Simple Bootstrap and Simulation Approaches to Quantifying Reliability of High-Dimensional Feature Selection

The Simplest Task

The Real Task

Bootstrapping a Dataset

Summary

Simple Bootstrap and Simulation Approaches to Quantifying Reliability of High-Dimensional Feature Selection

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Simplest Task: Estimate Association Between X_1 and Y With Precision

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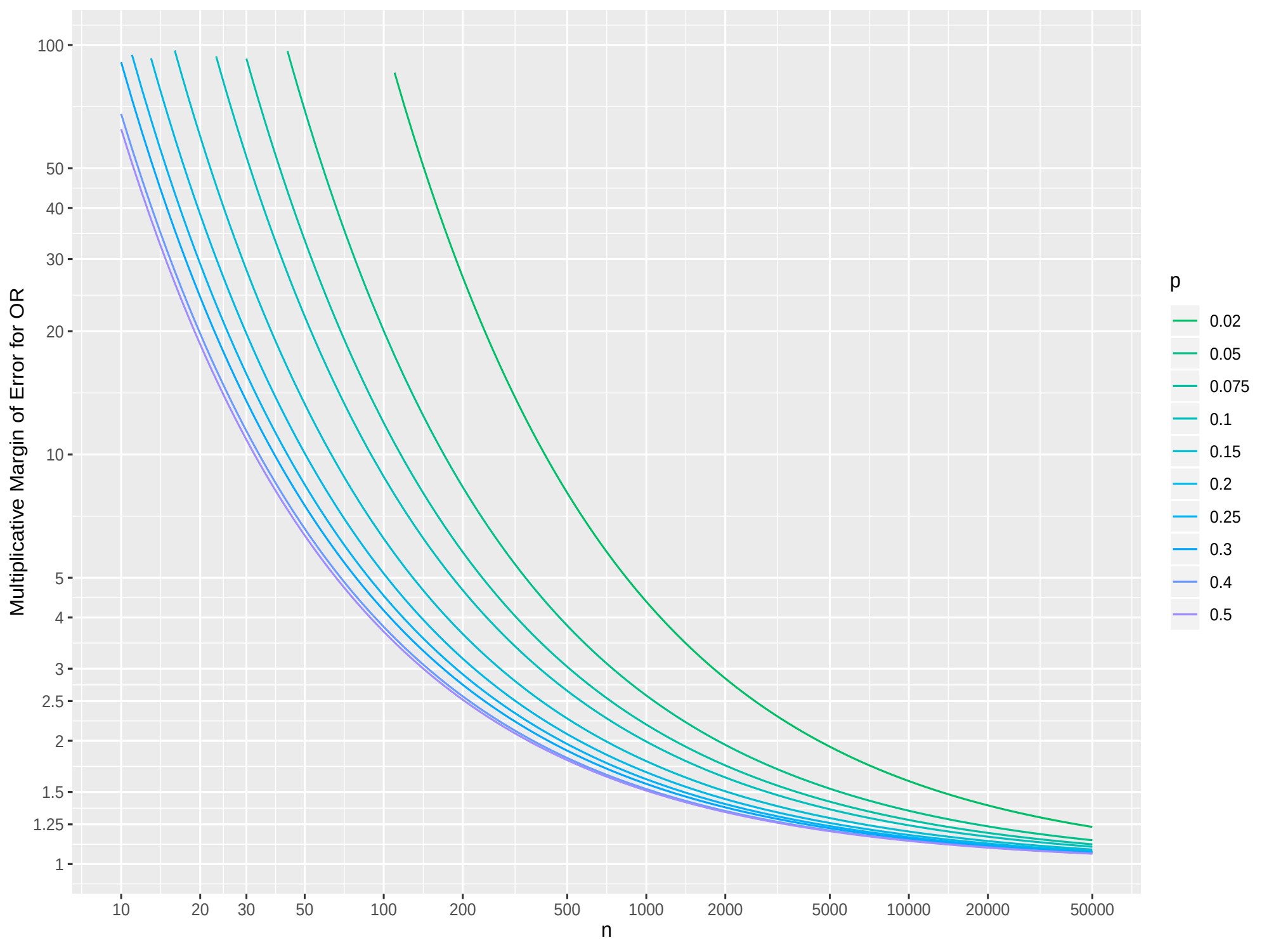
- Correlation coefficient, hazard ratio, odds ratio, etc.
- Consider multiplicative margin of error for an odds ratio
- Assume true $P(Y = 1)$ in each group be $\geq p$
- Assume total sample size n is split into $\frac{1}{10}$ of subjects with $X = 0$ and $\frac{9}{10}$ with $X = 1$
- MMOE = anti-log of half-width of 0.95 CL on log OR


Multiplicative Margin of Error for OR
100
50
40
30
20
10
5
4
3
2.5
2
1.5
1.25
1
10
20
30
50
100
200
500
1000
2000
5000
10000
20000
50000
n
p
0.02
0.05
0.075
0.1
0.15
0.2
0.25
0.3
0.4
0.5

The Real Task: High-Dimensional Modeling or Feature Selection

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Summary

- One-at-a-time feature selection from among large # candidate features
- Simultaneous modeling of large # features
- Ranking importance of features
- False discovery risks ignore false negative risks and precision of final estimates
- Use simple simulation to understand needed sample sizes

Controlling Margins of Error of Entire Set of OR Estimates

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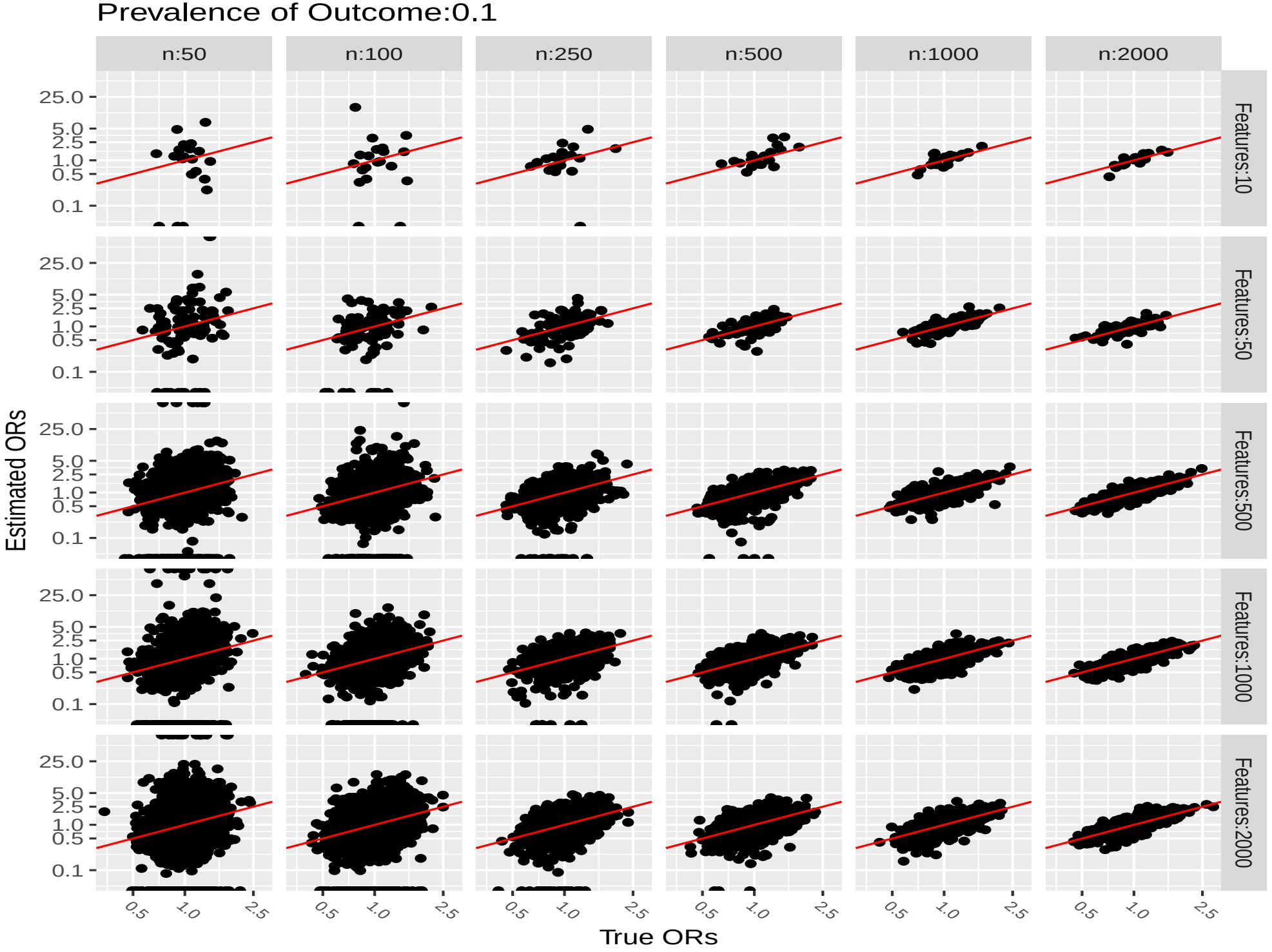
- Let $p = \#$ of candidate binary features
- Assume true log ORs have normal($\mu = 0, \sigma = 0.25$) distribution
- Want to
  - judge ability to jointly estimate p associations
  - rank order features by observed associations
- Y prevalence 0.1, X_i prev. $\sim U(0.05, 0.5)$


Prevalence of Outcome:0.1
n:50
n:100
n:250
n:500
n:1000
n:2000
Features:10
Features:50
Features:500
Features:1000
Features:2000
Estimated ORs
True ORs
25.0
5.0
2.5
1.0
0.5
0.1
0.5
1.0
2.5

Summarizing Multiplicative Errors in ORs

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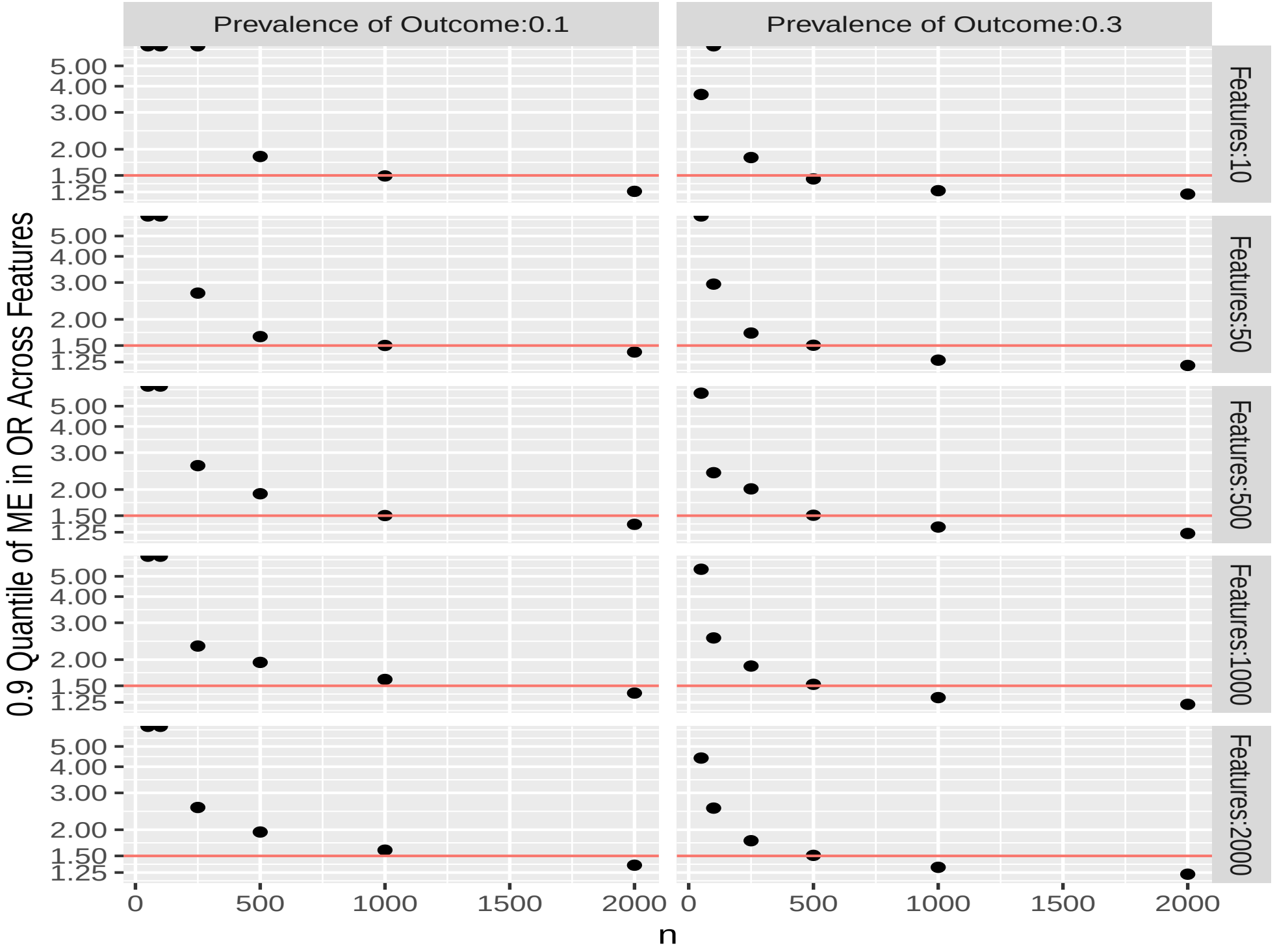
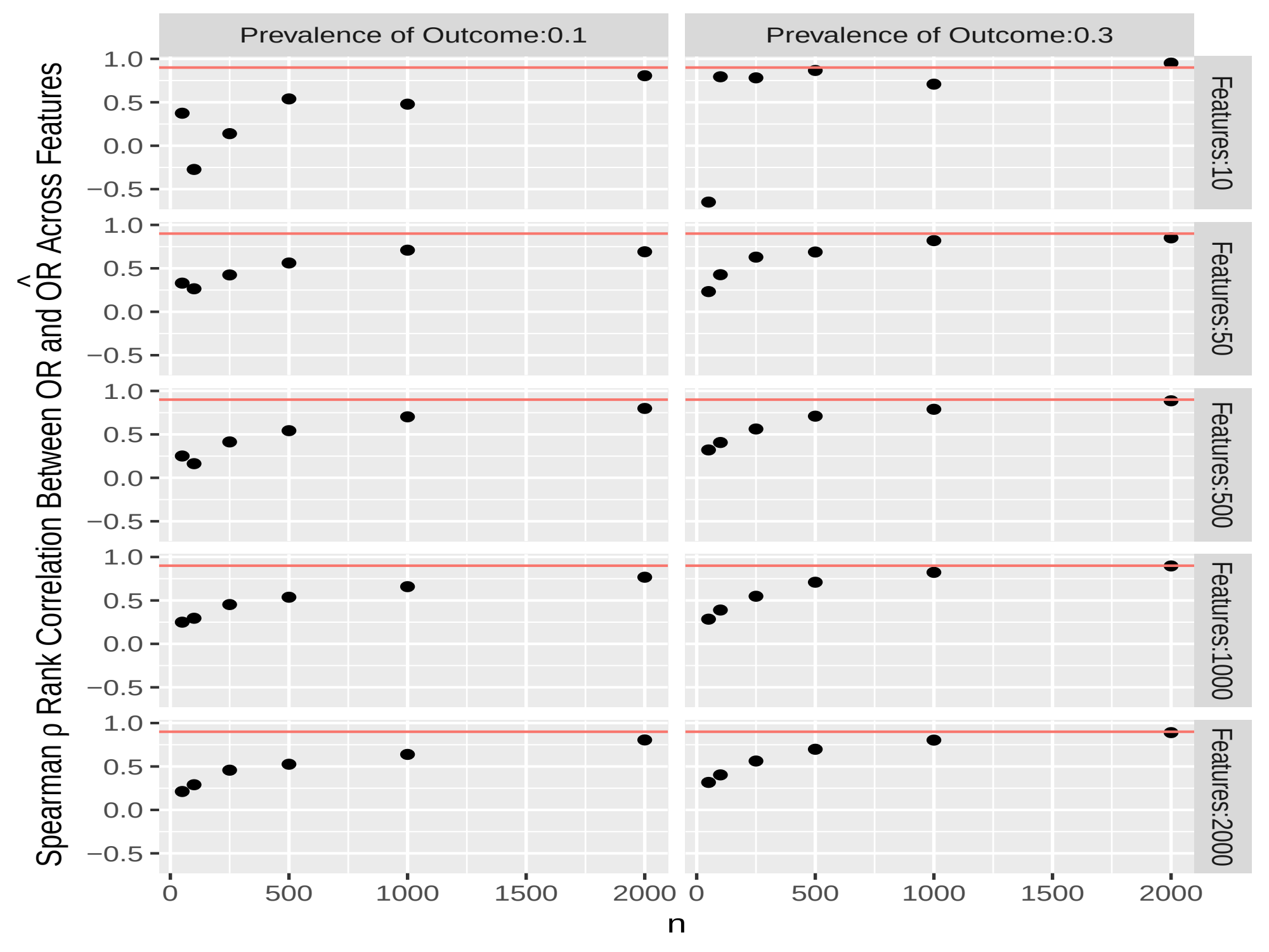
- ME = anti-log of estimate / true OR
- Compute 0.9 quantile of ME over whole set of estimated ORs
- Then compute Spearman rank correlation between estimated and true underlying ORs over whole set


Prevalence of Outcome:0.1
Prevalence of Outcome:0.3
Features:10
Features:50
Features:500
Features:1000
Features:2000
0.9 Quantile of ME in OR Across Features
5.00
4.00
3.00
2.00
1.50
1.25
0
500
1000
1500
2000
n


Prevalence of Outcome:0.1
Prevalence of Outcome:0.3
Features:10
Features:50
Features:500
Features:1000
Features:2000
Spearman ρ Rank Correlation Between OR and ÔR Across Features
n
1.0
0.5
0.0
−0.5
0
500
1000
1500
2000

Bootstrap Analysis for One Simulated Dataset

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Summary

- Are winning features really winners? Are losers really losers?
  - Compute confidence intervals for feature importance ranking
- What is the bias in an OR that passes the selection process?
- Bootstrap can take into account all sources of uncertainty
  - Actually underestimates instability compared to exact Bayesian credible intervals

Bootstrap Analysis, *continued*

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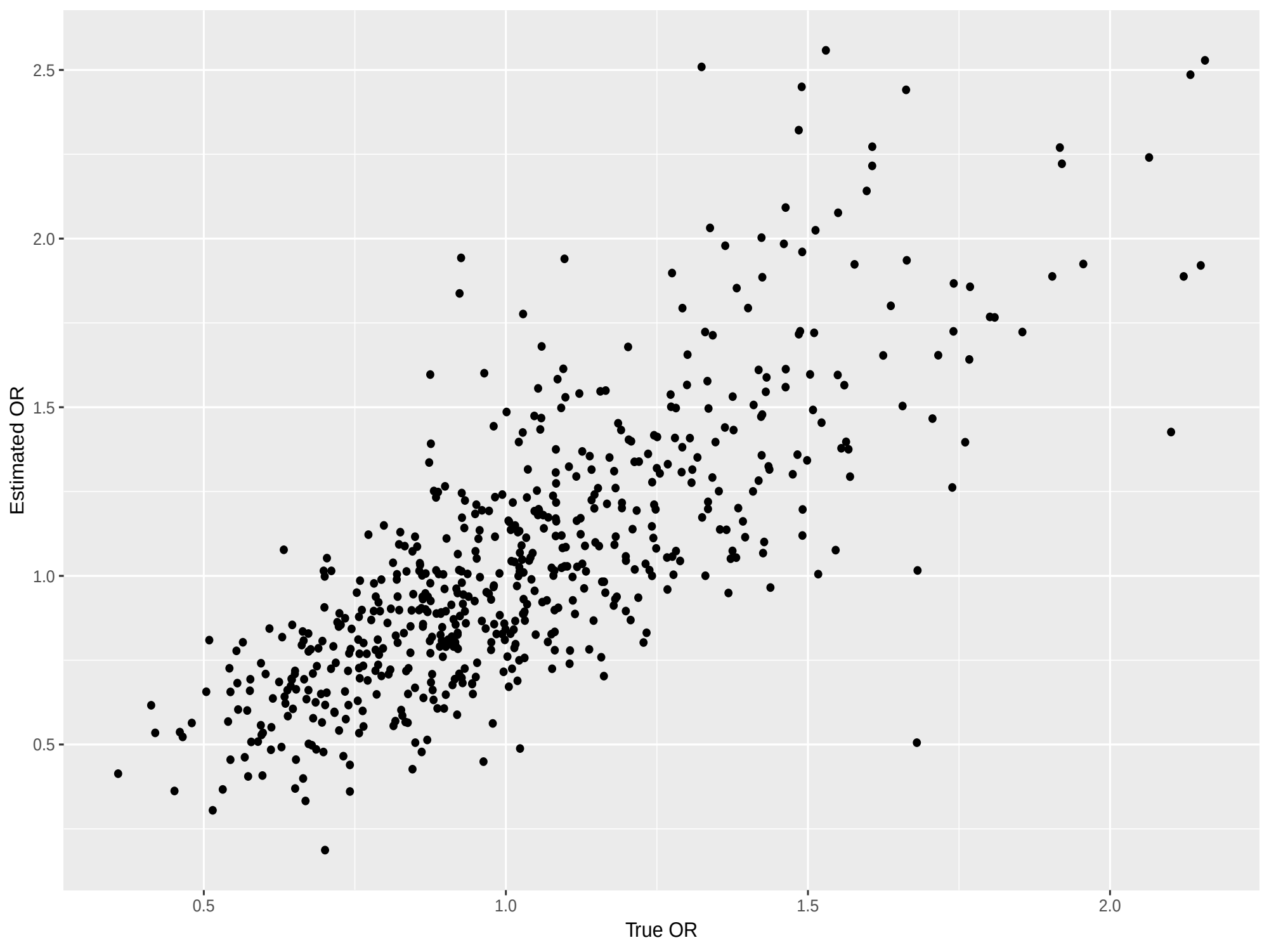
Summary

- Simulate data for 600 subjects with 600 candidate predictors
- Estimate bias in apparent lowest and apparent highest ORs
  - Find extreme estimated ORs in sample w/replacement
  - Compute dropoff when compared to same predictor in orig. sample
- Y has prevalence 0.2


Estimated OR
2.5
2.0
1.5
1.0
0.5
0.5
1.0
1.5
2.0
True OR

Features with Largest and Smallest Estimated ORs

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Largest observed OR

Estimated OR: 2.56, feature #1
true OR: 1.53, ME: $\times 1.67$

Smallest observed OR

Estimated OR: 0.19, feature #355
true OR: 0.7, ME: $\times 0.27$

Bootstrap Bias Estimates

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Largest OR

0.95 CL for rank: 440 600
Median bias: 1.64 Geometric mean bias: 1.69
True ME: 1.67

Bootstrap bias-corrected OR: 1.56
Original OR: 2.56 True OR: 1.53

Smallest OR

0.95 CL for rank: 1 45
Median bias: 0.24 Geometric mean bias: 0.11
True ME: 0.27

Bootstrap bias-corrected OR: 0.76
Original OR: 0.19 True OR: 0.7

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- Simple simulations and bootstrap can determine limits in information content from a sample of low or high-dimensional data
- Recognize that feature selection (not always recommended) is a ranking problem
- Bootstrap CLs for predictor ranks provide basis or caution in feature selection
- Bootstrap can estimate bias when selecting on extreme observed associations
- One can estimate the sample size so that data are unlikely to be tortured beyond the breaking point