

Classification

Statistical Learning
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Reference: Introduction to Statistical Learning Chapter 4

Outline

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2. Logistic regression: the basics
3. Interpreting a logit model
4. Estimating a logit model: MLE
5. KNN for classification
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7. Evaluating a classifier: likelihood and deviance
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Classification

- In classification, the target variable y is membership in a category $\{1, \dots, M\}$.
- Each observation is an observed class y_i , together with a vector of features x_i .
- The classification problem: given new x^\star , what is y^\star ?

Linear probability model

We'll start with binary classification (where y is 0 or 1).

Recall the basic form of a supervised learning problem:

$$E(y \mid x) = f(x)$$

Suppose the outcome y is binary (0/1). Then:

$$\begin{aligned} E(y \mid x) &= 0 \cdot P(y = 0 \mid x) + 1 \cdot P(y = 1 \mid x) \\ &= P(y = 1 \mid x) \end{aligned}$$

Conclusion: the expectation is a probability

Linear probability model

Now suppose we choose $f(x)$ to be a linear function of the features x_i :

$$\begin{aligned} P(y = 1 \mid x) &= f(x) = x \cdot \beta \\ &= \beta_0 + \sum_{j=1}^p x_{ij} \beta_j \end{aligned}$$

This is called the *linear probability model*: the probability of a “yes” outcome ($y = 1$) is linear in x_i .

LPM: spam classification

Let's revisit our spam classification problem:

- `spamfit.csv`: 3000 e-mails (40% spam) with 9 features.
- `spamttest.csv`: 601 testing e-mails for assessing performance.

First few lines of `spamfit`:

```
word.freq.remove word.freq.order word.freq.free word.freq.meeting
1                0                0.00                5.35                0
2                0                0.00                0.00                0
3                0                0.31                0.63                0
word.freq.re word.freq.edu char.freq.semicolon char.freq.exclamation
1                0                0                0                0.357
2                0                0                0                1.975
3                0                0                0                0.055
capital.run.length.average y
1                1.971 1
2                35.461 1
3                3.509 1
```

LPM: spam classification

Let's build a linear probability using all the available features for $P(\text{spam} \mid \mathbf{x})$ and examine the fitted coefficients:

```
# Recall: the dot (.) says "use all variables not otherwise named"
lm_spam1 = lm(y ~ ., data=spamfit)
coef(lm_spam1) %>% round(3)
```

| | |
|-----------------------|----------------------------|
| (Intercept) | word.freq.remove |
| 0.281 | 0.311 |
| word.freq.order | word.freq.free |
| 0.284 | 0.097 |
| word.freq.meeting | word.freq.re |
| -0.059 | -0.039 |
| word.freq.edu | char.freq.semicolon |
| -0.051 | -0.096 |
| char.freq.exclamation | capital.run.length.average |
| 0.229 | 0.001 |

LPM: spam classification

In-sample performance:

```
phat_train_spam1 = predict(lm_spam1, spamfit) # predicted probabilities
yhat_train_spam1 = ifelse(phat_train_spam1 > 0.5, 1, 0)
confusion_in = table(y = spamfit$y, yhat = yhat_train_spam1)
confusion_in
```

| | yhat | |
|---|------|-----|
| y | 0 | 1 |
| 0 | 1732 | 68 |
| 1 | 541 | 659 |

```
sum(diag(confusion_in))/sum(confusion_in) # in-sample accuracy
```

```
[1] 0.797
```


LPM: spam classification

Out-of-sample performance:

```
phat_test_spam1 = predict(lm_spam1, spamtest)
yhat_test_spam1 = ifelse(phat_test_spam1 > 0.5, 1, 0)
confusion_out = table(y = spamtest$y, yhat = yhat_test_spam1)
confusion_out
```

```
      yhat
y      0    1
0 372 13
1  98 118
```

```
sum(diag(confusion_out))/sum(confusion_out) # out-of-sample accuracy
```

```
[1] 0.8153078
```

LPM: spam classification

How well are we doing? Note that 60% of the training set isn't spam:

```
table(spamfit$y)
```

```
  0    1  
1800 1200
```

Thus “not spam” is the most likely outcome. So a reasonable baseline or “null model” is one that guesses “not spam” for every test-set instance.

LPM: spam classification

How well does this null model perform on the test set? It's about 64%, since it gets all the 0's right and all the 1's wrong:

```
table(spamtest$y)
```

```
 0    1  
385 216
```

```
385/sum(table(spamtest$y))
```

```
[1] 0.640599
```

LPM: spam classification

Our linear probability model had an 81.5% out-of-sample accuracy rate.

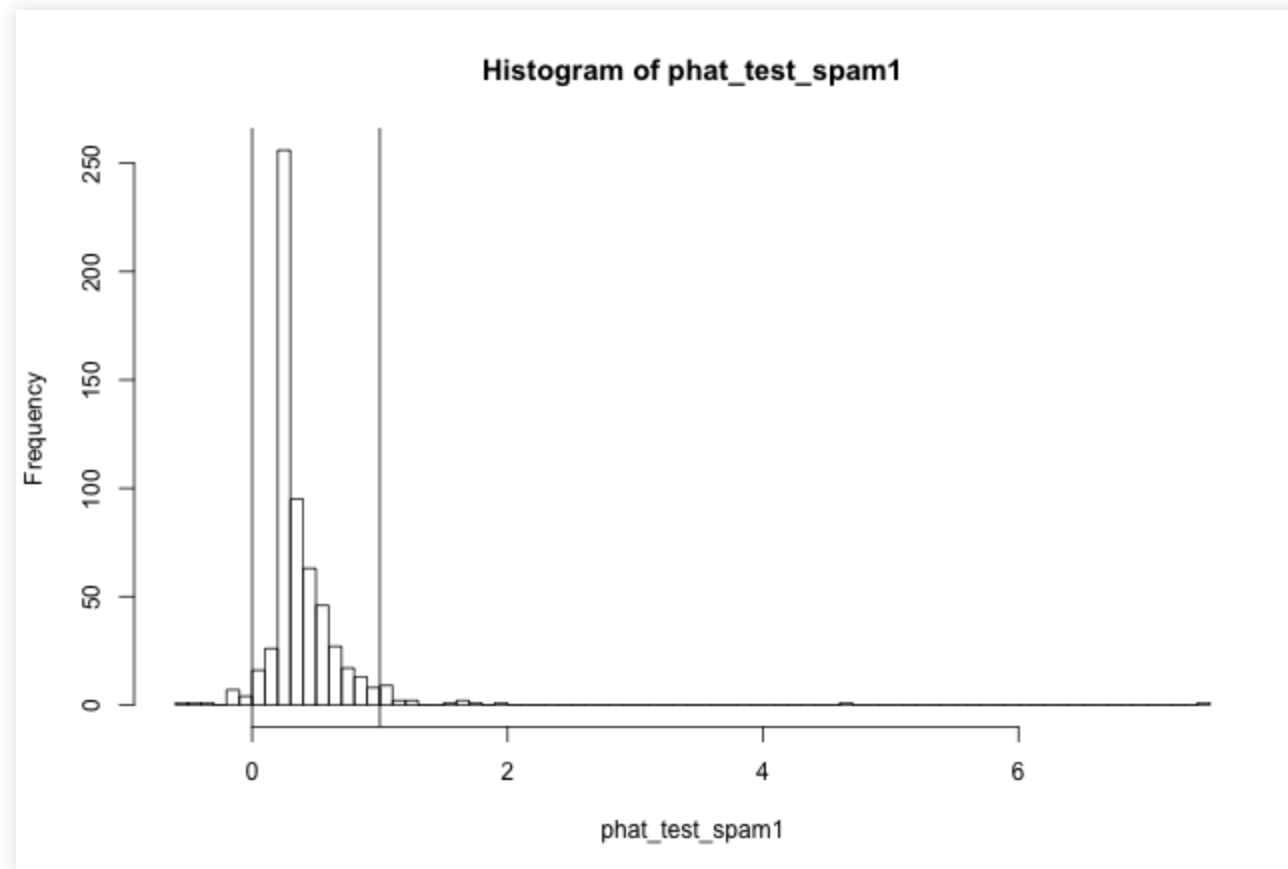
- Its absolute improvement over the null model is $\approx 81.5 - 64.1 = 17.4\%$.
- Its relative improvement, or *lift*, over the null model is $\approx 81.5/64.1 = 1.27$.

Comparing a model to a baseline or “null model” is often an important sanity check, especially in complicated problems.

- The null model might be one that knows nothing about x (as here).
- OR it might be a very simple model.

LPM: illegal probabilities

The linear probability model has one obvious problem: it can produce fitted probabilities that fall outside $(0,1)$. E.g. here is a histogram of predicted probabilities for the spam test set, where 34/601 predictions (5.6%) have this problem:



LPM: illegal probabilities

Recall the basic form of the linear probability model:

$$P(y = 1 \mid x) = x \cdot \beta$$

The core of the problem is this:

- the left-hand side needs to be constrained to fall between 0 and 1, by the basic rules of probabilities
- but the right-hand side is unconstrained – it can be any real number.

Modifying the LPM

A natural fix to this problem is to break our model down into two pieces:

$$P(y = 1 \mid x) = g(x \cdot \beta)$$

The inner piece, $f(x) = x \cdot \beta$, is called the *linear predictor*. It maps features x_i onto real numbers.

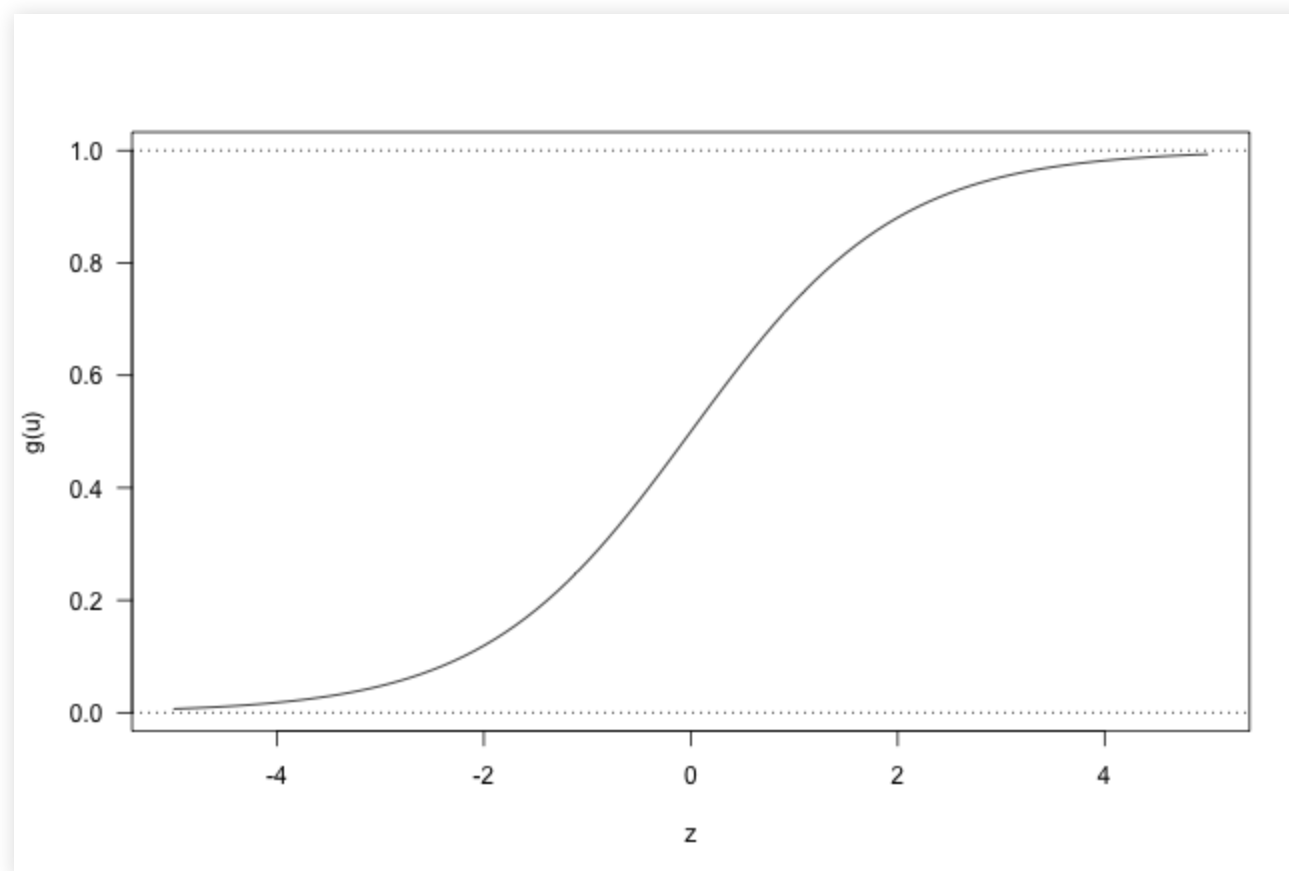
The outer piece, $g(z)$ is called a *link function*.

- It links the linear predictor $z_i \equiv f(x_i) = x_i \cdot \beta$ on the right to the probability on the left.
- It therefore must map real numbers onto the unit interval $(0,1)$.

Logistic regression

A standard choice is $g(z) = e^z / (1 + e^z)$.

- At $z = 0$, $g(z) = 0.5$.
- When $z \rightarrow \infty$, $g(z) \rightarrow 1$, and when $z \rightarrow -\infty$, $g(z) \rightarrow 0$.



Logistic regression

This is called the “logistic” or “logit” link, and it leads to the logistic regression model:

$$P(y = 1 \mid x) = \frac{\exp(x \cdot \beta)}{1 + \exp(x \cdot \beta)}$$

This is a very common choice of link function, for a couple of good reasons. One is interpretability: a little algebra shows that

$$\log \left[\frac{p}{1 - p} \right] = x \cdot \beta$$
$$\frac{p}{1 - p} = e^{x \cdot \beta}$$

so that it is a log-linear model for the *odds* of a yes outcome.

Logistic regression is easy in R

```
glm(y ~ x, data=mydata, family=binomial)
```

`glm` stands for “generalized linear model,” i.e. a linear model with a link function. The argument `family=binomial` tells R that `y` is binary and defaults to the logit link.

The response can take several forms:

- `y = 0, 1, 1, . . .` numeric vector
- `y = FALSE, TRUE, TRUE, . . .` logical
- `y = 'not spam', 'spam', 'spam', . . .` factor

Everything else is the same as in linear regression!

Logistic regression in your inbox

Let's fit a logit model to the spam data.

```
# Recall: the dot (.) says "use all variables not otherwise named"  
logit_spam1 = glm(y ~ ., data=spamfit, family='binomial')
```

```
Warning message:  
glm.fit: fitted probabilities numerically 0 or 1 occurred
```

We're warned that some emails are clearly spam or not spam (i.e. $p = 0$ or $p = 1$ up to floating-point numerical precision.) This warning is largely benign and isn't something to worry about.

Interpeting coefficients in LR

```
coef(logit_spam1)
```

| | |
|-----------------------|----------------------------|
| (Intercept) | word.freq.remove |
| -2.2381236 | 5.7161306 |
| word.freq.order | word.freq.free |
| 0.9168758 | 1.1018100 |
| word.freq.meeting | word.freq.re |
| -3.9106839 | -0.3800485 |
| word.freq.edu | char.freq.semicolon |
| -1.2632029 | -1.6941404 |
| char.freq.exclamation | capital.run.length.average |
| 2.2251096 | 0.3420581 |

Recall our model is

$$\text{Odds} = \frac{p}{1-p} = e^{\beta_0} \cdot e^{\beta_1 x_1} \dots e^{\beta_p x_p}$$

So e^{β_j} is an *odds multiplier* or *odds ratio* for for a one-unit increase in feature x_j .

Interpeting coefficients in LR

```
coef(logit_spam1)
```

| | |
|-----------------------|----------------------------|
| (Intercept) | word.freq.remove |
| -2.2381236 | 5.7161306 |
| word.freq.order | word.freq.free |
| 0.9168758 | 1.1018100 |
| word.freq.meeting | word.freq.re |
| -3.9106839 | -0.3800485 |
| word.freq.edu | char.freq.semicolon |
| -1.2632029 | -1.6941404 |
| char.freq.exclamation | capital.run.length.average |
| 2.2251096 | 0.3420581 |

The β for `char.freq.free` is 1.1. So having an extra `free` in an e-mail multiplies odds of spam by $e^{1.1} \approx 3$.

Interpeting coefficients in LR

```
coef(logit_spam1)
```

| | |
|-----------------------|----------------------------|
| (Intercept) | word.freq.remove |
| -2.2381236 | 5.7161306 |
| word.freq.order | word.freq.free |
| 0.9168758 | 1.1018100 |
| word.freq.meeting | word.freq.re |
| -3.9106839 | -0.3800485 |
| word.freq.edu | char.freq.semicolon |
| -1.2632029 | -1.6941404 |
| char.freq.exclamation | capital.run.length.average |
| 2.2251096 | 0.3420581 |

The β for `char.freq.semicolon` is -1.7. So having an extra semicolon in an e-mail multiplies odds of spam by $e^{-1.7} \approx 0.2$. (Down by a factor of five! Note to spammers: use more complex syntax.)

Interpeting coefficients in LR

```
coef(logit_spam1)
```

| | |
|-----------------------|----------------------------|
| (Intercept) | word.freq.remove |
| -2.2381236 | 5.7161306 |
| word.freq.order | word.freq.free |
| 0.9168758 | 1.1018100 |
| word.freq.meeting | word.freq.re |
| -3.9106839 | -0.3800485 |
| word.freq.edu | char.freq.semicolon |
| -1.2632029 | -1.6941404 |
| char.freq.exclamation | capital.run.length.average |
| 2.2251096 | 0.3420581 |

The β for `word.freq.remove` is 5.7. So having an extra `remove` in an e-mail multiplies odds of spam by $e^{5.7} \approx 300$.

Q: What is the odds multiplier for a coefficient of 0?

LR for spam: out-of-sample

```
logit_spam = glm(y ~ ., data=spamfit, family='binomial')
phat_test_logit_spam = predict(logit_spam, spamtest, type='response')
yhat_test_logit_spam = ifelse(phat_test_logit_spam > 0.5, 1, 0)
confusion_out_logit = table(y = spamtest$y, yhat = yhat_test_logit_spam)
confusion_out_logit
```

| | yhat | |
|---|------|-----|
| y | 0 | 1 |
| 0 | 358 | 27 |
| 1 | 51 | 165 |

We did better!

- Error rate $(51+27)/601 \approx 13\%$, or accuracy of 87%.
- Absolute improvement over LPM: $87 - 81.5 = 6.5\%$.
- Lift over LPM: $87/81.5 \approx 1.07$.

LR for spam: out-of-sample

We can take a slightly more nuanced look at the performance than simply calculating an overall accuracy/error rate. Three simple metrics you should know about:

- true positive rate (sensitivity, recall)
- the false positive rate (specificity)
- the false discovery rate (precision, positive predictive value)

LR for spam: true positive rate

The *true positive rate* (TPR): among spam e-mails ($y = 1$), how many are correctly flagged as spam ($\hat{y} = 1$)?

| | yhat | |
|---|------|-----|
| y | 0 | 1 |
| 0 | 358 | 27 |
| 1 | 51 | 165 |

Here the out-of-sample TPR is $165/(51 + 165) \approx 0.76$.

Synonyms for the TPR: sensitivity, recall.

LR for spam: false positive rate

The *false positive rate* (FPR): among non-spam e-mails ($y = 0$), how many are wrongly flagged as spam ($\hat{y} = 1$)?

| | yhat | |
|---|------|-----|
| y | 0 | 1 |
| 0 | 358 | 27 |
| 1 | 51 | 165 |

Here the out-of-sample FPR is $27/(27 + 358) \approx 0.07$.

Synonyms: *specificity* is the opposite of FPR, but conveys same information:

$$\text{Specificity} = 1 - \text{FPR}$$

So this procedure had a 93% out-of-sample specificity.

LR for spam: false discovery rate

The *false discovery rate* (FDR): among e-mails flagged as spam ($\hat{y} = 1$), how many were actually not spam ($y = 0$)?

| | yhat | |
|---|------|-----|
| y | 0 | 1 |
| 0 | 358 | 27 |
| 1 | 51 | 165 |

Here the out-of-sample FDR is $27/(27 + 165) \approx 0.14$.

Synonyms: The *precision/positive predictive value* is the opposite of FDR, but convey same information:

$$\text{Precision} = \text{Positive Predictive Value} = 1 - \text{FDR}$$

So this procedure had a 86% precision. Among flagged spam e-mails, 86% were actually spam.

Who uses these terms?

All these synonyms for the same error rates can be a pain! But their usage tends to be field-dependent.

- FPR, FNR, FDR: statistics, machine learning
- Sensivity, specificity, positive predictive value: medicine, epidemiology, and public health
- Precision and recall: database and search engine design, machine learning, computational linguistics

Solution: always go back to the confusion matrix! It tells the whole story. Ironically, the confusion matrix *avoids confusion* over terminology.

Estimating a logit model

A logistic regression model is fit by the principle of maximum likelihood: *choose the parameters so that the observed data looks as likely as possible.*

In LR, each outcome y_i is binary. By assumption:

$$P(y_i = 1 \mid x_i) = \frac{e^{x \cdot \beta}}{1 + e^{x \cdot \beta}}$$

$$P(y_i = 0 \mid x_i) = 1 - \frac{e^{x \cdot \beta}}{1 + e^{x \cdot \beta}} = \frac{1}{1 + e^{x \cdot \beta}}$$

Estimating a logit model

Recall that the likelihood function is the probability of the observed data as a function of the parameters. So we can write the likelihood contribution for observation i as:

$$L_i(\beta) = \left(\frac{e^{x \cdot \beta}}{1 + e^{x \cdot \beta}} \right)^{y_i} \cdot \left(\frac{1}{1 + e^{x \cdot \beta}} \right)^{1-y_i}$$

If $y_i = 1$, the second term gets zeroed out. Similarly, if $y_i = 0$, the first term gets zeroed out.

Estimating a logit model

The overall likelihood is then

$$L(\beta) = \prod_{i=1}^N L_i(\beta)$$

or on a log scale, to avoid numerical underflow:

$$\begin{aligned} l(\beta) &= \sum_{i=1}^N \log L_i(\beta) \\ &= \sum_{i=1}^N [y_i \cdot x_i \cdot \beta - \log(1 + e^{x_i \cdot \beta})] \end{aligned}$$

This quantity can be maximized as a function of β using an iterative numerical routine (typically Newton's method, sometimes gradient ascent or BFGS). Details for another course (feel free to ask me)!

KNN for classification

Another approach to classification: back to K-nearest-neighbors.

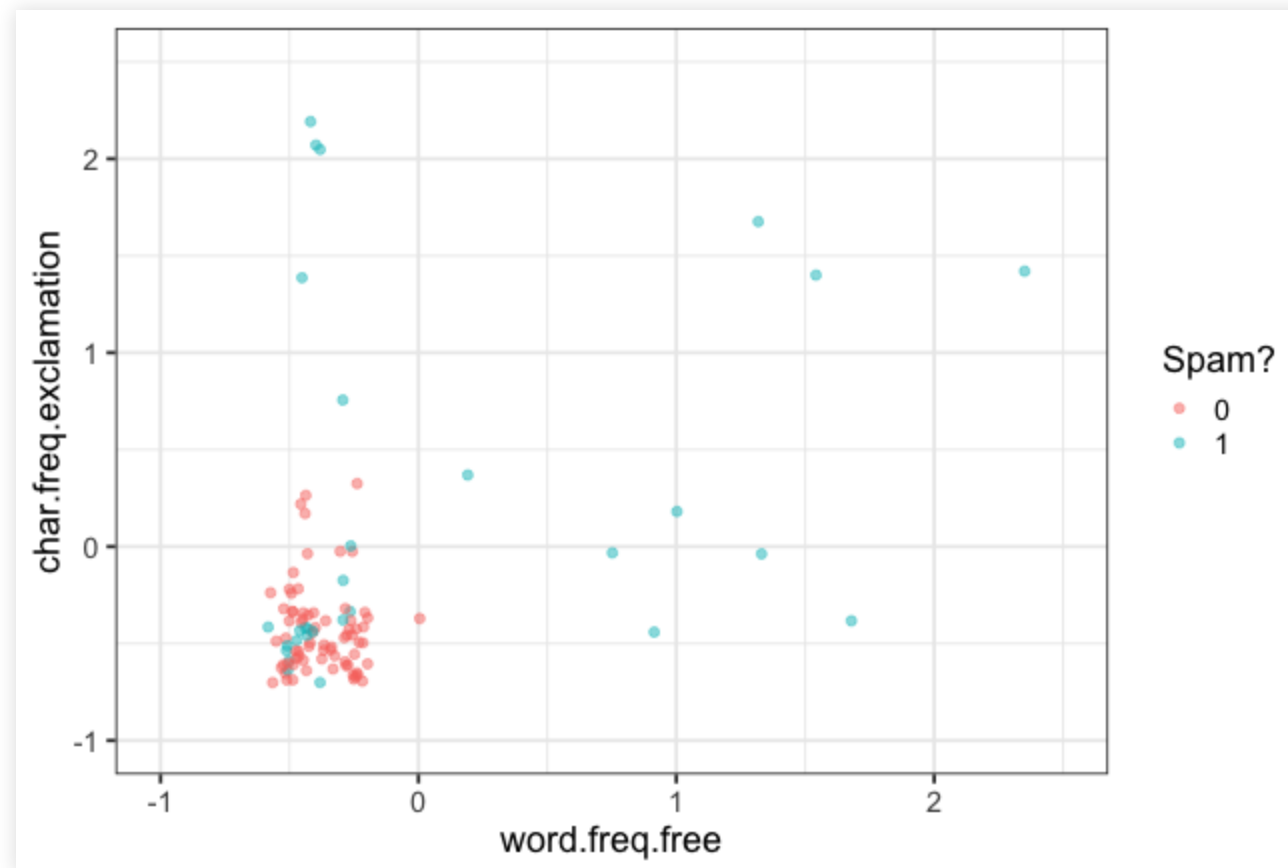
Super intuitive: what is the most common class around x^\star ?

- Nearness measured using some metric, typically Euclidean distance:

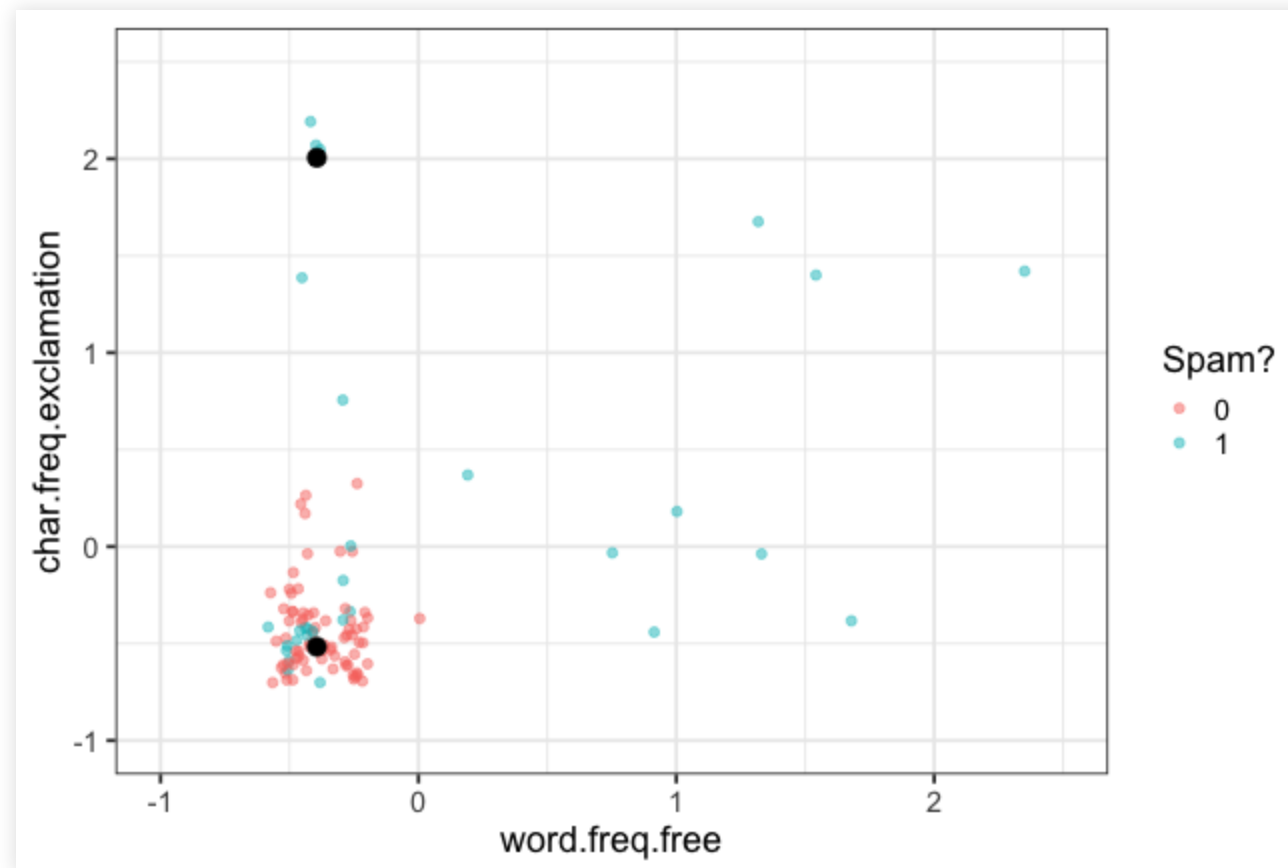
$$d(x, x') = \sqrt{\sum_{j=1}^p (x_j - x'_j)^2}$$

- Remember the importance of scaling your feature variables here! Typically we use distances scaled by $\text{sd}(x_j)$ rather than raw distances.

KNN for classification



KNN for classification



KNN for classification

In-class example: classifying glass shards for a recycling center

6 classes:

- WinF: float glass window
- WinNF: non-float window
- Veh: vehicle window
- Con: container (bottles)
- Tabl: tableware
- Head: vehicle headlamp

See `glass.R` on the class website!

Limitations of KNN for classification

Nearest-neighbor classification is simple, but limited.

- There is no good way to choose K . Train/test splits work, but they are unstable: different data \longrightarrow different K (perhaps very different).
- The classification can be very sensitive to K .
- All you get is a classification, with only rough probabilities. E.g. with $k = 5$, all probability estimates are multiple of 20%. Without accurate probabilities, it is hard to assess misclassification risk.
- But the basic idea is the same as in logistic regression: Observations with similar x 's should be classified similarly.

Multinomial logistic regression

In logistic regression, we get binary class probabilities.

In multi-class problems, the response is one of K categories. We'll encode this as $y_i = [0, 0, 1, \dots, 0]$ where $y_{ik} = 1$ if response i is in class $k \in \{1, \dots, K\}$.

In multinomial logistic regression (MLR), we fit a model for

$$E(y_{ik} \mid x_i) = P(y_{ik} = 1 \mid x_i) = g(x_i \cdot \beta_k)$$

That is, we fit regression coefficients for *each class*.

Multinomial logistic regression

In the MLR model, we construct this by analogy with the sigmoid link function (from binary LR) as follows:

$$\hat{p}_{ik} = P(y_{ik} = 1 \mid x_i) = \frac{e^{x_i \cdot \beta_k}}{\sum_{l=1}^K e^{x_i \cdot \beta_l}}$$

I like to think of this as each class vying to predict the outcome for x_i as its own, via a “rate and normalize” procedure:

- each class “rates” x_i as $e^{x_i \cdot \beta_k}$. The closer x_i is to the class-specific regression coefficient β_k , the bigger this rating is.
- Ratings \rightarrow probs: divide by the sum of the ratings across classes.
- This is often called the “softmax” function.

Multinomial logit: glass example

```
library(nnet)
n = nrow(fgl); n_train = 180
train_ind = sample.int(214, n_train, replace=FALSE)
ml1 = multinom(type ~ RI + Mg, data=fgl[train_ind,])
```

```
# weights: 24 (15 variable)
initial value 322.516704
iter 10 value 225.637114
iter 20 value 199.130574
iter 30 value 198.899834
final value 198.899720
converged
```

```
coef(ml1)
```

| | (Intercept) | RI | Mg |
|-------|-------------|------------|-------------|
| WinNF | 5.459371 | -0.2027355 | -1.59091718 |
| Veh | -1.016222 | -0.1188378 | -0.09264681 |
| Con | 7.444248 | -0.4911691 | -3.28404976 |
| Tabl | 6.571685 | -0.5274920 | -2.90523982 |
| Head | 8.190010 | -0.6817354 | -3.34953951 |

Multinomial logit: glass example

Fitted class probabilities for the first five test-set examples:

```
predict(ml1, fgl[-train_ind,], type='probs') %>%  
  head(5) %>%  
  round(3)
```

| | WinF | WinNF | Veh | Con | Tabl | Head |
|----|-------|-------|-------|-------|-------|-------|
| 1 | 0.788 | 0.080 | 0.132 | 0.000 | 0.000 | 0.000 |
| 18 | 0.719 | 0.166 | 0.114 | 0.001 | 0.001 | 0.000 |
| 19 | 0.575 | 0.285 | 0.129 | 0.003 | 0.004 | 0.004 |
| 26 | 0.443 | 0.401 | 0.121 | 0.008 | 0.013 | 0.014 |
| 27 | 0.438 | 0.411 | 0.116 | 0.008 | 0.013 | 0.014 |

Multinomial logit: glass example

How did we do?

```
y_test = fgl[-train_ind, 'type']
yhat_test = predict(ml1, fgl[-train_ind,], type='class')
conf_mat = table(y_test, yhat_test)
conf_mat
```

| | yhat_test | | | | | |
|--------|-----------|-------|-----|-----|------|------|
| y_test | WinF | WinNF | Veh | Con | Tabl | Head |
| WinF | 8 | 2 | 0 | 0 | 0 | 0 |
| WinNF | 4 | 9 | 0 | 0 | 0 | 1 |
| Veh | 1 | 1 | 0 | 0 | 0 | 0 |
| Con | 0 | 1 | 0 | 0 | 0 | 0 |
| Tabl | 0 | 1 | 0 | 0 | 0 | 1 |
| Head | 0 | 0 | 0 | 0 | 0 | 5 |

```
sum(diag(conf_mat)) / (n-n_train)
```

```
[1] 0.6470588
```

Evaluating a classifier: deviance

In making decisions, both costs and probabilities matter. E.g. if $P(y = 1 \mid x) = 0.3$, how would you respond differently if:

- x is word content of an e-mail and y is spam status?
- x is mammogram result and y is breast cancer status?
- x is DNA test and y is guilty/not guilty?

Different kinds of errors may have different costs. Thus it helps to de-couple two tasks: *modeling probabilities accurately* and *making decisions*.

This requires that we evaluate the performance of a classifier in terms its *predicted probabilities*, not its *decisions about class labels*.

Evaluating a classifier: likelihood

The natural way to do us is by calculating the *likelihood* for our model's predicted probabilities. Suppose that our classifier produces predicted probabilities \hat{p}_{ik} for each response i and class k . Then the likelihood is

$$\begin{aligned}\text{Like} &= \prod_{i=1}^n \prod_{l=1}^K \hat{p}_{il}^{y_{il}} \\ &= \prod_{i=1}^n \hat{p}_{i,k_i}\end{aligned}$$

where k_i is the observed class label for case i .

To get from the first to the second lines, notice that $y_{il} = 1$ for $l = k_i$, and zero otherwise.

Evaluating a classifier: log likelihood

On a log scale, this becomes

$$\text{loglike} = \sum_{i=1}^n \log \hat{p}_{i,k_i}$$

In words: we sum up our model's predicted log probabilities for the outcomes y_{i,k_i} that actually happened.

As with everything in statistical learning: we can calculate an in-sample or a out-of-sample log likelihood, and the out-of-sample is more important!

Q: what's the largest possible log likelihood for a classifier?

Evaluating a classifier: deviance

Sometimes we quote a model's *deviance* instead of its log likelihood.

The relationship is simple:

$$\text{deviance} = -2 \cdot \text{loglike}$$

Log likelihood measures *fit* (which we want to maximize), deviance measures *misfit* (which we want to minimize).

So the negative sign makes sense. But why the factor of 2? *Because of the analogy because least squares and the normal distribution.*

Evaluating a classifier: deviance

Remember back to an ordinary regression problem with normally distributed errors, $y_i \sim N(f(x_i), \sigma^2)$:

$$\text{Like} = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2}(y_i - f(x_i))^2\right\}$$

On a log scale, up to a constant not involving $f(x)$, this becomes:

$$\text{loglike} \propto -\frac{1}{2} \sum_{i=1}^n (y_i - f(x_i))^2 = -\text{RSS}/2$$

where RSS = residual sums of squares.

Deviance generalizes the notion of “residual sums of squares” to non-Gaussian models.

Bayes' Rule for classification

Recall Bayes' rule:

$$P(A \mid B) = \frac{P(A)P(B \mid A)}{P(B)}$$

You might remember that each of these terms has a name:

- $P(A)$: the prior probability
- $P(A \mid B)$: the posterior probability
- $P(B \mid A)$: the likelihood
- $P(B)$: the marginal (total/overall) probability

In classification, “A” is a class label and “B” is a set of features.

Bayes' Rule for classification

Bayes's rule:

$$P(y = k \mid x) = \frac{P(y = k) \cdot P(x \mid y = k)}{P(x)}$$

$P(y = k)$ is the prior probability for class k . We usually get this from the raw class frequencies in the training data. For example:

```
table(fgl[train_ind,]$type) %>% prop.table
```

| WinF | WinNF | Veh | Con | Tabl | Head |
|------------|------------|------------|------------|------------|------------|
| 0.33333333 | 0.34444444 | 0.08333333 | 0.06666667 | 0.03888889 | 0.13333333 |

Bayes' Rule for classification

Bayes's rule:

$$P(y = k \mid x) = \frac{P(y = k) \cdot P(x \mid y = k)}{P(x)}$$

$P(x)$ is the marginal probability of observing feature vector x . Notice it doesn't depend on k ! It's the same number for all classes.

Thus we usually write the posterior probabilities up to this constant of proportionality, without bothering to compute it:

$$P(y = k \mid x) \propto P(y = k) \cdot P(x \mid y = k)$$

(Note: often we do the actual computations on a log scale instead.)

Bayes' Rule for classification

Bayes's rule:

$$P(y = k \mid x) = \frac{P(y = k) \cdot P(x \mid y = k)}{P(x)}$$

The hard part is estimating the likelihood $P(x \mid y = k)$. In words: how likely is it that we would have observed feature vector x if the true class label were k ?

This is like regression in reverse! See `congress109_bayes.r` for a teaser example.

Naive Bayes

Recall that $x = (x_1, x_2, \dots, x_p)$ is a vector of p features. Our first strategy for estimating $P(x \mid y = k)$ is called “Naive Bayes.”

It's “naive” because we make the simplifying assumption that every feature x_j is *independent* of all other features:

$$\begin{aligned} P(x \mid y = k) &= P(x_1, x_2, \dots, x_p \mid y = k) \\ &= \prod_{j=1}^p P(x_j \mid y = k) \quad (\text{independence}) \end{aligned}$$

This simplifies the requirements of the problem: *just calculate the marginal distribution of the features*, i.e. $P(x_j \mid y = k)$ for all features j and classes k .

Naive Bayes: a small example

In `congress109.csv` we have data on all speeches given on the floor of the U.S. Congress during the 109th Congressional Session (January 3, 2005 to January 3, 2007).

Every row is a set of *phrase counts* associated with a single representative's speeches across the whole session. X_{ij} = number of times that rep i utter phrase j during a speech.

The target variable $y \in \mathcal{R}, \mathcal{D}$ is the party affiliation of the representative.

Naive Bayes: a small example

```
# read in data
congress109 = read.csv("../data/congress109.csv", header=TRUE, row.names=1)
congress109members = read.csv("../data/congress109members.csv",
header=TRUE, row.names=1)
```

Focus on a few key phrases and a few famous pols:

```
X_small = dplyr::select(congress109, minimum.wage, war.terror, tax.relief,
hurricane.katrina)
X_small[c('John McCain', 'Mike Pence', 'John Kerry', 'Edward Kennedy'),]
```

| | minimum.wage | war.terror | tax.relief | hurricane.katrina |
|----------------|--------------|------------|------------|-------------------|
| John McCain | 0 | 27 | 0 | 14 |
| Mike Pence | 0 | 12 | 1 | 11 |
| John Kerry | 12 | 16 | 13 | 23 |
| Edward Kennedy | 260 | 8 | 1 | 53 |

Naive Bayes: a small example

Let's look at these counts summed across all members in each party:

```
y = congress109members$party  
  
# Sum phrase counts by party  
R_rows = which(y == 'R')  
D_rows = which(y == 'D')  
colSums(X_small[R_rows,])
```

| | | | |
|--------------|------------|------------|-------------------|
| minimum.wage | war.terror | tax.relief | hurricane.katrina |
| 294 | 604 | 497 | 717 |

```
colSums(X_small[D_rows,])
```

| | | | |
|--------------|------------|------------|-------------------|
| minimum.wage | war.terror | tax.relief | hurricane.katrina |
| 767 | 237 | 176 | 1295 |

So we get the sense that some phrases are “more Republican” and some “more Democrat.”

Naive Bayes: a small example

To make this precise, let's build a simplified “bag of phrases” model for a Congressional speech:

- Imagine that every phrase uttered in a speech is a random sample from a “bag of phrases,” where each phrase has its own probability. (*This is the Naive Bayes assumption of independence.*)
- Here the bag consists of just four phrases: “minimum wage”, “war on terror”, “tax relief,” and “hurricane katrina”.
- Each class (R or D) has its own probability vector associated with the phrases in the bag.

Naive Bayes: a small example

We can estimate these probability vectors for each class from the phrase counts in the training data. For Republicans:

```
probhat_R = colSums(X_small[R_rows,])  
probhat_R = probhat_R/sum(probhat_R)  
probhat_R
```

| | | | |
|--------------|------------|------------|-------------------|
| minimum.wage | war.terror | tax.relief | hurricane.katrina |
| 0.1392045 | 0.2859848 | 0.2353220 | 0.3394886 |

And for Democrats:

```
probhat_D = colSums(X_small[D_rows,])  
probhat_D = probhat_D/sum(probhat_D)  
probhat_D
```

| | | | |
|--------------|------------|------------|-------------------|
| minimum.wage | war.terror | tax.relief | hurricane.katrina |
| 0.30989899 | 0.09575758 | 0.07111111 | 0.52323232 |

Naive Bayes: a small example

Let's now look at some particular member of Congress and try to build the “likelihood” for his or her phrase counts

```
X_small['Sheila Jackson-Lee',]
```

| | minimum.wage | war.terror | tax.relief | hurricane.katrina |
|--------------------|--------------|------------|------------|-------------------|
| Sheila Jackson-Lee | 11 | 15 | 3 | 66 |

Are Sheila Jackson-Lee's phrase counts $x = (11, 15, 3, 66)$ more likely under the Republican or Democrat probability vector?

Naive Bayes: a small example

Recall the Republican vector:

| | | | |
|--------------|------------|------------|-------------------|
| minimum.wage | war.terror | tax.relief | hurricane.katrina |
| 0.1392045 | 0.2859848 | 0.2353220 | 0.3394886 |

Under this probability vector:

$$\begin{aligned}P(x \mid y = R) &= P(x_1 = 11 \mid y = R) \\&\quad \times P(x_2 = 15 \mid y = R) \\&\quad \times P(x_3 = 3 \mid y = R) \\&\quad \times P(x_4 = 66 \mid y = R) \\&= (0.1392)^{11} \cdot (0.2860)^{15} \cdot (0.2353)^3 \cdot (0.3395)^{66} \\&= 3.765 \times 10^{-51}\end{aligned}$$

Naive Bayes: a small example

Now recall the Democratic vector:

| | | | |
|--------------|------------|------------|-------------------|
| minimum.wage | war.terror | tax.relief | hurricane.katrina |
| 0.30989899 | 0.09575758 | 0.07111111 | 0.52323232 |

Under this probability vector:

$$\begin{aligned}P(x \mid y = D) &= P(x_1 = 11 \mid y = D) \\&\quad \times P(x_2 = 15 \mid y = D) \\&\quad \times P(x_3 = 3 \mid y = D) \\&\quad \times P(x_4 = 66 \mid y = D) \\&= (0.3099)^{11} \cdot (0.0958)^{15} \cdot (0.0711)^3 \cdot (0.5232)^{66} \\&= 1.293 \times 10^{-43}\end{aligned}$$

Naive Bayes: a small example

Because these numbers are so tiny, it's much safer to work on a log scale:

$$\log P(x \mid y = k) = \sum_{j=1}^p x_j \log p_j^{(k)}$$

where $p_j^{(k)}$ is the j th entry in the probability vector for class k .

```
x_try = X_small['Sheila Jackson-Lee',]  
sum(x_try * log(probhat_R))
```

```
[1] -116.1083
```

```
sum(x_try * log(probhat_D))
```

```
[1] -98.75633
```

Naive Bayes: a small example

Let's use Bayes' rule (posterior \propto prior times likelihood) to put this together with our prior, estimated using the empirical class frequencies:

```
table(y) %>% prop.table
```

```
      y  
      D      I      R  
0.457466919 0.003780718 0.538752363
```

So:

$$P(R \mid x) \propto 0.539 \cdot (3.765 \times 10^{-51})$$

and

$$P(D \mid x) \propto 0.457 \cdot (1.293 \times 10^{-43})$$

Naive Bayes: a small example

- Turn this into a set of probabilities by normalizing, i.e. dividing by the sum across all classes:

$$P(D \mid x) = \frac{0.457 \cdot (1.293 \times 10^{-43})}{0.457 \cdot (1.293 \times 10^{-43}) + 0.539 \cdot (3.765 \times 10^{-51})} \approx 1$$

- So:
 1. Sheila Jackson-Lee is probably a Democrat, according to our model.
 2. The data completely overwhelm the prior! This is often the case in Naive Bayes models.

Naive Bayes: a bigger example

Turn to `congress109_bayes.R` to see a larger example of Naive Bayes classification, where we fit our model with all 1000 phrase counts.

Naive Bayes: summary

- Works by directly modeling $P(x \mid y)$, versus $P(y \mid x)$ as in logit.
- Simple and easy to compute, and therefore scalable to very large data sets and classification problems.
- Works even more with feature variables P than observations N .
- Often too simple: the “naive” assumption of independence really is a drastic simplification.
- The resulting probabilities are useful for classification purposes, but often not believable as probabilities.
- Most useful when the features x are categorical variables (like phrase counts!) Very common in text analysis.

Linear discriminant analysis

Linear discriminant analysis (LDA) has a similar motivation to Naive Bayes.

$$P(y = k \mid x) \propto p(y = k) \cdot p(x \mid y = k)$$

There are two key differences:

- LDA relaxes the assumption of independence.
- We explicitly model the multivariate *joint distribution* for vector x as a multivariate normal distribution:

$$p(x \mid y = k) = (2\pi)^{-p/2} \cdot |\Sigma_k|^{-1/2} \exp\{(x - \mu_k)' \Sigma_k^{-1} (x - \mu_k)\}$$

Written more concisely: $(x \mid y = k) \sim N(\mu_k, \Sigma_k)$, where (μ_k, Σ_k) are the mean vector and covariance matrix for class k .

- See `glass_LDA.R`