Model Selection: Information Criteria and Sparsity Approaches

CS 6190: Probabilistic Modeling

March 1, 2018

Linear Model Selection

Linear Model:

$$
\begin{aligned}
y &= X\beta + \epsilon \\
&= \beta_0 + x_1\beta_1 + x_2\beta_2 + \ldots + x_K\beta_K + \epsilon
\end{aligned}
$$

$$\epsilon \sim N(0, \sigma^2)$$

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$$

$$\epsilon \sim N(0, \sigma^2)$$

Model Selection Problem:

Which regressors, x_i, should we include in the model?

OASIS Brain Data

http://www.oasis-brains.org

```
> head(cdat[,-1])


  M.F Age MMSE CDR eTIV  nWBV RightHippoVol LeftHippoVol
1   F  73   27 0.5 1454 0.708          2896         2801
2   M  74   30 0.0 1636 0.689          2832         2578
3   F  81   30 0.0 1664 0.679          3557         3495
4   M  76   28 0.5 1738 0.719          3052         2770
5   M  82   27 0.5 1477 0.739          3421         3119
6   F  89   30 0.0 1536 0.715          3760         3167
```

MMSE: Mini-Mental State Exam

CDR : Clinical Dementia Rating

eTIV: Estimated Total Intracranial Volume

nWBV: Normalized Whole Brain Volume

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Hypotheses of interest:

- Hippocampal volume decreases with age

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Hypotheses of interest:

- Hippocampal volume decreases with age
- Lower hippocampal volume is also associate with cognitive decline (as measured by MMSE, CDR)

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```

What models do we use to test these hypotheses?

- Should we include all variables simultaneously (Age, MMSE, CDR)?
- Which covariates should we include (M.F, eTIV, nWBV)?

All models are wrong, but some are useful.

— George Box

Why not include all the variables we have?

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1. Danger of overfitting
2. Each parameter we estimate requires more data

Why not just include covariates that have a "significant" effect in the linear model?

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Let’s see!

Age Effects Only

```
> g1 = lm(RightHippoVol ~ Age, data = cdat)
> coef(summary(g1))

            Estimate Std. Error t value  Pr(>|t|)
(Intercept)  5660.19    361.858  15.642 9.477e-36
Age           -28.85      4.721  -6.111 5.668e-09
```

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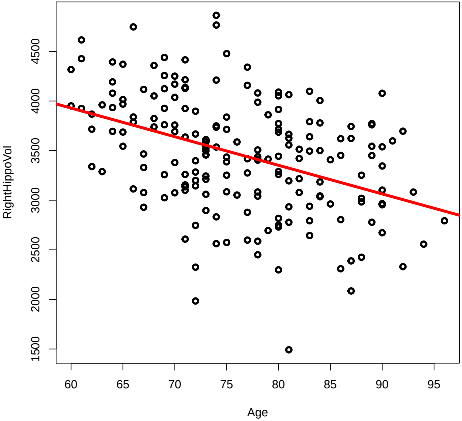
```

Age effect is significant

Age Effects Only

```
> plot(RightHippoVol ~ Age, data = cdat, lwd = 3)
> abline(g1, col = 'red', lwd = 4)
```



Adding Sex Covariate

```
> g2 = lm(RightHippoVol ~ Age + M.F, data = cdat)
> coef(summary(g2))

            Estimate Std. Error t value  Pr(>|t|)
(Intercept)  5595.85     362.07  15.455 3.847e-35
Age           -28.62       4.70  -6.088 6.437e-09
M.FM          137.93      81.56   1.691 9.249e-02
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```

Age effect is significant

Sex effect is significant

Adding Brain Volume Covariate

```
> g3 = lm(RightHippoVol ~ Age + M.F + nWBV, data = cdat)
> coef(summary(g3))

             Estimate Std. Error t value  Pr(>|t|)
(Intercept)  -509.99   1045.230 -0.4879 6.262e-01
Age           -10.23      5.228 -1.9570 5.186e-02
M.FM          220.60     75.666  2.9155 3.993e-03
nWBV         6338.75   1029.398  6.1577 4.524e-09
```

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```

Age effect is NOT significant

Sex effect is significant

Whole brain volume effect is significant

Adding Clinical Dementia Rating

```
> g4 = lm(RightHippoVol ~ Age + M.F + nWBV + CDR, data = cdat)
> coef(summary(g4))

            Estimate Std. Error t value  Pr(>|t|)
(Intercept)  1828.92   1077.497   1.697 9.133e-02
Age           -15.05      4.982  -3.021 2.878e-03
M.FM          237.85     70.921   3.354 9.692e-04
nWBV         3877.48   1074.262   3.609 3.960e-04
CDR          -496.90     95.796  -5.187 5.632e-07
```

Adding Clinical Dementia Rating

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> g4 = lm(RightHippoVol ~ Age + M.F + nWBV + CDR, data = cdat)
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Everything is significant!

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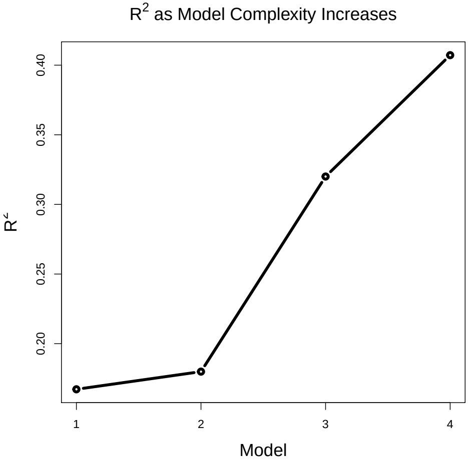
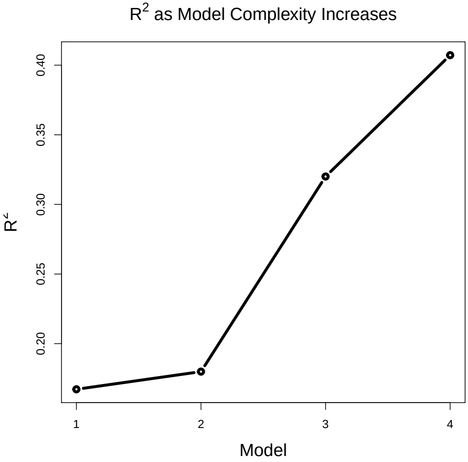
- Can't choose models based on p-values!
- Statistical significance can be manipulated by inclusion/exclusion of covariates
- Need a systematic and automatic method for selecting models
- Included variables and model selection procedure should be decided before analysis

Highest R^2 or Likelihood?



Highest R^2 or Likelihood?



R^2 always increases when you add covariates

Occam's Razor

Choose the simplest model that explains your data, i.e., the fewest parameters.

Akaike Information Criteria[1]

Pick the model that minimizes

$$\mathrm{AIC} = 2k - 2\ln(L)$$

k: number of parameters

L: log-likelihood

[1] Akaike, IEEE TAC, 1974

Akaike Information Criteria[1]

Pick the model that minimizes

$$\mathrm{AIC} = 2k - 2\ln(L)$$

k: number of parameters
L: log-likelihood

Tradeoff between

maximizing likelihood
and
minimizing number of parameters

[1] Akaike, IEEE TAC, 1974

AIC Under Gaussian Likelihood

If the model has normally-distributed errors,

$$\begin{aligned} \mathrm{AIC} &= 2k - 2\ln(L) \\ &= 2k + n\ln\left(\frac{1}{n}\sum_{i=1}^{n}\hat{\epsilon}_i{}^2\right) \end{aligned}$$

$\hat{\epsilon}_i$: estimated residual of ith data point

Motivation of AIC

- We want the best approximation of some "true" density $f(x)$.
- Given candidate models: $g_i(x|\theta_i)$

$$K(f, g_i) = \int f(x) \ln f(x) dx - \int f(x) \ln g_i(x|\theta_i) dx$$

Motivation of AIC

- We want the best approximation of some “true” density $f(x)$.
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- AIC approximates this KL divergence (up to a constant in g_i)

AICc: Bias-corrected AIC

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AICc: Bias-corrected AIC

- AIC has a first-order correction for bias
- The bias can still be significant for small n
- A second-order correction of the bias gives:

$$\mathrm{AICc} = \mathrm{AIC} + \frac{2k(k+1)}{n-k-1}$$

Nice Review Article on AIC

Burnham, K. P.; Anderson, D. R. (2004), “Multimodel inference: understanding AIC and BIC in Model Selection”, Sociological Methods and Research 33: 261-304.

R Package: `FindMinIC`

Install from CRAN:

```
> install.packages("FindMinIC")
```

- Tests all 2^K possible subsets of K regressors
- Ranks them based on AIC (or AICc, or BIC)
- Regressors can be fixed to always be included

OASIS Example Revisited

```
> aicModels = FindMinIC(
+   RightHippoVol ~ Age + CDR + MMSE + M.F + nWBV + eTIV,
+   data = cdat)
> print(summary(aicModels)$table[1:5,])

     AIC  formula
[1,] 2814 "+Age + CDR + eTIV + nWBV"
[2,] 2815 "+Age + CDR + MMSE + eTIV + nWBV"
[3,] 2816 "+Age + CDR + M.F + eTIV + nWBV"
[4,] 2817 "+Age + CDR + M.F + MMSE + eTIV + nWBV"
[5,] 2821 "+CDR + eTIV + nWBV"
```

OASIS Example Revisited

```
> summary(getFirstModel(aicModels))



Call:
lm(formula = RightHippoVol ~ +Age + CDR + eTIV + nWBV, data = tmp.gds)

Residuals:
    Min      1Q  Median      3Q     Max 
-1692.1  -258.1     9.3   285.0  1341.0 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) -862.449   1131.062   -0.76   0.4467    
Age          -13.822      4.671   -2.96   0.0035 ** 
CDR         -462.349     89.816   -5.15  6.8e-07 ***
eTIV           1.237      0.201    6.15  4.9e-09 ***
nWBV        5040.797   1033.980    4.88  2.4e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 423 on 183 degrees of freedom
Multiple R-squared:  0.478,Adjusted R-squared:  0.467 
F-statistic:   42 on 4 and 183 DF,  p-value: <2e-16
```

Model Selection via Sparsity

- Idea: force coefficients to zero by penalizing non-zero entries
- Sparse approximation:

  $$\hat{\beta} = \arg\min_{\beta} \|y - X\beta\|^2 + \lambda\|\beta\|_0.$$

  Using l_0 norm:

  $$\|\beta\|_0 = \text{“number of non-zero elements of } \beta\text{”}$$

- This is an NP-hard optimization problem

The lasso[2]

- The l_1 norm is a convex relaxation of the l_0 norm:

$$||\beta||_1 = \sum_{i=1}^{K} |\beta_i|$$

- The lasso estimator is

$$\hat{\beta} = \arg\min_{\beta} ||y - X\beta||^2 + \lambda ||\beta||_1$$

- This is now a convex optimization problem

[2] *Tibshirani, J. Royal. Statist. Soc B., 1996*

Adaptive Sparsity[3]

- Hierarchical prior on β:

$$\beta \sim N(0, \tau)$$
$$\tau \propto \frac{1}{\tau}$$

[3] *Figueiredo, PAMI 2003*

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- MAP estimation of β by EM algorithm

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Adaptive Sparsity[3]

- Hierarchical prior on β:

$$\beta \sim N(0, \tau)$$
$$\tau \propto \frac{1}{\tau}$$

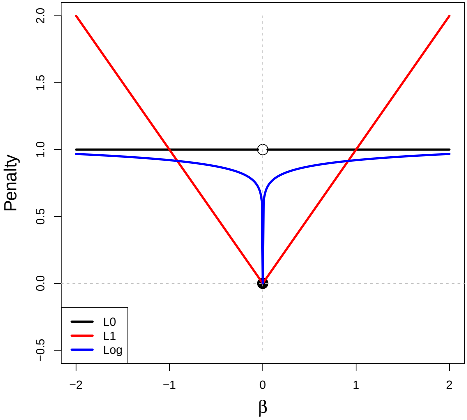
- Parameter-free Jeffreys' hyperprior on τ
- MAP estimation of β by EM algorithm
- After marginalizing τ, equivalent to a log penalty:

$$\log p(\beta) \propto \log(|\beta| + \delta) - \log(\delta)$$

(Need the $\delta > 0$ fudge factor for numerics)

[3] *Figueiredo, PAMI 2003*

Comparison of Penalty Functions



R Package: AdaptiveSparsity

Install from CRAN:

```
> install.packages(AdaptiveSparsity)
```

- Implements Figueiredo's adaptively sparse linear regression (`aslm`)
- Also has a method for estimating sparse Gaussian graphical models (`asggm`)[4]

[4] *Wong, Awate, Fletcher, ICML 2013*

OASIS Example Re-Revisited

```
> g = aslm(
+   RightHippoVol ~ Age + CDR + MMSE + M.F + nWBV + eTIV,
+   data = cdat)
> as.matrix(coef(g))


                  [,1]
(Intercept)      0.000
Age            -15.619
CDR           -477.447
MMSE             0.000
M.FM             0.000
nWBV          4284.793
eTIV             1.126
```

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Same coefficients chosen by AIC!

An Interesting Connection

Sparse approximation is **equivalent** to AIC!

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$$\hat{\beta} = \arg\min_{\beta} \|y - X\beta\|^2 + \lambda\|\beta\|_0$$

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Sparse approximation is **equivalent** to AIC!

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\begin{aligned}
\hat{\beta} &= \arg\min_{\beta} \|y - X\beta\|^2 + \lambda \|\beta\|_0 \\
&= \arg \min_{k, \|\beta\|_0 = k} -2 \ln L(\beta | y) + 2k, \quad \text{(setting } \lambda = 2\text{)}
\end{aligned}
$$

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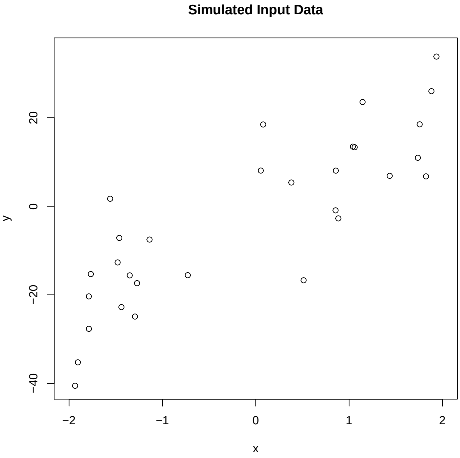
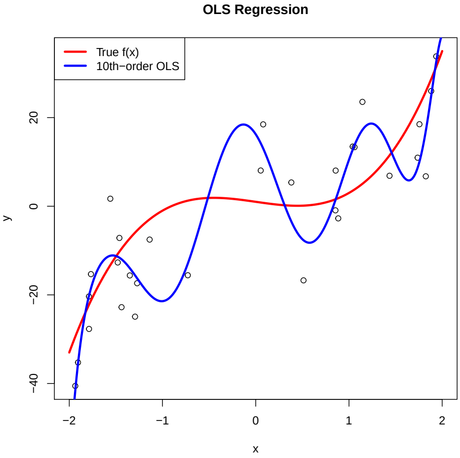
&= \arg\min_{k, \|\beta\|_0 = k} \mathrm{AIC}(\beta)
\end{aligned}
$$

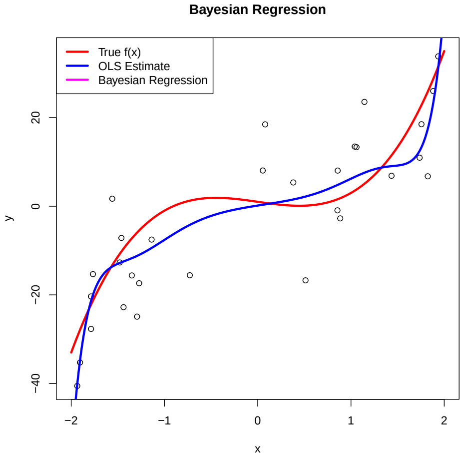
Polynomial Regression Example Revisited



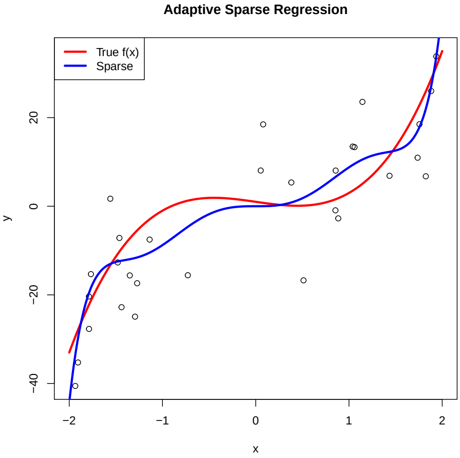
Ordinary Least Squares



Bayesian (Ridge) Regression



Adaptive Sparse Regression



Comparing Coefficient Estimates

```
> print(betaHat)

 [1]   16.238  -32.289 -107.265  106.119  152.427  -76.752
 [7]  -86.301   20.668   21.362   -1.805   -1.936

> print(betaPost)

 [1]  0.156257  3.350884 -0.737490  3.461802 -0.156540
 [6]  1.778690  0.058276 -2.150563 -0.004735  0.458031
[11] -0.002479

> print(betaSparse)

 [1]  0.000  0.000  0.000 16.616  0.000 -9.536  0.000
 [8]  1.692  0.000  0.000  0.000
```