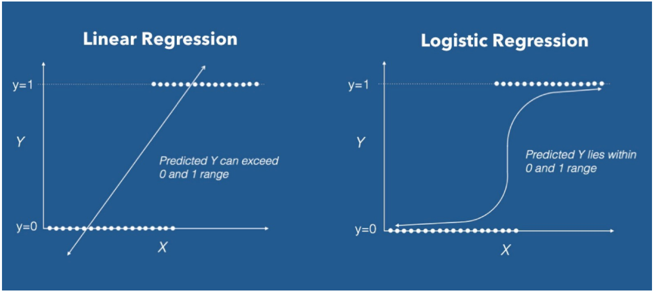
Regression

PSY-GS 8875 Behavioral Data Science



Overview: Week 2

Readings

- ESL Chapters: 3.1, 3.2, 4.4, and 4.4.1
- HML Chapters: 4.1-4.5 and 5.1-5.5
- Yarkoni and Westfall - 2017

Optional

- none

- Linear regression and **regression** metrics
- Logistic regression and **classification** metrics
- Gradient descent-style regression
- Activity: regression – new wine in old bottles

Linear Regression

Linear Regression

Goal: predict some outcome Y using some features X

- known as a "supervised learning" problem
- **supervised**: outcome is known and used in "learning"
- **learning**: estimation of model parameters

Linear Regression

What relationship does *linear* regression learn between Y and X?

Solves a *regression* problem

Linear Regression

What relationship does *linear* regression learn between Y and X?

Solves a *regression* problem

But how does it “learn” to solve this problem?

Linear Regression

Formally:

$$y_i = \sum_{i=1}^{n} X_i \beta_i + \epsilon_i$$

or

$$\mathbf{y} = \mathbf{X}\beta + \epsilon$$

ordinary least squares (OLS): estimate a line that minimizes the distance between $\mathbf{y}$ and $\widehat{\mathbf{y}}$

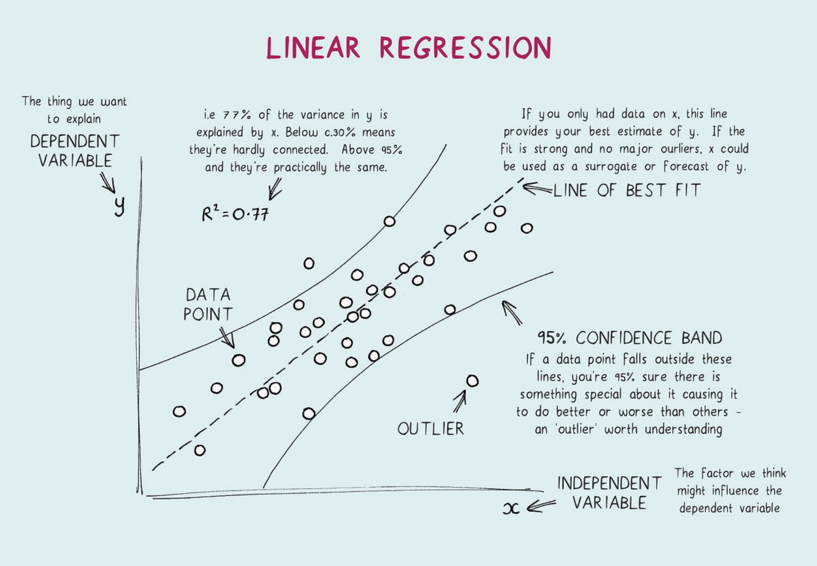
$$\widehat{\beta} = \arg\min_{\widehat{\beta}} \sum (\widehat{\mathbf{y}} - \mathbf{y})^2$$

Linear Regression

The OLS solution is a *closed-form* solution meaning can be solved analytically without any numerical optimization procedures such as Newton's method

$$\widehat{\beta} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

Linear Regression



Common Usage

- $R^2 = 1 - \frac{\sum(\hat{y}_i - y_i)^2}{\sum(y_i - \bar{y})^2}$
- $p < 0.05$ using $\hat{se}(\hat{b}) = \sqrt{\frac{n\hat{\sigma}^2}{n\sum x_i^2 - (\sum x_i)^2}}$
- Assumptions?

Linear Regression

Assumptions

- continuous outcome
- linear relationship between $\mathbf{y}$ and $\widehat{\mathbf{y}}$
- normality distributed errors (methods to check?)
- homoskedasticity or equal error variance (methods to check?)
- (lack of) multicollinearity (variance inflation factor or VIF > 5)

$$VIF_i = \frac{1}{1 - R_i^2},$$

where R_i^2 is each predictor treated as an outcome and predictor by all other predictors

R Example

Dataset

- Student math success in two Portegeuse schools [source]
- 395 students

```
# Load data
math <- read.csv("../../data/student_math/student_math_clean.csv")
```

Variables of Interest

Dependent Variable

- `final_grade`: math grade earned (0-20)

Independent Variables

- `study_time`: weekly study time ($1 = < 2$ hours, $2 =$ 2-5 hours, $3 =$ 5-10 hours, $4 = > 10$ hours)
- `class_failures`: number of past class failures (1-3; otherwise, 4)
- `school_support`: extra educational support (yes/no)
- `family_support`: extra family support (yes/no)
- `extra_paid_classes`: extra (outside of school) classes that were paid for (yes/no)
- `higher_ed`: wants to go to higher education (yes/no)
- `internet_access`: whether they had internet access at home (yes/no)
- `absences`: number of days absent from school (0-93)

```r
# Select variables
math_voi <- math[,c(
  "final_grade", "study_time", "class_failures",
  "school_support", "family_support", "extra_paid_classes",
  "higher_ed", "internet_access", "absences"
)]

# Set study time
replace_values <- 1:4
names(replace_values) <- unique(math_voi$study_time)
math_voi$study_time <- replace_values[math_voi$study_time]

# Set "yes/no" responses to numeric
math_voi[,4:8] <- ifelse(math_voi[,4:8] == "yes", 1, 0)

# Separate out outcome and predictors
Y <- as.matrix(math_voi[, 1])
X <- as.matrix(math_voi[, -1])
X <- cbind(1, X) # add intercept

# Compute betas (transposed for print)
t(solve(t(X) %*% X) %*% t(X) %*% Y)
```

```
              study_time class_failures school_support family_support
[1,] 8.386779  0.1957801      -2.036978      -1.071571      -0.700634
     extra_paid_classes higher_ed internet_access   absences
[1,]          0.3211003  1.945091       0.8606776 0.03396231
```

```r
# Linear model function
math_lm <- lm(final_grade ~ ., data = math_voi)

# Print summary
summary(math_lm)
```

```

Call:
lm(formula = final_grade ~ ., data = math_voi)

Residuals:
     Min       1Q   Median       3Q      Max 
-12.2968  -1.9497   0.2201   2.8957   8.1426 

Coefficients:
                   Estimate Std. Error t value         Pr(>|t|)    
(Intercept)         8.38678    1.24186   6.753 0.0000000000533 ***
study_time          0.19578    0.21229   0.922           0.3570    
class_failures     -2.03698    0.30520  -6.674 0.0000000000865 ***
school_support     -1.07157    0.64273  -1.667           0.0963 .  
family_support     -0.70063    0.46339  -1.512           0.1314    
extra_paid_classes  0.32110    0.46439   0.691           0.4897    
higher_ed           1.94509    1.03675   1.876           0.0614 .  
internet_access     0.86068    0.58458   1.472           0.1418    
absences            0.03396    0.02701   1.257           0.2094    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.244 on 386 degrees of freedom
Multiple R-squared:  0.1594,	Adjusted R-squared:  0.142 
F-statistic:  9.15 on 8 and 386 DF,  p-value: 0.00000000001514
```

Model Evaluation

- Usual suspects: R^2 and statistical significance
- More common in data science to use (root) mean square error

$$RMSE = \sqrt{\frac{\sum(\hat{y}_i - y)^2}{n}}$$

```
# Compute RMSE
sqrt(mean((predict(math_lm) - math_voi$final_grade)^2))
```

```
[1] 4.195114
```

Is that good?

Linear Regression

RMSE from the paper:

- neural networks: 4.41
- support vector machines: 4.37
- decision trees: 4.46
- random forest: 3.90

Seems like we did pretty good, right?

Linear Regression

RMSE from the paper:

- neural networks: 4.41
- support vector machines: 4.37
- decision trees: 4.46
- random forest: 3.90

Seems like we did pretty good, right?

There's a catch...

Linear Regression

- they held out data and were computing RMSE on the data *held out* (more on that next week)
- we had the knowledge of their better predictors and used those only (there were a lot of irrelevant predictors in the dataset)

Logistic Regression

Logistic Regression

Goal: predict some outcome Y using some features X

- known as a "supervised learning" problem
- **supervised**: outcome is known and used in "learning"
- **learning**: estimation of model parameters

Logistic Regression

What relationship does *logistic* regression learn between Y and X?

Logistic Regression

What relationship does *logistic* regression learn between Y and X?

Solves a *classification* problem

- classification: categorizing observations into two (or more) classes

Logistic Regression

Formally:

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\sum_{i=1}^{n} X_i \beta_i)}}$$

Conversely, it could be:

$$\sigma(z) = \frac{1}{1 + e^{-z}},$$

where

$$z = \sum_{i=1}^{n} X_i \beta_i$$

More on this notation when we cover neural networks. . .

Logistic Regression

Unlike linear regression, there isn't a closed-form solution for logistic regression

Instead, a numerical optimization method is used such as Newton's method:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

or iteratively reweighted least squares (IRLS):

$$\mathbf{w}_{k+1} = (\mathbf{X}^T \mathbf{S}_k \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{S}_k \mathbf{X} \mathbf{w}_k + \mathbf{y} - \mu_k),$$

where $\mathbf{S} = \text{diag}(\mu(i)(1 - \mu(i)))$ is a diagonal weighting matrix

Logistic Regression

The end goal is to seek a minimize of the difference between the predicted class (0 or 1) and the actual class

$$\widehat{\beta} = \arg\min_{\widehat{\beta}} \sum \log(1 + e^{(-\mathbf{yX}\beta)})$$

Assumptions?

Logistic Regression

Assumptions?

Fewer than linear regression but. . .

- (lack of) multicollinearity
- **balanced outcome** (i.e, 1s $\approx$ 0s)

R Example

Predicting whether a student had extra paid classes outside of school

```r
# Logistic regression function (don't forget to set 'family')
math_log <- glm(extra_paid_classes ~ ., data = math_voi, family = "binomial")

# Print summary
summary(math_log)
```

```
Call:
glm(formula = extra_paid_classes ~ ., family = "binomial", data = math_voi)

Coefficients:
                Estimate Std. Error z value    Pr(>|z|)
(Intercept)    -3.646498   1.145916  -3.182     0.00146 **
final_grade     0.014419   0.026773   0.539     0.59019
study_time     -0.138488   0.108597  -1.275     0.20222
class_failures -0.463546   0.191990  -2.414     0.01576 *
school_support -0.354765   0.325253  -1.091     0.27539
family_support  1.234305   0.234664   5.260 0.000000144 ***
higher_ed       2.405163   1.064476   2.259     0.02385 *
internet_access 0.755183   0.317798   2.376     0.01749 *
absences        0.002583   0.014899   0.173     0.86236
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 544.83  on 394  degrees of freedom
Residual deviance: 477.10  on 386  degrees of freedom
AIC: 495.1

Number of Fisher Scoring iterations: 5
```

Model Evaluation

- Usual suspects: pseudo-R^2 and statistical significance
- More common in data science to use confusion matrix metrics

Sources: [21][22][23][24][25][26][27][28][29] view · talk · edit

		Predicted condition			
	Total population $= P + N$	**Positive (PP)**	**Negative (PN)**	Informedness, bookmaker informedness (BM) $= TPR + TNR - 1$	Prevalence threshold (PT) $= \frac{\sqrt{TPR \times FPR} - FPR}{TPR - FPR}$
Actual condition	**Positive (P)**	**True positive (TP), hit**	**False negative (FN), type II error, miss, underestimation**	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{TP}{P} = 1 - FNR$	False negative rate (FNR), miss rate $= \frac{FN}{P} = 1 - TPR$
	Negative (N)	**False positive (FP), type I error, false alarm, overestimation**	**True negative (TN), correct rejection**	False positive rate (FPR), probability of false alarm, fall-out $= \frac{FP}{N} = 1 - TNR$	True negative rate (TNR), specificity (SPC), selectivity $= \frac{TN}{N} = 1 - FPR$
	Prevalence $= \frac{P}{P + N}$	Positive predictive value (PPV), precision $= \frac{TP}{PP} = 1 - FDR$	False omission rate (FOR) $= \frac{FN}{PN} = 1 - NPV$	Positive likelihood ratio (LR+) $= \frac{TPR}{FPR}$	Negative likelihood ratio (LR−) $= \frac{FNR}{TNR}$
	Accuracy (ACC) $= \frac{TP + TN}{P + N}$	False discovery rate (FDR) $= \frac{FP}{PP} = 1 - PPV$	Negative predictive value (NPV) $= \frac{TN}{PN} = 1 - FOR$	Markedness (MK), deltaP (Δp) $= PPV + NPV - 1$	Diagnostic odds ratio (DOR) $= \frac{LR+}{LR-}$
	Balanced accuracy (BA) $= \frac{TPR + TNR}{2}$	F_1 score $= \frac{2 PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) $= \sqrt{PPV \times TPR}$	Matthews correlation coefficient (MCC) $= \sqrt{TPR \times TNR \times PPV \times NPV} - \sqrt{FNR \times FPR \times FOR \times FDR}$	Threat score (TS), critical success index (CSI), Jaccard index $= \frac{TP}{TP + FN + FP}$

Wikipedia

Common Metrics

sensitivity: $\frac{TP}{TP+FP}$

specificity: $\frac{TN}{TN+FN}$

Accuracy: $\frac{TP+TN}{TP+FP+TN+FN}$

F1: $\frac{2TP}{2TP+FP+FN}$

Matthew's Correlation Coefficient (MCC or phi coefficient):

$$\frac{TP \times TN - FP \times FN}{\sqrt{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}}$$

Meet {caret}, your new best friend

Classification **a**nd **Re**gression **T**raining

```r
# Load {caret}
library(caret)

# Get predicted probabilities from model
math_probabilities <- predict(
  math_log, type = "response"
  # don't forget to set `type = "response"`
)

# Convert to classes
math_classes <- factor( # ensure 'factor' mode!
  ifelse(math_probabilities > 0.50, "yes", "no")
)

# Ensure 'factor' mode for actual!
math_actual <- factor( # ensure 'factor' mode!
  ifelse(math_voi$extra_paid_classes == 1, "yes", "no")
)

# Get confusion matrix
confusionMatrix(
  data = math_classes, # predicted
  reference = math_actual, # actual
  positive = "yes" # class = 1
)
```

Logistic Regression | Model Evaluation

```
Confusion Matrix and Statistics

          Reference
Prediction  no yes
       no  145  60
       yes  69 121

               Accuracy : 0.6734
                 95% CI : (0.6247, 0.7195)
    No Information Rate : 0.5418
    P-Value [Acc > NIR] : 0.00000006868

                  Kappa : 0.3448

 Mcnemar's Test P-Value : 0.4812

            Sensitivity : 0.6685
            Specificity : 0.6776
         Pos Pred Value : 0.6368
         Neg Pred Value : 0.7073
             Prevalence : 0.4582
         Detection Rate : 0.3063
   Detection Prevalence : 0.4810
      Balanced Accuracy : 0.6730

       'Positive' Class : yes
```

Kappa

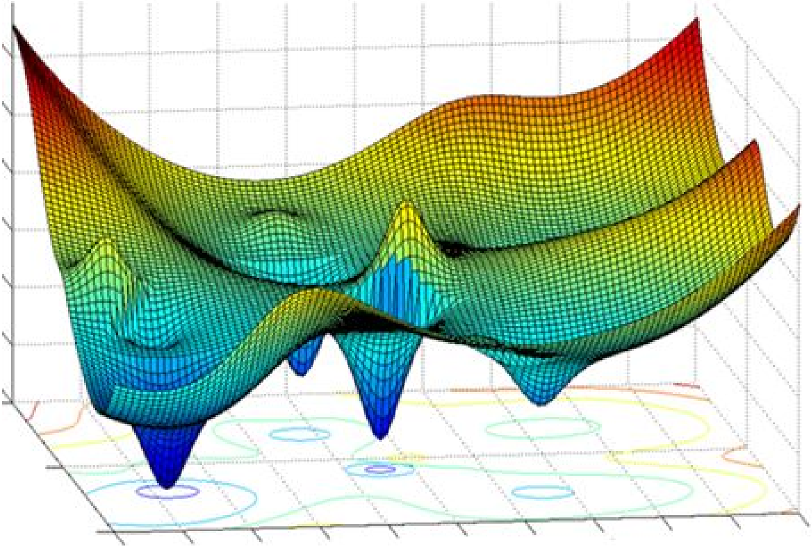
- Can be used to account for class imbalances
- Ranges from -1 (complete discordance) to 1 (complete concordance)
    - ≤ 0: no agreement
    - > 0.00: slight agreement
    - > 0.20: fair agreement
    - > 0.40: moderate agreement
    - > 0.60: substantial agreement
    - > 0.80: almost perfect agreement

✓ kappa $= 0.345$

Gradient Descent

Gradient Descent

Gradient Descent



Gradient Descent

- Numeric optimization method like Newton's method (or IRLS)
- Relatively simple to implement
- Computationally efficient for complex problems but inefficient relative to closed-form solutions or solutions amenable to Newton's method

Gradient Descent

Formally:

$$p_{n+1} = p_n - \eta \nabla f(p_n),$$

where

- η = learning rate (magnitude of "step" in direction of descent)
- p_n = current values (e.g., βs in regression)
- $\nabla f(p_n)$ = gradient $\frac{\mathbf{X}^T(\widehat{\mathbf{y}} - \mathbf{y})}{n}$

Gradient Descent

Gradient Descent for Linear Regression

$$p_{n+1} = p_n - \eta \nabla f(p_n),$$

p_n: $B_0 = 0$ and $B_1 = 0$

η: 0.1

$\nabla f(p_n)$: $B_0 = -2.851$ and $B_1 = -8.265$

p_{n+1}: $B_0 = 0.285$ and $B_1 = 0.826$

OLS: $B_0 = 2.970$ and $B_1 = 1.014$

Did we get closer or further away?

Gradient Descent

Gradient Descent for Linear Regression

$$p_{n+1} = p_n - \eta \nabla f(p_n),$$

p_n: $B_0 = 0.285$ and $B_1 = 0.826$

η: 0.1

$\nabla f(p_n)$: $B_0 = -2.663$ and $B_1 = -1.274$

p_{n+1}: $B_0 = 0.551$ and $B_1 = 0.954$

OLS: $B_0 = 2.970$ and $B_1 = 1.014$

Did we get closer or further away?

Gradient Descent for Linear Regression

$$p_{n+1} = p_n - \eta \nabla f(p_n),$$

p_n: $B_0 = 0.551$ and $B_1 = 0.954$

η: 0.1

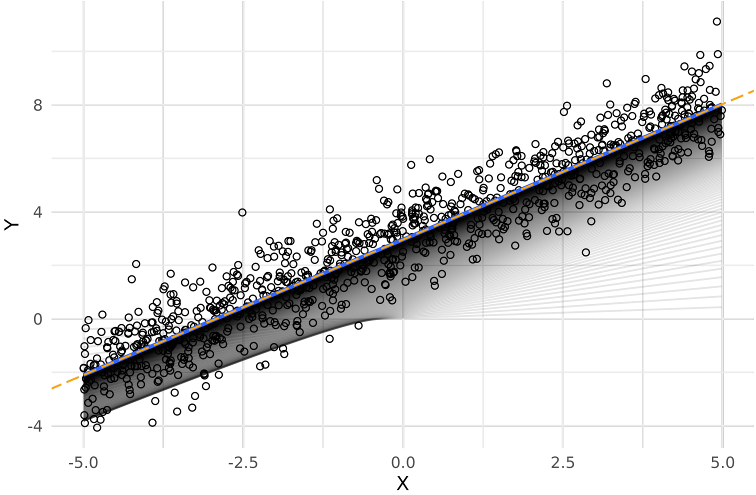
$\nabla f(p_n)$: $B_0 = -2.412$ and $B_1 = -0.223$

p_{n+1}: $B_0 = 0.793$ and $B_1 = 0.976$

OLS: $B_0 = 2.970$ and $B_1 = 1.014$

Did we get closer or further away?

Repeat for N iterations



Gradient Descent

How many iterations is enough?

- more complicated functions won't have closed-form solutions to check against (e.g., OLS)
- some criterion needs to be consulted for convergence
- change in criterion should stabilize (e.g., $\Delta_{criterion} < 0.001$ for n iterations)

Cost Functions

Mean square error (regression):

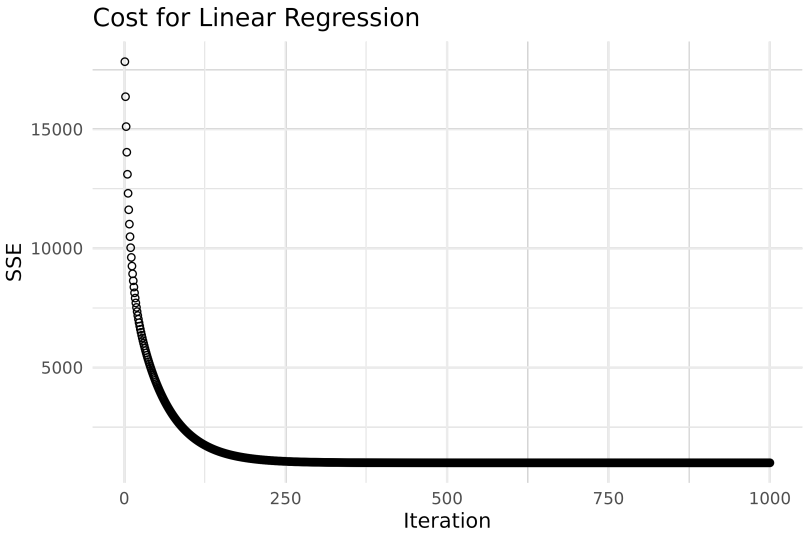
$$\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}$$

(Binary) cross-entropy loss (classification):

$$\frac{\sum_{i=1}^{n} -(y_i \log(\hat{y}_i) + (1 - y_i)(1 - \log(\hat{y}_i)))}{n}$$

These functions are sought to minimized

Gradient Descent



Gradient Descent

OLS: $B_0 = 2.970053$ and $B_1 = 1.013516$

GD: $B_0 = 2.969922$ and $B_1 = 1.013514$

Using 1000 iterations and $\eta = 0.01$

Iterations can be increased (21,401) and η (0.001) can be decreased to get closer and match OLS solution

In-class Activity

`regression.R`: new wine in old bottles

At Home Activity

Using the `student_math_clean.csv` data with the variables of interest used in these slides, get gradient descent linear and logistic regression parameters to match those presented in the slides

- Adjust `max_iter` and `learning_rate` as necessary
- Turn in final values of `max_iter` and `learning_rate` for the linear and logistic regression models to Brightspace

Readings for Next Week

Readings

- ESL Chapters: 7.10 and 7.11
- HML: Chapter 2
- Yarkoni - 2022

Optional

- Shen et al. - 2017