Direct Approach KEF

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Kernel Mean Embedding Estimation

Set the randomness seed.

```
# set the seed
seed <- 7
set.seed(seed)</pre>
```

Specfiy the True density

Set the mean and standard deviation of normal distribution P

```
# Set the mean and standard deviation of normal distribution P n=500 means = c(-2, 2) sds = c(1, 1.5) probabilities = c(0.3, 0.7)
```

Take Random samples

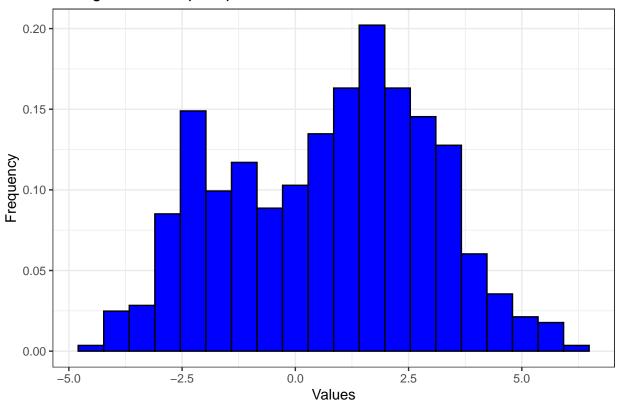
```
# vector of fixed points
vec_fixed_points <- sort(rnorm_mixture(n, means, sds, probabilities))

library(ggplot2)
# Assuming vec_fixed_points is your data
df <- data.frame(points = vec_fixed_points)

# Create the histogram with 20 breaks
ggplot(df, aes(x = points, y = ..density..)) +
geom_histogram(bins = 20, fill = "blue", color = "black") +
labs(title = "Histogram of sampled points", x = "Values", y = "Frequency")+
theme_bw()

## Warning: The dot-dot notation (`..density...`) was deprecated in ggplot2 3.4.0.
## i Please use `after_stat(density)` instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.</pre>
```

Histogram of sampled points



Find Gram Matrix of the sampled points

True Kernel Mean Embeddings

```
# Grid of 100 points from -10 to 10
u <- centering_param

lambda <- 1
# Kernel mean embedding be careful change the mean if change the mean of P

# Define the function f with point as a parameter</pre>
```

```
f <- function(x, point, lambda, probabilities, means, sds, centering_param) {</pre>
  base_measure_gaussian_mixture <- 0</pre>
  for (i in 1:length(probabilities)) {
    base_measure_gaussian_mixture <- base_measure_gaussian_mixture +</pre>
      probabilities[i] / (\operatorname{sqrt}(2 * \operatorname{pi}) * \operatorname{sds}[i]) * \exp(-(x - \operatorname{means}[i])^2 / (2 * \operatorname{sds}[i]^2)) *
      exp(-lambda/4*(x^2/centering_param + centering_param/3))
  }
 return ((lambda / 2) * (-abs(x - point) + (x^2 + point^2) / (2 * centering_param) + centering_param /
# Define a wrapper function to perform integration
integrate_for_point <- function(point, lambda, probabilities, means, sds, centering_param) {</pre>
  # Calculate the integral part
  integral_result <- integrate(function(x) f(x, point, lambda, probabilities,</pre>
                                                means, sds, centering_param),
                                 subdivisions = 10000, rel.tol = 1e-10,
                                 abs.tol = 1e-10, lower = -centering_param, upper = centering_param) $value
  additional_terms <- 0
  for (i in 1:length(probabilities)) {
    term1 <- probabilities[i] * lambda *</pre>
      (centering_param^2 + 6 * centering_param * point - 3 * point^2) *
      exp(lambda/24*(12*means[i]+4*centering_param+3*sds[i]^2*lambda))/ (24 * centering_param)
    term2 <- probabilities[i] * lambda *
      (centering_param^2 - 6 * centering_param * point - 3 * point^2) *
      exp(lambda/24*(-12*means[i]+4*centering_param+3*sds[i]^2*lambda))/ (24 * centering_param)
    erf_component1 <- erfc((2*(means[i] + centering_param)+ sds[i]^2*lambda )/ (2*sqrt(2) * sds[i]))</pre>
    erf_component2 <- erfc((2*(-means[i] + centering_param)+ sds[i]^2*lambda )/ (2*sqrt(2) * sds[i]))
    additional_terms <- additional_terms - (term1 * erf_component1) - (term2 * erf_component2)
  }
  result <- integral_result + additional_terms
  return(result)
}
# Apply the integration function to each element of grid_point
KME_true <- sapply(vec_fixed_points, integrate_for_point,</pre>
                    lambda = lambda,
                    probabilities = probabilities,
                    means = means,
                    sds = sds,
                    centering_param = centering_param)
# Data frame with true kernel mean embeddings
```

```
true_KME <- data.frame(vec_fixed_points, true_KME = KME_true)</pre>
```

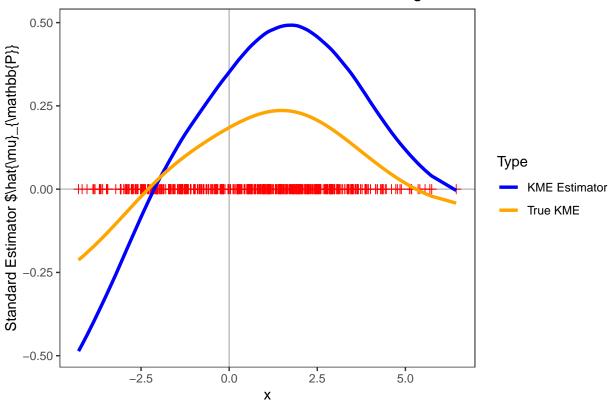
Kernel Mean Embedding Estimation: Standard Estimator

```
# Data frame with estimated kernel mean embedding
df_std <- data.frame(vec_fixed_points, standard_KME = colMeans(gram))
# Data frame for fixed points: adding e
df_fixed_points <- data.frame(x = vec_fixed_points, y = rep(0, length(vec_fixed_points)))</pre>
```

Kernel Mean Embedding Estimator

```
# Plot the results using ggplot
library(ggplot2)
# Create a combined data frame to handle both blue (standard) and orange (true KME) lines
df_combined <- rbind(</pre>
 data.frame(grid_points = df_std$vec_fixed_points, value = df_std$standard, line = "KME Estimator"),
  data.frame(grid_points = true_KME$vec_fixed_points, value = true_KME$true_KME, line = "True KME")
ggplot() +
  geom_hline(yintercept = 0, color = "gray", linetype = "solid", linewidth = 0.5) + # Add axis y = 0
  geom_vline(xintercept = 0, color = "gray", linetype = "solid", linewidth = 0.5) + # Add axis at x =
  geom_point(data = df_fixed_points, aes(x = x, y = y), color = 'red', size = 2 ,shape = 3) + # Plot x
  geom_line(data = df_combined, aes(x = grid_points, y = value, color = line), linewidth = 1.2) + # Plo
  labs(x = "x",
       y = "Standard Estimator $\\hat{\\mu}_{\\mathbb{P}}\",
       title = "Standard Estimator of Kernel Mean Embedding") +
  theme_bw() +
  theme(panel.grid = element_blank(), # Remove grid lines
       panel.grid.major = element_blank(),
       panel.grid.minor = element_blank()) +
  scale_color_manual(values = c("KME Estimator" = "blue", "True KME" = "orange")) + # Custom colors fo
  guides(color = guide_legend(title = "Type")) # Add a legend title
```

Standard Estimator of Kernel Mean Embedding



Pre calculations:

Find the shrinkage estimator of KME:

```
# Data frame with your data
df_reg <- data.frame(vec_fixed_points, regularized = results)</pre>
```

Shrinkage Estimator of Kernel Mean Embedding —-

Pre calculations:

LOOCV hyper parameter selection

```
loocv_values <- rep(0,length = length(lambda_grid))
### Use sapply to iterate over lambda_grid
loocv_values <- sapply(1:length(lambda_grid), function(i) {
   loocv_shr(gram = gram, lambda = lambda_grid[i], precomp_reg_inv = regularized_inverse_grid[[i]])
})

### Create a dataframe to store lambda values and their corresponding LOOCV errors
loocv_df <- data.frame(lambda = lambda_grid, loocv = loocv_values)

### Print the dataframe
print(loocv_df)</pre>
```

```
##
     lambda
               loocv
## 1
     1e-14 1.310779
      1e-13 1.292868
## 2
## 3
     1e-12 1.292174
## 4
     1e-11 1.292210
## 5
      1e-10 1.292202
## 6
      1e-09 1.292201
## 7
      1e-08 1.292201
## 8
      1e-07 1.292201
## 9
      1e-06 1.292201
## 10 1e-05 1.292201
## 11 1e-04 1.292201
## 12 1e-03 1.292209
## 13 1e-02 1.292821
```

```
## 14 1e-01 1.308502

## 15 1e+00 1.429393

## 16 1e+01 1.543056

## 17 1e+02 1.563978

## 18 1e+03 1.566249

## 19 1e+04 1.566501

## 20 1e+05 1.566501

## 21 1e+06 1.566503

## 22 1e+07 1.566503

## 23 1e+08 1.566503

## 24 1e+09 1.566503

## 25 1e+10 1.566503
```

CV hyper parameter selection

```
lambda_grid <- c(10^seq(-14,10,1))

cv_values <- rep(0,length = length(lambda_grid))
### Use sapply to iterate over lambda_grid

cv_values <- sapply(1:length(lambda_grid), function(i) {
    cross_validation(gram = gram, lambda = lambda_grid[i], folds_number = nrow(gram),estimator_type = "sh"
})

### Create a dataframe to store lambda values and their corresponding LOOCV errors

cv_df <- data.frame(lambda = lambda_grid, cv = cv_values)

### Print the dataframe

print(cv_df)</pre>
```

```
##
      lambda
## 1
       1e-14 1.292201
## 2
      1e-13 1.292201
## 3
       1e-12 1.292201
       1e-11 1.292201
## 4
## 5
       1e-10 1.292201
## 6
       1e-09 1.292201
## 7
       1e-08 1.292201
## 8
       1e-07 1.292201
## 9
       1e-06 1.292201
## 10
     1e-05 1.292201
      1e-04 1.292201
## 11
## 12
       1e-03 1.292209
## 13 1e-02 1.292821
## 14 1e-01 1.308502
## 15 1e+00 1.429393
## 16
      1e+01 1.543056
## 17 1e+02 1.563978
## 18 1e+03 1.566249
## 19 1e+04 1.566478
## 20
      1e+05 1.566501
## 21
     1e+06 1.566503
## 22
     1e+07 1.566503
## 23
       1e+08 1.566503
## 24 1e+09 1.566503
```

#save.image("C:/Users/rouda/OneDrive/Research/Codes/R/kef/examples/rdata_direct_brownian_3.RData")

Find the best hyper parameter and corresponding beta weights

```
merged_num_anal <- merge(cv_df,loocv_df,by = "lambda")

# Choose the best lambda with lowest loocv
lambda_shr <- cv_df[which.min(cv_df$cv),"lambda"]

# Calculate inverse of regularizer
inverse_regularizer <- solve(gram + n * lambda_shr*diag(n))

# 1_n vector
one_n <- rep(1,n)/n

# Find beta
beta_s <- sqrt(n) * inverse_regularizer %*% gram %*% one_n</pre>
```

Find the shrinkage estimator of KME

Merge all the KME estimators and plot

```
df_all <- merge(df_std,df_reg,by = "vec_fixed_points")
df_all <- merge(df_all,df_shr,by = "vec_fixed_points")
df_all <- merge(df_all,true_KME,by = "vec_fixed_points")

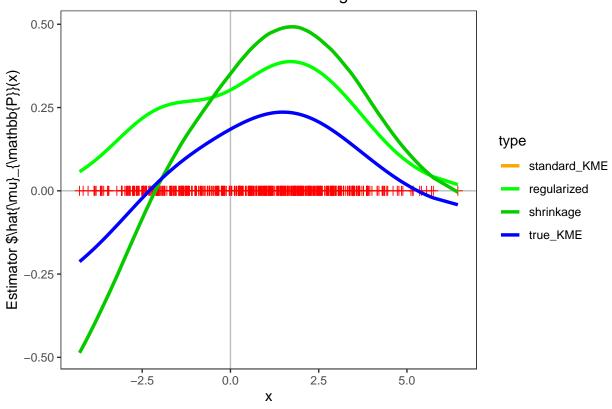
#save.image("C:/Users/rouda/OneDrive/Research/Codes/R/kef/examples/rdata_direct_4.RData")
library(tidyr)

#gather data from columns 2 and 3
df_long <- gather(df_all, key="type", value="estimation", 2:5)

df_long$type <- factor(df_long$type, levels = colnames(df_all)[-1])

# Data frame for fixed points:
df_fixed_points <- data.frame(x = vec_fixed_points, y = rep(0, length(vec_fixed_points)))</pre>
```

Estimator of Kernel Mean Embedding

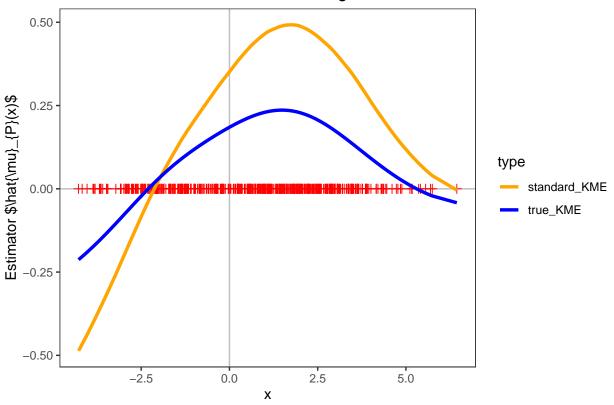


library(dplyr)

```
##
## Attaching package: 'dplyr'
## The following objects are masked from 'package:stats':
##
## filter, lag
## The following objects are masked from 'package:base':
##
```

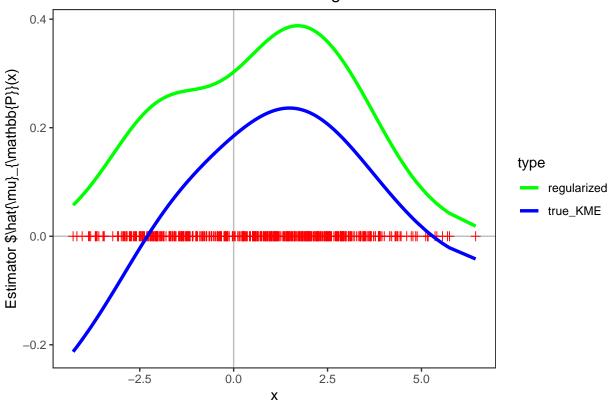
```
## intersect, setdiff, setequal, union
```

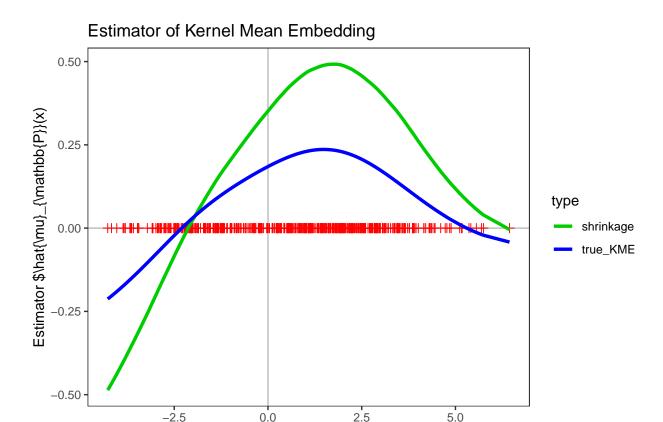
Estimator of Kernel Mean Embedding



```
theme(panel.grid = element_blank(), # Remove grid lines
    panel.grid.major = element_blank(),
    panel.grid.minor = element_blank()) + # Axis ticks color
scale_color_manual(values = c('green', 'blue')) # Customize colors
```

Estimator of Kernel Mean Embedding





Find the probabilities using KME and centered kernel

Х

The relationship for $\hat{\mu}(\mathbf{x}_i)$ is given by:

$$\hat{\mu}(\mathbf{x}_i) = \sum_{j=1}^n h(\mathbf{x}_i, \mathbf{x}_j) p_{\theta}(\mathbf{x}_j).$$

Furthermore, we can estimate $\hat{\mu}(\mathbf{x}_i)$ using methods like shrinkage or Bayesian approaches: Moreover, we can estimate $\hat{\mu}(\mathbf{x}_i)$ with methods like shrinkage methods provided by Gretton and colleagues. So we can say $\hat{\mathbf{p}}_{\theta} = \mathbf{H}_{samvle}^{-1} \hat{\mu}$

This allows us to form equations where only θ 's are unknown: So we can make equations that only θ 's are unknown, and we can find these parameters using estimated kernel mean embeddings.

Recall that the relationship for $p_{\theta}(\mathbf{x}_{j})$ is:

$$\hat{p}_{\theta}(\mathbf{x}_j) = \frac{\exp(\hat{\theta}_n(\mathbf{x}_j))}{\sum_{j=1}^n \exp(\hat{\theta}_n(\mathbf{x}_j))}.$$

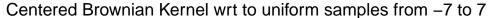
Specify the grid and centering grid

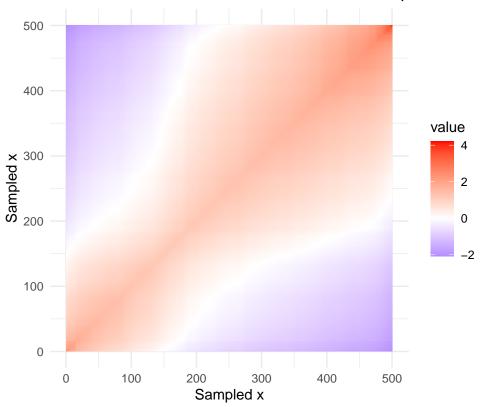
```
sampled_x <- vec_fixed_points
x_grid <- seq(-7,7,length.out = 1000)
# centering_grid <- sampled_x This doesn't work because using this centering grid the kernel mean embed
centering_grid <- runif(min = -7,max = 7,n = 1000)</pre>
```

Find Kernel Matrices:

\mathbf{H}_{sample} :

```
centered_kernel_mat_at_sampled <- centered_kernel_matrix(first_vec_kernel = sampled_x,</pre>
                                                          second_vec_kernel = sampled_x,
                                                          centering_grid = centering_grid,
                                                          hurst_coef = 0.5)
library(ggplot2)
library(reshape2)
## Warning: package 'reshape2' was built under R version 4.3.2
##
## Attaching package: 'reshape2'
## The following object is masked from 'package:tidyr':
##
       smiths
# Convert matrix to a data frame
matrix_df <- melt(centered_kernel_mat_at_sampled)</pre>
# Plot using ggplot2
ggplot(matrix_df, aes(Var1, Var2, fill = value)) +
  geom_tile() +
  scale_fill_gradient2(low = "blue", mid = "white", high = "red") +
 theme_minimal() +
  coord_fixed() + # Ensures the plot is square
  labs(title = "Centered Brownian Kernel wrt to uniform samples from -7 to 7", x = "Sampled x", y = "Sa
```

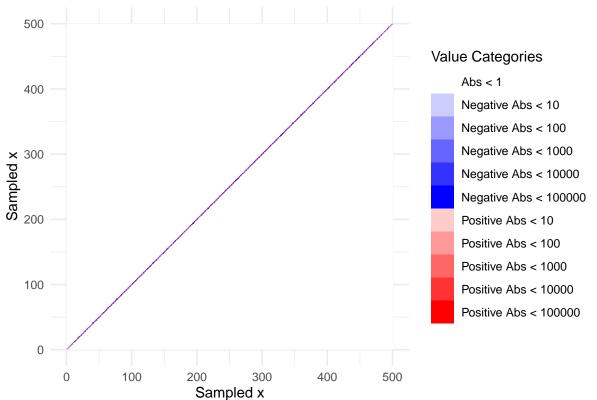




```
library(ggplot2)
library(reshape2)
library(dplyr)
# Convert matrix to a data frame
matrix_df <- melt(solve(centered_kernel_mat_at_sampled))</pre>
# Define the color categories based on the absolute value and sign of 'value'
matrix_df <- matrix_df %>%
  mutate(category = case_when(
    abs(value) < 1 ~ "Abs < 1",
    value > 0 & abs(value) < 10 ~ "Positive Abs < 10",</pre>
    value < 0 & abs(value) < 10 ~ "Negative Abs < 10",</pre>
    value > 0 & abs(value) < 100 ~ "Positive Abs < 100",</pre>
    value < 0 & abs(value) < 100 ~ "Negative Abs < 100",</pre>
    value > 0 & abs(value) < 1000 ~ "Positive Abs < 1000",</pre>
    value < 0 & abs(value) < 1000 ~ "Negative Abs < 1000",</pre>
    value > 0 & abs(value) < 10000 ~ "Positive Abs < 10000",</pre>
    value < 0 & abs(value) < 10000 ~ "Negative Abs < 10000",</pre>
    value > 0 & abs(value) < 100000 ~ "Positive Abs < 100000",</pre>
    value < 0 & abs(value) < 100000 ~ "Negative Abs < 100000",</pre>
    TRUE ~ "Other"
  ))
# Map the categories to colors
category_colors <- c(</pre>
```

```
"Abs < 1" = "white",
  "Positive Abs < 10" = rgb(1, 0, 0, alpha = 0.2),
  "Negative Abs < 10" = rgb(0, 0, 1, alpha = 0.2),
  "Positive Abs < 100" = rgb(1, 0, 0, alpha = 0.4),
  "Negative Abs < 100" = rgb(0, 0, 1, alpha = 0.4),
  "Positive Abs < 1000" = rgb(1, 0, 0, alpha = 0.6),
  "Negative Abs < 1000" = rgb(0, 0, 1, alpha = 0.6),
  "Positive Abs < 10000" = rgb(1, 0, 0, alpha = 0.8),
  "Negative Abs < 10000" = rgb(0, 0, 1, alpha = 0.8),
  "Positive Abs < 100000" = rgb(1, 0, 0, alpha = 1),
  "Negative Abs < 100000" = rgb(0, 0, 1, alpha = 1),
  "Other" = "black"
)
# Plot using ggplot2
ggplot(matrix_df, aes(Var1, Var2, fill = category)) +
  geom_tile() +
  scale_fill_manual(values = category_colors, name = "Value Categories") +
  theme_minimal() +
  coord_fixed() + # Ensures the plot is square
  labs(
   title = "Inverse Centered Brownian Kernel wrt to uniform samples from -7 to 7",
   x = "Sampled x", y = "Sampled x"
```

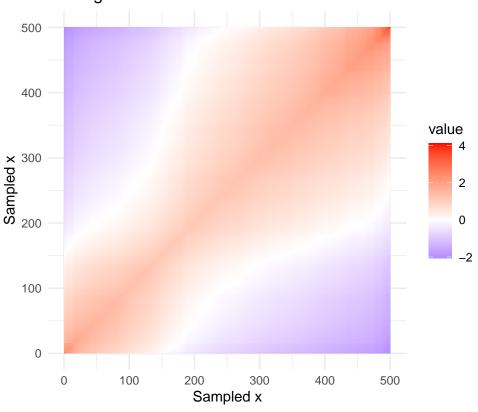
Inverse Centered Brownian Kernel wrt to uniform samples from -7 to 7



```
# Convert matrix to a data frame
matrix_df <- melt(gram)

# Plot using ggplot2
ggplot(matrix_df, aes(Var1, Var2, fill = value)) +
    geom_tile() +
    scale_fill_gradient2(low = "blue", mid = "white", high = "red") +
    theme_minimal() +
    coord_fixed() + # Ensures the plot is square
    labs(title = "Initial gram matrix centered wrt a uniform distribution from -7 to 7", x = "Sampled x",</pre>
```

Initial gram matrix centered wrt a uniform distribution from -7 to 7



```
# Positive Definiteness of centered_kernel_mat_at_sampled

# Get the eigenvalues
eigenvalues <- eigen(centered_kernel_mat_at_sampled)$values

# Check if all eigenvalues are positive
is_positive_definite <- all(eigenvalues > 0)
is_positive_definite

## [1] TRUE

# Check if the matrix is symmetric
is_symmetric <- all(centered_kernel_mat_at_sampled == t(centered_kernel_mat_at_sampled))
is_symmetric</pre>
```

Find the probabilities:

```
p <- solve(centered_kernel_mat_at_sampled) %*% df_all$regularized
sum(p)

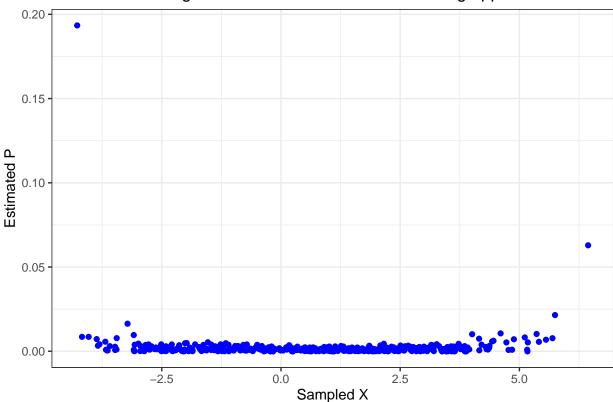
## [1] 4.743184

p <- p/sum(p)

plot_data <- data.frame(x = vec_fixed_points, prob = p)

ggplot(plot_data, aes(x,prob)) + geom_point(color = "blue") + labs(title = "Estimated P using estimated x = "Sampled X", y = "Estimated P") + theme_bw()</pre>
```

Estimated P using estimated Kernel Mean Embedding approximation



Find ln(p):

```
ln_p \leftarrow log(p - 2* min(p))
```

Find U weights:

```
one_n <- rep(1, length(sampled_x))
one_m <- rep(1, length(x_grid))

u_vec <- one_m %*% t(centered_kernel_mat_at_grid) %*% solve(centered_kernel_mat_at_sampled)</pre>
```

Find the θ 's:

```
C <- - as.vector(u_vec %*% ln_p) / as.vector(one_n %*% ln_p)
theta <- ln_p + C</pre>
```

Estimate the probabilities:

```
centered_kernel_self_grid <- diag(centered_kernel_mat_at_sampled)
estimated_p <- exp(theta + 0.5 * centered_kernel_self_grid)
sum(estimated_p,na.rm = T)
## [1] 2.941353</pre>
```

Show the result:

