DynamicBlocks: A Generalized ResNet Architecture

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Summary

Deep Residual Neural Networks (ResNets) have shown impressive performance on several image classification tasks (He et al. 2016). ResNets feature a skip connection, which has been observed to increase a model's robustness to vanishing and exploding gradients. ResNets also possess interesting theoretical properties; for example, the forward propagation through a ResNet can be interpreted as an explicit Euler method applied to a nonlinear ordinary differential equation (ODE) (Weinan 2017; Haber and Ruthotto 2017). Similarly, Ruthotto and Haber (2018) introduces a similar interpretation of convolutional ResNets as partial differential equations (PDE). These insights provide more theoretical insight along with new network architectures motivated by different types of differential equations, e.g., reversible hyperbolic network (Chang et al. 2018) or parabolic networks (Ruthotto and Haber 2018). Recent attention focuses on improving the time integrators used in forward propagation, e.g., higher-order single and multistep methods (Lu et al. 2018), black-box time integrators (Chen et al. 2018), and semi-implicit discretizations (Haber et al. 2019).

The primary goal of this toolbox is to facilitate further research and development in convolutional residual neural networks that are motivated by PDEs. To this end, we generalize the notation of ResNets, referring to each of its parts that amend a PDE interpretation (i.e., each set of several consecutive convolutional layers of fixed number of channels) as a `dynamic block`. A dynamic block can then be compactly described by a layer function and parameters of the time integrator (e.g., time discretization points). We provide the flexibility to model several state-of-the-art networks by combining several dynamic blocks (acting on different image resolutions and number of channels) through connective units (i.e., a convolutional layer to change the number of channels followed by a pooling layer).

Our `DynamicBlocks` toolbox provides a general framework to experiment with and apply more techniques from numerical differential equations in the context of ResNets. In its first version, we include capabilities to obtain a more general version of ResNet based on a forward Euler (Runge-Kutta 1) module that can handle arbitrary, non-uniform time steps. Furthermore, we include a fourth-order accurate Runge-Kuttta 4 block to demonstrate the generalizability of the architecture to accept other PDE solvers.

In the training, we primarily focus on discretize-optimize learning methods, which are popular in optimal control and whose favorable properties for ResNets have been shown in Gholami, Keutzer, and Biros (2019). However, dynamic blocks can also be employed in optimize-then-discretize approaches as in Neural ODEs (Chen et al. 2018).

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