Characterization of Transition States via Metastable Fuzzy Sets

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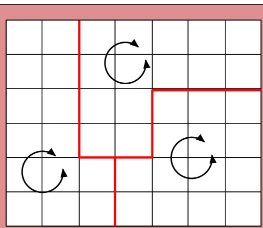
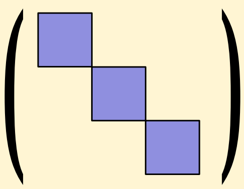


Ω

Problem: After discretization of Ω into m boxes find a decomposition into almost invariant sets based on a stochastic operator. Identify transition boxes.

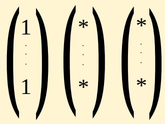
Idea: For every box compute the grade of membership to each of the k almost invariant sets, i.e. use metastable fuzzy sets instead of metastable crisp sets.



(m,m)−transition matrix T
"hidden" block diagonally dominant

spectrum of T with a gap after k=3

1.0 0.99 0.98 | 0.69 0.68 ...



basis of I_T

$\chi \in I_T \longrightarrow T\chi \approx \chi$

Properties of a solution S = $\{\chi_1, ..., \chi_k\}$

a) $\chi_i \in [0,1]^m \cap I_T, \quad i = 1, \ldots, k$

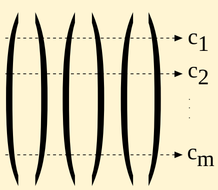
b) S is linear independent

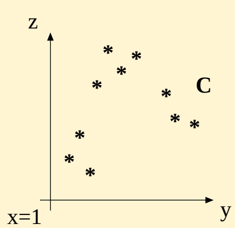
c) $\Sigma_{i=1}^{k} \chi_i = \mathbf{1}_\Omega$

d) $\chi_A, \chi_B \in [0,1]^m \cap I_T,\ \chi_A + \chi_B = \chi_i$
$\Rightarrow \{\chi_A, \chi_B\}$ linear dependent

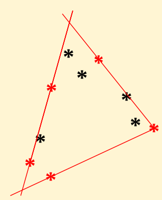
Linear transformation of a basis of I_T into a feasible solution S

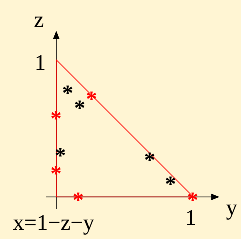
1. Projection of a basis of I_T





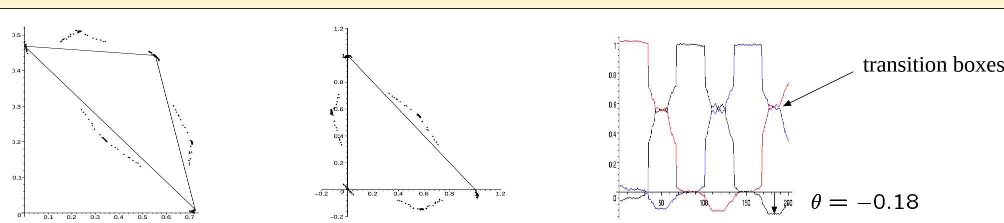
2. Find (k−1)−simplex V covering C (see prop. a−c), each facet of V includes at least (k−1) different points of C (see prop. d). Transform V into an unit simplex yielding a projection of S.





Indicator for the uniqueness of S

The choice of an outer simplex for the linear transformation is not unique if the convex hull of C is not a simplex. Therefore choose a maximal **inner** simplex and use the lowest value of χ_i as an indicator for the uniqueness of S (example: m=200, k=3).



2−dimensional projection | linear transformation | membership functions and indicator

References

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[2] T. Galliat, P.Deuflhard, R. Roitzsch and F. Cordes: Automatic Identification of Metastable Conformations via Self−Organized Neural Networks. *Computational Methods for Macromolecules: Challenges and Applications, Proceedings of 3rd International Workshop on Algorithms for Macromolecular Modelling, New York, Oct. 12−14, 2000,* T. Schlick and H.H. Gan, eds., *Lecture Notes in Computational Science and Engeneering, Vol.24,* Springer, 2002.

[3] M.Weber, T. Galliat: Characterization of Transition States in Conformational Dynamics using Fuzzy Sets. *ZIB−Report 02−12, March 2002.*

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