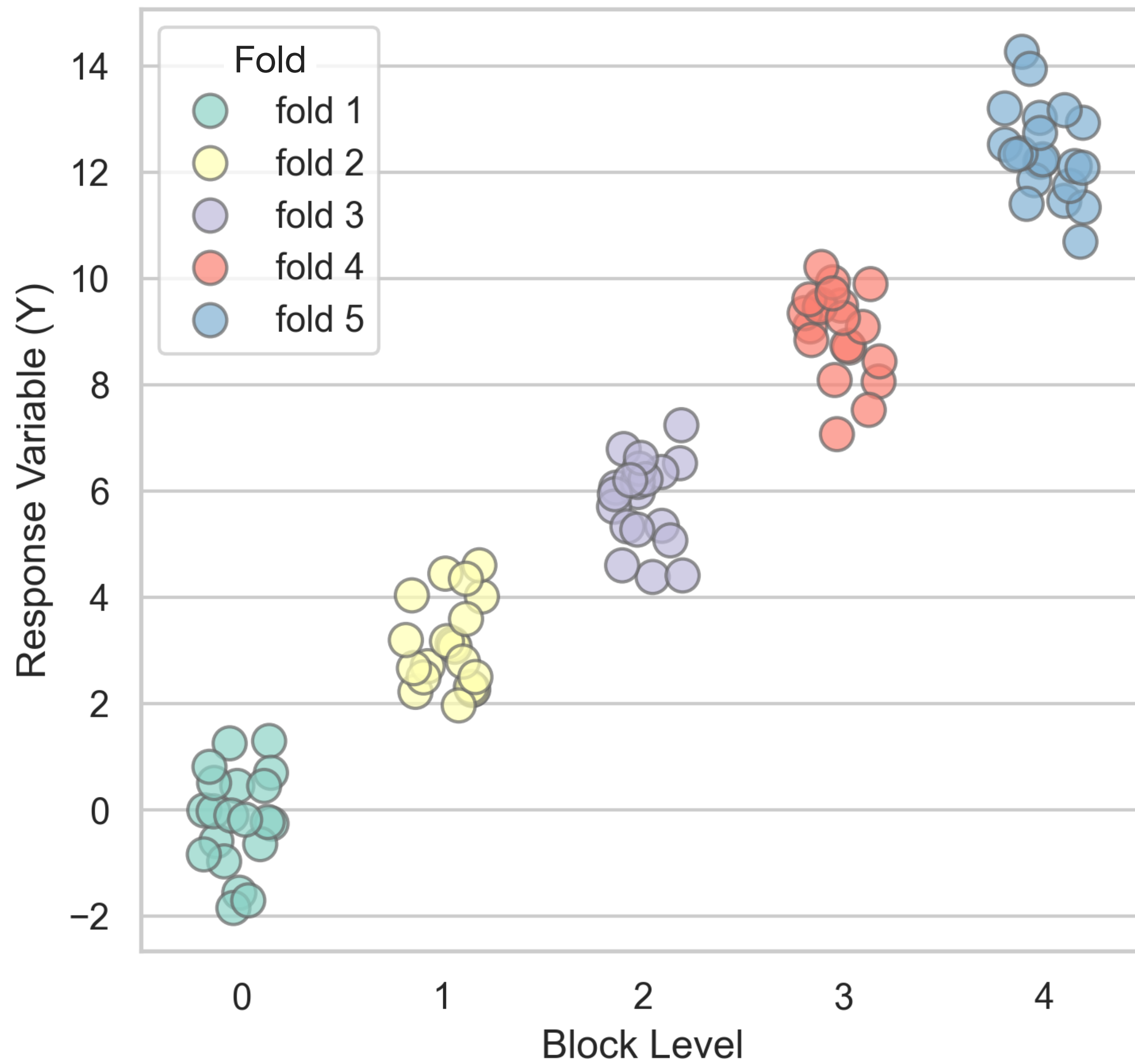
Block Cross Validation / Random Cross Validation