# Multiple (non) linear regression 

## Jiří Kléma

Department of Computer Science,<br>Czech Technical University in Prague

Lecture based on ISLR book and its accompanying slides


## Agenda

- Linear regression
- a simple model with a single predictor,
- parameters, interpretation, hypotheses testing,
- generalization towards multiple linear regression,
- special issues: qualitative predictors, outliers, collinearity,
- linear model selection and regularization
- subset selection,
- regularization $=$ shrinkage, lasso, ridge regression,
- choosing the optimal model, estimating test error,
- moving beyond linearity
- polynomial regression,
- step functions, splines,
- local regression,
- generalized additive models.


## Linear regression

- Assumption of linearity
- often simplifying assumption only
* true regression functions are rarely linear,
* still, the linear model extremely useful, both conceptually and practically,
- the simplification increases ability to learn
* helps to cope with the well-known curse of dimensionality,
- the simplification brings interpretability
* a reasonable number of parameters with clear meaning,
- good performance preserved in case of moderate violation
* linear models can be extended otherwise.



## Linear regression for the advertising data

- Consider the advertising data shown below, questions we might ask:
- is there a relationship between advertising budget and sales?
- how strong is the relationship between advertising budget and sales?
- which media contribute to sales?
- how accurately can we predict future sales?
- is the relationship linear?
- is there synergy among the advertising media?





## Simple linear regression using a single predictor $X$

- We assume a model

$$
Y=\beta_{0}+\beta_{1} X+\epsilon
$$

- where $\beta_{0}$ and $\beta_{1}$ are two unknown constants (coefficients, parameters),
- they represent the intercept and slope,
$-\epsilon$ is the error term, normally distributed with 0 mean, the same variance at every $X$, independent,
- we predict the future values of independent variable using

$$
\hat{y}=\hat{\beta}_{0}+\hat{\beta}_{1} x
$$

- where the hat symbol denotes an estimated value,
- $\hat{y}$ indicates a prediction of $Y$ on the basis of $X=x$.


## Estimation of the parameters by least squares

- Let $\hat{y}_{i}=\hat{\beta}_{0}+\hat{\beta}_{1} x_{i}$ be the prediction for $Y$ based on the $i$ th value of $X$,
- then $e_{i}=y_{i}-\hat{y}_{i}$ represents the $i$ th residual,
- we define the residual sum of squares (RSS) as

$$
R S S=e_{1}^{2}+e_{2}^{2}+\cdots+e_{m}^{2}=\sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\hat{\beta}_{1} x_{i}\right)^{2}
$$

- the least squares approach chooses $\hat{\beta}_{0}$ and $\hat{\beta}_{1}$ to minimize the RSS

$$
\begin{gathered}
\frac{\partial R S S}{\partial \hat{\beta}_{1}}=0 \rightarrow \hat{\beta}_{1}=\frac{\sum_{i=1}^{m}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sum_{i=1}^{m}\left(x_{i}-\bar{x}\right)^{2}} \\
\frac{\partial R S S}{\partial \hat{\beta}_{0}}=0 \rightarrow \hat{\beta}_{0}=\bar{y}-\hat{\beta}_{1} \bar{x}
\end{gathered}
$$

- where $\bar{x}$ and $\bar{y}$ are the sample means for $X$ and $Y$.


## Example: advertising data

- The least squares fit for the regression of sales onto TV
- a linear fit captures the essence of the relationship,
- although it is somewhat deficient in the left of the plot,
$-\hat{\beta}_{0}$ : no TV advertising, around 7 (thousand) units sold,
$-\hat{\beta}_{1}: \$ 1,000$ more spent on TV associated with selling $\sim 48$ additional units.



## Assessing the accuracy of the coefficient estimates

- Standard error of an estimator reflects how it varies under repeated sampling

$$
S E\left(\hat{\beta}_{1}\right)^{2}=\frac{\sigma^{2}}{\sum_{i=1}^{m}\left(x_{i}-\bar{x}\right)^{2}} \quad S E\left(\hat{\beta}_{0}\right)^{2}=\sigma^{2}\left(\frac{1}{m}+\frac{\bar{x}^{2}}{\sum_{i=1}^{m}\left(x_{i}-\bar{x}\right)^{2}}\right)
$$

- where $\sigma^{2}=\operatorname{Var}(\epsilon)$,
- residual standard error RSE is $\sigma$ estimate, $R S E=\sqrt{R S S /(m-2)}$.




## Coefficient confidence intervals

- Confidence interval (CI)
$-100(1-\alpha) \%$ confidence interval is a range of values that encompasses the true (unknown) population parameter in $100(1-\alpha) \%$ repeated sampling trials like this,
- there is approximately a $95 \%$ chance that the interval below will contain the true value of $\beta_{1}$ (under a scenario where we got repeated samples like the present sample)

$$
\left[\hat{\beta}_{1}-2 S E\left(\hat{\beta}_{1}\right), \hat{\beta}_{1}+2 S E\left(\hat{\beta}_{1}\right)\right]
$$

- a more precise (and general) Cl estimate is based on $1-\alpha / 2$ quantile of a t-distribution with ( $\mathrm{m}-2$ ) degrees of freedom

$$
\left[\hat{\beta}_{1}-t_{1-\alpha / 2, m-2} S E\left(\hat{\beta}_{1}\right), \hat{\beta}_{1}+t_{1-\alpha / 2, m-2} S E\left(\hat{\beta}_{1}\right)\right]
$$

- for the advertising data, the $95 \% \mathrm{Cl}$ for $\beta_{1}$ is [0.042, 0.053].


## Hypothesis testing

- The most common hypothesis test
- $H_{0}$ : there is no relationship between $X$ and $Y$,
$-H_{A}$ : there is some relationship between $X$ and $Y$,
- mathematically this corresponds to testing
$-H_{0}: \beta_{1}=0$ versus $H_{A}: \beta_{1} \neq 0$,
- the test stems from the standard error and t-statistic given by

$$
t=\frac{\hat{\beta}_{1}-0}{S E\left(\hat{\beta}_{1}\right)}
$$

- the statistic will have a t-distribution with m -2 degrees of freedom,
- the corresponding p -value is the probability of observing any value equal to $|t|$ or larger,
- both under the $H_{0}$ assumption, i.e., assuming $\beta_{1}=0$.


## Assessing the overall accuracy of the model

- R-squared gives the fraction of variance explained by the model

$$
R^{2}=\frac{T S S-R S S}{T S S}=1-\frac{R S S}{T S S}
$$

- where $T S S=\sum_{i=1}^{m}\left(y_{i}-\bar{y}\right)^{2}$ stands for the total sum of squares, - and $R S S=\sum_{i=1}^{m}\left(y_{i}-\hat{y}_{i}\right)^{2}$ stands for the residual sum of squares,
- while RSE mentioned earlier gives an absolute measure of its lack of fit,
- it can be shown that in this simple linear regression setting $R^{2}=r^{2}$,
- where $r$ is the correlation between X and Y .

$$
r=\frac{\sum_{i=1}^{m}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sqrt{\sum_{i=1}^{m}\left(x_{i}-\bar{x}\right)^{2}} \sqrt{\sum_{i=1}^{m}\left(y_{i}-\bar{y}\right)^{2}}}
$$

## Advertising data results: $\mathrm{X}=\mathrm{TV}, \mathrm{Y}=$ Sales

|  | Coefficient | Std. error | t-statistic | p-value |
| :---: | :---: | :---: | :---: | :---: |
| Intercept | 7.0325 | 0.4578 | 15.36 | $<0.0001$ |
| TV | 0.0475 | 0.0027 | 17.67 | $<0.0001$ |


| Quantity | Value |
| :---: | :---: |
| RSE | 3.26 |
| $R^{2}$ | 0.612 |
| F-statistic | 312.1 |

## Multiple linear regression

- Here, a following model is assumed

$$
Y=\beta_{0}+\beta_{1} X_{1}+\beta_{2} X_{2}+\cdots+\beta_{p} X_{p}+\epsilon
$$

- interpretation of the regression coefficients
$-\beta_{j}$ represents the average effect on $Y$ of a one unit increase in $X_{j}$, holding all other predictors fixed,
- it perfectly fits the balanced design where the predictors are uncorrelated,
- correlations among predictors cause problems
* the variance of all coefficients tends to increase, sometimes dramatically, * interpretations become hazardous, when $X_{j}$ changes, everything else changes,
- example: $Y=$ number of tackles by a football player in a season; $W$ and $H$ are his weight and height; fitted regression model is $\hat{Y}=b_{0}+.50 \mathrm{~W}-.10 \mathrm{H}$; how do we interpret $\hat{\beta}_{2}<0$ ?
- claims of causality should be avoided for observational data.


## Estimation of the parameters for multiple regression

- No principal changes from the simple model,
- the prediction formula is

$$
\hat{y}=\hat{\beta}_{0}+\hat{\beta}_{1} x_{1}+\hat{\beta}_{2} x_{2}+\cdots+\hat{\beta}_{p} x_{p}
$$

- the parameter estimates obtained by RSS minimization

$$
R S S=\sum_{i=1}^{m}\left(y_{i}-\hat{y}_{i}\right)^{2}=\sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\hat{\beta}_{1} x_{i 1}-\cdots-\hat{\beta}_{p} x_{i p}\right)^{2}
$$

- ordinary least squares estimation
- the most simple approach,
- generalized least squares
- allow efficient $\beta$ estimation when heteroscedascity or correlations are present.


## Categorical predictors

- So far, categorical and continuous independent variables treated separately
- often we need to study them concurrently, employ them in regression,
- for binary predictors we create a new $0 / 1$ variable $X_{i}$ with the resulting model

$$
y_{i}=\beta_{0}+\beta_{1} x_{i}+\epsilon_{i}=\left\{\begin{array}{l}
x_{i}=1: \beta_{0}+\beta_{1}+\epsilon_{i} \\
x_{i}=0: \beta_{0}+\epsilon_{i}
\end{array}\right.
$$

- interpretation: $\beta_{0}$ is the average outcome in the zero group, $\beta_{0}+\beta_{1}$ is the average outcome in the positive group, $\beta_{1}$ is the average difference in outcomes between groups,
- however, a - $1 / 1$ dummy variable could be introduced too

$$
y_{i}=\beta_{0}+\beta_{1} x_{i}+\epsilon_{i}=\left\{\begin{array}{l}
x_{i}=1: \beta_{0}+\beta_{1}+\epsilon_{i} \\
x_{i}=-1: \beta_{0}-\beta_{1}+\epsilon_{i}
\end{array}\right.
$$

- the predictions will be identical, $\beta$ values and interpretation change.


## Categorical predictors

- for predictors with $l$ levels we typically create $l-1$ dummy variables,
- e.g., ethnicity $\in\{$ Asian, Caucasian, African American $\}$ could be captured by

$$
x_{i 1}=\left\{\begin{array}{ll}
1 & \text { if } i \text { th person is Asian } \\
0 & \text { if } i \text { th person is not Asian }
\end{array} \quad x_{i 2}= \begin{cases}1 & \text { if } i \text { th person is Caucasian } \\
0 & \text { if } i \text { th person is not Caucasian }\end{cases}\right.
$$

- the level with no dummy variable (African American) is known as the baseline,
- the dummy variables appear in the regression equation
$y_{i}=\beta_{0}+\beta_{1} x_{i 1}+\beta_{2} x_{i 2}+\epsilon_{i}= \begin{cases}\beta_{0}+\beta_{1}+\epsilon_{i} & \text { if } i \text { th person is Asian } \\ \beta_{0}+\beta_{2}+\epsilon_{i} & \text { if } i \text { th person is Caucasian } \\ \beta_{0}+\epsilon_{i} & \text { if } i \text { th person is African American }\end{cases}$
- interpretation: $\beta_{0}$ is the average outcome in the baseline group, $\beta_{1}$ is the average outcome increase in the first group, $\beta_{2}$ is the average outcome increase in the second group (both wrt baseline).


## Interaction in the advertising data?

- Regular linear model is additive
- e.g., the average effect on sales of a one-unit increase in TV is always $\beta_{T V}$, regardless of the amount spent on radio,
- however, there is an interaction between TV and radio spending
- when advertising is split between the two media, the additive linear model tends to underestimate sales $\rightarrow$ there is synergy between the predictors.



## Modeling interactions

- Add an interaction term into the model, in the case of advertising problem

$$
\text { sales }=\beta_{0}+\beta_{1} \times \mathrm{TV}+\beta_{2} \times \text { radio }+\beta_{3} \times(\mathrm{TV} \times \text { radio })+\epsilon
$$

- in this model, the effect of TV changes with the value of radio (and vice versa)

$$
\begin{gathered}
\text { sales }=\beta_{0}+\left(\beta_{1}+\beta_{3} \times \text { radio }\right) \times \mathrm{TV}+\beta_{2} \times \text { radio }+\epsilon \\
\text { sales }=\beta_{0}+\beta_{1} \times \mathrm{TV}+\left(\beta_{2}+\beta_{3} \times \mathrm{TV}\right) \times \text { radio }+\epsilon
\end{gathered}
$$

- results of this model confirm the role of the interaction

|  | Coefficient | Std. error | t-statistic | p-value |
| :---: | :---: | :---: | :---: | :---: |
| Intercept | 6,7502 | 0.248 | 27.23 | $<0.0001$ |
| TV | 0.0191 | 0.002 | 12.70 | $<0.0001$ |
| radio | 0.0289 | 0.009 | 3.24 | 0.0014 |
| TV $\times$ radio | 0.0011 | 0.000 | 20.73 | $<0.0001$ |

## Modeling interactions - interpretation and hints

- The p-value for the interaction term TV $\times$ radio is extremely low
- indicating that there is strong evidence for $H_{a}: \beta_{3} \neq 0$,
- $R^{2}$ for the interaction model is $96.8 \%$
- compared to only $89.7 \%$ for the model using TV and radio without an interaction term,
$-\frac{96.8-89.7}{100-89.7}=69 \%$ of the variability in sales that remains after fitting the additive model has been explained by the interaction term,
- the coefficient estimates in the table suggest that
- increase in TV advertising of $\$ 1,000$ is associated with increased sales of $\left(\beta_{1}+\beta_{3} \times\right.$ radio $) \times 1000=19+1.1 \times$ radio units,
- If we include an interaction in a model
- we should also include the main effects (TV and radio in our case), even if the $p$-values associated with their coefficients are not significant.


## Some important questions

1. Is at least one of the $p$ predictors useful in predicting the response?
2. How well does the model fit the data?
3. Do all the predictors help to explain $Y$, or is only a subset of them useful?
4. Given a set of predictor values, what response value should we predict, and how accurate is our prediction?


## Is at least one predictor useful?

- Formally: $H_{0}: \beta_{1}=\beta_{2}=\cdots=\beta_{p}=0$ vs $H_{A}$ : at least one $\beta_{j} \neq 0$,
- this test is performed by computing the F -statistic

$$
F=\frac{(T S S-R S S) / p}{R S S /(m-p-1)}
$$

- in fact, we compare fit of the full (RSS) and intercept only model (TSS)
- technically, we compute the ratio between explained and unexplained variance of the full model,
- provided $H_{0}$ is true
- $E((T S S-R S S) / p)=E(R S S /(m-p-1))=\sigma^{2}$ and F is close to 1 ,
- the test is adjusted to the number of predictors $p$ and the sample size $m$,
- F-statistic is compared with quantiles of $F(p, m-p-1)$ distribution.


## F-distribution

- $\chi^{2}$ distribution with $d f$ degrees of freedom is the distribution of a sum of the squares of $d f$ independent standard normal random variables
- provided that $H_{0}$ holds, residuals should have normal distribution, zero mean and equal variance,
- consequently, $T S S, R S S$ as well as their additions and subtractions follow the $\chi^{2}$ distribution...
- F-distribution is any distribution obtained by taking the quotient of two $\chi^{2}$ distributions divided by their respective degrees of freedom,
- consequently, any F-distribution has two parameters corresponding to the degrees of freedom for the two $\chi^{2}$ distributions,
- given $X_{1} \sim \chi_{d f_{1}}^{2}$ and $X_{2} \sim \chi_{d f_{2}}^{2}$

$$
\frac{X_{1} / d f_{1}}{X_{2} / d f_{2}} \sim F_{d f_{1}, d f_{2}}
$$

## F-distribution in $\mathbf{R}$

- find the value of $F_{\alpha, g-1, N-g}$ : qf(alpha, df1, df2, lower.tail = F),
- find the p-value when knowing the observed $F$ value: pf (Fobs, df1, df2, lower.tail = F).


Statlect: The Digital Textbook

## Advertising data results: the full model

|  | Coefficient | Std. error | t-statistic | p-value |
| :---: | :---: | :---: | :---: | :---: |
| Intercept | 2.939 | 0.3119 | 9.42 | $<0.0001$ |
| TV | 0.046 | 0.0014 | 32.81 | $<0.0001$ |
| radio | 0.189 | 0.0086 | 21.89 | $<0.0001$ |
| newspaper | -0.001 | 0.0059 | -0.18 | 0.8599 |


| Correlations | TV | radio | newspaper | sales |
| :---: | :---: | :---: | :---: | :---: |
| TV | 1.0000 | 0.0548 | 0.0567 | 0.7822 |
| radio |  | 1.0000 | 0.3541 | 0.5762 |
| newspaper |  |  | 1.0000 | 0.2283 |
| sales |  |  |  | 1.0000 |


| Quantity | Value |
| :---: | :---: |
| RSE | 1.69 |
| $R^{2}$ | 0.897 |
| F-statistic | 570 |

## How well does the model fit the data?

- We have already seen that R-squared is a good quantifier for model fit, however
- it cannot show us whether the model is biased or not,
- features such as heteroscedasticity, non-linearity or outliers remain hidden,
- residual plot reveals these features
- most often it plots residuals as a function of predicted values,
- namely when having multiple independent variables.





[^0]
## Deciding on the important variables

- Selection cannot be directly based on the observed predictor p-values
- namely for large $p$, risk of false discoveries due to multiple comparisons,
- build and compare (a lot of) alternative models
- repetitive application of least squares on various reduced sets of predictors,
$-R S S$ and $R^{2}$ are not suitable for selecting the best model
* at least, among a collection of models with different numbers of predictors,
* they are related to the training error,
* the model containing all of the predictors will always have the smallest $R S S$ and the largest $R^{2}$.
- use a criterion that balances the training error and model size,
* to exemplify, Mallow's $C_{p}$, Akaike information criterion (AIC), Bayesian information criterion (BIC), adjusted $R^{2}$, and cross-validation (CV).


## Adjusted R-squared

- Unlike the $R^{2}$ statistic, it pays a price for unnecessary predictors,
- for a least squares model with $p$ variables

$$
\text { Adjusted } R^{2}=1-\frac{R S S /(m-p-1)}{T S S /(m-1)}
$$

- a maximization criterion (unlike $C_{p}$, AIC , and BIC ),
- a heuristic criterion, vaguely motivated in statistical theory,
- irrelevant variables bring a small decrease in RSS, this decrease is outweighed by decrease in $m-p-1$ (neither $T S S$ nor $m$ changes with p),
- a comparative measure, different meaning than $R^{2}$ (a measure of fit), can be e.g. negative.


## The ways to choose the optimal model

- Three classes of methods
- subset selection outlined before, search methods could be
* all subsets regression is not feasible, $\mathcal{O}\left(2^{p}\right)$,
* forward stepwise selection starts with the null model and gradually adds the variable that results in the lowest RSS, $\mathcal{O}\left(p^{2}\right)$,
* backward stepwise selection starts with the full model, gradually removes the variable with the largest p -value in the last model, i.e., the least significant one, $\mathcal{O}\left(p^{2}\right)$, cannot be used if $p>m$,
- dimension reduction - ordinary least squares regression in a L-dimensional subspace, see the lectures on dimension reduction,
- shrinkage - we fit a model involving all p predictors, but the estimated coefficients are shrunken towards zero relative to the least squares estimates, this shrinkage (also known as regularization) has the effect of reducing variance and can also perform variable selection.


## How regression got its name ...




Figure 8.8. Galton's graphical illustration of regression; the circles give the average heights for groups of children whose midparental heights can be read from the line $A B$. The difference between the line $C D$ (drawn by eye to approximate the circles) and $A B$ represents regression toward mediocrity. (From Galton, 1886a.)

## Shrinkage Methods

## - Ridge regression

- recall that the least squares fitting procedure estimates $\beta_{0}, \ldots, \beta_{p}$ with the values that minimize

$$
R S S=\sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\sum_{j=1}^{p} \hat{\beta}_{j} x_{i j}\right)^{2}
$$

- in contrast, the ridge regression coefficient estimates are the values that minimize

$$
\sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\sum_{j=1}^{p} \hat{\beta}_{j} x_{i j}\right)^{2}+\lambda \sum_{j=1}^{p} \hat{\beta}_{j}^{2}=R S S+\lambda \sum_{j=1}^{p} \hat{\beta}_{j}^{2}
$$

- where $\lambda \geq 0$ is a tuning parameter, to be determined separately, typically, CV is used,
$-\lambda \sum_{j} \hat{\beta}_{j}^{2}$ is a shrinkage penalty with the effect of shrinking the $\beta_{j}$ estimates towards zero.


## Shrinkage Methods

## - Ridge regression

- the standard least squares coefficient estimates are scale equivariant * multiplying $X_{j}$ by a constant $c$ simply leads to a scaling of the least squares coefficient estimates by a factor of $1 / c$.
* regardless of how the $j$ th predictor is scaled, $X_{j} \hat{\beta}_{j}$ will remain the same,
- in contrast, the ridge regression coefficient estimates can change substantially when multiplying a given predictor by a constant
* ridge regression should be applied after standardizing the predictors

$$
\tilde{x}_{i j}=\frac{x_{i j}}{\sqrt{\frac{1}{n} \sum_{i=1}^{n}\left(x_{i j}-\bar{x}_{j}\right)^{2}}}
$$

## Ridge regression improvement over least squares

- Bias-variance trade-off
- suppose we have fit a model $\hat{f}(x)$ to some training data,
- let $\left(x_{0}, y_{0}\right)$ be a test observation drawn from the same population,
- if the true model is $Y=f(X)+\epsilon$ (with $f(x)=E(Y \mid X=x)$ ) then

$$
\begin{gathered}
E\left(y_{0}-\hat{f}\left(x_{0}\right)\right)^{2}=\operatorname{Var}\left(\hat{f}\left(x_{0}\right)\right)+\left[\operatorname{Bias}\left(\hat{f}\left(x_{0}\right)\right)\right]^{2}+\operatorname{Var}(\epsilon) \\
\operatorname{Bias}\left(\hat{f}\left(x_{0}\right)\right)=E\left(\hat{f}\left(x_{0}\right)\right)-f\left(x_{0}\right)
\end{gathered}
$$

- the error can be decomposed into model variance, bias and irreducible error,
- typically as the flexibility of $\hat{f}$ increases, its variance increases, and its bias decreases,
- choosing the flexibility based on average test error amounts to a biasvariance trade-off.


## Ridge regression improvement over least squares

- Relationship between model flexibility and accuracy
- and the bias of the train error towards more flexible/overfit models.


Black curve is truth. Orange, blue and green curves/squares correspond to fits/models of different flexibility. Red curve on right is generalization error, grey curve is the training error.

## Ridge regression improvement over least squares




Simulated data with $n=50$ observations, $p=45$ predictors, all having nonzero coefficients. Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of $\lambda$ and the ration between the norms of ridge and ordinary regression coefficients. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.

## Shrinkage Methods

- The lasso
- ridge regression will include all $p$ predictors in the final model
* disadvantage, does not help in feature selection,
- lasso overcomes this problem by minimizing

$$
\sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\sum_{j=1}^{p} \hat{\beta}_{j} x_{i j}\right)^{2}+\lambda \sum_{j=1}^{p}\left|\hat{\beta}_{j}\right|=R S S+\lambda \sum_{j=1}^{p}\left|\hat{\beta}_{j}\right|
$$

* in statistical parlance, the lasso uses an $\ell_{1}$ penalty instead of an $\ell_{2}$ penalty applied in ridge regression,
- the $\ell_{1}$ penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when $\lambda$ is sufficiently large,
- the lasso yields sparse models and performs variable selection.


## The variable selection property of the lasso

- Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?
- One can show that the lasso and ridge regression coefficient estimates solve the problems minimize

$$
\min _{\hat{\beta}} \sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\sum_{j=1}^{p} \hat{\beta}_{j} x_{i j}\right)^{2} \text { subject to } \sum_{j=1}^{p}\left|\hat{\beta}_{j}\right| \leq s
$$

and

$$
\min _{\hat{\beta}} \sum_{i=1}^{m}\left(y_{i}-\hat{\beta}_{0}-\sum_{j=1}^{p} \hat{\beta}_{j} x_{i j}\right)^{2} \text { subject to } \sum_{j=1}^{p} \hat{\beta}_{j}^{2} \leq s
$$

- in other words, for every value of $\lambda$ there is some $s$ such that the alternative definitions lead to the same regression coefficient estimates.

Lasso and ridge regression: geometric interpretation


Lasso


Ridge regression

## Selecting the value of tuning parameter

- which $\lambda$ value (or equivalently, the value of the constraint $s$ ) is the best?
- employ cross-validation
- use fresh/unseen data to estimate the expected generalization error,
- calculate mean squared error $M S E_{T e}=\frac{R S S}{m}=\frac{1}{m} \sum_{i=1}^{m}\left(y_{i}-\hat{y}_{i}\right)^{2}$,
- in our case, proceed as follows
- choose a grid of $\lambda$ values,
- compute the cross-validation error rate for each value of $\lambda$,
- select either $\lambda_{\min }$ for which the cross-validation error is smallest,
- or select $\lambda_{1 \text { se }}$, the largest value of $\lambda$ such that error is within 1 standard error of the minimum,
- Finally, the model is re-fit
- using all of the available observations,
- and the selected value of the tuning parameter.


## Cross-validation

- the training error can dramatically underestimate the test error
- it is a positively biased estimate of the future generalization error,
- hold-out makes the most easy approach to model testing
- split the available data between train and validation set (70:30 ratio),
- sufficient for large data sets,
- $k$-fold cross-validation
- randomly split observations into $k$ folds of (approximately) equal size,
- in $k$ gradual runs perform training on $k-1$ folds and testing on the remaining fold (always different),
- eventually, $k$ estimates of the test error are averaged.



## Comparison between $\lambda_{\min }$ and $\lambda_{1 s e}$


$\lambda_{\text {min }}$ corresponds to the green line, always larger than $\lambda_{1 s e}$ which is in blue.

## Summary

- Multiple linear regression
- a simple model with the strong assumption of linearity,
- helps to understand concurrent effects on a target continuous variable,
- model selection and regularization may improve prediction and understanding
- neither ridge regression nor the lasso will universally dominate the other,
- lasso performs better when the response is a function of only a relatively small number of predictors, however ...
- . . . the number of predictors related to the response is never known a priori,
- cross-validation can help to decide which approach is better on a particular data set and select a value of the tuning parameter.


## The main references

:: Resources (slides, scripts, tasks) and reading

- G. James, D. Witten, T. Hastie and R. Tibshirani: An Introduction to Statistical Learning with Applications in R. Springer, 2014.
- K. Markham: In-depth Introduction to Machine Learning in 15 hours of Expert Videos. Available at R-bloggers.


[^0]:    Interpreting Residual Plots to Improve Your Regression (www.qualtrics.com): only the left-most residual plot meets the usual requirements.

