Nonconvex penalties: Algorithms and case studies

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Introduction

- In today's lecture, we will discuss the performance of nonconvex penalties with respect to the signal-to-noise ratio of the data-generating process, the most critical factor determining their success relative to the lasso
- We will then turn our attention to the details of model fitting, discussing algorithms for nonconvex penalties as well as the impact of nonconvexity on model-fitting

Signal to noise ratio

- For linear regression,

$$\begin{aligned}\mathrm{Var}(Y) &= \mathrm{Var}(\mathrm{E}(Y|X)) + \mathrm{E}(\mathrm{Var}(Y|X)) \\ &= \boldsymbol{\beta}^\top \mathrm{Var}(X)\boldsymbol{\beta} + \sigma^2\end{aligned}$$

- The first term in the sum is known as the *signal* and the second term the *noise*
- Thus, we may define the *signal-to-noise ratio*

$$\mathrm{SNR} = \boldsymbol{\beta}^\top \mathrm{Var}(X)\boldsymbol{\beta}/\sigma^2$$

SNR and R^2

- Recall that we have seen this decomposition before, in calculating R^2, which is also a function of the signal and noise
- In particular, note that

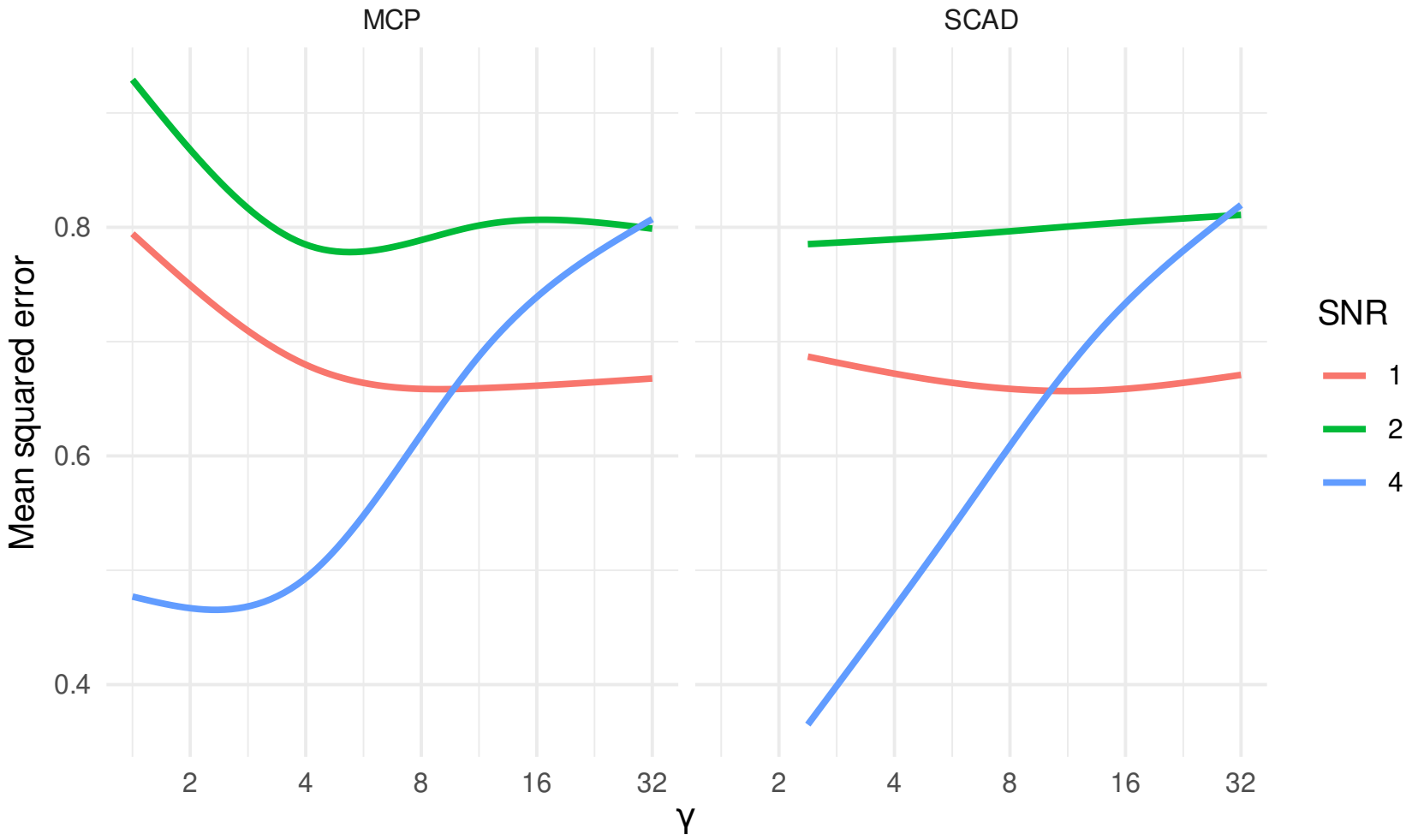
$$R^2 = \frac{\text{SNR}}{1 + \text{SNR}}$$

- As a general piece of advice, I strongly recommend considering the signal-to-noise ratio when designing simulations, and avoiding settings where SNR is, say, 50 ($R^2 = .98$); is this realistic?

Simulation: Setup

- To see the impact of SNR, let's set $n = 50$, $p = 100$, and let all features $\mathbf{x}_j$ follow independent, standard Gaussian distributions
- In the generating model, we set $\beta_1 = \beta_2 = \beta_3 = \cdots = \beta_6 \neq 0$ and $\beta_7 = \beta_8 = \cdots = \beta_{100} = 0$, varying the nonzero values of β_1 through β_6 to produce a range of signal to noise ratios
- For each data set, an independent data set of equal size was generated for the purposes of selecting the regularization parameter

Simulation: Results



Remarks

- The motivation of MCP/SCAD/etc. is to eliminate bias for large coefficients; it should not be a surprise, then, that the advantage of these methods only becomes apparent when some nonzero coefficients are large
- It is also worth noting that $\gamma \approx 3$ is generally a reasonable choice for MCP – its performance was never far from the best
- Also note that the SCAD is somewhat less sensitive to the choice of γ, in the sense that many values of γ produce rather lasso-like estimates

Algorithm

Letting $\tilde{z} = n^{-1}\mathbf{x}_j^\top \tilde{\mathbf{r}}_j$, F is the firm-thresholding operator, and T_{SCAD} is the SCAD-thresholding operator, the CD algorithm for MCP/SCAD is

repeat

for $j = 1, 2, \ldots, p$

$$\tilde{z}_j = n^{-1}\textstyle\sum_{i=1}^n x_{ij} r_i + \widetilde{\beta}_j^{(s)}$$

$$\widetilde{\beta}_j^{(s+1)} \leftarrow \begin{cases} F(\tilde{z}_j|\lambda,\gamma) & \text{for MCP, or} \\ T_{\text{SCAD}}(\tilde{z}_j|\lambda,\gamma) & \text{for SCAD} \end{cases}$$

$$r_i \leftarrow r_i - (\widetilde{\beta}_j^{(s+1)} - \widetilde{\beta}_j^{(s)})x_{ij} \text{ for all } i$$

until convergence

The algorithm is identical to our earlier algorithm for the lasso except for the step in which $\widetilde{\beta}_j$ is updated

Convergence

- Although the MCP and SCAD penalties are not convex functions, $Q(\beta_j|\boldsymbol{\beta}_{-j})$ is still convex
- As a result, the coordinate-wise updates are unique and always occur at the global minimum with respect to that coordinate
- **Proposition:** Let $\{\boldsymbol{\beta}^{(s)}\}$ denote the sequence of coefficients produced at each iteration of the coordinate descent algorithms for SCAD and MCP. For all $s = 0, 1, 2, \ldots$,

$$Q(\boldsymbol{\beta}^{(s+1)}) \leq Q(\boldsymbol{\beta}^{(s)}).$$

Furthermore, the sequence is guaranteed to converge to a local minimum of $Q(\boldsymbol{\beta})$.

Local linear approximation

- For MCP and SCAD, one can obtain closed-form coordinate-wise minima and use those solutions as updates
- An alternative approach, particularly useful in penalties that do not yield tidy closed-form solutions, is to construct a local approximation of the penalty about a point $\widetilde{\beta}$:

$$P(|\beta|) \approx P(|\widetilde{\beta}|) + \dot{P}(|\widetilde{\beta}|)(|\beta| - |\widetilde{\beta}|)$$

- Note that with this approximation, the penalty takes on the form of the lasso penalty (with $\dot{P}(|\widetilde{\beta}|)$ playing the role of the regularization parameter) plus a constant

LLA algorithm

- The approximation is applied in an iterative fashion: at the sth iteration, letting $\tilde{\lambda}_j = \dot{P}(|\beta_j^{(s-1)}|)$, the update is given by solving for the value minimizing

$$\frac{1}{2n}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \sum_{j=1}^{p} \tilde{\lambda}_j |\beta_j|$$

- Note that this equation is essentially identical to the one for the adaptive lasso; however, the adaptive lasso weights are assigned in a more or less ad hoc fashion based on an initial estimator, while the LLA modifications to λ are explicitly determined by the penalty function P

Remarks

- Like coordinate descent, the local linear approximation (LLA) algorithm is guaranteed to drive the objective function downhill with every iteration and to converge to a local minimum of $Q(\beta)$
- For MCP and SCAD, CD is more efficient, as it avoids the extra approximation introduced by LLA
- However, LLA is still quite efficient, and a valuable alternative when dealing with penalties without a simple solution in the one-dimensional case

Convexity challenges

- While the objective functions for SCAD and MCP are convex in each coordinate dimension, they are not convex over $\mathbb{R}^p$
- Thus, multiple minima may exist, each satisfying the KKT conditions
- Neither the CD or LLA algorithms are guaranteed to converge to the global minimum in such cases
- As we have discussed earlier, the existence of multiple minima poses problems, both numerically (convergence to an inferior solution) and statistically (increased variance as the solution jumps from one minima to another)

Global convexity

- It is worth noting that it is possible for the objective function Q to be convex with respect to $\boldsymbol{\beta}$ even though the penalty component is nonconvex
- Letting $c_{\min}$ denote the minimum eigenvalue of $\mathbf{X}^\top\mathbf{X}/n$, the MCP objective function is strictly convex if $\gamma > 1/c_{\min}$, while the SCAD objective function is strictly convex if $\gamma > 1 + 1/c_{\min}$
- In this case, the coordinate descent and LLA algorithms will converge to the unique global minimum of Q

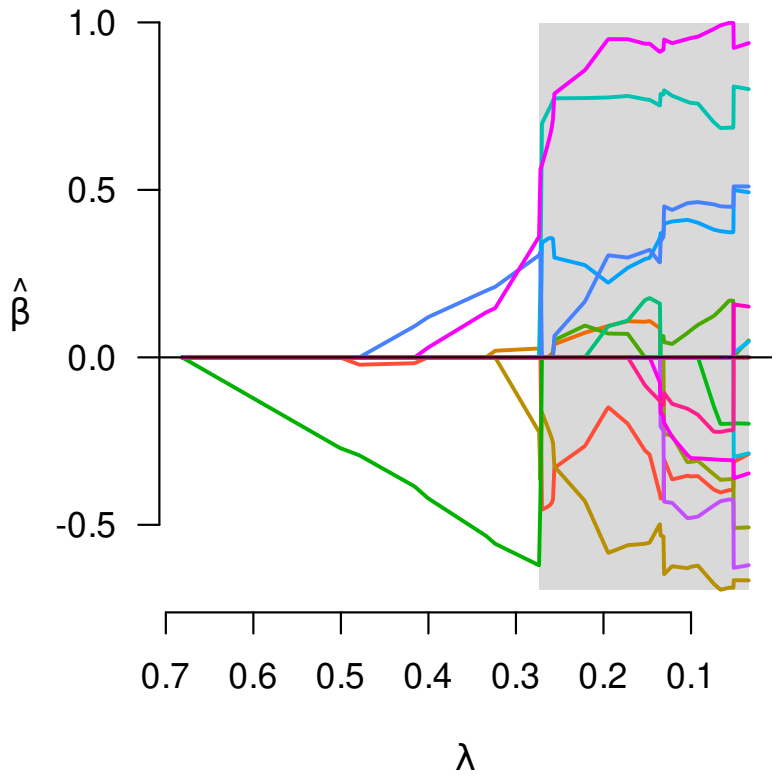
Is global convexity desirable?

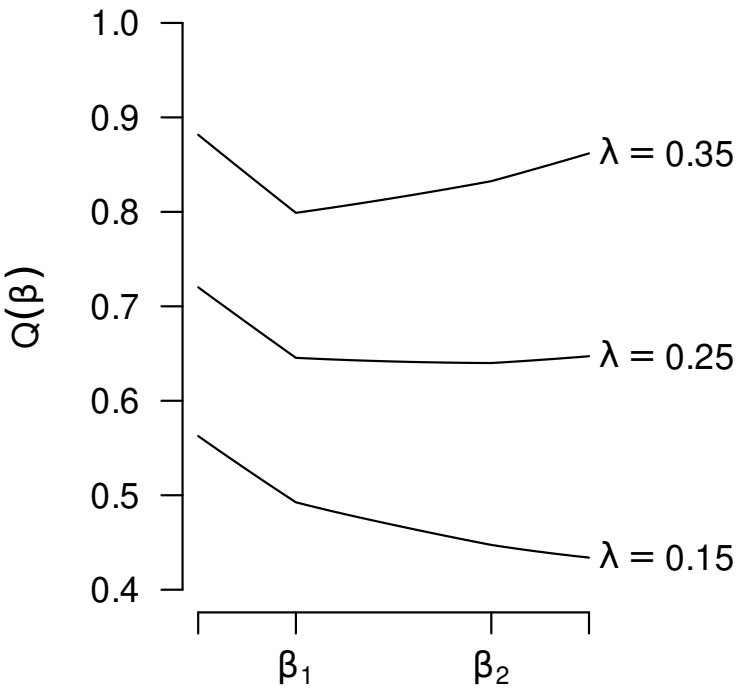
- However, obtaining strict convexity is not always possible or desirable; for example, in high-dimensional settings where $p > n$, $c_{\min} = 0$ and the MCP/SCAD objective functions cannot be globally convex
- Nevertheless, as we saw in the earlier simulations (where $p > n$), convex penalties do not necessarily outperform nonconvex in these scenarios
- For low signal-to-noise ratios there was indeed some benefit to increasing γ in an effort to make the objective function more convex; however, for larger SNR values, this strategy diminished estimation accuracy

Local convexity

- Although $Q(\boldsymbol{\beta})$ may not be convex over the entire p-dimensional parameter space (i.e., *globally convex*), it is still convex on many lower-dimensional spaces
- Some authors have advocated choosing solutions in the "locally convex" portion of the solution path (i.e., based on the minimum eigenvalues of the active features)
- Thus, local convexity of the objective function will not be an issue for large λ, but may cease to hold as λ is lowered past some critical value λ^*

Convexity diagnostic: Example (MCP)





Remarks

- As the figure indicates, when $\lambda = 0.35$, $\boldsymbol{\beta}_1$ clearly minimizes the objective function, whereas at $\lambda = 0.15$, $Q(\boldsymbol{\beta}_2) < Q(\boldsymbol{\beta}_1)$
- For $\lambda \approx 0.25$, however, the objective function is very broad and flat, indicating substantial uncertainty about which solution is preferable
- Calculation of the locally convex region (the unshaded region in the earlier figure) can be a useful diagnostic in practice to indicate which regions of the solution path may suffer from multiple local minima and discontinuous paths

Introduction

- Let us now revisit two high-dimensional studies from the previous topic and analyze them with our new reduced-bias approaches
- First, we consider an adaptive lasso model for the BRCA1 gene expression data
- As our initial estimator, let's use lasso estimates with λ chosen according to BIC:

```
fit <- ncvreg(X, y, penalty='lasso')
b <- coef(fit, which=which.min(BIC(fit)))[-1]
```

(using `ncvreg` for fitting due to its compatibility with `BIC`)

- Cross-validation would of course be a reasonable alternative

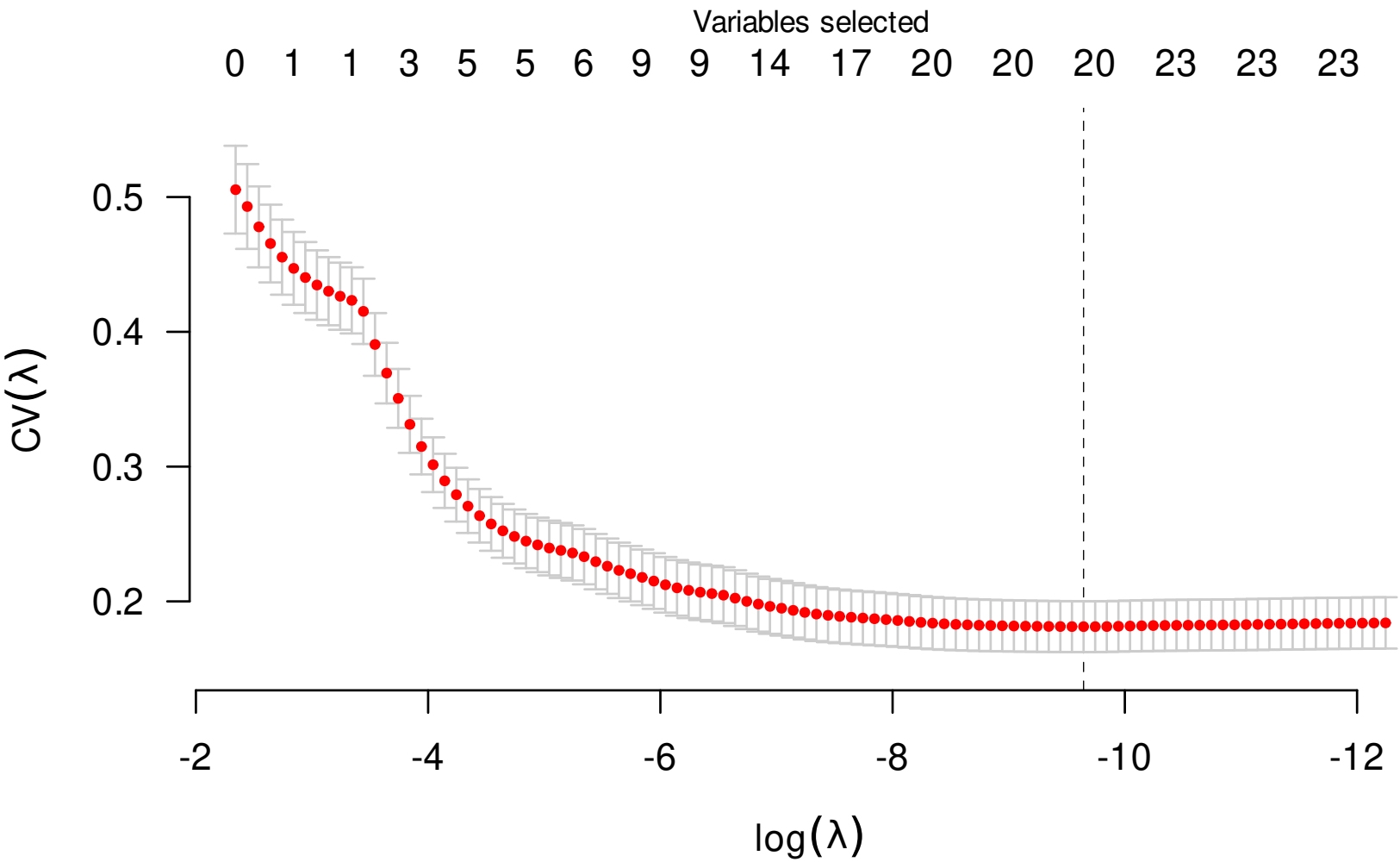
Adaptive lasso fit

Once we have the initial estimator, it may be tempting to fit an adaptive lasso model as follows:

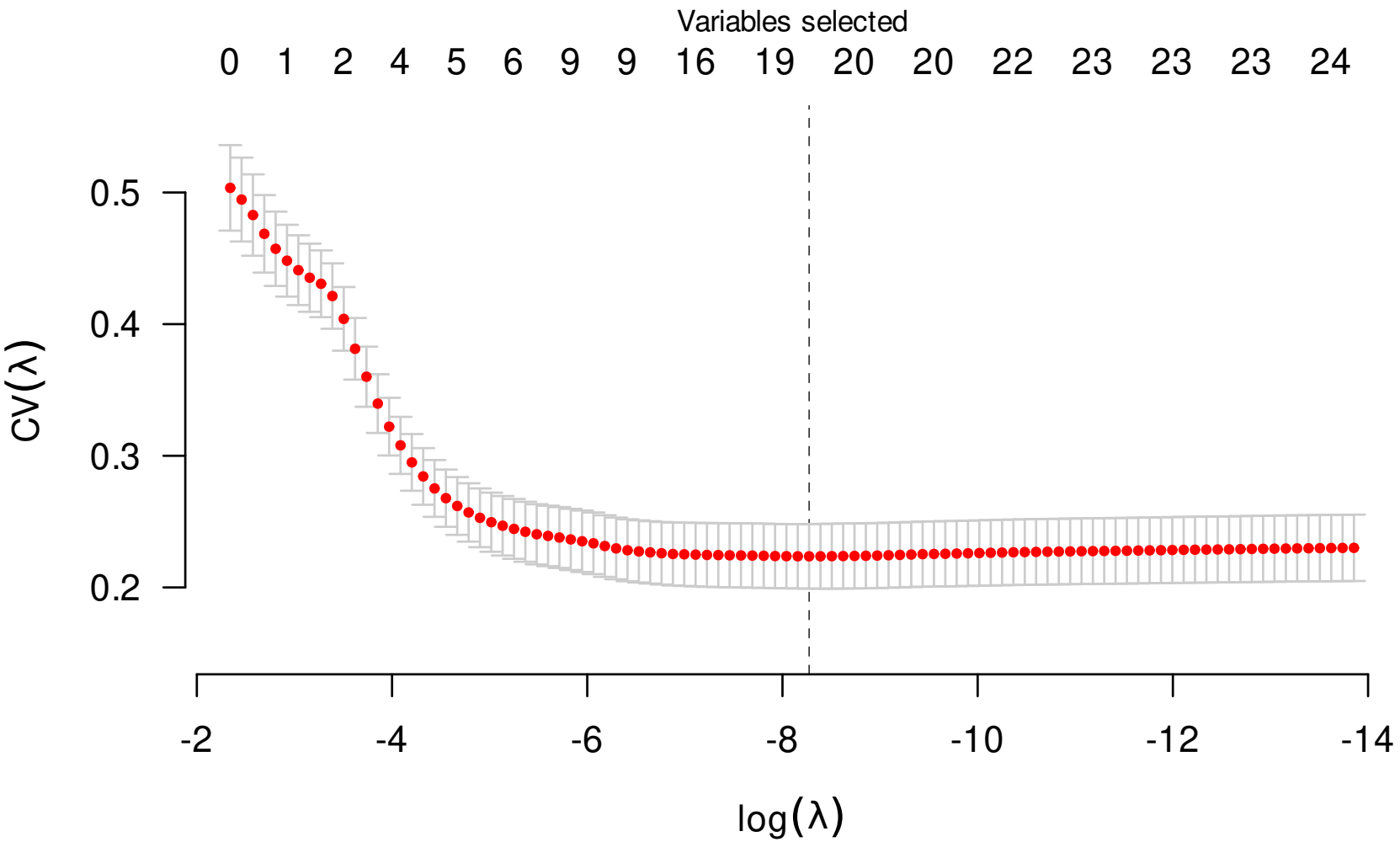
```
w <- abs(b)^(-1)    # Calculate weights
w <- pmin(w, 1e10) # cv.glmnet does not allow
                    # infinite weights
cvfit <- cv.glmnet(X, y, penalty.factor=w,
                    lambda.min=1e-5)
```

but caution is warranted

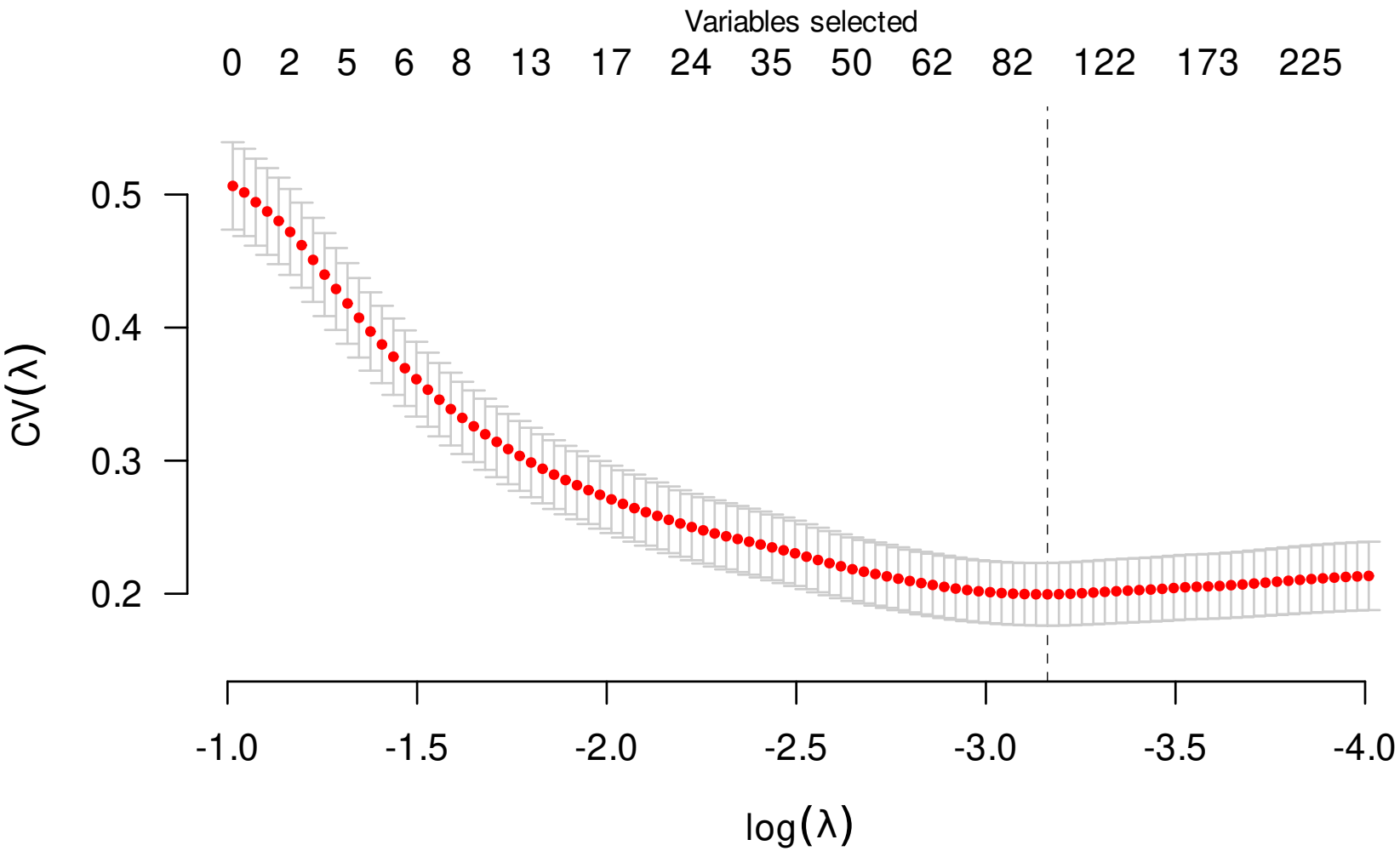
Adaptive lasso: Cross-validation (biased)



Adaptive lasso: Cross-validation (unbiased)



Regular lasso: Cross-validation



Source of bias

- In the first figure, the CV error is not estimated in an unbiased manner
- The reason is that the left-out fold is not truly external to the fitting procedure, as it was used to obtain an initial estimator
- As a result, prediction error is underestimated
- To obtain an (approximately) unbiased estimate of CV error, one must cross-validate the entire procedure, including the initial estimate

Remarks

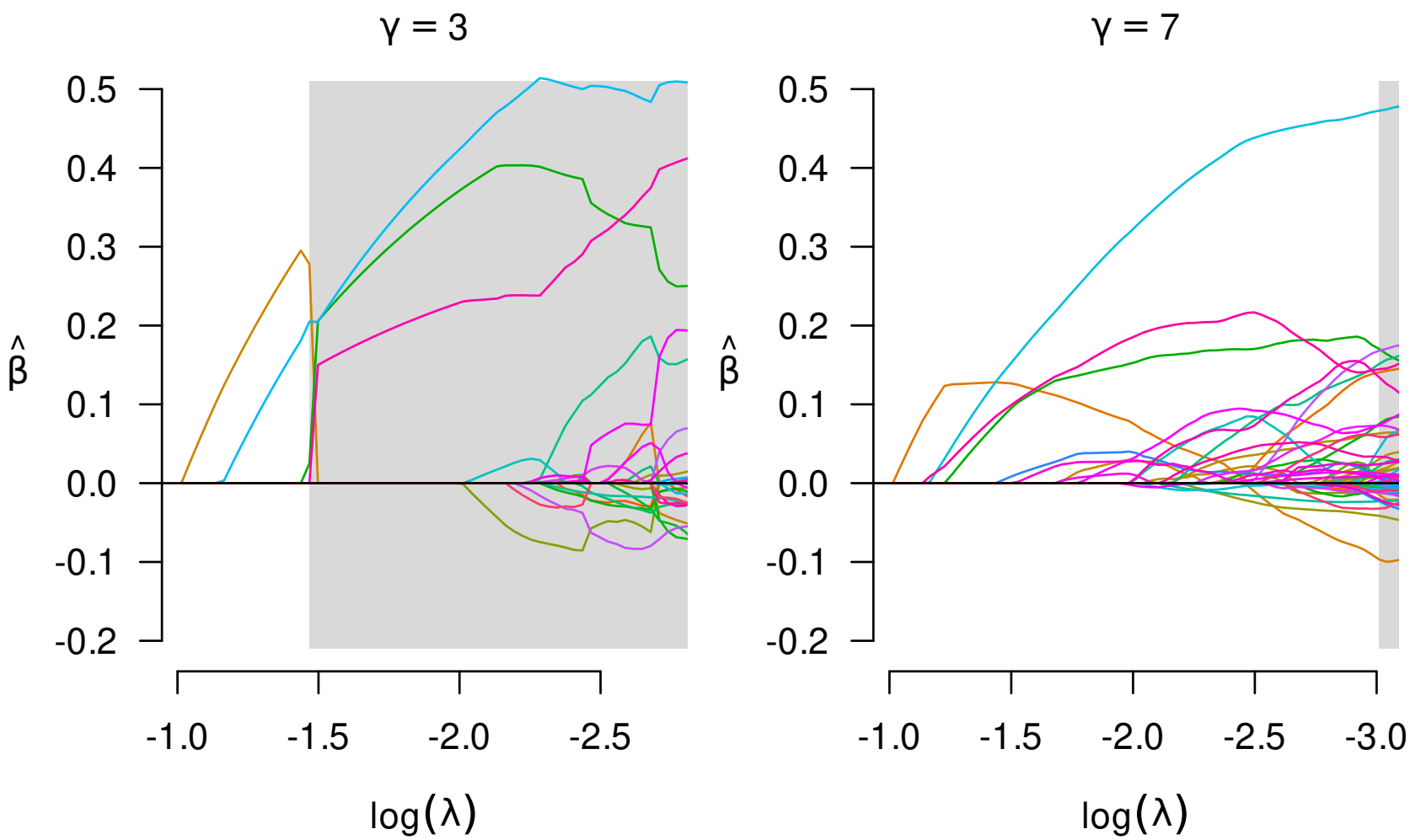
- CV errors:
  - Lasso: 0.20
  - Adaptive lasso (biased): 0.18
  - Adaptive lasso (unbiased): 0.22
- This is an important cautionary example to keep in mind for the adaptive lasso: flexible, two-stage methods have certain advantages in terms of simplicity, but are also easy to make mistakes with
- Unfortunately, while existing `R` packages can be used to fit adaptive lasso models, there are not currently any comprehensive software packages for the adaptive lasso (that I am aware of) that carry out full cross-validation

MCP analysis

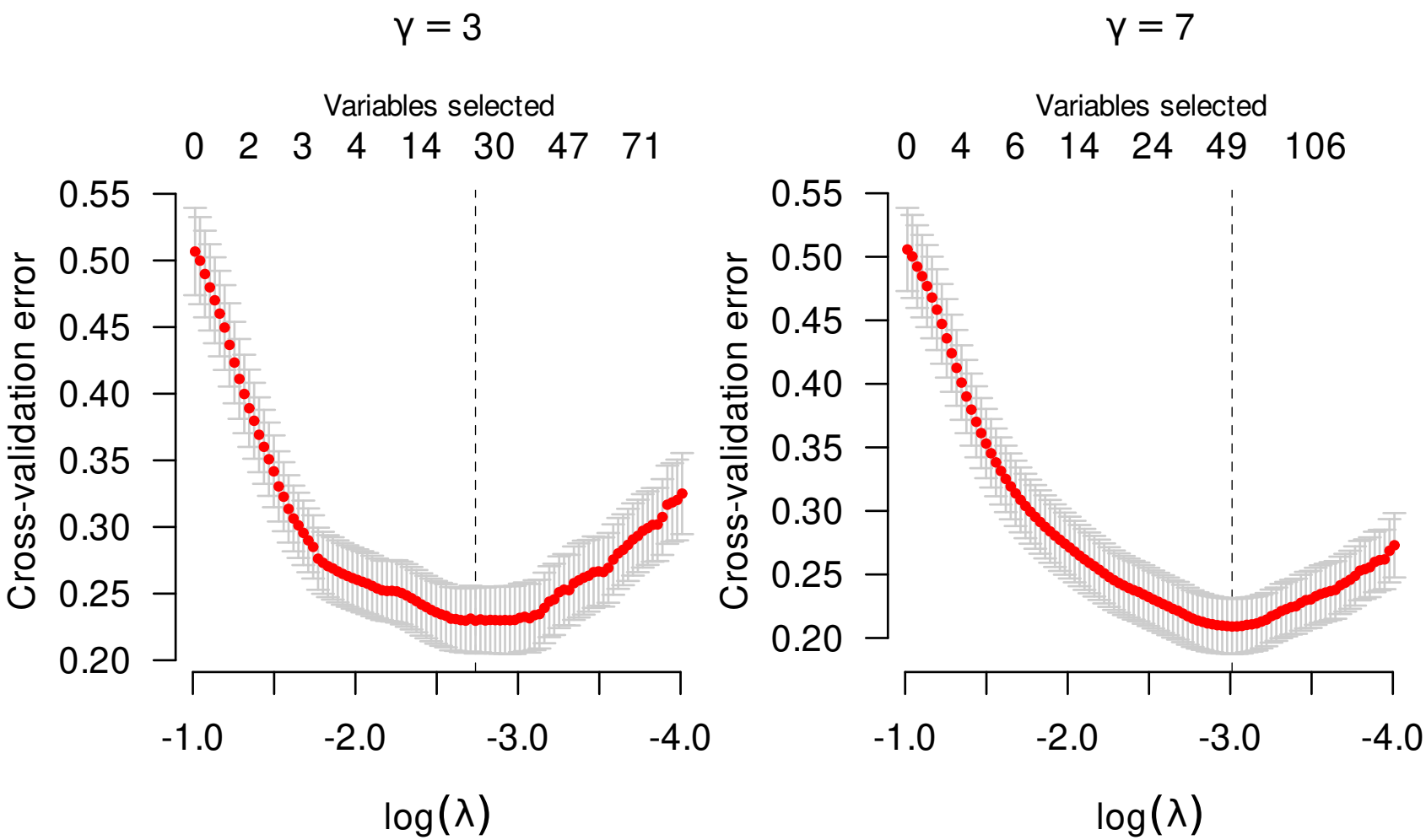
- MCP and SCAD achieve the adaptive lasso's goal of reducing the bias associated with the lasso, but do so in a single step and thus prove a bit more amenable to carrying out inference concerning predictive accuracy using cross-validation
- The `ncvreg` package is a widely used package for fitting MCP/SCAD penalized regression models; its syntax is fairly similar to `glmnet`
- Let's fit two penalized regression models to the BRCA1 data, one with $\gamma = 3$ and the other with $\gamma = 7$:

```
cvfit3 <- cv.ncvreg(X, y) # gam=3 is default
cvfit7 <- cv.ncvreg(X, y, gamma=7)
```

Results: MCP



CV Results: MCP



summary $(\gamma = 3)$

ncvreg provides a useful summary function for fitted CV objects:

```
summary(cvfit3)
# MCP-penalized linear regression with n=536, p=17322
# At minimum cross-validation error (lambda=0.0647):
# -----------------------------------------------
#   Nonzero coefficients: 23
#   Cross-validation error (deviance): 0.23
#   R-squared: 0.55
#   Signal-to-noise ratio: 1.21
#   Scale estimate (sigma): 0.479
```

summary $(\gamma = 7)$

And the equivalent summary for $\gamma = 7$:

```
summary(cvfit7)
# MCP-penalized linear regression with n=536, p=17322
# At minimum cross-validation error (lambda=0.0492):
# -----------------------------------------------
#   Nonzero coefficients: 53
#   Cross-validation error (deviance): 0.21
#   R-squared: 0.59
#   Signal-to-noise ratio: 1.42
#   Scale estimate (sigma): 0.457
```

Remarks

- For MCP with $\gamma = 7$, the minimum error is $\mathrm{CV} = 0.21$; very close to, although slightly larger than the $\mathrm{CV} = 0.20$ achieved by the lasso
- However, the MCP model selects far fewer features (49 compared to 96 for the lasso)
- The MCP model with $\gamma = 3$ selects an even more sparse model (32 features), although with a higher CV error ($\$\mathrm{CV}$=0.24) and greater local convexity concerns

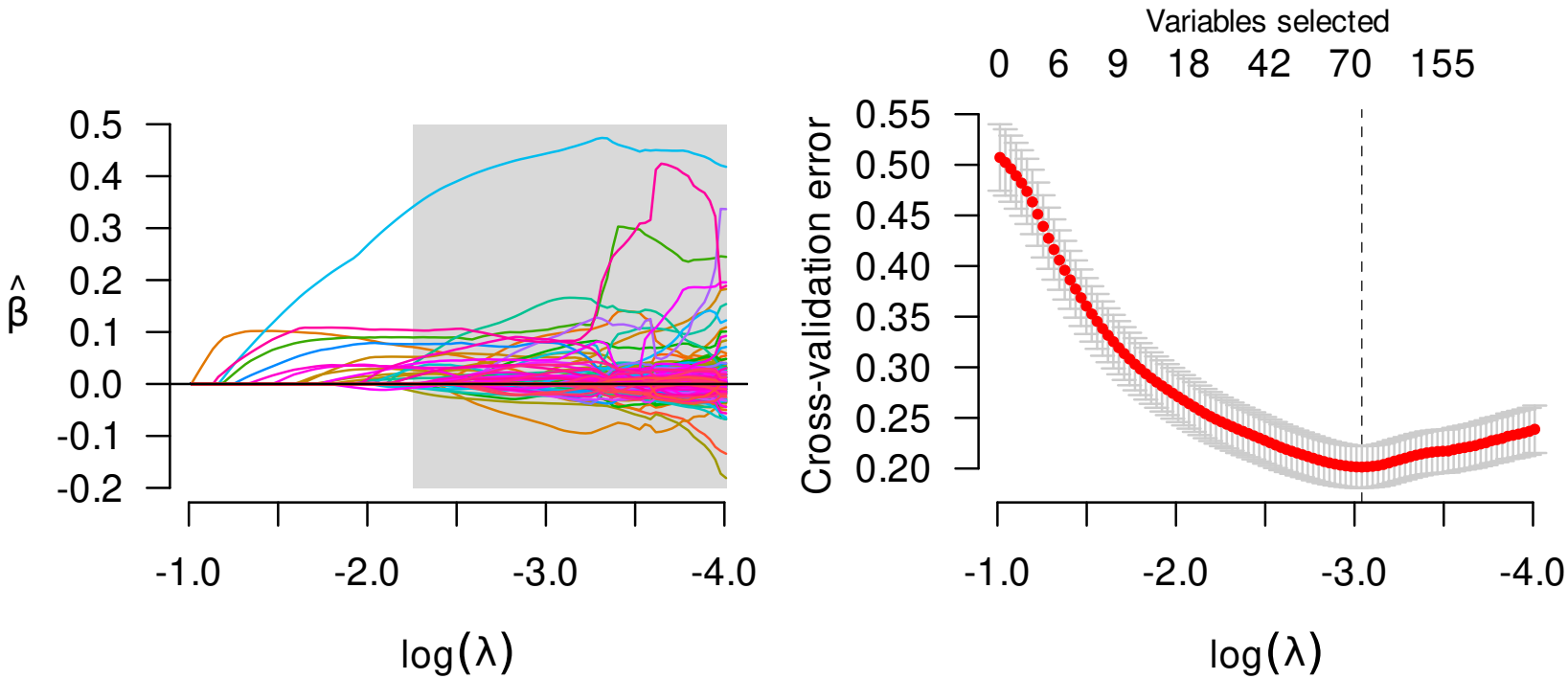
SCAD

Finally, let us fit a SCAD-penalized regression model to this data ($\gamma = 8$):

```
cvfit_scad <- cv.ncvreg(X, y, gamma=8, penalty='SCAD')
summary(cvfit_scad)
# SCAD-penalized linear regression with n=536, p=17322
# At minimum cross-validation error (lambda=0.0478):
# -----------------------------------------------
#   Nonzero coefficients: 79
#   Cross-validation error (deviance): 0.20
#   R-squared: 0.60
#   Signal-to-noise ratio: 1.51
#   Scale estimate (sigma): 0.449
```

Results: SCAD ($\gamma = 8$)

The SCAD results are more lasso-like than MCP is (as one would expect since the penalties are more similar)



Remarks

- This is just one example, but these results seen are fairly representative, in my experience
- The prediction performance (as estimated by cross-validation) is typically similar between MCP/SCAD/lasso, but there can be substantial differences in terms of the estimates themselves
- The main advantage in practice of MCP (or SCAD) is the ability to achieve that prediction performance using fewer features
- Finally, the results of SCAD are almost always in between those of MCP and lasso

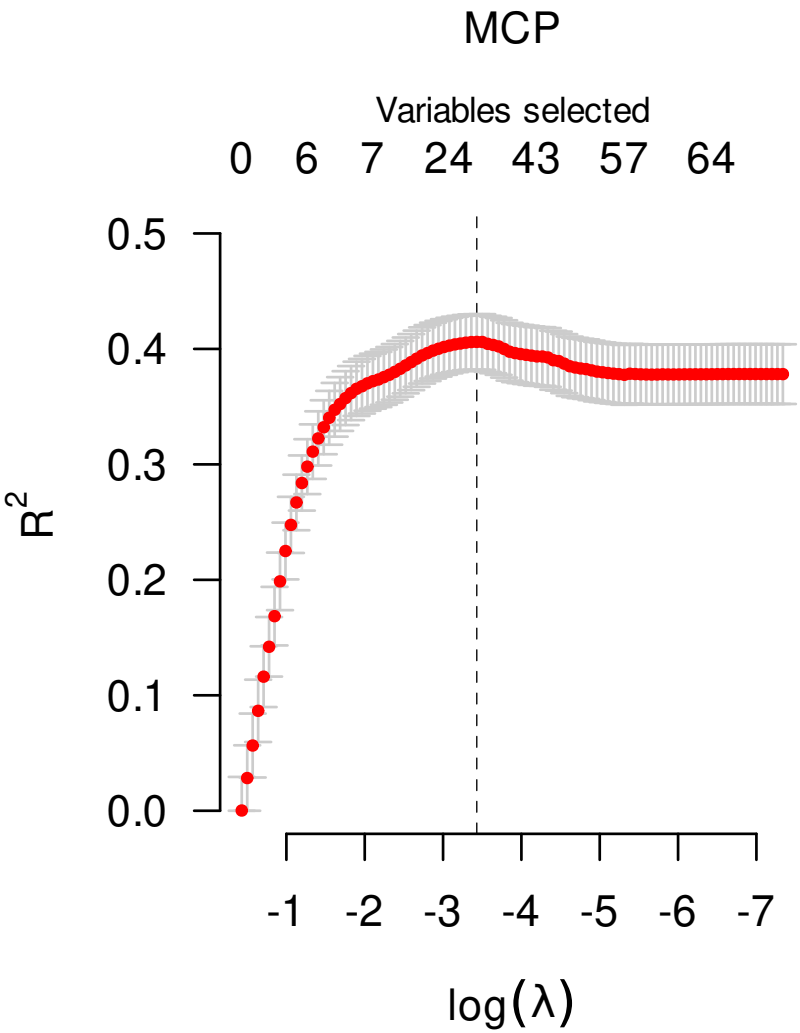
WHO-ARI: MCP

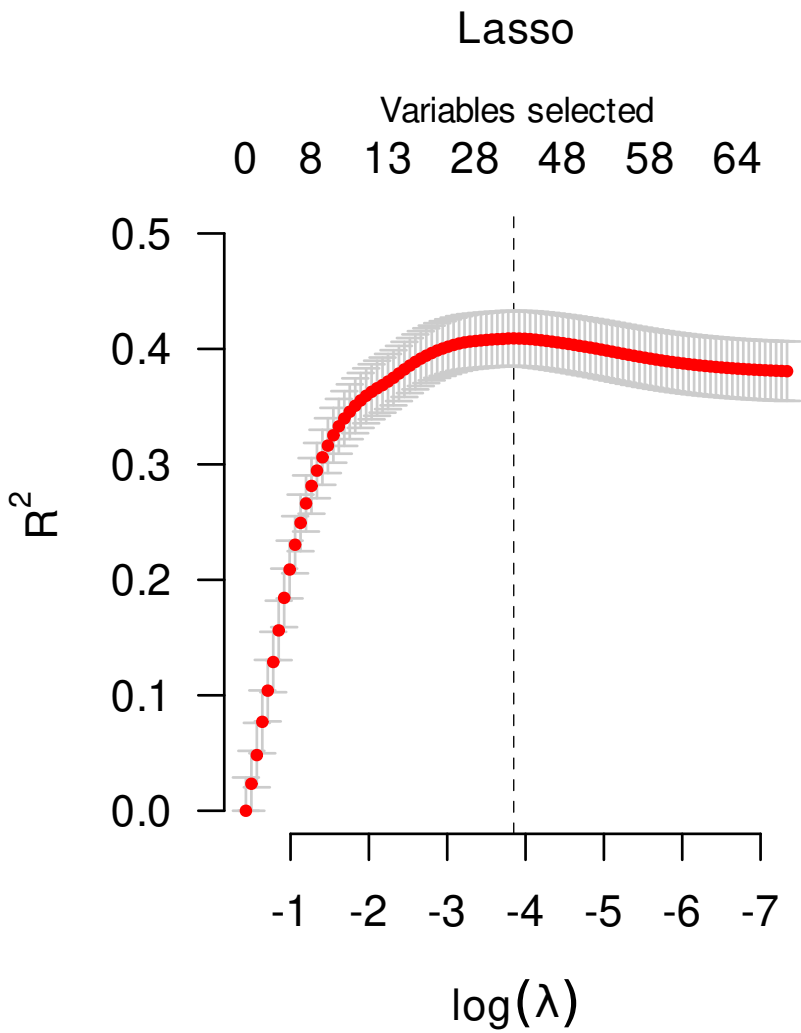
- Let us also revisit the WHO study of acute respiratory illness, which you have looked at a few times in your homework assignments
- Let us fit an MCP-penalized regression model to this data using $\gamma = 6$ and compare it to the fit of the lasso:

```
fold <- assign_fold(y, 10)
cvfit_mcp <- cv.ncvreg(XX, y, gam=6, fold=fold)
cvfit_las <- cv.ncvreg(XX, y, penalty="lasso",
                       fold=fold)
```

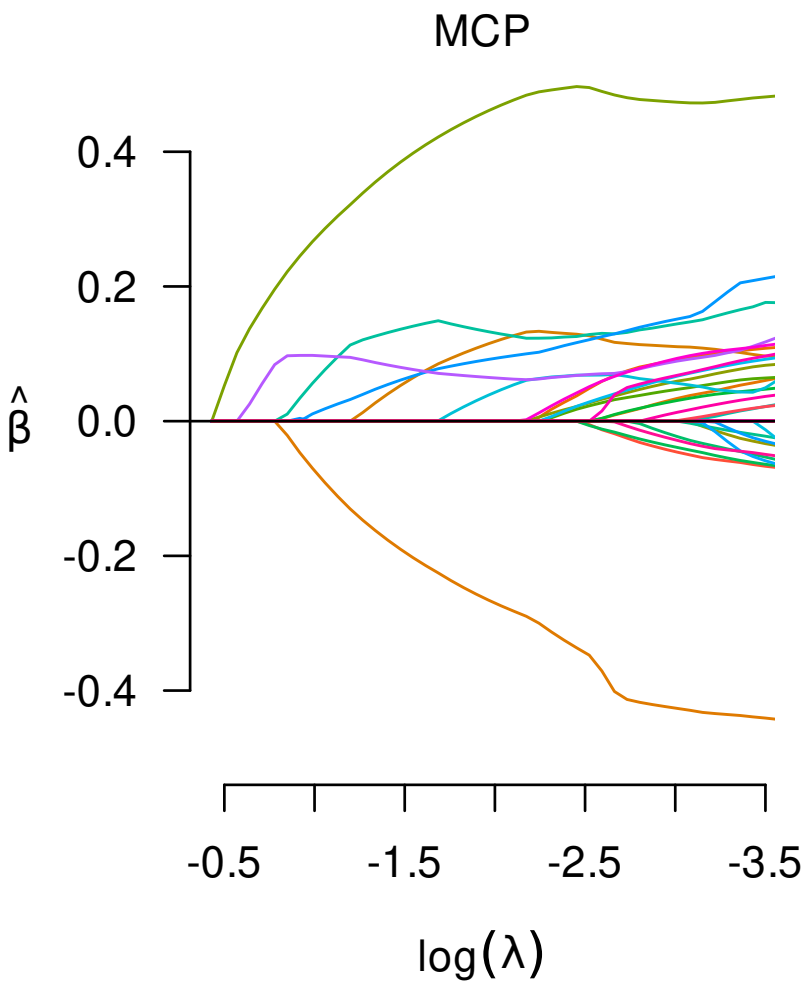
- When making these kinds of comparisons, keep the CV fold assignments the same, otherwise you risk mistaking the effect of different folds for the effect of the penalty

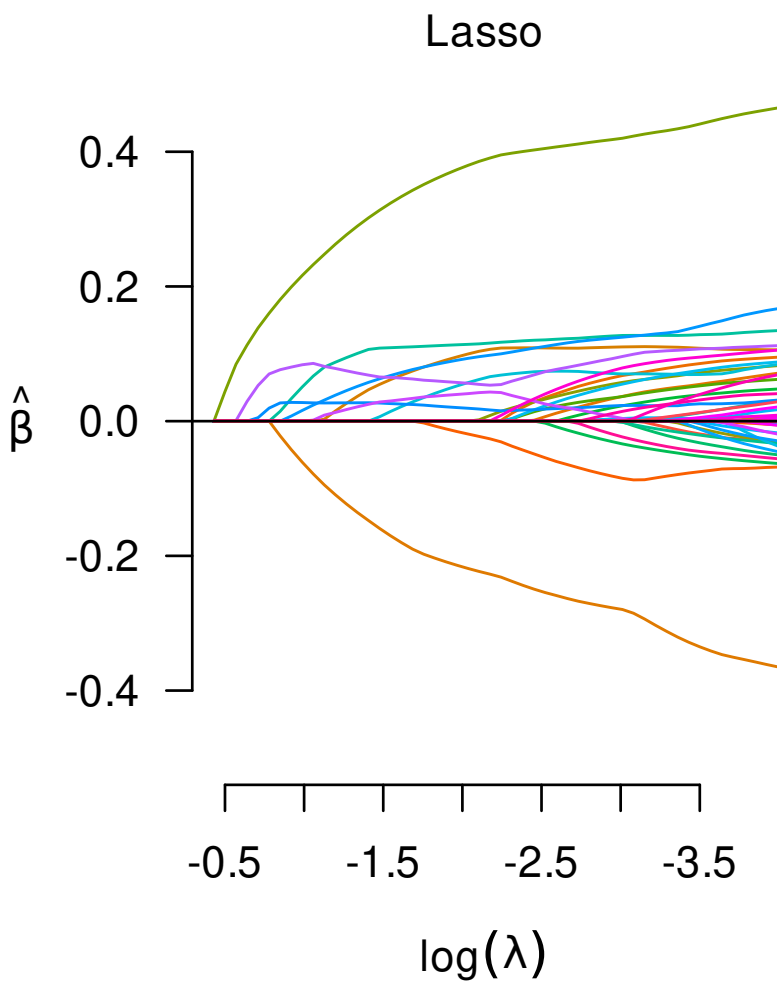
Results: CV


MCP
Variables selected
0 6 7 24 43 57 64
0.5
0.4
0.3
0.2
0.1
0.0
R^2
-1 -2 -3 -4 -5 -6 -7
log(λ)


Lasso
Variables selected
0 8 13 28 48 58 64
0.5
0.4
0.3
0.2
0.1
0.0
R^2
-1 -2 -3 -4 -5 -6 -7
log(λ)

Results: Coefficient path





Summary: MCP

```
summary(cvfit_mcp)
# MCP-penalized linear regression with n=816, p=66
# At minimum cross-validation error (lambda=0.0324):
# -----------------------------------------------
#   Nonzero coefficients: 26
#   Cross-validation error (deviance): 1.21
#   R-squared: 0.41
#   Signal-to-noise ratio: 0.68
#   Scale estimate (sigma): 1.099
```

Summary: Lasso

```
summary(cvfit_las)
# lasso-penalized linear regression with n=816, p=66
# At minimum cross-validation error (lambda=0.0213):
# -------------------------------------------------
#   Nonzero coefficients: 39
#   Cross-validation error (deviance): 1.20
#   R-squared: 0.41
#   Signal-to-noise ratio: 0.69
#   Scale estimate (sigma): 1.097
```