LASSO Regression

CMED6040 - Session 8

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Session 8 learning objectives

After this session, students should be able to

- Understand the bias-variance tradeoff in model selection
- Perform model selection using ridge, LASSO and elastic net regressions
- Recognize pros and cons of various model selection approaches

Model selection

Modelling an outcome variable on a set of predictor variables

- Select a subset of the candidate predictor variables
- Objective: simple, interpretable model with accurate predictions
- Goodness of fit
 - How similar the observed and predicted values are
 - Measured by R-squared, AIC, BIC, etc
- Parsimony
 - Occam's razor: for models with similar goodness of fit, the simpler one is preferred
- Data sets
 - Training set for developing the model
 - Testing set for examining the model in another data set

Example – polynomial regression

Consider a simple sinusoidal model

$$Y = 3\sin(X) + \varepsilon$$

where $\varepsilon \sim Normal(0, 1)$

Generate training data

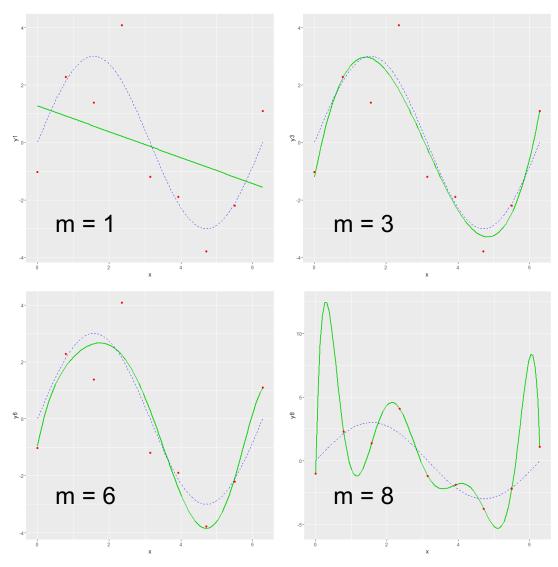
```
> set.seed(6789)
> x <- c(0:8) / 8 * 2 * pi
> y <- 3 * sin(x) + rnorm(n=9)
> data <- data.frame(x, y)</pre>
```

Fit a polynomial regression model

$$y = \alpha + \sum_{k=1}^{m} \beta_k x^k$$

Example – polynomial regression

Which model is the best?



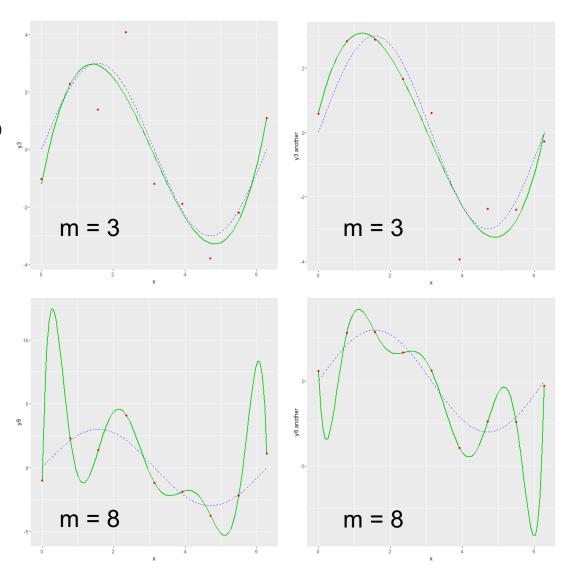
Over-fitting

- The model with m = 8 perfectly predicts the observed values, but...
- There are random fluctuations (or noise, errors) in the data
- Over-fitting causes the model to fit the noise rather than the actual underlying structure
- Too sensitive to the data that the fitted model would be very different if another set of training data is used
- May result in large prediction error if the model is applied to a set of testing data

Another training data set

• Generate training data

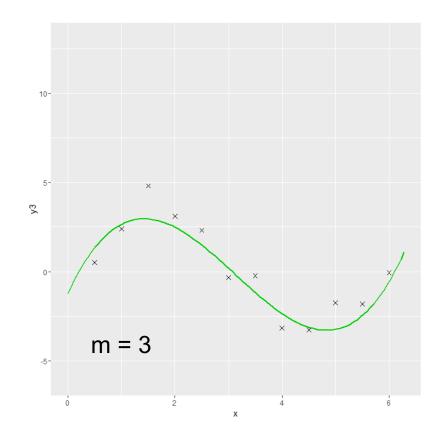
```
> set.seed(12345)
> x <- c(0:8) / 8 * 2 * pi
> y <- 3 * sin(x) + rnorm(n=9)
> another <- data.frame(x, y)</pre>
```

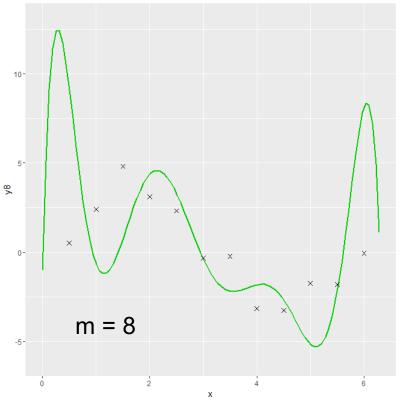


Testing data

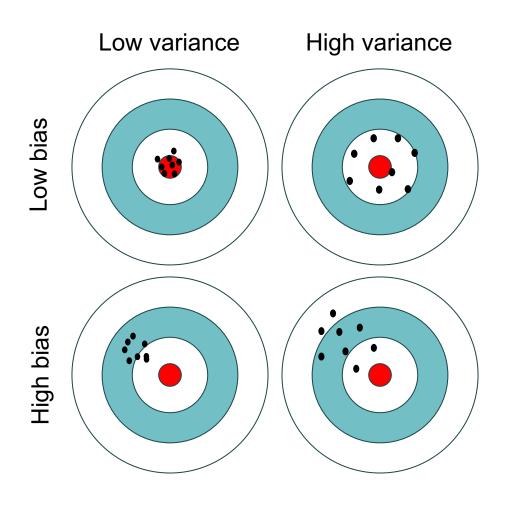
Generate testing data

```
> x <- c(1:12) / 2
> y <- 3 * sin(x) + rnorm(n=12)
> test <- data.frame(x, y)</pre>
```

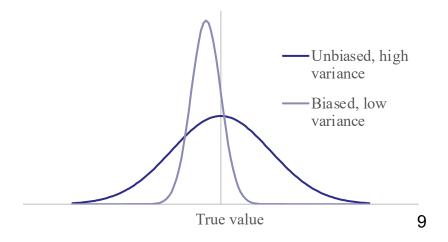




Bias and variance



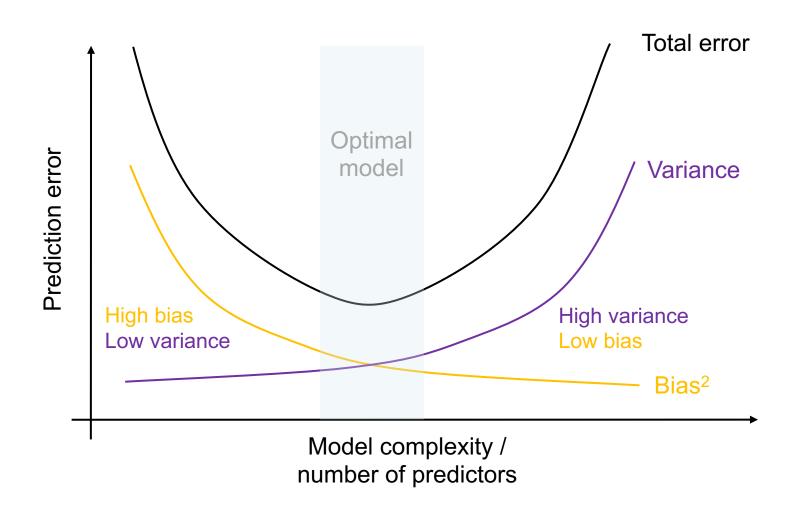
- Bias how far the predicted values deviated from the true
- Variance how scattered the predicted values are
- Ideally low bias and low variance
- But in practical there is a tradeoff between bias and variance



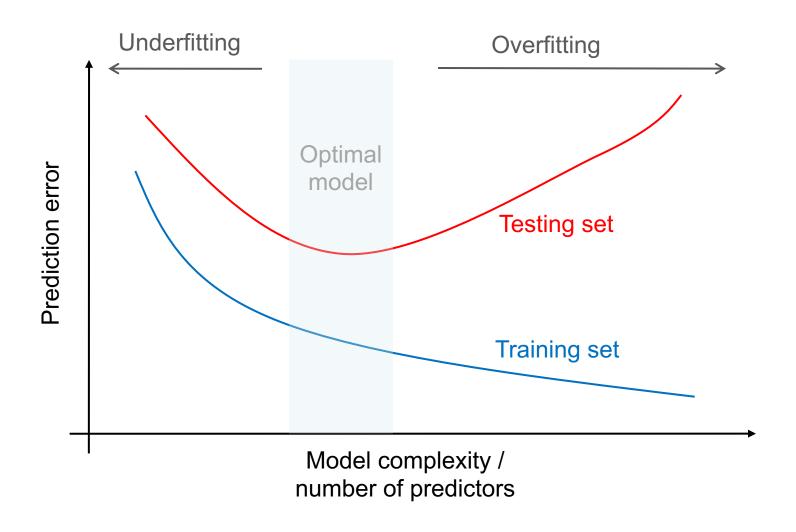
Bias-variance decomposition

- Observed value $Y = f(X) + \varepsilon$, where $E(\varepsilon) = 0$, $Var(\varepsilon) = \sigma^2$
- Predicted value $\hat{Y} = \hat{f}(X)$ is a random variable
- Bias = $f(X) E[\hat{f}(X)]$ = Expected difference between true and predicted
- Expectation of squared prediction error $E\left[\left(Y-\hat{Y}\right)^2\right]$ $= E \left| \left(f(X) + \varepsilon - \hat{f}(X) \right)^2 \right|$ $= E[\varepsilon^{2}] + 2E[\varepsilon(f(X) - \hat{f}(X))] + E[f(X) - \hat{f}(X)]^{2}$ (Grey part equals zero: $E\left[\varepsilon\left(f(X)-\hat{f}(X)\right)\right]=E\left[\varepsilon\right]E\left[\left(f(X)-\hat{f}(X)\right)\right]=0$) $= E[\varepsilon^2] + E\left[(f(X) - E[\hat{f}(X)] + E[\hat{f}(X)] - \hat{f}(X))^2 \right]$ (Grey part equals zero) $= E[\varepsilon^2] + E\left[\left(f(X) - E[\hat{f}(X)]\right)^2\right] + E\left[\left(\hat{f}(X) - E[\hat{f}(X)]\right)^2\right]$ (Grey part is constant) $\mathbb{E}\left[\left(f(X) - E[\hat{f}(X)]\right)\left(E[\hat{f}(X)] - \hat{f}(X)\right)\right] = \left(f(X) - E[\hat{f}(X)]\right)\mathbb{E}\left[\left(E[\hat{f}(X)] - \hat{f}(X)\right)\right] = 0$ $= \sigma^2 + (f(X) - E[\hat{f}(X)])^2 + Var(\hat{f}(X))$ = Noise² + Bias² + Variance

Bias-variance tradeoff



Training and testing sets



Example – Prostate cancer

 Source: Stamey, T.A., et al. (1989) Prostate specific antigen in the diagnosis and treatment of adenocarcinoma of the prostate: II. radical prostatectomy treated patients, Journal of Urology 141(5), 1076–1083.

Variable	Description [Level
Icavol	log(cancer volume)	Continuous	
lweight	log(prostate weight)	Continuous	
age	age	Continuous	
lbph	log(benign prostatic hyperplasia amount)	Continuous	
svi	seminal vesicle invasion	Categorical	1: Yes, 0: No
lcp	log(capsular penetration)	Continuous	
gleason	Gleason score	Continuous	
pgg45	percentage Gleason scores 4 or 5	Continuous	
lpsa	log(prostate specific antigen) (Outcome)	Continuous	

Data sets

Read data and assign factors

```
Prostate <- read.csv("prostate.csv")</pre>
```

Divide into training and testing sets

```
set.seed(23456)
TestingIndex <- sample(1:nrow(Prostate), 20)
Training <- Prostate[-TestingIndex, ]
Testing <- Prostate[TestingIndex, ]</pre>
```

Automated selection procedure

Backward selection

Automated selection procedure

Alternatives

A period "." means all other variables in the data set, a minus "—" excludes a variable

```
Alt <- lm(lpsa ~ . - age - svi, data = Training)
```

Add F-test or Chi-squared test in the output

```
Backward2 <- step(Full, direction = "backward", test = "F")
Backward3 <- step(Full, direction = "backward", test = "Chisq")</pre>
```

Forward and stepwise selection

Forward selection

Stepwise selection

Ordinary least squares

 At each step of the above selection procedures, the coefficients were found by ordinary least squares (OLS), i.e. minimizing the sum of squared residuals:

$$\sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2$$

- Unbiased
- Alternative: Penalized regression
 - Bias-variance trade-off: introduce bias to reduce variance

Penalized regression

Minimize the sum of squared residuals

$$\sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2$$

subject to a constraint

Ridge regression:
$$\sum_{j=1}^{p} \beta_j^2 \le t_1$$

LASSO regression:
$$\sum_{j=1}^{p} |\beta_j| \le t_2$$

where t_1 and $t_2 > 0$ are penalty parameters

No longer unbiased, but reduces the variance

Ridge regression

Minimize the sum of squared residuals subject to

$$\sum_{j=1}^{p} \beta_j^2 \le t$$

where t > 0 is a penalty parameter

• This is equivalent to find the set of coefficients β_j that minimizes the objective function with various non-negative values of λ :

$$\sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

- As $\lambda \to 0$, ridge coefficients \to OLS coefficients
- As $\lambda \to \infty$, ridge coefficients $\to 0$

Ridge and LASSO regression in R

- Package: glmnet
- glmnet(x, y, alpha, lambda, family...)
 - x: matrix of predictor variables
 - y: response variable
 - alpha: 0 = Ridge regression, 1 = LASSO regression
 - lambda: user-supplied λ values
 - family: Response type, e.g. "gaussian", "binomial", etc

Ridge regression

```
library(glmnet)
x <- model.matrix(lpsa ~ . - 1, data = Training)
v <- Training$lpsa</pre>
Ridge1 <- glmnet(x, y, alpha = 0, lambda = c(0.5, 1))
Ridge1
Call: glmnet(x = x, y = y, alpha = 0, lambda = c(0.5, 1))
    Df %Dev Lambda
[1,] 8 59.80 1.0
[2,] 8 64.06 0.5
coef(Ridge1)
                     s0
                                  s1
(Intercept) -0.1042577829 -0.309343110
lcavol 0.2846293551 0.366144109
lweight 0.3435344292 0.420581866
           -0.0004531201 -0.004340865
age
lbph
          0.0753331555 0.094017529
svi
        0.4579589510 0.534373698
lcp 0.0977048229 0.080735763
gleason 0.1222559227 0.128152107
           0.0031661125 0.003072614
pgq45
```

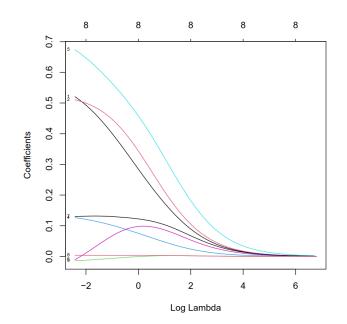
Ridge regression

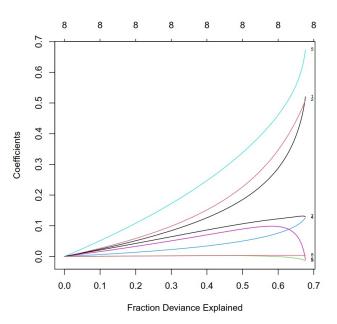
Not specifying λ

```
Ridge2 <- glmnet(x, y, alpha = 0)
plot(Ridge2, xvar="lambda", label=TRUE)
plot(Ridge2, xvar="dev", label=TRUE)</pre>
```

Magnitude of coefficients

- Decrease with λ, approach to (but not become) 0 due to the penalty λ $\sum_{i=1}^m eta_i^2$
- Overall, increase with the proportion of deviance explained





k-fold Cross-validation

- Randomly divide the data set into k (usually 10) equal-sized subsets
 - Use (k-1) subsets for estimation of model (training)
 - The remaining subset for computation of prediction error (testing)

Train	Train		Train	Test	⇒ 1 st prediction error			
Train	Train		Test	Train	⇒ 2 nd prediction error			
		:						
Train	Test		Train	Train	$ ight] \; ightrightarpoons \;$ (k-1) $^{ ext{th}}$ prediction error			
Test	Train		Train	Train	⇒ k th prediction error			

- Calculate the mean and standard error of mean squared error (MSE)
- Leave-one-out: k = sample size

Ridge regression

Cross-validation to determine λ

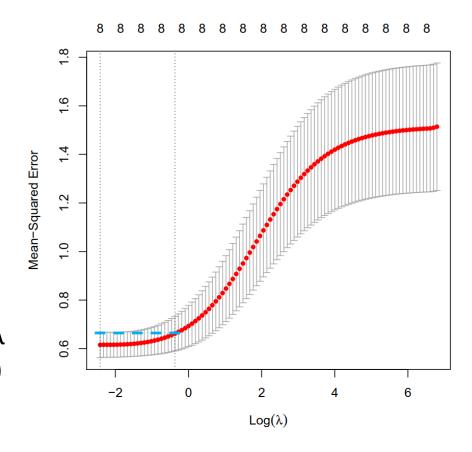
```
set.seed(56789)
Ridge2.cv <- cv.glmnet(x, y, alpha = 0)
plot(Ridge2.cv)</pre>
```

- Mean MSE (red dot) ± SE (vertical bar)
- Left vertical line: minimum MSE

```
min(Ridge2.cv$cvm)
[1] 0.615571
log(Ridge2.cv$lambda.min)
[1] -2.416623
```

• Right vertical line: maximum value of λ within 1 SE of the minimum (1-SE rule)

```
log(Ridge2.cv$lambda.1se)
[1] -0.3698812
```



Ridge regression

Coefficients by 1-SE rule

Predicted values on testing set

```
x.test <- model.matrix(lpsa ~ . - 1, data = Testing)
Ridge2.Pred <- predict(Ridge2, newx = x.test, s = Ridge2.cv$lambda.1se)</pre>
```

LASSO regression

- Ridge regression
 - Coefficients shrink towards but never reach 0
 - All predictor variables retain, cannot produce a parsimonious model
- LASSO = Least Absolute Shrinkage and Selection Operator
- Minimize the sum of squared residuals subject to

$$\sum_{j=1}^{p} |\beta_j| \le t$$

where t > 0 is a penalty parameter

Equivalent to the objective function:

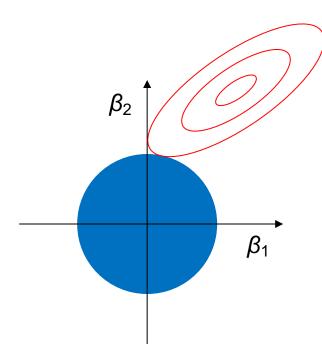
$$\sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

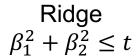
LASSO regression

• Same package glmnet as ridge regression, but alpha = 1

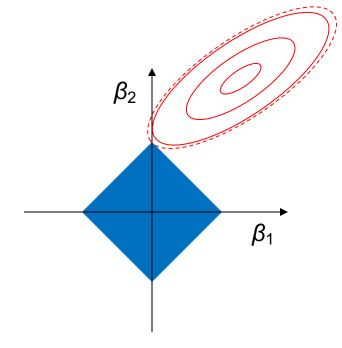
```
LASSO1 <- glmnet(x, y, alpha = 1, lambda = c(0.25, 0.5, 0.75, 1))
LASSO1
    Df
        %Dev Lambda
[1,] 0 0.00 1.00
[2,] 1 15.72 0.75
[3,] 1 36.75 0.50
[4,] 3 55.34 0.25
coef(LASSO1)
                 s0
                          s1
                                    s2
                                             s3
(Intercept) 2.473523 2.3139032 2.0333247 1.1850329
lcavol
                    0.1177542 0.3247419 0.4661090
lweight
                                       0.1598011
age
lbph
svi
                                       0.3314309
lcp
gleason
pgq45
```

Geometric interpretation





both β_1 and β_2 are non-zero



$$|\beta_1| + |\beta_2| \le t$$

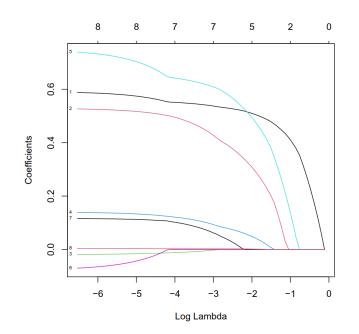
 β_1 or β_2 could be zero

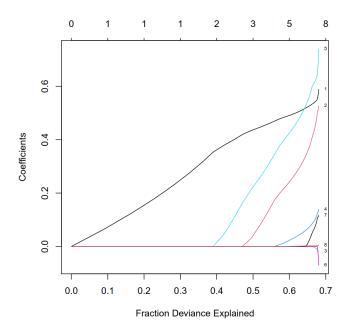
LASSO regression

```
LASSO2 <- glmnet(x, y, alpha = 1)
plot(LASSO2, xvar="lambda", label=TRUE)
plot(LASSO2, xvar="dev", label=TRUE)
```

Magnitude of coefficients

- Decrease with λ , same as ridge regression
- Become 0 one by one (x-axis on top); all become 0 as λ is large ($\lambda = 1$ in this example)
- Overall, increase with the proportion of deviance explained (only intercept when $\lambda = 1$)





LASSO regression

Cross-validation to determine λ

```
set.seed(54321)
LASSO2.cv <- cv.glmnet(x, y, alpha = 1)
plot(LASSO2.cv)</pre>
```

Minimum MSE

```
min(LASSO2.cv$cvm)
[1] 0.6172947
log(LASSO2.cv$lambda.min)
[1] -3.370219
```

1-SE rule

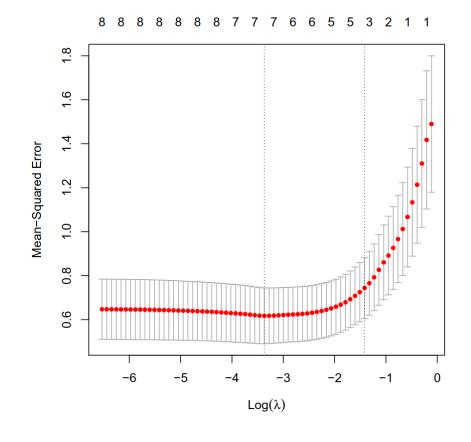
```
log(LASSO2.cv$lambda.1se)
[1] -1.416511
```

How many non-zero coefficients?

```
coef(LASSO2, s = LASSO2.cv$lambda.1se)
```

Export the predicted values for further analysis

```
LASSO2.Pred <- predict(LASSO2, newx = x.test, s = LASSO2.cv$lambda.1se)
```



Multicollinearity

- Grouped selection
 - A group of (usually correlated) predictor variables included in the model
- Create a new predictor variable which is the sum of two existing ones

```
Prostate.col <- Prostate
Prostate.col$new1 <- Prostate.col$lcavol + Prostate.col$lweight</pre>
```

OLS

Ridge

```
(Intercept) 0.2958473
lcavol 0.2510017
lweight 0.2103176
new1 0.2149762
```

Multicollinearity

Create another new variable which is nearly the sum of two existing ones

```
set.seed(234567)
Prostate.col$new2 <- Prostate.col$new1 + rnorm(nrow(Prostate.col), 0, 0.1)</pre>
```

OLS

Ridge

```
(Intercept) 0.2957072
lcavol 0.2495335
lweight 0.2072931
new2 0.2183987
```

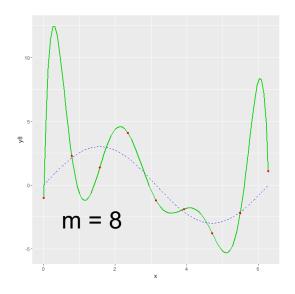
OLS is sensitive to multicollinearity

• Ridge regression is more robust

Number of predictors

- Recall the polynomial regression example
 - Sample size = 9
 - Perfectly fit when m = 8 (i.e. 9 parameters estimated)
 - What happen if $m \ge 9$?
- Prostate example

```
set.seed(21098)
SmallIndex <- sample(1:nrow(Prostate), 6)
Small <- Prostate[SmallIndex, ]</pre>
```



33

OLS

Coefficients:

(Intercept)	lcavol	lweight	age	lbph	svi
-5.67764	0.69457	0.70011	0.07270	-0.03293	NA
lcp	gleason	pgg45			
0.15074	NA	NA			

Number of predictors

Ridge and LASSO

```
x.Small <- model.matrix(lpsa ~ lcavol + lweight + age + lbph + svi + lcp +
                           gleason + pgg45 - 1, data = Small)
y.Small <- Small$lpsa
Small.Ridge \leftarrow glmnet(x.Small, y.Small, alpha = 0, lambda = c(0.1, 0.01))
coef(Small.Ridge)
Small.LASSO \leftarrow glmnet(x.Small, y.Small, alpha = 1, lambda = c(0.1, 0.01))
coef(Small.LASSO)
```

Ridge			LASSO		
	s0	s1		sO	s1
(Intercept)	-3.983189980	-3.34701545	(Intercept)	-4.61897188	-5.5170679541
lcavol	0.634838300	0.71370283	lcavol	0.62848146	0.6821712429
lweight	0.377882039	0.39886193	lweight	0.45130177	0.5797324637
age	0.052767193	0.04535218	age	0.06858169	0.0746291622
lbph	0.043633242	0.03597348	lbph	•	•
svi	•	•	svi	•	•
lcp	0.337259634	0.42433255	lcp	•	0.0129012020
gleason	0.156275254	0.12605415	gleason	•	
pgg45	0.005244347	0.00601659	pgg45	•	0.0005385419 ³⁴

Comparison

	OLS	Ridge	LASSO	
Bias	s Unbiased		Biased	
Variance	Larger variance	Smaller variance	Smaller variance	
Parsimony	Number of predictors cannot be reduced	Coefficients shrink but never reach 0, same number of predictors	Some coefficients shrink to 0, fewer predictors	
Multicollinearity	Sensitive to strongly correlated predictors	Robust and good for grouped selection	Some coefficients shrink to 0, good for excluding correlated predictors	
N < # of parameters	Not estimable	Estimable	Estimable	

Elastic net

- Objective functions:
 - Ridge minimizes $\sum_{i=1}^{N} (y_i \beta_0 \boldsymbol{x}_i^T \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} \beta_j^2$
 - LASSO minimizes $\sum_{i=1}^{N} (y_i \beta_0 \boldsymbol{x}_i^T \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} |\beta_j|$
- Averaging the two penalty functions, weighted by a parameter α :

$$- \lambda \left[(1 - \alpha) \sum_{j=1}^{p} \beta_j^2 + \alpha \sum_{j=1}^{p} |\beta_j| \right]$$

- When $\alpha = 0 \rightarrow \text{Ridge}$
- When $\alpha = 1 \rightarrow LASSO$
- − When $0 < \alpha < 1$ → Elastic net
- Recall the R codes for glmnet(x, y, alpha...)
 - alpha: 0 = Ridge regression, 1 = LASSO regression, 0 < α < 1 = Elastic net

Elastic net

Prostate example

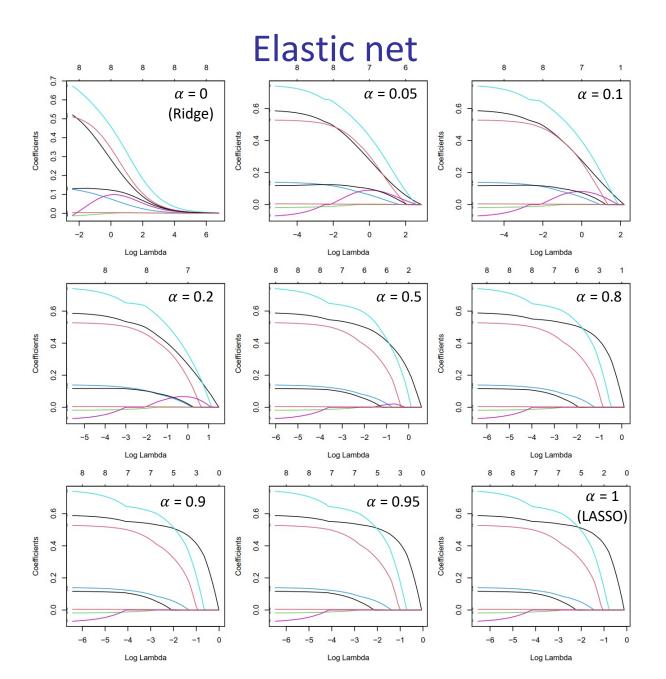
```
x <- model.matrix(lpsa ~ . - 1, data = Training)
y <- Training$lpsa
x.test <- model.matrix(lpsa ~ . - 1, data = Testing)</pre>
```

Using glmnet with various alpha values, without specifying lambda

```
library(glmnet)
Elastic000 <- glmnet(x, y, alpha = 0)
Elastic005 <- glmnet(x, y, alpha = 0.05)
Elastic010 <- glmnet(x, y, alpha = 0.1)
Elastic020 <- glmnet(x, y, alpha = 0.2)
Elastic050 <- glmnet(x, y, alpha = 0.5)
Elastic080 <- glmnet(x, y, alpha = 0.8)
Elastic090 <- glmnet(x, y, alpha = 0.9)
Elastic095 <- glmnet(x, y, alpha = 0.95)
Elastic100 <- glmnet(x, y, alpha = 1)</pre>
```

Plot the graphs of Coefficients again Log Lambda

```
plot(Elastic000, xvar="lambda", label=TRUE)
...
plot(Elastic100, xvar="lambda", label=TRUE)
```



Elastic net

Cross-validation to determine λ

```
set.seed(76543)
Elastic.cv <- cv.glmnet(x, y, alpha = 0.5)
plot(Elastic.cv)</pre>
```

Minimum MSE

```
min(Elastic.cv$cvm)
[1] 0.6108528
log(Elastic.cv$lambda.min)
[1] -2.956173
```

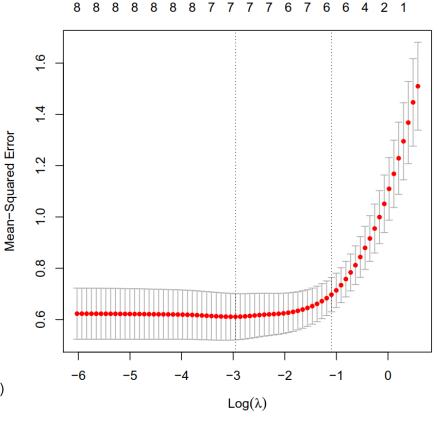
1-SE rule

```
log(Elastic.cv$lambda.1se)
[1] -1.095499
```

How many non-zero coefficients?

```
coef(Elastic050, s = Elastic.cv$lambda.1se)
```

Export the predicted values for further analysis



Application

Epidemiology of human infections with highly pathogenic avian influenza A(H7N9) virus in Guangdong, 2016 to 2017

M Kang 12, EHY Lau 23, W Guan 24, Y Yang 1, T Song 1, BJ Cowling 3, J Wu 1, M Peiris 45, J He 1, CKP Mok 45

Euro Surveill. 2017;22(27):pii=30568

TABLE 3

Multivariable logistic ridge regression analysis of risk factors for HPAI compared with LPAI A(H7N9) human infections (n=60)

Exposure	HPAI A(H7N9) infections AOR (95% CI)					
	Model 1	Model 2				
Raise backyard poultry	2.13 (1.02-6.06)	1.97 (1.01-6.33)				
Touched live poultry	2.11 (1.01-5.76)	Not entered				
Touched sick or dead poultry	Not entered	5.35 (1.09-32.60)				

AOR: adjusted odds ratio; CI: confidence interval; HPAI: highly pathogenic avian influenza; LPAI: low-pathogenic avian influenza.

- Sample size = 60 (9 HPAI vs 51 LPAI)
- Low power for OLS
- Not estimable if more than 9 predictors
- Ridge regression was used
- Another R package "ridge"

Application

Social contacts and the locations in which they occur as risk factors for influenza infection

Kin O. Kwok¹, Benjamin J. Cowling¹, Vivian W. I. Wei¹, Kendra M. Wu¹, Jonathan M. Read³, Justin Lessler⁴, Derek A. Cummings⁴, J. S. Malik Peiris^{1,2} and Steven Riley^{1,5}

Proc. R. Soc. B 2014; 281: 20140709.

Table 2. Regression model results from best subset analysis and group lasso regression.

- Used LASSO as sensitivity analysis
- To confirm the results from OLS where predictors were correlated
- Fixed $\lambda = 4$
- 95% CI constructed by bootstrap

	best sul	best subset							group lasso	
	baseline	e model		odel with variable only	best mo variable	odel with contact		odel with contact ation variables	estimate	95% CI ^b
age	0.942	(0.926 – 0.957)	0.939	(0.923-0.955)	0.942	(0.926-0.958)	0.939	(0.923 - 0.956)	0.945	(0.928-0.960)
district (ref Hong Kong Island)										
Kowloon East	1.06	(0.348 – 3.24)	1.03	(0.338-3.16)	1.06	(0.346-3.27)	1.03	(0.335 - 3.17)	1.00	(0.580 – 1.70)
Kowloon West	2.58	(0.915 – 7.29)	2.61	(0.918-7.41)	2.58	(0.905-7.37)	2.57	(0.898 - 7.38)	1.68	(1.00-3.96)
New Territories East	2.47	(1.04 – 5.87)	2.45	(1.03 – 5.83)	2.5	(1.05 – 5.97)	2.44	(1.02-5.84)	1.71	(1.11-3.35)
New Territories West	1.51	(0.584 - 3.89)	1.47	(0.567-3.81)	1.54	(0.592-4.01)	1.50	(0.574 - 3.91)	1.23	(0.828-2.23)
presence of child	2.49	(1.31 – 4.73)	2.47	(13 – 4.71)	2.49	(1.31-4.74)	2.46	(1.29-4.69)	2.06	(1.21-3.46)
number of locations (mean of maximum and minimum, per location)	_		1.16	(0.998-1.34)	_		1.15	(0.989 – 134)	1.08	(1.00 – 1.18)
contacts greater than 10 min (minimum, per 10 contacts)	_		_		1.10	(1.01 – 1.19)	_		1.03	(1.01 – 1.22)
contacts greater than 60 min (minimum, per 10 contacts)	_		_		_		1.09	(1.00-1.19)	1.04	(1.00-1.16)
AIC	402.3		400.7		400.3		399.3			
goodness-of-fit <i>p-</i> value ^a	0.38		0.31		0.25		0.28			
% of deviance explained	22.2		22.9		23.0		23.6			

^{*}Based on the le Cessie—van Houwelingen—Copas—Hosmer unweighted sum of squares test for global goodness of fit [15], calculated using the Irm package in R.

^bMiddle 95% of values from bootstrap refits in which the parameter was retained in the final model.