Gauss-Newton Natural Gradient for Physics-Informed Computational Fluid Dynamics

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We propose Gauss-Newton Natural Gradient (GNNG), a novel second-order optimization method based on Gauss-Newton's method in function space for the training of physics-informed neural networks (PINN). We give an infinite dimensional differential geometric interpretation of our method, explaining the algorithm's optimization dynamics in function space. More precisely, we have shown that the proposed method follows the function space updates up to an orthogonal projection on the model's tangent space. We demonstrate that – given appropriate integral discretization in the PINN formulation – the proposed method corresponds to the well-known Gauss-Newton method in parameter space. This leads to a matrix-free formulation that allows the applicability of the method to large network sizes.

Numerically, the proposed method demonstrates unprecedented accuracy of PINN solutions for the Navier-Stokes equations, achieving relative L^2 errors up to two orders of magnitude lower than those obtained with standard optimizers like Adam or BFGS, and reaching as low as 10^{-8}.