Memorandums on Old Type Programs for Paleomagnetism (seven programs contained in pmagt401.tar.gz nonuse of GMT)

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1 System environment and installation

Linux and gcc

Seven programs contained in ”pmagt401.tar.gz” are paleomagnetic tools with CUI (character user interface). They do only computations and do not use any of Generic Mapping Tools (GMT) of Wessel et al. (2013, 2019), while those in another archive ”pmagm302.tar.gz” utilize the GMT 6(5) tools. Hence, the programs in ”pmagt401.tar.gz” should work on terminals of most Linux systems. They are now working on ”Ubuntu 22.04” in which ”gcc 11.4.0” is installed, but other Linux environment should be OK. Some of the numerical algorithm used in the programs are adapted from those of Press et al. (1992).

Here, only the C sources are provided, which should be compiled by gcc. The programs are working on terminals in which TC shell ”tcsh ” is used as a login shell, but using other shell is probably OK. Use these programs at your own risk, although any problems have never been encountered. Nevertheless, you should be familiar with the minimum level of Unix commands such as ”ps ” and ”kill ” in case freeze of program occurs and ”Ctrl+C” does not work.

Installation

Put ”pmagt401.tar.gz” at a certain directory and extract by

```
tar xvfz pmagt401.tar.gz
```

”pmagt401” directory is created and enter to this directory by

```
cd pmagt401
```

Then compile the source files by

```
make
```

Executable files will be created under ”pmagt401/bin” directory. Copy them to your usual binary directory such as /usr/local/bin, etc. Each source directory, such as ”pmagt401/tmean-src”, contains one or more test data files which are usually named as ”t-*.d”.

Starting the program

Typing only the program name shows its usage to the display as the following example.

```
Usage: tmean file [-Ppc -Ddiff -L -H]
```

Starting the program with the option ”-H” (or, ”-h”) shows a simple help message as the example below. The message can be cleared by pressing ”Q” (or, ”q”).

```
HELP MESSAGE OF TMEAN
  Test of a common mean V1.2, H. Tanaka, 2018.
  Whether two scalar samples share a common mean is tested by
  Student’s t-test (common variance) or Welch’s t-test (different variances).

Usage:
  tmean file [-Ppc -Ddiff -L -H]

Options:
  P -- significance level (default: 0.05)
  D -- tests if mu1-mu2=diff (default: 0)
       (assign a negative diff for mu2>mu1)
  L -- lists original data at the last
  H -- help message
```

```
Input file:
  Data of sample 1 and sample 2 should be contained in a single file with
  one datum per line. They are divided by a line with first letter '>' or '<'.
  Lines with first letter '#' or '%' are comments and are ignored.

  Format:
  # comment line can be placed at any place
  X11 [notes ...] -- notes can be put after the datum
  X12
  X13
    ...
  >               -- this line separates two samples
  X21
  X22
  X23
   ...

Output:
  Results are written to stdout. To save them to a file,
  use redirect as "tmean in_file > out_file".
(Q to quit)
```

In the following sections, typical application of the programs are illustrated by using the test data files ”t-*.d” contained in each source directory ”pmagt401/*-src”.

2 Statistical test for means

2.1 Test of a common mean: tmean

”tmean” tests whether two scalar data (samples in statistics term) share a common population mean. The program uses the standard statistical methods which are illustrated in any text books of statistics. Student’s t-test is used when the two data share a common variance while Welch’s t-test is used when the variances of the two data are different. In the program, some numerical formulas are taken from Crow et al. (1960), Kohari (1973), and Press et al. (1992). Three files of test data are included in the directory ”tmean-src”; one is for Student’s t-test and other two are for Welch’s t-test.

Cases of common variance for Student’s t-test

The test data file ”t-tmean.d” includes weight of eggs before and after a hen was supplied by nutritional supplement (example from Kohari (1973)). To test if there is a weight difference, set the null hypothesis as [H0: $\mu_1 - \mu_2 = 0$], and carry out the test by typing

```
tmean t-tmean.d
```

the following test results are shown on the display.

```
Test of population means from two scalar samples:
  Data file: t-tmean.d,  Significance level: 0.0500,  Test if: mu1-mu2=0?
Null hypothesis H0; var1=var2 (Equal-Tails Test):
  F[5,9,0.0250]  var2/var1    p
     4.4844       1.0773   0.433
  H0 was NOT REJECTED, proceed to Student's t-test supposing common variance.
Null hypothesis H0; mu1-mu2=0 when var1=var2 (Equal-Tails Test):
  H0 was NOT REJECTED.
  tc[14,0.0250]      t        p
       2.1448      -1.1572   0.1333
Sample means:
  Sample  N   Mean        Stdev       Variance
     1   10   70.200      1.9810      3.9244
     2    6   71.400      2.0562      4.2280
```

To save the results to a file use the Unix’s re-direction as below.

```
tmean t-tmean.d > result.txt
```

In the first step of the test, common variance was tested by F-test using F-distribution. Because the null hypothesis of the common variance was not rejected, Student’s t-test was carried out in the second step.

As the null hypothesis H0, $\mu_1 = \mu_2$, was not rejected in the above test, you cannot say anything about the difference of μ_1 and μ_2. Probably the number of data is too small. Nevertheless, if the manufacturer of the supplement claims that the supplement increases the weight of eggs by 4 g or more, then, using ”-D” option, set the null hypothesis as [H0: $\mu_1 - \mu_2 = -4$] (negative value is because $\mu_2 - \mu_1 = 4$ is supposed), and carry out the test by typing

```
tmean -d-4 t-tmean.d
```

the results of this test are the following.

```
Test of population means from two scalar samples:
  Data file: t-tmean.d,  Significance level: 0.0500,  Test if: mu1-mu2=-4?
Null hypothesis H0; var1=var2 (Equal-Tails Test):
  F[5,9,0.0250]  var2/var1    p
```

```
     4.4844       1.0773   0.433
  H0 was NOT REJECTED, proceed to Student's t-test supposing common variance.
Null hypothesis H0; mu1-mu2=-4 when var1=var2 (Equal-Tails Test):
  H0 was REJECTED (NOT mu1-mu2=-4).
  tc[14,0.0250]      t        p
       2.1448      2.7000   0.0086
Sample means:
  Sample  N   Mean         Stdev        Variance
     1   10   70.200       1.9810       3.9244
     2    6   71.400       2.0562       4.2280
```

As H0 was rejected, we conclude that the manufacturer's claim is a fake.

Cases of different variances for Welch's t-test

"t-tmean2.d" and "t-tmean3.d" contain two random data of Gauss distribution in which the means and variances are different. To carry out the test to "t-tmean2.d", type as

```
tmean t-tmean2.d
```

and the following results are displayed.

```
Test of population means from two scalar samples:
  Data file: t-tmean2.d,  Significance level: 0.0500,  Test if: mu1-mu2=0?
Null hypothesis H0; var1=var2 (Equal-Tails Test):
  F[6,9,0.0250]  var1/var2    p
     4.3197       4.3875   0.024
  H0 was REJECTED, proceed to Welch's t-test when different variances.
Null hypothesis H0; mu1-mu2=0 when unequal variances (Equal-Tails Test):
  H0 was NOT REJECTED.
  tc[7.93,0.0250]    t        p
       2.3094      1.3477   0.1075
Sample means:
  Sample  N   Mean         Stdev        Variance
     1    7   72.067       16.445       270.43
     2   10   63.047       7.8509       61.637
```

Note that Welch's t-test was called in the program because the variances of the two data sets are different. In spite of quite different means, the null hypothesis H0, $\mu_1 = \mu_2$, was not rejected. This is because the variances are too large. Using the test data file "t-tmean3.d", the test will reject the null hypothesis of $\mu_1 = \mu_2$.

2.2 Test of a common mean direction: tmeandir

"tmeandir" tests whether two or more groups of unit vectors, distributed in the Fisher distribution, share a common mean direction. It is mainly used for the reversals test in paleomagnetism. The algorithm of the program and some of the numerical functions are based on McFadden & Lowes (1981), McFadden (1982), Fisher et al. (1987), McFadden & McElhinny (1990), and Press et al. (1992). There are four test data files in directory "tmeandir-src" which are named as "t-tmeandir#.d" where # is one of 1–4.

Only one datum in group 2

"t-tmeandir1.d" includes only one datum in group 2, and this single datum is tested whether it is from the same population of group 1. Test of an outlier is also made. To carry out the test, type as

```
tmeandir t-tmeandir1.d
```

and the following results are shown to the display (to save them to a file, use Unix's redirection).

```
Data file:
  t-tmeandir1.d
Case:
  two groups (1 DATUM ONLY in 2nd group, p = 0.050)
Null hypothesis H0; single group2 direction is from common mean group1:
  F[2,10,0.050]    G       p     gammc gamm0
     4.1028      4.0651  0.051   27.3  27.2
  H0 was NOT REJECTED (POSITIVE reversal test).
    CLASS: INDETERMINATEi
Test of outlier for the group2 single direction:
  gammc-out gamm0
     39.4    27.2
  NOT OUTLIER.
Group & total means:
  grp  n   incr   decr    R        k       a95
   1   6   51.0  351.2   5.8838   43.027  10.3
   2   1   25.7    4.3   1.0000   -1.000  -1.0
   T   7   47.5  353.7   6.7887   28.390  11.5
```

Single datum is not inconsistent with group 1, and not an outlier. Note that the difference angle γ_0 of 27.2° is only slightly smaller than the critical angle γ_c of 27.3°. Hence, if the significance level of 0.1 is assigned with "-P" option as

```
tmeandir -p0.1 t-tmeandir1.d
```

the null hypothesis is rejected and the negative reversal test is concluded as the following.

```
Data file:
  t-tmeandir1.d
Case:
  two groups (1 DATUM ONLY in 2nd group, p = 0.100)
Null hypothesis H0; single group2 direction is from common mean group1:
  F[2,10,0.100]    G       p     gammc gamm0
     2.9245      4.0651  0.051   23.0  27.2
  H0 was REJECTED (NEGATIVE reversal test).
Test of outlier for the group2 single direction:
  gammc-out gamm0
     34.8    27.2
  NOT OUTLIER.
```

```
Group & total means:
  grp  n   incr   decr    R         k       a95
   1   6   51.0  351.2   5.8838   43.027  10.3
   2   1   25.7    4.3   1.0000   -1.000  -1.0
   T   7   47.5  353.7   6.7887   28.390  11.5
```

The outlier test, however, still concludes that the single group2 direction is not an outlier with the significance level of 10%.

Two groups of normal directions

"t-tmeandir2.d" includes typical data of two groups in which the directional data are all normal. To carry out the test, type as

```
tmeandir t-tmeandir2.d
```

and we obtain the following results.

```
Data file:
  t-tmeandir2.d
Case:
  two groups (significance level = 0.050)
Null hypothesis H0; kappa1 = kappa2 (Equal-Tails Test):
  F[10,10,0.0250]  k1/k2    p
     3.7168       1.6204  0.229
  H0 was NOT REJECTED, proceed with test supposing common kappa.
Null hypothesis H0; common true mean when kappa1 = kappa2:
  F[2,20,0.050]    f      p      gammc gamm0
     3.4928      5.9423  0.009    7.9  10.3
  H0 was REJECTED (NEGATIVE reversal test).
Group & total means:
  grp  n   incr   decr    R         k       a95
   1   6   50.5    7.6   5.9694  163.576   5.3
   2   6   48.5  352.1   5.9505  100.950   6.7
   T  12   49.7  359.7  11.8722   86.080   4.7
```

The null hypothesis of the common mean direction was rejected, i.e. the result was a negative reversals test.

Reversed data in group 2

"t-tmeandir3.d" is the case in which group 2 data are the original reversed directions. In such a case "-R" option is used as

```
tmeandir -r t-tmeandir3.d
```

and we obtain the results below.

```
Data file:
  t-tmeandir3.d
Case:
  two groups (significance level = 0.050)
Null hypothesis H0; kappa1 = kappa2 (Equal-Tails Test):
  F[10,10,0.0250]  k2/k1    p
     3.7168       4.9632  0.009
  H0 was REJECTED. Simulation follows when kappa1 != kappa2.
Test by simulation (ni=2500) -- Null hypothesis H0; common true mean:
```

```
  Vc(p=0.050)   V0     gammc gamm0
    5.8998    2.0069   12.4   7.3
  H0 was NOT REJECTED (POSITIVE reversal test).
    CLASS: C
Group & total means (2nd group inverted):
  grp  n   incr   decr    R         k       a95
   1   6   51.3  355.6   5.8062   25.800  13.4
   2   6   48.6    6.1   5.9610  128.052   5.9
   T  12   50.1    1.0  11.7436   42.898   6.7
```

As the null hypothesis of a common kappa was rejected, computer simulation was used to test the common mean direction. Iteration was 2500 times but it can be changed by option ”-N”. The reversals test was positive, but classified to level C. Note that in the summary of the means, only the inverted one is shown for group 2.

Three groups

”t-meandir4.d” includes 3 groups. To test whether the three groups of directions are independent, type as

```
tmeandir t-tmeandir4.d
```

and the results are below.

```
Data file:
  t-tmeandir4.d
Case:
  multi groups (M=3, significance level = 0.050)
Null hypothesis H0: common kappa:
  Chi2[2,0.050]   G      p
     5.9915     1.0643  0.587
  H0 was NOT REJECTED, but a group with less than 5 data exists!
  Simulation follows supposing common kappa.
Test by simulation (ni=2500) -- Null hypothesis H0; common true mean:
  Vc(p=0.050)   V0
    9.5039    17.2254
  H0 was REJECTED (NOT common mean).
Group & total means:
  grp  n   incr   decr    R         k       a95
   1   6   48.7    0.8   5.9418   85.929   7.3
   2   6   57.9   12.2   5.9061   53.222   9.3
   3   4   61.6  355.4   3.9727  109.946   8.8
   T  16   55.5    3.6  15.7180   53.184   5.1
```

As the null hypothesis was rejected, three groups are independent. Note that computer simulation was made because data number of group 3 was less than 5.

3 Miscellaneous programs for paleomagnetism

3.1 Simple calculator for paleomagnetism: pcalc

Paleomagnetic measurement data are usually stored in a data file. To analyze them, we let a certain program read them and obtain the results which are output to another file (or a printout). However, we often need to do manual calculations. For such a case, "pcalc" provides a utility in which several miscellaneous calculations are available as a simple calculator.

The interactive calculator starts by typing "pcalc" with "-A" option which stands for "assorted". When table of items of calculation is displayed, type the item number which you want to do. Once you enter the level of each calculation, put necessary data manually. To end input of data, type "Return (Enter)" key. To return to the upper level, type "Q". In some calculations which reads more than one datum, the number of input data N is limited to $N <= 50$ (when input from a file, N is limitless).

Fisher statistics

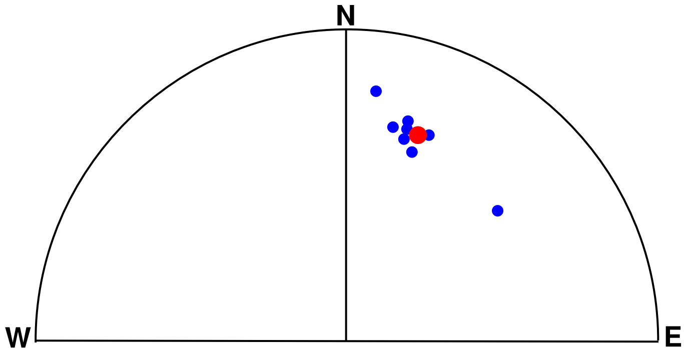
By selecting "Item 7" (Flds → Mean Fld), you can calculate a mean direction from several data using Fisher statistics. The following example illustrates a case of eight remanence directions.

```
pcalc -a
Miscellaneous Calculations in Paleomagnetism V3.3
  1: X,Y,Z  -> M,I,D    2: M,I,D   -> X,Y,Z
  3: Field  -> VGP      4: VGP     -> Field
  5: F,I    -> VDM      6: F,Lat   -> VADM
  7: Flds   -> Mean Fld 8: VGPs    -> Mean VGP
  9: I only -> Mean I   A: Lat,Lon -> IGRF
  B: Bingham statistics of Flds or VGPs
  C: Circle fitting of X-Y data points
(Q to quit) 7
Input data (N<=50): (Rtn--end, Q--cancel)
Slat,Slon? (Rtn to skip) 35.838 137.544
I,D_1? 32.9  16.1
I,D_2? 27.7  15.9
I,D_3? 36.2  49.4
I,D_4? 29.8  22.1
I,D_5? 20.5   6.8
I,D_6? 30.5  12.6
I,D_7? 29.4  16.0
I,D_8? 36.0  19.2
I,D_9?
 i      I      D     dev
 1    32.90  16.10   3.33
 2    27.70  15.90   4.33
 3    36.20  49.40  25.58
 4    29.80  22.10   2.70
 5    20.50   6.80  15.27
 6    30.50  12.60   5.72
 7    29.40  16.00   3.18
 8    36.00  19.20   5.10
 Slat    Slon    n   I      D       R      k      a95   Plat   Plon    dp     dm     asd
 35.84 137.54  8  30.90  19.24  7.851   46.84   8.18  64.31 270.81   5.10   9.13  11.91
Exclude one? (N or Rtn/Y)
Re-run? (N or Rtn/Y)
```

After the results are displayed, the program asks you if you wish to exclude one datum from the statistics. However, this function is not to encourage you to eliminate an inconvenient datum arbitrary. If you find a strange datum which might be an outlier, you should carry out the statistical test of outlier (McFadden, 1982) which is available by "tmeandir", and try to find physical reasons to the outlier.

Bingham statistics

The above input data used for "Item 7" (Flds $\rightarrow$ Mean Fld) are quite elongated as shown in the figure below, possibly due to failed elimination of the secondary remanence components.



Selecting "Item B" (Bingham statistics of Flds or VGPs) and supplying the same data, the following results are displayed together with Fisher statistics at the last (first a cautionary message appears, but just hit "Return (Enter)" to continue).

```
Bingham statistics:
  n     k1      k2      tau1   tau2   tau3
  8   -214.49 -15.43   0.02   0.27   7.71
  I3(Lat3) D3(Lon3)  I2(Lat2) D2(Lon2)  I1(Lat1) D1(Lon1)
     30.83   18.95     21.51  122.56     50.93  241.61
  a31     a32     a21     Xu      Xcp     Xcg
  2.44   9.25  14.04   35.83   24.93   57.41
Fisher statistics:
  n  Im(Latm) Dm(Lonm)   R       k     a95    Asd
  8   30.90    19.24    7.85   46.84   8.18  11.91
```

Among many parameters displayed, the direction of eigenvector $\mathbf{t}_3$ is shown under the head "I3(Lat3) D3(Lon3)". This is in excellent agreement with the mean direction of Fisher statistics which is obtained by "Item 7 " (or, that is shown under the head "Im(Latm) Dm(Lonm)"). However, it is noticed that there is a large elongation in the 95% confidence region as is known from a large difference of α_{31} and α_{32} which are shown under the head "a31 a32".

As the Bingham distribution is dependent on $\sin^2\theta$, you can analyze the combined data of normal and reversed directions. As a demonstration, try to recalculate the statistics with above data half of which are inverted by 180°. You will obtain identical results of Bingham statistics while Fisher statistics gives extremely small k and too large α_{95} to be determined.

The reason of displaying a cautionary message when "Item B" is selected is that the routine of the maximum likelihood estimate (MLE) of k_1 and k_2 sometimes fails to converge, especially for small number of extremely elongated data. If the process seems to be frozen, terminate it by Ctrl+C or kill command. Nevertheless, for typical paleomagnetic data with moderate dispersion, the process should easily converge.

Data input from a file: inclination only statistics

"pcalc" also reads input data from a file by using options other than "-A". In this case, the number N of input data is limitless but the interactive function such as excluding an outlier datum is not available. Hence, when using "pcalc" with options to read a data file, you can redirect the results to a file (but do not use redirection with option "-A"!). The following example of option "-I" shows inclination only statistics of the test data file "t-inc.d". "-L" option is also used to list the input data.

```
pcalc -i -l t-inc.d > result.txt
```

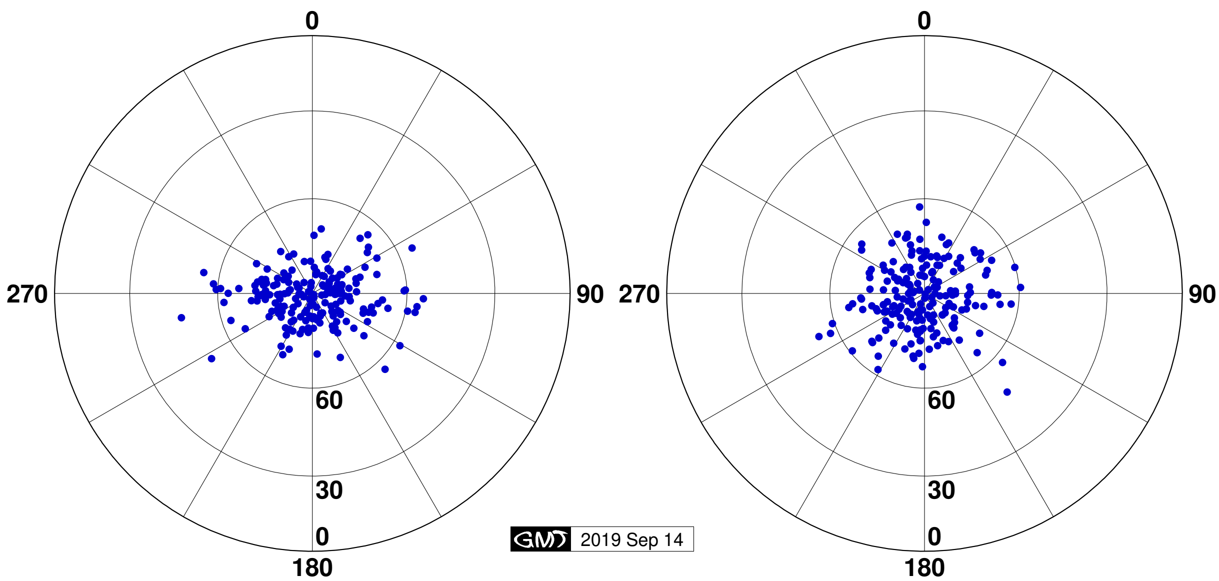
The content of the output file ”result.txt” is as the following.

```
Inclination only statistics of t-inc.d:
Arith. mean: Im= 68.78, km= 36.42
MLE estimations:
 n   Im      km     a95   iteration
 9  71.85   32.45   9.17      43
Input data:
 i    I      dev
 1  66.10  -5.75
 2  68.70  -3.15
 3  70.10  -1.75
 4  82.10  10.25
 5  79.50   7.65
 6  73.00   1.15
 7  69.30  -2.55
 8  58.80 -13.05
 9  51.40 -20.45
```

In this case, convergence of MLE estimations was quite rapid after 43 iterations. Depending on the data, however, the convergence might be bad and in that case a cautionary message is displayed.

Data input from a file: Bingham statistics

Three of nine test data files contained in the source directory ”pcalc-src” are for Bingham statistics. ”t-bingB.d” and ”t-bingF.d” contain 200 directions which are generated by random generator of Bingham and Fisher distributions, respectively (figures below). ”t-bingP.d” contains 18 data of girdle-like plane distribution.



Bingham distribution (k_1=−25, k_2=−10, N=200) Fisher distribution (k=30, N=200)

As an example of Bingham statistics from the test data file ”t-bingB.d”, type as

```
pcalc -b t-bingB.d
```

After hitting ”Return (Enter)” to the cautionary message shown, the following results are displayed.

```
Input file of Bingham statistics: t-bingB.d
Bingham statistics:
  n      k1      k2      tau1   tau2   tau3
 200   -29.79 -10.35   3.42   10.28 186.29
  I3(Lat3) D3(Lon3)  I2(Lat2) D2(Lon2)  I1(Lat1) D1(Lon1)
     88.75  171.94     -0.14   88.39      1.25  358.40
  a31     a32     a21      Xu      Xcp      Xcg
  1.34   2.32   8.59  805.87   66.66  911.16
Fisher statistics:
  n Im(Latm) Dm(Lonm)   R       k      a95    Asd
 200   88.73  171.89  192.82   27.72   1.93  15.51
```

In the results shown above, note that α_{32} is much larger than α_{31}, indicating elongation along the $\mathbf{t}_2$ direction. This is in good agreement with the shape of distribution shown in the left figure. It is also noted that the mean direction of Fisher statistics is in complete agreement with $\mathbf{t}_3$ direction.

It is also easy to obtain the statistics from "t-bingF.d" whose data distribution is shown in the right figure. However, for "t-bingP.d" which contains 18 girdle-like plane data, the program takes quite a long CPU time (eight seconds elapsed at Intel Core i-7 machine). During iteration, the display shows a message with increasing number like

```
** Wait 32 **
```

and convergence is attained after $\sim$80. If the number stops at a certain point, the process must be frozen. In such a case terminate the process by Ctrl+C or kill command.

Data input from a file: circle fitting

The last examples are circle fittings of 2-dimensional X-Y data ($N \geq 3$) by the method of Taubin (1991). Using a test data file "t-circ.d", type as

```
pcalc -c t-circ.d
```

The results of circle fitting are as the following.

```
Input file of circle fitting: t-circ.d
 N   X0         Y0         R          k          SSE
11 -4.687e-05  0.009647  1.035     0.9663     0.03994
```

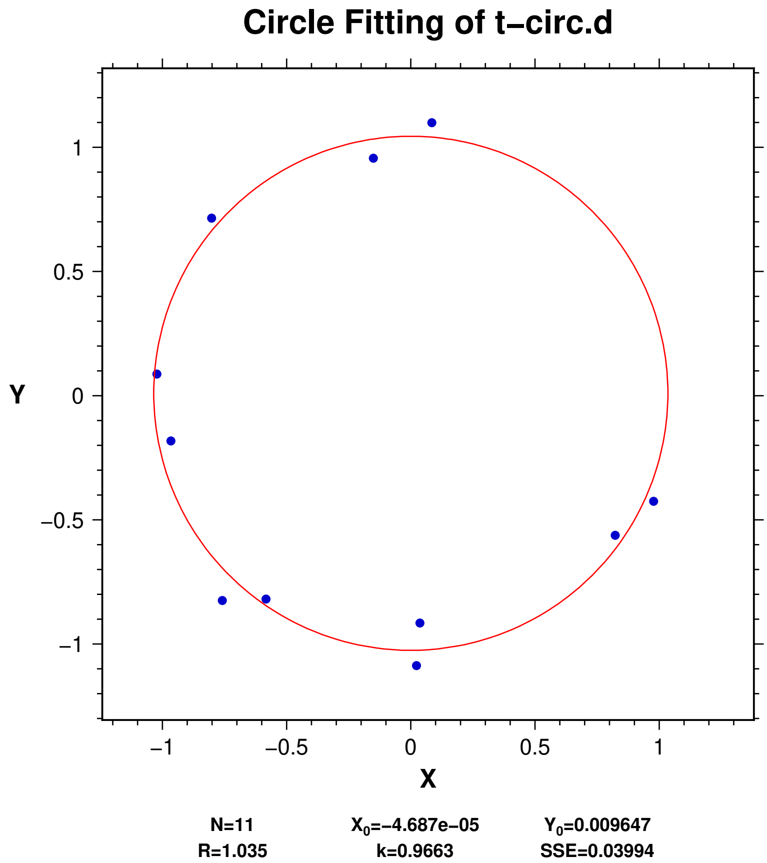
where (X_0, Y_0) and R are the circle center and the radius, respectively. k is a measure of the curvature extended from Paterson (2011) defined as,

$$k = \begin{cases} 1/R, & if \quad \bar{X} < X_0 \quad and \quad \bar{Y} < Y_0 \quad (concave\ up), \\ 1/R, & if \quad \bar{X} > X_0 \quad and \quad \bar{Y} < Y_0 \quad (concave\ up), \\ -1/R, & if \quad \bar{X} > X_0 \quad and \quad \bar{Y} > Y_0 \quad (concave\ down), \\ -1/R, & if \quad \bar{X} < X_0 \quad and \quad \bar{Y} > Y_0 \quad (concave\ down), \\ 0, & if \quad \bar{X} = X_0 \quad and \quad \bar{Y} = Y_0, \end{cases}$$

where $(\bar{X}, \bar{Y})$ is the centroid of the data. k was introduced to evaluate Thellier's paleointensity results. Hence, ignore it when general data are fitted to a circle as this example. SSE is the sum of the squares of the error, defined as,

$$SSE = \sum_{i=1}^{N} \left(\sqrt{(X_i - X_0)^2 + (Y_i - Y_0)^2} - R \right)^2 .$$

Figure next page shows the fitted circle together with the data. Such a figure can be drawn by using the program "pcirc" which is contained in another archive "pmagm302.tar.gz".



Another test data file "t-circ2.d" is provided to show a cautionary example. This file contains only four data points (1.1, 0), (0, 0.9), (-1.1, 0), (0, -0.9). The result from this file is as the following.

```
Input file of circle fitting: t-circ2.d
 N    X0          Y0          R           k           SSE
 4   0.000       0.000       1.005       0.000       0.04010
```

Note that the radius R of the fitted circle is slightly larger than the optimal value of 1. This is because the algorithm used by pcirc is to minimize the sum of the squares of "algebraic" distance $r_i^2 - R^2$ not the "geometric" distance $r_i - R$, where r_i is the distance of a data point from the center. It is known that the algebraic method is less accurate than the geometric one. Nevertheless, the former is simpler and practical due to its fast calculation speed.

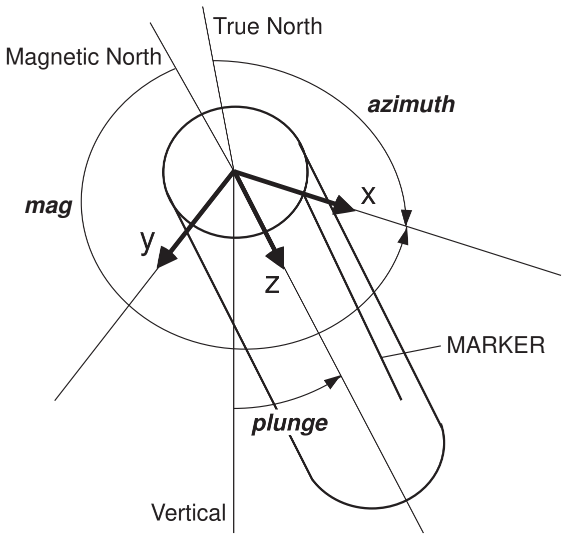
3.2 Core orientation by a sun compass: sunpmag

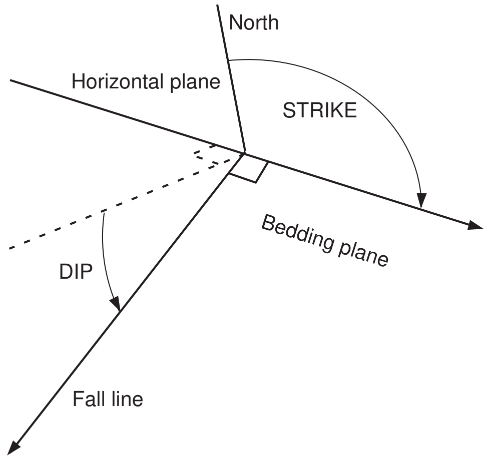
Orientation system and bedding attitude

The following figures illustrate the systems of core orientation and bedding attitude, which are used throughout the paleomagnetic programs including those in another archive ”pmagm302.tar.gz”.

In the orientation system (left figure), x-axis is in the horizontal plane. Azimuth of x-axis is measured clockwise from the north. Looking toward +x direction, y and z-axes are rotated clockwise by the angle plunge. This orientation system is applicable ONLY to the orientation device supplied by Natsuhara Giken.

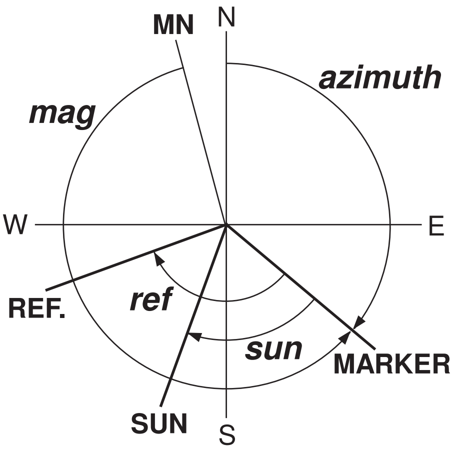
For the bedding attitude and its tilt correction (right figure), a standard system is used. Bedding strike is measured clockwise from the north. Looking toward the measured strike direction, dip angle is positive when the bedding plane is inclined clockwise. Note that the bedding plane of $(strike, dip)$ is equivalent to $(strike + 180°, -dip)$.





Azimuth of the core marker

”sunpmag” calculates *azimuth* of the marker of the sample which was collected with the orientation device described above. To convert the remanence vector from core coordinates to geographic coordinates, we need to know the angles *plunge* and *azimuth*. However, it is difficult to measure *azimuth* in the field because the true north is unknown. Hence, we measure one to three angles; *mag*, *sun*, and *ref* as shown in the figure below.



mag is the angle of the marker measured COUNTERCLOCKWISE from the magnetic north. *sun* is the sun’s direction (NOT its shadow) measured clockwise from the marker. *ref* is the direction of a reference measured clockwise from the marker. Another angle we need to know is the magnetic declination at the site. If the declination is available, it should be assigned as one of the site information such as the site latitude and longitude. If not available, the declination can be omitted, and in that case, ”sunpmag” calculates its IGRF or DGRF value corresponding to the date and site locality with altitude 0 km.

The astronomical algorithm of calculating the sun’s direction is taken from Yallop & Hohenkerk (2007) in which the claimed error is ∼0.6 minutes for the time span from 2000 BC to AD 2200. Declination is calculated by using the Gauss coefficients from IGRF-13 (IAGA Working Group V-MOD, 2020) with the geodetic system WGS84 up to n=m=10.

Input file format

The format of the input data file is as the following.

```
# lines beginning with "#" or "%", or blank line are ignored
$$ lat lon tzone [dec]
$ year month day [ref_azim]
core1-1 plun mag
core1-2 plun mag sun h m s
core1-3 plun mag ref
core1-4 plun mag sun h m s ref
        .
        .
$ year month day [ref_azim]
core2-1 plun mag sun h m s
        .
        .
$$ lat lon tzone [dec]
        .
        .
```

The line with ”$$” at the beginning is the locality information. The line with ”$” at the beginning indicates that the core orientation data follow from the next line. In the above explanation of the format, four cases of angle measurements are shown. The line of core1-1 shows the case of *plunge* and *mag* only. core1-2 shows the case of *plunge*, *mag*, *sun*, and time information. core1-3 is the case of *plunge*, *mag*, and *ref*. core1-4 is the case of all measurements. Second ”$” line indicates the beginning of another site under the same location. Second ”$$” line begins another locality. You can include lines with ”$” or ”$$” as many as you need. Simple descriptions of the input data are summarized as the following.

lat,lon	:	latitude and longitude in decimal
tzone	:	east positive time difference (ex., +9 for Japan)
dec	:	optional local declination (when omitted, the IGRF value used)
plun	:	plunge of the core (not used in the azimuth calculation)
ref_azim	:	optional reference azimuth (eastward from the true north)
mag	:	marker angle measured counterclockwise from the magnetic north
sun	:	sun angle measured clockwise from a marker (not the sun’s shadow)
ref	:	reference angle measured clockwise from a marker

To use ”sunpmag” type as,

```
sunpmag data-file
```

The results are printed out to stdout (display). To save them to a file, type as,

```
sunpmag data-file > out-file
```

To show the help message, type as,

```
sunpmag -h
```

Test data file "t-sunpmag.d" is included in the directory "pmagt401/sunpmag-src".

Example of output

An example of output from the test data file "t-sunpmag.d" is shown in the following, which is obtained from the orientation data taken in New Zealand in 1990. "Sld" (Standard longitude difference) at the first line is the time difference from Greenwich, which is +13 hours in New Zealand.

```
  Lat       Lon      Sld  Dec(1990.175)
-38.659  176.031   13.0   20.4

 Year Mon Day Ref_azm
 1990   3   5   105.0

 Core       Dip Sazim Mazim  dltMS Razim  dltMR  dltRS  Mag    Sun   Hr  Mn  Sc   Ref
NT56-1     73.5  92.1  90.9   -1.2    *      *      *   289.5 252.8 14   0  40    *
NT56-2     77.3  95.4  94.5   -1.0    *      *      *   285.9 247.8 14   4  25    *
NT56-3     77.9  93.7  91.6   -2.1    *      *      *   288.8 248.9 14   5  50    *
NT56-4     76.5  96.1  95.1   -1.1    *      *      *   285.3 245.8 14   7  25    *
NT56-5     69.3  70.8  69.4   -1.4  68.6    0.8   -2.2  311.0 262.8 14  27  20  36.4
NT56-6     71.8    *   70.7     *   70.1    0.6     *   309.7   *     *   *   *  34.9
NT56-7     82.8    *   82.8     *   82.0    0.8     *   297.6   *     *   *   *  23.0
NT56-8     86.8    *   91.9     *   90.2    1.7     *   288.5   *     *   *   *  14.8
```

As input of local declination was omitted, the declination was calculated by interpolating between DGRF1990 and DGRF1995 and its value 20.4 is shown under "Dec(1990.175)" in which fraction 0.175 corresponds to March 5. Reference azimuth 105.0 under "Ref_azim" is the value read from the topographic map. For each line of the core data, the figure under "Dip" is the same as the input datum *plunge*. Figures under "Sazim", "Mazim", and "Razim" are the azimuth values based on the measured angles *sun*, *mag*, and *ref*, respectively. Those under "dltMS" etc. are the differences between the calculated values of azimuth. The differences are quite small, indicating the small local magnetic anomaly and accurate measurements of the angles. Those under "Mag", "Sun", "Hr", etc. are the input data.

3.3 Main field elements from IGRF-13: igrf

"igrf" calculates elements of the geomagnetic main field at a specified site locality and date by using the Gauss coefficients from IGRF-13 (IAGA Working Group V-MOD, 2020). "pcalc" and "sunpmag" also include this function with limited conditions while "igrf" provides calculations with both geodetic and geocentric coordinate systems at a certain altitude or a radius from the earth's center. Inclusion of higher terms is limited to n=m=10 for the sake of simpler programming codes, although IGRF-13 provides coefficients up to n=m=13 for the time span from AD 2000 onward. Nevertheless, the elements values given from "igrf" should be accurate enough for paleomagnetic purposes. Differences from those for n=m=13 are 0.2–0.4° in declination and inclination, and 0.2–0.4% in total force excluding the regions near to the magnetic poles. If calculation with n=m=13 is necessary, you can use the programs provided by the geomagnetism groups (ex., URL: https://www.ngdc.noaa.gov/IAGA/vmod/igrf.html).

Interactive calculation

Starting the program by typing "igrf", the next message appears.

```
igrf
Main field calculation from IGRF-13 with n=m=10
  Rtn (Enter) to continue,
  U for usage,
  H for help message,
  Q to quit.
```

By typing Return, the interactive program begins. In default, geodetic system is adopted and date and site location formats are in decimal. In the next example of year 2019.5, Gauss coefficients are linearly interpolated between those of DGRF2015 and IGRF2020.

```
** Geodetic system adopted. **
Decimal year? (Q - quit) 2019.5
Altitude in km? (-10 ~ 500 km)
(Rtn - 0 km, Q - quit)
Decimal Lat, Lon? (Q - quit) 33.5 133.5

Year     altitude
2019.500    0.0
Latitude Longitude
 33.50    133.50
   X      Y      Z     F     I      D
 31373  -4135  35040 47214  47.91  -7.51
Decimal Lat, Lon? (Q - quit)
```

Options -Y and -D set the formats of "year, month, day" for the date and "degrees, minutes" for the site, respectively. Option -C sets the geocentric coordinate system. An example of these input formats is as the following.

```
igrf -y -d -c
** Geocentric system adopted. **
Year,Month,Day? (Q - quit) 2012 9 17
Geocentric distance in km? (3485~10000 km)
(Rtn - 6371.2 km, Q - quit) 6400
Lat_deg, Lat_min, Lon_deg, Lon_min? (Q - quit)
(Set "negative" only to "deg" for south & west values)
 64 26 -22 51
```

```
Year Mo Dy  radius
2012  9 17  6400.0
Lat-d Lat-m Lon-d Lon-m
  64    26   -22    51
   X       Y       Z      F      I       D
 12005  -3439  50113 51645  76.01 -15.99
Lat_deg, Lat_min, Lon_deg, Lon_min? (Q - quit)
(Set "negative" only to "deg" for south & west values)
```

Data input from a file

With -F option, ”igrf” reads dates and site locations from a file. In this case, the coordinate system is limited to geodetic and the format of the dates and site locations are automatically interpreted. The following is the results from the test data file ”t-igrf.d”.

```
igrf -f t-igrf.d
** IGRF elements from t-igrf.d **
** Geodetic system adopted. **

Year Mo Dy altitude
2020  5 15    0.2
Lat-d Lat-m Lon-d Lon-m
  33    24  -133    36
   X       Y       Z      F      I       D
 24192   5678  35552 43376  55.05  13.21
Latitude Longitude
 33.40    -133.60
   X       Y       Z      F      I       D
 24192   5678  35552 43376  55.05  13.21

Year     altitude
1991.330    0.5
Latitude Longitude
-20.20    145.50
   X       Y       Z      F      I       D
 31878   4301 -38672 50301 -50.25   7.68

Year Mo Dy altitude
2011 12  1    0.0
Lat-d Lat-m Lon-d Lon-m
  86    26   162    50
   X       Y       Z      F      I       D
   125    485  57247 57249  89.50  75.55

Year     altitude
2016.167    0.0
Latitude Longitude
-90.00      0.00
   X       Y       Z      F      I       D
   *       *   -52338 54944 -72.28   *
(At the poles X, Y, D are indefinite. H= 16722)
```

3.4 Convert Natsuhara SPIN2 files by sp2m & _sp2m

The programs ”sp2m” and ”_sp2m” transfer the Natsuhara’s SPIN2 measurements files to those for ”pdemag”, ”pdirec”, and ”pinte”. It is supposed that the input file format is that of Natsuhara Giken SPINNER 2000, which I used at the Marine Core Center of Kochi University from 2012 to 2015.

If error of reading a file happens, there would be two reasons, (1) the file format is different from that of SPINNER 2000, and (2) sample name or step data contains SPACE. Concerning to the latter problem, as ”sp2m” and ”_sp2m” treat the characters SPACE and ” as delimiters, any words including SPACE or ” are separated. For example, the program reads ”TH 1” as two words ”TH” and ”1”. So ”TH-1” or ”TH_1” should be used in this case. Test files ”*.txt” and ”_*.txt” are included in the source directories ”pmagt401/sp2m-src” and ”pmagt401/_sp2m-src”.

Case of new format file (”*.txt”): sp2m

”sp2m” takes the bedding attitude corrected directions in default. Using the three test files which contain measurements of thermal demagnetization, type as

```
sp2m thd1.txt thd2.txt thd3.txt > thd1-3.dmg
```

Content of the transferred file ”thd1-3.dmg” which can be analyzed by ”pdemag” is as the following.

```
# BED CORRECTED
$ thd1.txt 0.0 0.0 0.0 0.0
  20 6.589e-02  72.0  340.7
 200 6.475e-02  71.7  342.9
 300 6.226e-02  72.1  340.0
 400 5.732e-02  70.4  345.6
 450 5.254e-02  71.9  342.5
     ...
     ...
$ thd2.txt 0.0 0.0 0.0 0.0
  20 6.609e-02  55.4  344.0
 200 6.538e-02  55.6  341.3
     ...
     ...
$ thd3.txt 0.0 0.0 0.0 0.0
  20 2.651e-01  67.6  318.7
     ...
```

Using the test file ”nrm.txt”, to transfer the data to those with the format for ”pdirec”, type with ”-N” option,

```
sp2m -n nrm.txt > nrm.drc
```

As shown in the following content of ”nrm.drc”, directions in all coordinates are taken with ”-N” option. This file should be analyzed by ”pdirec”.

```
$ nrm.txt
    -1-1  71.3   53.1  42.2   33.6  40.1   37.5 -1.0 A 1  1.721e-02
    -2-1  70.7   52.6  48.2   59.5  44.3   62.8 -1.0 A 1  1.685e-02
    -3-1  55.8   74.9  40.0   26.9  38.4   30.8 -1.0 A 1  1.099e-02
    -4-1  70.0   68.2  38.2   75.6  33.6   77.0 -1.0 A 1  1.628e-02
    -5-1  38.4   59.2  44.1   96.8  39.1   97.0 -1.0 A 1  1.104e-02
    -6-1  40.6   69.5  45.6   97.1  40.6   97.4 -1.0 A 1  1.244e-02
        ...
        ...
```

Case of old format file ("_*.txt"): _sp2m

Concerning to the measurements data from Natsuhara's SPINNER 2000, it is recommended to use the file of old format "_*.txt" because it contains the information of orientation and bedding attitude which user inputted. In default, "_sp2m" takes only the data in core coordinates. Data of orientation and bedding are taken ONLY ONCE from the fist line (usually the NRM measurement as the first step). Hence, it is supposed that the next stage analysis by "pdemag" will calculate the in situ or tilt corrected directions. With "-N" option, "_sp2m" also takes the core coordinates data only. However, the orientation and bedding data are taken from every datum, and the in situ and tilt corrected directions are calculated. They are printed out to the display in the format for "pdirec".

Using the test files of thermal demagnetization, type as

```
_sp2m _thd1.txt _thd2.txt _thd3.txt > _thd1-3.dmg
```

Note that the data of orientation and bedding attitude are taken into "_thd1-3.dmg" as below.

```
$ _thd1.txt  132.6  75.0   10.0   5.0
  20  6.589e-02  19.8  111.3
 200  6.475e-02  20.6  111.3
 300  6.226e-02  19.6  111.4
 400  5.732e-02  22.0  112.2
 450  5.253e-02  20.4  111.2
     ...
     ...
$ _thd2.txt   47.4  76.8   10.0   5.0
  20  6.609e-02  47.0   72.0
 200  6.538e-02  47.8   73.9
     ...
     ...
$ _thd3.txt   62.9  89.1   10.0   5.0
  20  2.652e-01  25.6  100.0
     ...
```

To test "-N" option by using "_nrm.txt", type as

```
_sp2m -n _nrm.txt > _nrm.drc
```

With "-N" option, the results are the same with the case of "sp2m".

```
$ _nrm.txt
    -1-1  71.3   53.1  42.2   33.6  40.1   37.5 -1.0 A 1  1.721e-02
    -2-1  70.7   52.6  48.2   59.5  44.3   62.8 -1.0 A 1  1.685e-02
    -3-1  55.8   74.9  40.0   26.9  38.4   30.8 -1.0 A 1  1.099e-02
    -4-1  70.0   68.2  38.2   75.6  33.6   77.0 -1.0 A 1  1.628e-02
    -5-1  38.4   59.2  44.1   96.8  39.1   97.0 -1.0 A 1  1.104e-02
    -6-1  40.6   69.5  45.6   97.1  40.6   97.4 -1.0 A 1  1.244e-02
        ...
        ...
```

3.5 Summary of formulas

3.5.1 Core orientation and bedding tilt correction

To convert the remanence direction in core coordinates (X_C, Y_C, Z_C) to in situ direction (X_S, Y_S, Z_S), it is easier to consider in terms of rotation of the geographic coordinate system to core system by azimuth A and plunge P. The formula for the device of Natsuhara Giken is given as below.

$$
\begin{aligned}
\begin{pmatrix} X_S \\ Y_S \\ Z_S \end{pmatrix} &= \begin{pmatrix} \cos A & -\sin A & 0 \\ \sin A & \cos A & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos P & -\sin P \\ 0 & \sin P & \cos P \end{pmatrix} \begin{pmatrix} X_C \\ Y_C \\ Z_C \end{pmatrix} \\
&= \begin{pmatrix} \cos A & -\sin A \cos P & \sin A \sin P \\ \sin A & \cos A \cos P & -\cos A \sin P \\ 0 & \sin P & \cos P \end{pmatrix} \begin{pmatrix} X_C \\ Y_C \\ Z_C \end{pmatrix}
\end{aligned}
$$

To carry out tilt correction of the bedding attitude, strike α and dip β, it is easier to consider in terms of rotation of a vector. First rotate the vector by $(-\alpha, -\beta)$ and second rotate it by $(\alpha, 0)$. Hence, the formula of tilt corrected direction (X_T, Y_T, Z_T) is given as the following.

$$
\begin{aligned}
\begin{pmatrix} X_T \\ Y_T \\ Z_T \end{pmatrix} &= \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\beta & \sin\beta \\ 0 & -\sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} X_S \\ Y_S \\ Z_S \end{pmatrix} \\
&= \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha\cos\beta & \cos\alpha\cos\beta & \sin\beta \\ \sin\alpha\sin\beta & -\cos\alpha\sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} X_S \\ Y_S \\ Z_S \end{pmatrix}
\end{aligned}
$$

3.5.2 Field direction to pole position

Field direction (I, D) at a site (λ_S, ϕ_S) is transferred to a VGP at (λ_P, ϕ_P) by using the spherical trigonometry formulas.

$$
\begin{aligned}
&\tan p = 2\cot I, \\
&\sin\lambda_P = \sin\lambda_S \cos p + \cos\lambda_S \sin p \cos D, \\
&\sin(\phi_P - \phi_S) = \sin p \sin D / \cos\lambda_P.
\end{aligned}
$$

Let the solution of the last equation be β, ϕ_P is given by

$$
\begin{cases} \phi_P = \phi_S + \beta, & when \quad \cos p \geq \sin\lambda_S \sin\lambda_P \\ \phi_P = \phi_S + 180 - \beta. & when \quad \cos p < \sin\lambda_S \sin\lambda_P \end{cases}
$$

3.5.3 Pole to field direction

Given a VGP position (λ_P, ϕ_P), the field direction (I, D) observed at a site (λ_S, ϕ_S) is converse of the previous case and given by the following formulas.

$$
\begin{aligned}
&\cos p = \sin\lambda_S \sin\lambda_P + \cos\lambda_S \cos\lambda_P \cos(\phi_P - \phi_S), \\
&\tan I = 2\cot p, \\
&\cos D = (\sin\lambda_P - \sin\lambda_S \cos p)/(\cos\lambda_S \sin p).
\end{aligned}
$$

Using the solution δ ($0 \leq \delta \leq 180$) of the last equation, D is given by the following formulas.

$$
\begin{cases} D = \delta, & when \quad 0 \leq \phi_P - \phi_S \leq 180 \\ D = 360 - \delta. & when \quad 180 < \phi_P - \phi_S < 360 \end{cases}
$$

When the observation site is on the north or the south poles, ϕ_S and D are indeterminate. Nevertheless, "pcalc" defines D at the pole as the converged value of declination when the site is infinitesimally neared to the pole along the line of longitude ϕ_S. Hence, D is given at the poles as,

$$\begin{cases} D = 180 - (\phi_P - \phi_S), & when \quad \lambda_S = 90 \\ D = \phi_P - \phi_S. & when \quad \lambda_S = -90 \end{cases}$$

Another method to estimate the field direction from a VGP, which "pcalc" adopted, is to use the relation of the geocentric dipole and the degree 1 Gauss coefficients. Considering that a VGP is actually a south pole, we have to use an inverted pole position $(-\lambda_P, \phi_P - 180)$ to estimate the Gauss coefficients as

$$\begin{aligned} g_1^0 &= \frac{\mu_0 M}{4\pi a^3}\sin(-\lambda_P) = -\frac{\mu_0 M}{4\pi a^3}\sin\lambda_P, \\ g_1^1 &= \frac{\mu_0 M}{4\pi a^3}\cos(-\lambda_P)\cos(\phi_P - \pi) = -\frac{\mu_0 M}{4\pi a^3}\cos\lambda_P\cos\phi_P, \\ h_1^1 &= \frac{\mu_0 M}{4\pi a^3}\cos(-\lambda_P)\sin(\phi_P - \pi) = -\frac{\mu_0 M}{4\pi a^3}\cos\lambda_P\sin\phi_P, \end{aligned}$$

where μ_0, M, and a are permeability of free space, dipole moment, and the earth's radius, respectively. Using the geomagnetic potential of degree 1, the field components X, Y, Z (NS, EW, vertical, respectively) are given by

$$\begin{aligned} X &= -g_1^0\sin\theta_S + (g_1^1\cos\phi_S + h_1^1\sin\phi_S)\cos\theta_S, \\ Y &= g_1^1\sin\phi_S - h_1^1\cos\phi_S, \\ Z &= -2g_1^0\cos\theta_S - 2(g_1^1\cos\phi_S + h_1^1\sin\phi_S)\sin\theta_S, \end{aligned}$$

where $\theta_S = 90 - \lambda_S$.

3.5.4 VDM and VADM

Supposing that the paleomagnetic field was originated from a geocentric dipole, the dipole moment M is estimated from a paleointensity F and an inclination I or a paleolatitude λ as

$$\begin{aligned} M &= \frac{2\pi a^3 F}{\mu_0}\sqrt{1 + 3\cos^2 I}, \\ &= \frac{4\pi a^3 F}{\mu_0\sqrt{1 + 3\sin^2\lambda}}. \end{aligned}$$

The former is called a virtual dipole moment (VDM) which is estimated from the observed F and I. In the latter case, if λ is set to the present-day latitude λ_S of the observation site, it is called a virtual axial dipole moment (VADM).

3.5.5 Fisher statistics

In the statistics of Fisher (1953), the best estimate of the true mean direction of N paleodirections (I_i, D_i) is given by the vector sum $\mathbf{R}$ as

$$\begin{aligned} R_X &= \sum_{i=1}^{N}\cos I_i\cos D_i, \\ R_Y &= \sum_{i=1}^{N}\cos I_i\sin D_i, \\ R_Z &= \sum_{i=1}^{N}\sin I_i. \end{aligned}$$

and hence, the mean direction (I_m, D_m) is given by

$$\sin I_m = R_Z/R,$$
$$\tan D_m = R_Y/R_X.$$

The best estimate k of the precision parameter κ (for $\kappa > 3$) is given by

$$k = \frac{N-1}{N-R}.$$

The 95% confidence circle α_{95} around the mean direction is calculated by

$$\cos\alpha_{95} = 1 - \frac{N-R}{R}\left[\left(\frac{1}{0.05}\right)^{\frac{1}{N-1}} - 1\right].$$

Angular standard deviation S is defined as

$$S^2 = \frac{1}{N-1}\sum_{i=1}^{N}\theta_i^2,$$

where θ_i is the angular distance of i-th direction from the mean direction.

The mean field direction (I_m, D_m) observed at a certain site (λ_S, ϕ_S) is transferred to a VGP (λ_P, ϕ_P). About the equations to obtain the corresponding VGP, refer to the formulas at page 20. 95% confidence circle around the mean direction is also transferred to the error around the VGP. This error is approximated as the oval of 95% confidence by using two parameters dp and dm. dp is an error along the great circle passing through the site and pole and dm is the one perpendicular to the pass. they are given by

$$dp = \frac{\alpha_{95}}{2}(1 + 3\cos^2 p) = \alpha_{95}\frac{2}{1 + 3\cos^2 I_m},$$
$$dm = \alpha_{95}\frac{\sin p}{\cos I_m} = \alpha_{95}\frac{2}{\sqrt{1 + 3\cos^2 I_m}}.$$

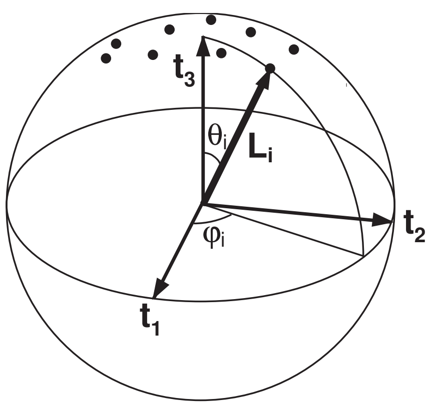
3.5.6 Bingham statistics

Statistics of Bingham (1974) is suitable to describe elongated distribution on the unit sphere. Here only the numerical procedure is described based on Onstott (1980) and Tanaka (1999). For a little more detailed explanation see this page (http://www.ne.jp/asahi/paleomagnetism.rock-magnetism/basics/pmag/dist/bingE.html).

Consider N unit vectors, $\mathbf{L}_i = (x_i, y_i, z_i)$ $(i = 1 \cdots N)$, which moderately scatter around the mean (Figure below). First, the following orientation matrix is calculated.

$$\mathbf{T} = \begin{pmatrix} \sum_{i=1}^N x_i^2 & \sum_{i=1}^N x_i y_i & \sum_{i=1}^N x_i z_i \\ \sum_{i=1}^N x_i y_i & \sum_{i=1}^N y_i^2 & \sum_{i=1}^N y_i z_i \\ \sum_{i=1}^N x_i z_i & \sum_{i=1}^N y_i z_i & \sum_{i=1}^N z_i^2 \end{pmatrix}.$$

Three eigenvalues of $\mathbf{T}$ are designated as τ_1, τ_2, τ_3 in the ascending order ($\tau_1 \le \tau_2 \le \tau_3$, $\tau_1 + \tau_2 + \tau_3 = N$), and corresponding eigenvectors as $\mathbf{t}_1$, $\mathbf{t}_2$, $\mathbf{t}_3$. The mean direction is given by $\mathbf{t}_3$, and the direction of elongation of the distribution is indicated by $\mathbf{t}_2$. Determination of eigenvalues and eigenvectors are carried out by using Jacobi's method described in Press et al. (1992).



Next step is to determine the Bingham's concentration parameters k_1 and k_2 ($k_1 \leq k_2 \leq 0$). The probability density of the Bingham distribution is given by

$$b(\theta, \varphi) = \frac{1}{4\pi d(k_1, k_2)} e^{(k_1 \cos^2 \varphi + k_2 \sin^2 \varphi) \sin^2 \theta},$$

where the normalization constant $d(k_1, k_2)$ is given by the next integration.

$$d(k_1, k_2) = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} e^{(k_1 \cos^2 \varphi + k_2 \sin^2 \varphi) \sin^2 \theta} \sin\theta d\theta d\varphi.$$

Given the N unit vectors $\mathbf{L}_i = (\theta_i, \varphi_i)$ ($i = 1 \cdots N$), the maximum likelihood estimates of k_1 and k_2 are determined by maximizing the next log-likelihood function,

$$F = -N \log 4\pi - N \log d(k_1, k_2) + k_1\tau_1 + k_2\tau_2.$$

Maximizing process is carried out by using Powell's method of Press et al. (1992) in which the maximum is sought starting from $k_1 = k_2 = 0$ to the negative directions of k_1 and k_2. At each of iteration, $d(k_1, k_2)$ is numerically determined by an integration routine.

Once k_1 and k_2 are determined, Bingham's 95% confidence radii around $\mathbf{t}_3$, α_{31} and α_{32} along $\mathbf{t}_1$ and $\mathbf{t}_2$ directions, respectively, are given by

$$\alpha_{31} = 2.45\sigma_{31}, \quad \alpha_{32} = 2.45\sigma_{32},$$

where σ_{ij} is given by

$$\sigma_{ij}^2 = \frac{1}{2(k_i - k_j)(\tau_i - \tau_j)}.$$

Bingham's test statistics of isotropy χ_U^2, polar circular symmetry χ_{CP}^2, and girdle circular symmetry χ_{CG}^2, are given by

$$\begin{aligned}
\chi_U^2 &= (15/2N)\left((\tau_1 - N/3)^2 + (\tau_2 - N/3)^2 + (\tau_3 - N/3)^2\right) \\
\chi_{CP}^2 &= (1/2)(\tau_1 - \tau_2)(k_1 - k_2) \\
\chi_{CG}^2 &= (1/2)(\tau_2 - \tau_3)k_2.
\end{aligned}$$

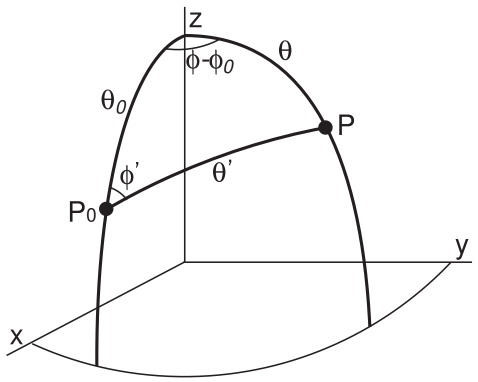
Each of the null hypotheses of isotropy, polar circular symmetry, and girdle circular symmetry is rejected with significance level $p = 0.05$, if each of the following condition is attained.

$$\begin{aligned}
\chi_U^2 &> \chi^2(\nu = 5, p = 0.05) = 11.07 \\
\chi_{CP}^2 &> \chi^2(\nu = 2, p = 0.05) = 5.991 \\
\chi_{CG}^2 &> \chi^2(\nu = 2, p = 0.05) = 5.991.
\end{aligned}$$

3.5.7 Inclination only statistics

Statistics of inclination only data was introduced to paleomagnetism in 1960's to analyze the paleomagnetic measurements from borecores which usually lack declinations. The first study which can be used as a computer algorithm was presented by Kono (1980). Among quite a few studies which followed, the method by McFadden & Reid (1982) has been the most used in the community. However, "pcalc" adopted the recent method of Arason & Levi (2010). The following are concise introduction to the inclination only statistics.

Using polar coordinates, consider a direction P(θ,ϕ) which is Fisher distributed around the true direction P$_0$(θ_0,ϕ_0). Let θ' and ϕ' be the polar angle of P from P$_0$ and the azimuthal angle of P around P$_0$, respectively, as shown in the figure.



The probability density of P around P_0 is given by

$$f(\theta', \phi')d\theta' d\phi' = \frac{\kappa}{4\pi \sinh \kappa} \exp(\kappa \cos \theta') \sin \theta' d\theta' d\phi'.$$

Using the spherical trigonometry as shown in the figure, variables (θ', ϕ') are transferred to (θ, ϕ) by the next equation,

$$\cos \theta' = \cos \theta_0 \cos \theta + \sin \theta_0 \sin \theta \cos(\phi - \phi_0).$$

Using the next relation,

$$\sin \theta' d\theta' d\phi' = \sin \theta d\theta d\phi,$$

the probability density is expressed in terms of (θ, ϕ) as

$$f(\theta, \phi)d\theta d\phi = \frac{\kappa}{4\pi \sinh \kappa} \exp[\kappa \cos \theta_0 \cos \theta + \kappa \sin \theta_0 \sin \theta \cos(\phi - \phi_0)] \sin \theta d\theta d\phi.$$

Now the problem is to find the probability density of θ when ϕ is not known, which is the marginal distribution $f(\theta)$. Integrating the last equation by ϕ, $f(\theta)$ is given by,

$$\begin{aligned} f(\theta)d\theta &= \frac{\kappa}{2\sinh \kappa} \exp(\kappa \cos \theta_0 \cos \theta) \frac{1}{2\pi} \int_0^{2\pi} \exp[\kappa \sin \theta_0 \sin \theta \cos(\phi - \phi_0)] d\phi \sin \theta d\theta, \\ &= \frac{\kappa \sin \theta}{2\sinh \kappa} \exp(\kappa \cos \theta_0 \cos \theta) I_0(\kappa \sin \theta_0 \sin \theta) d\theta, \end{aligned}$$

where $I_0(\cdot)$ is the modified Bessel function of the first kind of order 0.

When N colatitudes θ_i ($i = 1 \cdots N$) are given, the best estimates of θ_0 and κ are obtained by maximizing the following log-likelihood function

$$\begin{aligned} h(\theta, \kappa) &= \log \prod_{i=1}^{N} f(\theta_i), \\ &= \log \left[\left(\frac{\kappa}{2\sinh \kappa} \right)^N \prod_{i=1}^{N} \sin \theta_i \exp(\kappa \cos \theta_0 \cos \theta_i) I_0(\kappa \sin \theta_0 \sin \theta_i) \right], \\ &= N \log \left(\frac{\kappa}{2\sinh \kappa} \right) + \sum_{i=1}^{N} \log(\sin \theta_i) + \sum_{i=1}^{N} \kappa \cos \theta_0 \cos \theta_i + \sum_{i=1}^{N} \log(I_0(\kappa \sin \theta_0 \sin \theta_i)). \end{aligned}$$

Differences of the studies published so far are in the methods of approximating the above equation, especially the Bessel function part. Although I am not in the fields of theory or numerical calculations, I presume that the most reliable study is Arason & Levi (2010) in which detailed description was presented together with thorough comparison of the results among the previous studies.

3.5.8 International Geomagnetic Reference Field

Magnetic potential W of the geomagnetic field of internal origin is represented with the Gauss coefficients g_n^m and h_n^m as

$$W = a \sum_{n=1}^{\infty} \sum_{m=0}^{n} \left(\frac{a}{r}\right)^{n+1} P_n^m(\cos\theta)(g_n^m \cos m\phi + h_n^m \sin m\phi),$$

where a is the radius of the earth, (r, θ, ϕ) is an observation point in polar coordinates ($r \geq a$), and $P_n^m(\cos\theta)$ is quasi-normalized Schmidt function (associated Legendre polynomials). The geomagnetic field vector $\mathbf{B}$ at the observation point is given by

$$\mathbf{B} = -\nabla W.$$

Let X, Y, and Z be the northward, eastward, and vertical down components of $\mathbf{B}$, respectively. Noting that X, Y, and Z directions are $-\theta$, $+\phi$, and $-r$ directions, respectively, the three components are given by

$$X = \frac{1}{r}\frac{\partial W}{\partial \theta}, \quad Y = -\frac{1}{r\sin\theta}\frac{\partial W}{\partial \phi}, \quad Z = \frac{\partial W}{\partial r}.$$

Hence, three components of the geomagnetic field at the observation point (r, θ, ϕ) are calculated by

$$\begin{aligned}
X &= \sum_{n=1}^{\infty} \left(\frac{a}{r}\right)^{n+2} \sum_{m=0}^{n} (g_n^m \cos m\phi + h_n^m \sin m\phi) \frac{dP_n^m(\cos\theta)}{d\theta}, \\
Y &= \sum_{n=1}^{\infty} \left(\frac{a}{r}\right)^{n+2} \sum_{m=0}^{n} (g_n^m \sin m\phi - h_n^m \cos m\phi) \frac{mP_n^m(\cos\theta)}{\sin\theta}, \\
Z &= -\sum_{n=1}^{\infty} (n+1) \left(\frac{a}{r}\right)^{n+2} \sum_{m=0}^{n} (g_n^m \cos m\phi + h_n^m \sin m\phi) P_n^m(\cos\theta).
\end{aligned}$$

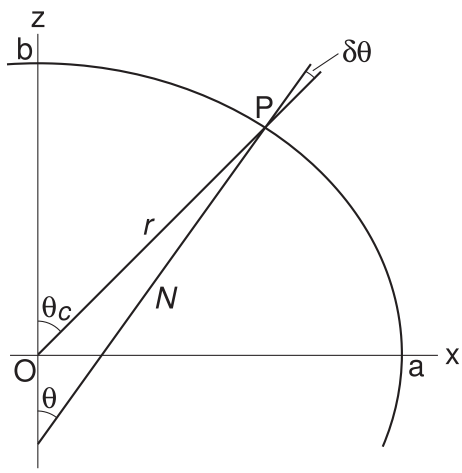
Programs ”igrf”, ”sunpmag”, and ”pcalc” take the Gauss coefficients for AD 1900–2020 from IAGA Working Group V-MOD (2020) and summation is carried out up to $n = m = 10$.

3.5.9 Geodetic and geocentric coordinate systems

Geomagnetic elements are calculated by using the above mentioned formulas which are defined on the geocentric coordinate system. It is preferable to transfer them to those expressed on the usual geographic (geodetic) coordinate system. The following summarize the relation of geodetic and geocentric coordinates systems.

Consider the earth of oblate spheroid with semi-axes a, a, and b ($a > b$). Using the geodetic colatitude θ of an observation point P, distances N and r in the figure are given by

$$\begin{aligned}
N^2 &= \frac{a^4}{a^2 \sin^2\theta + b^2 \cos^2\theta}, \\
r^2 &= \frac{a^4 \sin^2\theta + b^4 \cos^2\theta}{a^2 \sin^2\theta + b^2 \cos^2\theta}.
\end{aligned}$$



Orthogonal coordinates of the point P with altitude h (not shown in the figure) are given by

$$\begin{aligned} x &= (N+h)\sin\theta\cos\phi, \\ y &= (N+h)\sin\theta\sin\phi, \\ z &= \left(\frac{b^2}{a^2}N+h\right)\cos\theta. \end{aligned}$$

Using $r^2 = x^2+y^2+z^2$,

$$r^2 = \frac{a^4\sin^2\theta + b^4\cos^2\theta}{a^2\sin^2\theta + b^2\cos^2\theta} + h\left(h + 2\sqrt{a^2\sin^2\theta + b^2\cos^2\theta}\right).$$

Cosine and sine of the geocentric colatitude θ_c are

$$\begin{aligned} \cos\theta_c &= \frac{1}{r}\left(\frac{b^2}{a^2}N+h\right)\cos\theta, \\ \sin\theta_c &= \frac{N+h}{r}\sin\theta. \end{aligned}$$

Let unit vectors along r and N directions be $\mathbf{e}^c$ and $\mathbf{e}$, respectively, and their difference angle be $\delta\theta$. Cosine and sine of $\delta\theta$ are derived from $\mathbf{e}^c\mathbf{e}$ and $\mathbf{e}^c\times\mathbf{e}$, respectively. Hence,

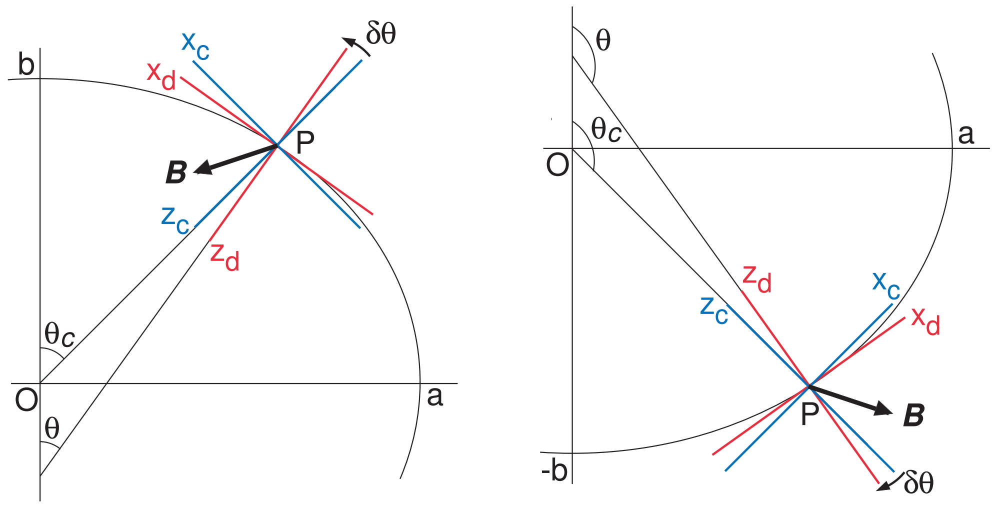
$$\begin{aligned} \cos\delta\theta &= \mathbf{e}^c\mathbf{e} = \sin\theta_c\sin\theta + \cos\theta_c\cos\theta, \\ &= \frac{h+\sqrt{a^2\sin^2\theta + b^2\cos^2\theta}}{r}. \\ \sin\delta\theta &= (\mathbf{e}^c\times\mathbf{e})_y = \sin\theta_c\cos\theta - \cos\theta_c\sin\theta, \\ &= \frac{(a^2-b^2)\sin\theta\cos\theta}{r\sqrt{a^2\sin^2\theta + b^2\cos^2\theta}}. \end{aligned}$$

As $\theta_c = \theta + \delta\theta$,

$$\cos\theta_c = \cos\theta\cos\delta\theta - \sin\theta\sin\delta\theta.$$

To summarize the procedure, given the observation point (θ, ϕ) with altitude h in geodetic system, the geocentric colatitude θ_c and the distance from the earth's center r are determined by using above equations. Setting $\phi_c = \phi$, field elements (X_c, Y_c, Z_c) at (r, θ_c, ϕ_c) are calculated. Those elements in the geodetic system (X, Y, Z) are obtained by rotating the local coordinate axes by $\delta\theta$ (see figure below).

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} \cos\delta\theta & 0 & \sin\delta\theta \\ 0 & 1 & 0 \\ -\sin\delta\theta & 0 & \cos\delta\theta \end{pmatrix} \begin{pmatrix} X_c \\ Y_c \\ Z_c \end{pmatrix}$$



Rotation of local coordinates from geocentric (blue) to geodetic (red) on northern (left) and southern (right) hemispheres (x:north, z:vertical down)

3.5.10 Circle fitting

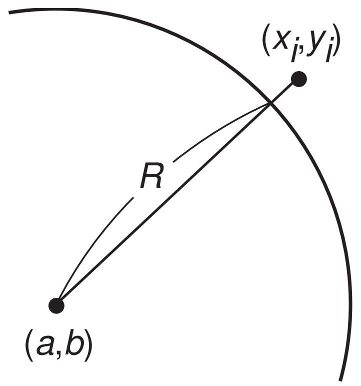
The program uses the method of Taubin (1991). This method seeks the circle parameters by minimizing the sum of the squares of "algebraic" distance $r_i^2 - R^2$ not the "geometric" distance $r_i - R$, where r_i and R are the distance of a data point from the center and the radius of the circle, respectively. Although the algebraic fits are less accurate than the geometric fits, Taubin's method is one of those improved over the classical ones such as Kasa (1976) (see, Chernov & Lesort 2005). The programming code used is adapted from the C++ routines given by Chernov (2012). The following are crude explanation of the theory.

Consider n observation points (x_i, y_i) $(i = 1, \cdots, n)$ which are fitted by a circle of radius R at the center (a, b). The geometric distance of an observation point from the arc of a circle is denoted as,

$$d_i = r_i - R,$$

where

$$r_i = \sqrt{(x_i - a)^2 + (y_i - b)^2}.$$



The geometric method seeks a, b, and R which minimize the sum of the squares of the distance d_i as,

$$\sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} \left(\sqrt{(x_i - a)^2 + (y_i - b)^2} - R \right)^2 .$$

However, this is a nonlinear problem which is quite difficult to solve. Although excellent programming codes of the geometric method are presented in Chernov (2012), here less accurate but simpler algebraic methods are considered. The algebraic distance is defined as,

$$f_i = r_i^2 - R^2.$$

Now the quantity to be minimized is,

$$\begin{aligned} \mathcal{F}_{\mathcal{K}} &= \sum_{i=1}^{n} f_i^2, \\ &= \sum_{i=1}^{n} (x_i^2 + y_i^2 - 2ax_i - 2by_i + a^2 + b^2 - R^2)^2. \end{aligned}$$

In the classical methods such as Kasa (1976), the parameters of the best fitted circle are easily obtained by the conventional least squares method by introducing new parameters as $A = -2a$, $B = -2b$, and $C = a^2 + b^2 - R^2$. For the details of the method, see this page (http://www.ne.jp/asahi/paleomagnetism.rock-magnetism/basics/pmag/circ/circ1E.html).

Unfortunately this method sometimes gives an answer biased toward a small R. According to Al-Sharadqah and Chernov (2009),

$$f_i = (r_i - R)(r_i + R) = d_i(2R + d_i) \approx 2Rd_i.$$

Hence the classical method minimizes,

$$\mathcal{F}_{\mathcal{K}} \approx 4R^2 \sum_{i=1}^{n} d_i^2,$$

and it often prefers to minimize R^2 rather than $\sum_{i=1}^{n} d_i^2$. To improve this,

$$\mathcal{F} = \frac{1}{4R^2}\mathcal{F}_{\mathcal{K}}$$

may be minimized. Taubin (1991) adopted the mean of r_i^2 for the denominator R^2. Hence, Taubin method minimizes,

$$\mathcal{F}_{\mathcal{T}} = \frac{\sum_{i=1}^{n}\left[(x_i-a)^2+(y_i-b)^2-R^2\right]^2}{4n^{-1}\sum_{i=1}^{n}\left[(x_i-a)^2+(y_i-b)^2\right]}.$$

In this method, the equation of the circle is denoted as,

$$A(x^2+y^2)+Bx+Cy+D=0.$$

The circle parameters a, b, and R are given by the new parameters as,

$$\begin{aligned} a &= -\frac{B}{2A}, \\ b &= -\frac{C}{2A}, \\ R^2 &= \frac{B^2+C^2-4AD}{4A^2}. \end{aligned}$$

As the parameters can be scaled by a scalar and considering that $B^2+C^2-4AD>0$, the following constraint can be imposed among the parameters.

$$B^2+C^2-4AD=1.$$

Using these notations, the above $\mathcal{F}_{\mathcal{T}}$ is represented as

$$\mathcal{F}_{\mathcal{T}} = \frac{\sum_{i=1}^{n}(Az_i+Bx_i+Cy_i+D)^2}{4A^2\bar{z}+4AB\bar{x}+4AC\bar{y}+B^2+C^2}$$

where $z_i = x_i^2+y_i^2$ and $\bar{x}=\frac{1}{n}\sum_{i=1}^{n}x_i$, etc. Considering the above constraint $B^2+C^2-4AD=1$, the problem is now equivalent to minimizing

$$\mathcal{F}_1 = \sum_{i=1}^{n}(Az_i+Bx_i+Cy_i+D)^2$$

on the constraint of

$$4A^2M_z+4ABM_x+4ACM_y+B^2n+C^2n=1,$$

where $M_x=\sum_{i=1}^{n}x_i$, etc. Using matrix notation, best fit parameters can be determined by minimizing,

$$\begin{aligned} \mathcal{F}_1 &= {}^t\alpha\mathbf{M}\alpha \\ &= \begin{pmatrix} A & B & C & D \end{pmatrix} \begin{pmatrix} M_{zz} & M_{xz} & M_{yz} & M_z \\ M_{xz} & M_{xx} & M_{xy} & M_x \\ M_{yz} & M_{xy} & M_{yy} & M_y \\ M_z & M_x & M_y & n \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}, \end{aligned}$$

on the constraint of,

$${}^t\alpha\mathbf{N}\alpha = \begin{pmatrix} A & B & C & D \end{pmatrix} \begin{pmatrix} 4M_z & 2M_x & 2M_y & 0 \\ 2M_x & n & 0 & 0 \\ 2M_y & 0 & n & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 1.$$

As this is a typical inverse problem, introducing a Lagrange multiplier η, the next equation is minimized.

$$\mathcal{F}_* = {}^t\alpha\mathbf{M}\alpha - \eta({}^t\alpha\mathbf{N}\alpha - 1).$$

$\partial\mathcal{F}_*/\partial\alpha = 0$ gives,

$$\mathbf{M}\alpha - \eta\mathbf{N}\alpha = 0.$$

This is an eigenvalue problem and η is obtained by

$$\det(\mathbf{M} - \eta\mathbf{N}) = 0.$$

Corresponding ${}^t\alpha = (A, B, C, D)$ is determined by solving

$$(\mathbf{M} - \eta\mathbf{N})\alpha = 0.$$

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