LINEARIZATION, DISCRETIZATION AND INTEGRATION IN VARIATIONAL FIELD THEORIES

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Abstract. We describe tools and techniques that allow to relate smooth variational principles to discrete ones, suitable for field theories that possess geometrical symmetries. We apply these objects to the generation of numerical integration schemes with energy preservation properties. The theory relies on the linearization of the geometrical configuration space using forward difference operators, the discretization of the space of independent variables using abstract cellular complexes, and the resolution of the Cauchy problem for a given initial conditions band, using the solution of several low-dimensional inverse optimization problems.

Introduction

In the present century there has been an extensive research on the construction of variational integrators for geometrical mechanical systems. These numerical schemes are used to integrate ordinary differential equations arising in mechanics, with a nice behavior regarding the symplectic structure and energy/momentum conservation laws of the mechanical system. These approaches don't follow a classical discretization of the differential equation that governs the trajectory $y(t)$ followed by the mechanical system, but rather a combined discretization of both the underlying geometrical structure on the configuration space Y and of the variational principle that characterizes these trajectories.

When one goes from mechanics (study of trajectories $y(t)$ modeled by a single independent "time" variable t) to the case of field theories (mappings $y(x)$ on several independent variables x), physically relevant fields $y(x)$ follow an specific variational principle. For physical reasons all principles and equations governing the system are invariant with respect to a given group of symmetries. Some of them can be used to reduce the number of dependent variables, and other ones lead to the identification of Noether conserved currents, which usually are presented as physical work-energy equilibrium laws.

General purpose numerical schemes for PDEs assume an affine structure on the dependent and independent variables, which may be useful to identify bounds of error propagation, but doesn't respect the physically relevant symmetries of the system under consideration, so that error bounds for energy or momentum frequently become too large. For field theories

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arising from a variational principle, better schemes are expected taking into consideration both numerical and geometrical aspects in the discretization.

As the geometrical elements arising in field theories carry symmetries that don't have affine nature, many of its fundamental properties disappear and one doesn't recover energy or momentum conservation, or work-energy equilibrium laws. This fact is already observed in geometrical mechanics, and can be controlled if one chooses appropriate linearization and discretization processes, so that the smooth variational principle with symmetries can be transformed into a new variational principle in a discrete space, preserving all the symmetries that were present in the original smooth model.

1. Linearization of geometrical structures

The most essential physical law of many field theories is not a system of partial differential equations, but the specific variational principle of least action that generates those equations. Physically observed fields are critical for a certain action functional $\mathbb{L}(y)$, obtained by integration on X of a Lagrangian density $L \cdot \mathrm{vol}$ that depends locally on $y(x)$. Usually the value of the Lagrangian density at any point $x \in X$ depends on the first order jet $j^1_x y$ of the mapping $y(x)$ at this point x. Higher order jets can be seen as first order jets of mappings with holonomy constraints. Any 1-jet $j^1_x y$ is a linear mapping $j^1_x y \colon T_x X \to T_y Y$ and comes from a linearization process of $y(x)$ at any point. The definition of Lagrangian density $L(j^1_x y)\,\mathrm{vol}_x$ on the space of 1-jets JY can be seen as a local linearization at x of the action $\mathbb{L}$.

A forward difference operator on a manifold Y is a mapping $\Delta \colon Y \times Y \to TY$ from a multi-point space to a tangent (vector) space, with specific properties. If such a linearization tool is chosen so that symmetries on Y commute with Δ, a symmetrical lagrangian density $L \cdot \mathrm{vol}$ generates a discrete Lagrangian function $L_d \colon Y^{\times n} \to \mathbb{R}$, defined on a multipoint space and preserving the symmetries of the original smooth Lagrangian given on the jet bundle JY. Difference operators can be used as fundamental tool to discretize Lagrangian density and, at the same time, allow for local measurements of error.

2. Discretization of fibered manifolds

As second step needed for the discretization of a variational principle, one may choose to substitute the action functional (integral of volume forms) depending on the smooth field by a discrete action functional (addition on discrete volume elements) of a discrete volume form locally depending on a discrete field.

Fields may differ by its geometrical nature. Some are scalar fields, but other ones are 1-forms, 2-forms, or densities (volume forms). A discretization process replaces arbitrary mappings $y(x)$ by a finite-dimensional subset of mappings, which may be characterized by its values at a finite number of points (the nodes of the discretization), or by its behaviour at a finite number of 1-cells, 2-cells ans son on.This can be done if we see the whole space X as composed of minimal (discrete) volume elements and work with minimal (discrete) line elements, surface elements, and so on. In many field theories the natural discrete analogue is that of an abstract cell complex.

We describe how a choice of cellular complex V, together with an immersion $x \colon V_0 \to X$ of its vertices as points on a manifold leads to notions of discrete bundles, and how to formulate discrete variational principles on such discrete bundles. We discuss then how a choice of forward difference operator relates differential calculus notions to discrete elements on a manifold and allows to create a discrete variational principle associated to a smooth one.

3. Integration of a discrete field

We review fundamental results of smooth variational theory that still hold on the discrete case, in particular the existence of discrete conserved quantities associated to its symmetries.

The problem of inverse optimization for a function $f(a, b)$ is the identification, for any value a, of the parameter b such that $f(x, b)$ takes minimum at the point a. In this section we relate the problem of integration of discrete Euler-Lagrange equations to a family of inverse optimization problems, and show how to apply this idea in the construction of variational integrators in field theories, with energy/momentum conservation properties.

The theory is illustrated with an example from elasticity theory.

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