1. Determinar la ecuación de calibración y comentarla brevemente.

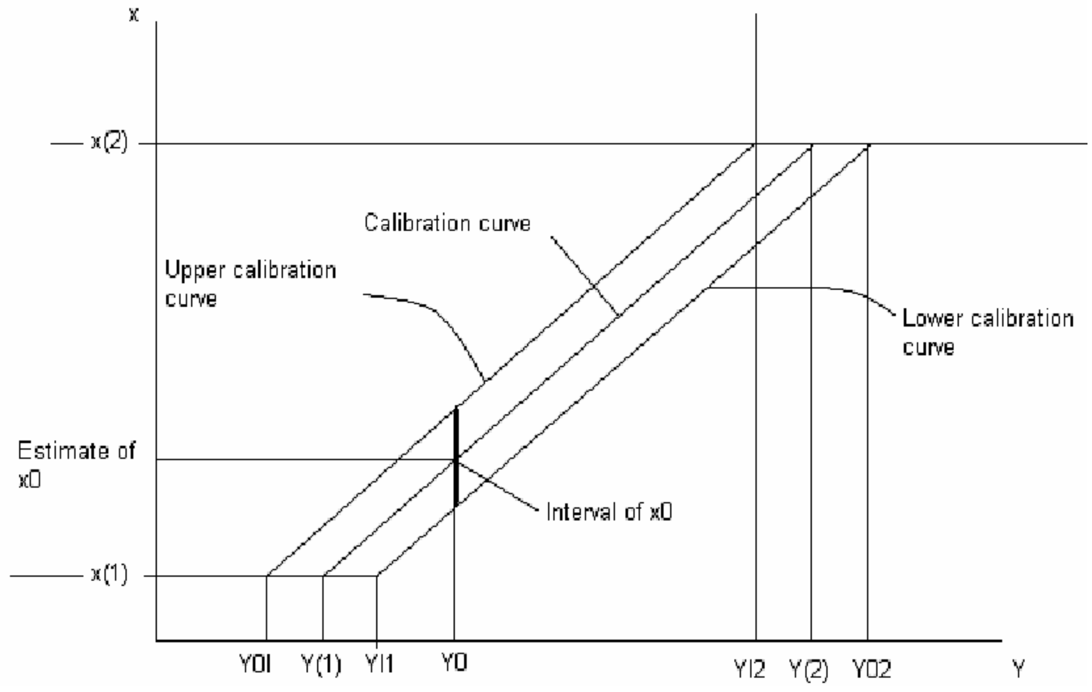
```
Coefficients: Uso do R[i]
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.006050   0.003721  -1.626    0.105
x            0.931153   0.003271 284.650   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Y = - 0,006050 + 0,931153 X

La media global $\hat{\beta}_0$ no es significativamente diferente de cero (p_valor > 0,1), mientras que la tasa de declive, $\hat{\beta}_1 = 0.931153$ es muy significativa. **X** representa la variable independiente, para muestras seleccionadas de carbono del experimento de calibración, y **Y** representa la variable dependiente, es la cantidad de carbono correspondiente.

2. Obtener el valor estimado del verdadero valor del contenido en carbono de las siguientes 4 muestras, así como la precisión en la estimación, en forma de desviación estándar e intervalo de confianza: 0,500; 1,000; 1,500; 2,000 i 2,5000.

Calibration Chart



Con el uso de los resultados de la pregunta número 1 y la expresión que hace referencia al intervalo de confianza (Thonnard, M. and Di Bucchianico, A. 2006)[ii] para las cuatro muestras, es posible estimar el valor real del contenido de carbono a través del intervalo de confianza para x0, para un determinado Y0.

$$IC(95\%) = \bar{x} + \frac{\hat{\beta}_1(\bar{Y}_0 - \bar{Y})}{a} \mp \frac{t_{\frac{\alpha}{2}:n+k-3}\,\hat{\sigma}}{a}\sqrt{a\left(\frac{1}{n}+\frac{1}{k}\right)+\frac{(\bar{Y}_0-\bar{Y})^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2}}$$

$$a = \hat{\beta}_1^{\,2} - \frac{\hat{\sigma}^2 t^2_{\frac{\alpha}{2}:n+k-3}}{\sum_{i=1}^{n}(x_i-\bar{x})^2}$$

```
>   x_mean<-mean(x);x_mean
[1] 0.76034

>   y_mean<-mean(y);y_mean
[1] 0.7019424

>   xi_xmean<-sum((x - x_mean)^2);xi_xmean
[1] 178.8741

>   reg1<-glm(formula = y ~ x);reg1
Coefficients:
(Intercept)            x
   -0.00605      0.93115

>   s_reg1<-summary(reg1);s_reg1

              Estimate     Std. Error    t value      Pr(>|t|)
(Intercept)  -0.006050     0.003721     -1.626        0.105
x             0.931153     0.003271     284.650       <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
    Null deviance: 155.5668  on 249  degrees of freedom

>   Yi_Ymean<-reg1$null.deviance;Yi_Ymean
[1] 155.5668

>   betas<-reg1$coefficients;betas
 (Intercept)             x
-0.006050489  0.931153022

>   b1<-betas[2];b1
       x
0.931153

>   Sb1<-s_reg1$coefficients[2,2];Sb1
[1] 0.003271219

>   S<-sqrt(Sb1^2*xi_xmean);S
[1] 0.04375054
```

Para un intervalo de confianza, dado
alpha=0.05
k=1; n=250
Y0=2.5

```
>   t_distr<-qt(1-alpha/2, n+k-3);t_distr
[1] 1.969576

>   a <- b1^2 - ((S^2)*(t_distr^2))/(xi_xmean);a
```

```
        x
0.8670044

>IC_inf<-round(x_mean+(b1*(Y0-y_mean))/a-((t_distr*S)/a)*sqrt(((Y0-
x_mean)^2/xi_xmean)+a*((1/n)+(1/k))),6)

>IC_sup<-round(x_mean+(b1*(Y0-y_mean))/a+((t_distr*S)/a)*sqrt(((Y0-
x_mean)^2/xi_xmean)+a*((1/n)+(1/k))),6)

             IC_inf   -  IC_sup
k=1,Y0=2.5 "(2.597809 ; 2.785059)"
```

llega a la conclusión de que:

```
> sqrt(Sb1^2*xi_xmean)
```

$\hat{\sigma}$ = 0.04375054

Intervalos de confianza para k=1,2…10, Y0 = (0.5; 1; 1.5; 2; 2.5)

```
> tabla
[[1]]
             IC_inf   -  IC_sup
k=1,Y0=0.5 "(0.450708 ; 0.636205)"
k=1,Y0=1   "(0.987705 ; 1.173196)"
k=1,Y0=1.5 "(1.524554 ; 1.710336)"
k=1,Y0=2   "(2.061254 ; 2.247624)"
k=1,Y0=2.5 "(2.597809 ; 2.785059)"

[[2]]
             IC_inf   -  IC_sup
k=2,Y0=0.5 "(0.477730 ; 0.609183)"
k=2,Y0=1   "(1.014728 ; 1.146173)"
k=2,Y0=1.5 "(1.551517 ; 1.683372)"
k=2,Y0=2   "(2.088099 ; 2.220780)"
k=2,Y0=2.5 "(2.624476 ; 2.758391)"

[[3]]
             IC_inf   -  IC_sup
k=3,Y0=0.5 "(0.489674 ; 0.597238)"
k=3,Y0=1   "(1.026674 ; 1.134227)"
k=3,Y0=1.5 "(1.563417 ; 1.671473)"
k=3,Y0=2   "(2.099908 ; 2.208970)"
k=3,Y0=2.5 "(2.636153 ; 2.746714)"

[[4]]
             IC_inf   -  IC_sup
k=4,Y0=0.5 "(0.496778 ; 0.590134)"
k=4,Y0=1   "(1.033779 ; 1.127122)"
k=4,Y0=1.5 "(1.570484 ; 1.664405)"
k=4,Y0=2   "(2.106901 ; 2.201978)"
k=4,Y0=2.5 "(2.643038 ; 2.739830)"

[[5]]
             IC_inf   -  IC_sup
k=5,Y0=0.5 "(0.501616 ; 0.585296)"
k=5,Y0=1   "(1.038617 ; 1.122284)"
k=5,Y0=1.5 "(1.575290 ; 1.659600)"
k=5,Y0=2   "(2.111641 ; 2.197238)"
k=5,Y0=2.5 "(2.647685 ; 2.735182)"
```

```
                 [[6]]
               IC_inf   -  IC_sup
k=6,Y0=0.5 "(0.505180 ; 0.581733)"
k=6,Y0=1   "(1.042181 ; 1.118720)"
k=6,Y0=1.5 "(1.578824 ; 1.656066)"
k=6,Y0=2   "(2.115117 ; 2.193761)"
k=6,Y0=2.5 "(2.651080 ; 2.731788)"

                 [[7]]
               IC_inf   -  IC_sup
k=7,Y0=0.5 "(0.507943 ; 0.578969)"
k=7,Y0=1   "(1.044946 ; 1.115956)"
k=7,Y0=1.5 "(1.581561 ; 1.653329)"
k=7,Y0=2   "(2.117802 ; 2.191076)"
k=7,Y0=2.5 "(2.653691 ; 2.729176)"

                 [[8]]
               IC_inf   -  IC_sup
k=8,Y0=0.5 "(0.510166 ; 0.576746)"
k=8,Y0=1   "(1.047169 ; 1.113732)"
k=8,Y0=1.5 "(1.583760 ; 1.651130)"
k=8,Y0=2   "(2.119952 ; 2.188926)"
k=8,Y0=2.5 "(2.655774 ; 2.727093)"

                 [[9]]
               IC_inf   -  IC_sup
k=9,Y0=0.5 "(0.512003 ; 0.574909)"
k=9,Y0=1   "(1.049007 ; 1.111894)"
k=9,Y0=1.5 "(1.585574 ; 1.649316)"
k=9,Y0=2   "(2.121723 ; 2.187156)"
k=9,Y0=2.5 "(2.657483 ; 2.725384)"

                 [[10]]
                IC_inf   -  IC_sup
k=10,Y0=0.5 "(0.513554 ; 0.573358)"
k=10,Y0=1   "(1.050558 ; 1.110343)"
k=10,Y0=1.5 "(1.587104 ; 1.647786)"
k=10,Y0=2   "(2.123211 ; 2.185668)"
k=10,Y0=2.5 "(2.658915 ; 2.723952)"
```

3. Obtener el valor mínimo que puede detectar el espectrómetro.

Utilizando el programa matemático Maple para obtener el límite de detección (xd) en cada medida, podemos obtener el valor de Y0 (= xd estimado) igualando a cero el límite inferior obtenido a través de la ecuación de Intervalo de Confianza; tenemos los siguientes valores mínimos:

Para k=1, Y0= 0.09260056203
Para k=2, Y0= 0.06749974693
Para k=3, Y0= 0.05642374795
Para k=4, Y0= 0.04984658782
Para k=5, Y0= 0.04537517149
Para k=6, Y0= 0.04208692155
Para k=7, Y0= 0.03954081927
Para k=8, Y0= 0.03749605019
Para k=9, Y0= 0.03580854776
Para k=10,Y0= 0.03438616465

Como se describe a continuación:

>

$$C\_inf \rightarrow x\_mean + \frac{b1\,(Y0 - y\_mean)}{a} + \frac{t\_distr\,S\,\sqrt{\frac{(Y0 - x\_mean)^2}{xi\_xmean} + a\left(\frac{1}{n} + \frac{1}{k}\right)}}{a} = 0$$

> $x\_mean := 0.76034$

$$x\_mean := 0.76034$$

> $b1 := 0.931153$

$$b1 := 0.931153$$

> $t\_distr := 1.969576$

$$t\_distr := 1.969576$$

> $S := 0.04375054$

$$S := 0.04375054$$

> $xi\_xmean := 178.8741$

$$xi\_xmean := 178.8741$$

> $a := 0.8670044$

$$a := 0.8670044$$

> $n := 250$

$$n := 250$$

> $k := 1$

$$k := 1$$

> IC_inf := x_mean + (b1*(Y0-y_mean))/a + t_distr*S/a*sqrt(((Y(
-x_mean)^2/xi_xmean) + a*((1/n) + (1/k)))

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0 - 0.76034)^2 + 0.8704724176}$$

> -solve(IC_inf)

$$0.09260056203$$

> $k := 2$

$$k := 2$$

> IC_inf := x_mean + (b1*(Y0-y_mean))/a + t_distr*S/a*sqrt(((Y(
-x_mean)^2/xi_xmean) + a*((1/n) + (1/k)))

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0 - 0.76034)^2 + 0.4369702176}$$

> -solve(IC_inf)

$$0.06749974693$$

> $k := 3$

$$k := 3$$

> $IC\_inf := x\_mean + (b1*(Y0-y\_mean))/a + t\_distr*S/a*\text{sqrt}(((Y($
> $-x\_mean)\hat{}2/xi\_xmean) + a*((1/n) + (1/k)))$

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0-0.76034)^2 + 0.2924694843}$$

> $-solve(\text{IC\_inf})$

$$0.05642374795$$

> $k := 4$

$$k := 4$$

> $IC\_inf := x\_mean + (b1*(Y0-y\_mean))/a + t\_distr*S/a*\text{sqrt}(((Y($
> $-x\_mean)\hat{}2/xi\_xmean) + a*((1/n) + (1/k)))$

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0-0.76034)^2 + 0.2202191176}$$

> $-solve(\text{IC\_inf})$

$$0.04984658782$$

> $k := 5$

$$k := 5$$

> $IC\_inf := x\_mean + (b1*(Y0-y\_mean))/a + t\_distr*S/a*\text{sqrt}(((Y($
> $-x\_mean)\hat{}2/xi\_xmean) + a*((1/n) + (1/k)))$

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0-0.76034)^2 + 0.1768688976}$$

> $-solve(\text{IC\_inf})$

$$0.04537517149$$

> $k := 6$

$$k := 6$$

> $IC\_inf := x\_mean + (b1*(Y0-y\_mean))/a + t\_distr*S/a*\text{sqrt}(((Y($
> $-x\_mean)\hat{}2/xi\_xmean) + a*((1/n) + (1/k)))$

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0-0.76034)^2 + 0.1479687509}$$

> $-solve(\text{IC\_inf})$

$$0.04208692155$$

> $k := 7$

$$k := 7$$

> $IC\_inf := x\_mean + (b1*(Y0-y\_mean))/a + t\_distr*S/a*\text{sqrt}(((Y($
> $-x\_mean)\hat{}2/xi\_xmean) + a*((1/n) + (1/k)))$

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0 - 0.76034)^2 + 0.1273257890}$$

\> -solve(IC_inf)

$$0.03954081927$$

\> k := 8

$$k := 8$$

\> IC_inf := x_mean + (b1*(Y0-y_mean))/a + t_distr*S/a*sqrt(((Y(-x_mean)^2/xi_xmean) + a*((1/n) + (1/k)))

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0 - 0.76034)^2 + 0.1118435676}$$

\> -solve(IC_inf)

$$0.03749605019$$

\> k := 9

$$k := 9$$

\> IC_inf := x_mean + (b1*(Y0-y_mean))/a + t_distr*S/a*sqrt(((Y(-x_mean)^2/xi_xmean) + a*((1/n) + (1/k)))

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0 - 0.76034)^2 + 0.09980183982}$$

\> -solve(IC_inf)

$$0.03580854776$$

\> k := 10

$$k := 10$$

\> IC_inf := x_mean + (b1*(Y0-y_mean))/a + t_distr*S/a*sqrt(((Y(-x_mean)^2/xi_xmean) + a*((1/n) + (1/k)))

$$IC\_inf := 0.0065072732 + 1.073988783\,Y0 + 0.09938820791\sqrt{0.005590524285\,(Y0 - 0.76034)^2 + 0.09016845760}$$

\> -solve(IC_inf)

$$0.03438616465$$

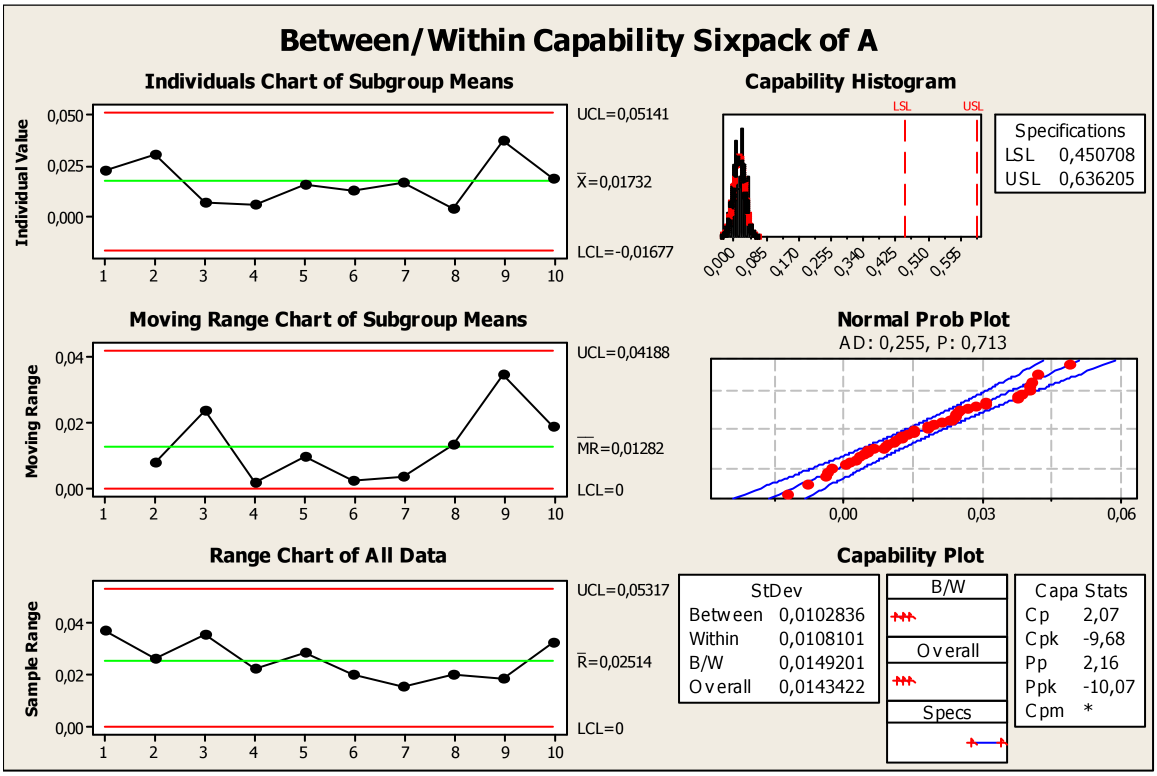
\>

4. ¿Muestran los datos algún comportamiento destacable?

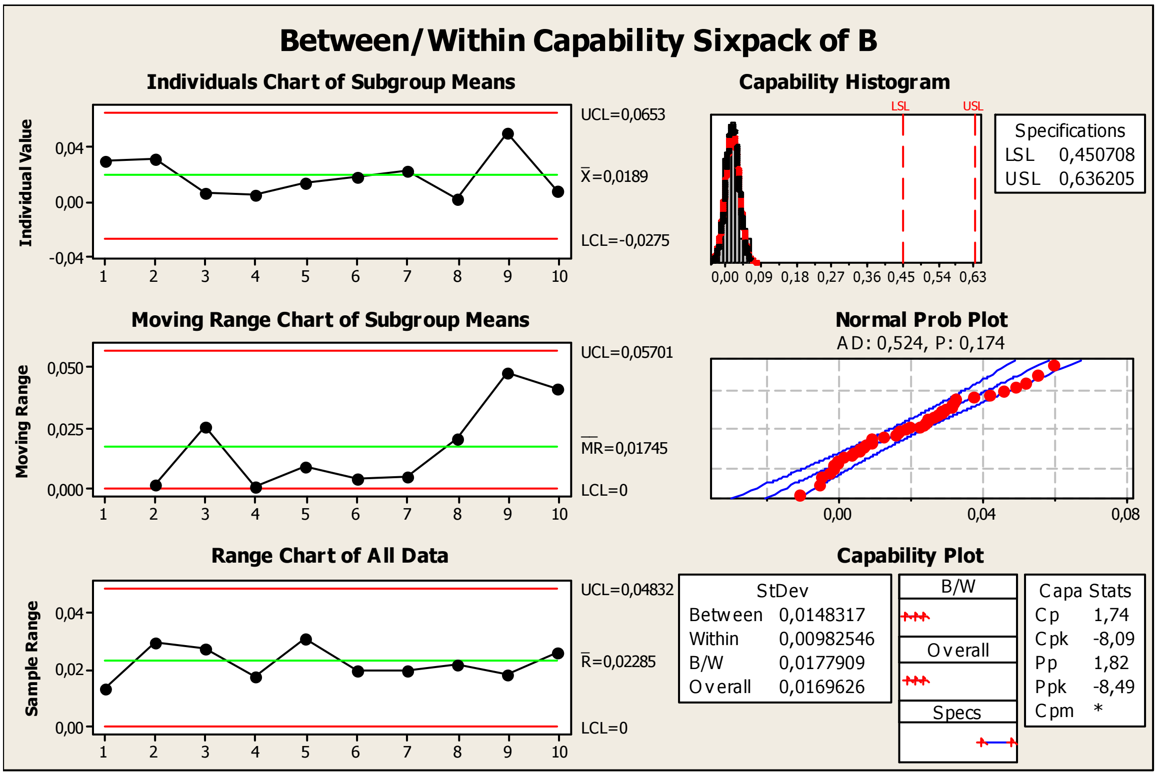
Los gráficos que siguen se refieren al estudio de las cinco muestras por separado. Para cada muestra, se les dio el límite inferir y superior del intervalo de confianza, de acuerdo a los datos:

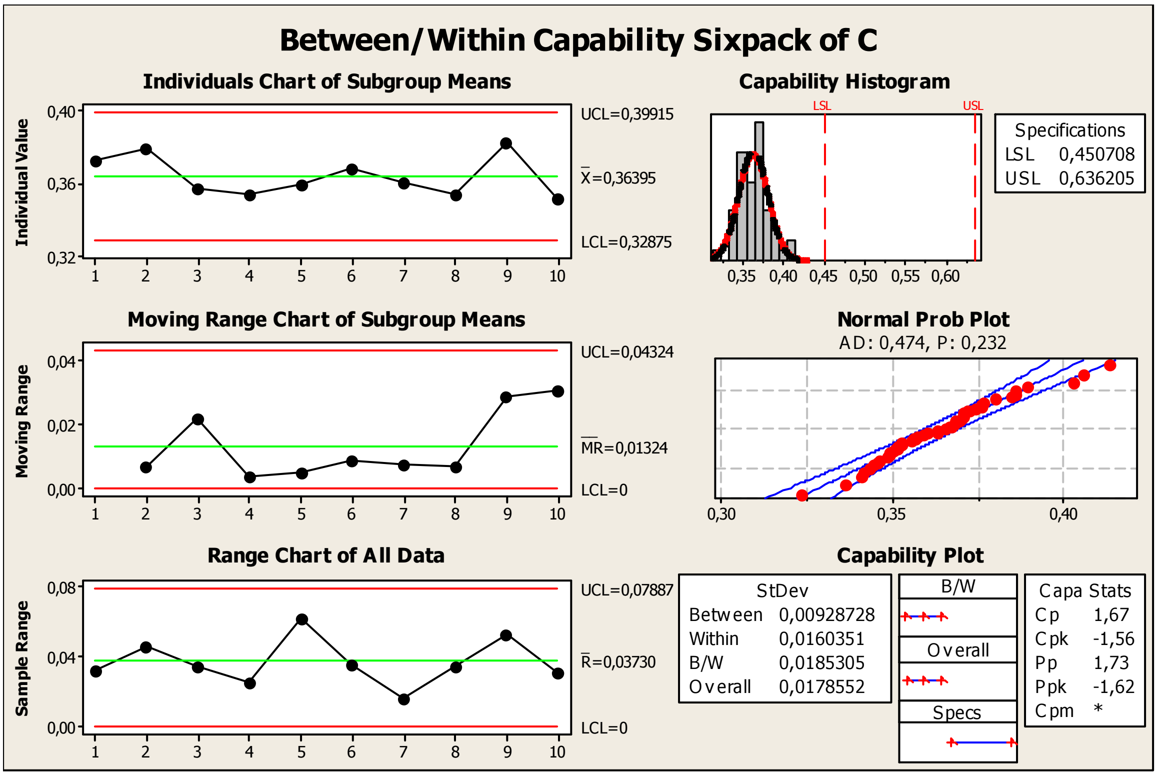
k=1
Y0=0.5
IC(95%)=(0.450708;0.636205)

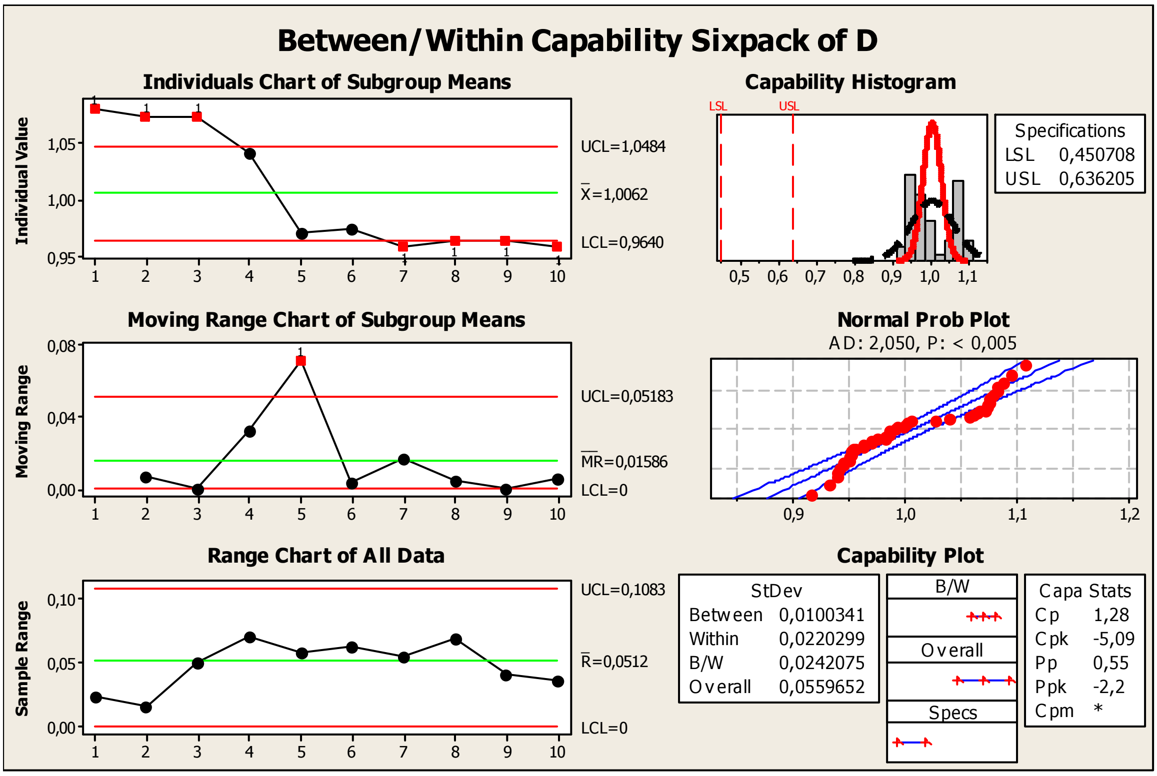
El resultado indica una distribución normal de las muestras A, B, C y E. Estas muestras se encuentran dentro del límite de control, es decir, no hay variaciones significativas en los resultados durante los 10 días. Dado que la muestra D presenta bastante inusual y es indicativo de que existe algún factor que influye en esta muestra, que tiene una distribución que no es normal, y está casi totalmente fuera de los límites de control, con una fuerte caída en los días 4 y 5, pasando del límite superior para el límite inferior del intervalo de confianza muy rápidamente. Otra cosa interesante es que en el día 9 las muestras A, B y C tienen un valor mayor, posiblemente algún factor también influyó en las tres muestras, en el día 9.

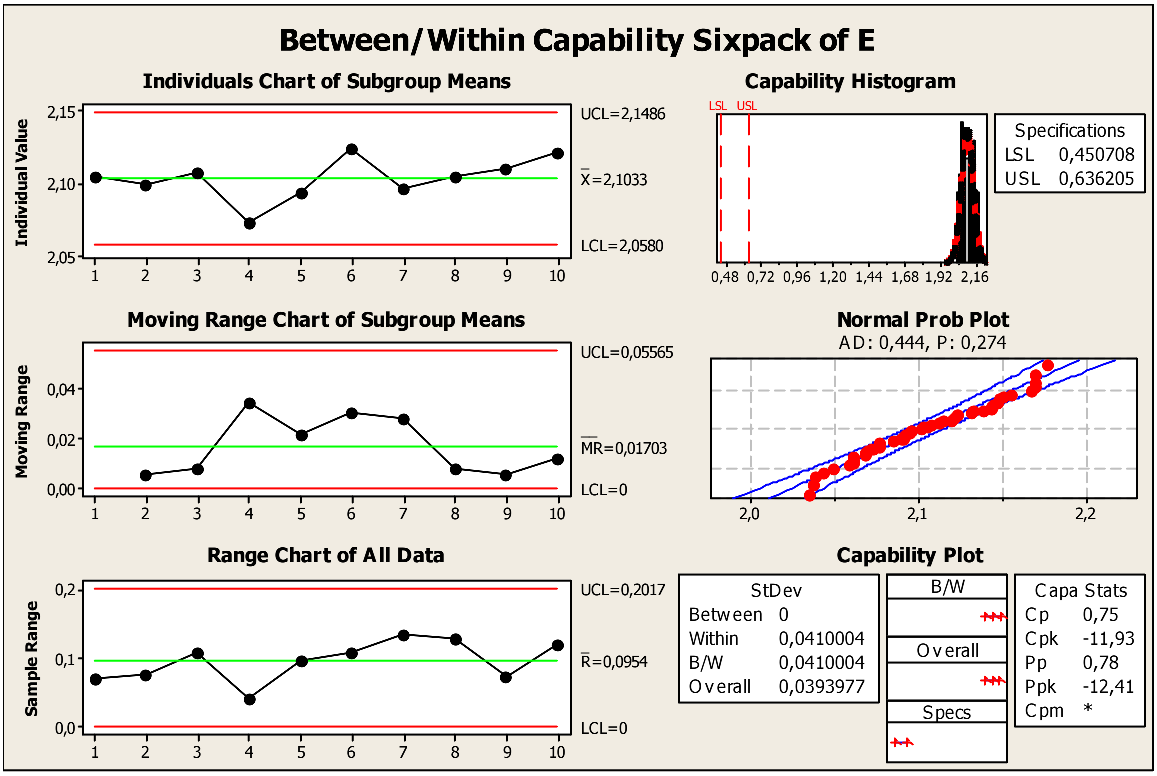


Cas 2.2: Calibratge d´un espectròmetre: (Parte 2)






Between/Within Capability Sixpack of D
Individuals Chart of Subgroup Means
UCL=1,0484
X̄=1,0062
LCL=0,9640
Capability Histogram
LSL USL
Specifications
LSL 0,450708
USL 0,636205
Moving Range Chart of Subgroup Means
UCL=0,05183
MR=0,01586
LCL=0
Normal Prob Plot
AD: 2,050, P: < 0,005
Range Chart of All Data
UCL=0,1083
R̄=0,0512
LCL=0
Capability Plot
StDev
Between 0,0100341
Within 0,0220299
B/W 0,0242075
Overall 0,0559652
B/W
Overall
Specs
Capa Stats
Cp 1,28
Cpk -5,09
Pp 0,55
Ppk -2,2
Cpm *


Between/Within Capability Sixpack of E
Individuals Chart of Subgroup Means
UCL=2,1486
X̄=2,1033
LCL=2,0580
Capability Histogram
LSL USL
Specifications
LSL 0,450708
USL 0,636205
Moving Range Chart of Subgroup Means
UCL=0,05565
MR=0,01703
LCL=0
Normal Prob Plot
AD: 0,444, P: 0,274
Range Chart of All Data
UCL=0,2017
R̄=0,0954
LCL=0
Capability Plot
StDev
Between 0
Within 0,0410004
B/W 0,0410004
Overall 0,0393977
B/W
Overall
Specs
Capa Stats
Cp 0,75
Cpk -11,93
Pp 0,78
Ppk -12,41
Cpm *

ANEXO – Código R.

```
A<-
c(0.0246,0.0032,0.0401,0.0248,0.0233,0.0151,0.0416,0.0229,0.0372,0.0382,0.0234,0.018,0.0062,-
0.0121,0.001,0.0025,0.0149,0.0183,-0.0037,-0.0028,-
0.0041,0.0211,0.0241,0.0124,0.024,0.0092,0.0049,0.0249,0.0087,0.0179,0.0112,0.0119,0.0266,0.0193,0.0151,0.0123,-
0.0078,0.0086,0.0043,0.0002,0.0303,0.0404,0.0486,0.0303,0.04,0.0283,0.0106,0.0048,0.0138,0.0373)
B<-
c(0.0275,0.0377,0.0246,0.0311,0.0289,0.0315,0.0285,0.0222,0.0519,0.0242,0.0089,0.0073,-
0.0108,0.0088,0.0162,0.0158,0.0056,0.0055,-0.0015,-
0.0006,0.0298,0.0037,0.0322,0.0013,0.0039,0.0285,0.0091,0.0088,0.0248,0.0186,0.0249,0.0122,0.0261,0.0198,0.0321,-
0.0049,-0.0052,0.0166,-0.0017,0.0067,0.0416,0.0459,0.0555,0.0492,0.0598,0.0237,-0.0024,-0.0005,0.0165,0.0059)
C<-
c(0.3575,0.3895,0.3799,0.3704,0.3664,0.3725,0.3767,0.413,0.3671,0.3679,0.3363,0.3601,0.3697,0.3704,0.3516,0.3683,0.359
,0.351,0.3494,0.3431,0.386,0.3461,0.3707,0.3238,0.3703,0.3556,0.3757,0.3739,0.3846,0.3492,0.3559,0.3628,0.363,0.3682,0
.3524,0.3569,0.3757,0.3485,0.3455,0.3412,0.4028,0.3655,0.3857,0.3524,0.4055,0.3503,0.3445,0.3414,0.3515,0.372)
D<-
c(1.073,1.0825,1.0711,1.0878,1.0949,1.0778,1.0664,1.0824,1.0704,1.077,1.0599,1.0754,1.0573,1.0721,1.1073,1.0047,1.0752
,1.0389,1.0639,1.0267,0.9996,0.9928,0.9514,0.9692,0.9417,0.9539,0.9977,1.0022,0.9822,0.939,0.9446,0.9316,0.9861,0.9851
,0.9449,0.9507,0.9818,0.9848,0.985,0.9157,0.9555,0.9692,0.9915,0.95,0.9513,0.9393,0.9628,0.9614,0.9494,0.9746)
E<-
c(2.1321,2.1385,2.0915,2.0941,2.068,2.0853,2.1476,2.0733,2.1194,2.0717,2.1428,2.1446,2.0371,2.0892,2.1226,2.1027,2.061
3,2.0608,2.0692,2.0684,2.0351,2.0766,2.1144,2.1127,2.1312,2.1688,2.1471,2.1689,2.0608,2.0762,2.1079,2.0946,2.0593,2.04
29,2.176,2.1666,2.1217,2.0391,2.1018,2.0903,2.0953,2.1205,2.1504,2.1049,2.0766,2.1695,2.1546,2.0903,2.0498,2.1427)

x<-c(rep(0.0158,50),rep(0.0299,50),rep(0.3710,50),rep(1.1447,50),rep(2.2403,50))
mean(x)==mean(c(0.0158,0.0299,0.3710,1.1447,2.2403))
y<-c(A,B,C,D,E)
n<-length(x);n
sum(A+B+C+D+E)
sum(x)
sum(y)

#################################################################
## Función Intervalo de Confianza para la Regresión Inversa ##
#################################################################

IC_Reg_Inv<-function(x=x,y=y,alpha=0.05,k=k,Y0=Y0)
{
  x_mean<-mean(x);x_mean
  y_mean<-mean(y);y_mean
  xi_xmean<-sum((x - x_mean)^2);xi_xmean

  reg1<-glm(formula = y ~ x);reg1
  s_reg1<-summary(reg1);s_reg1

  Yi_Ymean<-reg1$null.deviance;Yi_Ymean
  betas<-reg1$coefficients;betas
  b1<-betas[2];b1
  Sb1<-s_reg1$coefficients[2,2];Sb1
  S<-sqrt(Sb1^2*xi_xmean);S

  t_distr<-qt(1-alpha/2, n+k-3);t_distr
  a <- b1^2 - ((S^2)*(t_distr^2))/(xi_xmean);a

  IC_inf<-x_mean+(b1*(Y0-y_mean))/a-((t_distr*S)/a)*sqrt(((Y0-x_mean)^2/xi_xmean)+a*((1/n)+(1/k)))
  IC_sup<-x_mean+(b1*(Y0-y_mean))/a+((t_distr*S)/a)*sqrt(((Y0-x_mean)^2/xi_xmean)+a*((1/n)+(1/k)))
  IC<-cbind(paste("(",round(IC_inf,6)," ; ",round(IC_sup,6),")",sep=""));IC
  rownames(IC)<-c(paste("k=",k,",Y0=",Y0,sep=""))
  colnames(IC)<-c("  IC_inf   -  IC_sup")
  return(IC)
}

#questao 2
tabla=list()
for(i in 1:10)
{
  Y0_0.5<-IC_Reg_Inv(x=x,y=y,k=i,Y0=0.5);Y0_0.5
  Y0_1.0<-IC_Reg_Inv(x=x,y=y,k=i,Y0=1.0);Y0_1.0
  Y0_1.5<-IC_Reg_Inv(x=x,y=y,k=i,Y0=1.5);Y0_1.5
  Y0_2.0<-IC_Reg_Inv(x=x,y=y,k=i,Y0=2.0);Y0_2.0
  Y0_2.5<-IC_Reg_Inv(x=x,y=y,k=i,Y0=2.5);Y0_2.5
  tabla[[i]]<-rbind(Y0_0.5,Y0_1.0,Y0_1.5,Y0_2.0,Y0_2.5)
}
tabla

#Desviación Estándar
reg1<-glm(formula = y ~ x);reg1
s_reg1<-summary(reg1);s_reg1
x_mean<-mean(x);x_mean
y_mean<-mean(y);y_mean
xi_xmean<-sum((x - x_mean)^2);xi_xmean
t_distr<-qt(1-alpha/2, n+k-3);t_distr
Sb1<-s_reg1$coefficients[2,2];Sb1
S<-sqrt(Sb1^2*xi_xmean);S
Erro_max<-t_distr*S/sqrt(n);Erro_max
```

Referencias

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[i] Team, R.D.C. 2010, *R: A Language and Environment for Statistical Computing*, R Foundation for Statistical Computing, Vienna, Austria.

[ii] Thonnard, M. and Di Bucchianico, A. (2006). *Confidence intervals in inverse regression.* Technische Universiteit Eindhoven - Department of Mathematics and Computer Science)., http://alexandria.tue.nl/extra1/afstversl/wsk-i/thonnard2006.pdf.