

Re: Fast solution to very small eigenvalue problem

Source: <http://sci.tech-archive.net/Archive/sci.math.num-analysis/2004-06/0413.html>

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Date: 06/25/04

Date: 25 Jun 2004 11:10:49 +0100 (BST)

In article <avMcc.131446\$Gx4.109902@bgtnc04-news.ops.worldnet.att.net>, K. Doniger <k.doniger@ieee.org> wrote:

>>

>If this derives from a physical problem, perhaps you can use Rayleigh's
>variational principle.

The problem involves aligning molecules in 3D. The problem reduces down to constructing a symmetric 4x4 matrix from the atomic coordinates, and the eigenvector corresponding to the largest eigenvalue of that matrix is the rotation quaternion giving the best least-squares fit (see http://www.osc.edu/PET/CCM/skeleton/software/tested/source/qtrfit/qtrfit_theory.html, with the caveat that the matrix is depicted wrongly: it is actually symmetric)

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Mark Mackey

"The determined Real Programmer can write Fortran programs in any language."
- "Real Programmers don't use Pascal"