[3] Big Data: Model Selection

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[3] Making Model Decisions

Out-of-Sample vs In-Sample performance

Regularization paths and the lasso

OOS experiments and Cross Validation

Information Criteria

- AIC and the corrected AICc
- BIC and Bayesian model selection

Some basic facts about linear models

The model is always $\mathbb{E}[y|\mathbf{x}] = f(\mathbf{x}\beta)$.

- Gaussian (linear): $y \sim N(\mathbf{x}\beta, \sigma^2)$.
- ▶ Binomial (logistic): $p(y = 1) = e^{x\beta}/(1 + e^{x\beta})$.

$LHD(\hat{\beta})$ and $dev(\hat{\beta})$:

Likelihood (LHD) is $p(y_1|\mathbf{x}_1) \times p(y_2|\mathbf{x}_2) \cdots \times p(y_n|\mathbf{x}_n)$.

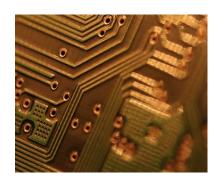
The Deviance (dev) is proportional to -log(LHD).

 $\hat{oldsymbol{eta}}$ is commonly fit to maximize LHD \Leftrightarrow minimize deviance.

Fit is summarized by $R^2 = 1 - \text{dev}(\hat{\beta})/\text{dev}(\beta = 0)$.

The only R^2 we ever really care about is out-of-sample R^2 .

Example: Semiconductor Manufacturing Processes



Very complicated operation Little margin for error.

Hundreds of diagnostics Useful or debilitating?

We want to focus reporting and better predict failures.

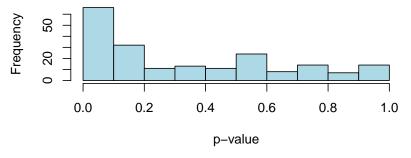
x is 200 input signals, *y* has 100/1500 failures.

Logistic regression for failure of chip *i* is

$$ho_i = exttt{p}(exttt{fail}_i | \mathbf{x}_i) = e^{lpha + \mathbf{x}_i oldsymbol{eta}}/(1 + e^{lpha + \mathbf{x}_i oldsymbol{eta}})$$

Semiconductor FDR Control

The full model has $R^2=0.56$ (based on binomial deviance). The p-values for these 200 coefficients:



Some are clustered at zero, the rest sprawl out to one. FDR of q=0.1 yields $\alpha=0.0122$ p-value rejection cut-off. Implies 25 'significant', of which approx 22-23 are true signals.

semiconductors

A *cut* model, using only these 25 signals, has $R_{cut}^2 = 0.18$. This is much smaller than the full model's $R_{tull}^2 = 0.56$.

In-Sample (IS) R^2 always increases with more covariates. This is exactly what MLE $\hat{\beta}$ is fit to maximize. But how well does each model predict *new* data?

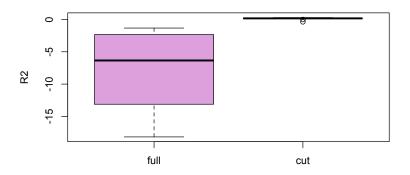
An out-of-sample (OOS) experiment

- split the data into 10 random subsets ('folds').
- ▶ Do 10x: fit model $\hat{\beta}$ using only 9/10 of data, and record R^2 on the left-out subset.

These OOS R^2 give us a sense of how well each model can predict data that it has not already seen.

OOS experiment for semiconductor failure

We gain predictive accuracy by *dropping* variables.



Cut model has mean OOS R2 of 0.09, about 1/2 in-sample R2.

The full model is terrible. It is overfit and worse than \bar{y} . Negative R2 are more common than you might expect.

OOS experimentation

All that matters is Out-of-Sample R^2 . We don't care about In Sample R^2 .

Using OOS experiments to choose the best model is called *cross validation*. It will be a big part of our big data lives.

Selection of 'the best' model is at the core of all big data. But before getting to selection, we first need strategies to build good sets of candidate models to choose amongst.

FDR as a selection tool?

A heretical way to think about 'q': a tuning parameter? Maybe we grab models for $q=0.1,0.2,\ldots$ and compare?

Problems with testing/FDR:

FDR theory requires *independence between tests*. This almost never holds. In regression, multicollinearity causes problems. Given two highly correlated *x*'s you're unsure which to use. You then get big p-values and neither variable is significant.

Regression p-values are based on the full model. This is probably a terrible model. e.g., p-values only exist for p < n.

Forward stepwise regression

Forward stepwise procedures: start from a simple 'null' model, and incrementally update fit to allow slightly more complexity.

Better than backwards methods

- ► The 'full' model can be expensive or tough to fit, while the null model is usually available in closed form.
- ▶ Jitter the data and the full model can change dramatically (because it is overfit). The null model is always the same.

Stepwise approaches are 'greedy': they find the best solution at each step without thought to global path properties.

Naive forward stepwise regression

The step () function in R executes a common routine:

- Fit all univariate models. Choose that with highest (IS) R² and put that variable − say x₍₁₎ − in your model.
- Fit all bivariate models including $x_{(1)}$ ($y \sim \beta_{(1)}x_{(1)} + \beta_j x_j$), and add x_j from one with highest R^2 to your model.
- ► Repeat: max R² by adding one variable to your model.

You stop when some model selection rule (AIC) is lower for the current model than for any of the models that add one variable.

Forward stepwise regression in R

Easiest way to step(): run null and full regressions.

```
null = glm(y ~ 1, data=D)
full = glm(y ~ ., data=D)
fwd = step(null, scope=formula(full), dir="forward")
scope is the biggest possible model.
```

Iterate for interactions: fwd2 = step(fwd, scope=.^2, ...

Example: semiconductors...

The problem with Subset Selection

```
step() is very slow (e.g., 90 sec for tiny semiconductors)
```

This is true in general with subset selection (SS):

Enumerate candidate models by applying maximum likelihood estimation for subsets of coefficients, with the rest set to zero.

SS is slow because adding one variable to a regression can change fit dramatically: *each model must be fit from scratch*.

A related subtle (but massively important) issue is stability.

MLEs have high *sampling variability*: they change a lot from one dataset to another. So which MLE model is 'best' changes a lot.

⇒ predictions based upon the 'best' model will be have high variance. And big variance leads to big expected errors.

Regularization

The key to contemporary statistics is regularization: depart from optimality to stabilize a system.

Common in engineering: I wouldn't drive on an optimal bridge.

We minimize deviance

$$\min - \frac{2}{n} \log \mathsf{LHD}(\beta)$$

Regularization

The key to contemporary statistics is regularization: depart from optimality to stabilize a system.

Common in engineering: I wouldn't drive on an optimal bridge.

We minimize deviance plus a cost on the size of coefficients.

$$\min - \frac{2}{n} \log \mathsf{LHD}(\boldsymbol{\beta}) + \lambda \sum_{k} |\beta_k|$$

This particular cost gives the 'lasso': the new least squares.

Decision theory: Cost in Estimation

Decision theory is based on the idea that choices have costs. Estimation and hypothesis testing: what are the costs?

Estimation:

Deviance is the cost of distance between data and the model.

Recall:
$$\sum_{i} (y_i - \hat{y}_i)^2 \text{ or } -\sum_{i} y_i \log(\hat{p}_i) - (1 - y_i) \log(1 - \hat{p}_i).$$

Testing:

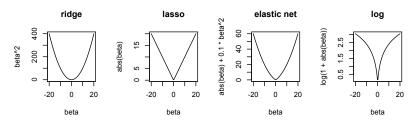
Since $\hat{\beta}_i = 0$ is *safe*, it should cost us to decide otherwise.

 \Rightarrow The cost of $\hat{\beta}$ is deviance plus a penalty away from zero.

[Sparse] Regularized Regression

$$\min \left\{ -\frac{2}{n} \log \mathsf{LHD}(\boldsymbol{\beta}) + \lambda \sum_{j} c(\beta_{j}) \right\}$$

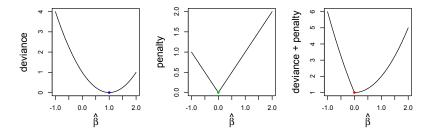
 $\lambda > 0$ is the penalty weight, c is a cost (penalty) function. $c(\beta)$ will be lowest at $\beta = 0$ and we pay more for $|\beta| > 0$.



Options: ridge β^2 , lasso $|\beta|$, elastic net $\alpha\beta^2 + |\beta|$, $\log(1 + |\beta|)$.

Penalization can yield automatic variable selection

The minimum of a smooth + pointy function can be at the point.



Anything with an absolute value (e.g., lasso) will do this.

There are MANY penalty options and far too much theory.

Think of lasso as a baseline, and others as variations on it.

Lasso Regularization Paths

The lasso fits $\hat{\beta}$ to minimize $-\frac{2}{n} \log \text{LHD}(\beta) + \lambda \sum_{j} |\beta_{j}|$. We'll do this for a *sequence* of penalties $\lambda_{1} > \lambda_{2}... > \lambda_{T}$.

Then we can apply model selection tools to choose best $\hat{\lambda}$.

Path estimation:

Start with big λ_1 so big that $\hat{\boldsymbol{\beta}} = \mathbf{0}$.

For $t = 2 \dots T$: update $\hat{\beta}$ to be optimal under $\lambda_t < \lambda_{t-1}$.

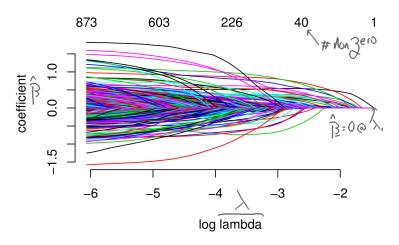
Since estimated $\hat{\beta}$ changes smoothly along this path:

- It's fast! Each update is easy.
- ▶ It's stable: optimal λ_t may change a bit from sample to sample, but that won't affect the model much.

It's a better version of forward stepwise selection.

Path plots

The whole enterprise is easiest to understand visually.



The algorithm moves *right to left*. The *y*-axis is $\hat{\beta}$ (each line a different $\hat{\beta}_i$) as a function of λ_t .

Example: Comscore web browser data

The previous plot is household log-online-spend regressed onto % of time spent on various websites (each β_i a different site).

Comscore (available via WRDS) records info on browsing and purchasing behavior for annual panels of households.

I've extracted 2006 data for the 1000 most heavily trafficked websites and for 10,000 households that spent at least 1\$.

Why do we care? Predict consumption from browser history. e.g., to control for base-level spending, say, in estimating advertising effectiveness. You'll see browser history of users when they land, but likely not what they have bought.

Add-on Packages for R

Much of R's capability comes from its packages, little pieces of purpose-specific statistical software.

You can add-on with the install.packages menu or cmd.

- ► A good mirror is http://cran.rstudio.com.
- ► You should 'install dependencies' when adding packages.
- ► Every package has a website on cran.r-project.org.

Today we'll be using

- gamlr: L0 to L1 penalized regression.
- Matrix: fancy sparse matrices.

Once installed, do (e.g.) library (gamlr) to use a package.

Lasso Software

There are many packages for fitting lasso regressions in R.

glmnet is most common. gamlr is my contribution. These two are very similar, and they share syntax.

Big difference is what they do beyond a simple lasso:.

```
glmnet does an 'elastic net': c(\beta) = |\beta| + \nu \beta^2. gamlr does a 'gamma lasso': c(\beta) \approx \log(\nu + |\beta|).
```

Since we stick mostly to lasso, they're nearly equivalent for us. gamlr just makes it easier to apply some model selection rules.

Both use the Matrix library representation for sparse matrices.

Diversion: Simple Triplet Matrices

Often, your data will be very sparse (i.e, mostly zeros). It is then efficient to ignore zero elements in storage.

A simple triplet matrix (STM) has three key elements:

The row 'i', column 'j', and entry value 'x'.

Everything else in the matrix is assumed zero.

For example:

$$\begin{bmatrix} -4 & 0 \\ 0 & 10 \\ 5 & 0 \end{bmatrix} \text{ is stored as } \begin{cases} i = 1, 3, 2 \\ j = 1, 1, 2 \\ x = -4, 5, 10 \end{cases}$$

The Matrix library provides STM storage and tools. See comscore.R for how to get data into this format.

Creating Sparse Design Matrices

For gamlr/glmnet you need to build your own design matrix i.e., what the $y \sim x1 + x2$ formula does for you inside glm.

In lecture 2 we saw how to do this with model.matrix for dense matrices. The sparse version works the same way.

Sparse Factor Designs

Under penalization, factor reference levels now matter!

We're shrinking effects towards zero, which means every factor effect is shrunk towards the reference level.

My solution is to just get rid of the reference level.

Then every factor level effect is shrunk towards a shared intercept, and only significantly distinct effects get nonzero $\hat{\beta}$.

In particular, code in <code>naref.R</code> makes NA, R's code for 'missing', the reference level for factors. This has the extra advantage of giving us a framework for missing data...

```
> demo <- naref(demo)
> levels(demo$region)
[1] NA "MW" "NE" "S" "W"
```

Running a lasso

Once you have your x and y, running a lasso is easy.

```
spender <- gamlr(xweb, log(yspend))
plot(spender) # nice path plot
spender$beta[c("mtv.com","zappos.com"),]</pre>
```

And you can do logistic lasso regression too

```
gamlr(x=SC[,-1], y=SC$FAIL, family="binomial")
```

You should make sure that y is numeric 0/1 here, not a factor.

Some common arguments

- verb=TRUE to get progress printout.
- ▶ nlambda: T, the length of your λ grid.
- ▶ lambda.min.ratio: λ_T/λ_1 , how close to MLE you get.

See ?gamlr for details and help.

Size Matters

Penalization means that scale matters. e.g., $x\beta$ has the same effect as $(2x)\beta/2$, but $|\beta|$ is twice as much penalty as $|\beta/2|$.

You can multiply β_j by $sd(x_j)$ in the cost function to standardize.

That is, minimize $-\frac{2}{n} \log LHD(\beta) + \lambda \sum_{j} \operatorname{sd}(x_{j}) |\beta_{j}|$.

 $\Rightarrow \beta_j$'s penalty is calculated per effect of 1SD change in x_j .

gamlr and glmnet both have standardize=TRUE by default. You only use standardize=FALSE if you have good reason. e.g., in today's homework. But usually standardize=TRUE.

Regularization and Selection

The lasso minimizes $-\frac{2}{n} \log LHD(\beta) + \lambda \sum_{j} |\beta_{j}|$.

This 'sparse regularization' auto-selects the variables.

Sound too good to be true? You need to choose λ .

Think of $\lambda > 0$ as a signal-to-noise filter: *like squelch on a radio.*

We'll use cross validation or information criteria to choose.

Path algorithms are key to the whole framework:

- * They let us quickly enumerate a set of candidate models.
- ⋆ This set is stable, so selected 'best' is probably pretty good.

Prediction vs Evidence

Testing is all about: *is this model true?*We want to know: *what is my best guess?*

None of your models will be 'true' for complicated HD systems. Instead, just try to get as close to the truth as possible.

Ask: which model does best in predicting unseen data?

- Overly simple models will 'underfit' available patterns.
- Complicated models 'overfit', and make noisy predictors.

The goal is to find the sweet spot in the middle.

Even in causal inference, we'll combine best-predicting models to obtain structural interpretation for a few chosen variables.

Model Selection: it is all about prediction.

A recipe for model selection.

- Find a manageable set of candidate models (i.e., such that fitting all models is fast).
- 2. Choose amongst these candidates the one with best predictive performance *on unseen data*.
- 1. is what the lasso paths provide.
- 2. Seems impossible! But it's not ...

First, define predictive performance via 'deviance'.

Then, we need to *estimate* deviance for a fitted model applied to *new independent observations* from the true data distribution.

Out-of-sample prediction experiments

We already saw an OOS experiment with the semiconductors. Implicitly, we were estimating predictive deviance (via R^2).

The procedure of using such experiments to do model selection is called Cross Validation (CV). It follows a basic algorithm:

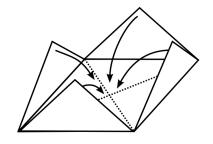
For
$$k = 1 \dots K$$
,

- ▶ Use a subset of $n_k < n$ observations to 'train' the model.
- Record the error rate for predictions from this fitted model on the left-out observations.

We'll usually measure 'error rate' as deviance. But alternatives include MSE, misclass rate, integrated ROC, or error quantiles. You care about both average and spread of OOS error.

K-fold Cross Validation

One option is to just take repeated random samples. It is better to 'fold' your data.



- Sample a random ordering of the data (important to avoid order dependence)
- Split the data into *K* folds: 1st 100/K%, 2nd 100/K%, etc.
- Cycle through K CV iterations with a single fold left-out.

This guarantees each observation is left-out for validation, and lowers the sampling variance of CV model selection.

Leave-one-out CV, with K = n, is nice but takes a long time. K = 5 to 10 is fine in most applications.

CV Lasso

The lasso path algorithm minimizes $-\frac{2}{n} \log \text{LHD}(\beta) + \lambda_t \sum_j |\beta_j|$ over the sequence of penalty weights $\lambda_1 > \lambda_2 \ldots > \lambda_T$.

This gives us a path of T fitted coefficient vectors, $\hat{\beta}_1 \dots \hat{\beta}_T$, each defining deviance for new data: $-\log p(\mathbf{y}^{new} \mid \mathbf{X}^{new} \hat{\beta}_t)$.

Set a sequence of penalties $\lambda_1 \dots \lambda_T$.

Then, for each of k = 1 ... K folds,

- Fit the path $\hat{\beta}_1^k \dots \hat{\beta}_T^k$ on all data *except* fold k.
- ▶ Get fitted deviance on left-out data: $-\log p(\mathbf{y}^k \mid \mathbf{X}^k \hat{\boldsymbol{\beta}}_t)$.

This gives us K draws of OOS deviance for each λ_t .

Finally, use the results to choose the 'best' $\hat{\lambda}$, then re-fit the model to *all of the data* by minimizing $-\frac{2}{n} \log \text{LHD}(\beta) + \hat{\lambda} \sum_{j} |\beta_{j}|$.

CV Lasso

Both gamlr and glmnet have functions to wrap this all up. The syntax is the same; just preface with cv.

```
cv.spender <- cv.gamlr(xweb, log(yspend))</pre>
```

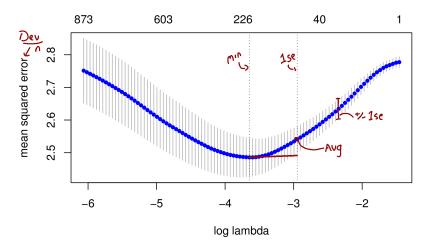
Then, coef (cv.spender) gives you \hat{eta}_t at the 'best' λ_t

- ▶ select="min" gives λ_t with min average OOS deviance.
- ▶ select="1se" defines best as biggest λ_t with average OOS deviance no more than 1SD away from the minimum.

1se is default, and balances prediction against false discovery. \min is purely focused on predictive performance.

CV Lasso

Again, the routine is most easily understood visually.



Both selection rules are good; 1se has extra bias for simplicity.

Problems with Cross Validation

It is time consuming: When estimation is not instant, fitting K times can become unfeasible even K in 5-10.

It can be unstable: imagine doing CV on many different samples. There can be large variability on the model chosen.

It is hard not to cheat: for example, with the FDR cut model we've already used the full *n* observations to select the 25 strongest variables. It is not surprising they do well 'OOS'. The rules: if you do something to the data, do it *inside* CV.

Still, some form of CV is used in most DM applications.

Alternatives to CV: Information Criteria

Many 'Information Criteria' out there: AICc, AIC, BIC, ...
These approximate distance between a model and 'the truth'.
You can apply them by choosing the model with minimum IC.

Most common is Akaike's AIC = Deviance + 2df.

df = 'degrees of freedom' used in your model fit. For lasso and MLE, this is just the # of nonzero $\hat{\beta}_j$.

For example, the summary.glm output reports

```
Null deviance: 731.59 on 1476 degrees of freedom Residual deviance: 599.04 on 1451 degrees of freedom AIC: 651.04
```

and many recommend picking the model with smallest AIC. Note the d.o.f. in R output is 'd.o.f. left after fit': n - df.

AIC overfits in high dimensions

The AIC is atually estimating OOS deviance: what your deviance would be on another *independent* sample of size *n*.

IS deviance is too small, since the model is tuned to this data. Some deep theory shows that IS - OOS deviance $\approx 2 \textit{df}$.

 \Rightarrow AIC \approx OOS deviance.

Its common to claim this approx (i.e., AIC) is good for 'big n'. Actually, its only good for big n/df.

In Big Data, df (# parameters) can be huge. Often $df \approx n$. In this case the AIC will be a bad approximation: it overfits!

AIC corrected: AICc

AIC approximates OOS deviance, but does a bad job for big df.

In linear regression an improved approx to OOS deviance is

AICc = Deviance +
$$2df\mathbb{E}\left[\frac{\sigma^2}{\hat{\sigma}^2}\right]$$
 = Deviance + $2df\frac{n}{n-df-1}$

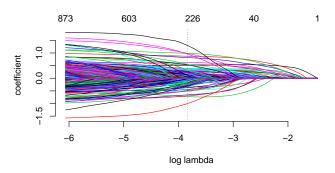
This is the corrected AIC, or AICc.

It also works nicely in logistic regression, or for any glm.

Notice that for big n/df, AICc \approx AIC. So *always* use AICc.

gamlr uses AICc

It's marked on the path plot



And it is the default for coef.gamlr

```
B <- coef(spender)[-1,]
B[c(which.min(B),which.max(B))]
    cursormania.com shopyourbargain.com
    -0.998143
    1.294246</pre>
```

Another option: Bayes IC

The BIC is Deviance + $\log(n) \times df$.

This looks just like AIC, but comes from a very different place.

 $BIC \approx -\log p(M_b|\text{data})$, the 'probability that model b is true'.

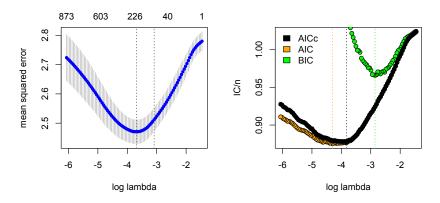
$$p(\textit{M}_\textit{b}|\text{data}) = \frac{p(\text{data}, \textit{M}_\textit{b})}{p(\text{data})} \propto \underbrace{p(\text{data}|\textit{M}_\textit{b})}_{\text{LHD}} \underbrace{p(\textit{M}_\textit{b})}_{\text{prior}}$$

The 'prior' is your probability that a model is true *before* you saw any data. BIC uses a 'unit-info' prior: $N\left[\hat{\beta}, \frac{2}{n} \text{var}(\hat{\beta})^{-1}\right]$

AIC[c] tries to approx OOS deviance.

BIC is trying to get at the 'truth'.

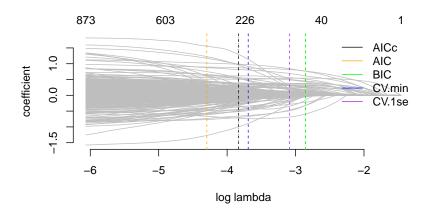
IC and CV on the Comscore Data



The take home message: AICc curve looks like CV curve.

In practice, BIC works more like the 1se CV rule. But with big *n* it chooses too simple models (it underfits).

IC and CV on the Comscore Data



With all of these selection rules, you get a range of answers. If you have time, do CV. But AICc is fast and stable. If you are worried about false discovery, tend towards BIC/1se.



Hockey Homework: what are individual players contributing?

A stat for player performance is the 'plus-minus' (PM).

PM is a function of goals scored while that player is on the ice: the number of goals for his team, minus the number against.

There is no accounting for teammates or opponents.

Due to 'line matching' this could make a big difference.

Can we build a better performance metric with regression?

Hockey Regression

Response is a binary 1 if home goal, 0 if away goal. Home players get an x-value of +1, and away players -1. Everyone off the ice is zero.

players (onice) home goal? AARON_DOWNEY ZIGMUND_PALFFY
$$1 \qquad \qquad 1 \qquad \qquad 1 \qquad \ldots \qquad 0 - 1 \ 0 \ \ldots \qquad 0$$

Our logistic regression plus-minus model is

$$\log \frac{p(y=1)}{1-p(y=1)} = \beta_0 + \sum_{\text{homeplayers}} \beta_j - \sum_{\text{awayplayers}} \beta_j$$

 β_j is j^{th} player's partial effect: When a goal is scored and player j is on ice, odds are multiplied by e^{β_j} that his team scored.

Hockey Regression

In addition to 'controlling' for the effect of who else is on the ice, we also want to control for things unrelated to player ability. (crowd, coach, schedule, ...)

We'll a 'fixed effect' for each team-season, $\alpha_{team,season}$. Also, special configurations (e.g., 5 on 4 power play) get α_{config} . So the full model has 'log odds that a goal was by home team'

$$eta_0 + lpha_{\textit{team}, \textit{season}} + lpha_{\textit{config}} + \sum_{\textit{homeplayers}} eta_j - \sum_{\textit{awayplayers}} eta_j$$

gamlr includes data on NHL goals from 2002/03-2012/13. The code to design and fit this model is in hockey_start.R. Via the free argument, only player β_k 's are penalized.

Homework due next lecture

- [1] Interpret AICc selected model from my nhlreg lasso. Just tell some stories about what the model tells you.
- [2] The gamlr run for nhlreg uses standardize=FALSE. Why did I do this? What happens if you do standardize?
- [3] Compare model selection methods for the nhlreg lasso. Consider both IC and CV (you'll want to create cv.nhlreg).
- [4] We've controlled our estimates for confounding information from team effects and special play configuration. How do things change if we ignored this info (i.e., fit a player-only model)? Which scheme is better (interpretability, CV, and IC)?
- [+] Can you translate player β_k effects into something comparable to classic Plus-Minus? How do things compare?