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# Equation-free analysis of agent-based models and systematic parameter determination

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## HIGHLIGHTS

- A systematic method to determine computational parameters for equation-free continuation.
- A simple and robust variance based procedure for root finding in stochastic systems.
- An equation-free tool that can interface with generic simulators and models.
- An equation-free continuation algorithm for agent-based models.
- Application of our continuation algorithm to examples in NetLogo.

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## ABSTRACT

Agent based models (ABM)s are increasingly used in social science, economics, mathematics, biology and computer science to describe time dependent systems in circumstances where a description in terms of equations is difficult. Yet few tools are currently available for the systematic analysis of ABM behaviour. Numerical continuation and bifurcation analysis is a well-established tool for the study of deterministic systems. Recently, equation-free (EF) methods have been developed to extend numerical continuation techniques to systems where the dynamics are described at a microscopic scale and continuation of a macroscopic property of the system is considered. To date, the practical use of EF methods has been limited by; (1) the over-head of application-specific implementation; (2) the laborious configuration of problem-specific parameters; and (3) large ensemble sizes (potentially) leading to computationally restrictive run-times.

In this paper we address these issues with our tool for the EF continuation of stochastic systems, which includes algorithms to systematically configuration problem specific parameters and enhance robustness to noise. Our tool is generic and can be applied to any 'black-box' simulator and determines the essential EF parameters prior to EF analysis. Robustness is significantly improved using our convergence-constraint with a corrector-repeat ($C^3R$) method. This algorithm automatically detects outliers based on the dynamics of the underlying system enabling both an order of magnitude reduction in ensemble size and continuation of systems at much higher levels of noise than classical approaches.

We demonstrate our method with application to several ABM models, revealing parameter dependence, bifurcation and stability analysis of these complex systems giving a deep understanding of the dynamical behaviour of the models in a way that is not otherwise easily obtainable. In each case we demonstrate our systematic parameter determination stage for configuring the system specific EF parameters.



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## 1. Introduction and motivation

Agent-based models (ABMs), also known as individual-based models, consist of individual entities (agents) which move and interact with each other according to a defined set of rules. They are increasingly used to model complex systems, where it is difficult to write down an explicit system-level description of macroscopic behaviour, and have been used in a wide range of disciplines such as social science and psychology [1,2], mathematics and network theory [3], policy making and economics [4–6], computer science [7–9] and biology [10–12]. Their increasing popularity has spawned a number of software packages specifically designed for the non-mathematicians/computer scientists to be able to construct their own ABM, for example SWARM [13] and NetLogo [14].

One significant challenge with ABMs is developing a systematic understanding of their behaviour; see Ref. [15] for a review. ABMs are typically stochastic in nature as a result of probabilistic interaction rules. Consequently, model behaviour is usually understood through repeatedly running simulations. Several analysis tools that aggregate repeated simulations are available but none can perform detailed analysis, if at all, on the macroscopic behaviour of a system. Moreover, popular tools such as `BehaviourSpace` [14] and MEME (http://mass.aitia.ai) perform parameter sweeps and multiple simulation runs, though the analysis must be performed in an external program; see Ref. [16] for a review. Others such as smartPLS (http://www.smartpls.de/) are designed for model verification rather than analysis of the dynamics.

Given the large number of parameters that are frequently embedded in the rules within an ABM, a repeated simulation approach is both time-consuming and inappropriate for some tasks [17]. The fact that the interaction rules at the microscopic (agent) level often lead to macroscopic (emergent) behaviour of the system as a whole, suggests that an alternative way to establish systematic ABM analysis is with the use of path-following techniques.

Numerical continuation (path-following) and bifurcation methods are well-established in their value in understanding deterministic systems and have been applied to problems in physics, chemistry, biology and engineering [18–23]. The ethos of path-following is fundamentally different from simulation. For example, consider an initial value problem defined by a map of the form

$$x^{n+1} = f(x^n, \lambda), \quad x \in \mathbb{R}^m, \ \lambda \in \mathbb{R}^p, \tag{1.1}$$

with $x^0 = a$, where $x^n$ describes the state at time $t_n$ and $\lambda$ are model parameters. A simulation approach involves starting at $t_0$ with $x^0 = a$ and iterating the map (1.1) to find a numerical approximation for the solution at $t_n$. Over time, for well-posed problems, the solution will evolve to a stable, attracting state which may be stationary, periodic or exhibit more complex dynamics such as chaos. For nonlinear maps, different attracting states may be observed for the *same* parameters but different *initial* conditions. Consequently, in order to build up a systematic description of system behaviour it is necessary to run multiple simulations—varying both parameters and initial conditions.

In a numerical continuation approach, the focus is typically on stationary (or periodic) solutions. In the case of stationary solutions, rather than time evolving to find $x^n$, stationary solutions to Eq. (1.1) are found by solving

$$\tilde{x} = f(\tilde{x}, \lambda), \tag{1.2}$$

for $\tilde{x}$. Having found a solution for one particular set of parameter values, the solution is 'followed' by stepping in parameters. This is both faster than stepping in the parameter and repeatedly finding stationary solutions using simulation, and has the advantage that both stable and unstable solutions can be found. While it is easy to think that unstable solutions are irrelevant as they are never seen as the direct outcome of a simulation, in fact they play an important part in the underpinning dynamical structure of a problem. The position of unstable solutions can explain the reason why different initial conditions lead to different results, and the presence of unstable stationary solutions is often observed in the transient behaviour of solutions. Moreover, the combination of stable and unstable branches at regime boundaries can explain behaviours such as tipping points, where stable solutions appear to 'vanish' as a parameter is slowly varied.

Typical numerical bifurcation packages for deterministic systems not only follow stationary and periodic solutions, but also detect changes in stability at each point along the solution branch [24,25]. Such changes are indicative of a bifurcation [26] where there are qualitative changes in the dynamics of the system. At bifurcations, new solutions can branch from the original, as occurs in transcritical or pitchfork bifurcations, or solutions may collide with each other and vanish, as occurs in saddle–node bifurcations (tipping points) [27]. Numerical methods have been constructed that allow for the automated switching from the current solution path to a bifurcating branch through perturbation [24], without the need to know the exact location of the bifurcation point [28]. Several packages exist for deterministic continuation, such as AUTO [29], XPPAUT [30], CONTENT [31], MATCONT [32] and DDE-BIFTOOL [33], all of which use similar algorithms [34] and contain bifurcation detection and branch switching functions.

Although continuation methods have been extensively used for deterministic systems, their application to stochastic systems is much more limited [25]. In the particular case of systems where a microscopic description of the system exists, but there is no equation for the macroscopic state, *equation-free* (EF) techniques [35] can be used to perform continuation of the system. These are based on the same principles as continuation for deterministic systems but the differential equations are replaced by an ensemble of appropriately initialised microscopic simulations and instead of following stationary solutions of the differential equation, stationary values of a representative statistic(s) are sought [20]. EF methods have been used as a platform for numerical continuation for a number of systems including: the FitzHugh–Nagumo and Lattice–Boltzmann