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Fast solvers for optimal control problems from pattern formation

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ABSTRACT

The modeling of pattern formation in biological systems using various models of reaction–diffusion type has been an active research topic for many years. We here look at a parameter identification (or PDE-constrained optimization) problem where the Schnakenberg and Gierer–Meinhardt equations, two well-known pattern formation models, form the constraints to an objective function. Our main focus is on the efficient solution of the associated nonlinear programming problems via a Lagrange–Newton scheme. In particular we focus on the fast and robust solution of the resulting large linear systems, which are of saddle point form. We illustrate this by considering several two- and three-dimensional setups for both models. Additionally, we discuss an image-driven formulation that allows us to identify parameters of the model to match an observed quantity obtained from an image.

1. Introduction

One of the fundamental problems in developmental biology is to understand how spatial patterns, such as pigmentation patterns, skeletal structures, and so on, arise. In 1952, Alan Turing [42] proposed his theory of pattern formation in which he hypothesized that a system of chemicals, reacting and diffusing, could be driven unstable by diffusion, leading to spatial patterns (solutions which are steady in time but vary in space). He proposed that these chemical patterns, which he termed morphogen patterns, set up pre-patterns which would then be interpreted by cells in a concentration-dependent manner, leading to the patterns that we see.

These models have been applied to a very wide range of areas (see, for example, Murray [27]) and have been shown to exist in chemistry [6,30]. While their applicability to biology remains controversial, there are many examples which suggest that Turing systems may be underlying key patterning processes (see [2,8,40] for the most recent examples). Two important models which embody the essence of the original Turing model are the Gierer–Meinhardt [14] and Schnakenberg models [39] and it is upon these models which we focus.[1] In light of the fact that, to date, no Turing morphogens have

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[1] Although the second model is commonly referred to as the Schnakenberg model, it was actually first proposed by Gierer and Meinhardt in [14] along with the model usually referenced as the Gierer–Meinhardt model – we therefore refer to the first and second models as '*GM*1' and '*GM*2' within our working.

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been unequivocally demonstrated, we do not have model parameter values so a key problem in mathematical biology is to determine parameters that give rise to certain observed patterns. It is this problem that the present study investigates.

More recently, an area in applied and numerical mathematics that has generated much research interest is that of PDE-constrained optimization problems (see [41] for an excellent introduction to this field). It has been found that one key application of such optimal control formulations is to find solutions to pattern formation problems [11,12], and so it is natural to explore this particular application here.

In this paper, we consider the numerical solution of optimal control (in this case parameter identification) formulations of these Turing models – in particular we wish to devise preconditioned iterative solvers for the matrix systems arising from the application of Newton and Gauss–Newton methods to the problems. The crucial aspect of the preconditioners is the utilization of saddle point theory to obtain effective approximations to the $(1,1)$-block and Schur complement of these matrix systems. The solvers incorporate aspects of iterative solution strategies developed by the first and second authors to tackle simpler optimal control problems in literature such as [32–35].

This paper is structured as follows. In Section 2 we introduce the Gierer–Meinhardt ($GM1$) and Schnakenberg ($GM2$) models that we consider, and outline the corresponding optimal control problems. In Section 3 we discuss the outer (Newton-type) iteration that we employ for these problems, and state the resulting matrix systems at each iteration. We then motivate and derive our preconditioning strategies in Section 4. In Section 5 we present numerical results to demonstrate the effectiveness of our approaches, and finally in Section 6 we make some concluding remarks.

2. A parameter identification problem

Parameter identification problems are crucial in determining the setup of a mathematical model, often given by a system of differential equations, that is best suited to describe measured data or an observed phenomenon. These problems are often posed as PDE-constrained optimization problems [20,41]. We here want to minimize an objective function of misfit type, i.e., the function is designed to penalize deviations of the function values from the observed or measured data. The particular form is given by [11,12]:

$$\begin{aligned}\mathcal{J}(u,v,a,b) = {} & \frac{\beta_1}{2}\,\|u(\mathbf{x},t)-\widehat{u}(\mathbf{x},t)\|^2_{L_2(\Omega\times[0,T])} + \frac{\beta_2}{2}\,\|v(\mathbf{x},t)-\widehat{v}(\mathbf{x},t)\|^2_{L_2(\Omega\times[0,T])} \\ & + \frac{\beta_{T,1}}{2}\,\|u(\mathbf{x},T)-\widehat{u}_T(\mathbf{x})\|^2_{L_2(\Omega)} + \frac{\beta_{T,2}}{2}\,\|v(\mathbf{x},T)-\widehat{v}_T(\mathbf{x})\|^2_{L_2(\Omega)} \\ & + \frac{\nu_1}{2}\,\|a(\mathbf{x},t)\|^2_{L_2(\Omega\times[0,T])} + \frac{\nu_2}{2}\,\|b(\mathbf{x},t)\|^2_{L_2(\Omega\times[0,T])}\,, \end{aligned} \tag{2.1}$$

where u, v are the *state variables*, and a, b the *control variables*, in our formulation. This is to say we wish to ensure that the state variables are as close as possible in the L_2-norm to some observed or desired states $\widehat{u}$, $\widehat{v}$, $\widehat{u}_T$, $\widehat{v}_T$, but at the same time penalize the enforcement of controls that have large magnitudes in this norm. The space–time domain on which this problem is considered is given by $\Omega\times[0,T]$, where $\Omega\subset\mathbb{R}^d$, $d\in\{2,3\}$.

Our goal is to identify the parameters of classical pattern formation equations such that the resulting optimal parameters allow the use of these models for real-world data. We here use models of reaction–diffusion type typically exploited to generate patterns seen in biological systems. The two formulations we consider are the $GM1$ model [14,27]:

$$\begin{aligned} u_t - D_u\Delta u - \frac{ru^2}{v} + au &= r, \quad \text{on } \Omega\times[0,T], \\ v_t - D_v\Delta v - ru^2 + bv &= 0, \quad \text{on } \Omega\times[0,T], \\ u(\mathbf{x},0)=u_0(\mathbf{x}), \quad v(\mathbf{x},0)&=v_0(\mathbf{x}), \quad \text{on } \Omega, \\ \frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} &= 0, \quad \text{on } \partial\Omega\times[0,T], \end{aligned} \tag{2.2}$$

and the $GM2$ model [14,27,39]:

$$\begin{aligned} u_t - D_u\Delta u + \gamma(u-u^2v) - \gamma a &= 0, \quad \text{on } \Omega\times[0,T], \\ v_t - D_v\Delta v + \gamma u^2v - \gamma b &= 0, \quad \text{on } \Omega\times[0,T], \\ u(\mathbf{x},0)=u_0(\mathbf{x}), \quad v(\mathbf{x},0)&=v_0(\mathbf{x}), \quad \text{on } \Omega, \\ \frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} &= 0, \quad \text{on } \partial\Omega\times[0,T], \end{aligned} \tag{2.3}$$

where r and γ are non-negative parameters involved in the respective models.

Both the $GM1$ and $GM2$ formulations are models of reaction–diffusion processes occurring in many types of pattern formation and morphogenesis processes [14,27,39]. The $GM1$ model relates to an "activator–inhibitor" system, whereas the $GM2$ model represents substrate-depletion. Within both models the variables u and v, the state variables in our formulation, represent the concentrations of chemical products. The parameters D_u and D_v denote the diffusion coefficients – typically