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Institut für Neutronenphysik und Reaktortechnik

FORTRAN-IV-Programs for Fitting Data to one or more Exponentials

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1. Summary

A brief description of the methods and a package of FORTRAN-IV-Subroutines together with main programs and sample problems are given for fitting data in the sense of least squares to one and several exponentials.
After a brief look at the given subroutines these can also be used without our main programs.

2. Introduction

Let data points (x_i, y_i) be given with associated weights p_i $(i = 1,\dots,n)$. We want to fit one of the following functions

$$f_1(x) = ae^{-bx}$$

$$f_2(x) = ae^{-bx} + c$$

$$f_3(x) = ae^{-bx} + cx + d \tag{1}$$

$$f_4(x) = \sum_{\substack{i=1 \\ i\equiv 1(2)}}^{j-1} a_i e^{-a_{i+1}x}$$

$$f_5(x) = a_1 + \sum_{\substack{i=2 \\ i\equiv 0(2)}}^{j-1} a_i e^{-a_{i+1}x}$$

to the data in the sense of least squares, that is to determine the parameters of the functions such that

$$S = \sum_{i=1}^{n} p_i (f_k(x_i) - y_i)^2 \tag{2}$$

$$(k = 1,2,3,4,5)$$

is a minimum.

3. Method for Models f_1, f_2, and f_3

The method for all three models is the same (published for f_2 in [1]). From the necessary conditions for S having a stationary point

$$\text{grad } S = 0 \qquad (3)$$

we eliminate the linearly appearing parameters a or a, c or a, c, d, respectively. Putting these expressions in the remaining equations of (3), we get one equation in one variable

$$F_k(b) = 0 \qquad (k = 1, 2, 3) \qquad (4)$$

Having found a zero of (4), we can also obtain the corresponding values for the linear parameters and have a stationary point of (2). By tabulating $F_k = F_k(b)$ and $S = S(b)$ this method allows to find intervals for all stationary points of S and therefore, if existing, the absolute minimum of S.
Subroutines for the functions F_k are listed below as F1, F2, and F3. The rootfinder is a simple bisection method and the corresponding subroutine has the name BISECT. The main program allows to find a zero of (4) with relative accuracy EPS and the corresponding linear parameters if an interval [B1, B2] is given with sign $F_k(B1) \neq$ sign $F_k(B2)$.

4. Programs for Models f_1, f_2, and f_3

The main program requires the following input data. (A new number means the beginning of a new card).

I.	IFF	If IFF $\geq$ 0 then go to II else end of input data

II.	N	Number of data points ($2 \leq N \leq 1000$)
	NG	Weighting:
		If NG > 0, the weights (P(I), I = 1,N) are read in.
		If NG = 0, the main program sets P(I) = 1. (I = 1,N)
		If NG < 0, the main program sets P(I) = 1./Y(I) (I = 1,N)
	NB	NB = 1 : model f_1
		NB = 2 : model f_2
		NB = 3 : model f_3
	B1 B2	Required interval for the exponent b. If sign $F_{NB}(B1)$ = sign $F_{NB}(B2)$ the main program is left without results
	EPS	Required relative accuracy parameter for b
III.	(X(I), I=1,N)	given abscissae
IV.	(Y(I), I=1,N)	given ordinates
V.	(P(I), I=1,N)	if NG > 0, given weights

Start at I.

An example for input data and the corresponding output is listed below.

```
C     MAINPROGRAM FOR FITTING WITH ONE EXPONENTIAL
      DIMENSION X(1000),Y(1000),P(1000)
      COMMON N,X,Y,P,A,C,D
      EXTERNAL F1,F2,F3
      KI=8
      KO=9
 1000 READ(KI,1)IFF
      IF(IFF)999,10,10
   10 READ(KI,1) N,NG,NB,B1,B2,EPS
      READ(KI,1)(X(I),I=1,N)
      READ(KI,1)(Y(I),I=1,N)
      IF(NG)14,12,11
   11 READ(KI,1)(P(I),I=1,N)
      GO TO 16
   12 DO 13  I=1,N
   13 P(I)=1.
      GO TO 16
   14 DO 15  I=1,N
   15 P(I)=1./Y(I)
   16 WRITE(KO,1)N
      IF(NB-2)17,18,19
   17 WRITE(KO,2)
      CALL BISECT(F1,B1,B2,B,EPS,KENN)
      C=0.
      D=0.
      GO TO 20
   18 WRITE(KO,3)
      CALL BISECT(F2,B1,B2,B,EPS,KENN)
      D=0.
      GO TO 20
   19 WRITE(KO,4)
      CALL BISECT(F3,B1,B2,B,EPS,KENN)
   20 H=0.
      IF(KENN)21,22,21
   21 WRITE(KO,5)
      GO TO 1000
   22 WRITE(KO,6) A,B,C,D
      WRITE(KO,7)
      DO 23  I=1,N
      H1=A*EXP(-B*X(I))
      IF(NB-2)24,25,26
   25 H1=H1+C
      GO TO 24
   26 H1=H1+C*X(I)+D
   24 H2=Y(I)-H1
      H=H+P(I)*H2*H2
      WRITE(KO,8)X(I),Y(I),H1,H2,P(I)
   23 CONTINUE
      WRITE(KO,9)H
      GO TO 1000
```

```
999 STOP
  1 FORMAT(1H1, 3H ZU,I4,61H DATEN WIRD EIN AUSGLEICH IM SINNE DER KLE
   1INSTEN QUADRATE MIT)
  2 FORMAT(1H ,16X,24HF(X)=A*EXP(-B*X) GEMACHT)
  3 FORMAT(1H ,16X,26HF(X)=A*EXP(-B*X)+C GEMACHT)
  4 FORMAT(1H ,15X,30HF(X)=A*EXP(-B*X)+C*X+D GEMACHT)
  5 FORMAT(1H0,38HANDERES INTERVALL (B1,B2) ERFORDERLICH)
  6 FORMAT(1H0,42HDIE WERTE FUER DIE GEFUNDEN PARAMETER SIND/
   11H0,4HA = ,E16.8/1H ,4HB = ,E16.8/1H ,4HC = ,E16.8/1H ,4HD = ,
   2E16.8)
  7 FORMAT(1H0,59H        X              Y              F(X)           Y-F(X)
   1       P/1H )
  8 FORMAT(1X,5E13.5)
  9 FORMAT(1H0,21HFEHLERQUADRATSUMME = ,E15.8)
```

```
      SUBROUTINE BISECT(F,B1,B2,B,EPS,KENN)
      F1=F(B1)
      F2=F(B2)
      IF(F1*F2)2,2,1
    1 KENN=1
      GO TO 8
    2 KENN=0
    3 B3=.5*(B1+B2)
      F3=F(B3)
      IF(F1*F3)5,5,4
    4 B=B2
      B2=B3
      F2=F3
      GO TO 6
    5 B=B1
      B1=B3
      F1=F3
    6 IF(ABS(B-B3)-EPS*ABS(B))7,3,3
    7 B=B3
    8 RETURN
```

```
      FUNCTION F2(B)
      DIMENSION X(1000),Y(1000),P(1000)
      COMMON N,X,Y,P,A,C,D
      H1=0.
      H2=0.
      H3=0.
      H4=0.
      H5=0.
      H6=0.
      H7=0.
      H8=0.
      DO 1 I=1,N
      S=X(I)
      U=EXP(-B*S)
      W=P(I)
      T=Y(I)
      Z1=W*U
      Z2=Z1*U
      Z3=Z1*T
      H1=H1+W
      H2=H2+Z1
      H3=H3+Z2
      H4=H4+W*T
      H5=H5+Z3
      H6=H6+Z1*S
      H7=H7+Z2*S
    1 H8=H8-Z3*S
      DET=1./(H1*H3-H2*H2)
      C=DET*(H3*H4-H2*H5)
      A=DET*(H1*H5-H2*H4)
      F2=H8+H6*C+H7*A
      RETURN
```

```
      FUNCTION F1(B)
      DIMENSION X(1000),Y(1000),P(1000)
      COMMON N,X,Y,P,A,C,D
      H1=0.
      H2=0.
      H3=0.
      H4=0.
      DO 1 I=1,N
      S=X(I)
      U=EXP(-B*S)
      W=P(I)
      T=Y(I)
      H6=W*T*U
      H5=W*U*U
      H1=H1+H6
      H2=H2+H5
      H3=H3+H6*S
    1 H4=H4+H5*S
      A=H1/H2
      F1=H3*H2-H1*H4
      RETURN
```

```
      FUNCTION F3(B)
      DIMENSION X(1000),Y(1000),P(1000)
      COMMON N,X,Y,P,A,C,D
      H1=0.
      H2=0.
      H3=0.
      H4=0.
      H5=0.
      H6=0.
      H7=0.
      H8=0.
      H9=0.
      H11=0.
      H12=0.
      H13=0.
      DO 1 I=1,N
      S=X(I)
      U=EXP(-B*S)
      W=P(I)
      T=Y(I)
      Z1=S*W
      Z2=U*W
      Z3=S*T
      H1=H1+W
      H2=H2+Z1
      H3=H3+Z2
      H4=H4+Z1*S
      H5=H5+Z1*U
      H6=H6+Z2*U
      H7=H7+W*T
      H8=H8+Z3*W
      H9=H9+Z2*T
      H11=H11+Z1*S*U
      H12=H12+Z1*U*U
    1 H13=H13+Z2*Z3
      P1=H4*H6-H5*H5
      P2=H6*H8-H5*H9
      P3=H5*H8-H4*H9
      Z1=H5*H3-H2*H6
      Z2=H2*H9-H3*H8
      Z3=H2*H5-H4*H3
      DET=1./(H1*P1+H2*Z1+H3*Z3)
      A=DET*(H7*Z3-H1*P3-H2*Z2)
      C=DET*(H1*P2+H7*Z1+H3*Z2)
      D=DET*(H7*P1-H2*P2+H3*P3)
      F3=D*H5+C*H11+A*H12-H13
      RETURN
```

Input data for sample problems

```
0
7  -1 1 1. 5. 1.-6
0. .5 1. 1.5 2. 2.5 3.5
15.+2 335. 75. 17. 4. .8 .1
0
9 0 2 .03 .07 1.-6
1. 2. 4. 5. 6. 7. 9. 11. 14.
9.7 9.3 8.7 8.5 8.2 8. 7.5 7. 6.5
0
10 -1 3 .6 2. 1.-6
0. 1. 2. 3. 4. 5. 6. 7. 8. 9.
13. 7. 5. 5. 5. 6. 6. 6.5 7. 7.5
-1
```

Output

```
ZU    7 DATEN WIRD EIN AUSGLEICH IM SINNE DER KLEINSTEN QUADRATE MIT
                F(X)=A*EXP(-B*X) GEMACHT

DIE WERTE FUER DIE GEFUNDEN PARAMETER SIND

A =    0.15009390E+04
B =    0.30000019E+01
C =    0.00000000E+00
D =    0.00000000E+00
```

X	Y	F(X)	Y-F(X)	P
0.00000E+00	0.15000E+04	0.15009E+04	-0.93900E+00	0.66667E-03
0.50000E+00	0.33500E+03	0.33490E+03	0.95550E-01	0.29851E-02
0.10000E+01	0.75000E+02	0.74727E+02	0.27279E+00	0.13333E-01
0.15000E+01	0.17000E+02	0.16674E+02	0.32612E+00	0.58824E-01
0.20000E+01	0.40000E+01	0.37204E+01	0.27956E+00	0.25000E+00
0.25000E+01	0.80000E+00	0.83014E+00	-0.30142E-01	0.12500E+01
0.35000E+01	0.10000E+00	0.41330E-01	0.58670E-01	0.10000E+02

```
FEHLERQUADRATSUMME =   0.62958709E-01
```

ZU 9 DATEN WIRD EIN AUSGLEICH IM SINNE DER KLEINSTEN QUADRATE MIT
F(X)=A*EXP(-B*X)+C GEMACHT

DIE WERTE FUER DIE GEFUNDEN PARAMETER SIND

A = 0.69868300E+01
B = 0.50000035E-01
C = 0.30239113E+01
D = 0.00000000E+00

X	Y	F(X)	Y-F(X)	P
0.10000E+01	0.97000E+01	0.96700E+01	0.30011E-01	0.10000E+01
0.20000E+01	0.93000E+01	0.93459E+01	-0.45856E-01	0.10000E+01
0.40000E+01	0.87000E+01	0.87442E+01	-0.44243E-01	0.10000E+01
0.50000E+01	0.85000E+01	0.84653E+01	0.34741E-01	0.10000E+01
0.60000E+01	0.82000E+01	0.81999E+01	0.11890E-03	0.10000E+01
0.70000E+01	0.80000E+01	0.79474E+01	0.52554E-01	0.10000E+01
0.90000E+01	0.75000E+01	0.74789E+01	0.21091E-01	0.10000E+01
0.11000E+02	0.70000E+01	0.70550E+01	-0.54960E-01	0.10000E+01
0.14000E+02	0.65000E+01	0.64935E+01	0.65334E-02	0.10000E+01

FEHLERQUADRATSUMME = 0.12437845E-01

ZU 10 DATEN WIRD EIN AUSGLEICH IM SINNE DER KLEINSTEN QUADRATE MIT
F(X)=A*EXP(-B*X)+C*X+D GEMACHT

DIE WERTE FUER DIE GEFUNDEN PARAMETER SIND

A = 0.96505729E+01
B = 0.13000013E+01
C = 0.43015678E+00
D = 0.35310334E+01

X	Y	F(X)	Y-F(X)	P
0.00000E+00	0.13000E+02	0.13182E+02	-0.18161E+00	0.76923E-01
0.10000E+01	0.70000E+01	0.65913E+01	0.40873E+00	0.14286E+00
0.20000E+01	0.50000E+01	0.51081E+01	-0.10813E+00	0.20000E+00
0.30000E+01	0.50000E+01	0.50168E+01	-0.16849E-01	0.20000E+00
0.40000E+01	0.50000E+01	0.53049E+01	-0.30490E+00	0.20000E+00
0.50000E+01	0.60000E+01	0.56963E+01	0.30367E+00	0.16667E+00
0.60000E+01	0.60000E+01	0.61159E+01	-0.11593E+00	0.16667E+00
0.70000E+01	0.65000E+01	0.65432E+01	-0.43208E-01	0.15385E+00
0.80000E+01	0.70000E+01	0.69726E+01	0.27419E-01	0.14286E+00
0.90000E+01	0.75000E+01	0.74025E+01	0.97476E-01	0.13333E+00

FEHLERQUADRATSUMME = 0.66660862E-01

5. Method for Models f_4 and f_5

The iterative method for minimizing S is the same for both models. We use the damped version of the GAUSS-NEWTON method derived in [2]. A brief description and an ALGOL procedure for this method can be found in [4]. The method has been described in particular and compared with other methods for fitting to sums of exponentials in [3] where also numerical experience and difficulties have been pointed out. Starting values for the required parameters must be given. Then the method only fails to converge to a stationary point of S if a certain matrix becomes singular [3]. In this case either the data are too bad or the number of exponentials too high or other starting values are necessary.

6. Programs for Models f_4 and f_5

A subroutine GAUSS (N, A, B, X, KK) must be made available which solves a linear systems of N equations Ax = b for x if A is not singular, otherwise it is left with KK = 1.

The main program requires the following input data:

I.	IFF	If IFF $\geq$ 0 then go to II else end of the input data
II.	N	Number of data points ($J \leq N \leq 500$)
	NG	Weighting (see 4.)

J	Number of parameters ($2 \leq J \leq 11$) If NOP $\neq$ 0, J must be even If NOP = 0, J must be odd
ITMAX	Maximal numbers of iterations to be performend (recommended : 20)
NOP	NOP $\neq$ 0 : model f_4 NOP = 0 : model f_5
III. - V.	see 4.
VI. (A(I), I = 1,J)	Starting values for the required parameters.

Start at I.

An example for input data and the corresponding output is given below.

```
      MAINPROGRAM FOR FITTING WITH SEVERAL EXPONENTIALS
      DIMENSION A(11),X(500),Y(500),G(500),FU(500),FELD(1863)
      COMMON FELD
      KI=8
      KO=9
 1000 READ(KI,1) IFF
      IF(IFF)999,10,10
   10 READ(KI,1)N,NG,J,ITMAX,NOP
      READ(KI,1)(X(I),I=1,N)
      READ(KI,1)(Y(I),I=1,N)
      IF(NG)12,12,11
   11 READ(KI,1)(G(I),I=1,N)
   12 READ(KI,1)(A(I),I=1,J)

      WRITE(KO,1)N
      IF(NOP)14,13,14
   13 WRITE(KO,2)
      GO TO 15
   14 WRITE(KO,3)
   15 WRITE(KO,4)J
      WRITE(KO,5) (A(I),I=1,J)

      CALL EXPO(A,X,Y,G,N,J,NG,NOP,FU,FM,ITMAX,IFEHL)

      WRITE(KO,6)ITMAX
      IF(IFEHL-1)17,16,17
   16 WRITE(KO,7)
      GO TO 1000
   17 WRITE(KO,8)(A(I),I=1,J)
      WRITE(KO,9)FM
      WRITE(KO,20)
      DO 18 I=1,N
      H=Y(I)-FU(I)
   18 WRITE(KO,21)X(I),Y(I),FU(I),H,G(I)
      GO TO 1000
  999 STOP

   21 FORMAT(1X,5E17.7)
   20 FORMAT(1H0,79H          X                    Y                    F(X)
     1          Y-F(X)               G/1H0)
    1 FORMAT(1H1,3H ZU,I4,62H  DATEN WIRD EIN AUSGLEICH IM SINNE DER KLE
     1INSTEN QUADRATE MIT)
    2 FORMAT(1H0,59HF(X)=A(1)+A(2)*EXP(-A(3)*X)+...+A(J-1)*EXP(-A(J)*X)
     1GEMACHT)
    3 FORMAT(1H0,54HF(X)=A(1)*EXP(-A(2)*X)+...+A(J-1)*EXP(-A(J)*X) GEMAC
     1HT)
    4 FORMAT(1H+,60X,7HMIT J =,I3)
    5 FORMAT(1H0,33HDIE EINGEGEBENEN STARTWERTE WAREN/1H0,(7E17.8/))
    6 FORMAT(1H0,4HNACH,I3,12H ITERATIONEN)
    7 FORMAT(1X,43HIST DIE FUNKTIONALMATRIX SINGULAER GEWORDEN/1H0,30HAN
     1DERE STARTWERTE ERFORDERLICH)
    8 FORMAT(1X,48HWURDEN FOLGENDE PARAMETER A(1),...,A(J) ERHALTEN/1H0,
     1(7E17.8/))
    9 FORMAT(1H0,26HDIE FEHLERQUADRATSUMME IST,E20.8/1H0)
```

```
      SUBROUTINE EXPO(A,X,Y,G,N,J,NG,NOP,FU,FM,ITMAX,IFEHL)
C
      DIMENSION A(2),A1(11),DA(11),B(11),X(2),Y(2),G(2),FU(2)
     1EN(27,27),DFDA(11,100),FELD(1863)
C
C     DIMENSION A(J),A1(J),DA(J),B(J),X(N),Y(N),G(N),FU(N),
C     EN(J,J),DFDA(J,N),FELD(1863)
C
      COMMON FELD
C
      EQUIVALENCE (FELD(1),DA(1)),(FELD(12),A1(1)),
     1(FELD(23),B(1)),(FELD(34),EN(1,1)),(FELD(763),DFDA(1,1))
C
      IF(NG)500,501,502
  500 DO 503 I=1,N
  503 G(I)=1.
      GO TO 502
  501 DO 504 I=1,N
  504 G(I)=1./Y(I)
  502 IFEHL=0
      IANZ=0
      RUND1=1.-1.E-5
      RUND2=1.+1.E-6
      S=1.E45
  300 IANZ=IANZ+1
      IDAE=0
      SUN=S*RUND1
      IF(IANZ-ITMAX)311,310,310
  310 IFEHL=-1
      GO TO 312
  311 S=0.
      DO 404 K=1,N
      IF(NOP)601,600,601
  601 HK=0.
      KK=2
      GOTO 602
  600 HK=A(1)
      DFDA(1,K)=1.
      KK=3
  602 DO 405 I=KK,J,2
      FH=EXP(-A(I)*X(K))
      DFDA(I-1,K)=FH
      DFDA(I,K)=-FH*A(I-1)*X(K)
      HK=HK+A(I-1)*FH
  405 CONTINUE
      FKT=HK
      HF=(Y(K)-FKT)
      S=S+G(K)*HF*HF
      IF(S-SUN)403,403,350
  403 FU(K)=HF*G(K)
  404 CONTINUE
      DO 302 I=1,J
      HF=0.0
      DO 303 K=1,N
  303 HF=HF+DFDA(I,K)*FU(K)
      B(I)=HF
  302 CONTINUE
      DO 304 I=1,J
      DO 304 K=1,J
      HF=0.0
      DO 305 L=1,N
```

```
  305 HF=HF+DFDA(I,L)*G(L)*DFDA(K,L)
      EN(I,K)=HF
  304 CONTINUE
      DO 340 I=1,J
  340 EN(I,I)=EN(I,I)*RUND2
C
      CALL GAUSS(J,EN,B,DA,IFEHL)
C
      IF(IFEHL-1)319,999,319
  319 DO 314 I=1,J
      A1(I)=A(I)
  314 A(I)=A(I)+DA(I)
      GO TO 300
  350 IF(IDAE-10)352,352,370
  352 IDAE=IDAE+1
      DO 354 I=1,J
  354 A(I)=(A(I)+1.5*A1(I))*.4
      GO TO 311
  370 DO 372 I=1,J
  372 A(I)=A1(I)
  312 FM=0.0
      DO 315 K=1,N
      IF(NOP)701,700,701
  701 HK=0.
      KK=2
      GOTO 702
  700 HK=A(1)
      KK=3
  702 DO 299 I=KK,J,2
  299 HK=HK+A(I-1)*EXP(-A(I)*X(K))
      FU(K)=HK
      FH=Y(K)-HK
      FM=FM+G(K)*FH*FH
  315 CONTINUE
      ITMAX=IANZ
  999 RETURN
```

Input data for sample problems

```
0
24  -1  5  20  0
.05 .1 .15 .2 .25 .3 .35 .4 .45 .5 .55 .6 .65 .7 .75 .8 .85 .9 .95 1. 1.05
1.1 1.15 1.2
2.51 2.04 1.67 1.37 1.12 .93 .77 .64 .53 .45 .38 .32 .27 .23 .2 .17 .15 .13
.11 .1 .09 .08 .07 .06
.05  3.  4.  1.  2.
0
24  -1  7  20  0
.05 .1 .15 .2 .25 .3 .35 .4 .45 .5 .55 .6 .65 .7 .75 .8 .85 .9 .95 1. 1.05
1.1 1.15 1.2
2.51 2.04 1.67 1.37 1.12 .93 .77 .64 .53 .45 .38 .32 .27 .23 .2 .17 .15 .13
.11 .1 .09 .08 .07 .06
.04  .4  7.  3.  4.  .4  .2
-1
```

Output

ZU 24 DATEN WIRD EIN AUSGLEICH IM SINNE DER KLEINSTEN QUADRATE MIT

Output

ZU 24 DATEN WIRD EIN AUSGLEICH IM SINNE DER KLEINSTEN QUADRATE MIT

F(X)=A(1)+A(2)*EXP(-A(3)*X)+...+A(J-1)*EXP(-A(J)*X) GEMACHT MIT J = 5

DIE EINGEGEBENEN STARTWERTE WAREN

0.50000000E-01 0.30000000E+01 0.40000000E+01 0.10000000E+01 0.20000000E+01

NACH 6 ITERATIONEN
WURDEN FOLGENDE PARAMETER A(1),...,A(J) ERHALTEN

0.16481979E-01 0.22634138E+01 0.48302326E+01 0.81100530E+00 0.25258549E+01

DIE FEHLERQUADRATSUMME IST 0.10763977E-03

X	Y	F(X)	Y-F(X)	G
0.5000000E-01	0.2510000E+01	0.2509042E+01	0.9582000E-03	0.1000000E+01
0.1000000E+00	0.2040000E+01	0.2042797E+01	-0.2797400E-02	0.1000000E+01
0.1500000E+00	0.1670000E+01	0.1668457E+01	0.1543500E-02	0.1000000E+01
0.2000000E+00	0.1370000E+01	0.1367265E+01	0.2734900E-02	0.1000000E+01
0.2500000E+00	0.1120000E+01	0.1124379E+01	-0.4378900E-02	0.1000000E+01
0.3000000E+00	0.9300000E+00	0.9280376E+00	0.1962430E-02	0.1000000E+01
0.3500000E+00	0.7700000E+00	0.7689150E+00	0.1084970E-02	0.1000000E+01
0.4000000E+00	0.6400000E+00	0.6396080E+00	0.3919600E-03	0.1000000E+01
0.4500000E+00	0.5300000E+00	0.5342326E+00	-0.4232550E-02	0.1000000E+01
0.5000000E+00	0.4500000E+00	0.4481062E+00	0.1893830E-02	0.1000000E+01
0.5500000E+00	0.3800000E+00	0.3774975E+00	0.2502500E-02	0.1000000E+01
0.6000000E+00	0.3200000E+00	0.3194284E+00	0.5716100E-03	0.1000000E+01
0.6500000E+00	0.2700000E+00	0.2715181E+00	-0.1518080E-02	0.1000000E+01
0.7000000E+00	0.2300000E+00	0.2318598E+00	-0.1859780E-02	0.1000000E+01
0.7500000E+00	0.2000000E+00	0.1989236E+00	0.1076440E-02	0.1000000E+01
0.8000000E+00	0.1700000E+00	0.1714791E+00	-0.1479110E-02	0.1000000E+01
0.8500000E+00	0.1500000E+00	0.1485350E+00	0.1465000E-02	0.1000000E+01
0.9000000E+00	0.1300000E+00	0.1292903E+00	0.7096900E-03	0.1000000E+01
0.9500000E+00	0.1100000E+00	0.1130965E+00	-0.3096470E-02	0.1000000E+01
0.1000000E+01	0.1000000E+00	0.9942681E-01	0.5731910E-03	0.1000000E+01
0.1050000E+01	0.9000000E-01	0.8785250E-01	0.2147500E-02	0.1000000E+01
0.1100000E+01	0.8000000E-01	0.7802334E-01	0.1976662E-02	0.1000000E+01
0.1150000E+01	0.7000000E-01	0.6965247E-01	0.3475340E-03	0.1000000E+01
0.1200000E+01	0.6000000E-01	0.6250420E-01	-0.2504197E-02	0.1000000E+01

ZU 24 DATEN WIRD EIN AUSGLEICH IM SINNE DER KLEINSTEN QUADRATE MIT

F(X)=A(1)+A(2)*EXP(-A(3)*X)+...+A(J-1)*EXP(-A(J)*X) GEMACHT MIT J = 7

DIE EINGEGEBENEN STARTWERTE WAREN

0.40000000E-01 0.40000000E+00 0.70000000E+01 0.30000000E+01 0.40000000E+01 0.40000000E+00
0.20000000E+00

NACH 17 ITERATIONEN
WURDEN FOLGENDE PARAMETER A(1),...,A(J) ERHALTEN

-0.17027122E+00 0.34304884E+00 0.72550936E+01 0.26363417E+01 0.39953116E+01 0.28568216E+00
0.25524708E+00

DIE FEHLERQUADRATSUMME IST 0.10502725E-03

X	Y	F(X)	Y-F(X)	G
0.5000000E-01	0.2510000E+01	0.2509427E+01	0.5733000E-03	0.1000000E+01
0.1000000E+00	0.2040000E+01	0.2042295E+01	-0.2294900E-02	0.1000000E+01
0.1500000E+00	0.1670000E+01	0.1668092E+01	0.1908500E-02	0.1000000E+01
0.2000000E+00	0.1370000E+01	0.1367276E+01	0.2724000E-02	0.1000000E+01
0.2500000E+00	0.1120000E+01	0.1124674E+01	-0.4673700E-02	0.1000000E+01
0.3000000E+00	0.9300000E+00	0.9284339E+00	0.1566150E-02	0.1000000E+01
0.3500000E+00	0.7700000E+00	0.7692519E+00	0.7480900E-03	0.1000000E+01
0.4000000E+00	0.6400000E+00	0.6397873E+00	0.2126900E-03	0.1000000E+01
0.4500000E+00	0.5300000E+00	0.5342224E+00	-0.4222390E-02	0.1000000E+01
0.5000000E+00	0.4500000E+00	0.4479279E+00	0.2072060E-02	0.1000000E+01
0.5500000E+00	0.3800000E+00	0.3772067E+00	0.2793270E-02	0.1000000E+01
0.6000000E+00	0.3200000E+00	0.3190962E+00	0.9037900E-03	0.1000000E+01
0.6500000E+00	0.2700000E+00	0.2712158E+00	-0.1215770E-02	0.1000000E+01
0.7000000E+00	0.2300000E+00	0.2316474E+00	-0.1647350E-02	0.1000000E+01
0.7500000E+00	0.2000000E+00	0.1988422E+00	0.1157830E-02	0.1000000E+01
0.8000000E+00	0.1700000E+00	0.1715471E+00	-0.1547080E-02	0.1000000E+01
0.8500000E+00	0.1500000E+00	0.1487465E+00	0.1253550E-02	0.1000000E+01
0.9000000E+00	0.1300000E+00	0.1296159E+00	0.3841400E-03	0.1000000E+01
0.9500000E+00	0.1100000E+00	0.1134853E+00	-0.3485290E-02	0.1000000E+01
0.1000000E+01	0.1000000E+00	0.9980949E-01	0.1905100E-03	0.1000000E+01
0.1050000E+01	0.9000000E-01	0.8814444E-01	0.1855560E-02	0.1000000E+01
0.1100000E+01	0.8000000E-01	0.7812810E-01	0.1871900E-02	0.1000000E+01
0.1150000E+01	0.7000000E-01	0.6946517E-01	0.5348300E-03	0.1000000E+01
0.1200000E+01	0.6000000E-01	0.6191457E-01	-0.1914570E-02	0.1000000E+01

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