Lecture 4: Linear Regression and Classification

STATS 202: Data Mining and Analysis

Linh Tran

tranlm@stanford.edu

Department of Statistics
Stanford University

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Announcements

- HW1 due Friday.
  - Can ask for regrades up to a week from grades being released.
  - Solutions will be posted on Tuesday.
- Use Piazza if you want to form study groups.
- Hw1 data is now on the course webpage.

Outline

- Regression issues
- Comparing linear regression to KNN
- More classification
  - Logistic regression
  - Linear/quadratic discriminant analysis

Recap

So far, we have:

- Defined Multiple Linear Regression
- Discussed how to estimate model parameters
- Discussed how to test the importance of variables
- Described one approach to choose a subset of variables
- Explained how to code dummy indicators

What are some potential issues?

Potential issues in linear regression

- Interactions between predictors
- Non-linear relationships
- Correlation of error terms
- Non-constant variance of error (heteroskedasticity)
- Outliers
- High leverage points
- Collinearity
- Mis-specification

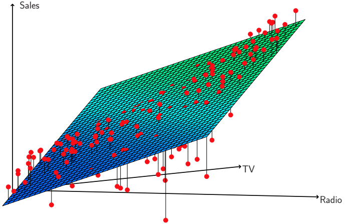
Interactions between predictors

Linear regression has an *additive* assumption, e.g.:

$$sales = \beta_0 + \beta_1 \cdot \texttt{tv} + \beta_2 \cdot \texttt{radio} + \epsilon \tag{1}$$

e.g. An increase of $ 100 dollars in TV ads correlates to a fixed increase in sales, independent of how much you spend on radio ads.

If we visualize the residuals, it is clear that this is false:



Interactions between predictors

One way to deal with this:

- Include multiplicative variables (aka interaction variables) in the model

$$sales = \beta_0 + \beta_1 \cdot tv + \beta_2 \cdot radio + \beta_3 \cdot (tv \times radio) + \epsilon \quad (2)$$

- Makes the effect of TV ads dependent on the radio ads (and vice versa)
- The *interaction variable* is high when both tv and radio are high

Interactions between predictors

Two ways of including interaction variables (in R):

- Create a new variable that is the product of the two
- Specify the interaction in the model formula

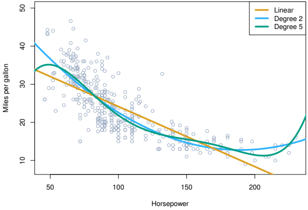
```
> lm.fit=lm(Sales~.+Income:Advertising+Price:Age,data=Carseats)
> summary(lm.fit)

Call:
lm(formula = Sales ~ . + Income:Advertising + Price:Age, data =
    Carseats)

Residuals:
   Min      1Q  Median      3Q     Max
-2.921  -0.750   0.018   0.675   3.341

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)         6.575565   1.008747    6.52  2.2e-10 ***
CompPrice           0.092937   0.004118   22.57  < 2e-16 ***
Income              0.010894   0.002604    4.18  3.6e-05 ***
Advertising         0.070246   0.022609    3.11  0.00203 **
Population          0.000159   0.000368    0.43  0.66533
Price              -0.100806   0.007440  -13.55  < 2e-16 ***
ShelveLocGood       4.848676   0.152838   31.72  < 2e-16 ***
ShelveLocMedium     1.953262   0.125768   15.53  < 2e-16 ***
Age                -0.057947   0.015951   -3.63  0.00032 ***
Education          -0.020852   0.019613   -1.06  0.28836
UrbanYes            0.140160   0.112402    1.25  0.21317
USYes              -0.157557   0.148923   -1.06  0.29073
Income:Advertising  0.000751   0.000278    2.70  0.00729 **
Price:Age           0.000107   0.000133    0.80  0.42381
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Non-linear relationships



Scatterplots between X and Y may reveal non-linear relationships

- **Solution**: Include polynomial terms in the model

$$
\begin{aligned}
MPG =& \beta_0 + \beta_1 \cdot horsepower \\
& + \beta_2 \cdot horsepower^2 \\
& + \beta_3 \cdot horsepower^3 + \ldots + \epsilon
\end{aligned} \tag{3}
$$

Non-linear relationships

In 2 or 3 dimensions, this is easy to visualize. What do we do when we have too many predictors?

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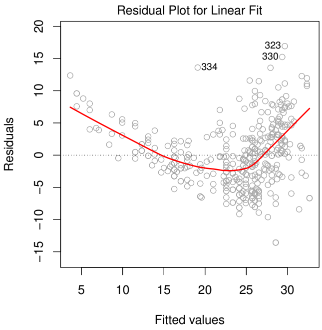
Plot the residuals against the response and look for a pattern:



Correlation of error terms

We assumed that the errors for each sample are independent:

$$y_i = f(x_i) + \epsilon_i : \epsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2) \tag{4}$$

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When it doesn't hold:

- Invalidates any assertions about Standard Errors, confidence intervals, and hypothesis tests

Example: Suppose that by accident, we double the data (i.e. we use each sample twice). Then, the standard errors would be artificially smaller by a factor of $\sqrt{2}$.

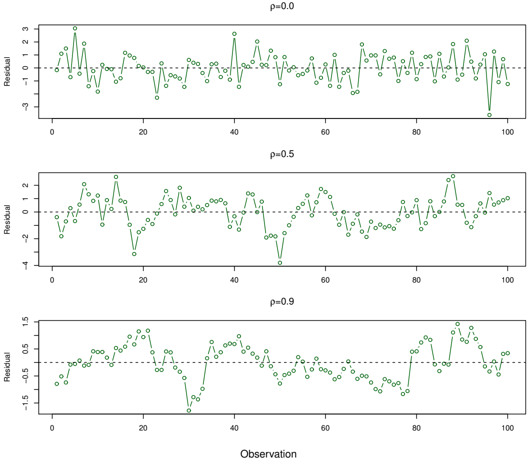
Correlation of error terms

Examples of when this happens:

- *Time series*: Each sample corresponds to a different point in time. The errors for samples that are close in time are correlated.
- *Spatial data*: Each sample corresponds to a different location in space.
- *Clustered data*: Study on predicting height from weight at birth. Suppose some of the subjects in the study are in the same family, their shared environment could make them deviate from $f(x)$ in similar ways.

Correlation of error terms

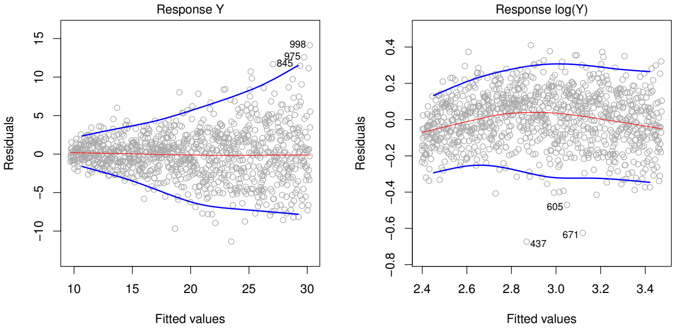
Simulations of time series with increasing correlations on ϵ_i.



Non-constant variance of error (heteroskedasticity)

The variance of the error depends on the input value.

To diagnose this, we can plot residuals vs. fitted values:



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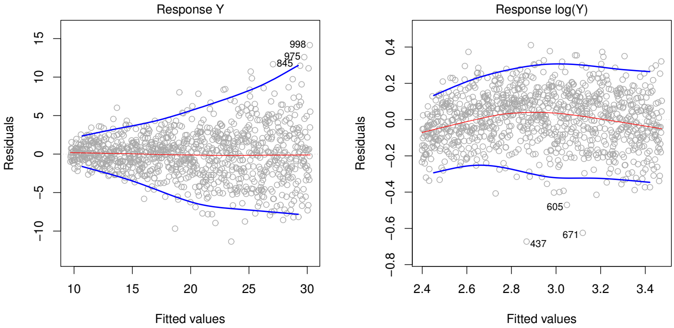
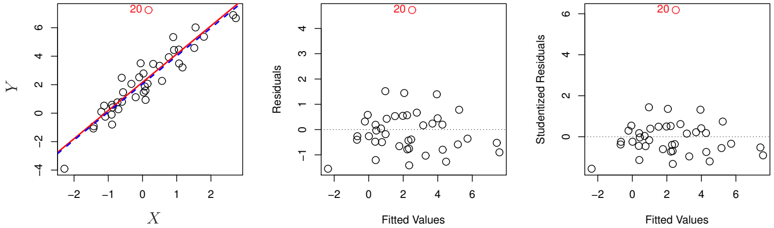


Solution: If the trend in variance is relatively simple, we can transform the response using a logarithm, for example.

Outliers

Outliers are points with very large errors, e.g.



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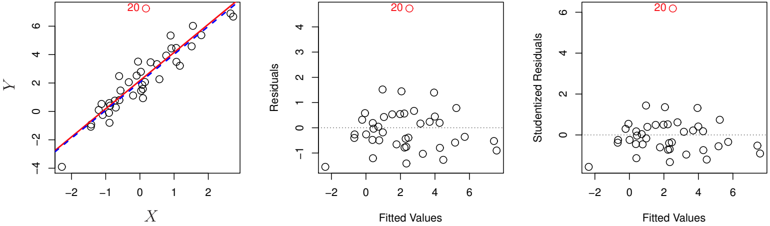


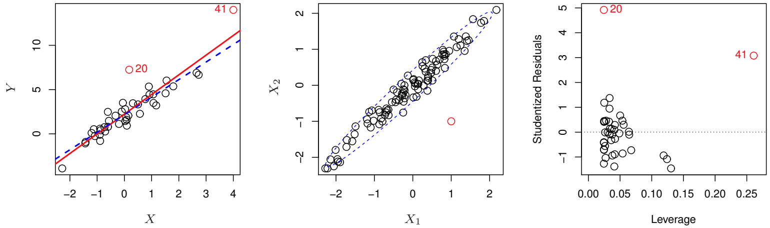
While they may not affect the fit, they might affect our assessment of model quality.

Possible solutions:

- If we believe an outlier is due to an error in data collection, we can remove it.

High leverage points

Some samples with extreme inputs have a large effect on $\hat{\beta}$.

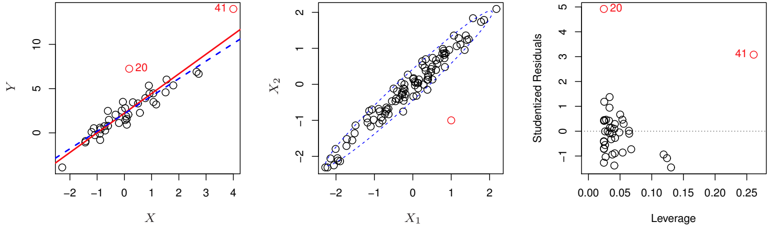


This can be measured with the *leverage statistic* or *self influence*:

$$h_{ii} = \frac{\partial \hat{y}_i}{\partial y_i} = (\underbrace{\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top}_{\text{Hat matrix})})_{i,i} \in \left[\frac{1}{n}, 1\right] \quad (5)$$

Values closer to 1 have high leverage.

Studentized residuals



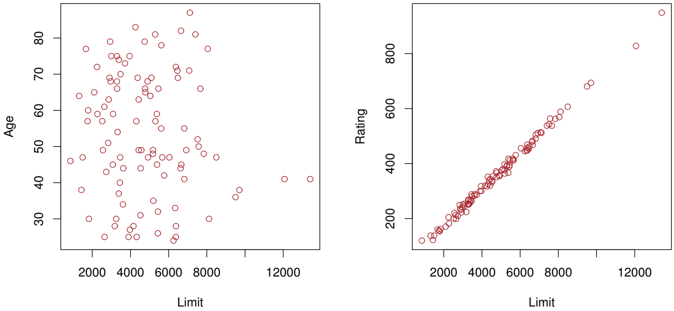
- The residual $\hat{\epsilon}_i = y_i - \hat{y}_i$ is an estimate for the noise ϵ_i
- The standard error of $\hat{\epsilon}_i$ is $\sigma\sqrt{1 - h_{ii}}$
- A studentized residual is $\hat{\epsilon}_i$ divided by its standard error
- It follows a Student-t distribution with $n - p - 2$ degrees of freedom

Collinearity

Two predictors are collinear if one explains the other well, e.g.

$$limit = a \times rating + b \tag{6}$$

i.e. they contain the same information



Problem: The coefficients become *unidentifiable*.

- i.e. different coefficients can mean the same fit

Collinearity

Problem: The coefficients become *unidentifiable*.

- i.e. different coefficients can mean the same fit

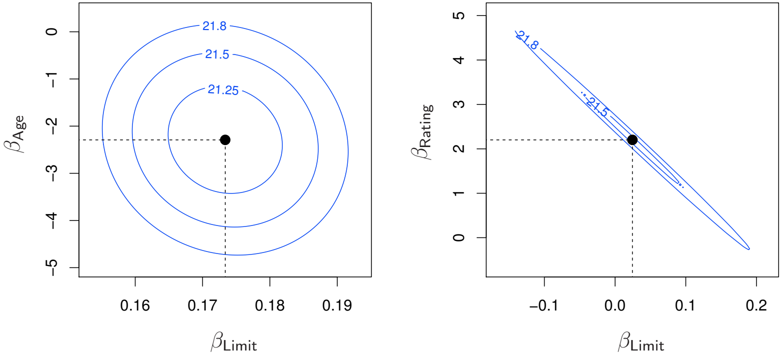
Example: using two identical predictors (`limit`):

$$\begin{aligned} \textit{balance} &= \beta_0 + \beta_1 \cdot \textit{limit} + \beta_2 \cdot \textit{limit} && (7) \\ &= \beta_0 + (\beta_1 + 100) \cdot \textit{limit} + (\beta_2 - 100) \cdot \textit{limit} && (8) \end{aligned}$$

The fit $(\hat\beta_0, \hat\beta_1, \hat\beta_2)$ is just as good as $(\hat\beta_0, \hat\beta_1 + 100, \hat\beta_2 - 100)$

Collinearity effect

Collinearity results in unstable estimates of β.



Recognizing collinearity

If 2 variables are collinear, we can easily diagnose this using their correlation.

A group of q variables is multilinear if these variables "contain less information" than q independent variables. Pairwise correlations may not reveal multilinear variables.

The Variance Inflation Factor (VIF) measures how necessary a variable is, or how predictable it is given the other variables:

$$VIF(\hat{\beta}_j) = \frac{1}{1 - R^2_{X_j|X_{-j}}}, \tag{9}$$

where $R^2_{X_j|X_{-j}}$ is the R^2 statistic for multiple linear regression of the predictor X_j onto the remaining predictors.

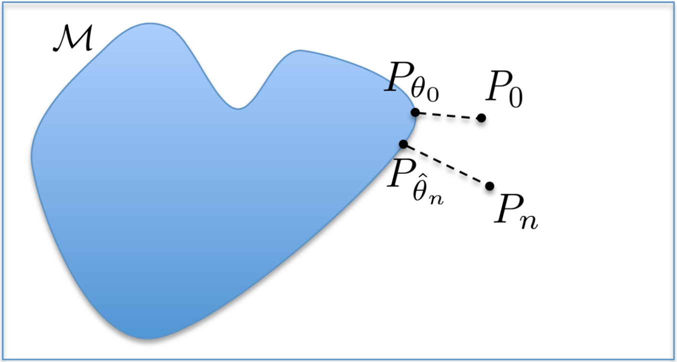
Dealing with collinearity

Three primary ways:

1. Drop one of the correlated features (e.g. Ridge/LASSO).
2. Combine the correlated features (e.g. PCA).
3. More data.

Mis-specification

What if our true distribution P_0 **isn't** linear?

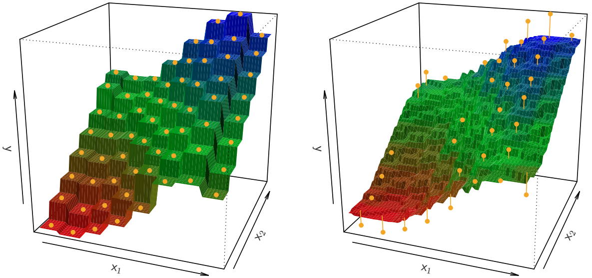


Estimates will still converge to a fixed value within our model, e.g.

$$\theta_0 \triangleq \arg\min_{\theta} D(P_\theta, P_0) : \theta = (\beta_0, ..., \beta_p) \tag{10}$$

Linear regression: prototypical parametric method
KNN regression: prototypical nonparametric method

$$\hat{f}_n(x) = \frac{1}{K} \sum_{i \in N_K(x)} y_i \tag{11}$$



Examples of KNN with $K = 1$ (left) and $K = 9$ (right)

Comparing Linear Regression to K-nearest neighbors

Linear regression: prototypical parametric method
KNN regression: prototypical nonparametric method Long story short:

- KNN is better when the function f_0 is not linear (and plenty of data)
  - **Question**: What if the true function f_0 IS linear?

Comparing Linear Regression to K-nearest neighbors

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- When n is not much larger than p, even if f_0 is nonlinear, linear regression can outperform KNN.

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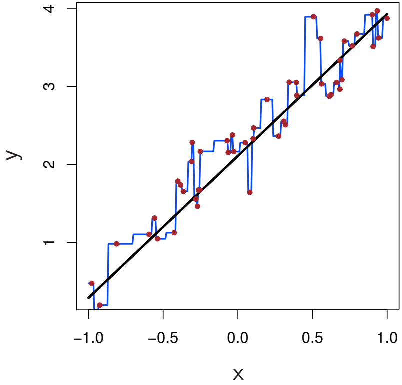
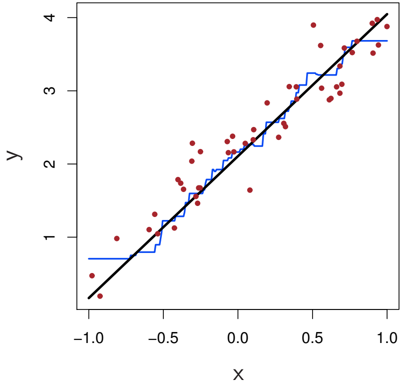
  - **Question**: What if the true function f_0 IS linear?
- When n is not much larger than p, even if f_0 is nonlinear, linear regression can outperform KNN.
- KNN has smaller bias, but this comes at a price of (much) higher variance (c.f. overfitting)

Comparing Linear Regression to K-nearest neighbors

KNN estimates for a simulation from a linear model

- True function f_0 is linear



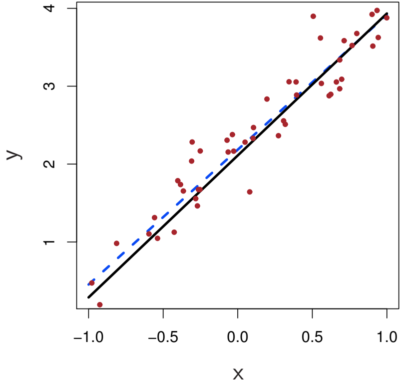


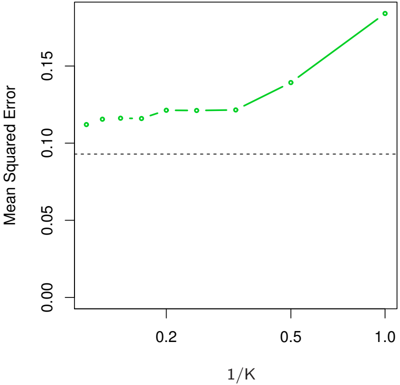
KNN fits with $K = 1$ (left) and $K = 9$ (right)

Comparing Linear Regression to K-nearest neighbors

Linear models dominate KNN

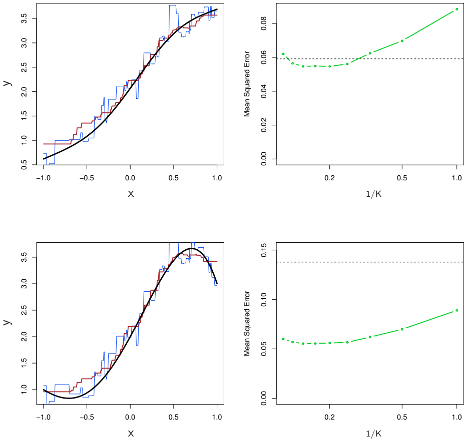
- We're able to gain statistical efficiency by taking advantage of the linear association





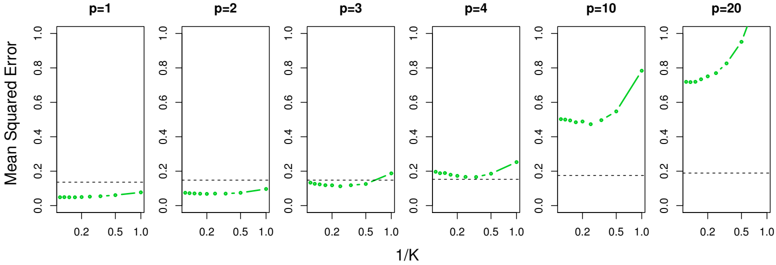
Comparing Linear Regression to K-nearest neighbors

Increasing deviations from linearity



Comparing Linear Regression to K-nearest neighbors

When there are more predictors than observations, linear regression dominates



When $p >> n$, each sample has no nearest neighbors, this is known as the curse of dimensionality.

- The variance of KNN regression is very large

Classification problems

Recall: Supervised learning with a *qualitative* or *categorical* response. As common (if not more) than regression

- *Medical diagnosis*: Given the symptoms a patient shows, predict which of 3 conditions they are attributed to
- *Online banking*: Determine whether a transaction is fraudulent or not, on the basis of the IP address, client's history, etc.
- *Web searching*: Based on a user's attributes and the string of a web search, predict which link a person will click
- *Online advertising*: Predict whether a user will click on an ad

Classification problems

Recall: In classification, the function f_0 we care about is

$$f_0 \triangleq \mathbb{P}_0[Y = y | X_1, X_2, ..., X_p] \tag{12}$$

To get a prediction, we use the Bayes Classifier:

$$\hat{y} = \arg\max_y \mathbb{P}_0[Y = y | X_1, X_2, ..., X_p] \tag{13}$$

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Example: Suppose $Y \in \{0, 1\}$. We *could* use linear model:

$$\mathbb{P}[Y = 1 | \mathbf{X}] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p \tag{14}$$

Problems:

- This would allow probabilities < 0 and > 1
- Difficult to extend to more than 2 categories

Logistic regression

An idea:
Let's apply a function to the result to keep it within $[0, 1]$

$$g^{-1}(z) = \frac{1}{1 + exp(-z)} \tag{15}$$

i.e.

$$\mathbb{P}[Y = 1|\mathbf{X}] = \frac{1}{1 + exp(-(\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p))} \tag{16}$$

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This is equivalent to modeling the log-odds, e.g.

$$\log \left[\frac{\mathbb{P}[Y = 1|\mathbf{X}]}{\mathbb{P}[Y = 0|\mathbf{X}]} \right] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p \tag{17}$$

n.b. $exp(\beta_j)$ is commonly referred to as the *odds-ratio* for X_j

Fitting a logistic regression

Let $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ..., (\mathbf{x}_n, y_n)$ be our training data.

In the linear model

$$\log\left[\frac{\mathbb{P}[Y=1|\mathbf{X}]}{\mathbb{P}[Y=0|\mathbf{X}]}\right] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p, \tag{18}$$

We don't actually observe the left side

- We observe $Y \in \{0, 1\}$, not probabilities
- This prevents us from using e.g. least squares to estimate our parameters

Fitting a logistic regression

Solution:
Let's try to maximize the probability of our training data

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$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{n} \mathbb{P}(Y = y_i | \mathbf{X} = \mathbf{x}_i) \tag{19}$$

$$= \prod_{i=1}^{n} p_i^{y_i} \cdot (1 - p_i)^{1-y_i} \tag{20}$$

where $p_i = g^{-1}(\beta_0 + \beta_1 x_{1,i} + \cdots + \beta_p x_{p,i})$

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where $p_i = g^{-1}(\beta_0 + \beta_1 x_{1,i} + \cdots + \beta_p x_{p,i})$

- We look for θ such that $\mathcal{L}(\boldsymbol{\theta})$ is maximized
- aka Maximum likelihood estimation (MLE)
- Has no closed form solution, so solved with numerical methods (e.g. Newton's method)

Note:
We typically deal with the log-likelihood:

$$
\begin{aligned}
\ell(\boldsymbol{\theta}) &= \log \mathcal{L}(\boldsymbol{\theta}) && (21)\\
&= \sum_{i=1}^{n} y_i \log(p_i) + (1 - y_i) \log(1 - p_i) && (22)\\
&= \sum_{k=0}^{1} \sum_{i=1}^{n} \mathbb{I}(Y_i = k) \log(\mathbb{P}(k|\mathbf{X} = \mathbf{x}_i)) && (23)
\end{aligned}
$$

Fitting a logistic regression

Given our loss function:

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} y_i \log(p_i) + (1 - y_i) \log(1 - p_i) \qquad (24)$$

Fitting a logistic regression

Given our loss function:

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} y_i \log(p_i) + (1 - y_i)\log(1 - p_i) \tag{24}$$

Where

$$p_i = \frac{1}{1 + \exp(-Z_i)} \tag{25}$$

$$Z_i = \mathbf{X_i}\beta \tag{26}$$

Fitting a logistic regression

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Where

$$p_i = \frac{1}{1 + \exp(-Z_i)} \tag{25}$$

$$Z_i = \mathbf{X_i}\beta \tag{26}$$

We can deriving the gradient using the chain rule:

$$\frac{\partial \ell(\boldsymbol{\theta})}{\partial \boldsymbol{\beta}} = \frac{\partial \ell(\boldsymbol{\theta})}{\partial p_i} \times \frac{\partial p_i}{\partial Z_i} \times \frac{\partial Z_i}{\partial \boldsymbol{\beta}} \tag{27}$$

Logistic regression in R

Estimating uncertainty

- We can estimate the Standard Error of each coefficient (e.g. using Fisher's information)

$$\mathbf{I_Y}(\beta) = -\mathbb{E}_\beta[\nabla^2 \ell(\beta)] \tag{28}$$

- The z-statistic (for logistic regression) is the equivalent of the t-statistic (in linear regression):

$$z = \frac{\hat{\beta}_j}{\hat{SE}(\hat{\beta}_j)} \tag{29}$$

- The p-values are test of the null hypothesis $\beta_j = 0$

Example fit

```
> glm.fit=glm(Direction~Lag1+Lag2+Lag3+Lag4+Lag5+Volume,
    data=Smarket,family=binomial)
> summary(glm.fit)

Call:
glm(formula = Direction ~ Lag1 + Lag2 + Lag3 + Lag4 + Lag5
    + Volume, family = binomial, data = Smarket)

Deviance Residuals:
   Min      1Q  Median      3Q     Max
 -1.45   -1.20    1.07    1.15    1.33

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.12600    0.24074   -0.52     0.60
Lag1        -0.07307    0.05017   -1.46     0.15
Lag2        -0.04230    0.05009   -0.84     0.40
Lag3         0.01109    0.04994    0.22     0.82
Lag4         0.00936    0.04997    0.19     0.85
Lag5         0.01031    0.04951    0.21     0.83
Volume       0.13544    0.15836    0.86     0.39
```

Example: Predicting credit card default

Predictors:

- `student`: 1 if student, 0 otherwise
- `balance`: credit card balance
- `income`: person's income

In this dataset there is *confounding*, but little collinearity

- Students tend to have higher balances. So, balance is explained by student, but not very well.
- People with a high balance are more likely to default.
- Among people with a given balance, students are less likely to default.

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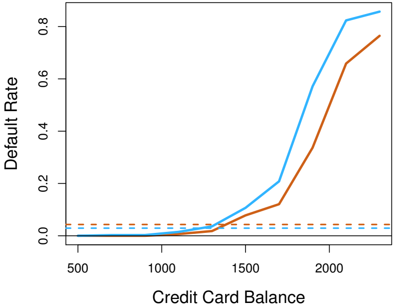

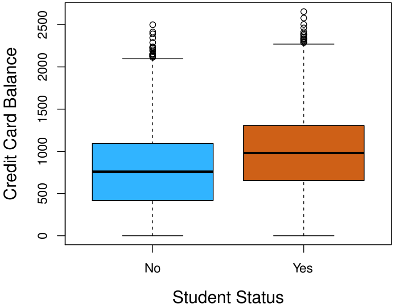

Example: Predicting credit card default

Logistic regression using only `balance`:

	Coefficient	Std. error	Z-statistic	P-value
`Intercept`	−10.6513	0.3612	−29.5	<0.0001
`balance`	0.0055	0.0002	24.9	<0.0001

Logistic regression using only `student`:

	Coefficient	Std. error	Z-statistic	P-value
`Intercept`	−3.5041	0.0707	−49.55	<0.0001
`student[Yes]`	0.4049	0.1150	3.52	0.0004

Logistic regression using all 3 predictors:

	Coefficient	Std. error	Z-statistic	P-value
`Intercept`	−10.8690	0.4923	−22.08	<0.0001
`balance`	0.0057	0.0002	24.74	<0.0001
`income`	0.0030	0.0082	0.37	0.7115
`student[Yes]`	−0.6468	0.2362	−2.74	0.0062

Some issues with logistic regression

- The coefficients become unstable when there is collinearity
  - This also affects the convergence of the fitting algorithm
- When the classes are well separated, the coefficients become unstable
  - This is always the case when $p \geq n - 1$.
- Sometimes may not converge
  - e.g. Needs more iterations

Linear Discriminant Analysis

A linear model (like logistic regression). Unlike logistic regression:

- Does not become unstable when classes are well separated
- With small n and $\mathbf{X}$ approximately normal, is stable
- Popular when we have > 2 classes

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High level idea:
Model distribution of $\mathbf{X}$ given Y, and apply Bayes' theorem, i.e.

$$\mathbb{P}(Y = k|\mathbf{X} = \mathbf{x}) = \frac{\pi_k f_k(\mathbf{x})}{\sum_{l=1}^{K} \pi_l f_l(\mathbf{x})} \tag{30}$$

- A common assumption is $f_k(\mathbf{x})$ is Gaussian

Example: $K = 2$ with Gaussian $f_k(\mathbf{x})$ and common σ^2

$$\mathbb{P}(Y = k|\mathbf{X} = \mathbf{x}) = \frac{\pi_k f_k(\mathbf{x})}{\sum_{l=1}^{K} \pi_l f_l(\mathbf{x})} \tag{31}$$

$$= \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)}{\sum_{l=1}^{2} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_l)^2\right)} \tag{32}$$

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Taking the log and rearranging gives:

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k) \quad (33)$$

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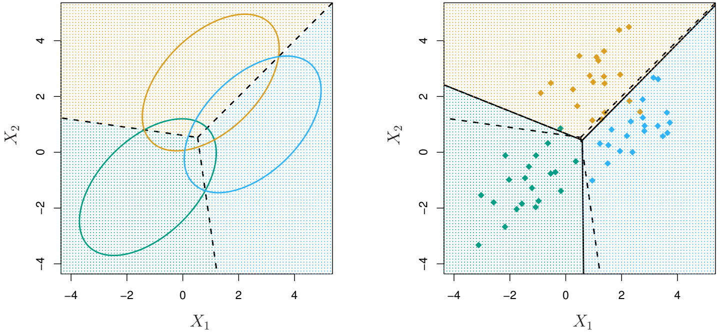
If $\pi_1 = \pi_2$, our Bayes Classifier is:

$$2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2 \tag{34}$$

Example of LDA



Quadratic Discriminant Analysis

Similar to LDA

- Assumes Gaussian $f_k(\mathbf{x})$
- Unlike LDA:
  - Assumes each class has its own covariance matrix $(\mathbf{\Sigma}_k)$

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$$\begin{aligned}\delta_k(x) &= -\frac{1}{2}(x-\mu_k)^\top \boldsymbol{\Sigma}_k^{-1}(x-\mu_k) - \frac{1}{2}\log|\boldsymbol{\Sigma}_k| + \log\pi_k \\ &= -\frac{1}{2}x^\top \boldsymbol{\Sigma}_k^{-1}x + x^\top \boldsymbol{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\mu_k^\top \boldsymbol{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\log|\boldsymbol{\Sigma}_k| + \log\pi_k \end{aligned} \tag{35}$$

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This results in more parameters to fit:

- LDA: Kp parameters
- QDA: $Kp(p+1)/2$ parameters

Assume a two-class setting with one predictor

Linear Discriminant Analysis:

$$\log\left[\frac{p_1(x)}{1-p_1(x)}\right] = c_0 + c_1 x \tag{36}$$

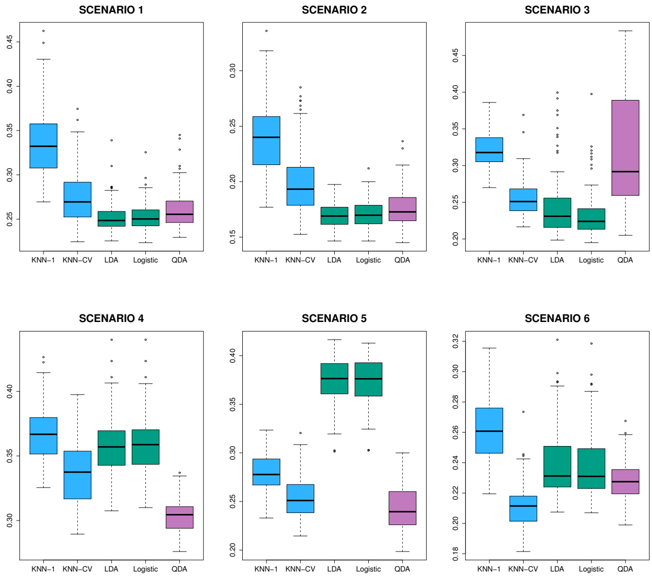
- c_0 and c_1 computed using $\hat{\mu}_0$, $\hat{\mu}_1$, and $\hat{\sigma}2$

Logistic regression:

$$\log\left[\frac{\mathbb{P}[Y=1|x]}{1-\mathbb{P}[Y=1|x]}\right] = \beta_0 + \beta_1 x \tag{37}$$

- β_0 and β_1 estimated using MLE

Comparison of classification methods



References

[1] ISL. Chapters 3-4.

[2] ESL. Chapters 3.