Constrained curve fitting with Bayesian neural networks

Curtis Taylor Peterson & Anna Hasenfratz
University of Colorado Boulder
curtis.peterson@colorado.edu

Introduction

Common to many analysis pipelines in lattice field theory is the need to fit data to a model that is determined only partially by a finite number of model parameters. Familiar examples include analyses of finite-size scaling (FSS) and ground state spectroscopy. Motivated by promising results in condensed matter physics [1], we conjecture that the expressivity of neural networks makes them good candidates for parameterizing the unknown component of such models. We test this conjecture by performing a curve collapse analysis of the 2nd-order finite-temperature phase transition of the 2D Ising model and the zero-temperature phase transition of the 4D massless $N_f/N_c = 8/3$ gauge-fermion system.

Network architecture & training

Architecture

- Full model $\mathcal{M}_N$ maps input features in $\mathbb{R}^{M_{in}} \times \mathbb{R}^{M_{out}}$ to output features in $\mathbb{R}^N$ given the model parameters $(\Theta) = \{\theta_1, \theta_{MLP}, \theta_{aux}\}$; see Fig. 1.
- $\{\theta_{aux}\}$ denote learnable parameters of a multilayer perception (MLP) that parameterize the a priori unknown component of the model, such as the scaling function in an FSS analysis or the infinite sum of excited-state exponentials in an analysis of hadron spectroscopy.
- $\{\theta_{aux}\}$ denote additional learnable parameters of the model, such as critical exponents or ground state energies/amplitudes, that enter the model function through explicitly-defined activation functions that act upon a combination of input features of the full network and output features of the MLP.

Training

- Training is performed by least-squares minimization of the augmented $\chi^2$ [2]

$$\chi^2_{aug} = \chi^2_{data} + \chi^2_{aux}$$

where $\chi^2_{data}$ and $\chi^2_{aux}$ include information from the covariance of the data & priors, respectively.

- Priors on the networks weights in $\{\theta_{MLP}\}$ provide a lever arm for controlling overfitting; equivalent to L2 regularization in the ML literature.

- Appropriate priors can be estimated using the empirical Bayes method

- We optimize $\chi^2_{data}$ using the “basin hopping” algorithm championed in Ref. [3]:
  1. Random perturbation of coordinates (8)
  2. Local minimization (trust region reflective)
  3. Metropolis accept/reject

Gradient flow coupling & FSS

The gradient flow coupling at smearing radius $\nu = \nu_0$ defined by

$$g(t, \nu_0, L) = \langle t + \nu_0 \rangle_{\nu_0, L}$$

can be utilized as a scaling variable for use in finite-size scaling [4].

- At a 1st/2nd-order phase transition, $g(t, \nu_0, L)$ is expected to scale as

$$g(t, \nu_0, L) \sim L^{\nu(\Theta, E(t_0, L))}$$

where $\nu = \nu_0/\nu_0$, signaling first order transition.

- At a Berezinskii–Kosterlitz–Thouless (BKT) transition the scaling is

$$g(t, \nu_0, L) \sim L^{\nu(\Theta, E(t_0, L))} \exp(-\zeta L^{1/\nu})$$

where $\nu \equiv \beta/\beta_0 - 1$.

References


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