

Jet transport for General Linear methods

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Estudiem la tècnica computacional anomenada “jet transport” per a la família d'integradors numèrics coneguts com a mètodes Generals Lineals (GLM), que generalitzen els reconeguts mètodes multipas lineals (LMM) i Runge–Kutta (RK). El jet transport és l'aplicació de l'aritmètica de sèries de potències truncades a un integrador numèric per tal d'obtenir la solució de les equacions variacionals (EV); és a dir, les equacions diferencials lineals que compleixen les derivades de la solució d'un problema de valor inicial (PVI). En particular, es discuteix la seva implementació i aplicacions.

Keywords: numerical integration, variational equations, stiff problems.

Abstract

The main subject of this thesis is to discuss how to apply the computational technique called jet transport to the family of numerical integrators known as General Linear methods. We also give instructions for its correct computational implementation, present numerical examples and applications. The content is organized into three chapters:

In the first chapter, we introduce General Linear methods (GLM), which are used for the numerical integration of initial value problems (IVP)

$$y'(x) = f(y(x)), \quad y(x_0) = y_0.$$

The formulation of an s -stage r -step General Linear method, for certain coefficient matrices $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{s \times s}$, $\mathbf{U} = [u_{ij}] \in \mathbb{R}^{s \times r}$, $\mathbf{B} = [b_{ij}] \in \mathbb{R}^{r \times s}$, $\mathbf{V} = [v_{ij}] \in \mathbb{R}^{r \times r}$, is the following

$$Y_i^{[n]} = h \sum_{j=1}^s a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, \quad i = 1, \dots, s,$$

$$y_i^{[n]} = h \sum_{j=1}^s b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, \quad i = 1, \dots, r.$$

They are a natural generalization of the well-known Runge–Kutta (RK) and Linear Multistep methods (LMM), and thus they use the information of several previous steps as well as several stages (additional computations per step). Throughout the chapter, we study the properties of local error, order, convergence, stability, consistency and the linear stability for the three families (i.e., LMM, RK and GLM) and observe that those of GLM generalize those of LMM and RK methods. For further reference, see [1] and [3].

In the second chapter, we introduce jet transport for computing the numerical solution of the variational equations (VE); i.e., the linear differential equations that are satisfied by the derivatives (up to any order, with respect to the initial conditions) of the solution of an initial value problem (IVP). Denoting the solution of the IVP as $y(x; x_0, y_0)$ and its derivative with respect to the initial conditions as $V(x) := D_{y_0}y(x; x_0, y_0)$, the first order variational equations are

$$\begin{aligned}y'(x) &= f(x, y(x)), & y(x_0) &= y_0, \\V'(x) &= D_y f(x, y(x))V(x), & V(x_0) &= I.\end{aligned}$$

Jet transport is the application to a numerical integrator of the technique called automatic differentiation, which is based on the observation that the jet (set of derivatives) of a multivariate function is codified by its Taylor expansion, so that high order derivatives of a function can be computed by using the arithmetic of truncated power series, which can be implemented in a computer. Consequently, jet transport can be understood as the application of the arithmetic of truncated power series to a numerical integrator in order to obtain the solution of variational equations. For further reference, see [2] and [4].

The rest of the second chapter is devoted to the presentation of our two main contributions. First, we prove that the numerical integration with a GLM of an IVP with jet transport of any order is equivalent to the numerical integration with the same GLM of the VE of the same order. Second, we derive the expressions that the coefficients of the jets must satisfy for them to be solutions of implicit systems. This allows jet transport to be applied to implicit General Linear methods; that is, those GLM that have an implicitly defined integration step, and which are of great utility in solving the so-called “stiff” problems.

The third chapter concludes the project by discussing the implementation and applications of the contents developed in the previous chapters. Given the complexity of GLM, we limit ourselves to presenting an efficient implementation of Runge–Kutta methods (both explicit and implicit) with jet transport. To show its applications, we use this implementation to determine the periodic orbit and the period of the van der Pol problem (which depends on a parameter that increases the stiffness of the problem). We also compute the power expansion of the Poincaré map of the periodic orbit with respect to the parameter.

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References

- [1] J.C. Butcher, General linear methods, *Acta Numerica* **15** (2006), 157–256.
- [2] J. Gimeno, À. Jorba, M. Jorba-Cuscó, N. Miguel, M. Zou, Numerical integration of high-order variational equations of ODEs, *Applied Mathematics and Computation* **442** (2023), 127743.
- [3] Z. Jackiewicz, *General Linear Methods for Ordinary Differential Equations*, Wiley, Hoboken, N.J., 2009.
- [4] À. Jorba, M. Zou, A Software Package for the Numerical Integration of ODEs by Means of High-Order Taylor Methods, *Experimental Mathematics* **14(1)** (2005), 99–117.