Model Selection

ISLR Chapter 6, GH 6 Chapter 24

Voting model with interactions and a subset of predictors

```r
# see code for variable coding
nes1992 = dplyr::select(nes1992, race,  black,
                        gender, educ, income, partyid,
                        ideo, vote)
vote.glm = glm(vote ~ (. -race)^2, data=nes1992,
               family="binomial")
```

Output

	Estimate	Std. Error
(Intercept)	-9.0E+14	2.2E+07
blackTRUE	-1.0E+15	2.4E+07
genderfemale	8.7E+14	2.1E+07
educhigh school graduate	-2.5E+15	2.5E+07
educsome college	-1.7E+15	2.7E+07
educcollege graduate	-1.9E+15	3.7E+07
educmissing	-1.7E+15	6.6E+07
income2	-2.1E+15	2.4E+07
income3	-2.0E+15	3.3E+07
income4	-3.0E+15	7.3E+07
income5	9.3E+14	8.0E+07
incomemissing	-1.0E+15	4.0E+07
partyidindependents	3.6E+15	4.7E+07
partyidrepublicans	7.6E+15	2.7E+07
partyidapolitical	-1.2E+15	1.0E+08
partyidmissing	6.0E+14	1.3E+08

Problems

- large coefficients
- large standard errors! instability
- very small p-values
- lots of NA's
- warnings glm.fit: algorithm did not converge
- warnings glm.fit: fitted probabilities numerically 0 or 1 occurred
- still have over-dispersion

Quasi-Separation (in Binary Data)

Collinearity

Possible Solutions

- Variable Selection: reduce the number of predictors
  - best subset selection of 2^p models (exhaustive enumeration)
  - step-wise selection (forward, backwards, step-wise, MCMC)
- Shrinkage: use all predictors, but the coefficients are shrunk towards 0
  - some shrinkage methods shrink coefficients to zero allowing variable selection (ad hoc)
- Shrinkage + variable selection
- Dimension Reduction: create new variables

Distinguish between goals of good predictions and learning the "true" model

Balancing Goodness of Fit and Model Complexity

Adjusted Deviance: deviance + number of parameters

- adding a variable with a parameter that is zero is expected to decrease the deviance by 1
- adding k variables (all with zero coefficients) is expected to reduce the deviance by k ($\mathsf{E}[\chi^2_k]$ variable)
- needs to be greater than 1
- How much bigger to improve predictions?

Akaike Information Criterion

AIC: deviance + 2 (number of parameters) + each predictor needs to reduce the deviance by 2 to improve the fit to new data

- True data generating model $f(y)$
- Candidate Model $p(y \mid \theta, \mathcal{M})$; estimate $p(y \mid \hat{\theta}, \mathcal{M})$
- measure closeness of candidate to truth by Kullback Leibler divergence

$$
\begin{aligned}
KL(f, \hat{p}_{\mathcal{M}}) &= \int \log \left[\frac{f(y)}{p(y \mid \hat{\theta}, \mathcal{M})} \right] f(y)\, dy \\
&= \int \log(f(y)) f(y)\, dy - \int \log(p(y \mid \hat{\theta}, \mathcal{M})) f(y)\, dy \\
&= C - \int \log(p(y \mid \hat{\theta}, \mathcal{M})) f(y)\, dy
\end{aligned}
$$

Estimating

Naive estimate of integral

$$
\begin{aligned}
K(f, \hat{p}_{\mathcal{M}}) &= C - \int \log(p(y \mid \hat{\theta}, \mathcal{M})) f(y)\, dy \\
&\approx C - \frac{1}{n} \sum_i \log(p(y_i \mid \hat{\theta}, \mathcal{M}))) \\
&= C - \frac{\ell(\hat{\theta}; \mathcal{M})}{n}
\end{aligned}
$$

Akaike showed that the bias was approximately $p_{\mathcal{M}}/n$

Correcting for bias, minimizing KL divergence is the same as minimizing

$$
-\frac{\ell(\hat{\theta}; \mathcal{M})}{n} + \frac{p_{\mathcal{M}}}{n}
$$

or multiplying by $2n$ we get the deviance $+\ 2p_{\mathcal{M}}$

$$
-2\ell(\hat{\theta}; \mathcal{M}) + 2p_{\mathcal{M}}
$$

Bayes Information Criterion (BIC or Schwarz Criterion)

Consider models $\mathcal{M}_1, \ldots \mathcal{M}_K$

Bayes Theorem: probability of model $\mathcal{M}$

$$p(\mathcal{M}_j \mid Y_1, \ldots, Y_n) = \frac{p(Y_1, \ldots, Y_n \mid \mathcal{M}_j) p(\mathcal{M}_j)}{\sum_k p(Y_1, \ldots, Y_n \mid \mathcal{M}_k) p(\mathcal{M}_k)}$$

Pick model that has highest posterior probability

What happened to θ?

$$\begin{aligned} p(Y_1, \ldots, Y_n \mid \mathcal{M}) &= \int p(Y_1, \ldots, Y_n \mid \theta, \mathcal{M}) p(\theta \mid \mathcal{M}) \, d\theta \\ &= \int \mathcal{L}(\theta) p(\theta \mid \mathcal{M}) \, d\theta \end{aligned}$$

Continue

Maximizing $p(\mathcal{M}_j \mid Y_1, \ldots, Y_n)$ is equivalent to picking $\mathcal{M}$ that maximizes

$$\log(p(Y_1, \ldots, Y_n \mid \mathcal{M}_j)) + \log(p(\mathcal{M}_j))$$

Taylor's series expansion of likelihood can be used to show this is approximately

$$\approx \ell_{\mathcal{M}_j}(\hat{\theta}) - \frac{p_{\mathcal{M}_j}}{2} \log(n)$$

Multiply by -2 to obtain BIC $=$ deviance $+$ log(n) (number of parameters)

Not necessarily the best predictive model! But the model that is most likely to be true given the data out of the collection of models under consideration.

R Packages/Functions

- `step` (base R, step-wise)
- `leaps::regsubsets` exhaustive Leaps & Bounds search AIC, BIC linear models
- `bestglim::bestglm` GLM's for AIC, BIC, LOOCV, others
- `BAS:bas.lm` or `BAS:bas.glm` AIC, BIC, more with exhaustive and MCMC as well as model averaging
- `BMA` samples based on leaps and MCMC

Stepwise

```
best.step = step(vote.glm, k=2)  # AIC
```

```
Start:  AIC=11197.27
vote ~ ((race + black + gender + educ + income + partyid +
    race)^2

                 Df Deviance     AIC
- educ:income    19    665.8   867.8
- educ:ideo      12    679.8   895.8
- educ:partyid    8    674.6   898.6
- income:ideo    15  10164.3 10374.3
- gender:partyid  2  10164.3 10400.3
- gender:income   5  10308.5 10538.5
<none>               10957.3 11197.3
- partyid:ideo    6  11461.9 11689.9
- black:partyid   2  12110.7 12346.7
- income:partyid 10  12254.8 12474.8
- black:educ      4  12326.9 12558.9
```

Final Model

```r
summary(best.step)
```

```
Call:
glm(formula = vote ~ black + gender + income + partyid + ic
    black:income + gender:partyid, family = "binomial", dat

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.4090  -0.3516  -0.2055   0.4019   3.3471

Coefficients: (1 not defined because of singularities)
                                  Estimate Std. Error z va
(Intercept)                       -3.64935    0.42549  -8.
blackTRUE                        -17.30639  612.84355  -0.
genderfemale                       0.75432    0.31208   2.
income2                            0.21476    0.37663   0.
income3                            0.07647    0.35021   0.
```

Stepwise

- each step pick the lowest IC model
- add/drop until no improvement
- output is the final model
- possible that forward, backwards, both lead to different final models.

Does not do exhaustive search

Example with bestglm (exhaustive)

```
library(bestglm)
nes1992sub = dplyr::select(nes1992, -race) %>%
          filter(partyid != "apolitical")
vote.AIC = bestglm(Xy=nes1992sub, family=binomial,
                   IC="AIC", RequireFullEnumerationQ = T)
```

```
Morgan-Tatar search since family is non-gaussian.
Note: factors present with more than 2 levels.
```

Notes: dataframe limited to variables under consideration with the response last

Best AIC

```
blackTRUE              -2.1791     0.4419  -4.931 8.20e-07 **
partyidindependents     1.5648     0.2876   5.440 5.32e-08 **
partyidrepublicans      3.8305     0.2037  18.801  < 2e-16 **
partyidmissing          1.0224     1.2645   0.809 0.418765
ideomoderate            0.5971     0.3590   1.663 0.096257 .
ideoconservative        1.6459     0.2215   7.431 1.07e-13 **
ideomissing             1.4722     0.4063   3.624 0.000291 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1767.29  on 1302  degrees of freedom
Residual deviance:  799.31  on 1295  degrees of freedom
AIC: 815.31

Number of Fisher Scoring iterations: 6
```

Best BIC

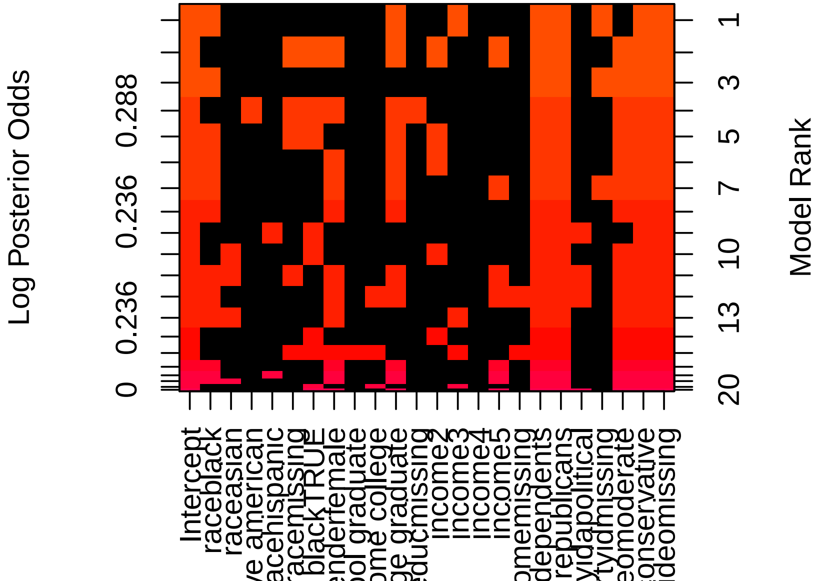
```
blackTRUE              -2.1791     0.4420  -4.931 8.20e-07 **
partyidindependents     1.5648     0.2876   5.440 5.32e-08 **
partyidrepublicans      3.8305     0.2037  18.801  < 2e-16 **
partyidapolitical     -12.2197   535.4112  -0.023 0.981791
partyidmissing          1.0224     1.2645   0.809 0.418765
ideomoderate            0.5971     0.3590   1.663 0.096257 .
ideoconservative        1.6459     0.2215   7.431 1.07e-13 **
ideomissing             1.4722     0.4063   3.624 0.000291 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1768.36  on 1303  degrees of freedom
Residual deviance:  799.31  on 1295  degrees of freedom
AIC: 817.31

Number of Fisher Scoring iterations: 12
```

BAS with AIC

```r
library(BAS)
# nes1992 = mutate(nes1992, vote=as.numeric(vote))
vote.BAS = bas.glm(vote ~ ., data=nes1992,
                   family=binomial(),
                   method="MCMC", n.models=20000,
                   betaprior=aic.prior(),
                   modelprior=uniform())
```

Top models

```r
image(vote.BAS, rotate=T)
```



summary

```r
summary(vote.BAS)
```

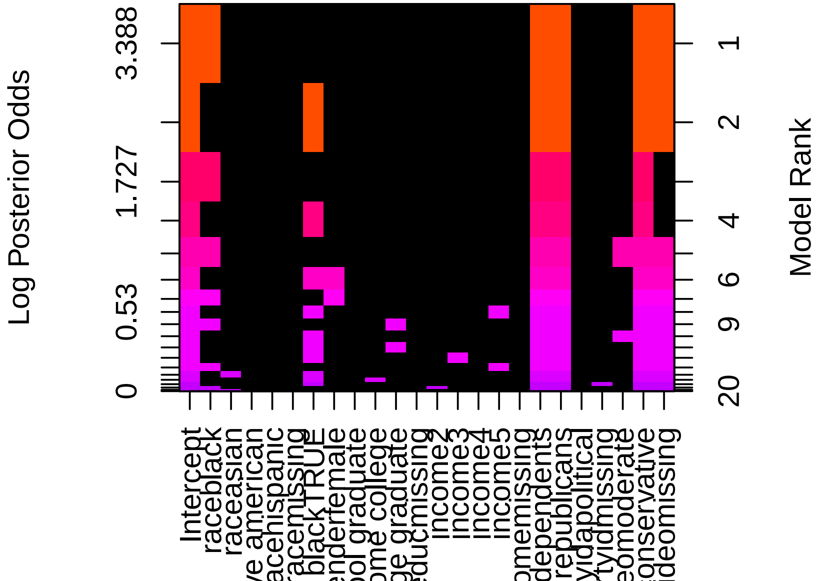
```
                           P(B != 0 | Y)    model 1      mo
Intercept                       1.000000  1.0000000    1.00
raceblack                       0.574300  1.0000000    0.00
raceasian                       0.320025  0.0000000    0.00
racenative american             0.263325  0.0000000    0.00
racehispanic                    0.351650  0.0000000    0.00
racemissing                     0.298150  0.0000000    1.00
blackTRUE                       0.580800  0.0000000    1.00
genderfemale                    0.539450  0.0000000    1.00
educhigh school graduate        0.309300  0.0000000    0.00
educsome college                0.332625  0.0000000    0.00
educcollege graduate            0.517525  1.0000000    1.00
educmissing                     0.333225  0.0000000    0.00
income2                         0.354225  0.0000000    1.00
income3                         0.359500  1.0000000    0.00
income4                         0.287975  0.0000000    0.00
```

BAS with BIC

```
library(BAS)
nes1992 = mutate(nes1992, vote=as.numeric(vote))
vote.BAS = bas.glm(vote ~ ., data=nes1992,
                   family=binomial(),
                   method="MCMC", n.models=20000,
                   betaprior=bic.prior(n = nrow(nes1992)),
                   modelprior=uniform())
```

Top models

```
image(vote.BAS, rotate=T)
```



BAS with BIC

```r
library(BAS)
#nes1992 = mutate(nes1992, vote=as.numeric(vote))
vote.BAS = bas.glm(vote ~ (. - race)^2, data=nes1992,
                   family=binomial(),
                   method="MCMC", n.models=20000,
                   betaprior=bic.prior(n = nrow(nes1992)),
                   modelprior=uniform())
```

Summary

- Various model selection criteria may not all agree on best model
- competing goals of finding the "true" model versus best for prediction
- exhaustive search is not always possible for big p
- Stochastic Search (more in lab)