Geometric Integration and Lie group methods, THREAD Network-wide training event 6

January 30, 2021

SECOND ASSIGNMENT. You have learned about discrete gradient methods for preserving invariants in ODEs. In this assignment you shall apply the same technique for a PDE. But it is then necessary to give some background information first. For a PDE, the first integral is usually an integral over the whole spatial domain of a function that depends not only on the solution $u(x,t)$, but also on its spatial derivatives, u_x, u_{xx} etc, so for instance with one space dimension we could have something like

$$H[u] = \int_{\mathbb{R}} G(u(x,t), u_x(x,t), u_{xx}(x,t), \ldots)\,\mathrm{d}x$$

What was in the ODE case the gradient of H is now replaced by the *variational derivative* $\frac{\delta H}{\delta u}$ which is defined through the relation

$$\frac{\partial}{\partial \varepsilon}\bigg|_{\varepsilon=0} H[u+\varepsilon v] = \left\langle \frac{\delta H}{\delta u}, v \right\rangle_{L^2}$$

Looking at the example

$$H[u] = \int_{\mathbb{R}} \left(\frac{1}{2}u_x^2 - u^3 \right)\,\mathrm{d}x \tag{1}$$

you may verify, using integration by parts and the fact that u must vanish at infinity

$$\frac{\delta H}{\delta u} = -u_{xx} - 3u^2 \tag{2}$$

The skew-symmetric matrix you saw in the ODE case has now been replaced by an operator which is skew-symmetric with respect to the L^2 inner product. For instance, one could choose

$$\mathcal{S} = \frac{\partial}{\partial x} \tag{3}$$

which is skew-symmetric with respect to the L^2 inner product. So we have arrived at the PDE itself, which is now written in the form

$$u_t = \mathcal{S}\,\frac{\delta H}{\delta u}. \tag{4}$$

Now, using the examples suggested above with invariant (1), and skew-symmetric operator (3), we would get, using (2) and (4), the KdV equation

$$u_t = -6uu_x - u_{xxx} \tag{5}$$

We shall be using the KdV equation as our case in this assignment. To make it simpler to implement, we also assume that we have periodic boundary conditions, i.e.

$$u(-L,t) = u(L,t), \quad \text{for all } t$$

and an initial condition of the form

$$u(x,0) = \frac{c}{2}\text{sech}^2(\frac{\sqrt{c}}{2}x)$$

Then the exact solution is $u(x,t) = \frac{c}{2}\text{sech}^2(\frac{\sqrt{c}}{2}(x-ct))$

Exercise. Let $\langle\cdot,\cdot\rangle_{\mathbb{R}^K}$ be the euclidean inner product.

1. Introduce a (uniform) grid in space $x_k = -L + k\Delta x$, $1 \leq k \leq K$, where $h = \frac{2L}{K}$.
2. Discretize the first integral H from (1) on this grid by
   (a) using a quadrature rule for the integral to get a discretization of the L_2 inner product (a rectangular rule is sufficiently accurate and gives $\Delta x\langle\cdot,\cdot\rangle_{\mathbf{R}^K} \approx \langle\cdot,\cdot\rangle_{L_2}$);
   (b) replacing the partial derivative in the integrand by finite difference quotients.

   The result is a function $H_d(\mathbf{u})$, where $\mathbf{u} \in \mathbb{R}^K$. For example, in the case of the discretization of the Hamiltonian of the KdV equation we have

$$H_d(\mathbf{u}) := \Delta x \sum_{j=1}^{K}\left[\left(\frac{u_{j+1}-u_j}{\Delta x}\right)^2 - u_j^3\right]$$

   $H_d : \mathbb{R}^K \to \mathbb{R}$, and introduce $\tilde{H}_d$ such that $H_d = \Delta x\, \tilde{H}_d$ for notational convenience.

3. Compute the variational derivative of the discrete Hamiltonian H_d with respect to the discrete L_2 inner product ($\Delta x\,\langle\cdot,\cdot\rangle_{\mathbb{R}^K} \approx \langle\cdot,\cdot\rangle_{L_2}$)

$$\begin{aligned}\frac{d}{d\epsilon}\bigg|_{\epsilon=0} H_d(u+\epsilon v) &= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \Delta x \sum_{j=1}^{K}\left[\left(\frac{u_{j+1}+\epsilon v_{j+1}-(u_j+\epsilon v_j)}{\Delta x}\right)^2 - (u_j+\epsilon v_j)^3\right] \\ &= \ldots \\ &= \Delta x\langle\nabla\tilde{H}_d, v\rangle_{\mathbb{R}^K}\end{aligned}$$

   where then $\nabla\tilde{H}_d$ is the usual gradient of $\tilde{H}_d$, and also $\nabla\tilde{H}_d$ is the variational derivative of H_d with respect to the discrete L_2 inner product (i.e. the sought approximation of the variational derivative $\frac{\delta H}{\delta u}$).

4. Discretize the operator $\mathcal{S}$ on the grid in such a way that a skew-symmetric matrix S is obtained.

5. You now solve the system of ODEs

$$\mathbf{u}_t = S\nabla\tilde{H}_d(\mathbf{u})$$

by an integral preserving method such as the AVF method

6. Implement this in MATLAB or Python or any other choice of programming language.

Suggested parameters: $K = 100$, $L = 10$, $c = 4$, $h = \Delta t = 0.05$.

To be handed in.

1. Document what you have done in 1–5 above, where you briefly describe how you have discretized H, your resulting H_d, write up the variational derivative of H_d with respect to the chosen discrete L_2 inner product. Give your skew-symmetric matrix S_d. Which is your choice of discrete gradient, give your $\overline{\nabla}H_d(\mathbf{u},\mathbf{v})$, and how does the complete method look like.

2. Supply a plot with linear axes where you show the numerical vs the exact solution at times $t = 1$ and $t = 50$.

3. Also hand in a plot which shows $H_d(\mathbf{u}^n)$ as a function of time ($t_n = n\Delta t$) for $n = 1000$ steps with stepsize $\Delta t = 0.05$.

Send your answers by e-mail to elena.celledoni@ntnu.no.