Runge-Kutta discretizations of singularly perturbed gradient equations

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Abstract

We analyze Runge-Kutta discretizations applied to singularly perturbed gradient systems. It is shown in which sense the discrete dynamics preserve the geometric properties and the longtime behavior of the underlying ordinary differential equation. If the continuous system has an attractive invariant manifold then numerical trajectories started in some neighbourhood (the size of which is independent of the step-size and the stiffness parameter) approach an equilibrium in a nearby manifold. The proof combines invariant manifold techniques developed by Nipp and Stoffer for singularly perturbed systems with some recent results of the second author on the global behavior of discretized gradient systems. The results support the favorable behavior of ODE methods for stiff minimization problems

1 Introduction

Dynamical systems with a gradient structure occur quite naturally when modelling systems that show a constant decay of some energy function. They also occur as auxiliary systems for minimization problems when searching for trajectories that approach a minimum. It is well known that the ω-limit sets of orbits in gradient systems consist of equilibria and the connecting orbits between them, see e.g. Hirsch, Smale (1974). In addition, these equilibria together with their unstable manifolds determine the general structure of the global attractor, see e.g. Hale and Raugel (1989).

Despite this seemingly simple situation gradient systems can show a rich transient and asymptotic behavior. Further analytic treatment of the systems is often impossible and

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numerical simulations become important in gaining a deeper understanding of the global behavior. Here the question arises which qualitative properties of the system are preserved by a numerical method. Some results about discretized gradient systems can be found for one-step methods in Stuart and Humphries (1994), (1996), Schropp (1995) and for linear multistep methods in Schropp (1997).

These results apply to nonstiff situations. In this paper we will treat the stiff gradient case. Such stiff systems occur quite often when the function f in the gradient system $\dot{x} = -\nabla f(x)$ arises from a highly nonlinear unconstrained minimization problem (see e.g. Schropp (1995), Schropp (1997)). In such a case the norm of the Jacobian typically becomes large, the allowed step sizes in the results of Humphries, Stuart (1994), Schropp (1995) tend to zero and the corresponding convergence theorems become useless for practical purposes.

In the present paper we analyze the behavior of Runge-Kutta discretizations applied to gradient equations of singular perturbation type. We prove global convergence of numerical trajectories for step sizes that are not restricted by the stiffness parameter. Moreover, the region of attraction will be a neighborhood of some invariant manifold that does not depend on both parameters.

We use the invariant manifold theorem of Nipp, Stoffer (1995) in order to reduce the discrete singularly perturbed problem to a parameter dependent regular problem. Our main result will then be obtained by a parameter dependent version of the global convergence properties for the nonstiff case, see Schropp (1995). Our results support the advantage of using stiff integrators on gradient systems for solving nonlinear least squares problems, see Schropp (1997). An illustrative example of this type will be given in section 2.

2 The main results

We consider a singularly perturbed autonomous system

$$\begin{aligned} \dot{x} &= f(x,y), \\ \epsilon\dot{y} &= g(x,y), \ 0 < \epsilon \ll 1 \end{aligned} \tag{2.1}$$

for $x \in \mathbb{R}^M$, $y \in \mathbb{R}^N$ and $\epsilon \in]0, \epsilon_0[$ of gradient type

$$f(x,y) \ := \ -\frac{\partial k}{\partial x}(x,y), \qquad g(x,y) \ := \ -\frac{\partial k}{\partial y}(x,y), \ \ k : \mathbb{R}^{M+N} \to \mathbb{R}. \tag{2.2}$$

Notice that (2.1) is in fact a gradient system as can be seen from the scaling

$$\xi = x, \quad \eta = \sqrt{\epsilon}y, \quad \kappa(\xi,\eta) = k(x, \frac{\eta}{\sqrt{\epsilon}}).$$

For the dynamical system (2.1) we assume the following

A1: The functions f, g are sufficiently smooth with globally bounded derivatives.