Functional Programming: Linear Model with RBF Feature Transform

Mathematical Set Up

Suppose we have a training matrix X with n observations and d features

$$X = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} \in \mathbb{R}^{n\times d}$$

and that we want to do a **feature transform** of this data using the Radial Basis Function. To do this, we

- choose b rows of X and we call them **centroids**

$$\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(b)}$$

- calculate using some heuristic a **bandwidth** parameter σ^2

And then, for every centroid we define a radial basis function as follows

$$\phi^{(i)}(\mathbf{x}) := \exp\left(-\frac{\parallel \mathbf{x} - \mathbf{x}^{(i)} \parallel^2}{\sigma^2}\right) \qquad \forall i \in \{1, \dots, b\} \quad \text{for } \mathbf{x} \in \mathbb{R}^d$$

We can therefore obtain a transformed data matrix as

$$\Phi := \begin{pmatrix} 1 & \phi^{(1)}(\mathbf{x}_1) & \phi^{(2)}(\mathbf{x}_1) & \cdots & \phi^{(b)}(\mathbf{x}_1) \\ 1 & \phi^{(1)}(\mathbf{x}_2) & \phi^{(2)}(\mathbf{x}_2) & \cdots & \phi^{(b)}(\mathbf{x}_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \phi^{(1)}(\mathbf{x}_n) & \phi^{(2)}(\mathbf{x}_n) & \cdots & \phi^{(b)}(\mathbf{x}_n) \end{pmatrix} \in \mathbb{R}^{n\times(b+1)}$$

Then we fit a **regularized** linear model so that **optimal parameters** are given by

$$\mathbf{w} := (\Phi^\top \Phi + \lambda I_n)^{-1} \Phi^\top \mathbf{y}$$

These parameters are usually found by solving the associated system of linear equations for $\mathbf{w}$

$$(\Phi^\top \Phi + \lambda I_n)\mathbf{w} = \Phi^\top \mathbf{y}$$

This will be one of the strategies that we'll see below. However, we are required to apply regularization with a very small regularization parameter λ. This hints at the fact that maybe we can simply set $\lambda = 0$ and then find $\mathbf{w}$ simply by finding the pseudoinverse of Φ

$$(\Phi^\top \Phi)^{-1} \Phi^\top$$

and then multiply this by $\mathbf{y}$ on the left. This approach looks more stable and can be implemented by setting `pseudoinverse=TRUE` in the function `make_predictor` defined in this document.

Parameters

In the following code chunk you can set up n the number of training observations, d the dimensionality of the input (i.e. the number of features), λ the regularization coefficient, m the number of testing observations, and b dimensionality of the data after the feature transform, which in this case corresponds to the number of centroids.

```
n <-  1000
d <-  2
lambda <-  0.00001
m <-  200
b <-  50
```

Training and Testing Sets

We work with synthetic data sets. For simplicity, we will generate X uniformly in an interval (which in this case is $[-4, 4]$) and then y will be taken to be a multivariate normal of each row of X. Note that we create a **factory of functions** to generate multivariate normal closures, yet the same behavior would be achieved writing up a simple function. The factory of functions is defined in order to work with the functional programming paradigm.

```
# Explanatory variable is uniformly distributed between -4 and 4, then reshaped
X <-  matrix(runif(n*d, min=-4, max=4), nrow=n, ncol=d)
# Factory of multivariate normal distributions
normal_factory <- function(mean_vector, cov_matrix){
  d <- nrow(cov_matrix)
  normal_pdf <- function(x){
    exponent <- -mahalanobis(x, center=mean_vector, cov=cov_matrix) / 2
    return(
      (2*pi)^(-d/2) * det(cov_matrix)^(-1/2) * exp(exponent)
    )
  }
}
# Closure will be our data-generating process for training and test response.
target_normal <- normal_factory(rnorm(d), diag(d))
y <- matrix(apply(X, 1, target_normal))
```

Similarly, create test data.

```
Xtest <- matrix(runif(m*d, min=-4, max=4), nrow=m, ncol=d)
ytest <- matrix(apply(Xtest, 1, target_normal))
```

Feature Transform Implementation

Define a function that, given a training data matrix X, finds the distance matrix containing all the pairwise distances squared, and then return the median of such distances. Essentially, it returns the badwidth squared σ^2.

```
compute_sigmasq <- function(X){
  # Compute distance matrix expanding the norm. Return its median
  Xcross <- tcrossprod(X)
```

```r
  Xnorms <- matrix(diag(Xcross), nrow(X), nrow(X), byrow=TRUE)
  return(median(Xnorms - 2*Xcross + t(Xnorms)))
}
```

Define a function that gets b random samples from the rows of an input matrix X, these will be the centroids.

```r
get_centroids <- function(X, n_centroids){
  # Find indeces of centroids
  idx <- sample(1:nrow(X), n_centroids)
  return(X[idx, ])
}
```

Construct a factory of Radial Basis Functions. The factory constructs an RBF, given a centroid and a σ^2.

```r
rbf <- function(centroid, sigmasq){
  rbfdot <- function(x){
    return(
      exp(-sum((x - centroid)^2) / sigmasq)
    )
  }
  return(rbfdot)
}
```

Finally, we can put all of these functions together to compute Φ and eventually make predictions.

```r
compute_phiX <- function(X, centroids, sigmasq){
  # Create a list of rbfdot functions and apply each of them to every row of X
  phiX <- mapply(
    function(f) apply(X, 1, f),
    apply(centroids, 1, rbf, sigmasq=sigmasq)
  )
  # Reshape phiX correctly
  phiX <- matrix(phiX, nrow(X), nrow(centroids))
  # Recall we need the first column to contain 1s for the bias
  return(cbind(1, phiX))  # this is a (n, d+1) matrix
}
```

Prediction

We're now ready to define a factory of functions that returns prediction functions.

```r
library(corpcor)
make_predictor <- function(X, y, lambda, n_centroids, pseudoinverse=FALSE){
  # Randomly sample centoids
  centroids <- get_centroids(X, n_centroids)
  sigmasq <- compute_sigmasq(X)
  # Get transformed data matrix
  phiX <- compute_phiX(X, centroids, sigmasq)
  # Find optimal parameters
  if (pseudoinverse){
    # This method works best cause it does automatic regularization with SVD
```

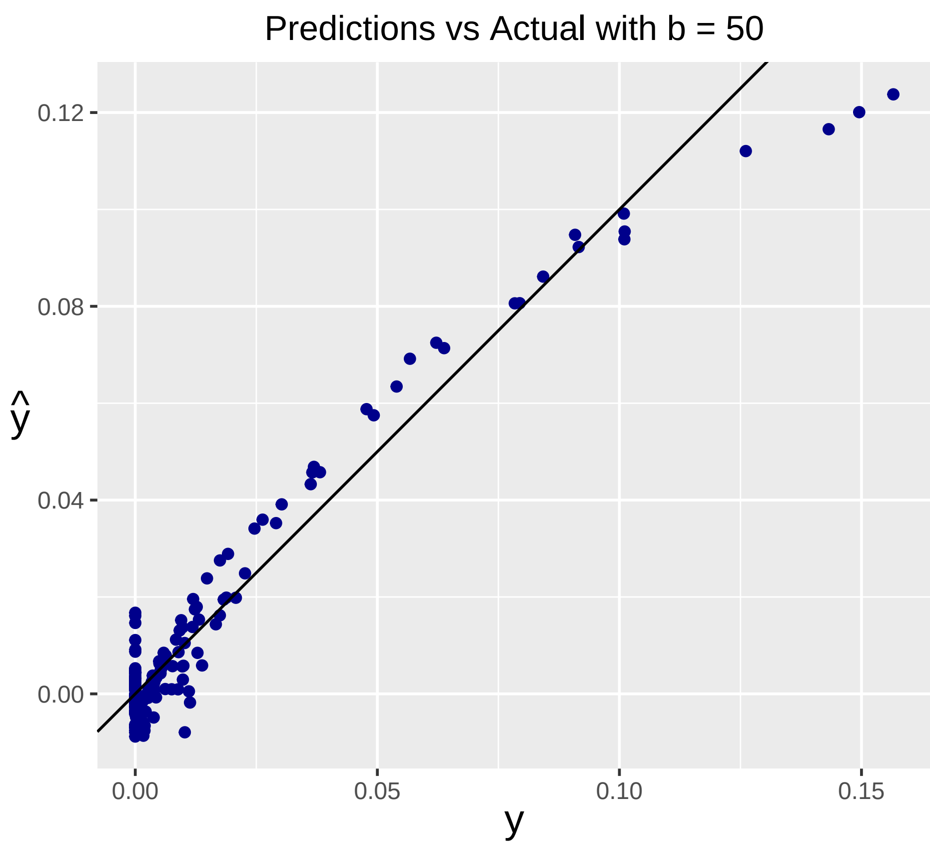
```r
    w <- pseudoinverse(phiX) %*% y
  } else {
    w <- solve(t(phiX)%*%phiX + lambda*diag(n_centroids+1), t(phiX) %*% y)
  }
  # Construct predictor closure for a new batch of testing data Xtest
  predictor <- function(Xtest){
    # Need to transform test data into a phi matrix
    phi_Xtest <- compute_phiX(Xtest, centroids, sigmasq)
    return(phi_Xtest %*% w)
  }
  return(predictor)
}
```

We can test its effectiveness now. Notice that in general we might need a lot of centroids to make this work.

```r
# Construct prediction functions. One with regularization, other with pseudoinv
predict <- make_predictor(X, y, lambda, n_centroids = b)
pseudo_predict <- make_predictor(X, y, lambda, n_centroids = b, pseudoinverse = TRUE)
# Get predictions
yhat <- predict(Xtest)
yhat_pseudo <- pseudo_predict(Xtest)
```

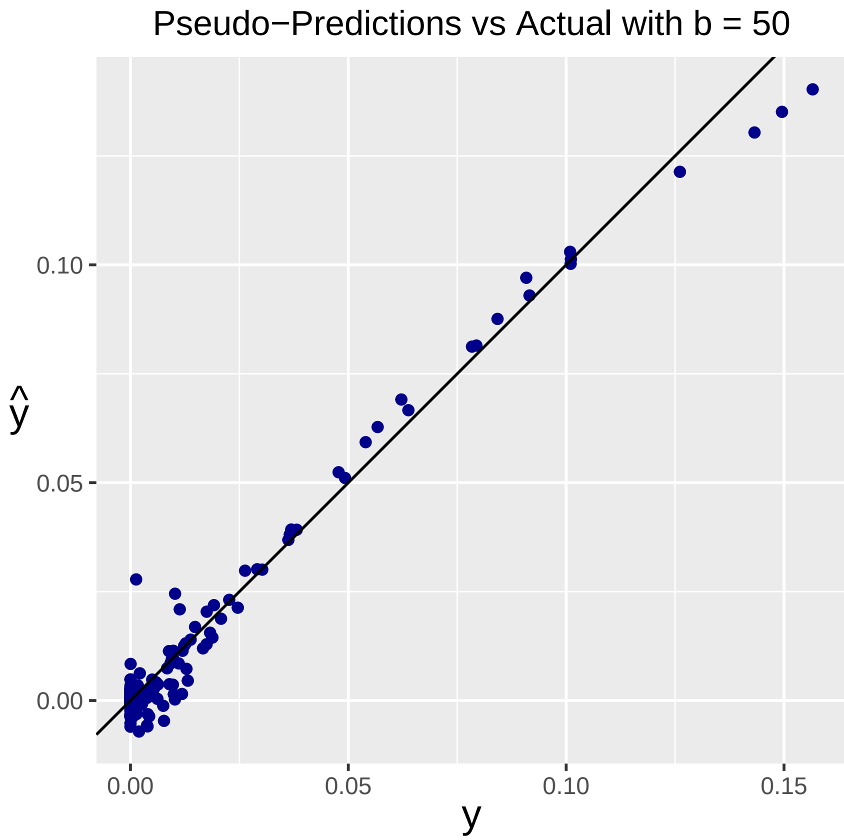
Predictions can be assessed by plotting predicted values against the true test values.

```r
library(ggplot2)
# Put data into a dataframe for ggplot2
df <- data.frame(real=ytest, pred=yhat, pseudo_pred=yhat_pseudo)
ggplot(data=df) +
  geom_point(aes(x=real, y=pred), color="darkblue") +
  geom_abline(intercept=0, slope=1) +
  ggtitle(paste("Predictions vs Actual with b =", b)) +
  theme(
    plot.title = element_text(hjust = 0.5),
    axis.title = element_text(size=15, face="bold"),
    axis.title.y = element_text(angle=0, vjust=0.5)
  ) +
  xlab(expression(y)) +
  ylab(expression(hat(y))) +
  coord_fixed()
```



Similarly, we can see the performance of our prediction using the pseudoinverse

```
ggplot(data=df) +
  geom_point(aes(x=real, y=pseudo_pred), color="darkblue") +
  geom_abline(intercept=0, slope=1) +
  ggtitle(paste("Pseudo-Predictions vs Actual with b =", b)) +
  theme(
    plot.title = element_text(hjust = 0.5),
    axis.title = element_text(size=15, face="bold"),
    axis.title.y = element_text(angle=0, vjust=0.5)
  ) +
  xlab(expression(y)) +
  ylab(expression(hat(y))) +
  coord_fixed()
```



Technical Note on Calculating the Bandwidth

To vectorize this operation, we aim to create a matrix containing all the squared norms of the difference between the vectors

$$D = \begin{pmatrix} \| \mathbf{x}_1 - \mathbf{x}_1 \|^2 & \| \mathbf{x}_1 - \mathbf{x}_2 \|^2 & \cdots & \| \mathbf{x}_1 - \mathbf{x}_n \|^2 \\ \| \mathbf{x}_2 - \mathbf{x}_1 \|^2 & \| \mathbf{x}_2 - \mathbf{x}_2 \|^2 & \cdots & \| \mathbf{x}_2 - \mathbf{x}_n \|^2 \\ \vdots & \vdots & \ddots & \vdots \\ \| \mathbf{x}_n - \mathbf{x}_1 \|^2 & \| \mathbf{x}_n - \mathbf{x}_2 \|^2 & \cdots & \| \mathbf{x}_n - \mathbf{x}_n \|^2 \end{pmatrix}$$

Notice that we can rewrite the norm of the difference between two vectors $\mathbf{x}_i$ and $\mathbf{x}_j$ as follows

$$\| \mathbf{x}_i - \mathbf{x}_j \|^2 = (\mathbf{x}_i - \mathbf{x}_j)^\top (\mathbf{x}_i - \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_i - 2\mathbf{x}_i^\top \mathbf{x}_j + \mathbf{x}_j^\top \mathbf{x}_j$$

Broadcasting this, we can rewrite the matrix D as

$$D = \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 - 2\mathbf{x}_1^\top \mathbf{x}_1 + \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_1^\top \mathbf{x}_1 - 2\mathbf{x}_1^\top \mathbf{x}_2 + \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_1^\top \mathbf{x}_1 - 2\mathbf{x}_1^\top \mathbf{x}_n + \mathbf{x}_n^\top \mathbf{x}_n \\ \mathbf{x}_2^\top \mathbf{x}_2 - 2\mathbf{x}_2^\top \mathbf{x}_1 + \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 - 2\mathbf{x}_2^\top \mathbf{x}_2 + \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_2^\top \mathbf{x}_2 - 2\mathbf{x}_2^\top \mathbf{x}_n + \mathbf{x}_n^\top \mathbf{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^\top \mathbf{x}_n - 2\mathbf{x}_n^\top \mathbf{x}_1 + \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_n^\top \mathbf{x}_n - 2\mathbf{x}_n^\top \mathbf{x}_2 + \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n - 2\mathbf{x}_n^\top \mathbf{x}_n + \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}$$

This can now be split into three matrices, where we can notice that the third matrix is nothing but the transpose of the first.

$$D = \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_1^\top \mathbf{x}_1 & \cdots & \mathbf{x}_1^\top \mathbf{x}_1 \\ \mathbf{x}_2^\top \mathbf{x}_2 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_2^\top \mathbf{x}_2 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^\top \mathbf{x}_n & \mathbf{x}_n^\top \mathbf{x}_n & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix} - 2 \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_1^\top \mathbf{x}_2 & \cdots & \mathbf{x}_1^\top \mathbf{x}_n \\ \mathbf{x}_2^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_2^\top \mathbf{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^\top \mathbf{x}_1 & \mathbf{x}_n^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix} + \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \\ \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}$$

The key is not to notice that we can obtain the middle matrix from X with a simple operation:

$$XX^\top = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_1^\top \mathbf{x}_2 & \cdots & \mathbf{x}_1^\top \mathbf{x}_n \\ \mathbf{x}_2^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_2^\top \mathbf{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^\top \mathbf{x}_1 & \mathbf{x}_n^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}$$

and then the first matrix can be obtained as follows

$$\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}_{n\times 1} \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}_{1\times n} = \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_1^\top \mathbf{x}_1 & \cdots & \mathbf{x}_1^\top \mathbf{x}_1 \\ \mathbf{x}_2^\top \mathbf{x}_2 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_2^\top \mathbf{x}_2 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^\top \mathbf{x}_n & \mathbf{x}_n^\top \mathbf{x}_n & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}$$

where

$$\operatorname{diag}\left[\begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_1^\top \mathbf{x}_2 & \cdots & \mathbf{x}_1^\top \mathbf{x}_n \\ \mathbf{x}_2^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_2^\top \mathbf{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^\top \mathbf{x}_1 & \mathbf{x}_n^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}\right] = \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \mathbf{x}_2^\top \mathbf{x}_2 & \cdots & \mathbf{x}_n^\top \mathbf{x}_n \end{pmatrix}_{1\times n}$$