Support Vector Machines

SYS 6018 | Spring 2023

svm.pdf

Contents

1 Support Vector Machines (SVM) Introduction

1.1 Required R Packages

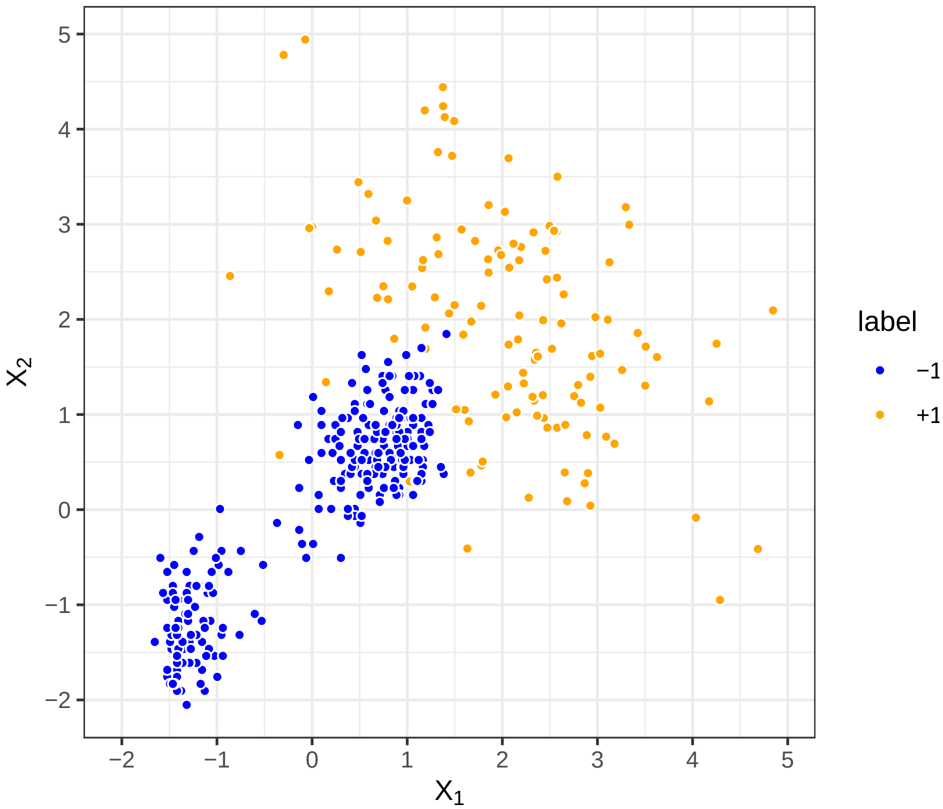
We will be using the R packages of:

- `tidyverse` for data manipulation and visualization
- `e1071` for the `svm()` functions

1.2 Example

Goal: find *best* line(s)/curve(s) to separate the two classes.

```
#> Error in rmvnorm(n1, mean = mu1, sigma = sigma1): unused argument (mean = mu1)
#> Error in rmvnorm(n2, mean = mu2, sigma = sigma2): unused argument (mean = mu2)
```



1.3 SVM as Loss + Penalty

Training Data: $\{(\tilde{y}_i, \mathbf{x}_i)\}_{i=1}^n$

- $\tilde{y}_i \in \{-1, +1\}$
- $\mathbf{x}_i^\mathsf{T} = [x_{i1}, x_{i2}, \ldots, x_{in}] \in \mathbb{R}^p$

Predictor Function: $f(x)$

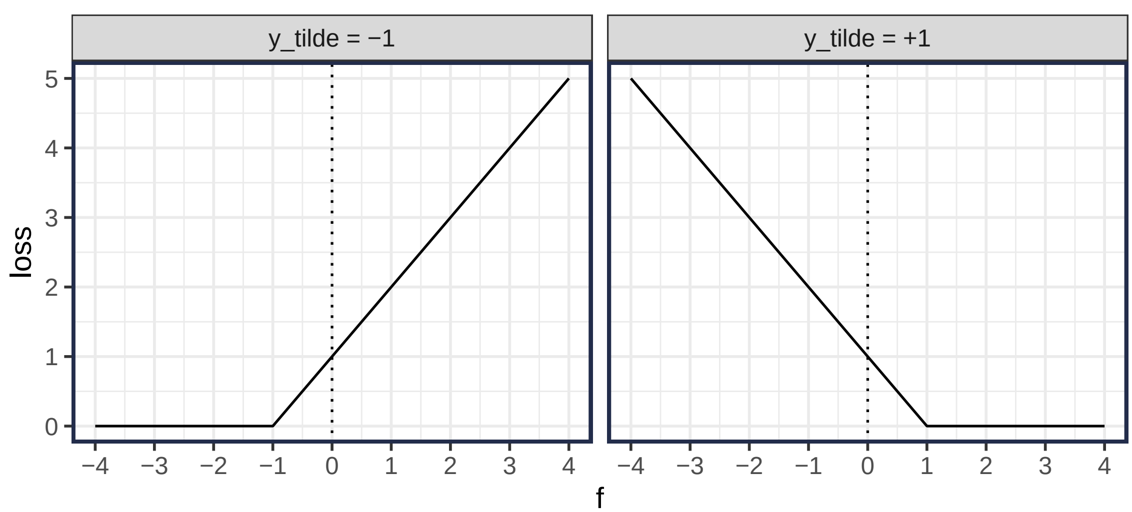
- Linear: $f(\mathbf{x}; \beta) = \beta_0 + \sum_{j=1}^p x_j \beta_j$
- Basis Expansion: $f(\mathbf{x}; \beta) = \beta_0 + \sum_{j=1}^d h_j(\mathbf{x}) \beta_j$
  - $h_j(\mathbf{x})$ transforms the raw x vector
  - Polynomial example: $h_1(\mathbf{x}) = x_1$, $h_2(\mathbf{x}) = x_1^2$, $h_3(\mathbf{x}) = x_2$, $h_4(\mathbf{x}) = x_2^2$, $h_5(\mathbf{x}) = x_1 x_2$
  - This is the connection to *kernels* that we will discuss later
- Let $f_i = f(\mathbf{x}_i)$

Classification:

- If $\hat{f}_i \geq 0$, then label as class $+1$
- If $\hat{f}_i < 0$, then label as class -1

Loss Function: Hinge Loss

$$L(\tilde{y}_i, f_i) = \max\{0, 1 - \tilde{y}_i f_i\}$$



Penalty Function: Ridge Penalty

$$\begin{aligned} P_\lambda(\beta) &= \frac{\lambda}{2} \sum_{j=1}^d \beta_j^2 \\ &= \lambda \|\beta\|^2 / 2 \end{aligned}$$

- This should have you thinking that the $\mathbf{x}$'s should be scaled!

Summary of SVM

1. Estimate *model parameters* β

$$\begin{aligned}\hat{\beta}_\lambda &= \arg\min_\beta \left\{ \sum_{i=1}^n \max\{0, 1 - \tilde{y}_i f_i(\beta)\} + \lambda \|\beta\|^2 / 2 \right\} \\ &= \arg\min_\beta \{\text{Hinge Loss}(\beta) + \lambda \text{ Penalty}(\beta)\}\end{aligned}$$

2. Label Class $+1$ if $\hat{f}_i \geq 0$, else label Class -1
   - This implicitly assumes a 0-1 loss (or equal cost FP and FN)
   - More generally, use threshold t that considers the costs of FP and FN
3. **Tuning Parameters**: besides the λ, SVM will also have tuning parameters related to the kernels (more to come on this).

1.4 SVM vs. Logistic Regression

The *linear* SVM is actually very similar to Logistic Regression (with Ridge Penalty).

Let $f_i(\beta) = \beta_0 + \sum_{j=1}^p x_j \beta_j$ be the log-odds.

- We also referred to this as $\gamma(\mathbf{x}_i)$ in previous notes.

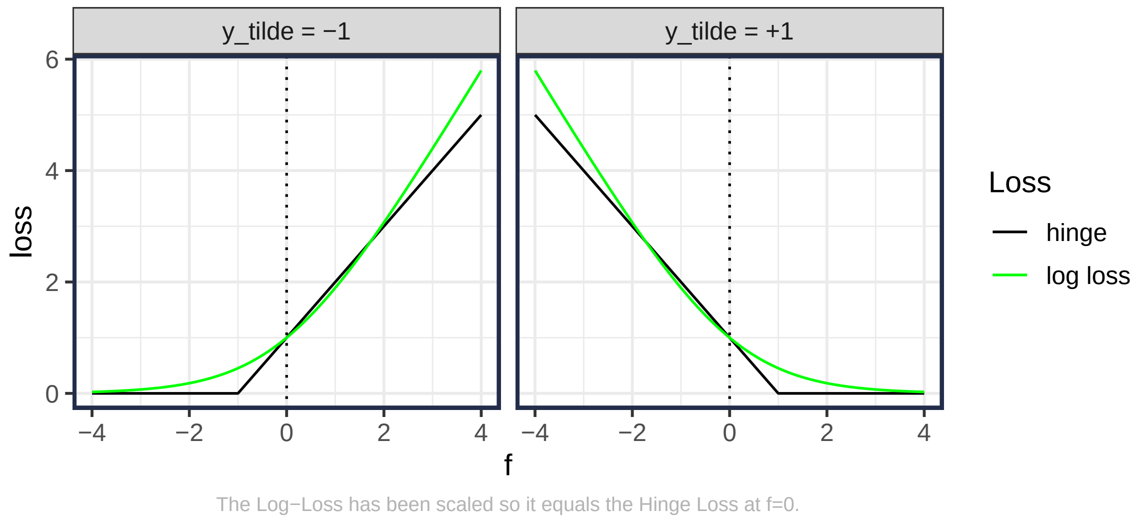
1. Estimate *model parameters* β
   - This assumes standardized $\mathbf{x}$'s

$$\begin{aligned}\hat{\beta}_\lambda &= \arg\min_\beta \left\{ \sum_{i=1}^n \log\left(1 + \exp\left(-\tilde{y}_i f_i(\beta)\right)\right) + \lambda \|\beta\|^2 / 2 \right\} \\ &= \arg\min_\beta \{\text{Log Loss}(\beta) + \lambda \text{ Penalty}(\beta)\}\end{aligned}$$

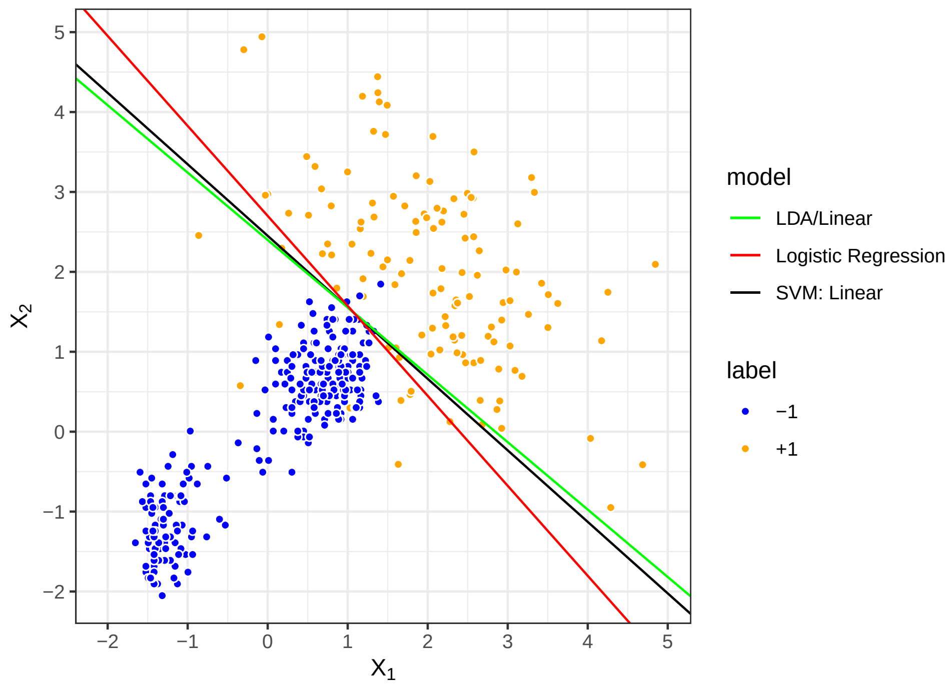
2. Label Class $+1$ if $\hat{f}_i \geq t$, else label Class -1
   - For some threshold t that considers the costs of FP and FN
   - If Cost(FP) = Cost(FN), the set $t = 0$, which is equivalent to $p(x) = 1/2$

Details of the Logistic Regression Loss Function

Note



1.5 Example: Compare Linear Classifiers



1.6 Three Representations of the Optimization Problem

1. **Penalized optimization**

$$\begin{aligned}\hat{\beta} &= \arg\min_{\beta} \{\text{Loss}(\beta) + \lambda \, \text{Penalty}(\beta)\} \\ &= \arg\min_{\beta} \{C \, \text{Loss}(\beta) + \text{Penalty}(\beta)\}\end{aligned}$$

   - where $C = \frac{1}{\lambda} > 0$ is an alternative strength of penalty
   - In SVM, C is referred to as the *cost*

2. **Constraint on Penalty**

$$\hat{\beta} = \arg\min_{\beta} \; \text{Loss}(\beta) \qquad \text{subject to} \;\; \text{Penalty}(\beta) \leq t$$

$$= \arg\min_{\beta:\, \text{Penalty}(\beta) \leq t} \text{Loss}(\beta)$$

3. **Constraint on Loss**

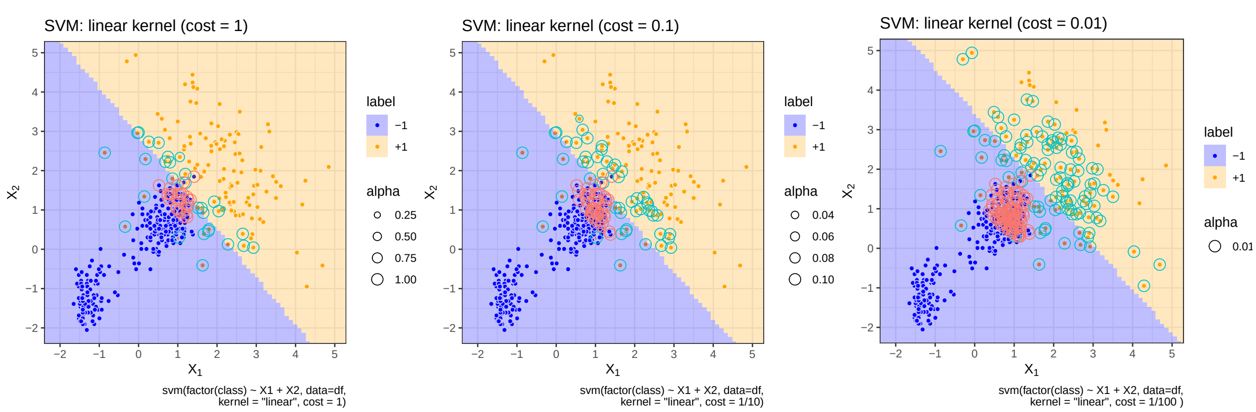
$$\hat{\beta} = \arg\min_{\beta} \; \text{Penalty}(\beta) \qquad \text{subject to} \;\; \text{Loss}(\beta) \leq M$$

$$= \arg\min_{\beta:\, \text{Loss}(\beta) \leq M} \text{Penalty}(\beta)$$

Note

There is a one-to-one relationship between all tuning parameters: λ, C, t, M.

1.7 Linear SVM



2 Kernels and Non-linear SVM

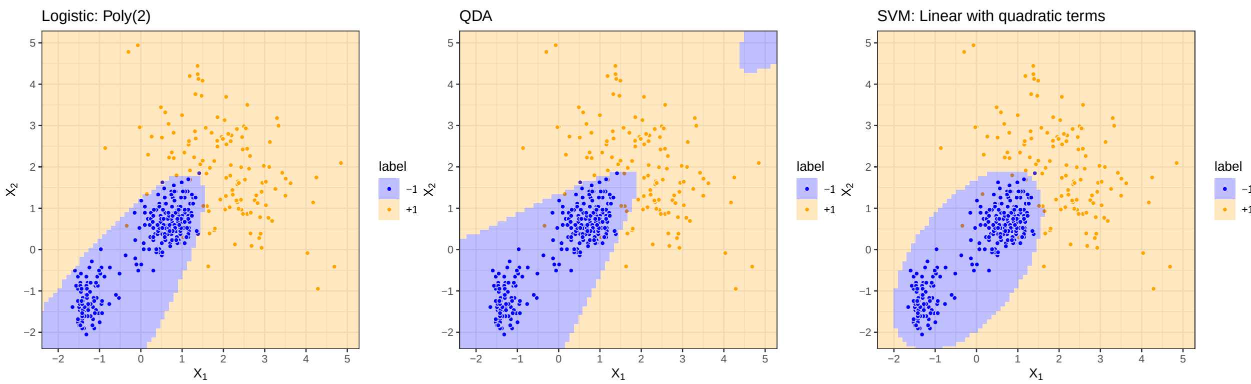
2.1 Basis Expansion

- Linear: $f(\mathbf{x}; \beta) = \beta_0 + \sum_{j=1}^{p} x_j \beta_j$
- Basis Expansion: $f(\mathbf{x}; \beta) = \beta_0 + \sum_{j=1}^{d} h_j(\mathbf{x}) \beta_j$
  - $h_j(\mathbf{x})$ transforms the raw $\mathbf{x}$ vector

2.1.1 Polynomial Expansion: Quadratic Terms

- Polynomial example: $h_1(\mathbf{x}) = x_1$, $h_2(\mathbf{x}) = x_1^2$, $h_3(\mathbf{x}) = x_2$, $h_4(\mathbf{x}) = x_2^2$, $h_5(\mathbf{x}) = x_1 x_2$
- $f(\mathbf{x}; \beta) = \beta_0 + \sum_{j=1}^{5} h_j(\mathbf{x}) \beta_j$

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



2.2 Alternative (Dual) Formulation

It turns out that the SVM solution for the model coefficients β can be written as

$$\hat{\beta}_j = \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \, h_j(\mathbf{x}_i)$$

- See ESL Eq. 12.17 if you are interested in the details.
- In this reformulation, the $\{\hat{\alpha}_i\}_{i=1}^{n}$ become the model parameters.
  - There is one model parameter for each observation!
  - $0 \le \alpha_i \le C$ (or $0 \le \alpha_i \le \frac{1}{\lambda}$)
  - But SVM will force most values to 0.
  - The observations with $\alpha_i > 0$ are called the *support vectors*
    - So the entire SVM model is a function of the support vectors only!
    - The support vectors are the observations on the wrong side of the margin.
- The decision function $\hat{f}(\mathbf{x})$ can be re-written

$$\begin{aligned}
\hat{f}(\mathbf{x}) &= f(\mathbf{x}; \hat{\beta}) \\
&= \hat{\beta}_0 + \sum_{j=1}^{d} h_j(\mathbf{x}) \hat{\beta}_j \\
&= \hat{\beta}_0 + \sum_{j=1}^{d} h_j(\mathbf{x}) \left[\sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \, h_j(\mathbf{x}_i) \right] \\
&= \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \left[\sum_{j=1}^{d} h_j(\mathbf{x}) h_j(\mathbf{x}_i) \right] \\
&= \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \, K(\mathbf{x}, \mathbf{x}_i)
\end{aligned}$$

  where

$$K(\mathbf{x}, \mathbf{x}_i) = \sum_{j=1}^{d} h_j(\mathbf{x}) h_j(\mathbf{x}_i) = \langle h(\mathbf{x}), h(\mathbf{x}_i) \rangle$$

  is called a **kernel** and measures the inner product, or *similarity* between x and x_i (observation i).

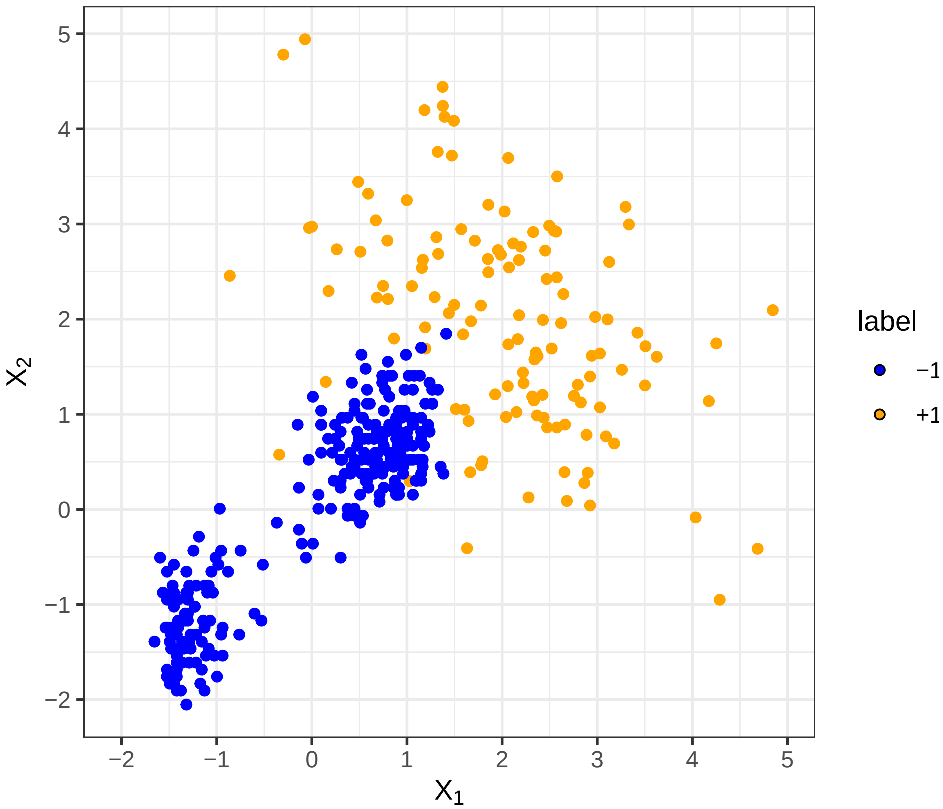
2.3 SVM in R

- The `svm()` function from the `e1071` package can implement SVM.
  - There is also a helpful `tune.svm()` to help you select the tuning parameters.
- The ISLR Lab in Section 9.6 has example R code.

2.4 Kernels

To help illustrate the difference between different kernels, let's look at slightly different data that won't be easy to classify using linear classifiers.

```
#> Error in rmvnorm(n1, mean = mu1, sigma = sigma1): unused argument (mean = mu1)
#> Error in rmvnorm(n2[1], mean = mu2, sigma = sigma2): unused argument (mean = mu2)
#> Error in rmvnorm(n2[2], mean = mu2.B, sigma = sigma2): unused argument (mean = mu2.B)
```

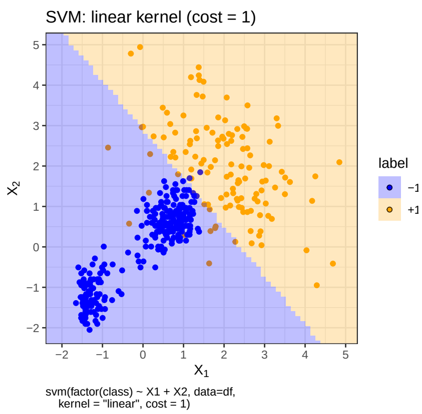


Three popular kernels (but there are many more) are the *linear*, *polynomial*, and *radial basis*

2.4.1 Linear Kernel

The *linear kernel* is

$$K(\mathbf{x}, \mathbf{u}) = \sum_{j=1}^{p} \mathbf{x}_j \mathbf{u}_j = \langle \mathbf{x}, \mathbf{u} \rangle$$



$$\hat{f}_{\text{linear}}(\mathbf{u}) = \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \, K(\mathbf{x}_i, \mathbf{u})$$

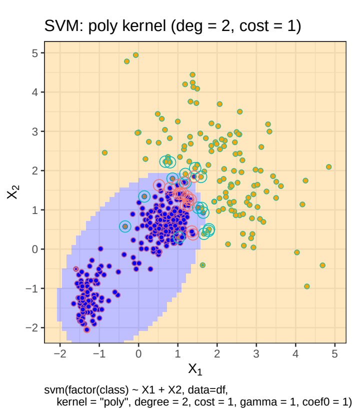
$$= \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \left(\sum_{j=1}^{p} \mathbf{x}_{ij} \mathbf{u}_j \right)$$

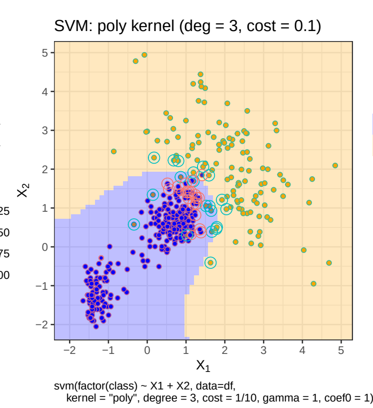
2.4.2 Polynomial Kernel

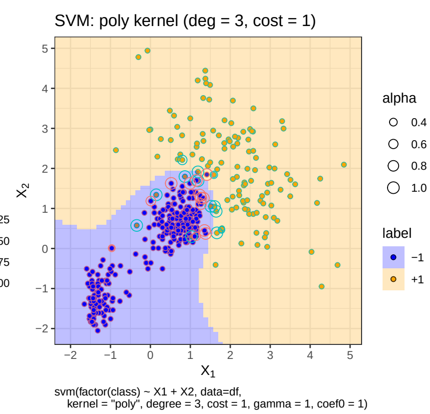
The *polynomial kernel* of degree `deg` is

$$K(\mathbf{x}, \mathbf{u}) = \left(1 + \sum_{j=1}^{p} \mathbf{x}_j \mathbf{u}_j \right)^{\text{deg}}$$

Note: in R, the ‘svm()‘ function from ‘e1071‘ package includes two other tuning parameters (`gamma` and `coef0`)







$$\hat{f}_{\text{poly}}(\mathbf{u}) = \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, y_i \, K(\mathbf{x}_i, \mathbf{u})$$

$$= \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, y_i \left(1 + \sum_{j=1}^{p} \mathbf{x}_j \mathbf{u}_j \right)^{\text{deg}}$$

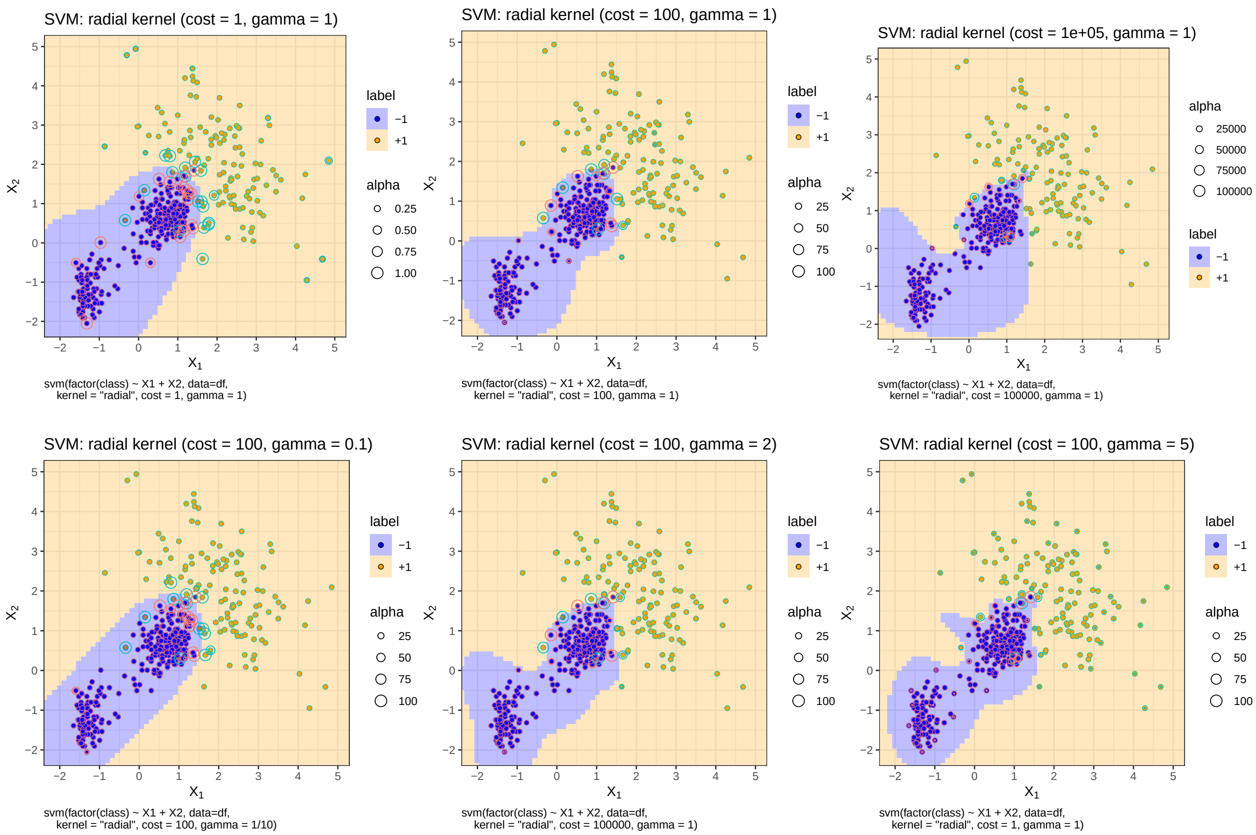
2.4.3 Radial Basis Kernel

The *Radial Basis Kernel* with parameter γ (`gamma`) is

$$K(\mathbf{x}, \mathbf{u}) = \exp\left(-\gamma \sum_{j=1}^{p} (\mathbf{x}_j - \mathbf{u}_j)^2\right)$$
$$= \exp\left(-\gamma \, dist^2(\mathbf{x}, \mathbf{u})\right)$$

where $dist^2(\mathbf{x}, \mathbf{u})$ is the *squared Euclidean distance* between $\mathbf{x}$ and $\mathbf{u}$.

- The Radial Basis kernel is large for test observations close to training observations.
- Notice that both `cost` and `gamma` are influential tuning parameters.



$$\hat{f}_{\text{radial}}(\mathbf{u}) = \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \, K(\mathbf{x}_i, \mathbf{u})$$
$$= \hat{\beta}_0 + \sum_{i=1}^{n} \hat{\alpha}_i \, \tilde{y}_i \, \exp\left(-\gamma \, dist^2(\mathbf{x}_i, \mathbf{u})\right)$$

2.5 Unbalanced Data

Three primary approaches:

1. Use weights corresponding to prior class probabilities
   - See the `class.weights` argument in `?svm`
   - Ensure the resulting score is what you want for unadjusted prediction.

$$\hat{\beta}_\lambda = \arg\min_{\beta} \left\{ \sum_{i=1}^{n} w_i \max\{0, 1 - \tilde{y}_i f_i(\beta)\} + \lambda \left\| \beta \right\|^2 / 2 \right\}$$

2. Use a threshold on the score
   - E.g., choose label = +1 if: $\hat{f}(\mathbf{x}) > t$
   - The $\hat{f}$ are the `decision.values` output of `predict.svm`
   - Its an attribute of the returned object
3. Sampling
   - under or over sample training data from one class to balance the label distribution.
   - The SVM (hinge) objective function is optimized at sign $[\Pr(Y = +1|X = x) - 1/2]$.
   - Ensure the resulting score is what you want for unadjusted prediction.

3 Appendix: R Code

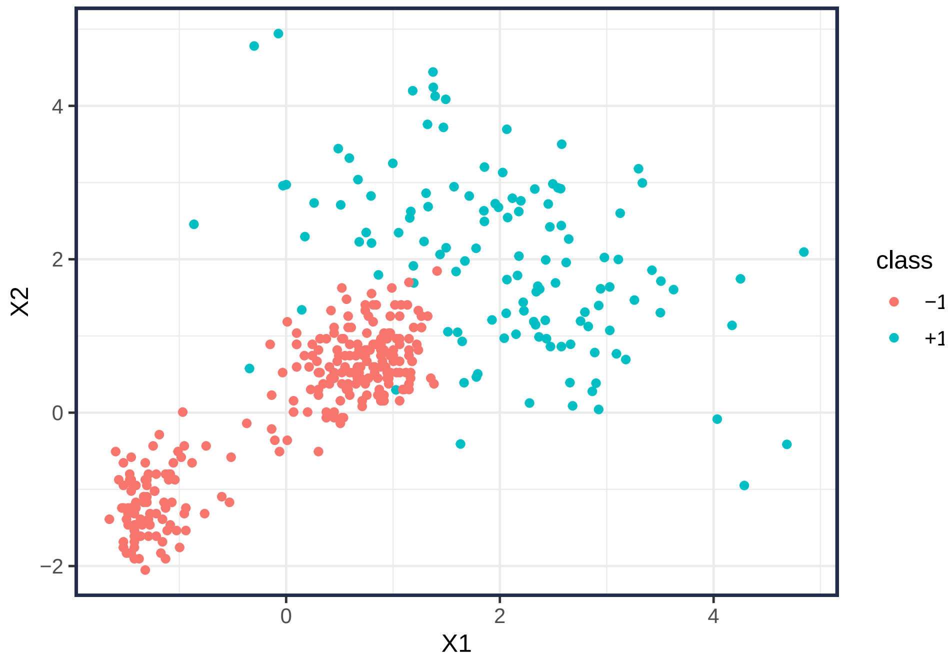
```
#--------------------------------------------------------------------#
# Create Data
#--------------------------------------------------------------------#
library(mvtnorm)

prior = c(.60, .40)
mu1 = c(2, 2)
mu2 = c(0, 0)
mu2.B = c(4, 4)
sigma1 = .5*matrix(c(2,-1, -1, 2), nrow=2)
sigma2 = .5*matrix(c(1,0,0,1), nrow=2)


set.seed(2020)
n = 200
n1 = rbinom(1, size=n, prob=prior[1])
n2 = n-n1
n2 = round(c(n2/2, n2/2))
X1 = rmvnorm(n1, mean=mu1, sigma = sigma1)
#> Error in rmvnorm(n1, mean = mu1, sigma = sigma1): unused argument (mean = mu1)
X2 = rmvnorm(n2[1], mean=mu2, sigma = sigma2)
#> Error in rmvnorm(n2[1], mean = mu2, sigma = sigma2): unused argument (mean = mu2)
X2 = rbind(X2, rmvnorm(n2[2], mean=mu2.B, sigma = sigma2))
#> Error in rmvnorm(n2[2], mean = mu2.B, sigma = sigma2): unused argument (mean = mu2.B)
labels = c("+1", "-1")


data_mix = bind_rows(
  !!labels[1] := as_tibble(X1, .name_repair = ~str_c("X", seq_along(.))),
  !!labels[2] := as_tibble(X2, .name_repair = ~str_c("X", seq_along(.))),
  .id = "class"
)


data_mix %>%
  ggplot(aes(X1, X2, color = class)) +
  geom_point()
```




```
#----------------------------------------------------------------------#
# Create Cross-Validation Folds
#----------------------------------------------------------------------#
set.seed(2022)
n.folds = 10
fold = sample(rep(1:n.folds, length=nrow(data_mix)))
```

```
#: using tidymodels
library(rsample)
set.seed(2022)
cv_folds = rsample::vfold_cv(data_mix, v = 10)
```

```
#----------------------------------------------------------------------#
# Polynomial SVM Example
#----------------------------------------------------------------------#
library(e1071)
fit = svm(factor(class) ~ X1 + X2,
    data = data_mix[fold != 1, ],    # hold out fold 1
    #: tuning parameters
    kernel = "poly",
    degree = 2,
    cost = 1
    )

# Notes:
# - svm() requires that the outcome variable be a "factor" for classification
#   problems.
# - the polynomial kernel only has cost and degree parameters
```

```
#: basic model summary
summary(fit)
#>
#> Call:
#> svm(formula = factor(class) ~ X1 + X2, data = data_mix[fold != 1,
#>     ], kernel = "poly", degree = 2, cost = 1)
#>
#>
```

```
#> Parameters:
#>    SVM-Type:  C-classification
#>  SVM-Kernel:  polynomial
#>        cost:  1
#>      degree:  2
#>      coef.0:  0
#>
#> Number of Support Vectors:  148
#>
#>  ( 73 75 )
#>
#>
#> Number of Classes:  2
#>
#> Levels:
#>  -1 +1

#: predictions
pred = predict(fit, data_mix[fold == 1,], decision.values = TRUE)

eval_data = tibble(
  outcome = data_mix$class[fold == 1],
  pred_hard = c(pred),
  pred_soft = as.numeric(attr(pred, "decision.values"))
)

# Notes:
# - using the `decision.values = TRUE` argument to get the scores. But set
#   to default of FALSE to just get the hard classifications
# - the scores can be used to create rank or threshold-based metrics like ROC
#   curves
# - There is also a way to get probability estimatates by setting
#   svm(..., probability = TRUE) and predict(..., probability = TRUE).
#   This attempts to convert scores to probabilities
```

```
#: evaluation
library(yardstick)
levs = c("+1", "-1")  # set outcome of interest at first level

eval_data %>%
  yardstick::roc_curve(truth = factor(outcome, levels=levs), estimate = pred_soft)
#> # A tibble: 42 x 3
#>   .threshold specificity sensitivity
#>        <dbl>       <dbl>       <dbl>
#> 1    -Inf         0                1
#> 2      -1.28      0                1
#> 3      -1.28      0.0370           1
#> 4      -1.27      0.0741           1
#> 5      -1.27      0.111            1
#> 6      -1.26      0.148            1
#> # ... with 36 more rows

eval_data %>%
  yardstick::accuracy(truth = factor(outcome, levels=levs),
                      estimate = factor(pred_hard, levels=levs))
#> # A tibble: 1 x 3
#>   .metric  .estimator .estimate
#>   <chr>    <chr>          <dbl>
```

```
#> 1 accuracy binary         0.825

# Notes:
# - the yardstick packages wants outcome variables and hard predictions be
#   "factors" with the outcome of interest as the first level
```

```
#---------------------------------------------------------------------#
# Radial basis SVM tuning parameter selection
#---------------------------------------------------------------------#
#: create function to fit, predict, and evaluate
eval_svm <- function(data_train, data_test, cost, gamma){

  #: fit
  fit = svm(factor(class) ~ X1 + X2,
            data = data_train,
            #: tuning parameters
            kernel = "radial",
            gamma = gamma,
            cost = cost
            )

  #: predict
  pred = predict(fit, data_test, decision.values = TRUE)

  #: evaluate
  eval_data = tibble(
    outcome = data_test$class,
    pred_hard = c(pred),
    pred_soft = as.numeric(attr(pred, "decision.values"))
  )

  levs = c("+1", "-1")  # set outcome of interest at first level

  auroc = eval_data %>%
    yardstick::roc_auc(truth = factor(outcome, levels=levs), estimate = pred_soft)

  accuracy = eval_data %>%
      yardstick::accuracy(truth = factor(outcome, levels=levs),
                          estimate = factor(pred_hard, levels=levs))

  bind_rows(auroc, accuracy) %>%
    mutate(cost, gamma)  # add tuning parameters

}
```

```
#: test it out
eval_svm(
  data_train = data_mix[fold != 1,],
  data_test = data_mix[fold == 1,],
  cost = 1,
  gamma = .1
)
#> # A tibble: 2 x 5
#>   .metric  .estimator .estimate  cost gamma
#>   <chr>    <chr>          <dbl> <dbl> <dbl>
#> 1 roc_auc  binary         0.974     1   0.1
#> 2 accuracy binary         0.95      1   0.1
```

```
#: using tidymodels
library(rsample)
eval_svm(
  data_train = training(cv_folds$splits[[1]]),
  data_test = testing(cv_folds$splits[[1]]),
  cost = 1,
  gamma = .1
)
#> # A tibble: 2 x 5
#>   .metric  .estimator .estimate  cost gamma
#>   <chr>    <chr>          <dbl> <dbl> <dbl>
#> 1 roc_auc  binary         0.974     1   0.1
#> 2 accuracy binary         0.95      1   0.1
```

```
#: create grid of tuning parameter values
tune_grid = expand_grid(
  cost = 10^(-2:2),
  gamma = c(.1, .5, 1)
)


#: loop over folds and grids
out = tibble()

for(k in unique(fold)){

  for(i in 1:nrow(tune_grid)){

    metrics = eval_svm(
      data_train = data_mix[fold != k,],
      data_test = data_mix[fold == k,],
      cost = tune_grid$cost[i],
      gamma = tune_grid$gamma[i]
    )

    out = bind_rows(out, metrics %>% mutate(fold = k) )
  }
}

#: average over folds

out %>%
  # calculate average performance over folds
  group_by(.metric, cost, gamma) %>%
  summarize(mu = mean(.estimate), .groups = "drop") %>%
  # spread data wider to see both metrics
  pivot_wider(names_from = .metric, values_from = mu) %>%
  # arrange by auc and then accuracy (if ties)
  arrange(desc(roc_auc), desc(accuracy))
#> # A tibble: 15 x 4
#>     cost gamma accuracy roc_auc
#>    <dbl> <dbl>    <dbl>   <dbl>
#> 1   0.1    1      0.972   0.995
#> 2   0.01   1      0.687   0.995
#> 3 100      0.5    0.975   0.994
#> 4   1      1      0.980   0.994
#> 5  10      0.5    0.980   0.992
#> 6  10      1      0.980   0.989
```

```
#> # ... with 9 more rows


# Notes:
# - can go back and modify grid to focus on best tuning region
```

```
#: using tidymodels and purrr

#: function to search over grid
eval_svm_grid <- function(data, grid){
  pmap_df(grid, function(cost, gamma) eval_svm(training(data), testing(data), cost, gamma))
}

# try it out
data = cv_folds$splits[[1]]
eval_svm_grid(data, head(tune_grid))
#> # A tibble: 12 x 5
#>   .metric  .estimator .estimate  cost gamma
#>   <chr>    <chr>          <dbl> <dbl> <dbl>
#> 1 roc_auc  binary         0.980  0.01   0.1
#> 2 accuracy binary         0.675  0.01   0.1
#> 3 roc_auc  binary         0.977  0.01   0.5
#> 4 accuracy binary         0.675  0.01   0.5
#> 5 roc_auc  binary         0.974  0.01   1
#> 6 accuracy binary         0.675  0.01   1
#> # ... with 6 more rows

#: loop over folds
map_df(cv_folds$splits, ~eval_svm_grid(data=.x, grid=tune_grid), .id="fold")
#> # A tibble: 300 x 6
#>   fold  .metric  .estimator .estimate  cost gamma
#>   <chr> <chr>    <chr>          <dbl> <dbl> <dbl>
#> 1 1     roc_auc  binary         0.980  0.01   0.1
#> 2 1     accuracy binary         0.675  0.01   0.1
#> 3 1     roc_auc  binary         0.977  0.01   0.5
#> 4 1     accuracy binary         0.675  0.01   0.5
#> 5 1     roc_auc  binary         0.974  0.01   1
#> 6 1     accuracy binary         0.675  0.01   1
#> # ... with 294 more rows
```