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Chaos in eigenvalue search methods

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ABSTRACT

Eigenvalue searches for multiplying systems emerge in several applications, encompassing the determination of the so-called alpha eigenvalues associated to the asymptotic reactor period and the adjustment of albedo boundary conditions or buckling in assembly calculations. Such problems are usually formulated by introducing a free parameter into a standard power iteration, and finding the value of the parameter that makes the system exactly critical. The corresponding parameter is supposed to converge to the sought eigenvalue. In this paper we show that the search for the critical value of the parameter might fail to converge for deep sub-critical systems: in this case, the search algorithm may undergo a series of period doubling bifurcations (leading to a multiplicity of solutions) instead of converging to a fixed point, or it may even crash. This anomalous behaviour is explained in terms of the mathematical structure of the search algorithm, which is shown to be closely related to the well-known logistic map for a few relevant applications illustrated in the context of the rod model. The impact of these findings for real-life applications is discussed, and possible remedies are finally suggested.

1. Introduction

A large class of problems emerging in nuclear reactor physics involve searching for the stationary state of a multiplying system by adjusting a control parameter (Bell and Glasstone, 1970; Azmy and Sartori, 2010). Examples include for instance the determination of the value of boron dilution or the control rod position that make the reactor exactly critical, all the other system parameters being kept constant. Similar searches are quite common also outside the realm of reactor control. Consider, for instance, the determination of the equilibrium temperature profile of reactor cores with thermal–hydraulics feedback (Cacuci, 1993; March-Leuba et al., 1984). The stationary solution of the coupled problem may be sought by alternatively iterating neutron transport and thermal–hydraulics solvers until they converge to a fixed point. There are no external control parameters in this case, but the temperature field may be seen to play the role of an adjustable parameter, whose shape at convergence makes the reactor critical. Other examples of *critical parameter searches* with iterative solution schemes arise in the context of the determination of the albedo at the core boundaries (Cho et al., 2009; Yun and Cho, 2010) or in reactor period calculations (Azmy and Sartori, 2010; Zoia et al., 2015; Nauchi, 2014).

Although inspired by their real-life counterparts (see, e.g., (Cacuci, 1993; March-Leuba et al., 1984)), for the purpose of this paper we will regard critical parameter searches as mathematical problems: we will assume that the reactor state can be described by the k-eigenvalue form of the linear Boltzmann equation (Goad and Johnston, 1959; Lewis and Miller, 1984; Lux and Koblinger, 1991), with a single free control parameter p. The presence of multiple control parameters, and the possible interactions between each other due to coupling mechanisms, will be neglected. For any value of p, there will be a spectrum $\sigma_p[k]$ of eigenvalues associated to the Boltzmann equation: starting from an arbitrary initial condition, the reactor will ultimately relax to its fundamental mode $\varphi_{k_0(p)}$, with associated fundamental eigenvalue $k_0(p)$. Both $\varphi_{k_0(p)}$ and $k_0(p)$ depend on the control parameter p. Formally speaking, the critical solution is usually sought by introducing iterative update schemes for the control parameter: the k-eigenvalue equation is solved for the fundamental eigenvalue $k_0(p)$ for a given p (for instance by power iteration), then p is progressively adjusted based on the value $k_0(p)$. If such a scheme ultimately converges to a fixed point, with corresponding fundamental eigenvalue $k_0(p) = k_0(p_c) = 1$, the resulting value of the control parameter is the sought solution $p = p_c$ that makes the system exactly critical.

One may be tempted to assume that such iterative schemes always converge to the fixed point $\{p = p_c, k_0(p_c) = 1\}$, assuming of course that it exists. Clearly, though, if the initial conditions of the iterative scheme are poorly chosen, the search may diverge or enter non-physical regions of the search space. Under these

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conditions, the fixed point p_c is never attained. However, even if a solution exists and suitable initial conditions are selected, the iterative scheme may still fail to converge.

In the context of reactor physics, the failure of the convergence to a fixed point has been first documented for the evolution of the neutron population in the presence of thermal–hydraulics feedback: in a series of pioneering works, the emergence of a chaotic behaviour via period-doubling bifurcations has been theoretically and numerically investigated, especially in relation to boiling water reactors (Cacuci, 1993; March-Leuba et al., 1984).

This phenomenon has been repeatedly observed and is widely documented also in the literature related to the numerical determination of the asymptotic reactor period (the so-called $\alpha - k$ iteration). For instance, simple iterative schemes for α eigenvalue search lead to abnormal code termination in sub-critical configurations (Hill, 1983). The same issue was later reported by many authors, and effective solutions have been proposed by resorting to operator or eigenvalue shifting techniques (Yamamoto and Miyoshi, 2003; Ye et al., 2006; Zoia et al., 2014, 2015).

It is perhaps worth observing that critical parameter searches are essentially root-finding problems for numerical functions. Thus, the whole apparatus of numerical root-finding methods can be in principle brought to bear in order to determine the value of the parameter p that makes the reactor critical. Many root-finding algorithms do guarantee convergence under weak assumptions. For instance, the class of bracketing methods (such as the bisection method or the *regula falsi* method) guarantee convergence if the initial conditions are suitably chosen (Traub, 1964; Householder, 1970; Ortega and Rheinboldt, 1970). However, it is not straightforward to apply bracketing methods to stochastic root-finding problems (Pasupathy and Kim, 2011).

The purpose of this paper is to provide insight into the reasons why some iterative schemes for criticality searches may fail to converge to the fixed-point solution, even when the latter exists and even when the search is seeded with appropriate initial conditions. While this paper addresses these questions in the framework of deterministic numerical solvers for the fundamental eigenvalue $k_0(p)$ and for the adjustment of the control parameter p, we actually also have in mind possible applications to eigenvalue searches with Monte Carlo codes. In this case, $k_0(p)$ is determined by the stochastic implementation of power iteration (by running a large number of cycles corresponding to successive neutron generations) and p is updated at the end of each cycle. In view of this consideration, we will mostly focus on update rules for p simple enough to depend on the value of $k_0(p)$ at the current cycle, without the need of storing in memory the past cycles. For the same reason, we will not consider methods based on derivatives of $k_0(p)$, which cannot be straightforwardly estimated in Monte Carlo schemes.

This paper is organized as follows. In Section 2 we begin by introducing the required notation and providing the general mathematical setup for eigenvalue searches. In particular, we will show that these problems can be formally recast into a discrete dynamical system, whose equilibrium point is the sought solution. In Section 3 we will provide a few numerical illustrations of eigenvalue searches in the context of the rod model, a simple system involving mono-energetic neutron transport. A broad class of eigenvalue problems associated to the rod model will be examined. We will show in particular under which conditions these searches may fail to converge, and display instead an oscillatory or even chaotic behaviour. Then, in Section 4 we will show that the mechanisms that lead to the failure of the eigenvalue search have a universal character (whose origins will be elucidated) and might thus more broadly emerge in real-life applications. Some remedies especially conceived in order to regularize the eigenvalue searches and possibly suppress the route to instabilities and chaos will be proposed and numerically tested in Section 5. Conclusions will be finally drawn in Section 6.

2. Definitions and notation

To fix the ideas, let us assume that the state of the reactor can be characterized in terms of the k-eigenvalue form of the linear Boltzmann equation, namely,

$$\begin{cases} \mathcal{L}\varphi_k = \frac{1}{k}\mathcal{F}\varphi_k, \\ \text{B.C.on}\varphi_k \end{cases} \tag{1}$$

where $\varphi_k = \varphi_k(\mathbf{x}, \mathbf{\Omega}, E)$ are the eigenfunctions of the angular neutron flux and k the associated eigenvalues,

$$\mathcal{L} = \mathbf{\Omega} \cdot \nabla_{\mathbf{x}} + \Sigma_t(\mathbf{x}, E) - \int d\mathbf{\Omega}' \int dE' \Sigma_s(\mathbf{x}, E') f_s(\mathbf{\Omega}', E' \to \mathbf{\Omega}, E) \tag{2}$$

is the net disappearance operator, with Σ_t the total cross section, Σ_s the scattering cross section, and f_s the scattering kernel, and

$$\mathcal{F} = \frac{\chi_f(E)}{4\pi} \int d\mathbf{\Omega}' \int dE' \nu_f(E') \Sigma_f(\mathbf{x}, E') \tag{3}$$

is the fission operator, with Σ_f the fission cross section, ν_f the average number of fission neutrons, and χ_f the fission spectrum (Bell and Glasstone, 1970). Boundary conditions (B. C.) on φ_k must be also assigned for Eq. (1). Although the existence of a dominant discrete eigenvalue k_0 with real part larger than those of all other eigenvalues in the spectrum $\sigma[k]$ and with non-negative associate eigenfunction φ_{k_0} has not been proven for arbitrary operators $\mathcal{L}$ and $\mathcal{F}$, domain shapes and boundary conditions, under rather mild assumptions it is reasonable to assume that the fundamental eigenpair $\left\{\varphi_{k_0}, k_0\right\}$ exists (Lewis and Miller, 1984; Lux and Koblinger, 1991). This means that the neutron population in the core, starting from arbitrary initial conditions, will eventually relax to a phase space distribution proportional to φ_{k_0}, and k_0 will asymptotically yield the ratio between population sizes at two successive generations. If $k_0 > 1$ the population will diverge; if $k_0 < 1$ the population will shrink; and if $k_0 = 1$ the population will stay constant, which precisely defines the critical state.

In many practical applications, one is only interested in determining the asymptotic behaviour of the core, the precise shape of the spectrum $\sigma[k]$ being of lesser importance. In this case, a widely adopted technique for assessing the dominant eigenpair $\left\{\varphi_{k_0}, k_0\right\}$ of Eq. (1) is the power iteration (Lewis and Miller, 1984; Lux and Koblinger, 1991). This method requires an ansatz $\varphi_k^{(0)}$ for the angular flux, and eventually converges to $\left\{\varphi_{k_0}, k_0\right\}$ by iterated application of the update rule

$$\varphi_k^{(n+1)} = \frac{1}{k^{(n)}} \mathcal{L}^{-1} \mathcal{F} \varphi_k^{(n)}, \tag{4}$$

with $k^{(n)} = |\varphi_k^{(n)}|/|\varphi_k^{(n-1)}|$ and $k^{(0)} = 1$, and the same boundary conditions as in Eq. (1). For sufficiently large n, the eigenvalue $k^{(n)}$ converges to k_0 as $k^{(n)} \simeq k_0 + c\left(\frac{k_1}{k_0}\right)^n + \cdots$, where c is a problem-dependent constant and k_1 is the eigenvalue corresponding to the first excited eigenmode. Correspondingly, the function $\varphi_k^{(n)}$ converges to the fundamental eigenmode φ_{k_0}. The power iteration scheme given in Eq. (4) can be solved by either deterministic or Monte Carlo methods (Lewis and Miller, 1984; Lux and Koblinger, 1991).