PARALLEL COMPUTATION OF FIXED POINTS ON NETWORKS OF NONLINEAR ODE

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SIAM Workshop on Network Science 2020
July 9–10 · Toronto

Summary

Fixed points of nonlinear network dynamics are important for determining asymptotic behavior of many real world dynamical systems. As network data becomes larger and the ability to parallelize numerical methods continues to define their scalability it consequently becomes necessary to develop parallel methods for numerical integration of network dynamics. We introduce a parallel algorithm for numerically integrating homogeneous nonlinear ordinary differential equations on networks.

Abstract

The problem of calculating fixed points of networks running homogeneous ordinary differential equations is broadly applicable to research including epidemic spreading [7], gene regulatory dynamics [1], and ecological dynamics [6]. While parallel methods for numerically integrating systems of ordinary differential equations exist [2][3] they require finite time windows and are not ideal for determining asymptotic fixed points. We introduce the general form of the equations considered here on the N-node graph $G = (V, E)$, also considered in [4][5].

$$\dot{x}_k(t) = f(x_k(t)) + \sum_{j=1}^{N} A_{kj} g(x_k(t), x_j(t)) \qquad (1)$$

Here $x_k(t)$ is the state of node k at time step t, and A_{kj} is the k-j^{th} entry of the network's adjacency matrix. $f(x_k(t))$ and $g(x_k(t), x_j(t))$ are non linear functions defined over the states of nodes in the network.

Our implementation relies on a mean field approximation of the network dynamics given in [5] to initially approximate long term behavior at the boundary of each compute rank allowing the ranks to evolve towards a steady state in parallel without the need for communication. Our method then uses multiple rounds of message passing to improve the initial fixed point estimates from each rank. We apply Euler's method for our implementation and provide evidence that this method recovers the true steady state of homogeneous network dynamics given a sufficient number of message passing rounds. This method entails applying an averaging operator over the system to reduce the system of N equations to one. Then the ambient network behavior outside of our considered subset is approximated by the steady state of this reduced system, which they refer to as x_{eff}. The reduced system takes the following form.

$$\dot{x} = f(x) + \beta g(x, x) \qquad (2)$$

Here β is the network resilience in the case of undirected networks, and the initial value of x is the degree weighted average of the initial node states on the network. We use this approximation to decouple each rank in our system allowing them to converge near their true serially computed steady states. Computationally, for this we consider each rank to be converged once two iterations are within some L_1 distance threshold ϵ of each other. While this initial estimate is relatively accurate it can be drastically improved by subsequently exchanging information between ranks. The process of converging and passing information is then repeated for increased accuracy.

Here we present accuracy results on two network test suites of 20 networks each. The sizes of these networks range between 100 and 2000 nodes. The networks consist of 20 Erdos Renyi random graphs with probability of connection $p = 0.05$ and 20 Barabási Albert networks with $m = 2$. On these networks we run two different systems of equations.

$$\dot{x}_k = -Bx_k^f + \sum_j A_{kj} R \frac{x_k^h}{x_k^h + 1} \qquad (3)$$

$$\dot{x}_k = -Bx_k + \sum_j A_{kj} R(1 - x_k) x_j \qquad (4)$$

System (3) arises from regulatory systems and gene expression [1], (4) arises from epidemic spreading processes [7].

In figure 1 and figure 2 we present the results from the basic meanfield approach where no additional iteration is done on each rank along with the results after ten additional converging iterations are done on each rank. The error ε we calculate is proportional to the serially calcu-

lated steady state $\mathbf{x}^*$ of the system given the initialization.

$$\varepsilon = \sum_{k=1}^{N} |\frac{x_k(t)}{x_k^*}| \tag{5}$$

We can see that the error is small for the tests with ten iterations of message passing to convergence. Furthermore a single round of computation to convergence without any message passing is low as well. Our results with respect to the basic meanfield approach mirror those expected from previous work [5] and our results adding additional iterations improve significantly upon them.

We also present scaling properties in figure 3 on a test suite of networks obtained from the Koblenz network repository. These networks range in size and homogeneity and we observe power law scaling. This suggests promising scalability for large networks.

Our data suggests significant accuracy when estimating steady states, however there is a discrepancy in performance between different network topologies. Further research estimating the error of this method on networks with varying parameters such as assortativity will be necessary in order to apply it to larger networks where serially computed fixed points can not be used for validation. Similarly, our data also suggests that the choice of equation affects error which is also worth further experimentation and analysis.

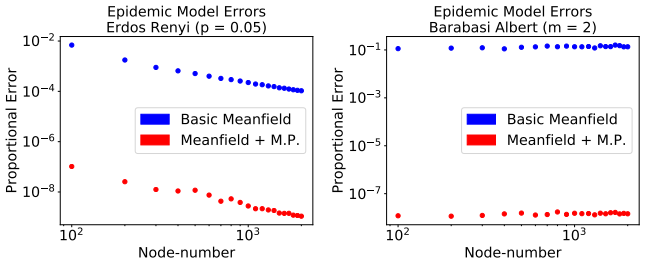

Figure 1: Error results for epidemic dynamics using the meanfield method (blue) and the meanfield method with message passing (red) for 20 random graphs with parameter $p = 0.05$ and 20 Barabási Albert networks with parameter $m = 2$. Meanfield plus message passing is iterated 10 times.

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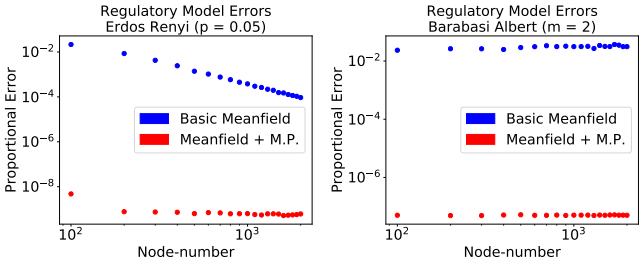

Figure 2: Error results for regulatory dynamics using the meanfield method (blue) and the meanfield method with message passing (red) for 20 random graphs with parameter $p = 0.05$ and 20 Barabási Albert networks with parameter $m = 2$. Meanfield plus message passing is iterated 10 times.

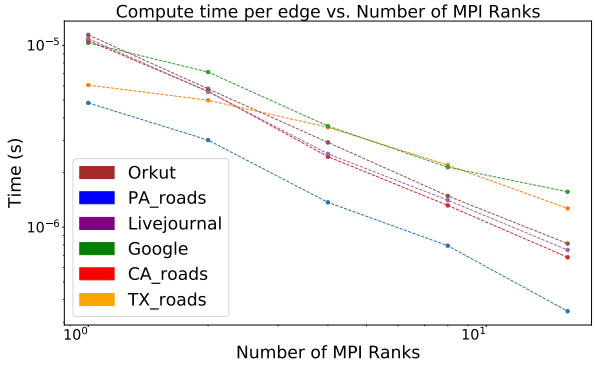

Figure 3: Computation time per edge versus the number of available MPI ranks are shown. Tests were run in serial up to 16 MPI ranks in subsequent powers of two. We see a clear power law scaling relationship on the test suite obtained from Koblenz.

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