Supplementary Information

Fighting Collinearity in QSPR Equations for Solution Kinetics with the Monte Carlo Method and Total Weighting

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Pascal code for MC confidence interval estimation

```
program regtemp (input,output);

  (* Nesta Versao o wi , calculado como no Constantinides, Pag. 570 *)
  (* Programa de Reg. Linear Multipla:
  (* Versao prov. p/ poder truncar as eq. *)
  (* alt no Z[i] *)
  (* versao alterada p/ 200 corridas e 67% IC *)
  (* DP do Aj calculado pelos Val. Medios dos coefic. *)

{N+}
{E+}
uses Printer,Crt,Dos;

Label  Voltar;

  Const
   FormFeed=#12; { para ejectar a p gina }
   NVarMax=10;
   NpontosMax=230;
Nvezes = 200;
   Perturb = 100.0;
   IC = 67;

 (*type
    Real= double;   *)
var
```

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```
i,j,k,l,m,n,Cont1,Transf,Expo,
n1,n2,n3,Flag2,Flag3,Nelim,aux1,aux2,
aux3,aux4,aux5,Continuar, N2Var,Imp,m1,
m2,npontos,npar,Eq,Code,Cpeso1     : integer;

baux,Qui2,r,Wtotal,Ymed,NAleat,YMed1,
corrV,SSE,SSR,Syy,VarAj,DpAj,corr2,corr,
corr2V,F,SomaZ,FV,Wtotal1,SigAux,
VarAji,Qui2i,DPAji,AleatMed,AleatVar       : Real;
    Uaux: Double;
pp,Pont,NVar,PesoEscrita                :String[20];
    Fich                              :String[60];

a,aM,a0,aMxy,AS2                        :Array[1..NVarMax,1..NVarMax] of Real;
b,c                                  :Array[1..NVarMax,1..NVarMax*2] of Real;
x                                    :Array[1..NVarMax,1..NPontosMax] of Real;
y,T,sig,YAux,Yaux1,Z,ZAux,w,ycalc,DeltaG,
    DeltaH,DeltaS, DeltaCp,SigDeltaG,
    SigDeltaH,SigDeltaS,SigDeltaCp          :Array[1..NPontosMax] of Real;
A0S2,A0M,A0M2,A0V,DPa                    :Array[1..NVarMax] of Real;
    U                                 :Array[1..1000] of Double;
    Elim                               :Array[1..NVarMax-1] of Integer;
FlagElim,Confirma,Col,Transfa,
Cpeso,RegTipo,RegTipo2,CalcErros         :Char;
{    aAux                               :array[1..NVarMax,1..NVarMax,1..Nvezes] of Real;}
    a0Aux                              :array[1..1,1..NVarMax,1..Nvezes] of Real;


 Procedure inicializa;

  Begin
for k:=1 to NVarMax do
   Begin
for j:= 1 to NVarMax do
     Begin
    (*  If Cont1=1 Then AM[k,j]:=0.0; *)
a[k,j]:=0;
a0[k,j]:=0;
c[k,j]:=0;
     End;
a0Aux[1,k,l]:=0.0;
   End;
```

```
for k:=1 to NVarMax do
   Begin
for j:= 1 to NVarMax do
     Begin
b[k,j]:=0;
     End;
   End;
  If (Flag2 = 0) Then
  Begin
for k:=1 to NPontosMax do
    Begin
      If (Cont1=1) Then
      Begin
        For i:=1 to NVarMax Do x[i,k]:=0.0;
sig[k]:=0.0;
      End;
y[k]:=0.0; w[k]:=0.0;
    End;
  End;
 End;

 Procedure invertematriz;
(* criar primeiro matriz com 'a' a esquerda e 'i' a direita *)

Begin
for i:= 1 to n  do
  Begin
for j:= 1 to n   do
Begin
b[i,j+n]:=0;
b[i,j]:=a[i,j];
    End;
b[i,i+n]:=1;
  End;

 (* operacoes sobre linhas para converter o lado esquerdo de b na matriz unidade *)
for k:=1 to n do
  Begin
if k=n then aux1:=1
else
     Begin
m:=k;
```

```
    (* encontrar o maximo *)
for i:=k+1 to n do
       Begin
        if abs(b[i,k]) > abs(b[m,k]) then m:=i;
       End;
if m=k then aux1:=1
else
       Begin
for j:=k to 2*n do
         Begin
baux:=b[k,j];
b[k,j]:=b[m,j];
b[m,j]:=baux;
          aux1:=1;
         End;
       End;
    End;
if aux1=1 then
    Begin
for j:=k+1 to 2*n do
      Begin
b[k,j]:=b[k,j]/b[k,k];
      End;
if k=1 then
      aux2:=1
else
      Begin
for i:=1 to k-1 do
        Begin
for j:=k+1 to 2*n do
          Begin
b[i,j]:=b[i,j]-b[i,k]*b[k,j];
          End;
        End;
if k=n then aux2:=2;
      End;
if aux2=1 then
for i:=k+1 to n do
         Begin
for j:=k+1 to 2*n do
          Begin
b[i,j]:=b[i,j]-b[i,k]*b[k,j];
```

```
          End;
        End;
  End;
 End;
for i:=1 to n do
   Begin
for j:=1 to n do
    Begin
b[i,j]:=b[i,j+n];
    End;
End;
End;

 Procedure guardarmatriz_a_em_c;
  (* guarda a matriz a na matriz c*)
var
i1,i2,i3: integer;

Begin
if (n1*n2<>0) then
     Begin
for i1:= 1 to n1 do
       Begin
for i2:=1 to n2 do
         Begin
c[i1,i2]:=a[i1,i2];
         End;
       End;
     End
else if (n1*n2=0) and  (n1<>0) then
for i1:=1 to n1 do
      Begin
c[i1,1]:=a[i1,1]
      End;
   End;

Procedure guardarmatriz_b_em_c;
  (* guarda a matriz b na matriz c*)
var
i1,i2,i3: integer;

Begin
```

```
if (n1*n2<>0) then
     Begin
for i1:= 1 to n1 do
       Begin
for i2:=1 to n2 do
         Begin
c[i1,i2]:=b[i1,i2];
         End;
       End;
     End
else if (n1*n2=0) and (n1 <>0) then
for i1:=1 to n1 do
      Begin
c[i1,1]:=b[i1,1];
      End;
End;


Procedure guardarmatriz_b_em_a;
  (* guarda a matriz b na matriz a*)
var
i1,i2,i3: integer;

Begin
if (n1*n2<>0) then
     Begin
for i1:= 1 to n1 do
       Begin
for i2:=1 to n2 do
         Begin
a[i1,i2]:=b[i1,i2];
         End;
       End;
     End
else if (n1*n2=0) and (n1 <>0) then
for i1:=1 to n1 do
      Begin
a[i1,1]:=b[i1,1];
      End;
     End;

Procedure guardarmatriz_c_em_b;
```

```
  (* guarda a matriz c na matriz b*)
var
i1,i2,i3: integer;

Begin
if (n1*n2)<>0 then
     Begin
for i1:= 1 to n1 do
       Begin
for i2:=1 to n2 do
         Begin
b[i1,i2]:=c[i1,i2];
         End;
       End;
     End
else if (n1*n2=0) and (n1 <>0) then
for i1:=1 to n1 do
      Begin
b[i1,1]:=c[i1,1];
      End;
End;


 Procedure multiplicamatriz;

 (* c=a x b; 'a' e' m1 por n1 e 'b' m2 por n2 e 'c' m1 por n2  *)

Begin
for i:=1 to m1 do
   Begin
for j:=1 to n2 do
    Begin
c[i,j]:=0;
for k:=1 to n1 do
      Begin
       c[i,j]:=c[i,j]+a[i,k]*b[k,j];
      End;
    End;
  End;
 End;
```

```
 Procedure imprimir;
  Begin
   Writeln;
for i:=1 to npar do
    Begin
for j:=1 to n do
      Begin
      (* Write(trunc(c[i,j]*1000 + 0.5)/1000,'    '); *)
      Write (c[i,j]:8:6,'   ');

      End;
     Writeln;
    End;
   Writeln;
  End;

Procedure LeFicheiros;

Var
Buf : Text;
  Result,l: Integer;
  Peso: Char;



Begin
  Result:=0;
  ClrScr;
GotoXY(5,10);
Write('               Nome Do Ficheiro (S/ EXTENSAO)? '  );
  Repeat
Readln(Fich);
(*  Fich:= 'c:\ruben\dados\rg012t1.dat';*)
 (*     Fich:= 'a:\numantln';*)
Fich := Fich + '.dat';
    Assign (Buf,Fich);
    (*$I-*)
Reset(Buf);
    (*$I+*)
    If IOresult <> 0 Then
      Begin
GotoXY(12,20);
```

```
Writeln('Esse Ficheiro nao existe !');
Delay(800);
       ClrScr;
     End
   Else Result:= 1;
  Until Result <> 0;
     Begin
       ClrScr;
j:=0;
GoToXY(1,1);
       For l:=1 To N2Var Do
Write('     X(',l,')  ');
Writeln('      Y        DP ');
Writeln( ' ');
       While Not Eof(Buf) Do
         Begin
j:= j+1;
           Begin
             If (RegTipo2 = '1') Then
             Begin
               For l:=1 To 1 Do
Read(Buf,x[l,j]);
               If RegTipo = '2' Then Readln(Buf,Z[j],sig[j])
else
               Begin
Readln(Buf,Z[j]);
w[j]:=1.0;
sig[j]:=1.0;
               End;
x[3,j]:=x[l,j];
x[2,j]:= ln(x[l,j]);
x[1,j]:=1/x[l,j];
               T[j]:=x[3,j];
GoToXY(1,2+j);
               For l:=1 To N2Var Do
               Write(x[l,j]:11);
Writeln(Z[j]:11,sig[j]:10);
             End
             Else If (RegTipo = '2') Then
           Begin
             For l:=1 To N2Var Do
Read(Buf,x[l,j]);
```

```
Readln(Buf,Z[j],sig[j]);
GoToXY(1,2+j);
            For l:=1 To N2Var Do
            Write(x[l,j]:11);
Writeln(Z[j]:11,sig[j]:10);
          End
          Else
          Begin
            For l:=1 To N2Var Do Read(Buf,x[l,j]);
Readln(Buf,Z[j]);
sig[j]:=1;
GoToXY(1,2+j);
            For l:=1 To N2Var Do
            Write(x[l,j]:11);
Writeln(Z[j]:11);

          End
        End;
        End;
      Npontos:= j;
Close(Buf);
End;
  For i:=1 To Npontos Do
  Yaux1[i]:=Z[i];
  For i:= 1 to 3 Do Writeln('  ');
Write('       Carregue numa tecla para continuar ');
Readln(pp); (* Readln(pp);  *)
Readln(pp);
End;

procedure dados;

  Var
Pontos,Aux5: Integer;

Label Truncar;

begin
   If (Flag2 = 0)  Then
   Begin
     (*GotoXY(20,3);
Writeln('Tipo de Regressao (1):  ');
```

```
GotoXY(20,6);
Writeln('(1)- Regressao p/ Eq. de Temperatura;  ');
GotoXY(20,7);
Writeln('(2)- Regressao Multipla;  ');
    Repeat Begin GoToXY(45,7); Read(RegTipo2); End
    Until (RegTipo2 = '1') or (RegTipo2 = '2');
    If (RegTipo2 = '1') Then
Begin
      GotoXY(8,9);
Write('Numero de Termos na Equacao (sem o Termo independente):');
Repeat Begin GoToXY(65,9); Readln(NVar); Val(NVar,N2Var,Code); End
      Until (N2Var in [1..5]);
    End
    Else *)
    Begin
     Regtipo2:='2';
     ClrScr;
GotoXY(12,3);
Write('Numero de Vari veis Independentes:');
    Repeat Begin GoToXY(50,3); Readln(NVar); Val(NVar,N2Var,Code); End
    Until (N2Var in [1..10]);
GotoXY(20,5);
    End;
Writeln('Tipo de Regressao :  ');
    GotoXY(20,6);
    Writeln('(1)- Regressao SEM Pesos;  ');
GotoXY(20,7);
Writeln('(2)- Regressao Pesada   ;  ');
    Repeat Begin GoToXY(45,7); Read(RegTipo); End
    Until (RegTipo = '1') or (RegTipo = '2');

GotoXY(20,10);
Writeln('Entrada de Pontos:');
GotoXY(20,11);
Writeln('(1)- Teclado ');
GotoXY(20,12);
Write('(2)- Ficheiro ');
    Repeat Begin GoToXY(45,12); Read(Pontos); End
Until (Pontos = 1) or (Pontos = 2);
    If (Pontos = 2) Then   (* se a entrada , por ficheiro *)
Begin
      If (RegTipo='2') Then  (* se a reg. , pesada *)
```

```
        Begin
          Writeln;
          Writeln;
Write( ' O Ficheiro Inclui (',N2Var+2,') Colunas (y, x(1..n) e D.P. de cada ponto) ?  (s/n)');
          Repeat
          Begin
GoToXY(70,15);
            Col:= ReadKey;
          End
          Until (UpCase(Col) ='N') or (UpCase(Col) = 'S');
          If (UpCase(Col)='N') Then
          Begin
ClrScr;
            GoTOXY(20,17);
Write('O seu Ficheiro Tem Apenas valores de y e x(1..n) ');
            GoTOXY(20,18);
Writeln('Nao , Poss¡vel Fazer Uma Regressao Pesada   ');
            GoTOXY(20,19);
Writeln('O Programa vai ler o Ficheiro. Em seguida introduza');
            GoTOXY(20,20);
Writeln('      os desvios padrao de cada um  ');
End;
          LeFicheiros;
          If (UpCase(Col)='N') and (RegTipo='2') Then
          Begin
            For j:=1 To Npontos Do
Begin
              ClrScr;
Write('Desvio Padrao do Ponto n§ ',j,': ');
Readln (sig[j]);
            End;
          End;
End
        Else LeFicheiros;(* se a reg. nao , pesada *)
      End
      Else If (pontos = 1) Then (* este else refere-se … opcao de entrada de pontos por teclado *)
      Begin
        Aux4:=3;

        ClrScr;
        GoToXY(10,2);
Write('numero de pontos ');Readln(npontos);
```

```
ClrScr;
Write('N§ ');
      For j:=1 To N2Var Do Write('   x(',j,')    ');
      If N2Var <=5 Then
        Begin
Write('   y(i)   ');
           If (RegTipo='2') Then Writeln('  sig(i)   ') else Writeln;
        End;
      If j=5 Then
         Begin
            Writeln;
GoToXY(4,2);
         End;
      If N2Var > 5 Then
      Begin
GoToXY(57,2);
         Write ('    y(i)   ');
         If RegTipo='2' Then Write('    sig(i)');
         Writeln;
      End;
      For i:=1 to Npontos do
       Begin
GoToXY(1,Aux4);
Write(i);
Aux5:=5;
        For j:=1 To N2Var Do
Begin
          If j=6 Then
            Begin
               Aux5:=5;
               Aux4:=Aux4+1;
            End;
GoToXY(Aux5,Aux4);
          Read(x[j,i]);
          Aux5:=Aux5+11;
GoToXY(Aux5,WhereY-1);
        End;
        If N2Var >5 Then Aux5:=59;
GoToXY(Aux5,WhereY);
Read(z[i]);
        (* GoToXY(30,Aux4); *)
        (*Write(' y(',i,')= ');*)
```

```
          Aux5:=Aux5+11;
GoToXY(Aux5,WhereY-1);
          If (RegTipo='1') Then Writeln
          Else
          If (RegTipo='2') Then Readln(sig[i]);
          Aux4:= Aux4+1;
         End;
     End;
Writeln( '  ');
(*  End; *)

   (*         ---   Crit,rios de Peso ----          *)

For i:= 1 to 25 Do Writeln('  ');
    If (RegTipo = '2')  THEN
    Begin
GotoXY(10,15);
Writeln ('              Crit,rio de peso :');
Writeln ('              (1) - Wi = 1/sig(y(i))^2');
      Writeln ('              (2) - Wi = (y(i)/sig(y(i)))^2');
      Writeln ('              (3) - Wi = 1/y(i)^2');
      Repeat Begin
GoToXY(50,18);
      CPeso:=ReadKey;
      End; Until (Cpeso ='1') or (Cpeso='2') or (Cpeso='3');
    End
    Else
    If (RegTipo = '1') Then
Begin
      Writeln (' Cada Ponto fica com peso 1');
For i:=1 to npontos do Begin sig[i]:=1.0; w[i]:=1.0; End;
    End;
   Npar:= N2Var+1;
GotoXY(18,20);
   If (N2Var > 1) Then
Begin
     Write   ('Quer Truncar a equacao ? (s/n) ');
Repeat Begin GotoXY(50,20); Read (FlagElim) End ;
     Until (UpCase(FlagElim) = 'S') or(UpCAse(FlagElim) = 'N') ;
     If (UpCase(FlagElim) = 'S') Then
     Begin
      ClrScr;
```

```
      For k:=1 To NVarMax-1 Do Elim[k]:=0;
      If (Npar = 3) Then
      Begin
GoToXY(20,8);
Writeln(' a0  +  a1*x1  +  a2*x2   ');
GoToXY(20,9);
Writeln('       (1)       (2)       ');
      End
      Else If (Npar = 4) Then
      Begin
GoToXY(20,8);
Writeln(' a0  +  a1*x1  +  a2*x2  +  a3*x3 ');
GoToXY(20,9);
Writeln('       (1)       (2)       (3)  ');
      End
      Else If (Npar = 5) Then
      Begin
GoToXY(20,8);
Writeln(' a0  +  a1*x1  +  a2*x2  +  a3*x3  +  a4*x4 ');
GoToXY(20,9);
Writeln('      (1)       (2)       (3)     (4)   ');
      End
      Else If (Npar = 6) Then
      Begin
GoToXY(20,8);
       Writeln(' a0  +  a1*x1  +  a2*x2  +  a3*x3  +  a4*x4  +  a5*x5  ');
GoToXY(20,17);
Writeln('(1)      (2)       (3)       (4)       (5)  ');
      End
      Else If (Npar = 7) Then
      Begin
GoToXY(20,3);
Writeln(' a0 + a1*x1 + a2*x2 + a3*x3 + a4*x4 + a5*x5 + a6*x6 ');
GoToXY(20,10);
Writeln('(1)     (2)     (3)     (4)     (5)     (6) ');
      End
      Else If (Npar = 8) Then
      Begin
GoToXY(20,3);
Writeln('a0 + a1*x1 + a2*x2 + a3*x3 + a4*x4 + a5*x5 + a6*x6 + a7*x7');
GoToXY(20,9);
Writeln('(1)     (2)     (3)     (4)     (5)     (6)     (7) ');
```

```
        End
        Else If (Npar = 9) Then
        Begin
GoToXY(20,2);
Writeln('a0 + a1*x1 + a2*x2 + a3*x3 + a4*x4 + a5*x5 + a6*x6 + a7*x7 + a8*x8');
GoToXY(20,8);
Writeln('(1)    (2)    (3)    (4)    (5)    (6)    (7)    (8) ');
        End
        Else If (Npar = 10) Then
        Begin
GoToXY(20,1);
Writeln('a0 + a1*x1 + a2*x2 + a3*x3 + a4*x4 + a5*x5 + a6*x6 + a7*x7 + a8*x8 + a9*x9');
GoToXY(20,7);
Writeln('(1)    (2)    (3)    (4)    (5)    (6)    (7)    (8)    (9) ');
        End
        Else If (Npar = 11) Then
        Begin
GoToXY(20,1);
Writeln('a0 + a1*x1 + a2*x2 + a3*x3 + a4*x4 + a5*x5 + a6*x6 + a7*x7 + a8*x8 + a9*x9 + a10*x10');
GoToXY(20,7);
Writeln('(1)    (2)    (3)    (4)    (5)    (6)    (7)    (8)    (9)    (10) ');
        End;

GoTOXY(20,13);
Write('Quantos Termos Quer Truncar ?');
Repeat Begin GoToXY(51,13); Read(Nelim); End
        Until (Nelim >= 1) and (Nelim <= Npar-2);
        Writeln;
k:=1;
        Truncar:
        For k:=1 To Nelim Do
        Begin
GoTOXY(20,16);
Write('Eliminar Termo N§: ');
Readln(Elim[k]);
GoTOXY(38,16);
Writeln('   ');
        End;
GoTOXY(20,18);
        If (Nelim = 1) Then
Write( 'O Termo a Eliminar ,: (',Elim[k],')')
        Else
```

```
Begin
Write( 'Os Termos a Eliminar sao: ');
For k:=1 To Nelim Do
Write('(',Elim[k],')   ');
        End;
Writeln(' ');
GoToXY(30,20);
Write('Confirma ? (s/n)');
Repeat Begin GotoXY(48,20); Read (Confirma) End ;
     Until (UpCase(Confirma) = 'S') or(UpCAse(Confirma) = 'N') ;
     If (UpCase(Confirma) = 'N') Then
     GoTo Truncar;
     ClrScr;
     End;
   End;
   End
   Else Eq:=1;
   If (UpCase(FlagElim) = 'S') Then
   Begin
    For k:=1 To N2Var Do
    Begin
      For i:=1 To Npontos Do
      Begin
if (Elim[k] > 0) Then
        Begin
          For j:= Elim[k] To N2Var Do x[j,i]:=x[j+1,i];
          If (i=Npontos) Then
          Begin
(*            For j:= k To N2Var Do Elim[j]:=Elim[j+1]-1;*)
Npar:= Npar-1;
            N2Var:=Npar-1;
          End;
End;
      End;
    End;


n:= Npar;
For i:=1 to npontos do For l:= Npar to NVarMax do x[l,i]:=0;
End;

   ClrScr;
```

```
Writeln('Transformacao da vari vel dependente: ');
Writeln(' ');
Writeln('              1 - s/ transformacao;');
Writeln('              2 - ln (y);');
Writeln('              3 - y^n);');
Writeln('              4 - (1/y)^n);');
Write('              5 - exp(y);');
Readln(Transf);
   If (Transf=2) Then
   Begin
ClrScr;
     GoToXY(10,20);
Write('Logaritmo (N)atural ou (D)ecimal ?');
GotoXY(10,40);
Readln(TransfA);
   End
   Else If (Transf=3) or (Transf=4) Then
Begin
     ClrScr;
     GoToXY(10,20);
Write('Valor do expoente `n` ');
GotoXY(10,50);
Readln(expo);
   End;
 End;

Procedure Transforma;


 Begin
  For i:=1 To Npontos do
  Begin
   If (Transf = 1) Then
   Begin
y[i]:= Z[i]
   End
   Else
   If (Transf = 2) Then
   Begin
     If (UpCase(TransfA) = 'D') Then
begin
     (* If (Z[i] <=0) Then Z[i] := 2e-29;*)
```

```
y[i]:= ln(Z[i])/ln(10)
end
     Else
y[i]:= ln(Z[i])
   End
   Else
   If (Transf = 3) Then
    Begin
      For j:=2 To n Do
      Begin
        If (j=2) Then y[i]:= Z[i]*Z[i]
        Else y[i]:=y[i]*Z[i];
      End;
    End
   Else
   If (Transf = 4) Then
    Begin
      For j:=1 To n Do
      Begin
        If (j=1) Then y[i]:= 1/Z[i]
          Else y[i]:=y[i]*1/Z[i];
      End;
    End
    Else If (Transf = 5) Then y[i]:=exp(z[i]);
  End;
 End;

Procedure Somas;

Type
   Pointer1 = ^ItensDoPointer1;
   ItensDoPointer1 = Record
                Somay    : Real;
                SomaYX   : Array [1..10] of Real;
                SomaX    : Array [1..10] of Real;
                SomaXX   : Array [1..10,1..10] of Real;
                End;
var
SomaAux : Pointer1;
    Aux,SigAux, UMaxAbs,ProdMinAbs: Real;
 Begin
   SomaAux:=Nil;
```

```
New(SomaAux);
   Wtotal:=0.0;
   Wtotal1:=0.0;
   Somaz:=0.0;
   If Aux5=1 Then
     Begin
        AleatMed:=0.0;
        AleatVar:=0.0;
        Naleat:=0.0;
     End;
If (Aux5>1) Then

   (* Redimensionar os val. aleat¢rios p/ o factor de perturbacao escolhido *)
Begin
     If Aux5=2 Then
     Begin
       For k:=1 To  1000 do U[k]:=U[k]*1e8;
(* determinar o UmaxAbsoluto *)
       UmaxAbs:=U[1];
For k:=2 to Npontos Do If Abs(U[k]) > Abs(U[k-1]) Then UMaxAbs:=Abs(U[k]);
(* determinar o produto minimo Perturb*Z[i] *)
       ProdMinAbs:=U[1];
       For k:=2 to Npontos Do If Abs(Perturb*Z[k])< Abs(Perturb*Z[k-1]) Then ProdMinAbs:=Abs(Perturb*Z[k]);
     {UAux:=U[Aux5]*1e8;
     For i:=1 To Npontos Do
     While (Abs(UAux) > Abs(Perturb*Z[i]))
      Do UAux:=UAux/10;  }
(*While UMaxAbs > ProdMinAbs Do For k:=1 To  1000 do U[k]:=U[k]/10;*)
     (*  For k:=1 To 1000 Do Write (U[k],'  ');*)
      For k:=1 To 1000 Do If Abs(U[k])> ProdMinAbs then
      For j:=1 to 1000 Do Begin k:=1;U[j]:=U[j]/10;End;
     End;
     For i:=1 to Npontos Do
     Begin
     If Transf=2 Then
     Begin
     (* Begin
if ZAux[i] + U[i] <=0 Then
         Begin
          For k:=1 To 1000 Do U[k]:=U[k]/10;
i:=1
End;       *)
```

```
        Z[i]:= ZAux[i] + U[i];
k:=Nvezes;
repeat Z[i]:= ZAux[i] + U[i+k+100];k:=k+1; until z[i] >0;
         UAux:=U[i];
{repeat Z[i]:= ZAux[i] + UAux; UAux:=UAux/10; Until Z[i] >0;}
      (* if Z[i]<=0 Then Z[i]:=1e-15        ;  *)
         AleatMed:=AleatMed + UAux;
AleatVar:=AleatVAr + UAux*UAux;
         Naleat:=Naleat +1;
End;
     End;
    End
    Else
    Begin
      For i:=1 To Npontos Do
      Begin
        ZAux[i]:= Z[i];
      End;
    End;
    For i:= 1 to npontos do
    Begin
      If (Flag2 = 0) Then
If(Cpeso = '1') Then
w[i]:= 1/(sig[i]*sig[i])
      Else
If(Cpeso = '2') Then
       Begin
sigaux:=sig[i]/Z[i];
w[i]:= 1/(sigaux*sigaux);
        End
      Else
If(Cpeso = '3') Then
w[i]:= 1/y[i]
      Else
w[i]:= 1.0;
      Wtotal1:= Wtotal1 + w[i];
End;
    Wtotal1:= Wtotal1/Npontos;
    Transforma;
With  SomaAux^ Do
    Begin
        Somay:=0.0;
```

```
        For j:= 1 to Npar Do
           Begin
            SomaX[j]:=0.0;
            SomaYX[j]:= 0.0;
            For k:=1 to Npar Do
               Begin
                 If (k >=j) Then
SomaXX[j,k]:= 0.0;
               End;
        End;
    For i:=1 To npontos do
    Begin
w[i]:=w[i]/Wtotal1;
        If (Cont1=1) Then Yaux[i]:=y[i];
        Wtotal:= Wtotal + w[i];
        SomaY:=SomaY+y[i]*w[i];

      For j:= 1 to Npar Do
        Begin
SomaX[j]:=SomaX[j]+x[j,i]*w[i];
          SomaYX[j]:= SomaYX[j] + (w[i]*y[i]*x[j,i]);
For k:=1 to Npar Do
          Begin
           If (k >=j) Then
SomaXX[j,k]:= SomaXX[j,k] + w[i]*x[j,i]*x[k,i];
          End;
        End;
    End;
{ X1med:= SomaX[1]/Wtotal;}
    Ymed:= Somay/ Wtotal;
if Aux5=1 Then Ymed1:=Ymed;
    Begin
a[1,1]:=Wtotal;
b[1,1]:=SomaY;
    For i:=2 to Npar do
    Begin
a[1,i]:=SomaX[i-1];
a[i,1]:=a[1,i];
For j:= i to Npar do
     Begin
a[i,j]:=SomaXX[i-1,j-1];
a[j,i]:=a[i,j];
```

```
      End;
b[i,1]:=SomaYX[i-1];
    End;

     End;
    End;
Dispose(SomaAux);
 End;




 Procedure OrdeRejeita;

Var

  a0Aux2,aAux2:   Real;
j,k,l,mm:    Integer;

Begin
  If (Aux5 <= Nvezes) Then
  Begin
     For k:=1 to npar do
     Begin
a0Aux[1,k,Aux5]:= a0[1,k];
       For j:=1 To Npar Do
      (* aAux[j,k,Aux5]:=a[j,k];*)
     End;
  End;

  If (Aux5 = Nvezes ) Then
  Begin
       For k:= 1 To Npar Do
       Begin
l:=1;
         Repeat
           For mm:= 1 To Nvezes-l Do
           Begin
if (a0Aux[1,k,l+mm] < a0Aux[1,k,l]) Then
Begin
a0Aux2:= a0Aux[1,k,l];
```

```
a0Aux[1,k,l]:=a0Aux[1,k,l+mm];
a0Aux[1,k,l+mm]:=a0Aux2;
End;
          (* For j:=1 To npar Do
           Begin
if (aAux[j,k,l+mm] < aAux[j,k,l]) Then
             Begin
               aAux2:= aAux[j,k,l];
aAux[j,k,l]:=aAux[j,k,l+mm];
aAux[j,k,l+mm]:=aAux2;
End;
           End; *)
         End;
l:=l+1;
       Until l = Nvezes;
     End;
 (*AleatMed:=0;
 For j:= 1 To Aux5  Do
   Begin
    For i:=1 To Npontos Do
    Begin
      AleatMed:= AleatMed + AleatAux[j,i];
    End;
End  *)
AleatVar:=(Naleat*AleatVar-AleatMed*AleatMed)/(Naleat*(Naleat-1));
 AleatMed:=AleatMed/Aux5;

 End;
End;

Procedure coeficientes;

 Var
Aux5a :Extended;

 Begin
 For i:= 1 to 25 Do Writeln('  ');
 If (Aux5=1) Then
 Begin
   For k:=1 To NVarMax Do
    Begin
      A0M[k]:=0;
```

```
A0M2[k]:=0;
A0S2[k]:=0;
       For j:=1 To NVarMax Do
       Begin
AS2[j,k]:=0.0;
AMxy[j,k]:=0.0;
       End;
     End;
  End;

for j:=1 to npar do
    Begin
a0[1,j]:= c[j,1];
     (* a0aux[cont1]:=a0[1,3]; *)
   (* Writeln ('a0[1,',j,']',a0[1,j]);Readln(pp);*)
End;
   (* Writeln('     y        y calc    (  y calc- y  )^2                          ');*)

SSE := 0;SSR := 0;Syy := 0;Qui2:=0;
for k:= 1 to npontos do
Begin
     Ycalc[k]:= a0[1,1];
     For j:=2 to Npar do Ycalc[k]:=Ycalc[k]+a0[1,j]*x[j-1,k];
SSE := SSE + W[k] * (Y[k] - Ycalc[k]) * (Y[k] - Ycalc[k]);
Syy := Syy + W[k] * (Y[k] - Ymed) * (Y[k] - Ymed);
Qui2:= Qui2 + w[k]*(Ycalc[k]-y[k])*(Ycalc[k]-y[k]);
End;

(*    For j:=1 To Npar Do
Begin
       A0M2[j]:=A0M2[j] + a0[1,j]*a0[1,j];*) (* Somas dos QUADRADOS dos coefic. a0 *)
(*       A0M[j]:=A0M[j]+a0[1,j]; *) (* Somas dos coefic. a0 *)
  (*    End; *)
SSE := SSE;
VarAj := SSE / (Npontos - (npar-1) - 1);
DpAj := SQRt(ABS(VarAj));
Syy := ABS(Syy );
SSR := Syy - SSE;
corr2 := SSR / Syy;
Corr := SQRT(ABS(corr2));
F := (corr2 / (npar-1)) / ((1 - corr2) / (Npontos - (npar - 1)-1));
    (* aqui multiplica-se por 1/Npontos... pq , o somat. do vector pesos *)
```

```
    If (Cont1=1) Then
    Begin
      {qui2i e DPaji guardam os valores de qui2 e DpAj p/ a 1¦ reg }
       DPAji:=DPAj;
       VarAji:=VArAj;
       Qui2i:=Qui2;
corr2V:=corr2;
corrV:=corr;
      FV:= F;
For l:=1 To Npar Do
      Begin
        For k:=1 To NPar Do
        Begin
          a0V[k]:=a0[1,k];
        End;
      End;
    End;
  (*  For k:= 1 to npontos do
Writeln(y[k]:6:4,'   ',ycalc[k]:6:4,'  ',(ycalc[k]-y[k])*(ycalc[k]-y[k]):6:4);
Writeln('a0=',a0[1,1]);
Readln(pp);Readln(pp);   *)

   OrdeRejeita;

   If (Aux5=Nvezes) then
   Begin
For l:= 34 To 167  Do    (* N§ DE CORR: > 200 e IC de 67%*)
Begin
       For j:=1 To Npar Do
Begin
         A0M[j]:=A0M[j]+a0Aux[1,j,l];  (* Somas dos coefic. a0 *)
If l<80 Then gotoxy(1,l-33) else
if (l>80) and (l < 136)  then gotoxy(20,l-80) else
gotoxy (40,l-136);
Write(a0Aux[1,j,l]);
A0M2[j]:=A0M2[j] + a0Aux[1,j,l]*a0Aux[1,j,l]; (* Somas dos QUADRADOS dos coefic. a0 *)
For k:=1 To Npar Do
         Begin
           If (k <> j) Then
           Begin
             (* AM[k,j]:=AM[k,j]+aAux[k,j,l];   Somas dos coefic. ai  *)
             AMxy[k,j]:=AMxy[k,j] + a0Aux[1,k,l]*a0Aux[1,j,l];
```

```
          End;
        End;
      End;
    End;
    Aux5:=134;  (*Trunc(IC*Nvezes/100); *)
Aux5a:=(aux5-1);
    Aux5a:=Aux5a*Aux5;
For k:=1 To NPar Do
   Begin
A0S2[k]:= (Aux5*A0M2[k]-(A0M[k]*A0M[k]))/Aux5a;
    (*  Aux5a:=(0.9*aux5)-1; *)(* ALTERAR P/ INT de CONF DIF de 95% *)
    (*  Aux5a:=Aux5a*(0.9*Aux5);
     A0S2[k]:= (((0.9*Aux5)-1)*A0M2[k]-(A0M[k]*A0M[k]))/Aux5a;
A0M[k]:=A0M[k]/(0.9*Aux5); *)
     For j:= 1 To Npar Do
     If (k <>j ) Then
     Begin
AS2[j,k]:= (AMxy[j,k]-((1/Aux5)*A0M[j]*A0M[k]))/(Aux5-1);
      (*If (j=1) and (k=2) Then AS2[j,k]:= -AS2[j,k];
      If (j=2) and (k=1) Then AS2[j,k]:= -AS2[j,k];
      If (j=1) and (k=3) Then AS2[j,k]:= -AS2[j,k];
      If (j=3) and (k=1) Then AS2[j,k]:= -AS2[j,k];     *)
      (* AMxy[j,k]:=AMxy[j,k]/Aux5;*)
     End;

   End;
for k:= 1 to npar do A0M[k]:=A0M[k]/(Aux5);

SSE:=0.0;Syy:=0.0;Qui2:=0.0;
for k:= 1 to npontos do

Begin
    Ycalc[k]:= a0M[1];
    For j:=2 to Npar do Ycalc[k]:=Ycalc[k]+a0M[j]*x[j-1,k];
SSE := SSE + W[k] * (Yaux[k] - Ycalc[k]) * (Yaux[k] - Ycalc[k]);
Syy := Syy + W[k] * (Yaux[k] - Ymed1) * (Yaux[k] - Ymed1);
    Qui2:= Qui2 + w[k]*(Ycalc[k]-yaux[k])*(Ycalc[k]-yaux[k]);
End;
SSE := SSE;
VarAj := SSE / (Npontos - (npar-1) - 1);
DpAj := SQRt(ABS(VarAj));
Syy := ABS(Syy );
```

```
SSR := Syy - SSE;
corr2 := SSR / Syy;
Corr := SQRT(ABS(corr2));
F := (corr2 / (npar-1)) / ((1 - corr2) / (Npontos - (npar - 1)-1));
    (* aqui multiplica-se por 1/Npontos... pq , o somat. do vector pesos *)
  (*  Qui2:=Qui2i;
    DpAj:=DPAji;
    VarAj:=VarAji;  *)

End;
     Aux5:= Aux5+1;
 End;

Procedure Aleatorios;
{Numeros aleatorios gerados de acordo com o artigo do Shadd}
(* Uses Crt; *)
Const
   X= 0000100003;
Type
  Real= Extended;
Var
  Umed,Umed2,Umed3      :Real;


Begin
  ClrScr;
U[1]:=0123456789;
  Umed:=0.0;
  Umed2:=0.0;
Umed3:=0.0;
l:=1;
  For i:= 2 To 1000 Do   {Estava Nvezes q. , o n§ de corridas em cada caso}
Begin
   U[i]:= X*U[i-1];
   If (i=1) Then U[i]:= U[i]/1e10
Else U[i]:=U[i]/1e11;
   U[i]:= Frac(U[i])*1e9;
Umed:=Umed+U[i];
l:=l+1;
  (* If l= 25 Then Begin Readln(l); l:=1; End; *)
  End;
   Umed:=Umed/1000;
```

```
  For i:= 1 To 1000 Do
  Begin
    U[i]:= U[i]/Umed;       (* -5e8;  *)
    Umed2:=Umed2+U[i];
  End;
    Umed2:=Umed2/1000;
  For i:= 1 To 1000 Do
  Begin
    U[i]:= U[i]- Umed2;       (* -5e8;  *)
    Umed3:=Umed3+U[i];
 (*     Writeln('U[',i,']= ',U[i]); *)
  End;
  Umed3:=Umed3/1000;
(*  Writeln('Umedfin',Umed3);          *)
(* EscreveFich; *)
End;

Procedure EscreveFich;

Var
  Buf            :Text;
Erro,Aux6       :Integer;
Apagar,Fich3    : Char;
  Fich4          : String [60];
Begin
  Repeat
Write(' Quer Escrever o resultado p/ um Ficheiro ? (s/n)');
Readln(Fich3);
  Until (UpCase(Fich3) = 'S') or (UpCase(Fich3) = 'N');
  If (UpCase(Fich3)= 'S') Then
  Begin
Write(' Nome do Ficheiro (c/ direct¢rio e SEM extensao)');
Readln (Fich4);
    Fich4:= Fich4 + '.dat';
    Assign (Buf,Fich4);
    {$I-}
    Reset (Buf);
    Erro:= IoResult;
    {$I+}
    If Erro=0 Then
    Begin
Write(Fich4);
```

```
Write(' j  existe!  Apagar(s/n): ');
     Readln(Apagar);
If UpCAse(Apagar)='S' Then
     Begin
Close(Buf);
ReWrite(Buf);
Writeln('Aleat foi apagado');
     End;
  End;
  Begin
ReWrite(Buf);
    Begin
Writeln(Buf,'  ');
Write(Buf,'Programa:  RegMCM5.pas            ','Ficheiro:  ',Fich);
Writeln(Buf,'      Tipo de Reg:   ',PesoEscrita);
     For j:=1 to 2 Do
Writeln(Buf,'  ');
Writeln(Buf, '            equacao calculada :');
     For j:=1 to 2 do
Writeln(Buf,'  ');
Writeln(Buf,'    ');
Write(Buf,'y = ');
j:=0;
  Aux6:= Round(N2Var/3 + 0.4);
  Repeat
     For i:= 1 To 3 Do
     Begin
          If i+j<=NPar Then
          Begin
               If (i>1) Then If (a0M[i+j] >0 ) Then Write(Buf,' + ') Else Write (Buf,'  ');
Write(Buf,a0M[i+j]:13);
               If (i>1) Then Write(Buf,'*x',i-1+j);
          End;
           If (i=NPar) or ((Npar>3) and (i=3)) Then
           Begin
Writeln(Buf,' ');
                For k:=1 to NPar Do If (k<=3) and (k+j <=NPar) Then Write (Buf,'   ñ',DPa[k+j]:13);
           End;
     End;
Writeln(Buf,' '); Writeln(Buf,' ');
j:=j+3;
Write(Buf,'   ');
```

```
  Until j >=NPar;
    (*  Write(Buf,' y = ',a0M[1]:13);
      If (Npar=2) Then
      Begin
        If (a0M[2] >0 ) Then Write(Buf,' + ') Else Write(Buf, '  ');
Writeln(Buf,a0M[2]:13,'*x1 ');
Writeln(Buf,'    ñ ',DpA1:13,'  ñ ',DpA2:13);
    End
    Else
    If (Npar=3) Then
    Begin
      If (a0M[2] >0 ) Then Write(Buf,' + ') Else Write(Buf, '  ');
Write(Buf,a0M[2]:13,'*x1 ');
      If (a0M[3] >0 ) Then Write(Buf,' + ') Else Write(Buf, '  ');
Writeln(Buf,a0M[3]:13,'*x2 ');
Writeln(Buf,'    ñ ',DpA1:13,'   ñ ',DpA2:13,'   ñ ',DpA3:13);
    End
    Else
    If (Npar=4) Then
    Begin
      If (a0M[2] >0 ) Then Write(Buf,' + ') Else Write(Buf, '  ');
Write(Buf,a0M[2]:13,'*x1 ');
      If (a0M[3] >0 ) Then Write(Buf,' + ') Else Write(Buf,'  ');
Write(Buf,a0M[3]:13,'*x2 ');
      If (a0M[4] >0 ) Then Write(Buf,' + ') Else Write(Buf,'  ');
Writeln(Buf,a0M[4]:13,'* x3 ');
Writeln(Buf,'    ñ ',DpA1:13,'   ñ ',DpA2:13,'   ñ ',DpA3:13,'  ñ ',
      DpA4:13);
    End
    Else
    If (Npar=5) Then
    Begin
      If (a0M[2] >0 ) Then Write(Buf,' + ') Else Write(Buf,'  ');
Write(Buf,a0M[2]:13,'*x1 ');
      If (a0M[3] >0 ) Then Write(Buf,' + ') Else Write(Buf,'  ');
Write(Buf,a0M[3]:13,'*x2 ');
      If (a0M[4] >0 ) Then Write(Buf,' + ') Else Write(Buf,'  ');
Write(Buf,a0M[4]:13,'*x3 ');
      If (a0M[5] >0 ) Then Write(Buf,' + ') Else Write(Buf,'  ');
Writeln(Buf,a0M[5]:13,'*x4  ');
Writeln(Buf,'   ñ ',DpA1:13,'  ñ ',DpA2:13,'   ñ ',DpA3:13,'        ñ ',
      DpA4:13,'      ñ ',DpA5:13);
```

```
   End
   Else
   Begin
    If (a0M[2] >0 ) Then Write(Buf,' + ') Else Write (Buf,' ');
Write(Buf,a0M[2]:13,'*x1 ');
    If (a0M[3] >0 ) Then Write(Buf,' + ') Else Write (Buf,' ');
Write(Buf,a0M[3]:13,'*x2 ');
    If (a0M[4] >0 ) Then Write(Buf,' + ') Else Write (Buf,' ');
Writeln(Buf,a0M[4]:13,'*x3 ');
    If (a0M[5] >0 ) Then Write(Buf,'    + ') Else Write (Buf,' ');
Write(Buf,a0M[5]:13,'*x4 ');
    If (a0M[6] >0 ) Then Write(Buf,' + ') Else Write (Buf,'  ');
Writeln(Buf,a0M[6]:7,'*x5 ');
    Writeln (Buf,'  ñ ',DpA1:13,'  ñ ',DpA2:13,'   ñ ',DpA3:13,'        ñ ',
    DpA4:13,'      ñ ',DpA5:13,'      ñ ',DpA6:13);
   End; *)
Writeln(Buf,'  ');
Writeln(Buf,'  ');
Writeln(Buf,'         desvio padrao =',DpAj:13);
Writeln(Buf,'         Qui2 = ',Qui2:13);
Writeln(Buf,'         r = ',corr:9:8);
Writeln(Buf,'         r2 =',corr2:9:8);
Writeln(Buf,'         valor F(',(npar-1) , ',', Npontos - (npar-1) - 1, ')= ', F:6:2);
Writeln(Buf,'         numero de it =',Nvezes);
Writeln(Buf,'         Perturbacao = ',Perturb:6:3);
Writeln(Buf,'         ValorMedio dos n§s Aleat. =',AleatMed:13);
Writeln(Buf,'         Desv. Padrao dos n§s Aleat. =',sqrt(abs(AleatVar)):13);
   For j:=1 to 4 do
Writeln(Buf,'  ');
   Writeln (Buf, '            Matriz var-covar           ');
Writeln(Buf,' ');
   For k:= 1 to npar Do
   Begin
    For j:= 1 to npar Do Write (Buf,'  ',a[k,j]*VarAj:13);
Writeln(Buf,'');
   End;
   For j:=1 to 4 do
Writeln(Buf,'  ');
   If (2 = 2) Then
   Begin
    If RegTipo2='2' Then
    Begin
```

```
        If (transf = 2) Then
        Begin
        If (UpCase(TransfA) = 'D') Then
           Writeln (Buf, '                ln kexp        ln kcalc        ln kcalc-ln kexp')
        Else
           Writeln (Buf, '                log kexp       log kcalc       log kcalc-log kexp');
        End;
Writeln(Buf,'    ');
        For j:=1 to npontos do
        Writeln (Buf,'      ',yaux[j]:18:5,ycalc[j]:18:5,(ycalc[j]-yaux[j]):18:5);
Writeln(Buf,' ');
     End;
   End;
   Imp:=0;
 End;
   If RegTipo2='1' Then
   Begin
     For j:=2 To Npontos+1 Do
  (* Writeln(Buf,U[i],a0aux[i]);  *)
(*    Writeln(Buf,U[i]);*)
Writeln(Buf, T[j-1]:6:2,' ',1e-3*DeltaG[j-1]:8:2,' ñ',1e-3*SigDeltaG[j-1]:7:2,' ',1e-3*DeltaH[j-1]:7:2,
' ñ',1e-3*SigDeltaH[j-1]:6:2,",
DeltaS[j-1]:10:2,' ñ',SigDeltaS[j-1]:7:2,' ', DeltaCp[j-1]:8:2,' ñ',SigDeltaCp[j-1]:7:2);
End;
End;
Close(Buf);
End;
End;

Procedure EscrevResult1;

 Var
  Flag1,AuxX,AuxY:  Integer;
 Begin
  For i:=1 To Npar Do
  Begin
a0[1,i]:=A0M[i];
  DPA[i]:= Sqrt(Abs(A0S2[i]));
End;
  Writeln;
  Writeln ( 'equacao calculada :');
Write('y = ');
```

```
  For i:= 1 To NPar Do
    Begin
      If (i=1) Then Write(a0M[i]:13)
      Else If (i>1) or (j>0) Then
      Begin
        If (a0M[i] >0 ) Then Write(' + ') Else Write ('  ');
Write(a0M[i]:13);
      End;
      If (i>1) Then Write('*x',i-1);
      AuxX:=WhereX;
      AuxY:=WhereY;
GoToXY(AuxX-15,AuxY+1);
      Write (' ñ',DPa[i]:13);
GoToXY(AuxX,AuxY);
      If (i=4) or (i=8) Then GoToXY(4,AuxY+3);
  End;
GoToXY(1,AuxY+3);
End;
  (*Write('y = ',a0[1,1]:13);
  If (Npar=2) Then
  Begin
    If (a0[1,2] >0 ) Then Write(' + ') Else Write ('  ');
Writeln(a0[1,2]:13,'*x1 ');
    Writeln ('  ñ ',DpA1:13,'   ñ ',DpA2:13);
  End
  Else
  If (Npar=3) Then
  Begin
    If (a0[1,2] >0 ) Then Write(' + ') Else Write ('  ');
Write(a0[1,2]:13,'*x1 ');
    If (a0[1,3] >0 ) Then Write(' + ') Else Write ('  ');
Writeln(a0[1,3]:13,'* x2 ');
    Writeln ('  ñ ',DpA1:13,'   ñ ',DpA2:13,'   ñ ',DpA3:13);
  End
  Else
  If (Npar=4) Then
  Begin
    If (a0[1,2] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,2]:13,'*x1');
    If (a0[1,3] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,3]:13,'*x2 ');
    If (  a0[1,4] >0 ) Then Write(' + ') Else Write ('  ');
```

```
Writeln(a0[1,4]:13,'*x3 ');
   Writeln ('  ñ ',DpA1:13,'   ñ ',DpA2:13,'   ñ ',DpA3:13,'  ñ ',
   DpA4:13);
  End
  Else
  If (Npar=5) Then
  Begin
   If (a0[1,2] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,2]:13,'*x1 ');
   If (a0[1,3] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,3]:13,'* x2 ');
   If (a0[1,4] >0 ) Then Write(' + ') Else Write (' ');
Writeln(a0[1,4]:13,'* x3 ');
   If (a0[1,5] >0 ) Then Write(' + ') Else Write (' ');
Writeln(a0[1,5]:13,'* x4 ');
   Writeln ('  ñ ',DpA1:13,'  ñ ',DpA2:13,'   ñ ',DpA3:13,'          ñ ',
   DpA4:13,'   ñ ',DpA5:13);
  End
  Else
  Begin
   If (a0[1,2] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,2]:13,'*x1 ');
   If (a0[1,3] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,3]:13,'* x2 ');
   If (a0[1,4] >0 ) Then Write(' + ') Else Write (' ');
Write(a0[1,4]:13,'* x3     ');
   If (a0[1,5] >0 ) Then Write('    + ') Else Write (' ');
Write(a0[1,5]:13,'* x4 ');
   If (a0[1,6] >0 ) Then Write(' + ') Else Write ('  ');
Writeln(a0[1,6]:13,'*x5 ');
   Writeln ('  ñ ',DpA1:13,'  ñ ',DpA2:13,'   ñ ',DpA3:13,'       ñ ',
   DpA4:13,'      ñ ',DpA5:13,'      ñ ',DpA6:13);

  End;
 End;  *)



Procedure EscrevResult2;
 Begin
   Writeln ('desvio padrao =',DpAj:13);
```

```
Writeln('Qui2 = ',Qui2:13);
   Writeln ('r = ',corr:9:8);
   Writeln ('r2 =',corr2:9:8);
   Writeln ('valor F(',(npar-1) , ',', Npontos - (npar-1) - 1, ')= ', F:6:2);
Writeln(' ');
Write('       Carregue numa tecla para continuar ');
Readln(pp);
  ClrScr;

{ For k:=1 to 5 Do
     Begin
a0[1,k+2]:=a0[1,k+1];
       If (k=2) or (k>npar+1) Then a0[1,k]:=0;

       For i:= 1 To 5 Do
       Begin
         If (i=k) Then
           If (i> 1) Then
a[i+1,k+1]:=a[i,k]

         Else
If(i=1) Then a[1,k+1]:=a[1,k]
         Else
a[i+1,k+1]:=a[i,k];
         If (i=2) or (k=2) Then a[i,k]:=0.0;
       End;
       If (i>npar+1) or (k>npar+1) Then a[i,k]:=0.0;
     End;      }
  If (FlagElim='t') Then
  Begin
a[3,1]:=a[2,1];
a[1,3]:=a[1,2];
a[3,3]:=a[2,2];
a0[1,3]:=a0[1,2];
a[2,1]:=0.0;       {GENERALIZAR E INCLUIR VAR. AUX. P/ GUARDAR OS}
a[1,2]:=0.0;       {VALORES ORIGINAIS POR CAUSA DA IMPRESSAO;}
a[2,2]:=0.0;       {NA PARTE DA IMPRESSAO TAMB • M • PRECISO ALTERAR}
a[3,2]:=0.0;
a[2,3]:=0.0;
a0[1,2]:=0.0 ;
    A0s2[3]:=A0s2[2];
    A0s2[2]:=0.0;
```

```
    Npar:=3;
End;
Writeln('                    Matriz var/covar');
  aux3:=3;
GoToXY(15,aux3);
  For k:= 1 to Npar Do
  Begin
    For j:= 1 to npar Do
    Begin
      If k=j Then
      Begin
aM[k,j]:= as2[k,j];
Write  (a0S2[k]:13,'  ');
      End
      Else
Write  (as2[k,j]:13,'  ');
    End;
Writeln(' ');
    aux3:= aux3+1;
GoToXY(15,aux3);
  End;
  Writeln;
Writeln('Carregue numa tecla para continuar ');
Readln(pp);
  ClrScr;
 End;

(*Procedure impressora;

var
   Flag1,Aux6,Res:   Integer;

 Begin


Writeln(Lst,'  ');
Write(Lst,'Programa: RegMCM5B.pas     ','Ficheiro:  ',Fich);
Writeln(Lst,'   Tipo de Reg:  ',PesoEscrita);
For j:=1 to 2 Do
Writeln(Lst,'  ');
Writeln(Lst, '             equacao calculada :');
Writeln(Lst,'    ');
```

```
Write(Lst,'y = ');
j:=0;
  Aux6:= Round(N2Var/3 + 0.4);
  Repeat
     For i:= 1 To 3 Do
     Begin
        If i+j<=NPar Then
        Begin
           If (i>1) Then If (a0M[i+j] >0 ) Then Write(Lst,' + ') Else Write (Lst,'  ');
Write(Lst,a0M[i+j]:13);
           If (i>1) Then Write(Lst,'*x',i-1+j);
        End;
         If (i=NPar) or ((Npar>3) and (i=3)) Then
         Begin
Writeln(Lst,' ');
            For k:=1 to NPar Do If (k<=3) and (k+j <=NPar) Then Write (Lst,'   ñ',DPa[k+j]:13);
         End;
     End;
Writeln(Lst,' '); Writeln(Lst,' ');
j:=j+3;
Write(Lst,'   ');
  Until j >=NPar;
(*  For j:=1 to 2 do
Writeln(Lst,'  ');
Writeln(Lst,'    ');
Write(Lst,' y = ',a0M[1]:13);
  If (Npar=2) Then
  Begin
   If (a0V[2] >0 ) Then Write(Lst,' + ') Else Write(Lst, '  ');
Writeln(Lst,a0M[2]:13,'*x1 ');
Writeln(Lst,'    ñ ',DpA1:13,'  ñ ',DpA2:13);
  End
  Else
  If (Npar=3) Then
  Begin
    If (a0M[2] >0 ) Then Write(Lst,' + ') Else Write(Lst, '  ');
Write(Lst,a0M[2]:13,'*x1 ');
    If (a0M[3] >0 ) Then Write(Lst,' + ') Else Write(Lst, '  ');
Writeln(Lst,a0M[3]:13,'*x2 ');
Writeln(Lst,'    ñ ',DpA1:13,'   ñ ',DpA2:13,'   ñ ',DpA3:13);
  End
  Else
```

```
  If (Npar=4) Then
  Begin
    If (a0M[2] >0 ) Then Write(Lst,' + ') Else Write(Lst, '  ');
Write(Lst,a0M[2]:13,'*x1 ');
    If (a0M[3] >0 ) Then Write(Lst,' + ') Else Write(Lst,'  ');
Write(Lst,a0M[3]:13,'*x2 ');
    If (a0M[4] >0 ) Then Write(Lst,' + ') Else Write(Lst,'  ');
Writeln(Lst,a0M[4]:13,'* x3 ');
Writeln(Lst,'    ñ ',DpA1:13,'   ñ ',DpA2:13,'   ñ ',DpA3:13,'  ñ ',
    DpA4:13);
  End
  Else
  If (Npar=5) Then
  Begin
    If (a0M[2] >0 ) Then Write(Lst,' + ') Else Write(Lst,'  ');
Write(Lst,a0M[2]:13,'*x1 ');
    If (a0M[3] >0 ) Then Write(Lst,' + ') Else Write(Lst,'  ');
Write(Lst,a0M[3]:13,'*x2 ');
    If (a0M[4] >0 ) Then Write(Lst,' + ') Else Write(Lst,'  ');
Write(Lst,a0M[4]:13,'*x3 ');
    If (a0M[5] >0 ) Then Write(Lst,' + ') Else Write(Lst,'  ');
Writeln(Lst,a0M[5]:13,'*x4  ');
Writeln(Lst,'   ñ ',DpA1:13,'  ñ ',DpA2:13,'   ñ ',DpA3:13,'       ñ ',
    DpA4:13,'     ñ ',DpA5:13);
  End
  Else
  Begin
    If (a0M[2] >0 ) Then Write(Lst,' + ') Else Write (Lst,' ');
Write(Lst,a0M[2]:13,'*x1 ');
    If (a0M[3] >0 ) Then Write(Lst,' + ') Else Write (Lst,' ');
Write(Lst,a0M[3]:13,'*x2 ');
    If (a0M[4] >0 ) Then Write(Lst,' + ') Else Write (Lst,' ');
Writeln(Lst,a0M[4]:13,'*x3 ');
    If (a0M[5] >0 ) Then Write(Lst,'    + ') Else Write (Lst,' ');
Write(Lst,a0M[5]:13,'*x4 ');
    If (a0M[6] >0 ) Then Write(Lst,' + ') Else Write (Lst,'  ');
Writeln(Lst,a0M[6]:7,'*x5 ');
    Writeln (Lst,'  ñ ',DpA1:13,'  ñ ',DpA2:13,'   ñ ',DpA3:13,'       ñ ',
    DpA4:13,'     ñ ',DpA5:13,'     ñ ',DpA6:13);
End;(* )
Writeln(Lst,'  ');
Writeln(Lst,'  ');
```

```
Writeln(Lst,'        desvio padrao =',DpAj:13);
Writeln(Lst,'        Qui2 = ',Qui2:13);
Writeln(Lst,'        r = ',corrV:9:8);
Writeln(Lst,'        r2 =',corr2V:9:8);
Writeln(Lst,'        valor F(',(npar-1) , ',', Npontos - (npar-1) - 1, ')= ', FV:6:2);
Writeln(Lst,'        numero de it =',Nvezes);
 For j:=1 to 4 do
Writeln(Lst,'  ');
 Writeln (Lst, '            Matriz var-covar            ');
Writeln(Lst,' ');
  For k:= 1 to Npar Do
  Begin
    For j:= 1 to npar Do
    Begin
      If k=j Then
      Begin
aM[k,j]:= as2[k,j];
Write  (Lst,a0S2[k]:13,'  ');
      End
      Else
Write  (Lst,as2[k,j]:13,'  ');
    End;
Writeln(Lst,' ');
  End;
  For i := 1 to 4 do
Writeln(Lst,' ');

 If (Imp = 2) Then
 Imp:=0;
 Begin
   If (transf = 2) Then
      Begin
        If (UpCase(TransfA) = 'D') Then
        Writeln (Lst, '              log yexp         log ycalc       log ycalc-log yexp        peso')
        Else
        Writeln (Lst, '              ln yexp        ln ycalc         ln ycalc-ln yexp          peso');
      End
Else  Writeln (Lst, '            Yexp              Ycalc          Ycalc - Yexp          Peso');
Writeln(Lst,'    ');
   For j:=1 to npontos do
   Writeln (Lst,'      ',yaux[j]:18:5,ycalc[j]:18:5,(ycalc[j]-yaux[j]):18:5, w[j]:18:5);
Writeln(Lst,' ');
```

```
Writeln(Lst, Formfeed);
 End;
 Imp:=0;


 (* Writeln('Carregue numa tecla para continuar ');
Readln(pp);  *)
(* End;              *)

Procedure Factiv;

Const
  RG =8.314;
Var
Const1,q1,q2,q3,q4,q5: Extended ;
Flag1         : Integer;
Begin
Const1:= ln(6.62618e-34/1.38066e-23);
For j:= 1 to npontos do
Begin
   If (Eq = 1) Then
   Begin
     DeltaG[j]:= -RG*T[j]*(Const1 + (Yaux[j]-ln(T[j])));
     DeltaS[j]:= RG*(a0[1,1] + a0[1,3] - 1 + (a0[1,3] -1) * ln(T[j]) +
              2*a0[1,4]*T[j] + 3*a0[1,5]*Sqr(T[j]) + Const1);
     DeltaH[j]:= -RG * (a0[1,2] + (1-a0[1,3])*T[j] - a0[1,4]*Sqr(T[j])-
               2*a0[1,5]*T[j]*Sqr(T[j]));
     DeltaCp[j]:= -RG* (1-a0[1,3] - 2*a0[1,4]*T[j] - 6*a0[1,5]*Sqr(T[j]));
   SigDeltaG[j]:= RG*T[j]*sig[j]/Yaux1[j];
q1 := A0s2[1] + Sqr(1 + ln(T[j])) * A0s2[3] +
                2*(1+ln(T[j]))*aS2[1,3] + 4*Sqr(T[j])*A0s2[4];
q2 :=   + 9*Sqr(T[j])*Sqr(T[j])*A0s2[5] + 4*T[j]*(aS2[1,4]);
          q3:=    + 6*Sqr(T[j])*(aS2[1,5]) + 4*T[j]*(1+ln(T[j])) *
                  (aS2[3,4]) + 6*Sqr(T[j])*(1+ln(T[j]))*(aS2[3,5]);
          q4:=    + 12*T[j]*Sqr(T[j])*(aS2[4,5]);
   SigDeltaS[j] := Abs(RG*Sqrt(Abs(q1+q2+q3+q4)));
If (SigDeltaS[j]> 0.2*DeltaS[j]) Then SigDeltaS[j]:= 0.2*DeltaS[j];
q1:= A0s2[2] + Sqr(T[j])*A0s2[3] + Sqr(T[j])*Sqr(T[j])*
A0s2[4] + 4*Sqr(T[j])*Sqr(T[j])*Sqr(T[j])*A0s2[5];
          q2:=  -2*T[j]*(aS2[2,3]) - 2*Sqr(T[j])*(aS2[2,4]);
          q3:= -4*Sqr(T[j])*T[j]*(aS2[2,5]) + 2*Sqr(T[j])*T[j]*
                  (aS2[3,4]) + 4*Sqr(T[j])*Sqr(T[j])*(aS2[3,5]);
```

```
          q4:= 4*Sqr(T[j])*Sqr(T[j])*T[j]*(aS2[4,5]);
     SigDeltaH[j]:= Abs(RG*Sqrt(Abs(q1+q2+q3+q4)));
          q1:= A0s2[3] + 4*Sqr(T[j])*A0s2[4] + 36*Sqr(T[j])*Sqr(T[j])*A0s2[5];
          q2:= 4*T[j]*(aS2[3,4]) + 12*Sqr(T[j])*(aS2[3,5]);
          q3:= 24*Sqr(T[j])*T[j]*(aS2[4,5]);
                SigDeltaCp[j]:=RG*Sqrt(Abs( q1+q2+q3));
   End
   Else
   Begin
     DeltaG[j]:= -RG*T[j]*(Const1 + (Yaux[j]-ln(T[j])));
     DeltaS[j]:= RG*(Const1 - 1 - ln(T[j]) + a0[1,1]- a0[1,3]/Sqr(T[j])
              -2*a0[1,4]/(Sqr(T[j])*T[j])- 3*a0[1,5]/(Sqr(T[j])*Sqr(T[j])));
     DeltaH[j]:= -RG*(T[j] +a0[1,2] + 2*a0[1,3]/T[j] + 3*a0[1,4]/Sqr(T[j])  +
              4*a0[1,5]/(Sqr(T[j])*T[j]));
     DeltaCp[j]:= -RG*(1-2*a0[1,3]/Sqr(T[j]) - 6*a0[1,4]/(Sqr(T[j])*T[j]) -
               12*a0[1,5]/(Sqr(T[j])*Sqr(T[j])));
     SigDeltaG[j]:= RG*T[j]*sig[j]/Yaux1[j];
          q1:=  A0s2[1] + A0s2[3]/(Sqr(T[j])*Sqr(T[j])) + A0s2[4]*4/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j]));
          q2:=  A0s2[5]*9/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j])*Sqr(T[j])) - aS2[1,3]*2/Sqr(T[j]);
          q3:=  -aS2[1,4]*4/(Sqr(T[j])*T[j]) -  aS2[1,5]*6/(Sqr(T[j])*Sqr(T[j]))
              +aS2[3,4]*4/(Sqr(T[j])*Sqr(T[j])*T[j]);
          q4:=  aS2[3,5]*6/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j]))+
aS2[4,5]*12/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j])*T[j]);
     SigDeltaS[j]:= Abs(RG*Sqrt(Abs(q1+q2+q3+q4)));
     (* SigDeltaS[j]:=SigDeltaS[j]/100; *)
          q1:=  A0s2[2] + A0s2[3]*4/Sqr(T[j]) + A0s2[4]*9/(Sqr(T[j])*Sqr(T[j]));
          q2:=  A0s2[5]*16/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j])) +
aS2[2,3]*4/T[j] + aS2[2,4]*6/Sqr(T[j]);
          q3:=  aS2[2,5]*8/(Sqr(T[j])*T[j]) +  aS2[3,4]*12/(Sqr(T[j])*T[j]);
          q4:=  aS2[3,5]*16/(Sqr(T[j])*Sqr(T[j]))+
aS2[4,5]*24/(Sqr(T[j])*Sqr(T[j])*T[j]);
     SigDeltaH[j]:= Abs(RG*Sqrt(Abs(q1+q2+q3+q4)));
          q1:=   A0s2[3]*4/(Sqr(T[j])*Sqr(T[j])) + a0s2[4]*36/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j]));
          q2:=   A0s2[5]*144/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j])*Sqr(T[j]))+
aS2[3,4]*24/(Sqr(T[j])*Sqr(T[j])*T[j]);
          q3:=  + aS2[3,5]*48/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j]))+
aS2[4,5]*144/(Sqr(T[j])*Sqr(T[j])*Sqr(T[j])*T[j]);
     SigDeltaCp[j]:= Abs(RG*(Sqrt(Abs(q1+q2+q3))));
   End
end;
Writeln('Carregue numa tecla para continuar ');
readln(pp);
```

```
  ClrScr;
GotoXY(15,7);
Writeln( 'Func”es Termodin ƒmicas de Activacao:');
GotoXY(1,9);
  Writeln ('Temp        DeltaG        DeltaH        DeltaS        DeltaCp');
GotoXY(2,11);
  Writeln (' /K        /kJmol-1      /kJmol-1      /Jmol-1K-1    /Jmol-1K-1');
Writeln(' ');
  Flag1:=1;
  For j:= 2 to Npontos+1 Do
 Begin
  If (Flag1 = 1) Then
Writeln(T[j-1]:6:2,' ',1e-3*DeltaG[j-1]:8:2,' ñ',1e-3*SigDeltaG[j-1]:7:2,' ',1e-3*DeltaH[j-1]:7:2,
' ñ',1e-3*SigDeltaH[j-1]:6:2,",
DeltaS[j-1]:10:2,' ñ',SigDeltaS[j-1]:7:2,' ', DeltaCp[j-1]:8:2,' ñ',SigDeltaCp[j-1]:7:2);
  If (Abs(T[j] - T[j-1]) < 1e-5) Then Flag1:=0 Else Flag1:=1;
 End;

End;

(* PROGRAMA PRINCIPAL *)

Begin
 ClrScr;
 Aux5:=1;
 Cont1:=1;
 For i:= 1 to 30 Do Writeln('  ');
 Flag2:=0;
 Voltar:   (* Volta aqui p/ novo conj. de dados  ou p/ reutilizar *)
inicializa;
dados;
 Flag3:=0;
 For Cont1:=1 To Nvezes Do
 Begin
n:= npar;
   If (Cont1>1) Then     Inicializa;
   (* For j:=1 To 5 Do c[j,1]:=0.0; *)
    ClrScr;
GotoXY(10,10);
Write('Cont= ',Cont1);
    If (Aux5=1) Then Aleatorios;
    Somas;
```

```
   (* Writeln('matriz X`X= '); *)
    n1:=n;
    n2:=n;
    n3:=0;
    guardarmatriz_a_em_c;
m:=n;
   (* imprimir;          (*          escrever X'X
Writeln('Carregue numa tecla para continuar ');
Readln(pp);                *)
    guardarmatriz_b_em_c;
    Writeln;
    (*   Writeln('vector das constantes '); *)
n:=1;
    (* imprimir;                  escrever vector constantes *)
    (* Writeln('Carregue numa tecla para continuar ');
Readln(pp);  *)
n:=m;
invertematriz;     { ao inverter b inverte-se a }
    guardarmatriz_b_em_a; { a , agora o seu prćprio inverso }
    guardarmatriz_c_em_b;
                    (*multiplicar o inverso pelo vector das constantes *)
    m1:=n;
    n1:=n;
    m2:=n;
    n2:=1;
multiplicamatriz;
                  (* o resultado esta em c: escrever c *)
m:=n;
n:=1;
    (* Writeln('vector solucao = '); *)
    (* imprimir; Readln(pp); *)
coeficientes;
    (* Writeln('Carregue numa tecla para continuar ');
Readln(pp);  *)

    (* Gerar Conj. de Resultados a Partir dos Par. Determinados na 1¦ Reg. *)
    (*         H  que guardar os valores experim. verdadeiros *)

    For k:=1 To Npontos Do
    Begin
      Z[k]:=0.0;
      For j:= 2 To NPar Do  Z[k]:= a0V[j] * x[j-1,k] + z[k] ;
```

```
      Z[k]:= a0V[1] + Z[k];
      (* ALTERAR AQUI PARA OUTRAS TRANSF *)

      If (Transf = 2) Then
If(UpCase(TransfA) = 'D') Then
      Begin
        Z[k]:= exp(Z[k]*ln(10));
      End
      Else Z[k]:= exp(Z[k]);
    End;
    Flag3:=1;
 End;
 ClrScr;
 For k:=1 To Npontos Do
 Begin
   Ycalc[k]:=0.0;
   For j:= 2 To NPar Do  Ycalc[k]:= a0M[j] * x[j-1,k] + Ycalc[k] ;
   Ycalc[k]:= a0M[1]+ Ycalc[k];
 End;
 EscrevResult1;
 EscrevResult2;
 EscreveFich;
 {escrevefich;}
 If (RegTipo2 = '1') Then Factiv;
(* Writeln('              Quer Imprimir ?');
Writeln('              (0) - Nao;          ');
Writeln('              (1) - Sem Res¡duos; ');
Write  ('              (2) - Com Res¡duos; ');
 Repeat
 Read (Imp);
 Until Imp in [0,1,2];
 If (Imp = 1) or (Imp =2) Then Impressora;
Writeln('Carregue numa tecla para continuar ');
Readln(pp);             *)
 For i:= 1 to 25 Do Writeln('  ');
GoToXY(10,10);
Writeln('(1) - Trabalhar os mesmos resultados com outra equacao;');
Writeln('         (2) - Trabalhar outro conjunto de resultados;');
Write  ('         (3) - Acabar;');
 Repeat Read(Continuar) Until Continuar in [1,2,3];
 If (Continuar = 1) Then
 Begin
```

```
  Flag2:= 1;
  GoTo Voltar;
End
Else
If (Continuar = 2) Then
Begin
  ClrScr;
  Flag2:=0;
  GoTo Voltar;
  End
Else
End.
```