

Superimposition Errors in the IMP3D Software

January 23, 2006

H.D.Sheets, Dept. of Physics, Canisius College, 2001 Main St. Buffalo, NY 14208
sheets@canisius.edu

Thanks to a query from Jonathan Britton (U. Toronto), I have discovered that I have made a substantial in the programming of the Partial Procrustes Superimposition in the IMP3D programs. The same superimposition function was used throughout the IMP3D series, and thus affects all programs in the series.

Impact

Since this error was in a very fundamental part of any operation on shape, all results obtained with the IMP3D series should be regarded as suspect and rechecked. Users of IMP3D are strongly urged to download the revised versions posted on my website at: <http://www2.canisius.edu/~sheets/moremorph.html>. There are corrected versions of all IMP3D programs with compile dates of 1/23/06 or later.

Details of the Error

The error was in the calculation of the rigid rotation of a specimen in 3D to match to a reference form. The rotation matrix is calculated by using a singular value decomposition, the proper calculation of the rotation matrix H necessary to orient the specimen Y on the reference X is obtained by computing:

$$A = Y'X$$

And then obtaining the singular value decomposition of A

$$A = USV'$$

From which we can obtain the estimate of the rotation H

$$H = UV'$$

The error made in the earlier IMP3D programs was to use $A = Y \setminus X$, where \setminus is the MATLAB division operator. This approach yields incorrect results in many cases.

I also checked the performance of the current (fixed) SVD based calculation of H by using a numerical estimation procedure to minimize the summed squared inter-landmark distances between X and HY , where H is the standard 3D rotational matrix in terms of

the angles of rotation alpha, beta and gamma about the z, x and y axes respectively as detailed in Slice (1996, the White Book, page 182). This procedure used a simplex method to determine the values of alpha, beta and gamma that minimized the procrustes distances, and returned results identical (within the machine precision) to those obtained using the corrected SVD method.

Additional Error in Goodall's F-test

In addition to the error in the Superimposition common to all IMP3D programs, it appears that changes to the Simple3D version (*IMP: Simple3D 4/12/05 Variant Version with Variance Statistics*) introduced an additional error into the Goodall's F-test in this program. The introduced error squared all the distances used in the calculation. This has been corrected in the latest version.

How Did This Happen?

I should have caught this programming error prior to release of the software. Unfortunately, for the simulated test data I had available, the error does not appear. The correct superimposition calculation and my original incorrect method give the same answer for my test data, but Dr. Britton's data clearly illustrated the error. The programs needed to be checked with multiple data sets, which I simply did not do adequately.

I find it difficult to express my level of dismay and alarm at this error, and the difficulties it has caused others. I had created and posted the IMP3D programs (which are adaptations of the 2D IMP software) in an effort to support and encourage the study of morphology in three dimensions. I do hope my efforts have done more good than harm.

Please don't hesitate to contact me if you have questions about this error, or other aspects of IMP software.

-Dave Sheets