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ALGORITHM 32

# CONSTRUCTION OF POLYNOMIAL VALUES ORTHOGONAL ON A GIVEN SET OF A ONE-DIMENSIONAL VARIABLE

**1. Procedure declaration.** Procedure *orthonw* is an auxiliary procedure used in calculations dealing with

a. polynomial approximation of a given set of some response variable $y$,

b. the trend-decomposition of variance due to between-class-variation.

This procedure should be called repeatedly for $k = 0, 1, \ldots$ and the values of $pa$ must not be destroyed between successive calls.

Data:

$p$ — actual degree of the polynomial,

$n$ — number of values in array $x$,

$w[1:n]$ — weights for the values of array $x$ (number of observations for each value of $x$),

$x[1:n]$ — array of values of the independent variable $x$,

$pl[1:n]$ — values of the polynomial of degree $p-1$, generated during the preceding call of *orthonw* (undefined for $p = 0$),

$pa[1:n+6]$ — auxiliary array containing the values of the polynomial of degree $p-2$ (undefined for $p = 0$).

Results:

$pl[1:n]$ — values of the polynomial of degree $p$ evaluated for the values given in array $x$,

$pa[1:n+6]$ — values of the polynomial of degree $p-1$ evaluated for the values given in array $x$, and constants necessary for further calculations of expected values and coefficients of regression,

*ifault* — error indicator:

0 — no error,

1 — the call of *orthonw* does not succeede in the appropriate order,

2 — there are at least two identical values in array $x$,

3 — the normalizing divisor is less than $10^{-50}$.

**2. Method used.** Given the set of values $x_1, x_2, \ldots, x_n$ with weights $w_1, w_2, \ldots, w_n$, the aim of the procedure is to find, for $k = 0, 1, \ldots, n-1$, sets of values $p_k(x_1), p_k(x_2), \ldots, p_k(x_n)$ such that, for $i = 1, 2, \ldots, n$,

a. $p_k(x_i)$ is the value of a polynomial of degree $k$ evaluated for $x_i$,

b. the following conditions of orthonormality hold:

$$\sum_{i=1}^{n} w_i p_j(x_i) p_k(x_i) = \begin{cases} 1 & \text{for } j = k, \\ 0 & \text{for } j \neq k. \end{cases}$$

The $p_j(x_i)$ are evaluated by the use of recurrent formulas which can be found in Ralston [4] and, for the case of equal weights, also in Cooper [3]. The procedure uses the formulas

$$p_0(x_i) = \frac{1}{\sqrt{\sum_{i=1}^{n} w_i}}, \qquad p_1(x_i) = \frac{x_i - A}{\sqrt{\sum_{i=1}^{n} w_i (x_i - A)^2}},$$

where $A$ is the weighted average of the $x$-values,

$$A = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i},$$

$$C_{r+1} p_{r+1}(x_i) = \big(p_1(x_i) - A_{r+1}\big) - B_{r+1} p_{r-1}(x_i)$$

$$\text{for } 1 < r \leqslant n-1 \text{ and } i = 1, \ldots, n$$

with constants $A_{r+1}$, $B_{r+1}$ and $C_{r+1}$ satisfying the following relations:

$$C_{r+1} = \sqrt{\sum_{i=1}^{n} w_i p_{r+1}^2(x_i)},$$

$$A_{r+1} = A + \sum_{i=1}^{n} w_i p_1(x_i) p_r^2(x_i),$$

$$B_{r+1} = \sum_{i=1}^{n} w_i p_1(x_i) p_{r-1}(x_i) p_r(x_i).$$

The first call of *orthonw* with $p = 0$ calculates the sum of weights

$$S = \sum_{i=1}^{n} w_i$$

and stores it as $pa[n+3]$. The values of $pl[i]$ and $pa[i]$ are set equal to $1/\sqrt{A}$ for $i = 1, \ldots, n$. The value of *ifault* is set equal to 2 if there are at least two identical values of $x$. Otherwise, *ifault* is set equal to 0.

```
procedure orthonw(p,n,w,x,pl,pa,ifault);
 value p,n;
 integer p,n,ifault;
 array w,x,pl,pa;
 begin
  integer m,i,j;
  real ss,d1,d2,a,z;
  m:=p-1;
  if p=0
   then
   begin
    a:=0.0;
    for i:=1 step 1 until n do
     a:=a+w[i];
    pa[n+3]:=a;
    z:=1.0/sqrt(a);
    for i:=1 step 1 until n do
     pl[i]:=pa[i]:=z;
    for i:=2 step 1 until n do
     for j:=1 step 1 until i-1 do
      if x[i]=x[j]
       then
       begin
        ifault:=2;
        go to konorthon
       end x[i]=x[j];
    ifault:=0;
    go to konorthon
   end p=0
   else
```

```
if p=1
 then
 begin
  d2:=d1:=ss:=0.0;
  for i:=1 step 1 until n do
   ss:=ss+x[i]×w[i];
  a:=pa[n+2]:=ss/pa[n+3];
  ss:=0.0;
  for i:=1 step 1 until n do
   begin
    pl[i]:=x[i]-a;
    ss:=ss+w[i]×pl[i]↑2
   end i
 end p=1
 else
 begin
  if abs(m-pa[n+1])<₁₀-50
   then
   begin
    ifault:=1;
    go to konorthon
   end p>1;
  d1:=d2:=0.0;
  a:=pa[n+2];
  for i:=1 step 1 until n do
   begin
    ss:=(x[i]-a)×w[i]×pl[i];
    d2:=d2+ss×pa[i];
    d1:=d1+ss×pl[i]
   end i;
```

```
            ss:=0.0;
            for i:=1 step 1 until n do
             begin
              z:=pl[i];
              pl[i]:=-d2×pa[i]+(x[i]-a-d1)×pl[i];
              pa[i]:=z;
              ss:=ss+w[i]×pl[i]↑2
             end i;
            if ss<₁₀-50
             then
             begin
              ifault:=3;
              go to konorthon
             end ss<₁₀-50
          end p>1;
      pa[n+4]:=ss:=1/sqrt(ss);
      for i:=1 step 1 until n do
       pl[i]:=pl[i]×ss;
      pa[n+1]:=p;
      pa[n+5]:=(a+d1)×ss;
      pa[n+6]:=d2×ss;
    konorthon:
     end orthonw
```

The second call of *orthonw* with $p = 1$ supplies the values of $p_1(x_i)$ for $i = 1, \dots, n$, and sets $pa[n+1]$, $pa[n+4]$, $pa[n+5]$ and $pa[n+6]$ as described below for $p > 1$.

Further calls of *orthonw*, for $p = 2, \dots, n-1$, provide the values of $p_{r+1}(x_i)$, $1 < r \leqslant n-1$.

After the entry with $p = r+1$ the values of *pl*, representing polynomials of degree $r$, are removed into the auxiliary array *pa*, and new values of orthogonal polynomials of degree $r+1$ are calculated. The actual value $p-1 = r$ is compared with the stored value $pl[n+1]$. If both values do not agree, the error indicator *ifault* is set equal to 1 and further calculations are not executed. Moreover, when $C_{r+1} < 10^{-50}$, the error indicator *ifault* is set equal to 3 and further calculations are not executed. Otherwise, the constants necessary for further calculations are stored as follows:

$$pa[n+1] = p, \quad pa[n+4] = 1/C_{r+1},$$
$$pa[n+5] = A_{r+1}/C_{r+1}, \quad pa[n+6] = B_{r+1}/C_{r+1}.$$

**3. Certification.** Let $n = 3$, $w_1 = w_2 = w_3 = 1$, $x_1 = 1$, $x_2 = 2$, $x_3 = 3$. Polynomials of first and second degrees can be constructed. Their values are the following:

$$p_1(x_1) = -0.707,\ p_1(x_2) = 0.000,\ p_1(x_3) = 0.707,$$
$$p_2(x_1) = 0.408,\ p_2(x_2) = -0.816,\ p_2(x_3) = 0.408.$$

Further examples of an application of procedure *orthonw* are presented in [1] and [2].

## References

[1] A. Bartkowiak, *Test for difference in trends in a two-factor experiment with repeated measurements*, this fascicle, p. 335-342.
[2] — *Use of orthogonal components in tests for trend*, this fascicle, p. 343-356.
[3] B. E. Cooper, *The use of orthogonal polynomials, Algorithm AS 10*, Appl. Statist. 17 (1969), p. 283-287.
[4] A. Ralston, *A first course in numerical analysis*, McGraw Hill, New York 1965.

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## GENEROWANIE WIELOMIANÓW ORTOGONALNYCH NA DANYM ZBIORZE WARTOŚCI ZMIENNEJ NIEZALEŻNEJ

STRESZCZENIE

Dany jest zbiór $(x_1, \ldots, x_n)$ zawierający $n$ wartości zmiennej $x$. Każdej wartości $x_i$ jest przypisana waga $w_i$ $(i = 1, \ldots, n)$.

Procedura *orthonw* generuje dla sukcesywnych wartości $j$ $(j = 0, 1, \ldots, n-1)$ wartości $p_j(x_i)$ ortogonalne na danym zbiorze, tj. takie, że

$$\sum_{i=1}^{n} w_i p_j(x_i) p_k(x_i) = \begin{cases} 1 & \text{dla } j = k, \\ 0 & \text{dla } j \neq k. \end{cases}$$

Wielomiany te mają zastosowanie przy aproksymacji obserwowanej zmiennej za pomocą funkcji wielomianowej, w szczególności pozwalają w prosty sposób ocenić statystyczną istotność poszczególnych składników.

Dane:

$p$ — stopień wielomianu,
$n$ — liczba wartości w tablicy $x$,
$w[1:n]$ — wagi dla wartości tablicy $x$ (liczba obserwacji dla każdej wartości),
$x[1:n]$ — tablica wartości zmiennej niezależnej,
$pl[1:n]$ — wartości wielomianu stopnia $p-1$, wygenerowanego przy poprzednim wywołaniu procedury *orthonw* (nieokreślone dla $p = 0$),
$pa[1:n+6]$ — tablica pomocnicza, zawierająca wartości wielomianu stopnia $p-2$ (nieokreślona dla $p = 0$).

Wyniki:

$pl[1:n]$ — wartości wielomianu stopnia $p$, obliczonego dla danych tablicy $x$,
$pa[1:n+6]$ — wartości wielomianu stopnia $p-1$, obliczonego dla danych tablicy $x$ oraz pewne stałe, potrzebne do dalszego obliczania wartości oczekiwanych i współczynników regresji,
*ifault* — wskaźnik błędu, przyjmujący następujące wartości:
0 — gdy błędu nie ma,
1 — gdy procedurę *orthonw* wywołano w niewłaściwym porządku,
2 — gdy tablica $x$ zawiera co najmniej dwie identyczne wartości,
3 — gdy czynnik normalizujący jest mniejszy niż $10^{-50}$.

Procedura *orthonw*, podobnie jak procedura *orthon* [1], opiera się na wzorach rekurencyjnych, co umożliwia oszczędne korzystanie z pamięci operacyjnej maszyny.