

Module 6 Part 2: Sparse Regression

Monday, November 27, 2023 14:26



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Module 6, part II: Sparse regression and shrinkage

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Module 6, part II: Sparse regression and shrinkage

Reading

- Sections 3.3 - 3.4 in Elements of Statistical Learning II (ESL II) (Hastie et al)
- Section 6.5 in Introduction to Statistical Learning (ISL) (James et al)

Concepts

- Ridge regression and L2 norm
- Sparsity
- Lasso and L1 norm
- Selecting the penalty / CV
- Correlated Variables and Elastic Net
- Bonferroni Correction

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Motivation

In modern applications, p is often very large relative to n .

A study is "high dimensional" if p is large. \rightarrow large # predictors

There are a number of considerations:

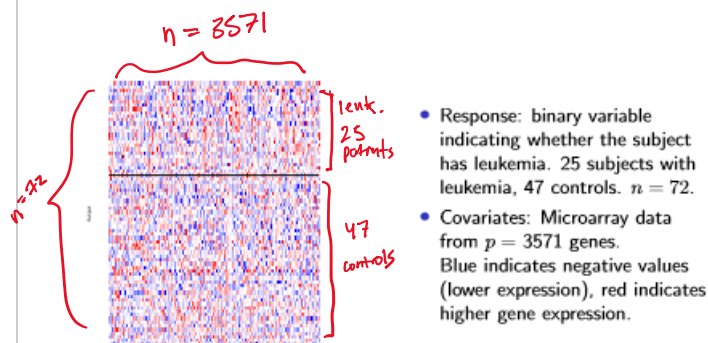
1. Predictive Ability: OLS has low bias but high variance. Can we sacrifice bias to achieve lower variance, and thus greater accuracy?
2. Interpretability: with large p , our goal is to identify important variables. It would be helpful to have a model that does this, rather than rely upon forward/backward selection procedures and p-values.
3. Moreover, when $p > n$, we can't use multiple regression – OLS estimators are not unique.

In $(X'X)^{-1}X'Y$, $p > n$ then $(X'X)$ not invertible

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Motivating dataset: gene expression in leukemia



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Review: Bias-Variance Trade-off

$$\begin{aligned} E\{g(\mathbf{x}_i) - \hat{g}(\mathbf{x}_i)\}^2 &= E[\{g(\mathbf{x}_i) - E\hat{g}(\mathbf{x}_i) + E\hat{g}(\mathbf{x}_i) - \hat{g}(\mathbf{x}_i)\}^2] \\ &= [g(\mathbf{x}_i) - E\hat{g}(\mathbf{x}_i)]^2 + E[\hat{g}(\mathbf{x}_i) - E\hat{g}(\mathbf{x}_i)]^2 \\ &= (\text{Bias of } \hat{g}(\mathbf{x}_i))^2 + \text{Variance of } \hat{g}(\mathbf{x}_i) \end{aligned}$$

where $\hat{g}(\mathbf{x}_i)$ is the estimate of $E(Y|\mathbf{x}_i) = g(\mathbf{x}_i)$.

Here, $g(\mathbf{x}_i) = \mathbf{x}_i'\beta$.

When estimating a large number of parameters, we may overfit the data.

Sacrifice some bias to reduce variance, improve overall accuracy.

To estimate more parameters accurately, you need more data. A rough rule of thumb is 10 observations / parameter.

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Model Complexity

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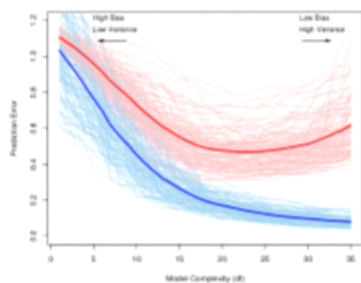


FIGURE 7.1. Behavior of test sample and training sample error as the model complexity is varied. The light blue curves show the training error E_T , while the light red curves show the conditional test error E_{Tc} for 100 training sets of size 50 each, as the model complexity is increased. The solid curves show the expected test error E_{Tc} and the expected training error $E[E_T]$.

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Review

We discussed penalized regression in Module 5.

Recall the ridge regression penalty from M5.2:

$$\operatorname{argmin}_{\beta} \sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 + \lambda \|\beta\|_2^2$$

Here, λ is the **penalty**.

This problem can be equivalently formulated as

$$\operatorname{argmin}_{\beta} (\mathbf{Y} - \mathbf{X}\beta)'(\mathbf{Y} - \mathbf{X}\beta) \quad \text{with constraint } \beta' \beta \leq C$$

where there exists a one-to-one mapping between λ and C .

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Closed-form solution

We derived the solution, which has a very convenient closed form:

$$\hat{\beta} = (\mathbf{X}'\mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}'\mathbf{Y}$$

for some positive number λ .

Note:

- When $\lambda = 0$, $\hat{\beta}$ becomes the ordinary least squares estimate. So no penalization is present ($C = \infty$).
- When $\lambda \rightarrow \infty$, $(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I})^{-1}$ becomes small, so $\hat{\beta} \rightarrow \mathbf{0}$.
- $(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I})$ is positive definite for $\lambda > 0$, so we can invert it even if $p > n$!

a positive
definite matrix

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Important details

The penalty λ is unfair if the predictors are not on the same scale.

Consequently, we **scale** the columns of \mathbf{X} to have **unit variance**. Then the penalty for each coefficient is equitable.

We often do not want to penalize the intercept:

$$\operatorname{argmin}_{\beta} \sum_{i=1}^n (y_i - \beta_0 - \mathbf{x}_i' \beta)^2 + \lambda \|\beta\|_2^2$$

where β_0 is not penalized.

Similarly, we can center all columns of $\mathbf{X} \in \mathbb{R}^{n \times p}$ and center y . Then $\hat{\beta}_0 = 0$. So one approach is to **center** your data and then penalize all terms.

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Ridge regression versus sparsity

For variable selection, it would be nice to have estimates of β that include **exact zeros**.

↳ "sparsity" = lots of β 's equal to zero

If $\hat{\beta}_j \neq 0$, x_j is selected.

If $\hat{\beta}_j = 0$, x_j is not important.

→ drawback of ridge: All $\hat{\beta}_j \neq 0$. can only approach 0. does not achieve variable selection

Although $\hat{\beta}^{\text{Ridge}}$ may have reduced MSE relative to $\hat{\beta}^{\text{OLS}}$, it does not help us too much with variable selection.

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Norms

We can measure the length of a vector using different metrics.

Ridge regression uses the squared L_2 norm, which is also called the Euclidean norm.

For a vector $\beta \in \mathbb{R}^d$, an L_p norm has the general form

$$\|\beta\|_p = \left(\sum_{j=1}^d |\beta_j|^p \right)^{1/p}$$

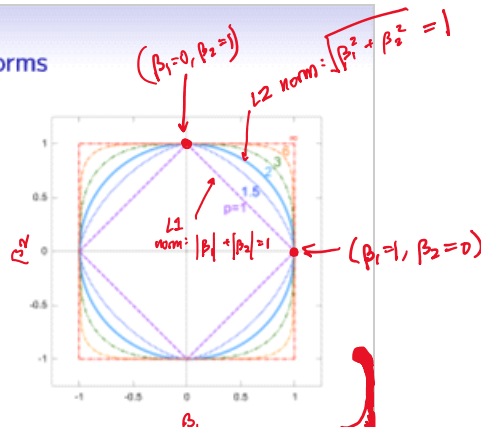


Figure: Illustration of the unit circles of some p norms for $p=1$: sum norm, $p=1.5$, $p=2$: Euclidean norm, $p=3$, $p=6$, $p=\infty$: max norm in two dimensions from https://en.wikipedia.org/wiki/Lp_space#/media/File:Vector-p-Norms.q111.svg

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Lasso

We will assume all covariates and y are centered so that we don't need to estimate the intercept.

We will also assume they are scaled.

Let's consider using a different norm, the L_1 norm.

$$\hat{\beta}^{Lasso} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 + \lambda \|\beta\|_1$$

where $\|\beta\|_1 = \sum_{j=1}^p |\beta_j|$.

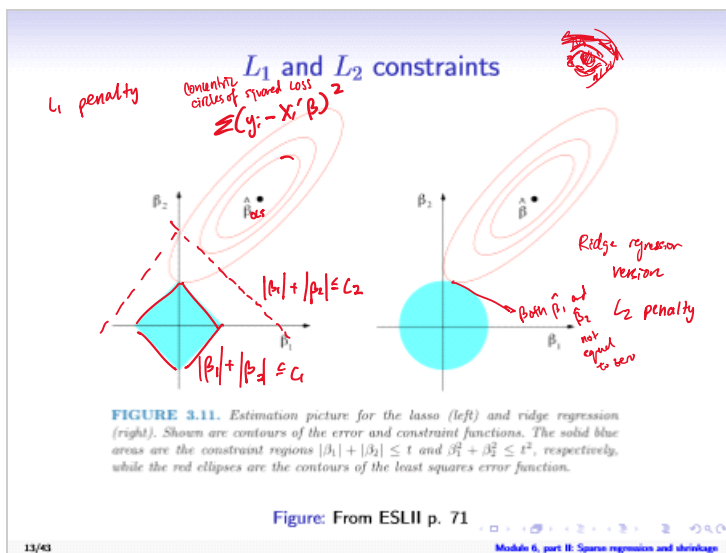
Statisticians call this the **LASSO**: Least absolute shrinkage and selection operator.

This penalty is chosen because it induces **sparsity**.

Sparsity is when we have many zeros and a relatively small number of non-zeros.

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Lasso

Why does the Lasso induce sparsity?

For $\|\beta\|_1 \leq C$, the L_1 constraint creates sharp points at the boundary corresponding to $(\beta_1, \beta_2) = (C, 0)$, $(0, C)$, $(-C, 0)$, and $(0, -C)$.

For $\beta = (\beta_1, \beta_2)$, consider where the contours of $(Y - X\beta)'(Y - X\beta)$ intersect the constraint.

For sufficiently small C , i.e., large λ , the constraint leads to the selection of either β_2 or β_1 .

In contrast, the smooth circle from the ridge regression, $\beta_1^2 + \beta_2^2 = C$, is tangent to the contours of $(Y - X\beta)'(Y - X\beta)$ at $\beta_1 \neq 0$ and $\beta_2 \neq 0$.

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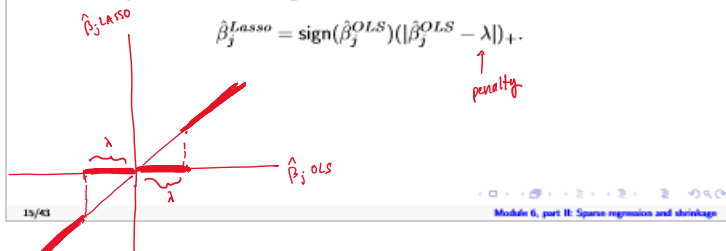
Obtaining Lasso estimates

Unfortunately, there is no closed form solution for the Lasso.

Fortunately, it is convex problem.

In the R package `glmnet`, there are efficient ways to calculate the solutions for a set of λ_k .

In the **special case** of orthogonal and standardized covariates, we have



Perspectives on Lasso and Ridge: Orthonormal covariates

Estimator	Formula
Best subset (size M)	$\hat{\beta}_j \cdot I(\hat{\beta}_j \geq \hat{\beta}_{(M)})$
Ridge	$\hat{\beta}_j / (1 + \lambda)$
Lasso	$\text{sign}(\hat{\beta}_j)(\hat{\beta}_j - \lambda)_+$

Hard-thresholding

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Figure: Table 3.4 from ESL II. Closed forms for Best Subset, Ridge, and Lasso for the **special case** of orthonormal covariates.

Ridge Regression and Bayes Estimates

In the Bayesian framework, $f(\beta|y) \propto f(y|\beta)f(\beta)$.

Let's assume a Gaussian likelihood with variance σ^2 and independent mean-zero Gaussian priors on β with common variance τ^2 :

$$f(\beta|y) \propto (2\pi\sigma^2)^{-n/2} \exp \left\{ -\sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 / (2\sigma^2) \right\} \\ \times (2\pi\tau^2)^{-p/2} \exp \left\{ -\sum_{j=1}^p \beta_j^2 / (2\tau^2) \right\}$$

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Bayesian Perspective on Ridge Regression

Assumes σ^2 and τ^2 are given.

On the log scale, and dropping constants, the maximum a posteriori estimate (i.e., mode) is obtained as

$$\begin{aligned}\hat{\beta}^{MAP} &= \underset{\beta}{\operatorname{argmax}} \quad -\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 - \frac{1}{2\tau^2} \sum_{j=1}^p \beta_j^2 \\ &= \underset{\beta}{\operatorname{argmin}} \quad \sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 + \lambda \sum_{j=1}^p \beta_j^2.\end{aligned}$$

for $\lambda = \sigma^2 / \tau^2$.

Thus, $\hat{\beta}^{Ridge}$ can be derived from the Bayesian perspective in which the prior distribution is **Gaussian** and the **prior precision** determines the degree of shrinkage.

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Bayesian Perspective on the Lasso

The Laplace distribution (also called double exponential) is a shrinkage prior.

For mean zero, $f(\beta_j) = \frac{1}{2\tau} \exp(-|\beta_j|/\tau)$, which has variance $2\tau^2$.

absolute value

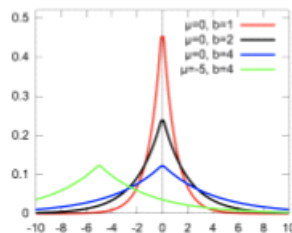


Figure: https://en.wikipedia.org/wiki/Laplace_distribution

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Bayesian Perspective on the Lasso

Then we have

$$\begin{aligned}\hat{\beta}^{MAP} &= \underset{\beta}{\operatorname{argmax}} \quad -\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 - \frac{1}{2\tau} \sum_{j=1}^p |\beta_j| \\ &= \underset{\beta}{\operatorname{argmin}} \quad \sum_{i=1}^n (y_i - \mathbf{x}_i' \beta)^2 + \lambda \sum_{j=1}^p |\beta_j|.\end{aligned}$$

for $\lambda = \sigma^2 / \tau$.

Thus, we again see a stronger prior (smaller τ) leads to greater shrinkage. For sufficiently large τ , we get variable selection.

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Selecting λ : Cross-validation

Recall from M5.2:

- In K -Fold CV, the data are divided into K subsets

$$MSE_k = \frac{1}{n/K} \sum_{i \in S_k} (y_i - \hat{y}_i^{-S_k})^2$$

$$CV = \widehat{MSE} = \frac{1}{K} \sum_{k=1}^K MSE_k$$

- Each partition has a training dataset with $(K-1) * n/K$ observations and test dataset with n/K observations.
- Then the model is fit K times.
- LOOCV is a special case where the number of folds is n .

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K-fold Cross-Validation

$$MSE_k = \frac{1}{n/K} \sum_{i \in S_k} (y_i - \hat{y}_i^{-S_k})^2$$

$$CV = \widehat{MSE} = \frac{1}{K} \sum_{k=1}^K MSE_k$$



Figure: R Tibshirani Lecture notes, <http://www.stat.cmu.edu/~ryantibs/datamining/lectures/18-val1.pdf>.

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Prediction error to choose λ

Note: the goal of CV is to improve prediction.

The resulting choice of λ may not be optimal for addressing our goal, which is to select the most important covariates.

CV tends to over-select the number of parameters. i.e. λ_{min} is too small

There are heuristics such as the one standard error rule:

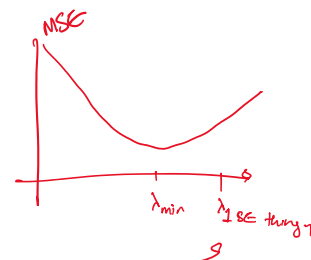
- Find λ_{min} using 10-fold CV.
- Estimate the variance of the CV using each fold's MSE_k as a sample:

$$SE = \sqrt{\frac{1}{K} \sum_{k=1}^K (MSE_k - \widehat{MSE})^2}$$

- Increase λ to result in an MSE that is $+1$ SE of CV for λ_{min} .

a little bit of overfitting

because of this



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Correlated covariates

It turns out that variable selection via the Lasso is **sensitive to correlation** between your covariates.

For two correlated covariates, Lasso picks one but not the other, e.g., $\hat{\beta}_1$ is set to zero while $\hat{\beta}_2$ is not.

For small samples, which variable is chosen can be arbitrary.

Ridge regression is less sensitive to correlation between covariates, and shrinks covariates together.

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Variable Selection Methods for Correlated Covariates

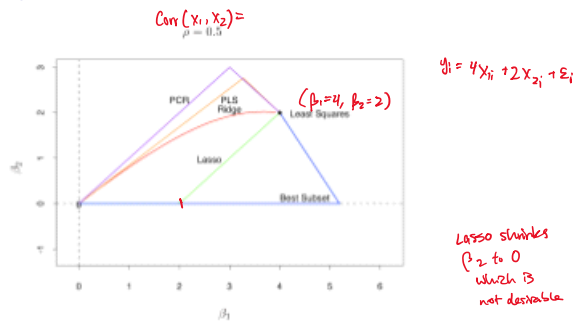


Figure: Figure 3.18 from ESL II. Correlation between x_1 and x_2 is 0.5. The true regression coefficients are (4, 2). Note that Ridge and Lasso are estimated over a continuous range of λ , whereas other methods correspond to the discrete steps selecting 0, 1, or 2 variables.

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Elastic Net \rightarrow Stanford

The **elastic net** offers a middle ground and uses a combination of the two. For $\alpha \in (0, 1)$,

$$\hat{\beta}^{ELNet} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^n (y_i - x_i' \beta)^2 + \lambda \sum_{j=1}^p (\alpha |\beta_j| + (1-\alpha) \beta_j^2)$$

Handwritten notes: α Lasso penalty, $1-\alpha$ Ridge penalty, λ in the software

Elastic net tends to shrink some coefficients to zero, like the lasso, but shrinks correlated covariates together, like ridge.

In the R package `glmnet`, the penalty is $\lambda \sum_{j=1}^p \{\alpha |\beta_j| + (1-\alpha) \beta_j^2 / 2\}$.

According to the vignette, when variables are correlated in groups, $\alpha = 0.5$ tends to result in variables in the group either all selected or dropped.

Note in `glmnet`, $\alpha = 0$ = ridge, $\alpha = 1$ = Lasso.

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GLM Elastic Net

We can also use penalized regression in the generalized linear model framework. Let ℓ be the log density of y_i .

$$\hat{\beta}^{ELNet} = \underset{\beta}{\operatorname{argmin}} \quad \underbrace{- \sum_{i=1}^n \ell(y_i; \mathbf{x}_i' \beta)}_{\text{log likelihood}} + \underbrace{\lambda \sum_{j=1}^p (\alpha |\beta_j| + (1 - \alpha) \beta_j^2)}_{\text{penalty (L1 and L2)}}.$$

Note that rather than penalizing the squared loss, here we penalize the negative log-likelihood.

With the penalty, the objective function is maximized at smaller values of β_j relative to the MLE.

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Module 6, part II: Sparse regression and shrinkage

Cross-validation and loss functions

For Gaussian data, we used the PMSE in cross-validation:

$$\sum_{i=1}^n (y_i - \hat{y}_i)^2.$$

In GLMs, we use the negative log likelihood, which is often multiplied by two and called the **deviance**:

$$D = -2 \sum_{i=1}^n \ell(y_i; \mathbf{x}_i' \beta)$$

Note that for iid Gaussian data with variance 1, the deviance equals $\sum_{i=1}^n (y_i - \hat{y}_i)^2$.

For CV, we can use the deviance in place of PMSE. Other options are available.

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The R package glmnet

The R package `glmnet` contains a function, also called `glmnet`

Some of the options are listed below:

`library(glmnet)`
`glmnet(x, y, family = c("gaussian", "binomial", "poisson", "multinomial",
 "cox", "mgauddisian"), alpha = 1, nlambda = 100,
 lambda = NULL, standardize = TRUE, intercept = TRUE,`

A key parameter here is α : the elastic net mixing parameter with $0 \leq \alpha \leq 1$. The penalty is defined as

$$\frac{1 - \alpha}{2} \|\beta\|_2^2 + \alpha \|\beta\|_1$$

$\alpha=1$ is the lasso penalty, and $\alpha=0$ the ridge penalty.

Standardizes data by default.

No "data" argument.

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Leukemia Dataset: Ridge Regression

```
> x = Leukemia$x
> y = Leukemia$y
> model.ridge = glmnet(x,y,alpha=0,family = 'binomial')
> print(model.ridge)

Call: glmnet(x = x, y = y, family = "binomial", alpha = 0)

    Df  %Dev Lambda
1  3571  0.00 409.30
2  3571 18.35 390.70
3  3571 19.01 372.90
4  3571 19.69 356.00
5  3571 20.38 339.80
6  3571 21.09 324.40
7  3571 21.82 309.60
8  3571 22.56 296.60
9  3571 23.32 282.10
10 3571 24.09 269.30
```

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Module 6, part II: Sparse regression and shrinkage

Leukemia Dataset: Ridge Regression

```
> dim(coef(model.ridge))
[1] 3572 100
> coef(model.ridge)[1:10,1:5]
10 x 5 sparse Matrix of class "dgCMatrix"
      s0      s1      s2      s3      s4
(Intercept) -6.312718e-01 -6.449201e-01 -6.459674e-01 -6.470840e-01 -6.482734e-01
V1 -4.780168e-38 -1.203411e-04 -1.259193e-04 -1.317424e-04 -1.378195e-04
V2 3.994960e-38 8.906586e-05 9.273885e-05 9.654906e-05 1.004888e-04
V3 9.777714e-38 2.086957e-04 2.169559e-04 2.254734e-04 2.342506e-04
V4 3.692679e-38 7.792437e-05 8.089428e-05 8.394169e-05 8.706528e-05
V5 -9.494342e-39 -1.533100e-05 -1.579680e-05 -1.626987e-05 -1.675012e-05
V6 -3.815336e-38 -1.003254e-04 -1.050186e-04 -1.099108e-04 -1.150079e-04
V7 -7.641146e-38 -1.80051e-04 -1.878006e-04 -1.958899e-04 -2.042796e-04
V8 -8.192134e-38 -1.976823e-04 -2.064352e-04 -2.155335e-04 -2.249867e-04
V9 2.647430e-38 4.418512e-05 4.547821e-05 4.677791e-05 4.808161e-05
```

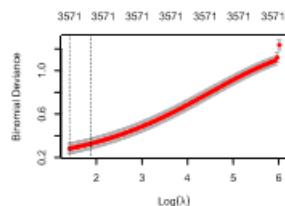
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Leukemia Dataset: Ridge Regression

Fit model using 10-fold CV to select lambda:

```
> set.seed(123)
> cv.model.ridge = cv.glmnet(x,y,alpha=0,family='binomial')
> plot(cv.model.ridge)
```



The default values of lambda did not work.

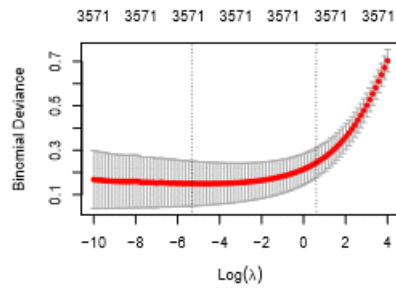
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Leukemia Dataset: Ridge Regression

Refit using smaller values of lambda to get a minimum:

```
> lambda = exp(seq(4,-10,length=100))
> cv.model.ridge = cv.glmnet(x,y,alpha=0,lambda = lambda,family='binomial')
> cv.model.ridge$lambda.min
[1] 0.00462795
> cv.model.ridge$lambda.1se
[1] 1.833195
```

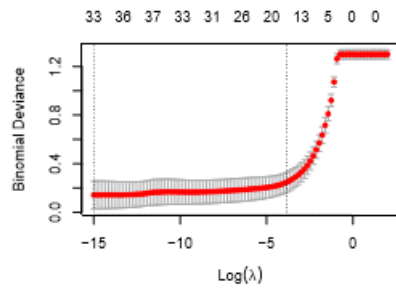


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Leukemia Dataset: Lasso

```
> set.seed(123)
> lambda = exp(seq(2,-15,length=100))
> cv.model.lasso = cv.glmnet(x,y,alpha=1,lambda=lambda,family='binomial')
> plot(cv.model.lasso)
```



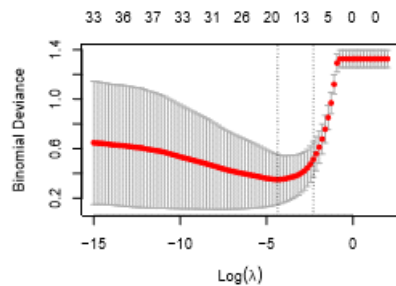
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Leukemia Dataset: Lasso

Unfortunately, the CV estimate can be highly variable.

This is running the same code but using a different random partition of the data into folds:



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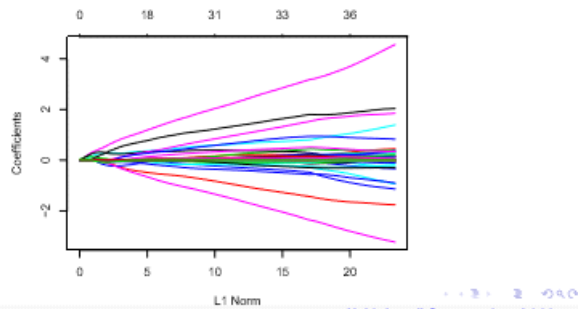
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Coefficient Paths

We can also look at coefficient paths.

These plot the coefficients across the grid of λ .

Variables that enter the model first are more important (when using standardization).



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Leukemia Dataset: Elastic Net

For elastic net, a typical default is $\alpha = 0.5$.

You could try to perform a 2D-CV varying λ and α , but this is computationally costly and may not work very well due to high CV variability.

Elastic net with $\alpha = 0.5$ is a good default for high-dimensional regression. Tends to be more reliable than lasso, and unlike ridge, achieves variable selection.

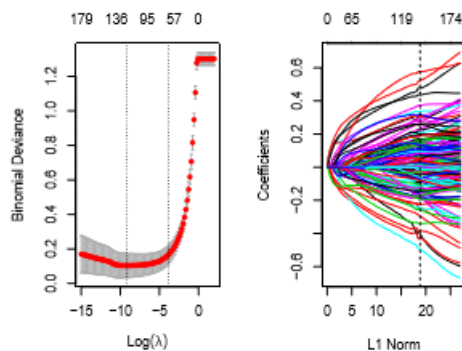
To select fewer variables, increase α .

```
> set.seed(123)
> cv.model.elnet = cv.glmnet(x,y,alpha=0.5,lambda=lambda,family='binomial')
> elnet.estimates = coef(cv.model.elnet,s=cv.model.elnet$lambda.min)
> model.elnet = glmnet(x,y,alpha=0.5,lambda=lambda,family='binomial')
> plot(model.elnet)
> abline(v=sum(abs(elnet.estimates)),lty=2)
```

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Leukemia Dataset: Elastic Net



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What about inference?

Inference in the Lasso and penalized regression is an active area of research.

Recent distributional results are available when conditioning on the selection event: Lee, J. D., Sun, D. L., Sun, Y., & Taylor, J. E. (2016). Exact post-selection inference, with application to the lasso. *The Annals of Statistics*, 44(3), 907-927.

Since we are also choosing the tuning parameter via cross-validation, "conditioning on the selection event" is not incorporating all sources of uncertainty.

Another promising approach is "knockoffs," where you create "knockoffs" of X unrelated to Y and estimate the distribution of test statistics from these knockoffs: Barber, R. F., Candès, E. J., & Samworth, R. J. (2020). Robust inference with knockoffs. *Annals of Statistics*, 48(3), 1409-1431.

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Other issues with inference

For elastic net and lasso using `glmnet`, we have replaced inference with variable selection and CV.

A common approach to large p (high dimensional) studies is to conduct thousands of univariate tests.

E.g., t tests for comparing cancer and control in gene expression.

Multiple comparisons is a problem: when conducting thousands of tests, we need to consider the probability that we falsely reject null hypotheses.

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Note on Bonferroni Correction

When we conduct many hypothesis tests, we increase the chance of false detections.

Let H_1, \dots, H_m be a family of null hypothesis tests, and p_1, \dots, p_m their associated p-values.

Here we use m instead of p predictors due to notational conflict.

The **family-wise error rate** is the probability of at least one false positive.

Let $m_0 < m$ be the number of true null hypotheses.

We control the FWER if

$$P \left\{ \bigcup_{j=1}^{m_0} (H_j \text{ is rejected} \mid H_j \text{ is true}) \right\} < \alpha.$$

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Bonferroni correction, cont.

The Bonferroni correction is popular in part due to its simplicity: let $\alpha^* = \alpha/m$, where α is typically 0.05.

$$\begin{aligned} P\left\{\bigcup_{j=1}^{m_0} (p_j \leq 0.05/m)\right\} &\leq \sum_{j=1}^{m_0} P(p_j \leq 0.05/m) \\ &= m_0 * 0.05/m \\ &\leq m * 0.05/m \\ &= 0.05. \end{aligned}$$

So when we control the individual tests at α^* , the FWER is less than or equal to α .

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Module 6, part II: Sparse regression and shrinkage

Bonferroni Correction, cont.

The Bonferroni Correction is a very conservative approach to correcting for multiple comparisons in variable selection.

It is often *too* conservative, and we will not find much (or even any) signal for very large p .

Other methods can be more powerful: controlling the false discovery rate (FDR), which is the proportion of falsely rejected null hypotheses, i.e., among the set of rejected null hypotheses, what proportion were in fact Type 1 errors.

There are also more powerful approaches to FWER, particularly under some types of dependence.

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