Predictive Bias and Calibration

DS 6030 | Fall 2023

calibration.pdf

Contents

1 Probability Modeling

1.1 Data

```
#: Load Data, Create binary column (y)
data(Default, package="ISLR")
Default = Default %>% as_tibble() %>%
  mutate(y = if_else(default == "Yes", 1L, 0L), .after=default)
```

default	y	student	balance	income
No	0	No	1384.9	40131
Yes	1	Yes	1889.3	22652
Yes	1	Yes	1740.8	18161
Yes	1	Yes	2123.4	23836
No	0	Yes	856.7	15523
No	0	No	310.1	31446
No	0	No	1248.9	31960
Yes	1	No	1823.6	44260

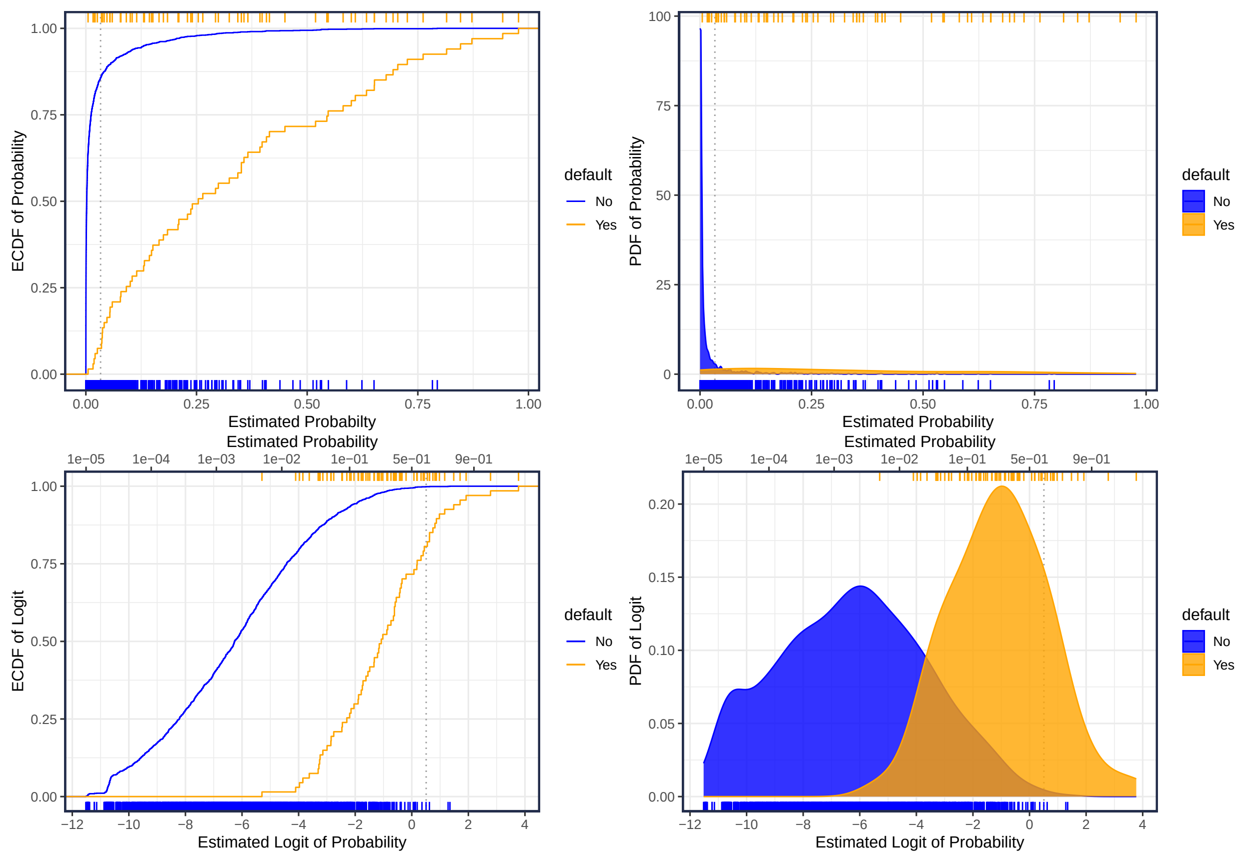
```
#: train/test split
set.seed(2019)
test = sample(nrow(Default), size=2000)
train = -test
```

1.2 Logistic Regression

```
#: fit logistic regression model on training data
fit_lr = glm(default~student + balance + income, family='binomial',
             data = Default[train, ])
```

1.3 Predictive Performance

```
#: table of predictions and true values
tbl_lr = Default[test,]  %>%
  mutate(
    g = factor(y, c(0,1)),
    p_hat = predict(fit_lr, ., type="response"),
    gamma_hat = predict(fit_lr, ., type="link"),
  )
```



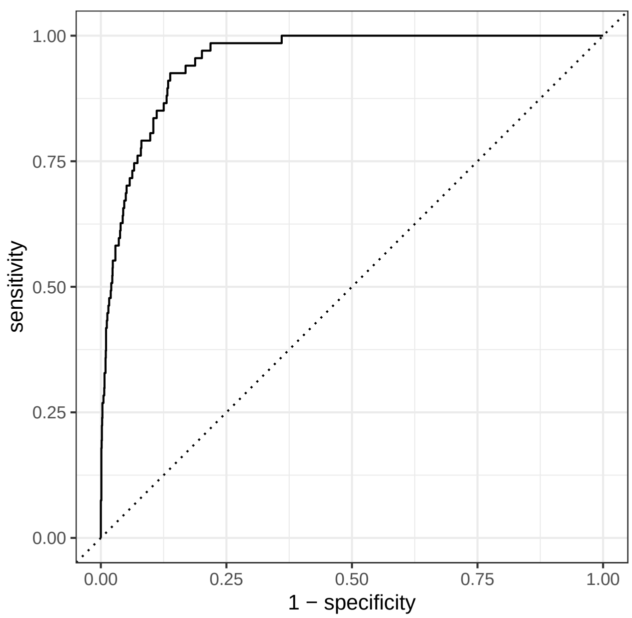

```r
#: Threshold of 1/2
tbl_lr %>%
  mutate(Y_hat = ifelse(p_hat > 1/2, 1L, 0L)) %>%
  count(y, Y_hat)
#> # A tibble: 4 x 3
#>       y Y_hat     n
#>   <int> <int> <int>
#> 1     0     0  1922
#> 2     0     1    11
#> 3     1     0    48
#> 4     1     1    19
```

```r
#: Threshold of 1/4
tbl_lr %>%
  mutate(Y_hat = ifelse(p_hat > 1/4, 1L, 0L)) %>%
  count(y, Y_hat)
#> # A tibble: 4 x 3
#>       y Y_hat     n
#>   <int> <int> <int>
#> 1     0     0  1891
#> 2     0     1    42
#> 3     1     0    33
#> 4     1     1    34
```

```r
library(yardstick)
roc_curve(tbl_lr, truth = g, p_hat, event_level="second") %>%
  autoplot()
```

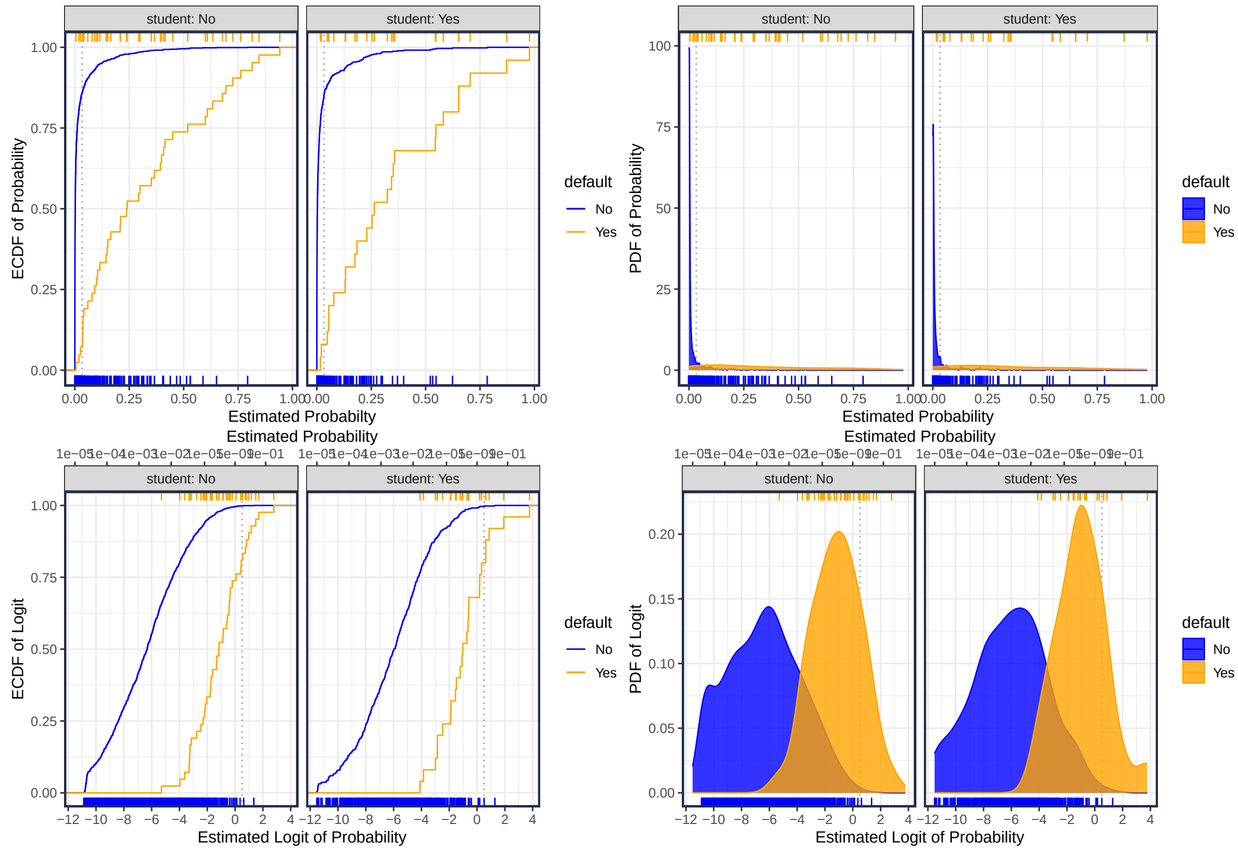
thres	$\hat{P}$	$\hat{N}$	FP	FN
0.1	178	1822	128	17
0.2	101	1899	62	28
0.3	59	1941	29	37
0.4	39	1961	17	45
0.5	30	1970	11	48
0.6	18	1982	4	53
0.7	10	1990	2	59
0.8	5	1995	0	62
0.9	2	1998	0	65

n	log_loss	brier	mae	auroc
2000	0.082	0.023	0.046	0.951



1.4 Performance by Group

All performance scores can also be assessed at the group level (i.e., over subsets of the features). Here we explore the predicted output by `Student` status.




```
#: Threshold of 1/2
tbl_lr %>%
  mutate(Y_hat = ifelse(p_hat > 1/2, 1L, 0L)) %>%
  count(student, y, Y_hat)
#> # A tibble: 8 x 4
#>   student     y Y_hat     n
#>   <fct>   <int> <int> <int>
#> 1 No          0     0  1356
#> 2 No          0     1     6
#> 3 No          1     0    31
#> 4 No          1     1    11
#> 5 Yes         0     0   566
#> 6 Yes         0     1     5
#> # i 2 more rows
```

```
#: Threshold of 1/4
tbl_lr %>%
  mutate(Y_hat = ifelse(p_hat > 1/4, 1L, 0L)) %>%
  count(student, y, Y_hat)
#> # A tibble: 8 x 4
#>   student     y Y_hat     n
#>   <fct>   <int> <int> <int>
#> 1 No          0     0  1334
#> 2 No          0     1    28
#> 3 No          1     0    22
```

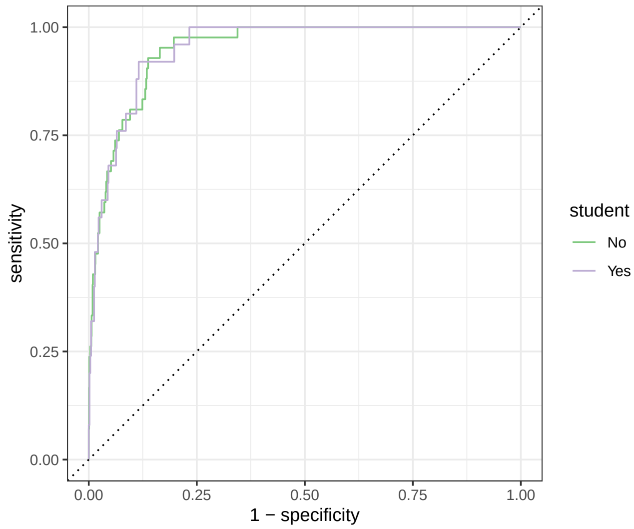
```
#> 4 No            1      1     20
#> 5 Yes           0      0    557
#> 6 Yes           0      1     14
#> # i 2 more rows
```

thres	student	$\hat{P}$	$\hat{N}$	FP	FN
0.1	No	114	1290	83	11
0.2	No	63	1341	39	18
0.3	No	38	1366	20	24
0.4	No	26	1378	12	28
0.5	No	17	1387	6	31
0.6	No	11	1393	2	33
0.7	No	6	1398	1	37
0.8	No	3	1401	0	39
0.9	No	1	1403	0	41

thres	student	$\hat{P}$	$\hat{N}$	FP	FN
0.1	Yes	64	532	45	6
0.2	Yes	38	558	23	10
0.3	Yes	21	575	9	13
0.4	Yes	13	583	5	17
0.5	Yes	13	583	5	17
0.6	Yes	7	589	2	20
0.7	Yes	4	592	1	22
0.8	Yes	2	594	0	23
0.9	Yes	1	595	0	24

student	n	log_loss	brier	mae	auroc
No	1404	0.076	0.021	0.042	0.949
Yes	596	0.096	0.028	0.054	0.951

```
library(yardstick)
tbl_lr %>% group_by(student) %>%
  roc_curve(truth = g, p_hat, event_level="second") %>%
  autoplot() + scale_color_brewer(type = "qual")
```


sensitivity
1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
1 − specificity
student
No
Yes

2 Predictive Bias and Calibration

A risk model is said to be *calibrated* if the predicted probabilities are equal to the true risk (probabilities).

$$\Pr(Y = 1 \mid \hat{p}(x) = p) = p \qquad \text{for all } p$$

To evaluate the calibration of a model's predictions, we need to estimate the proportion of the observations with $Y = 1$ and $\hat{p} \approx p$.

Calibration *plots* can be used to measure drift, fairness, and model/algorithmic bias. We could for example use binning (regressograms/histograms), kNN, smoothing, or isotonic regression.

2.1 Binning

Here is an example of binning. I'll partition the predictions such that there are 10 groups of equal width.

```
tbl_grp = tbl_lr %>%
  mutate(grp = cut_width(p_hat, width = .1, boundary = 1)) %>%
  group_by(grp) %>%
  summarize(
    n = n(),
    lower = min(p_hat),
    upper = max(p_hat),
    p_hat = mean(p_hat),
    n_y = sum(y),
    # bayesian (uniform prior)
    p_y = (n_y+1) / (n+2), # posterior mean
    beta_lower = qbeta(.025, n_y+1, n-n_y+1),
    beta_upper = qbeta(.975, n_y+1, n-n_y+1),
    # frequentist
    p_y_bar = mean(y),
    moe = 1.96*sqrt(p_y_bar*(1-p_y_bar)/n)
  )
```

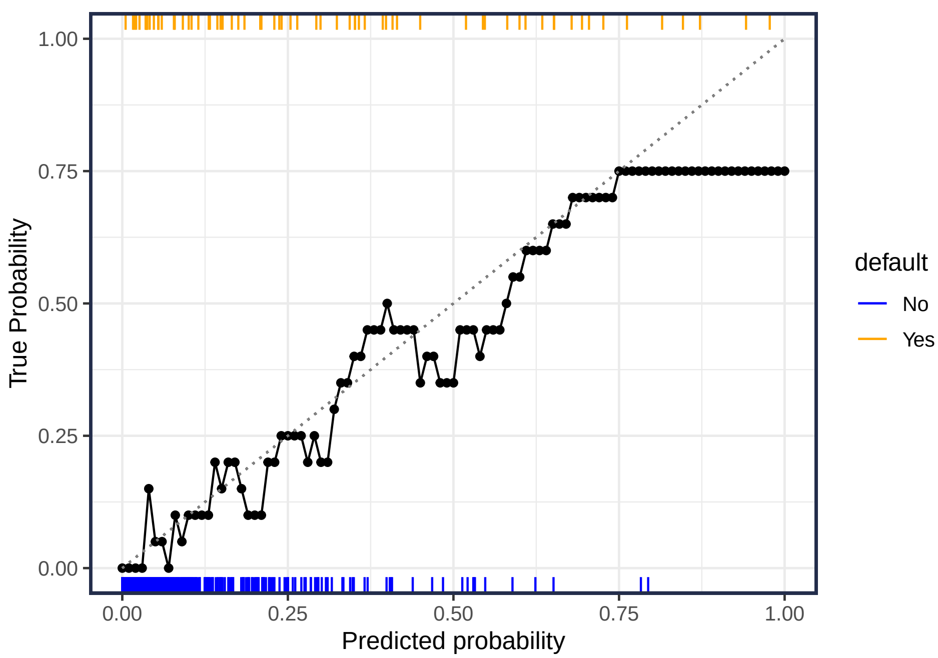
grp	n	lower	upper	p_hat	n_y	p_y	beta_lower	beta_upper	p_y_bar	moe
[0,0.1]	1822	0.000	0.100	0.009	17	0.010	0.006	0.015	0.009	0.004
(0.1,0.2]	77	0.100	0.199	0.141	11	0.152	0.082	0.238	0.143	0.078
(0.2,0.3]	42	0.202	0.299	0.242	9	0.227	0.118	0.360	0.214	0.124
(0.3,0.4]	20	0.301	0.399	0.348	8	0.409	0.218	0.616	0.400	0.215
(0.4,0.5]	9	0.404	0.484	0.431	3	0.364	0.122	0.652	0.333	0.308
(0.5,0.6]	12	0.513	0.600	0.546	5	0.429	0.192	0.684	0.417	0.279
(0.6,0.7]	8	0.609	0.694	0.649	6	0.700	0.400	0.925	0.750	0.300
(0.7,0.8]	5	0.705	0.794	0.754	3	0.571	0.223	0.882	0.600	0.429
(0.8,0.9]	3	0.815	0.872	0.845	3	0.800	0.398	0.994	1.000	0.000
(0.9,1]	2	0.942	0.978	0.960	2	0.750	0.292	0.992	1.000	0.000

```
tbl_grp %>%
  ggplot(aes(p_hat, p_y)) +
    geom_rect(aes(xmin=lower, xmax=upper,
                  ymin=beta_lower,
                  ymax=beta_upper)
             ) +
  geom_point() +
```

```
  geom_linerange(aes(xmin=lower, xmax=upper)) +
  geom_segment(x=0,xend=1, y=0, yend=1, linetype = 3, color = "grey50") +
  labs(x = "Predicted probability", y = "True Probability") +
  geom_rug(data = . %>% filter(y==0),
           aes(x=p_hat, color=default), sides="b",
           inherit.aes = FALSE) +
  geom_rug(data = . %>% filter(y==1),
           aes(x=p_hat,color=default), sides="t",
           inherit.aes = FALSE)  +
  scale_color_manual(values=c(Yes="orange", No="blue"))
#> Error in `geom_rug()`:
#> ! Problem while computing layer data.
#> i Error occurred in the 5th layer.
#> Caused by error in `filter()`:
#> i In argument: `y == 0`.
#> Caused by error:
#> ! object 'y' not found
```

2.2 Nearest Neighbor

K-nearest neighbor:



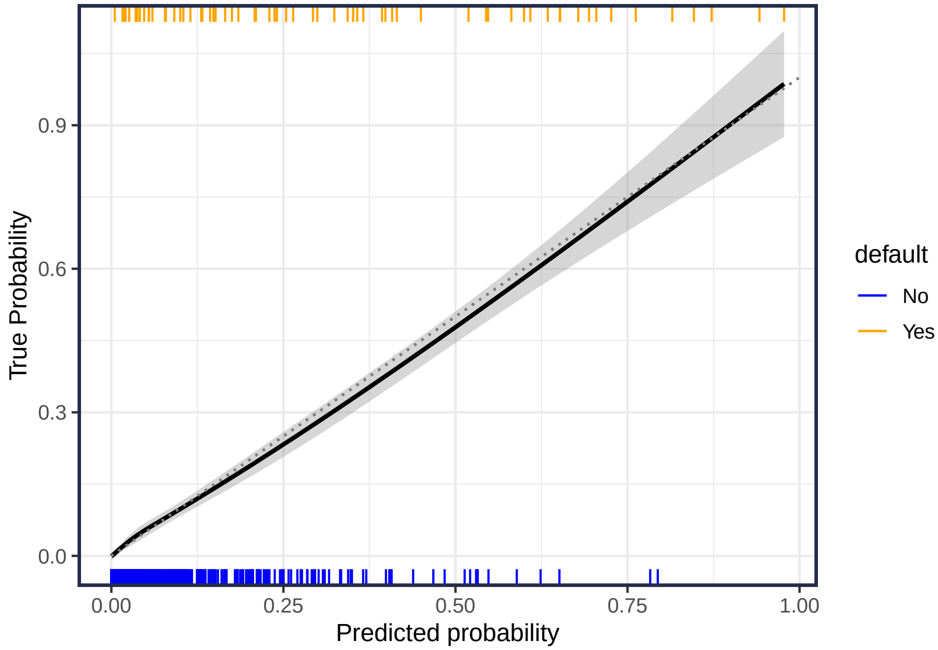
But knn is not expected to work well at the edges ($\hat{p}$ close to 0 or 1).

2.3 Smoothing splines

Using smoothing splines (brier score loss):

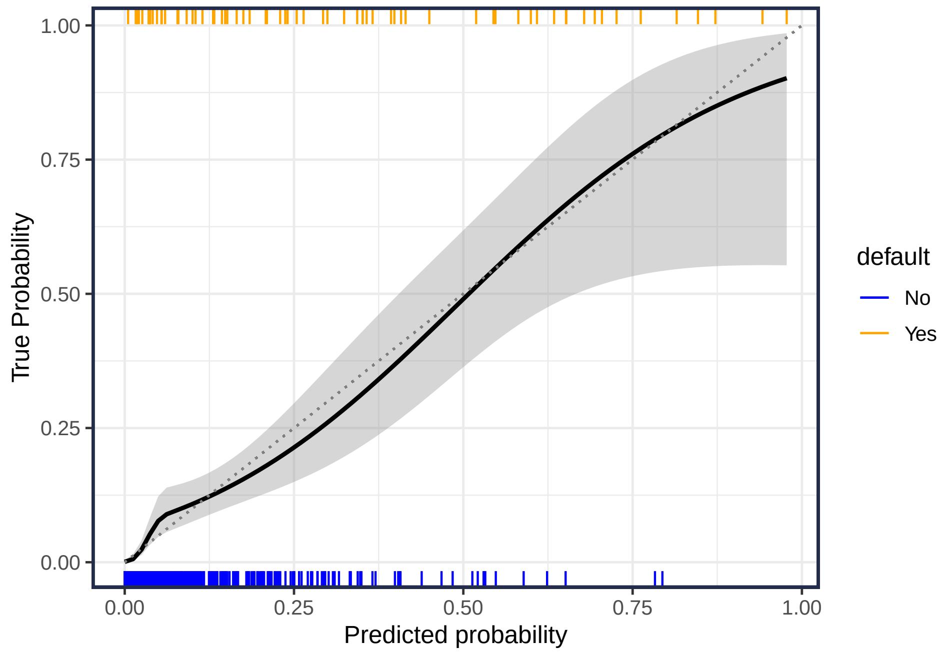
```
#: The Regular geom_smooth() uses an MSE (brier score) loss
tbl_lr %>%
  ggplot(aes(p_hat)) +
  geom_smooth(aes(y = y), color="black") +
  geom_segment(x=0,xend=1, y=0, yend=1, linetype = 3, color = "grey50") +
  geom_rug(data = . %>% filter(y==0), aes(color=default), sides="b") +
  geom_rug(data = . %>% filter(y==1), aes(color=default), sides="t") +
```

```
  scale_color_manual(values=c(Yes="orange", No="blue")) +
  labs(x = "Predicted probability", y = "True Probability")
```



Using smoothing splines (log-loss):

```
#: Here we use family argument in geom_smooth() to force log-loss
tbl_lr %>%
  ggplot(aes(p_hat)) +
  geom_smooth(aes(y = y),
              method = "gam",
              method.args = list(family = binomial()),
              color="black") +
  geom_segment(x=0,xend=1, y=0, yend=1, linetype = 3, color = "grey50") +
  geom_rug(data = . %>% filter(y==0), aes(color=default), sides="b") +
  geom_rug(data = . %>% filter(y==1), aes(color=default), sides="t") +
  scale_color_manual(values=c(Yes="orange", No="blue")) +
  labs(x = "Predicted probability", y = "True Probability")
```



2.4 Summary

It looks like the logistic regression model is decently calibrated for *overall* calibration (i.e., aggregated). The predicted probabilities are suitably close to the observed proportions in a test set. That is, with 2000 test observations there is not enough evidence to suggest clear predictive bias.

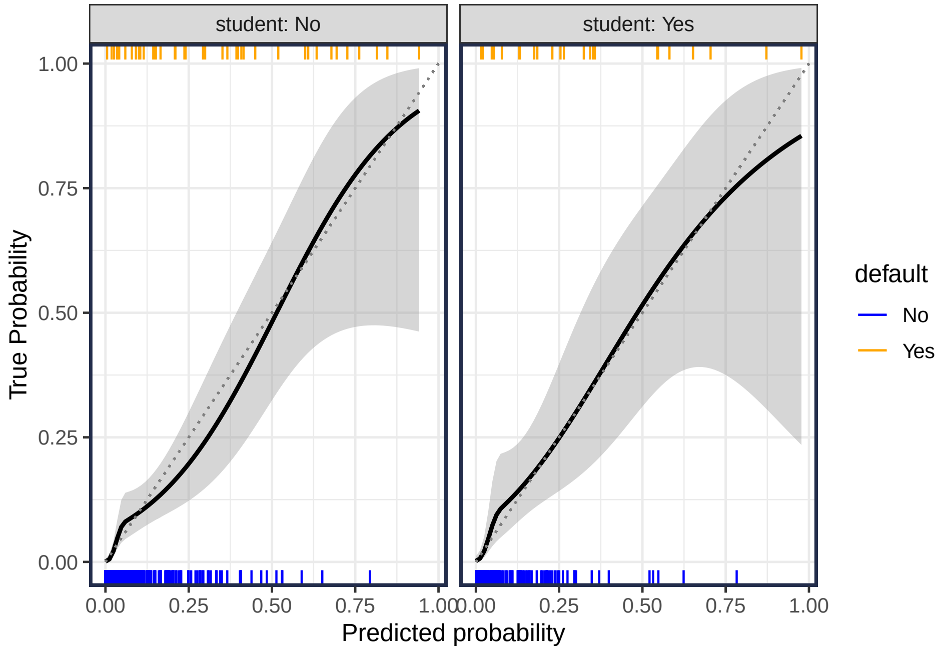
But, does predictive performance and calibration hold for all groups?

2.5 Calibration by group

Consider comparing the predictive performance of our models for Students and Non-Students.

$$\Pr(Y = 1 \mid \hat{p}(x) = p, X = x) = p \qquad \text{for all } p \text{ and } x$$

```
tbl_lr %>%
  ggplot(aes(p_hat)) +
  geom_smooth(aes(y = y),
              method = "gam",
              method.args = list(family = binomial()),
              color="black") +
  geom_segment(x=0,xend=1, y=0, yend=1, linetype = 3, color = "grey50") +
  labs(x = "predicted probability", y = "true - predicted") +
  geom_rug(data = . %>% filter(y==0), aes(color=default), sides="b") +
  geom_rug(data = . %>% filter(y==1), aes(color=default), sides="t") +
  scale_color_manual(values=c(Yes="orange", No="blue")) +
  labs(x = "Predicted probability", y = "True Probability") +
  facet_wrap(~student, labeller = label_both) # <--- Faceting
```


student: No
student: Yes
True Probability
1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
Predicted probability
default
No
Yes

3 Testing for Calibration

The main idea is to test the (null) hypothesis that

$$\Pr(Y = 1 \mid \hat{p}(x) = p) = p \qquad \text{for all } p$$

or equivalently,

$$\Pr(Y = 1 \mid \hat{p}(x)) - \hat{p}(x) = 0 \qquad \text{for all } \hat{p}$$

The plots shown above visually explore the hypothesis. We can also take a model-based approach.

3.1 Logistic Regression

For a calibrated model the estimated $\hat{p}(x)$ should be close to the true $p(x)$,

$$p(x) \approx \hat{p}(x)$$
$$\text{logit } p(x) \approx \text{logit } \hat{p}(x)$$

To test this, we introduce a bias term $b(x)$ and test for $b(x) = 0 \; \forall x$.

$$\text{logit } p(x) = b(x) + \text{logit } \hat{p}(x)$$

Notice the above expression is the same form as logistic regression.

This means we can use logistic regression to test for mis-calibration (predictive bias). To do this, use logit $\hat{p}(x)$ as an *offset* in the logistic regression model. An *offset* is a term that has a fixed weight/coefficient of 1.

We also need to specify the form of the bias term before we can test it. We give a few examples below.

3.2 Linear bias

To check for linear deviation, we specify the bias term as $b(x) = \beta_0 + \beta_1 \text{logit } \hat{p}(x)$.

$$\text{logit } p(x) = \beta_0 + \beta_1 \text{logit } \hat{p}(x) + (\text{logit } \hat{p}(x))$$

Fit on a hold-out set, and check how far β_0 and β_1 are from 0.

```
calibrated = glm(y~gamma_hat + offset(gamma_hat),
    family = binomial,
    data = tbl_lr)
# Note that gamma_hat = logit(p_hat)

calibrated %>% summary()
#>
#> Call:
#> glm(formula = y ~ gamma_hat + offset(gamma_hat), family = binomial,
#>     data = tbl_lr)
#>
#> Coefficients:
#>                Estimate Std. Error z value Pr(>|z|)
```

```
#> (Intercept) -0.02237    0.22027   -0.10     0.92
#> gamma_hat    0.00589    0.09235    0.06     0.95
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>     Null deviance: 326.02  on 1999  degrees of freedom
#> Residual deviance: 326.02  on 1998  degrees of freedom
#> AIC: 330
#>
#> Number of Fisher Scoring iterations: 8
```

No significance suggests not enough evidence to reject null of no bias against linear bias.

3.3 Non-linear bias

We can introduce splines to detect non-linear deviations:

```
glm(y~splines::bs(gamma_hat, df = 3) + offset(gamma_hat),
    family = binomial,
    data = tbl_lr) %>%
  summary()
#> Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
#>
#> Call:
#> glm(formula = y ~ splines::bs(gamma_hat, df = 3) + offset(gamma_hat),
#>     family = binomial, data = tbl_lr)
#>
#> Coefficients:
#>                                 Estimate Std. Error z value Pr(>|z|)
#> (Intercept)                        -27.0       22.5   -1.20     0.23
#> splines::bs(gamma_hat, df = 3)1     43.7       36.7    1.19     0.23
#> splines::bs(gamma_hat, df = 3)2     18.4       15.3    1.21     0.23
#> splines::bs(gamma_hat, df = 3)3     30.5       26.1    1.17     0.24
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>     Null deviance: 326.02  on 1999  degrees of freedom
#> Residual deviance: 323.50  on 1996  degrees of freedom
#> AIC: 331.5
#>
#> Number of Fisher Scoring iterations: 12
```

Again, no significance suggests not enough evidence to reject null of no bias against non-linear bias (although we could try other smoothing).

3.4 Bias in predictors

We can also see if the predictions should be adjusted for regions in features space.

Including an interaction term too.

```
glm(y ~ student + student:gamma_hat +  offset(gamma_hat),
    family = binomial,
    data = tbl_lr) %>%
  summary()
#>
#> Call:
#> glm(formula = y ~ student + student:gamma_hat + offset(gamma_hat),
```

```
#>     family = binomial, data = tbl_lr)
#>
#> Coefficients:
#>                      Estimate Std. Error z value Pr(>|z|)
#> (Intercept)          -0.07335    0.27616   -0.27     0.79
#> studentYes            0.14052    0.45795    0.31     0.76
#> studentNo:gamma_hat   0.00509    0.11489    0.04     0.96
#> studentYes:gamma_hat  0.00368    0.15511    0.02     0.98
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>     Null deviance: 326.02  on 1999  degrees of freedom
#> Residual deviance: 325.81  on 1996  degrees of freedom
#> AIC: 333.8
#>
#> Number of Fisher Scoring iterations: 8
```

```
glm(y ~ splines::bs(balance, 3) +  offset(gamma_hat),
    family = binomial,
    data = tbl_lr) %>%
  summary()
#>
#> Call:
#> glm(formula = y ~ splines::bs(balance, 3) + offset(gamma_hat),
#>     family = binomial, data = tbl_lr)
#>
#> Coefficients:
#>                          Estimate Std. Error z value Pr(>|z|)
#> (Intercept)                -15.55      15.59   -1.00     0.32
#> splines::bs(balance, 3)1    26.26      26.97    0.97     0.33
#> splines::bs(balance, 3)2     9.37       9.26    1.01     0.31
#> splines::bs(balance, 3)3    18.40      19.45    0.95     0.34
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>     Null deviance: 326.02  on 1999  degrees of freedom
#> Residual deviance: 324.29  on 1996  degrees of freedom
#> AIC: 332.3
#>
#> Number of Fisher Scoring iterations: 12
```

```
glm(y ~ splines::bs(income, 3) +  offset(gamma_hat),
    family = binomial,
    data = tbl_lr) %>%
  summary()
#>
#> Call:
#> glm(formula = y ~ splines::bs(income, 3) + offset(gamma_hat),
#>     family = binomial, data = tbl_lr)
#>
#> Coefficients:
#>                         Estimate Std. Error z value Pr(>|z|)
#> (Intercept)                0.435      1.038    0.42     0.68
#> splines::bs(income, 3)1   -0.756      2.829   -0.27     0.79
#> splines::bs(income, 3)2   -0.299      1.646   -0.18     0.86
#> splines::bs(income, 3)3   -1.104      2.564   -0.43     0.67
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
```

```
#>     Null deviance: 326.02  on 1999  degrees of freedom
#> Residual deviance: 325.07  on 1996  degrees of freedom
#> AIC: 333.1
#>
#> Number of Fisher Scoring iterations: 7
```

The logistic regression model appears well-calibrated. This isn't surprising as the log-loss metric encourages good calibration.

However, we could still get poor calibration due to over-fitting, drift, or mis-specification.

4 SVM Calibration

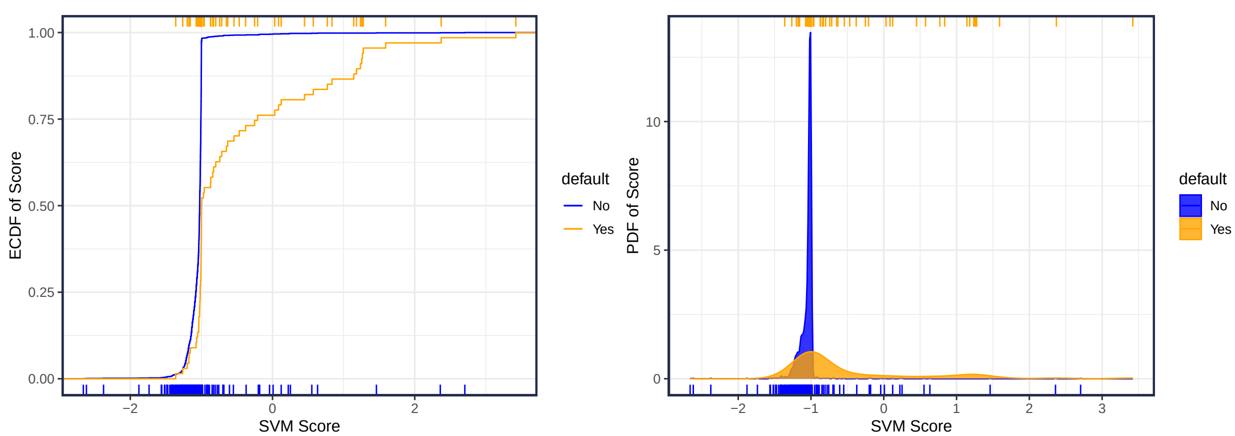
4.1 SVM Modeling

```
library(kernlab)
#: Radial basis kernel
fit_svm = ksvm(default~student + balance + income,
               data = Default[train, ],
               scaled = TRUE,         # be sure to scale the predictors
               kernel = "rbfdot",     # kernel
               sigma = .01, C = 100, # tuning parameters
               )
```

```
#: table of predictions and true values
tbl_svm = Default[test,]  %>%
  mutate(
    g = factor(y, c(0,1)),
    score = predict(fit_svm, ., type = "decision")[,1],
    class = predict(fit_svm, ., "response"),
  )
```

SVMs don't naturally output a probability, but rather a score (or `decision`) value that indicates the observations' distance to the decision boundary. We called the SVM score output $\hat{f}(x)$ in the class notes.

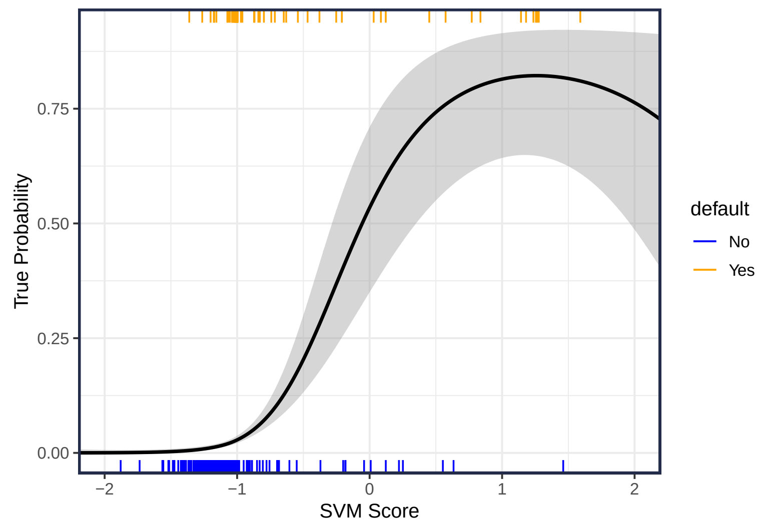
default	y	student	balance	income	g	score	class
No	0	Yes	1026.1	16431	0	-1.023	No
No	0	Yes	1378.2	20120	0	-1.002	No
No	0	No	487.1	55459	0	-1.156	No
No	0	Yes	1252.1	13861	0	-0.999	No
No	0	No	0.0	30208	0	-1.004	No
No	0	No	921.3	25350	0	-1.046	No



Let's check out how well the SVM scores map to a probability. Here I'll go with the smoothing spline approach (log-loss):

```
#: Here we use family argument in geom_smooth() to force log-loss
tbl_svm %>%
  ggplot(aes(score)) +
  geom_smooth(aes(y = y), n=1000,
              method = "gam",
              method.args = list(family = binomial()),
```

```
              color="black") +
  geom_rug(data = . %>% filter(y==0), aes(color=default), sides="b") +
  geom_rug(data = . %>% filter(y==1), aes(color=default), sides="t") +
  scale_color_manual(values=c(Yes="orange", No="blue")) +
  labs(x = "SVM Score", y = "True Probability") +
  scale_x_continuous(breaks = seq(-5, 5, by=1)) +
  coord_cartesian(xlim = c(-2, 2))
```



4.2 SVM Calibration

Let $\hat{f}_i = \hat{f}(x_i)$ be the score output from an SVM model. Platt's idea was to fit a logistic regression model using $\hat{f}(x)$ as the predictor variable. The *calibrated probabilities* are the predictions from this model. That is:

$$\text{logit}(p(x)) = \beta_0 + \beta_1 \hat{f}(x)$$

or

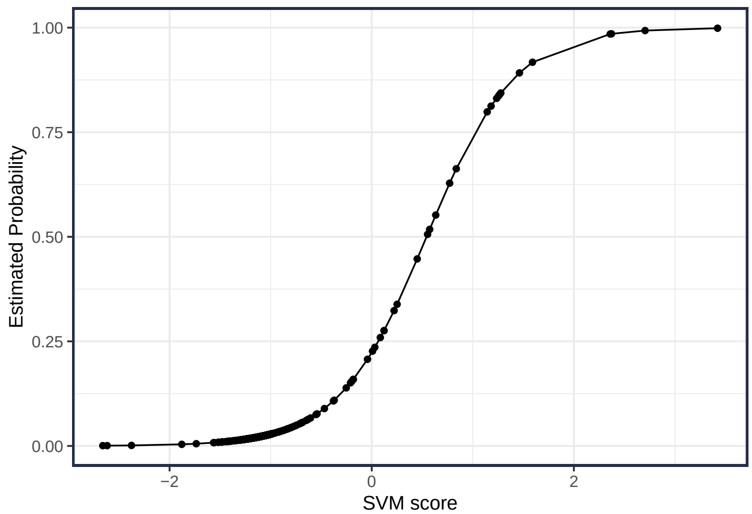
$$p(x) = 1/\left(1 + e^{-(\beta_0 + \beta_1 \hat{f}(x))}\right)$$

```
calibrated_svm = glm(y~score, family="binomial", data = tbl_svm)
summary(calibrated_svm)
#>
#> Call:
#> glm(formula = y ~ score, family = "binomial", data = tbl_svm)
#>
#> Coefficients:
#>              Estimate Std. Error z value Pr(>|z|)
#> (Intercept)    -1.246      0.294   -4.24  2.2e-05 ***
#> score           2.297      0.289    7.95  1.9e-15 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>     Null deviance: 586.82  on 1999  degrees of freedom
#> Residual deviance: 492.90  on 1998  degrees of freedom
```

```
#> AIC: 496.9
#>
#> Number of Fisher Scoring iterations: 6
```

```
tbl_svm = tbl_svm %>%
  mutate(
    p_hat = predict(calibrated_svm, ., type="response"),
    gamma_hat = log(p_hat) - log(1-p_hat)
  )
```

```
tbl_svm %>%
  ggplot(aes(score, p_hat)) +
  geom_point() +
  geom_line() +
  labs(x = "SVM score", y = "Estimated Probability")
```



Notice that when the SVM score is zero ($\hat{f}(x) = 0$), the estimated probability is 0.25; this is pretty far from the expected 0.50.

Sketch of SVM Calibration System

4.2.1 Testing Calibration

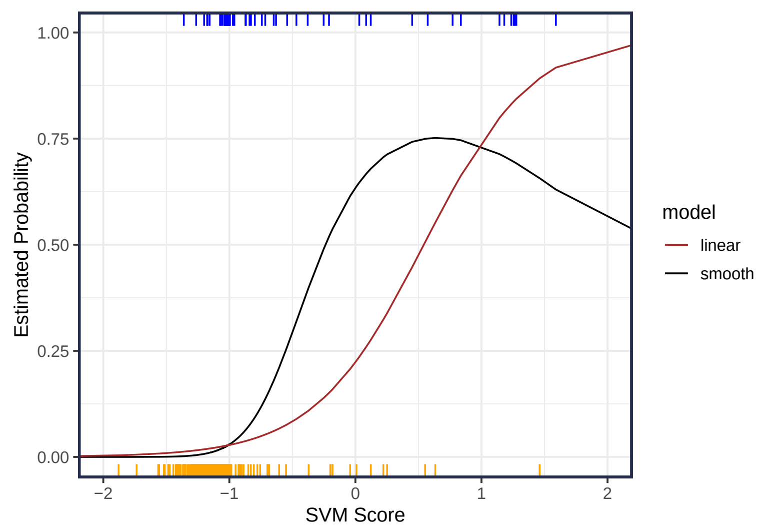
How well did Platt's method work? Is the 2 parameter logistic transformation sufficiently complex?

We can for test this, just like we did earlier. However, we are going to see a problem with using splines!

```
calibrated_svm_2 = glm(y~splines::bs(score, df=3),
                       family="binomial", data = tbl_svm)
summary(calibrated_svm_2)
#>
#> Call:
#> glm(formula = y ~ splines::bs(score, df = 3), family = "binomial",
#>     data = tbl_svm)
#>
#> Coefficients:
#>                             Estimate Std. Error z value Pr(>|z|)
#> (Intercept)                   -24.41       4.51   -5.41  6.4e-08 ***
#> splines::bs(score, df = 3)1    39.84       9.89    4.03  5.7e-05 ***
#> splines::bs(score, df = 3)2    19.36       2.33    8.31  < 2e-16 ***
#> splines::bs(score, df = 3)3    25.87       5.87    4.41  1.0e-05 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>     Null deviance: 586.82  on 1999  degrees of freedom
#> Residual deviance: 463.51  on 1996  degrees of freedom
#> AIC: 471.5
#>
#> Number of Fisher Scoring iterations: 7
```

Notice that the bspline with 3 df (4 edf with intercept) has statistically significant terms. But what does this non-linear calibration look like?

```r
tbl_svm %>%
  ggplot(aes(score)) +
  geom_line(aes(y = p_smooth, color = "smooth")) +
  geom_line(aes(y = p_hat, color = "linear")) +
  geom_rug(data = . %>% filter(y==0), color = "orange", sides="b") +
  geom_rug(data = . %>% filter(y==1), color = "blue", sides="t") +
  scale_color_manual(name = "model", values=c(smooth="black", linear="brown")) +
  labs(x = "SVM Score", y = "Estimated Probability") +
  scale_x_continuous(breaks = seq(-5, 5, by=1)) +
  coord_cartesian(xlim = c(-2, 2))
```



That dip doesn't look good! It suggests a non-monotonic transformation which is not appealing. It would mean an individual that SVM classifies as a default ($\hat{f} < 0$) could actually be given a higher probability that someone that SVM scored higher!

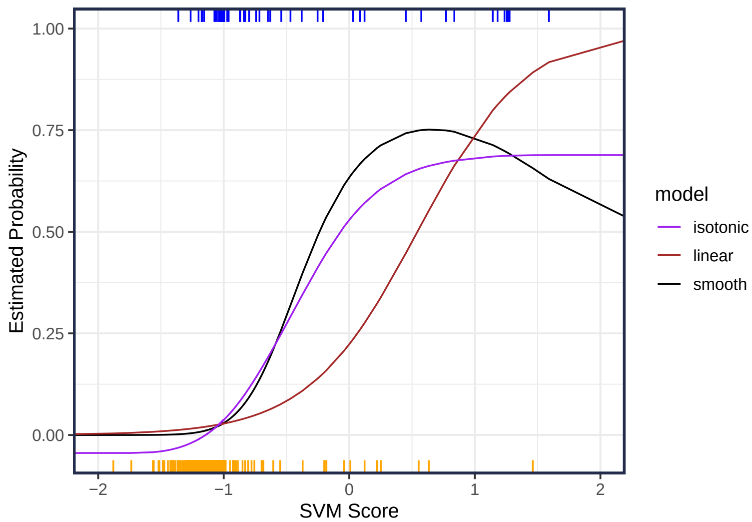
4.2.2 Isotonic Calibration

Enter isotonic (or monotonic) splines. These are special splines that produce a monotonic prediction; something perfect for our application.

```r
library(scam)
iso = scam(y~s(score, bs="mpi"), data=tbl_svm)
summary(iso)
#>
#> Family: gaussian
#> Link function: identity
#>
#> Formula:
#> y ~ s(score, bs = "mpi")
#> <environment: 0x559268a2a3d0>
#>
#> Parametric coefficients:
#>             Estimate Std. Error t value Pr(>|t|)
#> (Intercept)  -0.0443     0.0080   -5.54  3.5e-08 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> Approximate significance of smooth terms:
#>           edf Ref.df    F p-value
```

```
#> s(score)    3       3 157  <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> R-sq.(adj) =  0.1905   Deviance explained = 19.2%
#> GCV score = 0.026274  Scale est. = 0.026222  n = 2000
```

```
tbl_svm %>%
  ggplot(aes(score)) +
  geom_line(aes(y = p_smooth, color = "smooth")) +
  geom_line(aes(y = p_hat, color = "linear")) +
  geom_line(aes(y = p_iso, color = "isotonic")) +
  geom_rug(data = . %>% filter(y==0), color = "orange", sides="b") +
  geom_rug(data = . %>% filter(y==1), color = "blue", sides="t") +
  scale_color_manual(name = "model",
                     values=c(smooth="black", linear="brown",
                              isotonic = "purple")) +
  labs(x = "SVM Score", y = "Estimated Probability") +
  scale_x_continuous(breaks = seq(-5, 5, by=1)) +
  coord_cartesian(xlim = c(-2, 2))
```



It does appear that the more complex isotonic smoother deviates from the logistic, but with only 3 edf in the smoothing portion, it isn't too different.

4.2.3 Hold-out data

Calibration with Validation Data

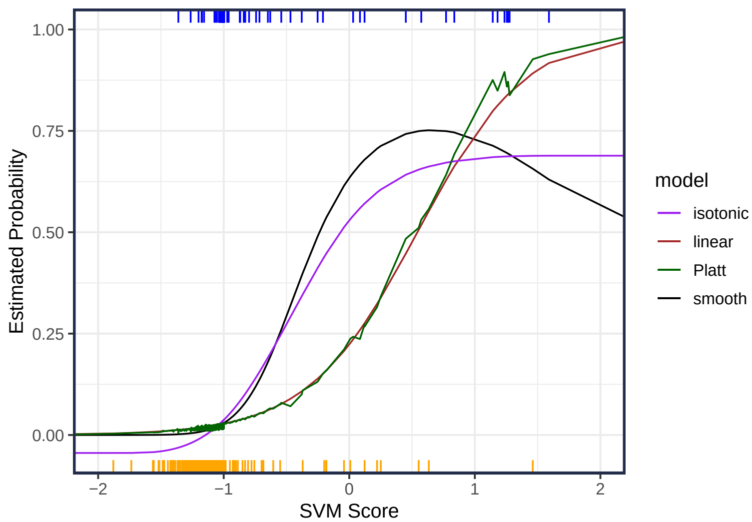
4.2.4 Built-in Calibration

Set `prob.model=TRUE` in the `ksvm()` function to get probability estimates. Note that this uses 3-fold cross-validation to predict out-of-sample scores. Then uses weighted logistic regression to estimate the calibration function.

```
library(kernlab)
#: Radial basis kernel
fit_svm = ksvm(default~student + balance + income,
               data = Default[train, ],
               prob.model = TRUE, # ** Need to set to TRUE to get probabilities
               scaled = TRUE,        # be sure to scale the predictors
               kernel = "rbfdot",    # kernel
               sigma = .01, C = 100, # tuning parameters
               )
```

```
#: table of predictions and true values
tbl_svm = tbl_svm %>%
  mutate(
    p_ksvm = predict(fit_svm, ., type = "probabilities")[,"Yes"]
  )
```

```r
tbl_svm %>%
  ggplot(aes(score)) +
  geom_line(aes(y = p_smooth, color = "smooth")) +
  geom_line(aes(y = p_hat, color = "linear")) +
  geom_line(aes(y = p_iso, color = "isotonic")) +
  geom_line(aes(y = p_ksvm, color = "Platt")) +
  geom_rug(data = . %>% filter(y==0), color = "orange", sides="b") +
  geom_rug(data = . %>% filter(y==1), color = "blue", sides="t") +
  scale_color_manual(name = "model",
                     values=c(smooth="black", linear="brown",
                              isotonic = "purple", Platt="darkgreen")) +
  labs(x = "SVM Score", y = "Estimated Probability") +
  scale_x_continuous(breaks = seq(-5, 5, by=1)) +
  coord_cartesian(xlim = c(-2, 2))
```



It matches pretty closely to just implementing logistic regression on the in-sample data.