Additional functions for transforming soil particlesize distributions

Wei Shangguan

September 30, 2010

1 Load the soiltexture package

The soiltexture package can be installed from CRAN with the following commands:

```
install.packages("soiltexture")
   And loaded with the following commands:
   require( "soiltexture" )
   require( "drc" )

'drc' has been loaded.

Please cite R and 'drc' if used for a publication,
for references type 'citation()' and 'citation('drc')'.
```

2 Transforming soil texture data using many Particle-Size Distribution models (from 3 or more particle size classes)

TT.text.transf.Xm() is used to transform soil texture data from 3 or more particle size classes using various Particle-Size Distribution (PSD) models. The drc package and its associate packages(lattice,magic,nlme, plotrix) are required in the PSD model fitting.Compared to TT.text.transf(), the following check is not needed (and not done):

• When the 1st value of input tri.data and output particle size classes limits is 0, The 2nd value of the output particle size classes limits must be higher or equal to the 2nd value of the input particle size classes limits."

We need first to create a dummy dataset with more than 3 particle size classes:

```
"SAND" = c(90, 32, 70, 70, 20, 10, 10, 10, 20, 10, 70, 10)
  Transform this data frame from 4 particle size classes to 3 particle size classes:
res <- TT.text.transf.Xm(</pre>
     tri.data = my.text4,
     base.ps.lim = c(0,1,50,2000),
     dat.ps.lim = c(0,2,30,60,2000),
     psdmodel
                 ="AD"
)
#
round( res[,1:6], 3 )
             1-50 50-2000 f0:(Intercept) b:(Intercept)
 [1,] 4.341 4.651 91.007
                                      0.584
                                                     0.364
 [2,] 59.657 6.931
                     33.412
                                      0.807
                                                     0.148
                                      0.763
 [3,] 13.657 14.860
                     71.483
                                                     0.477
 [4,] 3.408 23.472
                     73.119
                                                     0.412
                                      0.571
 [5,] 24.116 49.480
                     26.403
                                      0.619
                                                     0.265
 [6,] 4.472 81.324
                     14.283
                                      0.521
                                                     0.318
 [7,] 24.365 62.043 13.594
                                                     0.255
                                      0.620
 [8,] 44.507 41.646 13.848
                                      0.721
                                                     0.189
[9,] 63.849 14.739 21.412
                                      0.833
                                                     0.171
[10,] 74.779 11.981 13.240
                                      0.874
                                                     0.087
[11,] 11.934 15.826 72.239
                                                     0.361
                                      0.611
[12,] 46.495 39.835 13.677
                                      0.731
                                                     0.183
      c:(Intercept)
 [1,]
              4.276
[2,]
              3.211
[3,]
              1.314
 [4,]
              1.630
 [5,]
              4.298
 [6,]
              9.084
 [7,]
              6.745
[8,]
              5.920
[9,]
              1.102
[10,]
              4.801
[11,]
              1.989
[12,]
              5.533
round( res[,7:ncol(res)], 3 )
     r0:(Intercept)
 [1,]
               0.613 0.783
 [2,]
               0.138 0.000
               0.773 0.003
 [3,]
               0.179 0.000
 [4,]
 [5,]
               0.039 0.000
```

"CSILT" = c(03,04,05,10,30,45,30,25,05,10,07,23),

```
[6,] 0.032 0.018
[7,] 0.031 0.000
[8,] 0.035 0.000
[9,] 0.090 0.000
[10,] 0.052 0.000
[11,] 0.231 0.000
[12,] 0.035 0.000
```

The first 3 columns are the predicted values with a sum not equal to 100% (can be normalised by TT.normalise.sum.X()). The following 4 columns are the fitted PSD model parameters. And the last column is the Residual Sum of Squares (deviance). Note that the transforming results may be slightly different even with the same function parameters. This is cause by the nature of drc package in fitting dose-response models.

Sometimes, the fitting will failed for the iteration is not converged or some errors and warnings happened. These can be ignored, as you can get the transforming results.

The following PSD models are implemented: Anderson (AD), Fredlund4P (F4P), Fredlund3P (F3P), modified logistic growth (ML), Offset-Nonrenormalized Lognormal (ONL), Offset-Renormalized Lognormal (ORL), Skaggs (S), van Genuchten type(VG), van Genuchten modified, Weibull (W), Logarithm(L), Logistic growth (LG), Simple Lognormal (SL), Shiozawa and Compbell (SC). The performance of PSD models is influenced by many aspects like soil texture class, number and position (or closeness) of observation points, clay content etc. The latter four PSD models perform worse than the former ten. The AD, F4P, S, and W model is recommended for most of texture classes. And it will be even better to compare several different PSD models and using the results of the model with the minimum residual sum of squares. Except S and W models, all the PSD models could be used to predict the content below the minimum input limit. The "psdmodel" option could be changed to any other of the above models:

```
res <- TT.text.transf.Xm(</pre>
    tri.data
                 = my.text4,
    base.ps.lim = c(0,1,50,2000),
                = c(0,2,30,60,2000),
    dat.ps.lim
                 = "ML"
    psdmodel
)
round( res[,1:6], 3 )
        0 - 1
               1-50 50-2000 a: (Intercept) b: (Intercept)
[1,]
      4.941
             3.947
                     91.113
                                     19.476
                                                    13.341
[2,] 59.849
             6.848
                     33.302
                                     0.675
                                                     5.740
[3,] 14.721 13.805
                     70.984
                                     6.473
                                                     4.910
      4.413 22.512
                                     53.869
                                                     7.420
[4,]
                     72.511
[5,] 24.466 46.833
                     28.700
                                     3.162
                                                    62.763
[6,] 4.376 76.265
                                     26.148
                                                    57.096
                     19.359
```

```
[7,] 24.185 58.851
                                     3.259
                                                   72.585
                     16.964
 [8,] 44.788 38.541
                                                  180.302
                      16.671
                                     1.238
[9,] 64.027 14.560
                     21.321
                                     0.615
                                                     4.399
[10,] 74.978 11.682
                     13.340
                                     0.334
                                                  249.075
[11,] 12.405 15.396
                                     8.171
                                                    5.553
                     71.925
[12,] 46.747 37.139
                     16.114
                                     1.146
                                                  144.538
      c:(Intercept)
 [1,]
              1.013
 [2,]
              0.983
 [3,]
              0.549
 [4,]
              0.304
 [5,]
              1.140
 [6,]
              0.834
 [7,]
              1.090
 [8,]
              1.534
[9,]
              0.563
              1.927
[10,]
[11,]
              0.527
[12,]
              1.467
round( res[,7:ncol(res)], 3 )
[1] 0.000 0.000 1.669 1.071 0.000 0.000 0.000 0.000 0.011 0.000
[11] 0.205 0.000
```

Because the current PSD model fitting is quite time-consuming and some models are not always successful for all soils, you can change the PSD model, or optimization method potentially at the cost of some accuracy. The default "omethod" option (i.e. "all") is to run all methods and choose the best results with minimum residual sum of squares. The optional methods are "Nelder-Mead", "BFGS", "CG", "L-BFGS-B", "SANN" (see optim() for details.)

```
res <- TT.text.transf.Xm(</pre>
    tri.data
                = my.text4,
    base.ps.lim = c(0,1,50,2000),
    dat.ps.lim = c(0,2,30,60,2000),
                = "ML",
    psdmodel
                = "SANN"
    omethod
)
round( res[,1:6], 3 )
              1-50 50-2000 a:(Intercept) b:(Intercept)
        0 - 1
[1,] 4.731
            4.231
                                   20.873
                    91.027
                                                   7.161
[2,] 59.849 6.849
                    33.302
                                    0.675
                                                   5.740
[3,] 14.721 13.805
                    70.985
                                    6.473
                                                   4.911
[4,] 4.415 22.509
                    72.513
                                   53.781
                                                   7.420
[5,] 24.466 46.834
                                                  62.764
                    28.700
                                    3.162
[6,] 4.376 76.264
                    19.360
                                   26.146
                                                  57.091
[7,] 24.186 58.850
                                    3.259
                                                  72.608
                    16.964
```

```
[8,] 44.788 38.541 16.671
                                     1.238
                                                 180.303
[9,] 64.026 14.561 21.321
                                                   4.396
                                     0.615
[10,] 74.978 11.682 13.340
                                     0.334
                                                 249.151
[11,] 12.410 15.390 71.926
                                    8.166
                                                   5.552
[12,] 46.745 37.142 16.113
                                    1.146
                                                 144.522
     c:(Intercept)
[1,]
             0.767
[2,]
              0.983
 [3,]
              0.549
 [4,]
              0.304
 [5,]
              1.140
 [6,]
              0.834
 [7,]
              1.090
[8,]
              1.534
[9,]
              0.563
[10,]
              1.927
[11,]
              0.527
[12,]
              1.467
round( res[,7:ncol(res)], 3 )
[1] 0.091 0.000 1.669 1.071 0.000 0.000 0.000 0.000 0.011 0.000
[11] 0.205 0.000
```

3 Normalizing soil texture data (sum of X texture classes)

 $\mathtt{TT.normalise.sum.X()}$ is similar to $\mathtt{TT.normalise.sum()}$. But it normalize the sum of the X (X>1) texture classes instead of 3. The option $\mathtt{tri.data}$ should be a data.frame with only soil texture data (no additional extra columns should be present).

```
my.text5 <- data.frame(
    "CLAY" = c(05,60,15,04.9,25,05,25,45,65,75,13,47),
    "FSILT" = c(02,04.3,10,15,25,40,35,20,10,05,10,20),
    "CSILT" = c(03,04,05,10,30,45,30,25,05,10,07.2,23.3),
    "SAND" = c(90.5,32,70,70,20.3,10.9,9.3,9.4,20,10,70,10)
) #
#
res <- TT.normalise.sum.X(
    tri.data = my.text5,
    residuals = TRUE
) #

[1] 100.5 100.3 100.0 99.9 100.3 100.9 99.3 99.4 100.0 100.0
[11] 100.2 100.3
#
res</pre>
```

	CLAY	FSILT	CSILT	SAND	residuals
[1,]	4.975124	1.990050	2.985075	90.049751	0.5
[2,]	59.820538	4.287139	3.988036	31.904287	0.3
[3,]	15.000000	10.000000	5.000000	70.000000	0.0
[4,]	4.904905	15.015015	10.010010	70.070070	-0.1
[5,]	24.925224	24.925224	29.910269	20.239282	0.3
[6,]	4.955401	39.643211	44.598612	10.802775	0.9
[7,]	25.176234	35.246727	30.211480	9.365559	-0.7
[8,]	45.271630	20.120724	25.150905	9.456740	-0.6
[9,]	65.000000	10.000000	5.000000	20.000000	0.0
[10,]	75.000000	5.000000	10.000000	10.000000	0.0
[11,]	12.974052	9.980040	7.185629	69.860279	0.2
[12,]	46.859422	19.940179	23.230309	9.970090	0.3