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The BASIC Program to Analyse the Polymodal Frequency Distribution

into Normal Distributions with Marquardt's Method

by

Tatsuro AKAMINE

Abstract

The algorithm of this program is Marquardt's method. Gauss' elimination method is used to solve the simultaneous linear equations. Each parameter is scaled during calculation for faster convergence. User inputs the data and initial values of the parameters. It is adequate for convergence to set $\lambda=10000$ or larger.

The method analysing the polymodal frequency distribution into normal distribution enables by plotting the frequencies in the medium values of the classes to perform a resolution to the regression curve method based on the least square. Akamine (1982) prepared the program of the Gauss-Seidel method. As the memory was reduced to the minimum for a small-size computer, there was a drawback of slow convergence.

The performance of small computers has risen remarkably in recent times and it became possible to prepare programs with more rapid convergence. The present program based on the Marquardt method is rapid

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in convergence and good in stability. The machine used is the PC 8801 (NEC), but if the memory is satisfactory, less advanced machines may be used.

Calculation Method

We will call F the given frequency distribution, m the number of classes, h the width of the classes, a the smallest class value and b the greatest value. If we call n the number of normal distributions to be analysed, then the sought formula f , the residual function d^2 are:

$$f = \sum_{i=1}^n K_i \cdot N(\mu_i, \sigma_i, x) \quad \dots\dots\dots (1)$$

$$N(\mu_i, \sigma_i, x) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp \left\{ -\frac{(x-\mu_i)^2}{2\sigma_i^2} \right\}$$

$$d^2 = \sum_{x=a}^b d_x^2 = \sum_x (F-f)^2 \quad \dots\dots\dots (2)$$

$$b = a + (m-1)h$$

(Fig. 1).

From (1) we have:

$$\begin{cases} \frac{\partial f}{\partial K_i} = N(\mu_i, \sigma_i, x) \\ \frac{\partial f}{\partial \mu_i} = K_i \cdot N(\mu_i, \sigma_i, x) \cdot \frac{x-\mu_i}{\sigma_i^2} \\ \frac{\partial f}{\partial \sigma_i} = K_i \cdot N(\mu_i, \sigma_i, x) \cdot \frac{(x-\mu_i)^2 - \sigma_i^2}{\sigma_i^3} \end{cases}$$

1. The Gauss-Seidel and the Gauss-Newton methods

With a primary approximation of (1), we have:

$$\Delta f \approx \sum_i \left\{ \frac{\partial f}{\partial K_i} \Delta K_i + \frac{\partial f}{\partial \mu_i} \Delta \mu_i + \frac{\partial f}{\partial \sigma_i} \Delta \sigma_i \right\}$$

If rearranging here the parameters K_i , μ_i , σ_i we express by

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$\alpha_i = (i = 1-3n)$, we obtain:

$$\Delta f \approx \sum_i \frac{\partial f}{\partial \alpha_i} \Delta \alpha_i$$

If we substitute this in (2), then:

$$d^2 = \sum_x \left\{ F - \left(f + \Delta f \right) \right\}^2 = \sum_x \left(d_x - \sum_i \frac{\partial f}{\partial \alpha_i} \Delta \alpha_i \right)^2$$

If we use here the least square method, then:

$$\frac{\partial d^2}{\partial \alpha_j} = -2 \sum_x \left(d_x - \sum_i \frac{\partial f}{\partial \alpha_i} d_{\alpha_i} \right) \frac{\partial f}{\partial \alpha_j} = 0$$

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From this we obtain the following simultaneous equation:

$$\left(\sum_x \frac{\partial f}{\partial \alpha_i} \frac{\partial f}{\partial \alpha_j} \right) (d_{\alpha_i}) = \left(\sum_x d_x \frac{\partial f}{\partial \alpha_i} \right) \dots \textcircled{3}$$

This we call a normal equation and abbreviate as

$$A \Delta \alpha = b$$

This is solved by the Gauss-Newton method which seeks $\Delta \alpha_i$. In fact, however, the methods not using directly the normal equation are more precise and adopted by apparatus such as the large computers (Nakagawa-Koyanagi 1982). We used here the method solving the normal equation by the elimination method of Gauss. However, as the coefficient queue consists of symmetric positive fixed values, the computation is performed in an upper triangular queue (Togawa 1971).

As the parameters are moved one at a time in the Gauss-Seidel method, because of $\Delta \alpha_j = 0$ ($j \neq i$), $\textcircled{3}$ becomes:

$$\sum_x \left(\frac{\partial f}{\partial \alpha_i} \right)^2 d_{\alpha_i} = \sum_x \left(d_x \frac{\partial f}{\partial \alpha_i} \right)$$

and the solution is easy. When explained in the case of 2 variables, Fig. 2 is obtained and we see that the convergence is slow.

In this regard, with linear patterns a solution is obtained at once in the Gauss-Newton method as with regression straight lines. With non-linear patterns, repetition is necessary because of the error due to linear pattern approximation. However, convergence is extremely rapid in the vicinity of the solution. Farther away from the solution there is occurrence of vibration and dispersion.

In order to compare both methods, we analysed the data of porgy body length composition by Tanaka (1956). With the Gauss-Seidel method it

takes 500 iterations to reach a perfect convergence. With the Gauss-Newton method, a perfect convergence is reached after 5 or less iterations. However in the latter method, there is vibration and dispersion with ordinary early values, and so for the early values we used values calculated 5 times by the Gauss-Seidel method.

2. Steepest descent method

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Calling the parameter α_i , (2) yields:

$$\frac{\partial d^2}{\partial \alpha_i} = -2 \sum_x d_x \frac{\partial f}{\partial \alpha_i} \dots\dots\dots (4)$$

If we assume:

$$g = \left(-\frac{\partial d^2}{\partial \alpha_i} \right)$$

then the vector g is the normal of the equal-height surface of d^2 and faces the direction of the valley bottom (Fig. 4). We call g the steepest descent vector. Thus we put

$$\Delta \alpha_i = \left(\sum_x d_x \frac{\partial f}{\partial \alpha_i} \right) k$$

and by taking a suitable k we repeat the calculation until the solution is reached. Generally one provides a suitable early value k_0 and when $\Delta d^2 < 0$, there is acceleration by $k_{n+1} = k_n * 1.2$. When $\Delta d^2 > 0$, there is acceleration by $k_{n+1} = k_n / 2$ and one proceeds anew (Ruckdeschel 1982).

If we take a method similar to the Gauss-Seidel method, then from

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$$\begin{aligned} \Delta f &= \sum_i \frac{\partial f}{\partial \alpha_i} \Delta \alpha_i = \left\{ \sum_i \frac{\partial f}{\partial \alpha_i} \left(\sum_x d_x \frac{\partial f}{\partial \alpha_i} \right) \right\} k \\ &= \beta_s k \\ d^2 &= \sum_x \left\{ F - (f + \Delta f) \right\}^2 = \sum_x (d_x - \beta_s k)^2 \\ \frac{\partial d^2}{\partial k} &= 0 \quad k \text{ is found through } k = \frac{\sum_x d_x \beta_x}{\sum_x \beta_x^2} \end{aligned}$$

However, no convergence takes place by this alone. The reason is that because of $\frac{\partial f}{\partial K_i} < \frac{\partial f}{\partial \mu_i}$, $\frac{\partial f}{\partial \sigma_i}$, K_i does not change at all. So we performed scaling with $\alpha_i' = \frac{\alpha_i}{a_i}$. We obtain at this time

$$\begin{aligned} \frac{\partial f}{\partial \alpha_i'} &= \frac{\partial f}{\partial \alpha_i} \frac{\partial \alpha_i}{\partial \alpha_i'} = a_i \cdot \frac{\partial f}{\partial \alpha_i} \\ \Delta \alpha_i &= a_i \cdot \Delta \alpha_i' \end{aligned}$$

We chose here α_i and used the value of α_i at this time. Consequently all parameters of every scale become 1 (Fig. 5). With this scaling there is a fair improvement of convergence. In simple cases, this will do but in this case the convergence is slow and not practical (Table 1). The reason is that although the steepest descent direction is locally the optimum direction, it is not necessarily a good general direction (Nakagawa, Koyanagi 1982). Thus the steepest descent method is stable but its characteristic is a slow convergence.

3. The Marquardt method

The Marquardt method combines the mutually opposite Gauss-Newton method and the steepest descent method. When comparing (3) and (4) we have $b = g$. Thus:

$$(A + \lambda I) \Delta \alpha = b$$

We pose I : unit sequence. When λ is large, $\lambda I \Delta \alpha = b$ is approximated and as $\Delta \alpha = (1/\lambda)b$, we have the steepest descent method. When λ is small $A \Delta \alpha = b$ is approximated and we have the Gauss-Newton method. Consequently, we take a large λ early value and as it grows smaller, the solution is reached. When in the Marquardt method $\Delta d^2 < 0$, λ is decreased by $\lambda = \lambda/\nu$. When $\Delta d^2 \geq 0$, λ is increased by $\lambda = \lambda \cdot \nu$ and the procedure is repeated. Generally $\nu = 2$ (Shimazu 1979). There is a method to obtain Δd^2 through primary approximation by

$$\Delta d^2 \approx -2 \sum_i d_i \left(\sum_i \frac{\partial f}{\partial \alpha_i} \Delta \alpha_i \right)$$

but vibration and dispersion occurred. The reason seems to be that the non-rectilinear pattern characteristic is strong and the error large with a primary approximation. Here we find Δd^2 directly by $\Delta d^2 = d_{n+1}^2 - d_n^2$ and use this for the determination.

Example of application

Using a PC 8801, we analysed the data of Tanaka. The results are shown in Table 1. When λ is taken above 1,000, the convergence is extremely good. When λ is taken at 100 or lower, $\lambda \rightarrow \infty$ after the 2nd time and a stop p. 57 is reached. The reason seems to be that because λ is too small, the contribution of λ is small and with the first computation, there is a change due to the Gauss-Newton method and a stoppage point is entered.

In the Marquardt method one must take a large λ and start in a condition close to the steepest descent method. In this case λ decreases regularly and one converges on the solution. When to the contrary λ increases regularly, the solution is neared or λ becomes too small and a stop point or another very small point is entered so that one has to stop. In this program, λ is continuous and one stops when a 10-fold increase takes place.

As for the value of λ , a number around 10,000 is appropriate. With PC 8801, when things went well, one iteration took about 3 min 25 s.

Discussion

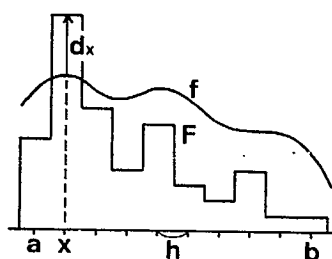
Generally d^2 converges relatively fast but the convergence of the various parameters is slow. The reason seems to be that in the vicinity of the solution, the value of the deviation-inducing functions of the various parameters came close to 0 and this is a common characteristic seen in the various kinds of optimization methods. Consequently it is preferable not to put excessive faith in the calculated values of the parameters (Ruckdeschel 1982).

The method seeking the regression curve by the least square method is explained in detail by Nakagawa and Koyanagi (1982). For this, complex large programs must be prepared for use by large computers, as in the presented SALS. However, as program to be used with small computers, this

level of program seems to be appropriate. With regard to data not suited to this program, it is preferable to proceed with large computers. It also appears that the method determining by integrals the residual functions as proposed by Shimazu (1979) takes too much time with small computers.

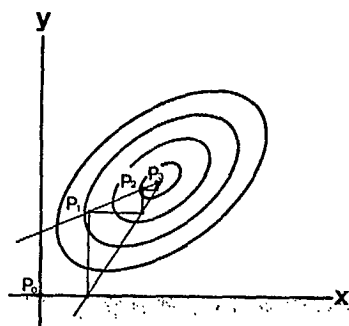
This program may be applied to most regression curves. It is also possible to find the partial differences by difference approximation and to make the program universally usable. When, however, one considers things such as the fact that the convergence becomes less stable because of the errors, it seems preferable to make a new preparation each time.

At the close of this article I want to thank Kiyohide ISHIOKA, chief researcher at the marine resources department of the Southwest Sea Regional Fisheries Laboratory as well as Fumihiko KATO, chief researcher at the resources department at the Sea of Japan Regional Fisheries Laboratory for their encouragement and advice.



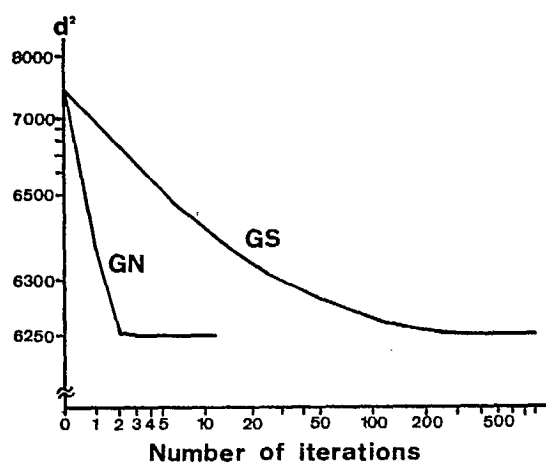
第1図 変数の説明
Fig. 1. Illustration of variables.

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第2図 パラメータ数が2の場合の Gauss-Seidel 法の収束

Fig. 2. Convergence of Gauss-Seidel method in the case of 2 parameters.

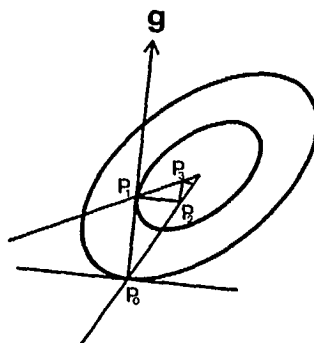


第3図 d^2 の収束状態

GS: Gauss-Seidel 法 GN: Gauss-Newton 法 データ: キダイの例
初期値: Gauss-Seidel 法で5回反復計算

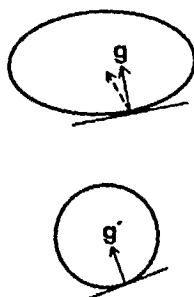
Fig. 3. Convergence of d^2 .

GS: Gauss-Seidel method. GN: Gauss-Newton method. Data: the example of porgy. Initial values: after 5 iterations of Gauss-Seidel method.



第4図 パラメータ数が2の場合の最急降下法の収束

Fig. 4. Convergence of steepest descent method in the case of 2 parameters.



第5図 パラメータのスケールリング
 g : 最急降下ベクトル
 g' : スケールリングしたパラメータの最急降下ベクトル

Fig. 5. Scaling of parameters.
 g : steepest descent vector.
 g' : steepest descent vector of scaled parameter.

Table 1. Convergence of d^2 .

Number of iterations	Marquardt's method		Gauss-Seidel method	Steepest descent method
	$\lambda=1000$	$\lambda=10^4$		
0	798925	798925	798925	798925
1	30880	21717	95838	638443
2	6784	9405	25020	579662
3	6282	7646	11443	520681
4	6251	6810	8309	492315
5	6250	6530	7364	465906
6	6250	6453	6987	440723
7		6401	6802	417380
8		6359	6695	395116
9		6329	6626	374430
10		6300	6577	354749
11		6273	6539	336417
12		6257	6508	319014
13		6251	6481	302771
14		6250	6458	287377
15		6250	6439	272987
16			6421	259367
17			6406	246620
18			6392	234566
19			6380	223274
20			6370	212604

プログラムリスト (キダイのデータの入力例)
 Program list (DATA: the example of porgy)

```

0  REM
10 REM POLYMODAL 3
20 REM
30 REM
40 REM ニュウロク
50 READ NND,MCM,NCL,CWD,NIT,LAMBDA,NU
60 PRINT "キダイ7" / "ノ カス" = ; NND
70 PRINT "サイショク / カイキウチ" = ; MCM
80 PRINT "カイキウ / カス" = ; NCL
90 PRINT "カイキウ / ハ" = ; CWD
100 PRINT "ハナフクサ" = ; NIT
110 PRINT "LAMBDA" = ; LAMBDA
120 PRINT "NU" = ; NU
130 PRINT
140 STOP
150 N3=3*NND
160 DIM F(NCL),X(NCL),DX(NCL),BIBUN(N3),ND(NND,NCL)
170 DIM HENSU(N3),KEISU(N3,N3),TEISU(N3),ZOBUN(N3),HENSU2(N3)
180 FOR K=1 TO NCL
190   X(K)=MCM+(K-1)*CWD
200   READ F(K)
210   PRINT "F(" ; X(K) ; ") = " ; F(K)
220 NEXT K
230 PRINT
240 STOP
250 FOR I=1 TO NND
260   S3=I:S2=S3+NND:S1=S2+NND
270   READ HENSU(S1),HENSU(S2),HENSU(S3)
280   PRINT "I=" ; I
290   PRINT "メソッド" ; HENSU(S1), "アイキ" ; HENSU(S2), "7" ; HENSU(S3)
300 NEXT I
310 STOP
320 REM タイム
330 P9=.398942:P8=-.5
340 FOR I=1 TO N3
350   HENSU2(I)=HENSU(I)
360 NEXT I
370 GOSUB *CLD2
380 D2=D3
390 PRINT "D2=" ; D2
400 PRINT
410 FOR KK1=1 TO NIT+1
420   REM タイム
430   FOR I=1 TO N3
440     TEISU(I)=0
450     FOR J=1 TO N3
460       KEISU(I,J)=0
470     NEXT J:NEXT I
480   REM ヨウ
490   FOR K=1 TO NCL
500     FOR I=1 TO NND
510       S3=I:S2=S3+NND:S1=S2+NND
520       P1=HENSU(S1):P2=X(K)-HENSU(S2):P3=HENSU(S3)
530       P6=ND(I,K)
540       BIBUN(S1)=P6/P1*HENSU(S1)
550       BIBUN(S2)=P6*P2/P3/P3*HENSU(S2)
560       BIBUN(S3)=P6*(P2*P2-P3*P3)/P3/P3/P3*HENSU(S3)
570     NEXT I
580     D1=DX(K)

```

```

770 REM タイム
780 FOR I=1 TO N3
790   TEISU(I)=TEISU(I)+D1*BIBUN(I)
800   FOR J=1 TO N3
810     KEISU(I,J)=KEISU(I,J)+BIBUN(I)*BIBUN(J)
820   NEXT J:NEXT I:NEXT K
830 LAMBDA2=0
840 K2=0
850 *REP
860 K2=K2+1
870 IF K2>11 GOTO *OWARI
880 PRINT
890 PRINT "LAMBDA=" ; LAMBDA
900 PRINT
910 FOR I=1 TO N3
920   KEISU(I,I)=KEISU(I,I)+LAMBDA-LAMBDA2
930 NEXT I
940 REM タイム ショウキ
950 FOR I=1 TO N3-1
960   FOR K=I+1 TO N3
970     Q1=KEISU(I,K)/KEISU(I,I)
980     TEISU(K)=TEISU(K)-Q1*TEISU(I)
990     FOR J=K TO N3
1000      KEISU(K,J)=KEISU(K,J)-Q1*KEISU(I,J)
1010   NEXT J:NEXT K:NEXT I
1020 REM ヨウ タイム
1030 ZOBUN(N3)=TEISU(N3)/KEISU(N3,N3)
1040 FOR I=N3-1 TO 1 STEP -1
1050   T1=TEISU(I)
1060   FOR J=I+1 TO N3
1070     T1=T1-ZOBUN(J)*KEISU(I,J)
1080   NEXT J
1090   ZOBUN(I)=T1/KEISU(I,I)
1100 NEXT I
1110 FOR I=1 TO N3
1120   ZOBUN(I)=ZOBUN(I)*HENSU(I)
1130   HENSU2(I)=HENSU(I)+ZOBUN(I)
1140 NEXT I
1150 GOSUB *CLD2
1160 IF D3>D2 THEN LAMBDA2=LAMBDA:LAMBDA=LAMBDA*NU:GOTO *REP
1170 REM タイム
1180 LAMBDA=LAMBDA/NU
1190 D2=D3
1200 FOR I=1 TO N3
1210   HENSU(I)=HENSU2(I)
1220 NEXT I
1230 GOSUB *SHUTU
1240 NEXT KK1
1250 *OWARI
1260 END
1500 *CLD2
1510 D3=0
1520 FOR K=1 TO NCL
1530   F1=0
1540   FOR I=1 TO NND
1550     S3=I:S2=S3+NND:S1=S2+NND
1560     P1=HENSU2(S1):P2=X(K)-HENSU2(S2):P3=HENSU2(S3)
1570     ND(I,K)=P9*P1/P3*EXP(P8*P2*P2/P3/P3)
1580     F1=F1+ND(I,K)
1590   NEXT I
1600   D1=F(K)-F1
1610   DX(K)=D1
1620   D3=D3+D1*D1
1630 NEXT K
1640 RETURN
2000 *SHUTU

```

```

2010 REM シミュレーション
2020 PRINT "D2=";D2
2030 PRINT
2040 PRINT "ハンフックスウ=";KK1
2050 FOR I=1 TO NND
2060   PRINT "I=";I
2070   S3=I:S2=S3+NND:S1=S2+NND
2080   PRINT "メンセキ=";HENSU(S1),"エイセン=";HENSU(S2),"フアンサン=";HENSU(S3)
2090 NEXT I
2100 RETURN
3000 DATA 5,7.5,29,1,20,10000,2
3010 DATA 7,79,509,2240,2341,623,476,1230,1439,921,448,512,719,673
3020 DATA 445,341,310,228,168,140,114,64,22,0,2,2,0,0,1
3030 DATA 5000,11,1,4000,15.5,1,3000,20,1.5,1000,24,1.5,500,27,1.5

```

変数の説明

Correspondence of variables

NND : number of normal distributions	D3 : d_{n+1}^2
MCM : minimum class mark	HENSU (I) : $\alpha_{i,n}$
NCL : number of classes	HENSU 2 (I) : $\alpha_{i,n+1}$
CWD : class width	BIBUN (I) : $\frac{\partial f}{\partial \alpha_i}$
NIT : number of iterations	KEISU (I, J) : $\sum_x \frac{\partial f}{\partial \alpha_i} \frac{\partial f}{\partial \alpha_j}$
F(K) : F	TEISU (I) : $\sum_x d_x \frac{\partial f}{\partial \alpha_i}$
X(K) : x	ZOBUN (I) : $\Delta \alpha_i$
DX(K) : d_x	ND (J, K) : $K_i \cdot N(\mu_i, \sigma_i, x)$
D2 : d_n^2	

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