Algorithms

J. G. HERRIOT, Editor

ALGORITHM 295
EXPONENTIAL CURVE FIT [E2]

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procedure expfit (x, y, p, n, ca, ce, eps, a, b, c, s, fx, exit);
  value n, ca, ce, eps;  integer n;  real ca, ce, eps, a, b, c, s;
  label exit;  array x, y, p, fx;
comment  If the method of least squares is used to determine
  the parameters a, b, c of a curve f(x) = a + be^{-cx} which approxi-
  mates n data points (x_i, y_i) with associated weights p_i, then

                    s(a, b, c) = Σ_{i=1}^{n} p_i(y_i − f(x_i))²        (I)

  must be a minimum. A necessary condition for this is that

                    ∂s/∂a = ∂s/∂b = ∂s/∂c = 0.                        (II)

  Usually (see [1]) it is attempted to solve this system of nonlinear
  equations by an iterative method which is based upon the
  linearization of f in (II) and the convergence of which depends
  on the given starting values for a, b, c.
    A simpler and more effective way which can always be chosen
  if there is only one nonlinear parameter in f is the following:
  It is always possible to eliminate a = a(c) and b = b(c) from the
  equations ∂s/∂a = 0 and ∂s/∂b = 0 and to put these expressions
  into ∂s/∂c = 0. This gives only one equation in one variable

                    F(c) := ∂s/∂c (a(c), b(c), c) = 0.

  If a value c' is calculated with F(c') = 0 then the corresponding
  values of a and b are obtained from a' = a(c') and b' = b(c').
    The following procedure is based upon this idea which is fully
  treated in [2]. It allows to find a triple (a, b, c) which solves (II)
  if you make available a nonlocal procedure Rootfinder which is
  able to get a zero c of a function F(c) in the interval [ca, ce] with
  the relative accuracy eps, if sign (F(ca)) ≠ sign (F(ce)) otherwise
  leaving to the global label exit. As the above F(c) is discontinu-
  ous at c = 0, [ca, ce] must not contain 0. [The speed and efficiency
  of the algorithm depend on the choice of the procedure Root-
  finder. REF.]
    Most of the symbols are self-explanatory. The array fx finally
  contains the values a + be^{-cx_i};
begin integer i;  real t, u, v, w, fc, h0, h1, h2, h3, h4, h5, h6, h7;
  procedure fronc (c, fc);  value c;  real c, fc;
  comment  computes for a given c the value fc = F(c) and
    a = a(c), b = b(c);
  begin h0 := h1 := h2 := h3 := h4 := h5 := h6 := h7 := 0;
    for i := 1 step 1 until n do
    begin
      t := x[i];  u := exp(−c×t);  v := p[i];  w := y[i];
      h0 := h0 + v;  h1 := h1 + u × v;  h2 := h2 + u × u × v;
      h3 := h3 + v × w;  h4 := h4 + u × v × w;
      h5 := h5 + t × u × v;
      h6 := h6 + t × u × u × v;  h7 := h7 − u × v × w × t
    end i;
    t := 1.0/(h0×h2−h1×h1);  a := t × (h2×h3−h1×h4);
    b := t × (h0×h4−h1×h3);  fc := h7 + (h5×a+h6×b)
  end fronc;
  Rootfinder (fronc, ca, ce, eps, c, exit);  t := 0;
  for i := 1 step 1 until n do
  begin
    v := fx[i] := a + b × exp(−c×x[i]);  v := v − y[i];
    t := t + p[i] × v × v
  end i;
  s := t
end expfit
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REFERENCES:
1. DEILY, G. R. Algorithm 275, Exponential curve fit. *Comm. ACM 9* (Feb. 1966), 85.
2. OBERLÄNDER, S. Die Methode der kleinsten Quadrate bei einem dreiparametrigen Exponentialansatz. *ZAMM 43* (1963), 493–506.

ALGORITHM 296
GENERALIZED LEAST SQUARES FIT BY ORTHOGONAL POLYNOMIALS [E2]

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procedure LSFITUW (f, x, w, m, k, si, p, l, al, be, s);  value m, k;
  integer m, k;  array f, w, si, p, x, al, be, s;  Boolean l;
comment  LSFITUW accepts m observations x[i], f[i], i = 1, 2,
  · · ·, m each with its associated weight w[i]. The weights should
  be provided inversely proportional to the standard error of the
  observations.
    x[1] should be algebraically the smallest abscissa and x[m] the
  largest.
    The coefficients of the best fitting polynomial of degree k or
  less, where k < m − 1, are obtained in p[0:k], with p[0] the
  independent term. si[0:k] contains the measures of the goodness
  of fit of each polynomial tested. The si[t] are examined suc-
  cessively and the best polynomial is chosen of degree h if h is
  the first value of t found such that si[h] < si[h+1] provided
  that si[j] > 0.6 × si[h] for k ≧ j > h + 1. If h is the first value
  of t found such that si[h] < si[h+1] but then a j is found that
  satisfies si[j] ≦ 0.6 × si[h] for j > h + 1 the procedure will choose
  the polynomial of degree j as best fit.
    If an h such that si[h] < si[h+1] is not found then the poly-
  nomial is chosen of degree k. LSFITUW uses the procedure
  POLYX (a, b, c, d, n) [Algorithm 29, Comm. ACM 3 (Nov. 1960),
  604] to transform its results from the interval (−2,2) to the
  interval (x[1], x[m]).
    Normally l should be false but if the choice made is to be
  overruled after consideration of the si and the best fitting
  polynomial is required to be strictly of degree k, then l should be
  true.
    The programming is as outlined by G. E. Forsythe, [J. Soc.
  Indust. Appl. Math. 5 (1957), 74–88] and originally programmed
  by J. G. Mackinney [Algorithm 28/29, Comm. ACM 3 (Nov.
  1960), 604]. LSFITUW incorporates remarks made by D. B.
  MacMillan [Comm. ACM 4 (Dec. 1961), 544].
    The variables in the paper of Forsythe have been abbreviated
  as follows.
    al[i] is alpha[i], be[i] is beta[i], si[i] is (sigma[i]) ↑ 2, s[i] is
  the same, om is omega, lw is w[i, i], tw is w[i+1, i+1],
  ctp[j] is the coefficient of x ↑ j in This (the current)
  orthogonal polynomial, clp[j] is the coefficient of x ↑ j in
  the Last (previous) orthogonal polynomial, cp[j] is the co-
  efficient of x ↑ j in the most recently calculated polynomial
  of best fit, tp[i] is the value at x[i] of the present orthogonal
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        polynomial, lp[i] is the value at x[i] of the last orthogo-
        nal polynomial, simin is the least value of (sigma[i]) ↑ 2
        found so far, swx becomes false as soon as (sigma[i+1]) ↑
        2 ≧ (sigma[i]) ↑ 2 one time, comp becomes true if swx
        is false and some (sigma[i]) ↑ 2 < 0.6 × simin;
egin integer i, j; real du, delsq, om, lw, tw, simin, a, b;
 array clp, cpsave, cp[0:k], clp[-1:k], lp, tp[1:m];
   Boolean swx, comp;
 comment initialization;
 for i := 0 step 1 until k do cp[i] := 0; simin := 0;
 swx := true; be[0] := clp[0] := clp[-1] := delsq := om := 0;
   clp[0] := 1; tw := 0; comp := false;
 for i := 1 step 1 until m do
 begin
   delsq := delsq + w[i] × f[i] ↑ 2; tp[i] := 1;
   lp[i] := 0; om := om + w[i] × f[i]; tw := tw + w[i]
 end;
 s[0] := cp[0] := om/tw; delsq := delsq - s[0] × om;
   si[0] := delsq/(m-1);
 comment transformation of abscissa;
 a := 4/(x[m]-x[1]); b := - 2 - a × x[1];
 for i := 1 step 1 until m do x[i] := a × x[i] + b;
 comment main computation loop;
 for i := 0 step 1 until k - 1 do
 begin
   du := 0;
   for j := 1 step 1 until m do du := du + w[j] × x[j] × tp[j] ↑ 2;
   al[i + 1] := du/tw; lw := tw; tw := om := 0;
   for j := 1 step 1 until m do
   begin
     du := be[i] × lp[j];
     lp[j] := tp[j];
     tp[j] := (x[j]-al[i+1]) × tp[j] - du;
     tw := tw + w[j] × tp[j] ↑ 2;
     om := om + w[j] × f[j] × tp[j]
   end;
   be[i+1] := tw/lw; s[i+1] := om/tw;
   delsq := delsq - s[i+1] × om; si[i+1] := delsq/(m-i-2);
   if l then go to L1;
   if ¬ comp then
   begin
     if swx then
     begin
     if si[i+1]≧ si[i] then
       begin
         comment higher power appears not to improve fit;
         swx := false;
         simin := si[i];
         for j := 0 step 1 until k do
           cpsave[j] := cp[j]
       end;
       go to L1
     end;
     if si[i+1] < 0.6 × simin then comp := true;
     comment termination of main loop at superior fit to first
       one found;
     comment recursion to obtain the coefficients cp of the
       polynomial of best fit of degree i + 1;
L1:  for j := 0 step 1 until i do
     begin
       du := clp[j] × be[i];
       clp[j] := ctp[j];
       ctp[j] := clp[j-1] - al[i+1] × ctp[j] - du;
       cp[j] := cp[j] + s[i+1] × ctp[j]
     end;
     cp[i+1] := s[i+1]; ctp[i+1] := 1; clp[i+1] := 0;
     if ¬ (comp ∨ swx) then
       begin
         if i = k - 1 then
         for j := 0 step 1 until k do
           cp[j] := cpsave[j]
       end
     end
   end end of main computation loop. Transformation of poly-
     nomial follows;
   POLYX(a, b, cp, p, k)
end LSFITUW
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Algorithms Policy • Revised August, 1966

(Includes Fortran)

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insymbol	*inreal*	*outarray*	*ininteger*
outsymbol	*outreal*	*outboolean*	*outinteger*
length	*inarray*	*outstring*	

If only one channel is used by the program for output, it should be designated by 1 and similarly a single input channel should be designated by 2. Examples:

outstring (1, '*x*='); *outreal* (1,*x*);
for *i* := 1 **step** 1 **until** *n* **do** *outreal* (1,*A*[*i*]);
ininteger (2, *digit* [17]):

For FORTRAN programs, input and output should be achieved as described in the ASA preliminary report on FORTRAN and Basic FORTRAN.

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