Integrating Multilevel Graph Partitioning with Hierarchical Set Oriented Methods for the Analysis of Dynamical Systems

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Abstract

Dynamical systems from real applications are usually very complex and difficult to handle. Recently, the combination of hierarchical set oriented methods and of multilevel graph partitioning methods has been used for the analysis of the almost invariant sets of the system which are a key characteristic of dynamical systems. Both approaches include their own multilevel mechanisms. In this paper we interlock these multilevel approaches by integrating graph partitioning techniques directly in the hierarchical set oriented paradigm. Our experimental results show that this interlocked approach leads us to a robust and successful method for analyzing the almost invariant sets. It is important to mention that the work in this direction not only incorporates the handling of continuous and discrete structures but also requires the interlock between numerical, algebraic and graph theoretic concepts.

The analysis of dynamical systems arising from real applications is usually very complex. Often, analytical methods can not be applied and one has to use numerical techniques in order to work with the dynamical system. In particular, in the last ten years a set oriented approach has been developed which allows the analysis of dynamically relevant structures in the dynamical system such as macroscopic features [1]. Initially, algebraic based methods have been applied to analyze the so obtained discrete dynamical systems [7, 9, 10]. One step further on, set oriented numerical methods open the field by transforming the discretized structure into a graph based setting. Thus, graph algorithms were then applied in order to analyze the dynamical systems [5, 9].

A map $f : X \to X$ on a compact subset $X \subset \mathbb{R}^n$ defines a discrete dynamical system

$$x_{k+1} = f(x_k),\ k = 0, 1, \dots \ .$$

Almost invariant sets of a dynamical system are an important characteristic for analyzing the macroscopic dynamics. An almost invariant set is a subset of state space where typical trajectories stay for a long period of time before they enter other parts of the state space. Recently, the identification of these sets has successfully been used both in the context of the approximation of chemical conformations for molecules [5, 6] and in explaining transport phenomena in dynamical astronomy [3, 4]. In applications it is important to find out the number as well as the positions of these relevant sets.

Let m be the Lebesgue measure and for a set $S \subset X$ let $\rho(S) = \frac{m(f^{-1}(S)\cap S)}{m(S)}$ be the transition probability that a set S maps into itself. Now we have to solve the following problem.

Problem 1 (Continuous) *For some fixed* $p \in \mathbb{N}^+$ *find a collection of pairwise disjoint sets* $\mathcal{S} = \{S_1, \dots, S_p\}$ *with* $\bigcup_{1\le i\le p} S_i = X$ *and* $m(S_i) > 0$, $1 \le i \le p$, *such that*

$$\rho(\mathcal{S}) := \frac{1}{p}\sum_{i=1}^{p} \rho(S_i) \to \max \ .$$

The use of set oriented numerical methods in combination with graph algorithmic techniques has been proposed for the identification of the number and location of almost invariant sets in state space [3, 5]. In this setting the dynamical system is approximated by a box covering of the region of interest, that is, a finite collection $\mathcal{B} = \{B_1, \dots, B_b\}$ of boxes, such that $X = \bigcup_{i=1}^{b} B_i$ and $m(B_i \cap B_j) = 0$ for $i \neq j$.

In practice this box covering can be created by using a subdivision scheme as described in [1]. The dynamics on the such discretized phase space can be approximated in terms of a transition matrix $P_{\mathcal{B}}$, whose entries are the transition probabilities between the boxes:

$$P_{\mathcal{B}} = (p_{ij}), \quad \text{where} \quad p_{ij} = \frac{m(f^{-1}(B_i) \cap B_j)}{m(B_j)}, \quad 1 \le i, j \le b. \tag{1}$$

Therefore, our goal in the discretized setting is to solve the following problem with μ being the natural invariant measure on $\mathcal{B}$.

Problem 2 (Boxes) *For some fixed* $p \in \mathbb{N}^+$ *find a collection of pairwise disjoint sets* $\mathcal{S} = \{S_1, \ldots, S_p\}$ *with* $\bigcup_{1 \le i \le p} S_i = \mathcal{B}$ *and* $\mu(S_k) > 0$, $1 \le i \le p$, *such that*

$$\rho(\mathcal{S}) = \frac{1}{p}\sum_{k=1}^{p} \rho(S_k) = \frac{1}{p}\sum_{k=1}^{p} \frac{\sum_{B_i, B_j \subset S_k} p_{ij} \cdot \mu(B_j)}{\sum_{B_j \subset S_k} \mu(B_j)} \to \max \ .$$

The optimization problem 2 can be translated into the question of finding an optimal cut in a graph. Let $G = (V, E)$ be a graph with vertex set $V = \mathcal{B}$ and directed edge set $E = E(\mathcal{B}) = \{(B_1, B_2) \in \mathcal{B} \times \mathcal{B} : f(B_1) \cap B_2 \neq \emptyset\}$. The function $vw : V \to \mathbb{R}$ with $vw(B_i) = \mu(B_i)$ assigns a weight to the vertices and the function $ew : E \to \mathbb{R}$ with $ew((B_i, B_j)) = \mu(B_i)p_{ji}$ assigns a weight to the edges. Clearly, a partition of $\mathcal{B}$ corresponds to a partition of V and vice versa. One can easily model the problem as a graph partitioning problem minimizing the *internal costs* of a partition S as following.

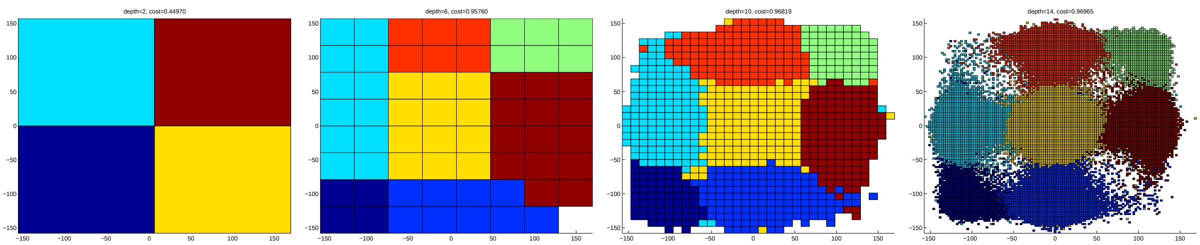
Problem 3 (Graph) *For some fixed* $p \in \mathbb{N}^+$ *find a collection of pairwise disjoint sets* $\mathcal{S} = \{S_1, \ldots, S_p\}$ *with* $\bigcup_{1 \le i \le p} S_i = V$ *and* $vw(S_i) > 0$, $1 \le i \le p$, *such that*

$$\rho(\mathcal{S}) = C_{int}(\mathcal{S}) = \frac{1}{p}\sum_{i=1}^{p} \frac{\sum_{(v,w) \in E; v,w \in S_i} ew(\{v, w\})}{\sum_{v \in S_i} vw(v)} \to \max \ . \tag{2}$$

Both, the construction of the sets as box coverings as well as the most efficient graph partitioning heuristics exhibit approaches based on multilevel strategies. The hierarchical set oriented approach provides a natural multilevel structure [1, 2]. Here, starting with one large box on an initial level, the boxes are subdivided from one level to the next one until a desired status of detail is achieved. Note that the structure of the box covered sets progresses from a coarse to a fine resolution. Additionally, the most efficient graph partitioning approaches take massively use of the multilevel graph partitioning paradigm. Here, the initial level consist of the graph which is then coarsened on each further level by simultaneously and independently contracting some vertex sets until a small number of vertices is achieved. After partitioning of this small graph the partition is then projected back on the graphs on the same levels until a partition of the initial graph is achieved. Note that the structure of the graph progresses from a fine to a coarse and then back to a fine resolution.

So far, the multilevel structures of the set oriented approach and the multilevel structure of the graph partitioning approach have been used independently. In this research we interlock both multilevel structures in the following way. Starting with an initial box collection $\mathcal{B}_0$ consisting only of one box which covers our focus of interest, we perform four steps on each level k, $k \ge 1$. First, we subdivide the boxes of $\mathcal{B}_{k-1}$ and select boxes to obtain $\mathcal{B}_k$. Second, we compute the transition matrix P_k and the measure μ_k. Third, we project $\mathcal{S}_{k-1}$ to a partition $\mathcal{S}_k$ of $\mathcal{B}_k$. Fourth, we locally optimize $\mathcal{S}_k$ with respect to C_{int}.

We illustrate the approach with an example which is a Hybrid Monte Carlo simulation of a Pentane at a temperature of 300K, see [7, 5]. Here we consider a time series with respect to the torsion angles in order to identify distinct conformations of the molecule. The time series had been produced in advance using the HMC Toolbox [8]. Based on the entries in the times series we are then able to produce box coverings on prescribed levels of refinement and the transition matrices. So, we are working with the same time series all the time. The resulting graphs are partitioned into seven almost invariant sets. The figure shows the boxes on different levels with boxes/vertices of the same part having identical colors.



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