Models

Prediction and overfitting

Prof. Dr. Jan Kirenz

The following content is based on Mine Çetinkaya-Rundel's excellent book Data Science in a Box

Prediction

Goal: Building a spam filter

- Data: Set of emails and we know if each email is spam/not and other features
- Use logistic regression to predict the probability that an incoming email is spam
- Use model selection to pick the model with the best predictive performance
- Building a model to predict the probability that an email is spam is only half of the battle! We also need a decision rule about which emails get flagged as spam (e.g. what probability should we use as out cutoff?)
- A simple approach: choose a single threshold probability and any email that exceeds that probability is flagged as spam

A multiple regression approach

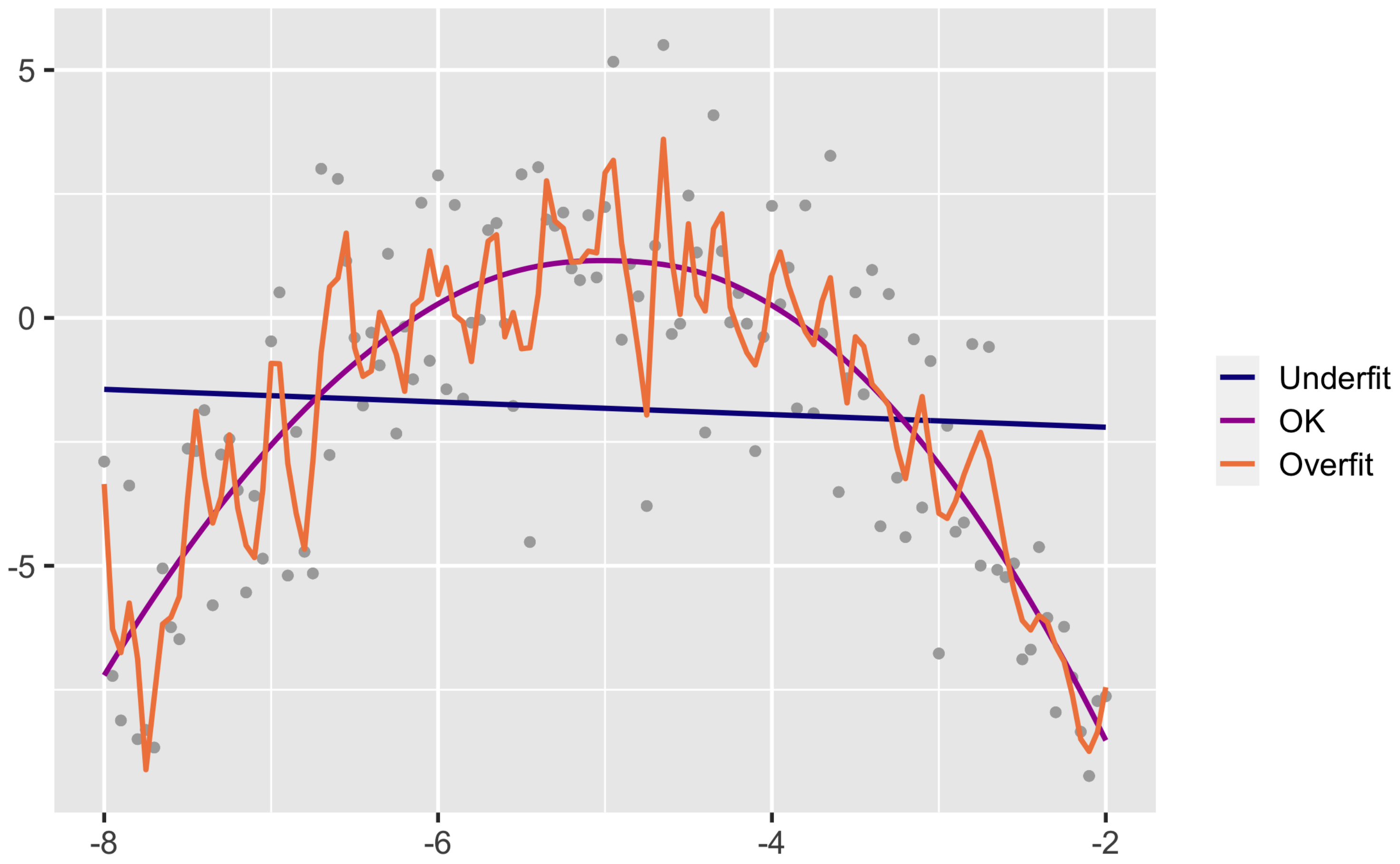
Output   Code

```
## # A tibble: 22 x 5
##    term        estimate std.error statistic  p.value
##    <chr>          <dbl>     <dbl>     <dbl>    <dbl>
##  1 (Intercept) -9.09e+1   9.80e+3  -0.00928 9.93e- 1
##  2 to_multiple -2.68e+0   3.27e-1  -8.21    2.25e-16
##  3 from        -2.19e+1   9.80e+3  -0.00224 9.98e- 1
##  4 cc           1.88e-2   2.20e-2   0.855   3.93e- 1
##  5 sent_email  -2.07e+1   3.87e+2  -0.0536  9.57e- 1
##  6 time         8.48e-8   2.85e-8   2.98    2.92e- 3
##  7 image       -1.78e+0   5.95e-1  -3.00    2.73e- 3
##  8 attach       7.35e-1   1.44e-1   5.09    3.61e- 7
##  9 dollar      -6.85e-2   2.64e-2  -2.59    9.64e- 3
## 10 winneryes    2.07e+0   3.65e-1   5.67    1.41e- 8
## 11 inherit      3.15e-1   1.56e-1   2.02    4.32e- 2
## 12 viagra       2.84e+0   2.22e+3   0.00128 9.99e- 1
## 13 password    -8.54e-1   2.97e-1  -2.88    4.03e- 3
## 14 num_char     5.06e-2   2.38e-2   2.13    3.35e- 2
## 15 line_breaks -5.49e-3   1.35e-3  -4.06    4.91e- 5
## 16 format      -6.14e-1   1.49e-1  -4.14    3.53e- 5
## 17 re_subj     -1.64e+0   3.86e-1  -4.25    2.16e- 5
## 18 exclaim_subj  1.42e-1  2.43e-1   0.585   5.58e- 1
## 19 urgent_subj  3.88e+0   1.32e+0   2.95    3.18e- 3
## 20 exclaim_mess  1.08e-2  1.81e-3   5.98    2.23e- 9
## 21 numbersmall -1.19e+0   1.54e-1  -7.74    9.62e-15
## 22 numberbig   -2.95e-1   2.20e-1  -1.34    1.79e- 1
```

Prediction

- The mechanics of prediction is **easy**:
  - Plug in values of predictors to the model equation
  - Calculate the predicted value of the response variable, $\hat{y}$
- Getting it right is **hard**!
  - There is no guarantee the model estimates you have are correct
  - Or that your model will perform as well with new data as it did with your sample data

Underfitting and overfitting



Spending our data

- Several steps to create a useful model: parameter estimation, model selection, performance assessment, etc.

- Doing all of this on the entire data we have available can lead to **overfitting**

- Allocate specific subsets of data for different tasks, as opposed to allocating the largest possible amount to the model parameter estimation only (which is what we've done so far)

Splitting data

Splitting data

- **Training set:**
  - Sandbox for model building
  - Spend most of your time using the training set to develop the model
  - Majority of the data (usually 80%)
- **Testing set:**
  - Held in reserve to determine efficacy of one or two chosen models
  - Critical to look at it once, otherwise it becomes part of the modeling process
  - Remainder of the data (usually 20%)

Performing the split

```r
# Fix random numbers by setting the seed
# Enables analysis to be reproducible when random numbers are used
set.seed(1116)

# Put 80% of the data into the training set
email_split <- initial_split(email, prop = 0.80)

# Create data frames for the two sets:
train_data <- training(email_split)
test_data  <- testing(email_split)
```

Peek at the split

```r
glimpse(train_data)
```

```
## Rows: 3,137
## Columns: 21
## $ spam         <fct> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ to_multiple  <dbl> 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0,…
## $ from         <dbl> 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,…
## $ cc           <int> 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 2, 1, 0,…
## $ sent_email   <dbl> 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 1, 0,…
## $ time         <dttm> 2012-01-01 07:16:41, 2012-01-01 08:03:59…
## $ image        <dbl> 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0,…
## $ attach       <dbl> 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0,…
## $ dollar       <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 5,…
## $ winner       <fct> no, no, no, no, no, no, no, no, no, no, n…
## $ inherit      <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ viagra       <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ password     <dbl> 0, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 1,…
## $ num_char     <dbl> 11.370, 10.504, 13.256, 1.231, 1.091, 4.8…
## $ line_breaks  <int> 202, 202, 255, 29, 25, 193, 237, 69, 79, …
## $ format       <dbl> 1, 1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 1, 1, 1,…
## $ re_subj      <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 1, 0,…
## $ exclaim_subj <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1,…
## $ urgent_subj  <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ exclaim_mess <dbl> 0, 1, 48, 1, 1, 1, 18, 1, 1, 0, 10, 4, 10…
## $ number       <fct> big, small, small, none, none, big, small…
```

```r
glimpse(test_data)
```

```
## Rows: 784
## Columns: 21
## $ spam         <fct> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ to_multiple  <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0,…
## $ from         <dbl> 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,…
## $ cc           <int> 0, 0, 0, 2, 0, 0, 0, 0, 2, 0, 0, 7, 0, 0,…
## $ sent_email   <dbl> 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0,…
## $ time         <dttm> 2012-01-01 17:00:32, 2012-01-01 19:12:00…
## $ image        <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ attach       <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ dollar       <dbl> 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 8,…
## $ winner       <fct> no, no, no, no, no, no, no, no, no, no, n…
## $ inherit      <dbl> 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ viagra       <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ password     <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ num_char     <dbl> 7.773, 2.643, 0.869, 13.890, 4.560, 2.192…
## $ line_breaks  <int> 192, 68, 25, 225, 64, 85, 10, 57, 97, 39,…
## $ format       <dbl> 1, 1, 1, 1, 1, 1, 0, 1, 0, 0, 0, 0, 1, 1,…
## $ re_subj      <dbl> 0, 0, 0, 1, 0, 0, 1, 0, 1, 1, 0, 1, 0, 0,…
## $ exclaim_subj <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1,…
## $ urgent_subj  <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
## $ exclaim_mess <dbl> 6, 0, 2, 0, 0, 3, 0, 5, 1, 3, 3, 0, 4, 32…
## $ number       <fct> small, small, small, small, none, big, sm…
```

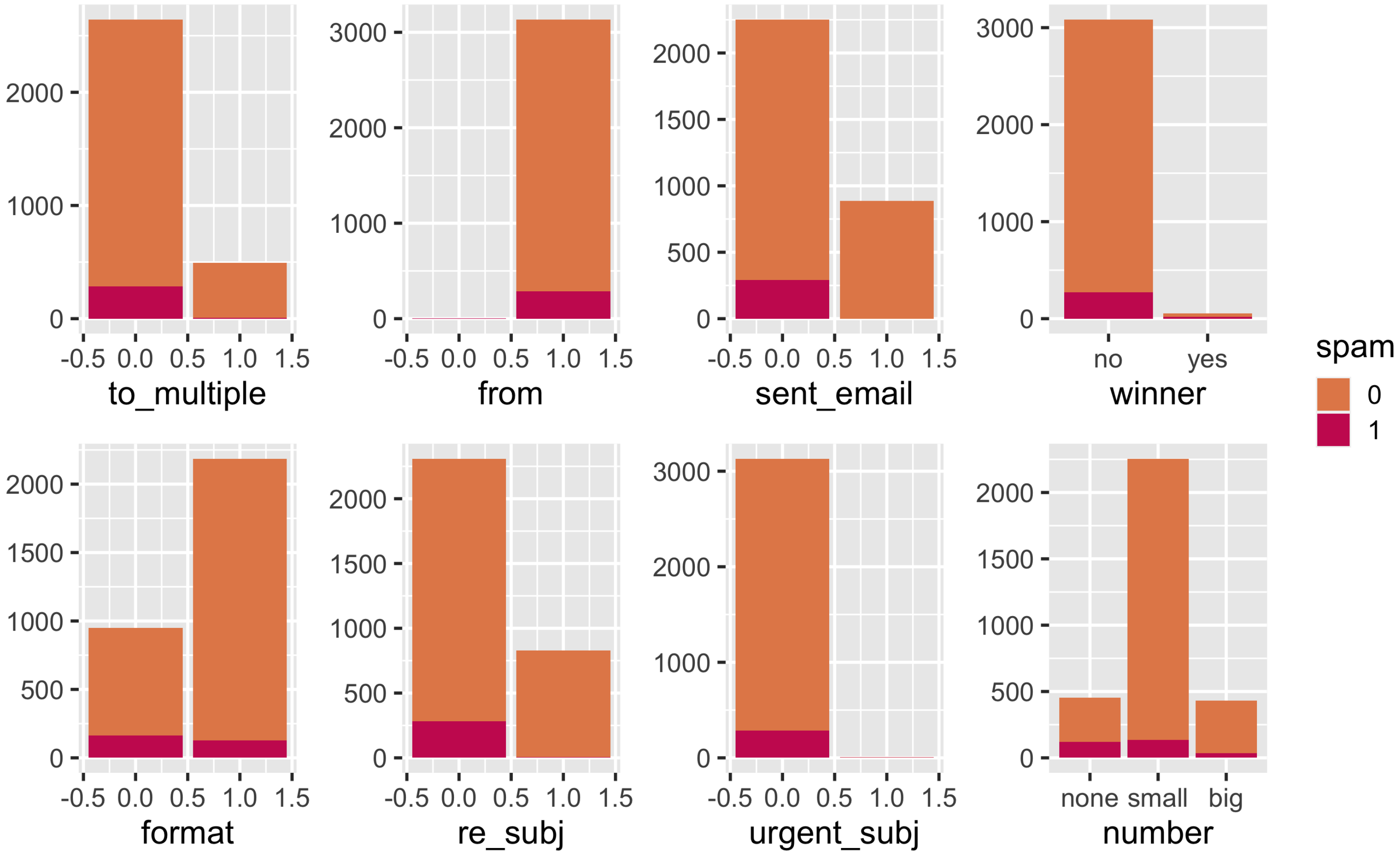
Modeling workflow

Fit a model to the training dataset

```
email_fit <- logistic_reg() %>%
  set_engine("glm") %>%
  fit(spam ~ ., data = train_data, family = "binomial")
```

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

Categorical predictors



`from` and `sent_email`

- `from`: Whether the message was listed as from anyone (this is usually set by default for regular outgoing email)

```
train_data %>%
  count(spam, from)
```

```
## # A tibble: 3 x 3
##   spam   from     n
##   <fct> <dbl> <int>
## 1 0         1  2847
## 2 1         0     3
## 3 1         1   287
```

- `sent_email`: Indicator for whether the sender had been sent an email in the last 30 days

```
train_data %>%
  count(spam, sent_email)
```

```
## # A tibble: 3 x 3
##   spam  sent_email     n
##   <fct>      <dbl> <int>
## 1 0              0  1962
## 2 0              1   885
## 3 1              0   290
```

Numerical predictors

```
##
## ── Variable type: numeric ─────────────────────────────────────────────────────────────────
##    skim_variable spam  n_missing complete_rate      mean       sd   p0      p25     p50     p75   p100
##  1 to_multiple   0             0             1   0.171      0.377  0       0       0       0       1
##  2 to_multiple   1             0             1   0.0207     0.143  0       0       0       0       1
##  3 from          0             0             1   1          0      1       1       1       1       1
##  4 from          1             0             1   0.990      0.101  0       1       1       1       1
##  5 cc            0             0             1   0.416      2.77   0       0       0       0      68
##  6 cc            1             0             1   0.345      2.02   0       0       0       0      23
##  7 sent_email    0             0             1   0.311      0.463  0       0       0       1       1
##  8 sent_email    1             0             1   0          0      0       0       0       0       0
##  9 image         0             0             1   0.0562     0.510  0       0       0       0      20
## 10 image         1             0             1   0.00690    0.0829 0       0       0       0       1
## 11 attach        0             0             1   0.128      0.765  0       0       0       0      21
## 12 attach        1             0             1   0.193      0.574  0       0       0       0       2
## 13 dollar        0             0             1   1.54       5.19   0       0       0       0      64
## 14 dollar        1             0             1   0.655      2.63   0       0       0       0      36
## 15 inherit       0             0             1   0.0351     0.237  0       0       0       0       6
## 16 inherit       1             0             1   0.0690     0.560  0       0       0       0       9
## 17 viagra        0             0             1   0          0      0       0       0       0       0
## 18 viagra        1             0             1   0          0      0       0       0       0       0
## 19 password      0             0             1   0.126      1.09   0       0       0       0      28
## 20 password      1             0             1   0.0138     0.143  0       0       0       0       2
## 21 num_char      0             0             1  11.2       14.3    0.003   1.86    6.83   15.4    165.
## 22 num_char      1             0             1   4.60      13.0    0.001   0.503   1.08    3.20   174.
## 23 line_breaks   0             0             1 244.       317.     2      42     136     320.    3589
## 24 line_breaks   1             0             1  88.8      265.     1      14      22.5    63.8   3729
## 25 format        0             0             1   0.724      0.447  0       0       1       1       1
## 26 format        1             0             1   0.434      0.497  0       0       0       1       1
## 27 re_subj       0             0             1   0.289      0.453  0       0       0       1       1
## 28 re_subj       1             0             1   0.0207     0.143  0       0       0       0       1
## 29 exclaim_subj  0             0             1   0.0780     0.268  0       0       0       0       1
## 30 exclaim_subj  1             0             1   0.0862     0.281  0       0       0       0       1
## 31 urgent_subj   0             0             1   0.00105    0.0324 0       0       0       0       1
## 32 urgent_subj   1             0             1   0.0103     0.101  0       0       0       0       1
## 33 exclaim_mess  0             0             1   6.02      41.2    0       0       1       5    1203
```

Fit a model to the training dataset

```r
email_fit <- logistic_reg() %>%
  set_engine("glm") %>%
  fit(spam ~ . - from - sent_email - viagra, data = train_data, family = "binomial")
```

```r
email_fit
```

```
## parsnip model object
##
## Fit time:  24ms
##
## Call:  stats::glm(formula = spam ~ . - from - sent_email - viagra, family = stats::binomial,
##     data = data)
##
## Coefficients:
##  (Intercept)   to_multiple            cc          time         image        attach        dollar
##   -8.251e+01    -3.114e+00     2.130e-02     6.173e-08    -1.412e+00     3.871e-01    -7.115e-02
##    winneryes       inherit      password      num_char   line_breaks        format       re_subj
##    2.134e+00     3.569e-01    -9.737e-01     5.793e-02    -6.367e-03    -7.715e-01    -3.050e+00
## exclaim_subj   urgent_subj  exclaim_mess   numbersmall     numberbig
##    2.350e-01     3.866e+00     1.200e-02    -6.915e-01     1.174e-01
##
## Degrees of Freedom: 3136 Total (i.e. Null);  3118 Residual
## Null Deviance:	    1933
## Residual Deviance: 1402 	AIC: 1440
```

Predict outcome on the testing dataset

```
predict(email_fit, test_data)
```

```
## # A tibble: 784 x 1
##   .pred_class
##   <fct>
## 1 0
## 2 0
## 3 0
## 4 0
## 5 0
## 6 0
## # … with 778 more rows
```

Predict probabilities on the testing dataset

```
email_pred <- predict(email_fit, test_data, type = "prob") %>%
  bind_cols(test_data %>% select(spam, time))

email_pred
```

```
## # A tibble: 784 x 4
##   .pred_0 .pred_1 spam  time
##     <dbl>   <dbl> <fct> <dttm>
## 1   0.942 0.0581  0     2012-01-01 17:00:32
## 2   0.920 0.0804  0     2012-01-01 19:12:00
## 3   0.904 0.0960  0     2012-01-01 19:23:44
## 4   0.997 0.00304 0     2012-01-02 01:54:46
## 5   0.833 0.167   0     2012-01-02 02:58:14
## 6   0.849 0.151   0     2012-01-02 03:05:45
## # … with 778 more rows
```

A closer look at predictions

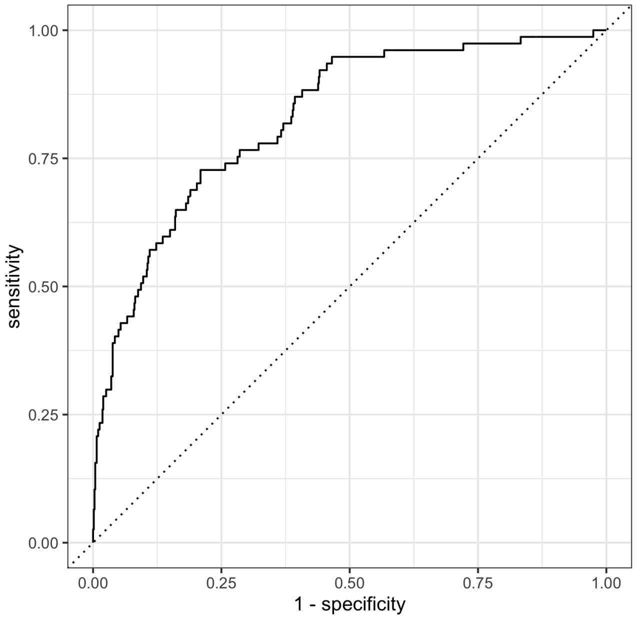
```
email_pred %>%
  arrange(desc(.pred_1)) %>%
  print(n = 10)
```

```
## # A tibble: 784 x 4
##    .pred_0 .pred_1 spam  time
##      <dbl>   <dbl> <fct> <dttm>
##  1  0.0381   0.962 1     2012-03-27 07:17:01
##  2  0.205    0.795 1     2012-02-21 09:34:56
##  3  0.408    0.592 0     2012-02-03 14:25:39
##  4  0.412    0.588 1     2012-03-10 23:43:58
##  5  0.448    0.552 1     2012-02-14 20:45:19
##  6  0.462    0.538 1     2012-02-04 16:54:23
##  7  0.469    0.531 0     2012-01-12 03:00:16
##  8  0.472    0.528 1     2012-01-25 17:17:54
##  9  0.477    0.523 1     2012-03-21 03:00:30
## 10  0.486    0.514 1     2012-03-16 22:39:28
## # … with 774 more rows
```

Evaluate the performance

Receiver operating characteristic (ROC) curve[+] which plot true positive rate vs. false positive rate (1 - specificity)

```r
email_pred %>%
  roc_curve(
    truth = spam,
    .pred_1,
    event_level = "second"
  ) %>%
  autoplot()
```



[+]Originally developed for operators of military radar receivers, hence the name.

Evaluate the performance

Find the area under the curve:

```
email_pred %>%
  roc_auc(
    truth = spam,
    .pred_1,
    event_level = "second"
  )
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 roc_auc binary         0.828
```