

Non-perturbative renormalization for the neural network-QFT correspondence

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In collaboration with:

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Outline: 1. Motivations

Motivations

NN-QFT correspondence

Renormalization group in NN-QFT

Conclusion

Why a QFT?

Problems with neural networks:

- ▶ black box: very hard to understand the meaning of NN computation
- ▶ loss landscape problem: loss function non-convex and very rough, hard to find (global) minimum (related to spin glass)
[1412.0233, Choromanska et al.; 1712.09913, Li et al.]
- ▶ training can be complicated (expensive computationally, convergence issues. . .)
- ▶ hyperparameter tuning (find architecture / best parameters): mostly trial and errors or random optimization

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→ develop tools to improve analytical understanding of neural network building and training

[See also talks by: Roberts, Halverson, Maiti, Yang, Silverstein. . .]

Plan

NN-QFT correspondence

For a very general class of architectures, it is possible to associate a quantum field theory (QFT) to a neural network (NN).

[2008.08601, Halverson-Maiti-Stoner (HMS)] (see also [2106.00694, HMS; 2106.10165, Roberts-Yaida-Hanin; 2109.13247, Grosnevor-Jefferson...])

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In this talk [[2108.01403](#), HE-Lahoche-Samary]:

- ▶ describe the NN-QFT correspondence
- ▶ establish RG flow for the QFT
- ▶ provide numerical results

Main “experimental” result

Varying the standard deviation of the weight distribution induces an RG flow in the space of neural networks.

Outline: 2. NN-QFT correspondence

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Neural network

- ▶ fully connected neural network (one hidden layer)

$$f_{\theta, N} : \mathbb{R}^{d_{\text{in}}} \rightarrow \mathbb{R}^{d_{\text{out}}}$$

$$f_{\theta, N}(x) = W_1 \left(g(W_0 x + b_0) \right) + b_1$$

width N , activation function g

parameters (weights and biases) $\theta = (W_0, b_0, W_1, b_1)$

$$W_0 \sim \mathcal{N}(0, \sigma_W^2 / d_{\text{in}}), \quad W_1 \sim \mathcal{N}(0, \sigma_W^2 / N)$$

$$b_0, b_1 \sim \mathcal{N}(0, \sigma_b^2)$$

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- ▶ change of perspective
 - ▶ consider **statistical ensemble** of neural networks defined by **distribution in parameter space**
 - ▶ specific NN = sample from distribution
 - ▶ dual description: parameter dist. + architecture induces **distribution in function space**
 - ▶ training = change parameter dist. = flow in function space

Note: no training in this talk

Large N limit, Gaussian process and free QFT

Large N limit = infinite layer width:

- ▶ NN (function) distribution drawn from **Gaussian process** (GP) with kernel K (consequence of central limit theorem) [Neal '96]
- ▶ generalize to most architectures [1910.12478, Yang] and training

Large N limit, Gaussian process and free QFT

Large N limit = infinite layer width:

- ▶ NN (function) distribution drawn from **Gaussian process** (GP) with kernel K (consequence of central limit theorem) [Neal '96]
- ▶ generalize to most architectures [1910.12478, Yang] and training
- ▶ log likelihood

$$S_0[f] = \frac{1}{2} \int d^{d_{\text{in}}} x d^{d_{\text{in}}} x' f(x) \Xi(x, x') f(x'), \quad \Xi := K^{-1}$$

- ▶ n -point correlation (Green) functions (fixed by Wick theorem)

$$G_0^{(n)}(x_1, \dots, x_n) := \int df e^{-S_0[f]} f(x_1) \cdots f(x_n)$$

→ looks like a free QFT

Finite N and interactions

- ▶ for finite N , non-GP \Rightarrow deviations of Green functions

$$\Delta G^{(n)} := G^{(n)} - G_0^{(n)}$$

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$$S[f] = S'_0[f] + S_{\text{int}}[f]$$

- ▶ free action $S'_0[f]$ **unknown**

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- ▶ n -point Green functions

$$G^{(n)}(x_1, \dots, x_n) := \int df e^{-S[f]} f(x_1) \cdots f(x_n)$$

- ▶ effective (IR) 2-point function **exactly known** ($G^{(2)}$ N -indep.)

$$G^{(2)}(x, y) = K(x, y) = G_0^{(2)}(x, y)$$

- ▶ N -scaling [2008.08601, HMS; 2108.01403, HE-Lahoche-Samary]

$$G_c^{(2n)} = O\left(\frac{1}{N^{n-1}}\right)$$

Summary of NN-QFT correspondence

	QFT	NN / GP
x	spacetime points	data-space inputs
p	momentum space	dual data-space
$f(x)$	field	neural network
$K(x, y)$	propagator	Gaussian kernel
S_0	free action	log-likelihood
	interactions	non-Gaussian corrections

GaussNet

Setup in this talk and [2108.01403, HE-Lahoche-Samary]:

- ▶ take $d_{\text{out}} = 1$
- ▶ translation-invariant activation function (exp: element-wise)

$$g(W_0x + b_0) = \frac{\exp(W_0x + b_0)}{\sqrt{\exp\left[2\left(\sigma_b^2 + \frac{\sigma_W^2}{d_{\text{in}}} x^2\right)\right]}}$$

(stricly speaking, activation func. + normalization)

- ▶ GP kernel [2008.08601, HMS]

$$K(x, y) := \sigma_b^2 + K_W(x, y), \quad K_W(x, y) = \sigma_W^2 e^{-\frac{\sigma_W^2}{2d_{\text{in}}} |x-y|^2}$$

- ▶ note: [2008.08601, HMS] also considers ReLU and Erf functions

Numerical setup

[2008.08601, HMS; 2108.01403, HE-Lahoche-Samary]

- ▶ $d_{\text{in}} = 1, \sigma_b = 1, N \in \{2, 3, 4, 5, 10, 20, 50, 100, 500, 1000\}$
- ▶ n_{bags} distinct statistical ensembles of n_{nets} networks each
- ▶ “experimental” Green functions

$$\bar{G}_{\text{exp}}^{(n)}(x_1, \dots, x_n) := \frac{1}{n_{\text{bags}}} \sum_{A=1}^{n_{\text{bags}}} G_{\text{exp}}^{(n)}(x_1, \dots, x_n) \Big|_{\text{bag } A}$$

$$G_{\text{exp}}^{(n)}(x_1, \dots, x_n) := \frac{1}{n_{\text{nets}}} \sum_{\alpha=1}^{n_{\text{nets}}} f_{\alpha}(x_1) \cdots f_{\alpha}(x_n)$$

$$\Delta G_{\text{exp}}^{(n)} := \bar{G}_{\text{exp}}^{(n)} - G_0^{(n)}, \quad m_n := \frac{\Delta G_{\text{exp}}^{(n)}}{G_0^{(n)}}$$

- ▶ $x^{(1)}, \dots, x^{(6)} \in \{-0.01, -0.006, -0.002, 0.002, 0.006, 0.01\}$
→ evaluate Green functions for all inequivalent combinations

Effective action

- ▶ numerical results

$$\forall N : m_2 \approx 0, \quad \forall n \geq 2 : m_{2n} = O\left(\frac{1}{N}\right)$$

- ▶ extract single number $\langle |m_n| \rangle$: average $|m_n(x_1, \dots, x_n)|$ over all combinations of points
- ▶ compare with background: standard deviation of $G_{\text{exp}}^{(n)}$ over all bags, then average over all combinations of points
(compare statistical deviation and deviation from free result)

Effective action

- ▶ numerical results

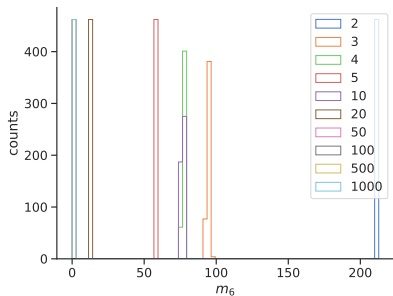
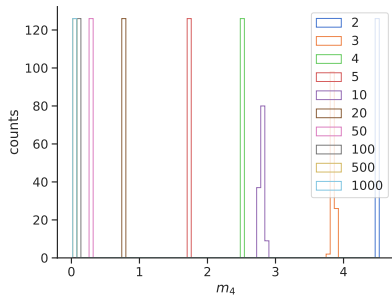
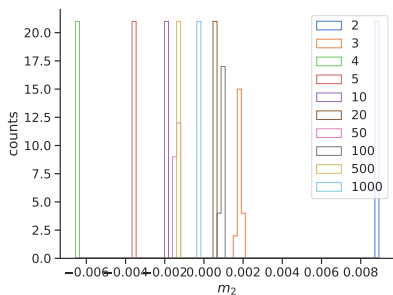
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- ▶ compare with background: standard deviation of $G_{\text{exp}}^{(n)}$ over all bags, then average over all combinations of points
(compare statistical deviation and deviation from free result)
- ▶ compute 1PI action with quartic and sextic interactions:

$$\Gamma = \Gamma_0 + \frac{u_4}{4!} \int d^{d_{\text{in}}} x f(x)^4 + \frac{u_6}{6!} \int d^{d_{\text{in}}} x f(x)^6$$

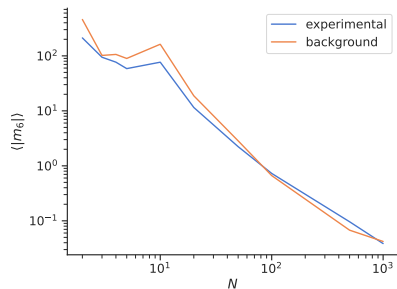
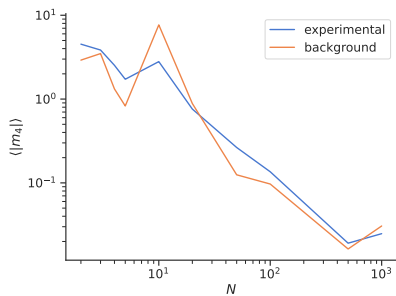
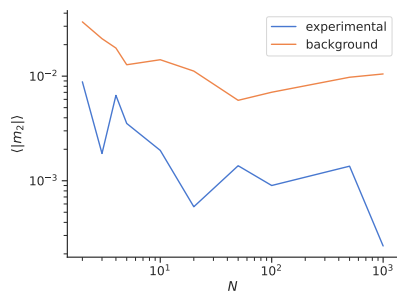
reminder: Γ_0 defined by K

Green function deviations: histogram



$\sigma_W = 1$
 $n_{bags} = 20$
 $n_{nets} = 30000$

Green function deviations: mean values

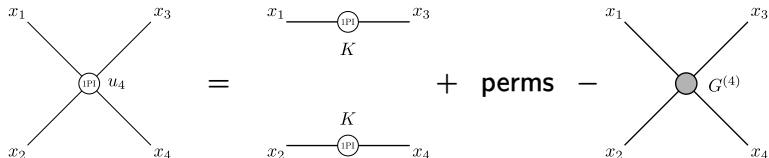


$$\sigma_W = 1$$
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Extract quartic coupling

[2008.08601, HMS; 2108.01403, HE-Lahoche-Samary]

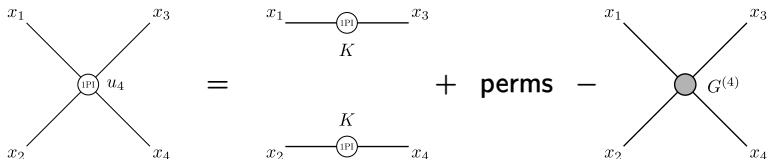
- ▶ 4-point Feynman diagrams (1PI \rightarrow no loops)



Extract quartic coupling

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- ▶ measure u_4 from $G_{\text{exp}}^{(4)}$

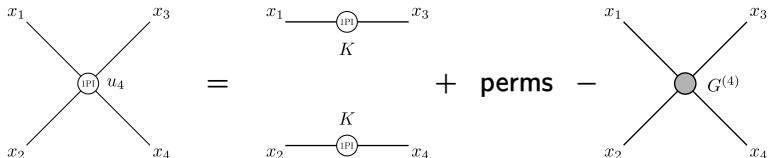
$$u_4(x_1, x_2, x_3, x_4) = - \frac{\Delta G_{\text{exp}}^{(4)}(x_1, x_2, x_3, x_4)}{N_K(x_1, x_2, x_3, x_4)}$$

$$N_K := \int d^{d_{\text{in}}} x K_W(x, x_1) K_W(x, x_2) K_W(x, x_3) K_W(x, x_4)$$

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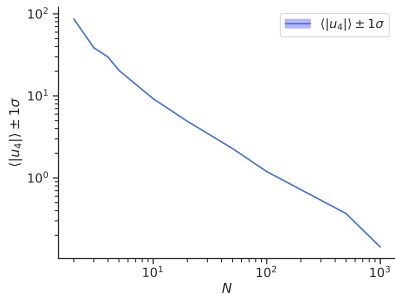
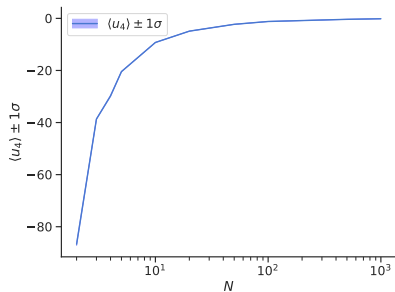
- ▶ measure u_4 from $G_{\text{exp}}^{(4)}$

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- ▶ result: $u_4 \approx \text{constant} < 0$
 \rightarrow need $u_6 > 0$ for path integral stability

Quartic coupling



$$\sigma_W = 1, \quad n_{\text{bags}} = 30, \quad n_{\text{nets}} = 30000$$

Outline: 3. Renormalization group in NN-QFT

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Renormalization group in NN-QFT

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Non-perturbative RG

- ▶ partition function and microscopic action

$$Z[j] := e^{W[j]} := \int d\phi e^{-S[\phi] - j \cdot \phi}$$

$S[\phi]$ encodes **microscopic (UV) physics**

Non-perturbative RG

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- ▶ classical field and 1PI effective action

$$\varphi(x) := \frac{\delta W}{\delta j}, \quad \Gamma[\varphi] := j \cdot \varphi - W[j]$$

$\Gamma[\varphi]$ encodes **effective (IR) physics**

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- ▶ renormalization group (RG) flow:
 - ▶ organize theory according to length scales
 - ▶ integrate degrees of freedom (dof) step by step
→ flow in the theory space
 - ▶ connect UV to IR
- ▶ review: [[cond-mat/0702365](#), Delamotte]

Wilson RG: momentum-shell integration

- ▶ split field in slow and fast modes with respect to scale k

$$\phi(\mathbf{p}) = \phi_{<}(\mathbf{p}) + \phi_{>}(\mathbf{p}), \quad \begin{cases} \phi_{<}(\mathbf{p}) := \theta(|\mathbf{p}| < k) \phi(\mathbf{p}) \\ \phi_{>}(\mathbf{p}) := \theta(|\mathbf{p}| \geq k) \phi(\mathbf{p}) \end{cases}$$

- ▶ kinetic operator decomposes

$$\Xi(\mathbf{p}) = \Xi_{<}(\mathbf{p}) + \Xi_{>}(\mathbf{p}), \quad \begin{cases} \Xi_{<}(\mathbf{p}) := \theta(|\mathbf{p}| < k) \Xi(\mathbf{p}) \\ \Xi_{>}(\mathbf{p}) := \theta(|\mathbf{p}| \geq k) \Xi(\mathbf{p}) \end{cases}$$

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- ▶ **Wilsonian effective action** for $\phi_{<}$

$$\begin{aligned} \mathcal{S}_{\text{eff}}[\phi_{<}] &:= \frac{1}{2} \phi_{<} \cdot \Xi_{<} \cdot \phi_{<} + \mathcal{S}_{\text{eff,int}}[\phi_{<}] \\ e^{-\mathcal{S}_{\text{eff,int}}[\phi_{<}]} &:= \int d\phi_{>} e^{-\frac{1}{2} \phi_{>} \cdot \Xi_{>} \cdot \phi_{>} - \mathcal{S}_{\text{int}}[\phi_{<} + \phi_{>}]} \end{aligned}$$

$\phi_{<}$ background, $\phi_{>}$ fluctuations

Wilson–Polchinski RG

- ▶ hard cutoff not convenient, use smooth regulator

$$\Xi_k(p) := R_k(p) \Xi(p), \quad R_k(p) \rightarrow \begin{cases} 1 & p \ll k \\ 0 & p \gg k \end{cases}$$

- ▶ measure factorization \Rightarrow field decomposition

$$\begin{aligned} \phi(p) &= \chi(p) + \Phi(p) \\ \int d\phi e^{-\frac{1}{2}\phi \cdot \Xi \cdot \phi} &= \left(\int d\chi e^{-\frac{1}{2}\chi \cdot \Xi_k \cdot \chi} \right) \times \left(\int d\Phi e^{-\frac{1}{2}\Phi \cdot (\Xi - \Xi_k) \cdot \Phi} \right) \end{aligned}$$

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- ▶ effective action at scale k (UV cut-off for χ)

$$e^{-S_{\text{int},k}[\chi]} := \int d\Phi e^{-\frac{1}{2}\Phi \cdot (\Xi - \Xi_k) \cdot \Phi - S_{\text{int}}[\chi + \Phi]}$$

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- ▶ Polchinski equation

$$k \frac{dS_{\text{int},k}}{dk} = \int \frac{d^d p}{(2\pi)^d} k \frac{d\Xi_k(p)}{dk} \left[\frac{\delta^2 S_{\text{int},k}}{\delta\chi(p)\delta\chi(-p)} - \frac{\delta S_{\text{int},k}}{\delta\chi(p)} \frac{\delta S_{\text{int},k}}{\delta\chi(-p)} \right]$$

Wetterich formalism

- ▶ non-perturbative truncation with Polchinski equation difficult
→ Wetterich formalism
- ▶ regularize path integral

$$Z_k[j] := e^{W_k[j]} := \int d\phi e^{-S[\phi] - \frac{1}{2}\phi \cdot R_k \cdot \phi - j \cdot \phi}$$

- ▶ R_k cutoff function s.t. $W_{k=\infty} = S$, $W_{k=0} = W$

$$R_{k=\infty}(p) = \infty, \quad R_{k=0}(p) = 0, \quad R_k(|p| > k) \approx 0$$

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- ▶ effective average action at scale k (IR cutoff for φ)

$$\varphi(x) := \frac{\delta W_k}{\delta j}, \quad \Gamma_k[\varphi] := j \cdot \varphi - W_k[j] - \frac{1}{2} \varphi \cdot R_k \cdot \varphi$$

- ▶ Legendre transform requires correction to satisfy:

$$\Gamma_{k=0}[\varphi] = \Gamma[\varphi], \quad \Gamma_{k=\infty}[\varphi] = S[\varphi]$$

Wetterich equation

- ▶ Wetterich equation

$$\frac{d\Gamma_k}{dk} = \frac{1}{2} \frac{dR_k}{dk} \text{tr} (\Gamma_k'' + R_k)^{-1}$$

Γ_k'' second derivatives of Γ w.r.t. φ

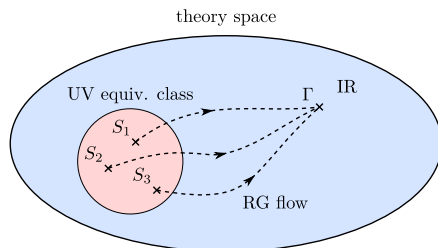
- ▶ solving requires approximation
 - ▶ restrict theory space to finite-dimensional subspace
 - ▶ derivative / local potential expansion
- ▶ non-perturbative formalism, finite coupling constants
- ▶ large N expansion: keeping up to $\phi^{2n} \leftrightarrow O(1/N^{n-1})$ effects

RG for NN-QFT

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→ similar to RG flow

RG for NN-QFT

- ▶ machine learning: find patterns in large dataset, ignoring noise
→ similar to RG flow
- ▶ action: effective (IR) known, microscopic (UV) unknown
 - ▶ opposite as usual, need to reverse flow
 - ▶ since information is lost, no 1-to-1 map UV / IR
 - ▶ but any microscopic theory in IR universality class is fine



(Note: [2008.08601, Halverson-Maiti-Stoner] defines RG flow w.r.t. IR cutoff)

Momentum space 2-point function

- ▶ momentum space propagator

$$K(p) = (\sigma_W^2)^{1 - \frac{d_{\text{in}}}{2}} \left(\frac{d_{\text{in}}}{2\pi} \right)^{\frac{d_{\text{in}}}{2}} \exp \left[- \frac{d_{\text{in}}}{2\sigma_W^2} p^2 \right]$$

- ▶ momentum expansion (derivatives subleading in IR, $|p| \rightarrow 0$)

$$K(p) \approx \frac{Z_0^{-1}}{m_0^2 + p^2 + O(p^2)}, \quad m_0^2 := \frac{2\sigma_W^2}{d_{\text{in}}}$$

→ can be used in deep IR

- ▶ typical mass scale → correlation length $\xi := m_0^{-1}$

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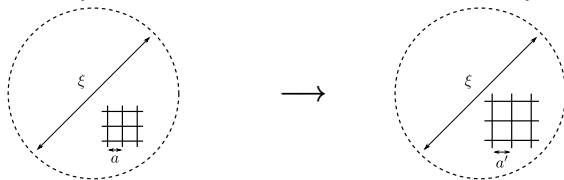
→ can be used in deep IR

- ▶ typical mass scale → correlation length $\xi := m_0^{-1}$
- ▶ two possible RG scales: a_0^{-1} (machine precision) and m_0
- ▶ effective action: kinetic term + local potential

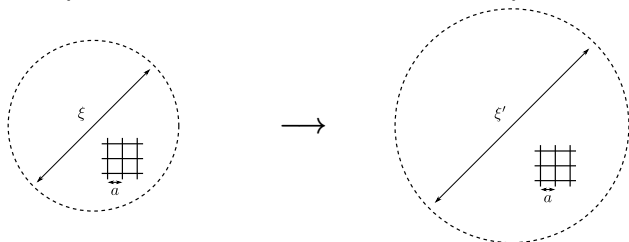
$$\Gamma_k = \Gamma_{k,0} + \frac{u_4(k)}{4!} \int d^{d_{\text{in}}} x \varphi(x)^4 + \frac{u_6(k)}{6!} \int d^{d_{\text{in}}} x \varphi(x)^6$$

Passive / active RG

- ▶ **passive RG**: keep $m_0 = \xi^{-1}$ fixed, vary $k = a^{-1} \leq a_0^{-1}$
(keep neural network fixed, vary data)



- ▶ **active RG**: keep a_0 fixed, vary $k = m \geq m_0$
(keep data fixed, vary neural network)



Active RG

- ▶ propagator looks like zero-momentum propagator with UV regulator with scale k

$$K_k(p) := \frac{e^{-p^2/k^2}}{k^2}, \quad k^2 := \frac{2\sigma_W^2}{d_{\text{in}}}$$

- ▶ changing $\sigma_W \approx$ changing UV cutoff k
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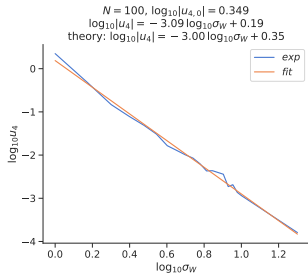
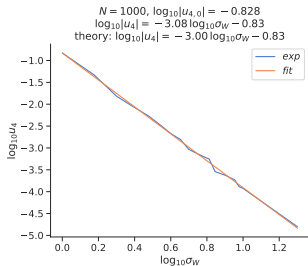
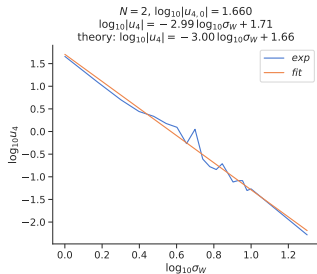
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- ▶ flow equations

$$\sigma_W \frac{du_4}{d\sigma_W} = (4 - d_{\text{in}}) u_4, \quad \sigma_W \frac{du_6}{d\sigma_W} = (6 - 2d_{\text{in}}) u_6$$

Results: active RG



$$\sigma_W \in \{1.0, 1.5, \dots, 10, 20\}$$

$$n_{\text{bags}} = 30, \quad n_{\text{nets}} = 30000$$

Outline: 4. Conclusion

Motivations

NN-QFT correspondence

Renormalization group in NN-QFT

Conclusion

Conclusion and outlook

Achievements:

- ▶ additional checks of the NN-QFT correspondence
- ▶ map of the possible theory space
- ▶ passive and active RG flow equations for neural networks
- ▶ change in standard deviation = RG flow
- ▶ numerical tests of the equations

Conclusion and outlook

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- ▶ additional checks of the NN-QFT correspondence
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Future directions:

- ▶ increase d_{in} , d_{out} , and order in N expansion; large d_{in} limit
- ▶ consider more general architectures
- ▶ extend to non-translation invariant kernels (ReLU...) using 2PI formalism [2102.13628, Blaizot-Pawlowski-Reinosa]
- ▶ numerical tests for passive RG flow
- ▶ investigate non-locality and random tensor models