Hybrid modeling of hyperbolic systems of equations for fluid flows

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Machine Learning [1] is the new revolution in applied sciences. A recent major breakthrough [2] is meteorology modeling [3] with hybrid models. Hybrid models are based on the coupling of a standard PDE fluid model with a Neural Network representation of sources.

A possible model for fluid flow around the earth can be inferred from [2, 3]. It is a set of Euler/Boussinesq/St Venant-like system of equations with Coriolis force (in abstract form)

$$\left\{ \begin{array}{ll} \partial_t U + \mathcal{L}(U, \partial_x U, \partial_{xx} U, \dots) = S_\theta^{NN}(\alpha), & \theta = \text{all Neural Network weights}, \\ U(x,0) = \beta, & \text{initial data at time } t = 0, \end{array} \right. \tag{1}$$

where one has a large dataset of observations $\mathcal{D} = \{(\alpha_i, \beta_i, \gamma_i) \mid 1 \le i \le N \text{ with } 1 \ll N\}$. The initial solution is β, the current observations are α and the final solution is γ. The Neural Network modeling of the sources $S_\theta^{NN}(\alpha)$ can be reinterpreted as a local subgrid model. A cost function evaluated at given final time $T > 0$ is written as

$$J(\theta) = \frac{1}{N} \sum_i \int_{x \in \Omega} |U(x, T : \alpha_i, \beta_i, \theta) - \gamma_i|^2 \, dx \qquad (+ \text{ many other terms}).$$

The function J must be auto-differentiable with respect to the weights θ so that one can train/minimize it and obtain a quasi-optimal value θ_{opt}. The critical mathematical issue [3] is that the discrete solution $U_{h,\Delta t}(x, n\Delta t : \alpha_i, \beta_i, \theta)$ of the hyperbolic model must be auto-differentiable as well.

A simple example is the 1D advection equation $\partial_t u + a\partial_x u = 0$ with the upwind scheme $\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+\frac12}^n - u_{j-\frac12}^n}{\Delta x} = 0$. The flux $u_{j+\frac12}^n = G_a(u_j^n, u_{j+1}^n)$ follows the characteristic lines: $G_a(\alpha, \beta) = \alpha$ if $a > 0$ and $G_a(\alpha, \beta) = \beta$ if $a \le 0$. The time steps are composed one after the other. What matters is the regularity of the flux where $R(x) = \max(0, x)$ is a notation for the ReLU function $F(a, \alpha, \beta) = aG_a(\alpha, \beta) = R(a)\alpha - R(-a)\beta$. The observation is that the upwind scheme, and so any numerical scheme which follows the characteristic lines, contains the ReLU function which evidently is not differentiable at the origin.

This observation was also done in [6] for hybrid modeling of geophysical flows.

I will review some recent mathematical and numerical advances [4, 5] which establish a functional setting for auto-differentiability of the upwind scheme and a possible route for the development of discrete hybrid models for fluid flows.

References

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