Electronic Transactions on Numerical Analysis.
Volume 29, pp. 46-69, 2008.

ISSN 1068-9613.

ETNA
Kent State University
etna@mcs.kent.edu

AN SVD APPROACH TO IDENTIFYING METASTABLE STATES OF MARKOV CHAINS*

DAVID FRITZSCHE†, VOLKER MEHRMANN‡, DANIEL B. SZYLD§, AND ELENA VIRNIK‡

Abstract. Being one of the key tools in conformation dynamics, the identification of metastable states of Markov chains has been subject to extensive research in recent years, especially when the Markov chains represent energy states of biomolecules. Some previous work on this topic involved the computation of the eigenvalue cluster close to one, as well as the corresponding eigenvectors and the stationary probability distribution of the associated stochastic matrix. More recently, since the eigenvalue cluster algorithm may be nonrobust, an optimization approach was developed. As a possible less costly alternative, we present an SVD approach of identifying metastable states of a stochastic matrix, where we only need the singular vector associated with the second largest singular value. We also introduce a concept of block diagonal dominance on which our algorithm is based. We outline some theoretical background and discuss the advantages of this strategy. Some simulated and real numerical examples illustrate the effectiveness of the proposed algorithm.

Key words. Markov chain, stochastic matrix, conformation dynamics, metastable, eigenvalue cluster, singular value decomposition, block diagonal dominance

AMS subject classifications. 15A18, 15A51, 60J10, 60J20, 65F15

---

*Received October 9, 2006. Accepted for publication October 15, 2007. Published online on January 28, 2008. Recommended by A. Frommer. This work was supported in part by DFG Research Center MATHEON in Berlin, by the U.S. National Science Foundation under grant CCF-0514489, and by the U.S. Department of Energy under grant DE-FG02-05ER25672.

†Bergische Universität Wuppertal, Fachgruppe Mathematik, Gaußstraße 20, 42119 Wuppertal, Germany (david.fritzsche@math.uni-wuppertal.de).

‡Technische Universität Berlin, Institut für Mathematik, Straße des 17. Juni 136, 10623 Berlin, Germany (mehrmann,virnik@math.tu-berlin.de).

§Temple University, Department of Mathematics, 1805 North Broad Street, Philadelphia, PA 19122-6094, USA (szyld@temple.edu).