Multiple regression - information criteria for large data bases

November 14, 2023

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$$\hat{\sigma}^2 = s^2 = \frac{||Y - X\hat{\beta}_{LS}||^2}{n-p} = \frac{RSS}{n-p}$$

Selection of important variables

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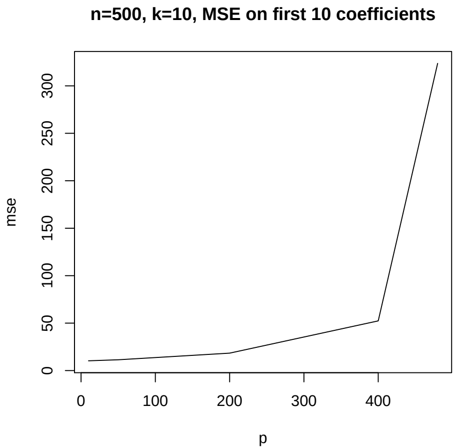
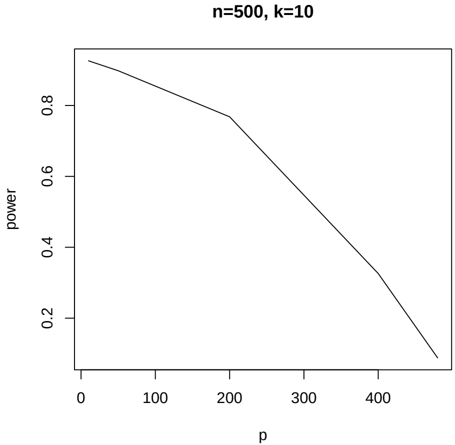
But $(X'X)^{-1}$ has the inverse Wishart distribution and the expected values of the elements on the diagonal are equal to $\frac{n}{n-p-1}$ and become very large as p approaches n.

Inflation of MSE



Loss of Power



Model selection

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Also, RSS is not a good measure of the prediction error.

Training and prediction error

Let's consider a new sample

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$RSS = ||Y - \hat{Y}||^2$ measures the fit in the training sample, i.e. it depends on the specific realization of the noise term ϵ - this is overfitting. PE measures the fit with respect to the true expected value of Y, which indeed is an indication of predictive properties for different noise terms.

Prediction error

Fact 1:

$$E(RSS) = PE - 2\sum_{i=1}^{n} Cov(\hat{y}_i, y_i)$$

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Proof:

$$E(\hat{y}_i - y_i)^2 = E((\hat{y}_i - \mu_i) - (y_i - \mu_i))^2$$

$$= E(\hat{y}_i - \mu_i)^2 + \sigma^2 - 2Cov(\hat{y}_i, y_i) = PE_i - 2Cov(\hat{y}_i, y_i)$$

Prediction error for a linear operator

If $\hat{Y} = M_{n \times n} Y$ then

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$$PE = E(RSS) + 2\sigma^2 Tr(M)$$

In least squares estimation

$$M = X(X'X)^{-1}X'$$

is the matrix of the orthogonal projection on the space spanned by columns of X and $Tr(M) = rank(X)$.

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Leave-one-out cross-validation:

$$CV = \sum_{i=1}^{n}(Y_i - \hat{Y}[i])^2 = \sum_{i=1}^{n}\left(\frac{Y_i - \hat{Y}_i}{1 - M_{ii}}\right)^2$$

Akaike Information Criterion

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$$AIC(M_k) = \ln L(X, \hat{\theta}_{MLE}) - k$$

Akaike Information Criterion in Linear Regression

$\epsilon_1 = Y_1 - X_1\beta, \ldots, \epsilon_n = Y_n - X_n\beta$ - iid from $N(0, \sigma^2)$, $\beta \in R^k$

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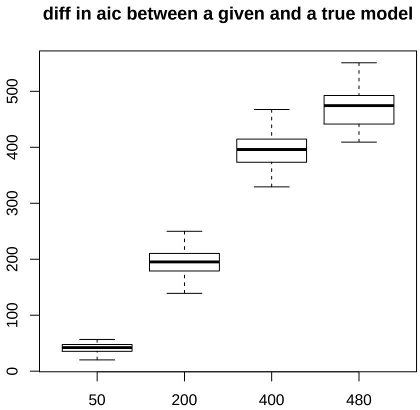
Maximizing AIC corresponds to minimizing $RSS + 2\sigma^2 k$

Properties of AIC (1)

In our example AIC identifies the true model among 5 models with different dimensions, $p = 500$, $k = 10$.



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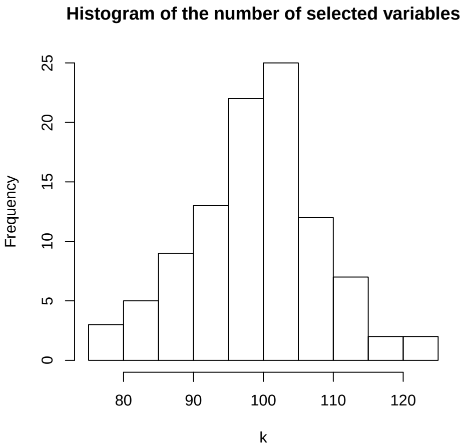
More complicated heuristics: genetic algorithms, simulated annealing etc.

Can we use AIC to select important variables in large data bases ?

bigstep - *R* library with many different search strategies, optimizing a variety of model selection criteria; $p = 500$, $k = 10$.



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$$RSS = Y'Y - \hat{\beta}'\hat{\beta} = Y'Y - \sum_{i=1}^{k} \hat{\beta}_i^2$$

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In our simulations $\hat{k} \approx 100$ due to additional disturbance by the sample correlations between columns of the design matrix and using the form of AIC with unknown σ

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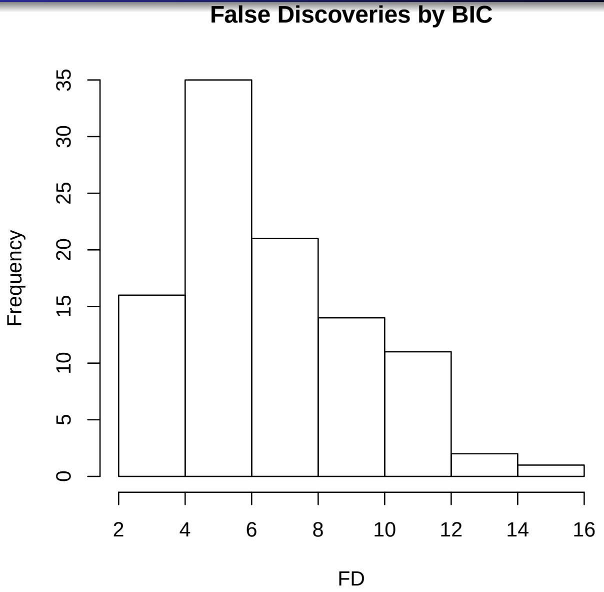
Thus we expect to see on average $p_0 * 0.013 = 490 * 0.013 \approx 6.5$ false discoveries

False Discoveries by BIC



Solution - multiple testing correction

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Here the expected number of false discoveries is smaller than 1 and decreases with p

Modified BIC

In mBIC (Bogdan et al. 2004) the penalty depends on p and n,

$$mBIC = RSS + \sigma^2 k \left(\log n + 2 \log \left(\frac{p}{C} \right) \right) \quad ,$$

where C is the prior expected number of nonzero regression coefficients. In the lack of the prior knowledge the value $C = 4$ is suggested. It is motivated by controlling FWER.

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mBIC2 (Żak-Szatkowska and Bogdan (CSDA, 2011), Frommlet et al. (2011))

$$mBIC2 := RSS + \sigma^2(k\log(n) + 2k\log(p/4) - 2\log(k!) \quad .$$

The last relaxing term comes from the BH correction :
$\Phi^{-1}\left(1 - \frac{i\alpha}{2p}\right) = \sqrt{2\log(p/i)}(1 + o_p)$

$$\sum_{i=1}^{k} 2\log(p/i) = 2k\log p - 2\log(k!)$$

Simulation results for GWAS (Frommlet, Ruhaltinger, Twarog and Bogdan, 2011, CSDA)

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- Simulation scenario:
  β_j equally distributed between 0.27 and 0.66

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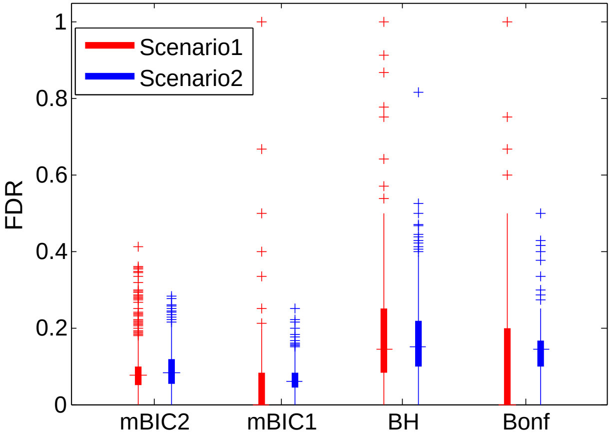
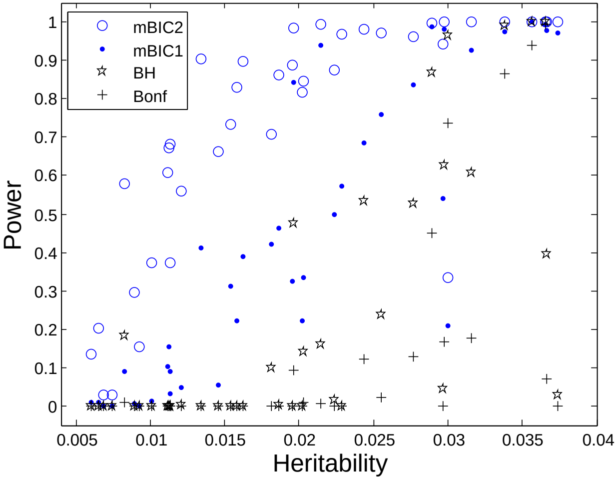
4. False positive - correlation with a causal SNP<0.9

FDR



Power



mBIC2
mBIC1
BH
Bonf
Power
Heritability
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04