# 1-. Theoretical/Kernel density function on a histogram

```
(Example 1.1-Exercises Bank)
```

#### Histogram:

```
hist( data, breaks = whatever, xlab = "", ylab = "", main = "",
    prob = TRUE)
```

#### How to plot theoretical density function on a histogram:

## How to plot the Kernel Density Function on a histogram:

```
lines( density(data, bw = value),
lwd = 2, col = "red")
```

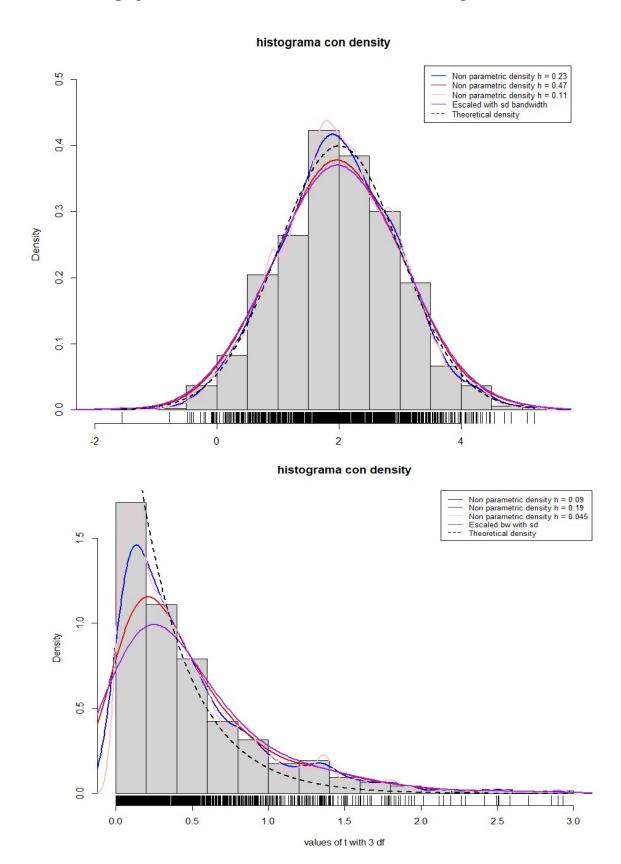
#### How to add a legend

```
legend( "position_legend",
    legend = c(names_in_legend),
    col = c(color_of_lines),
    lty = c(lines_types),
    cex = size legend)
```

#### Different ways for bw:

```
fx = density(data)
1-. density(data, bw = fx$bw*2)
2-. density(data, bw = fx$bw*0.5)
3-. density(data, bw = sd(data)/2)
Note: more bw smoother, less bw squigglier..
(Check Exercise 3 Chapter 1)
```

Note: Remember KDE is worse for distrubution like the Exponential (picture 2). That's why the exponential converges to infinity when it tends to 0. Conversely, it works very good for function such as normal (picture 1).



# 1-. Montecarlo:

## Montecarlo Integral:

$$\int_{a}^{b} f(x) dx$$

```
1-. realizations = runif(M, a , b)
2-. We evaluate these realizations
for (i in 1:M) {
    sum = 0
    sum = sum + f(realizations[i])
```

Basic Montecarlo Example:

<u>Montecarlo:</u> we know ahead of calculating anything the underlying distribution of the data.

```
M = 1000
storage = numeric(M) # Storing results for each montecarlo iteration
for (i in 1:M) {
    # We need to generate different noise in each iteration
    noise = rnorm(1000, mean = 10, sd = 2)
    # We add that noise to whatever, for example
    Y = true_theta*x + noise
    # And now we calculate what we are interested in...
    ...
}
```

**Note:** remember Montecarlo is based on CLT (Central Limit Theorem). So that, the more M or the more N we have the better our estimation will be. (Check exercise  $3\ b)\ 2019)$ 

```
Moreover, if we are trying to estimate the sd of a distribution Sd(storage) = sd(distribution) / root(N) (CLT) (check 02_Rscrip_L14) (We should know ahead of calculating anything sd of the distribution)
```

#### How to make a good boxplot

#### Statistics of interest for Montecarlo

```
1-. Bias: estimated value - real value
2-. Percentage of bias: (estimated value - real value) / real value
3-. Variance/sd: var(storage) or sd(storage)
4-. MSE: Bias^2 + Variance or mean( (estimated - real)^2 )
```

## Using abline

```
abline(h = horizontal line, v = vertical line, lwd = 2, col = "red")
```

# Storages variables

```
1-. storage = numeric(K)
2-. Storage = matrix(NA, nrow = nrow, ncol = ncol)
```

```
Non-parametric confidence interval
```

```
Ex) for a 95%
quantile(data, prob = c(0.025, 0.975))
```

<u>2-. Bootstrap:</u> We learn from the data without assiming an underlying distribution.

Bootstrap  ${\bf relies}$  on the assumption that the sample appropriately represents the underlying distribution.

Bootstrap takes an average of 63.4% of the data in each iteration.

```
Example of an easy bootstrap:

B = 100

storage = numeric(B) or matrix(NA, nrow = nrow, ncol = ncol)

n = nrow(data)

for (b in 1:B) {

    # We are generating a sample WITH REPLACEMENT

    temporal.index = sample(1:n, n, replace = TRUE)

    # We use the indeces now..

    temporal.data = data[temporal.index,]

    # We calculate whatever we wanted now...

...

}
```

Caution: We generate the indeces just ONCE in each iteration

```
Useful command if they are asking for lm (inside the loop)
```

```
temp.lm = lm(y \sim x , data = dat, subset = temp.index)
```

#### Function apply

```
apply(whatever, 2(columns) or 1(rows), mean/sd/median...)
```

## Statistics of interest for Bootstrap

- 1-. Bias: estimated value value (taking all data)
- 2-. Percentage of bias: (estimated value value\_all\_data) /
  value\_all\_ data
- 3-. Variance/sd: var(storage) or sd(storage)
- **4-. MSE:** Bias^2 + Variance or mean( (estimated real)^2)

## Bootstrap confidence intervals

♦ Naïve or Non-Parametric interval:

$$(q_L, q_M)$$
 = quantile(storage, c(0.025,0.975)) - 95%

♦ Studentized CI

Bootstrap\_estimate +- 
$$t_{N-1,1-alpha/2} * se(boostrap_{estimate})$$

♦ Bootstrap CI

$$(2*value_{all_{data}}-q_{\rm M}, \qquad 2*value_{all_{data}}-q_{\rm L})$$
 (check exercise 3 part c) Assignment 1)

## 3-. Cross Validation:

- 1-. LOO: using as many folds as your data's rows has
  - ullet We use only one point for testing in each iteration and n-1 points for training.
  - ♦ We are OVERFITTING
  - ♦ Each point is tested just once.

### 2-. K-FOLD CV: (most important)

- lack We have k-folds of the same lengths
- lack Each point is just tested once
- lack The samleer sample, the smallet k-fold
- ♦ We'd like to have 70% training 30% testing

An easy K-fold Cross Validation

```
n = nrow(data)
Shuffle the data
data = data[sample(1:n, n, replace = F),]
Number of folds
K = 10
folds = cut(1:n, K, labels = F)
storage = numeric/matrix...
# Loop all over folds
for (k in 1:K){
    train.set = which(folds != k)
    test.set = which(folds == k)
    # And now we make whatever...
# But usually we fit a model with the training data and we check
```

errors with the test set (predictions...)

## 3-. Repeated K-fold CV:

```
An example is as follows:
n = nrow(data)
R = 10 \# repetitions
K = 10 \# Number of folds
folds = cut(1:n, K, labels = F) # folds
storages =...
# First loop
for (r in 1:R) {
      # Shuffle the data en each repetition
      Data = data[sample(1:n, n, replace = F),]
      for (k in 1:K) {
            train.set = which(folds != k)
            test.set = which(folds == k)
            # And now we make whatever...
            # But usually we fit a model with the training data and we
check errors with the test set (predictions...)
            # To store something changes
            storage[k + (r-1)*K] = whatever...
(Check exercise 3.7 Exercises Bank)
4-.Out-of-Bag Bootstrap:
Since in bootstrap we are generally taking 63.4% of the data. We will
use 63.4 training set and the remaining for test.
```

(Example 03 Out of Bag Boots Kfold - Chapter 03)

## 1-. Polynomial Regression

 $y \sim a + b*exp(c*x)$ 

 $y \sim log(a*b)/c$ 

```
We are constructing here a polynomial with ideally (N-1) degrees
R code:
polynomial = lm(y \sim x + I(x^2) + ... + I(x^r))
Plotting it
lines(x, fitted(polynomial), ...) # it has fitted values
Predicting with the polynomial
We use the coefficients
cc = coef(polynomial)
new = seq(min, max, length = 1)
y.pred = cc[1] + cc[2]*new + cc[3]*new^2 + ... + cc[r+1]*new^r
2-. NLS
R code:
model.nls = nls(y ~ formula,
      start = list(a = a1, b = b1, ...)) # Parameters involved in the
formula
Formula ex:
```

```
How to plot it
```

```
1-. lines(x, fitted(nls.model),...)
2-. curve(coeficients*x, ...)
Predict with it
We use the coefficients
cc = coef(nls.model)
new = seq(min, max, length = 1)
y.pred = coefficients*x
3-. OPTIM
(Example in 02_Optim.R - Chapters)
It should have three functions associated:
   1. Model: it will have the expression of your model.
Ex: (for a model y \sim \exp(theta*x)
model <- function(x, theta) {</pre>
  \ensuremath{\text{\#}} Here if we had more than one parameter we could use
  \# a = theta[1]
  \# b = theta[2]
  return(theta*x)
}
```

Important: this function must have theta as 1st parameter and return
a single value

2. Criterion: it will have the criterion to minimize such as MSE,

RMSE or whatever...

```
Ex:
crit <- function(theta,x,y){</pre>
  # RSS in this case...
  return( sum((y-model(x,theta))^2)
   3. Optim: we use optim function
Ex:
(optim.out <- optim(par=c(3), fn=crit, x=x, y=y,
                    method="L-BFGS-B",
                    lower=c(0.01), upper=c(3.05)))
Note: par could have been par = c(theta 1, theta 2, ...), as many
parameters as we have.
(See an example with more than one parameter in Exercise-11 Shiny
Apps)
Result: we can obtain the estimations for the parameters using
                             optim.out$par
Plot it
Since we have the coefficients we can use curve
curve(expression using par coefficients, lwd = ..., col = "")
4-. Grid Search
(Example 03_02_Grid_Search - Chapter 03)
In this scenario we are going to build a grid and then we are gonna
evaluate or criterion to see which point in the grid has the minimum
value associated.
R Code:
2-D grid search: when we have to optimize two parameters (i.e a and b)
L = length
a.grid = seq(min value, max value, length=L)
```

```
b.grid = seq(min_value, max_value, length=L)
# Storage
crt = matrix( NA , nrow = L, ncol = L)
# Loop all over the grid
for(i in 1:L) {
  for(j in 1:L) {
   crit[i,j] = crit(c(a.grid[i],a.grid[j], x, y)
 }
# We find the minimum
ij.best = which.min(crit.values)
ij.best = arrayInd(ij.best, .dim=dim(crt))
# grid search solutions:
a.best = a.grid[ij.best[1]]
b.best = b.grid[ij.best[2]]
# 3-D Plot grid search
persp(a.grid, b.grid, crt, col = "..", theta = angle)
contour(a.grid, b.grid, crt)
Note: this grid search is not only useful with optim it can be used
for splines as well...
(Example 02 2018 2019 - Winter 2018)
5-. Regularization: they are techniques to reduce the
overfitting of glm/lm. (i.e. they will increase a little
the train error but will reduce test error)
(Exercise 07 Exercise.R Exercises Bank Chapter 3)
We are going to stand out three regularization techniques.
R Code FOR ALL OF THEM:
```

They DO NOT HAVE FITTED VALUES

library(glmnet)

CAUTION: all of these three model requires  ${\bf x}$  (predictors) TO BE A MATTRX

xm = as.matrix(x)

We can tune the parameter lamda by grid search or using CV:

cv.l = cv.glmnet(xm[i.train,],y[i.train],grouped=FALSE)

#### Plot them

They have coefficients so go ahead with them with curve

Calculate training errors (since they do no have fitted values)

yh.r = predict(lasso/ridge/elastic ,newx=xm[train.set,])

#### Predict with them

yh.p = predict( lasso/ridge/elastic , newx = xm[-train.set,])

### 1-. Ridge

$$J_1(\theta) = \sum_{i=1}^{n} (Y_i - \theta_0 - \theta_1 X_{1,i} - \dots - \theta_p X_{p,i})^2 + \lambda \sum_{j=1}^{p} \theta_j^2$$

This technique does not drop from the model any variables.

R Code:

2-. LASSO

$$J_2(\theta) = \sum_{i=1}^{n} (Y_i - \theta_0 - \theta_1 X_{1,i} - \dots - \theta_p X_{p,i})^2 + \lambda \sum_{j=1}^{p} |\theta_j|$$

This technique is ABLE TO RULE OUT VARIABLES FROM THE MODEL.

R Code:

3-. Elastic Net

$$J_3(\theta) = \sum_{i=1}^n (Y_i - \theta_0 - \theta_1 X_{1,i} - \dots - \theta_p X_{p,i})^2 + \lambda_1 \sum_{j=1}^p \theta_j^2 + \lambda_2 \sum_{j=1}^p |\theta_j|$$

This technique is capable to drop variables from the model.

Is less strict than LASSO

R Code:

In this chapter we are trying to estimate the underlying distribution. So all the techninques are **NON-PARAMETRIC**.

These models WON'T HAVE COEFFICIENTS since we are estimates the underlying distribution...

#### 1-. Local Polynomial Regression

Although both of them has the capability of predict, their predictions will be PLAIN and so we would consider Splines insetead. (i.e. their prediction are far away from reality)

(03 B-Splines P-Splines (and predicting from polynomial regression).R)

## Lowess (1 vs 1)

CAUTION: lowess sorts the x values

It has fitted values lw\$y

#### R code:

```
lw = lowess(x, y)
```

#### Plot it

# Remember that lowess sorts the x values...

```
lines(sort(x), low$y # fitted values, col='red', lwd=3)
```

#### Predict with lowess

# We need to use approx since lowess is **not capabale to predict values outside its range** 

#### Interpolation

```
pred.low = approx(low$x, low$y, xout=newx, rule=2)$y
```

```
(don't care about warnings)
```

## Loess (1 vs many)

CAUTION: check output values are in the same order as input values

lo\$x - x ; lo\$y - y ; # It should give u all 0s

It has fitted values lo\$fitted

R code:

Span

By 0 to jittery
0.5 suitable

1 to smooth

lo = loess(y  $\sim$  x1 + x2 + ... + x\_n, span = value, degree = degree)

#### Plot it

# Remember that lowess sorts the x values...
points(x, lo\$fitted, col='navy', pch=15)

#### Predict with loess (Important)

#### Interpolation

pred.low = approx(lo\$x, lo\$fitted, xout=newx, rule=2)\$y

(don't care about warnings)

Note: we could have used for loess predict

pred.lo = predict(lo, newdata=data.frame(x=newx))

## 2-. Splines

They are very common when it comes to predict values outside our predictors' range such as temporal series... Since their predictions are more realistic than the local polynomial.

(Check that difference in:  $03\_B-Splines\_P-Splines$  (and predicting from polynomial regression).R)

There are mainly 2 types of splines: B and P Splines

#### **B-Splines**

Here is a cubic B-Spline with 3+J knots.

 $S(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \sum_{j=1}^{J} \alpha_j (x - x_j)^{3+}$ 

Total knots = degree of the spline + internal knots

#### R Code

library(splines)

#### Process:

1-. Set the B Spline (basis)

BM = bs(x, knots = c(knot\_1, knot\_2,...), df = degree\_Bspline # default
3)

With the knots we can control the tailance.

Note: usually the knots are the quantiles of  $\boldsymbol{x}$ 

Ex) knots = quantile(x, prob = c(0.25, 0.5, 0.75))

Plot the basis

```
matplot(x,BM,xlab="x",ylab="Spline basis",main="total_knots-basis", t
= 'b')
2-Fit a linear model y ~ BM
lm.out = lm(mM~BM) # of course it has fitted values
coef(lm.out) # Will have as many coefficients as knots has
Plot it
points(x, fitted(lm.out), t='1', col="red", lwd = 3)
Predict with it
pred = predict(lm.out, newdata = data_frame)
P-splines
They give us even a better tailance than B-Splines.
R Code
They have fitted values
# Smooth spline with spar set with CV
p1 = smooth.spline(age, mF, cv = TRUE)
par = p1\$spar
p2 = smooth.spline(age, mF, spar = par/2) # different spar
CAUTION: We need to check that they have the same order than x.
p1$x - x # should give u all 0s
If not we just need to sort {\bf x}
```

#### Plot it

```
points(x, fitted(P.spline), pch=15, col='navy')
```

#### Predicting

```
pred.pspline = predict(P.spline, x=newx)
```

# Other models

## lm / glm

The unique difference between both is that **lm uses least squares** and **glm uses maximum likelihood**.

#### Predict

```
pred = predict(lm/glm.model , newdata = should_be_dataframe)
```