Renormalization Group as a Koopman Operator

William T. Redman

University of California, Santa Barbara

wredman@ucsb.edu

Abstract

Koopman operator theory - a nonlinear dynamical systems theory - is shown to be directly related to the renormalization group. This observation allows us to compute critical exponents of classical spin systems from observables alone, making no assumptions of translation invariance, broadening the number of problems renormalization group theory can be applied to.

Introduction

Understanding the behavior of complex systems with many components is a central problem in all areas of science. In physics, the study of phase transitions and critical phenomena led to the development of the renormalization group (RG), one of the most successful tools in theoretical physics [1–4]. By turning disparate physical problems into dynamical systems problems, it enabled a coherent understanding of the universality of critical exponents and allowed a controlled, albeit difficult, manner in which to compute them.

Given its success, there has been interest in applying the RG framework to problems beyond traditional physics. A recent example was the discovery that there is an exact mapping between the RG and deep neural networks (DNNs) based on Restricted Boltzmann Machines (RBMs) [5]. As emphasized in [5], while there has been considerable development of RG theory, the majority of it has been focused on systems with symmetries (e.g. spin models that are translationally invariant). How the RG framework can be extended to compute things of interest for more complicated, non-symmetric systems, such as RBM DNNs, is an important open question that likely requires a new approach.

A recent advance in nonlinear dynamical systems theory has been the development of Koopman operator theory (KOT). While KOT is based a foundation of rigorous mathematical theory, there are a number of effective, data driven algorithms inspired by KOT that extract the dynam-
ics underlying a wide range of physical systems. Intriguingly, KOT has been indirectly linked with the RG in several different areas. Seminal work by Goldenfeld and colleagues showed that the RG could be used to find the asymptotics to partial differential equations (PDEs) [6, 7]. KOT has also been used to discover the dynamics of PDEs [8]. The RG has been used as a way to extend principal component analysis and perform dimensionality reduction [9], something KOT has also been directly related to [10, 11]. Recent work showed that applying normal form theory to the RG equations allowed for better classification of the universality of systems and gives nonlinear corrections to the RG critical exponents [12]. KOT has also been shown to have connections to normal form theory [13, 14]. Finally, the RG has been shown to have a direct mapping to RBM DNNs [5], and KOT has been used to develop novel machine learning techniques [15–17].

These connections between the RG and KOT motivated us to look more closely at the two. Does there exist a direct link between them? As we show below, the RG is, in fact, a Koopman operator.

This paper is organized as follows. We start by providing a brief overview of basic KOT. This will allow us to show that, by definition, the RG is a Koopman operator. We include references to a number of recent theoretical and applied works that provide more details about KOT for the interested reader. We next show that we can successfully use a KOT inspired algorithm to compute the critical exponents of the Ising model and the three-state Potts model in 2D. We show that our algorithm relies solely on measuring single observables, and does not rely on any explicit calculation of how applying the RG changes coupling constants. We compare these results to standard Monte Carlo RG (MCRG) approaches. We find that our method performs similarly, while requiring less information about the exact RG flow, and can be considerably faster. These encouraging results lead us to end by speculating about the possible uses that this KOT RG approach might have in other fields. In particular, we suggest that the calculation of critical exponents for more complex systems, such as DNNs, where connections between units change and become inhomogenous with training, will be possible for the first time. These critical exponents would give new insight into how architecture affects performance of DNNs, and could lead to better optimized networks.

1 KOT and its connection to the RG operator

KOT is a spectral dynamical systems theory that was first developed by Bernard Koopman in 1931 in the context of classical mechanics [18], and then later expanded upon by Koopman
and John von Neumann [19]. It continued to be a subject of limited interest, especially as it
is connected to Perron-Frobenius operator theory for measure preserving systems. However,
it has seen a great increase in attention over the past two decades as a wave of new data
driven methods [20–24] and underlying mathematical theory [23,25,26], allowed it to be applied
to the dynamics of fluids [27–30], and the study of power grids [31,32], logistics [33], urban
insurgency [34], and building energy [35].

The key insight in KOT is the fact that there exists an infinite linear operator, the Koopman
operator (also called the composition operator), whose spectrum provides information on the
dynamics of nonlinear systems. The Koopman operator,

\[ U_t \], is defined, to be the time evolution
operator of a given observable \( g \)

\[ U^t(g(x_0)) = g(S^t(x_0)) \] (1)

where \( S^t \) is the dynamics that act on the observable \( g \) [23]. Time here can either be discrete or
continuous.

The block spin RG is defined to be a map in the infinite space of possible Hamiltonians with
coupling constants \( (K_1, K_2, ...) \), which we refer to as K-space from now on [36]. In particular,
the RG transformation, \( R_b \), acting on a Hamiltonian with coupling constants \( K_0 = (K_1, K_2, ...) \)
is equivalent to finding the coupling constants to the coarse grained Hamiltonian, which can be
done \( n \) times

\[ R_b^n H(K_0) = H(T^n(K_0)) \] (2)

where \( T \) is the transformation from one point in K-space to another following the chosen blocking
procedure.

With this, we see that the RG is definitionally a Koopman operator, defining the flow in the
infinite dimensional K-space. Because the Hamiltonian defines the values of all the observables
that we might be interested in (such as magnetization), we can hope that we can apply KOT
methods to successfully measure the critical exponents of these observables. Although we are
only considering the block spin RG here, the Wilsonian (momentum space) RG, which integrates
over continuous degrees of freedom, is, definitionally, a continuous Koopman operator.

While there are a number of powerful KOT methods, the finite section method is especially
useful for calculating the critical exponents of the block spin RG [23]. It approximates the
Koopman operator, \( \tilde{U} \), using the data matrix, \( F \), which is comprised of the first \( n \) time points
of \( m \) observables \( g_1, \ldots, g_m \) (i.e. \( F = [g_1, \ldots, g_m] \)). In particular,

\[
\tilde{U} = F^+ F'
\]  

(3)

where \( F' \) is the data matrix shifted one time step forward and \( F^+ \) is the Moore-Penrose pseudoinverse (i.e. \( F^+ = (F^\dagger F)^{-1} F^\dagger \)) \cite{23}. Note that if we are only considering a single observable, \( \tilde{U} \) is also the approximation for its spectrum.

Results

Having found that the RG operator is a Koopman operator in K-space, we turned our attention to seeing whether we could use tools imported from KOT to calculate critical exponents of the 2D Ising model and the 2D three-state Potts model.

We started by considering the magnetization, \( m \), which scales as

\[
m \sim t^{-\beta}
\]  

(4)

near the critical manifold, where \( t \) is the difference between the critical temperature and actual temperature (i.e. \( t = T_c - T \)) \cite{36}.

To calculate \( \beta \), we first equilibrated our spin systems using standard Monte Carlo approaches \cite{37}. We then performed block spin renormalizations with \( b^2 \) spins in each block \( n_R \) times, measuring the magnetization after each renormalization (see Supplemental Material). This gave us \( n_R + 1 \) values of \( m \). We used the finite section method (as discussed in the previous section) to calculate \( \beta \) as

\[
\beta = \log(\lambda) / \log(b)
\]  

(5)

where \( \lambda = (m_0, ..., m_{n_R-1})^+ \ast (m_1, ..., m_{n_R})^T \) and \( m_i \) is the magnetization of the spin system after \( i \) block spin renormalizations.

The error in estimating \( \beta \) using this method, as a function of where the system was started in K-space, is shown in Fig. 1a. The existence of the critical manifold is shown by the regions in K-space where the error is low. The fixed points found previously \cite{38,39}, which used more coupling constants, lie along, or very close, to this region, suggesting our method is indeed able to correctly calculate \( \beta \) in the correct region of K-space.

We compared this method to standard Monte Carlo RG (MCRG) methods \cite{37,39,41}. These methods approximate the RG transformation near the fixed point Hamiltonian, \( H^* \), by the
Figure 1: **Error in approximating β for the 2D Ising model**  
(a) Error in approximating β using the KOT finite section method.  
(b) Error in approximating β using the MCRG method, while fixing η = 0.125. This effectively limits our computation to the even K-space.  
(c) Renormalization “time” averaged magnetization in (K₂, K₄) space. This serves as a proxy for the RG flow.  
(d) same as (c), but for the flow in the (K₂, h) space.  
(e) Error in approximating β using the MCRG method, setting h = 0 (as we did in (a)). Note that for all error subplots, the values were set to a maximum value of 100% (yellow).

Linearization

\[ T_{\alpha\beta} = \left[ \frac{\partial K^{(n+1)}_{\alpha}}{\partial K^{(n)}_{\beta}} \right]_{H^*} \]  

where \( \frac{\partial K^{(n+1)}_{\alpha}}{\partial K^{(n)}_{\beta}} \) can be solved for using the chain rule and certain identities that require computing spin-spin correlations [41, 42]. If the matrix T is constructed by using only even interactions in the fixed point Hamiltonian (i.e. \( K_2, K_4, \) etc.), the critical exponent \( \nu \) will be given by the largest eigenvalue of T. If T is instead constructed by using only odd interactions (or in the case of [41], one even and one odd interaction), the critical exponent \( \eta \) will be given by the largest eigenvalue of T. The remaining critical exponents are found using standard critical exponent relationships [36] (see Supplemental Material).

Note that the MCRG requires knowledge of the RG flow in both the odd and even K-spaces to compute β, whereas the finite section method does not. If we ignore some of the information, for instance, if we fix the odd interaction to be 0 (as we did when we computed β using the finite section method), we get error over a considerable range of K-space when computing β (Fig 1e). This is because the flow in the odd K-space is different from that in the even K-space (Fig. 1c,d). Fixing the value of η to it’s exact value of 0.125 [36] and only searching the even K-space, we were able to compute β with similar (but better) performance compared to our KOT method (Fig. 1b). Similar results are seen when evaluating β in the 2D three-state Potts model (see Fig. S1 Supplemental Material).
Note that our KOT method, which performed nearly as well as standard MCRG methods, does not require any explicit calculation of how $K$ changes when applying the block spin RG. This property shows the power of recognizing the RG as a Koopman operator: simply by recording an observable (here, the magnetization, but in principle any observable) as we renormalize, we can recover the underlying dynamics in the form of a critical exponent. This then removes the constraint of only being able to work on systems where solutions for the linearization of $T, \partial K_{(n+1)}^{(n+1)} / \partial K_{(n)}^{(n)}$, has been worked out. This means that the KOT method allows for the calculation of critical exponents even in systems that are not translationally invariant, as long as a coarse graining block spin RG exists for some more complex systems. Because such blocking methods exist, this is not a particularly strong requirement (e.g. [43]).

**Discussion**

We started by connecting the renormalization group to a powerful nonlinear dynamical systems theory, Koopman operator theory, an insight that was suggested by the fact that KOT and the RG have both been shown to be related to the asymptotics of partial differential equations [6–8], principal component analysis [9–11], normal form theory [12–14], and machine learning [5,15–17]. We showed that, by definition, the RG is a Koopman operator in the infinite dimensional coupling constant space. The fact that KOT has been successfully applied to understanding the dynamics of a wide range of systems in a data driven manner [20,27,29,32–35], led us to investigate whether we could import KOT methods to successfully evaluate critical exponents, and whether these methods would afford us benefits that standard Monte Carlo RG methods cannot.

We showed that, for both the 2D Ising model and the 2D three-state Potts model, the finite section method allowed for an evaluation of $\beta$ that was close to as good as that of standard MCRG methods on the critical manifold [37,39–41], yet required less information about the RG flow. This is because the MCRG methods use knowledge of the RG flow in odd and even K-space, whereas the KOT method does not. Additionally, our method was significantly faster for computing the critical exponent $\beta$, as we only had to measure the magnetization at each renormalization “time” point, whereas the MCRG methods required computing spin-spin correlations over a lengthy time period (see Supplemental Material).

While the robust calculation of $\beta$ in K-space is encouraging, and shows a possible use the KOT RG method may play in calculating critical exponents of systems that MCRG methods have struggled with, the real advantage of using the KOT method comes from that fact that it
does not rely on any explicit formulation of the RG transformation in terms of $K$. This greatly broadens the range of problems that we can calculate the RG critical exponents of. The example of deep neural networks is particularly exciting. While the fact that DNNs undergo a phase transition in rate-distortion space has been appreciated since at least the landmark paper \[44\], it has not yet, to our knowledge, been possible to calculate the corresponding critical exponents of such networks and their information flow. Such critical exponents could offer new insight into how architecture affects performance of DNNs, and could lead to better optimized networks. With the KOT RG, such a computation is simple for a Restricted Boltzmann Machine DNN - by measuring the information bottleneck (IB) distortion of each layer, we can use the finite section method to calculate the critical exponent (as we did in this paper), all without worrying about the fact that the trained weights of the network are not translationally symmetric. This will be the subject of future work.

This work highlights the power that applying techniques developed in the field of nonlinear dynamical systems offers when working with the RG. We see our work very much in the same spirit as the recent success in using normal form theory to predict and classify nonlinear generalizations of scaling functions \[12\]. Given the connection of KOT with normal form theory and nonlinear systems in general \[13,14\], it would be interesting to see whether our method could be used to provide numerical predictions of what universality families systems belong to \[12\].

KOT is an exciting, powerful, and growing theory and we hope that this work will help increase it’s use as a tool for physicists.

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