Title: A Study of Neural Network Field Theories

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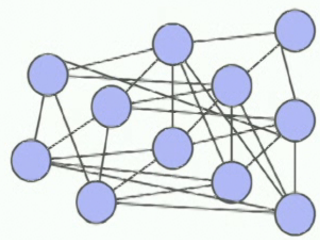
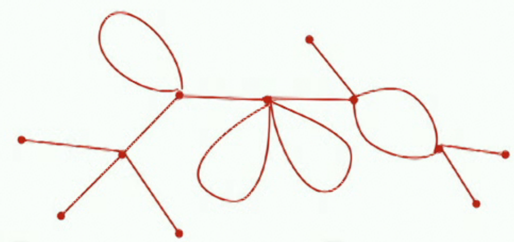
Abstract: The backbones of modern-day Deep Learning, Neural Networks (NN), define field theories on Euclidean background through their architectures, where field interaction strengths depend on the choice of NN architecture width and stochastic parameters. Infinite width limit of NN architectures, combined with independently distributed stochastic parameters, lead to generalized free field theories by the Central Limit Theorem (CLT). Small and large deviations from the CLT, due to finite architecture width and/or correlated stochastic parameters, respectively give rise to weakly coupled field theories and non-perturbative non-Lagrangian field theories in Neural Networks. I will present a systematic exploration of Neural Network field theories via a dual framework of NN parameters: non-Gaussianity, locality by cluster decomposition, and symmetries are studied without necessitating the knowledge of an action. Such a dual description to statistical or quantum field theories in Neural Networks can have potential implications for physics.

A Study of Neural Network Field Theories

Anindita Maiti





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Based on arxiv: 2008.08601, 2106.00694 & 22xx.xxxxx (w/ Jim Halverson, Matt Schwartz, Mehmet Demirtas & Keegan Stoner)

What are Neural Networks?

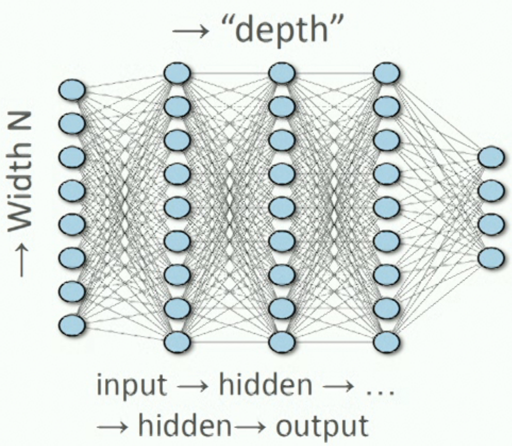
Backbones of Deep Learning.

Outputs are functions of inputs, with continuous learnable parameters $\boldsymbol{\theta}$ and discrete hyperparameter N.

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

Generate NN outputs multiple times, outputs get drawn from same distribution.

Fully Connected Feedforward NN :



$$z_i^l(x) = b_i^l + \sum_{j=1}^{N} W_{ij}^l x_j^l(x)$$

$$x_j^l = \sigma(z_j^{l-1}(x))$$

Statistical perspective: Field Theories are defined by distributions on field / function space (via Feynman path integral).

Action S[ϕ] is the 'log-likelihood'

$$Z = \int D\phi \, e^{-S[\phi]}$$

Punchlines

- Ensembles of Neural Network outputs behave as Euclidean Field Theories.
- Some limits in Neural Network architectures correspond to Free Field Theories. Deviations turn on interaction terms.
- Small & large deviations lead to weakly coupled & non-perturbative Neural Network Field Theories, respectively.
- NNs also have a dual “parameter distributions + architecture” framework.
- Symmetries, connected correlators, partition function, and locality via cluster decomposition can be studied in this dual framework; knowledge of action isn’t necessary.

Motivations

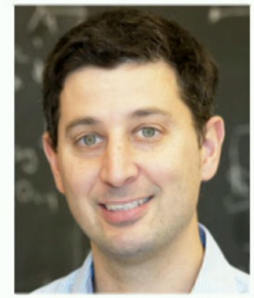
- Ongoing work to find NN architectures corresponding to known Euclidean Field Theory actions at initialization.
- A new approach to simulate field theories on lattice on computer, without involving NN "learning" dynamics.
- Bypassing NN learning saves computational resources.
- If Osterwalder-Schrader axioms are satisfied by Euclidean correlators of NN output ensembles, then these NN architectures correspond to QFTs. [Halverson 2021]
- Combinations of such NN architectures would result in field theories with actions similar to that of the Standard Model.

References & Related Works

Based on:

1. arXiv:2008.08601
2. arXiv:2106.00694
3. arXiv:22xx.xxxxx (to appear)

Jim Halverson



Matt Schwartz

Related Works:

[Halverson 2021],
[Erbin, Lahoche, Dine 2021],
[Grosvenor, Jefferson 2021],
[Lee, Bahri, Novak, Schoenholz, Pennington, Sohl-Dickstein 2017],
[Yang 2019],
[Roberts, Yaida, Hanin 2021],
[Yaida 2019].

Mehmet Demirtas

Keegan Stoner

Outline

- **Field Theories in Neural Networks**
  - Free Field Theories in Neural Networks
  - Wilsonian EFT in Neural Networks
  - Non-Perturbative Neural Network Field Theories
- **Study of NN Field Theories via Dual Parameter Space**
  - Symmetry in NN Field Theories
  - Connected Correlators in Field Theories
  - Locality via Cluster Decomposition
  - Partition Function of NN Field Theory

Free Field Theories in Neural Networks

Infinite NN architecture width and Independent, Identical Parameters: NN output is a sum over infinite i.i.d. variables. By Central Limit Theorem (CLT) such outputs are drawn from Gaussian distribution.

GP / asymptotic NN	Free QFT
input x	external space or momentum space point
kernel $K(x_1, x_2)$	Feynman propagator
asymptotic NN $f(x)$	free field
log-likelihood	free action S_{GP}

NNGP Field Density: $P[f] \sim \exp\left[-\frac{1}{2}\int d^{d_{\text{in}}}x\, d^{d_{\text{in}}}x'\, f(x)\Xi(x,x')f(x')\right]$

$$\int d^{d_{\text{in}}}x'\, K(x,x')\,\Xi(x',x'') = \delta^{(d_{\text{in}})}(x-x'')$$

Wilsonian EFT in Neural Networks

NGP / finite NN	Interacting QFT
input x	external space or momentum space point
kernel $K(x_1, x_2)$	free or exact propagator
network output $f(x)$	interacting field
non-Gaussianities	interactions
non-Gaussian coefficients	coupling strengths
log probability	effective action S

ML framework ⟶ a large number of NN parameters, very complex system.

EFT framework is simpler: some interactions are more relevant.

Small deviations from NNGP, caused by (i) large width, (ii) small correlations in NN parameters ⟶ described by EFT.

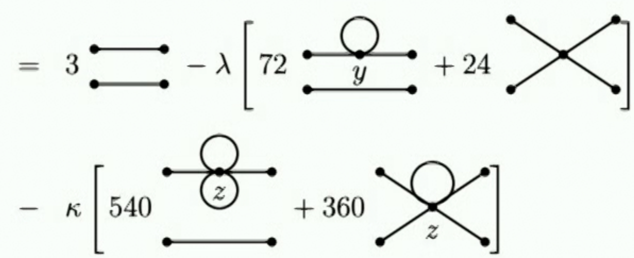
Wilsonian EFT action: $S = S_{\mathrm{GP}} + \Delta S$

$$\Delta S = \int d^{d_{\mathrm{in}}}x \; [g\, f(x)^3 + \lambda\, f(x)^4 + \alpha\, f(x)^5 + \kappa\, f(x)^6 + \dots]$$

See [Erbin, Lahoche, Dine 2021] for an alternate field theory close to NNGP.

Feynman diagrams for correlation functions of NN outputs:

$G^{(4)}(x_1, x_2, x_3, x_4)$



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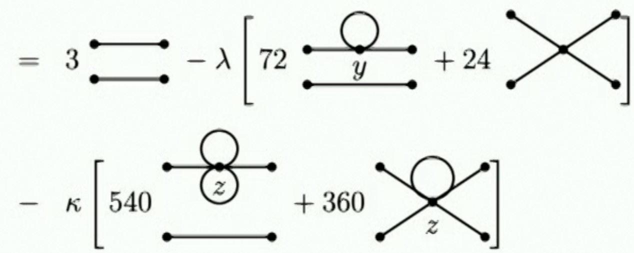

Non-Perturbative Neural Network Field Theories

(i) Small width, (ii) large parameter correlations violate Central Limit Theorem by large amounts.

Leads to non-perturbative field theories in NN output ensembles, with actions often unknown.

$$f_{\theta,N}(x) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} h_i(x)$$

$h_i(x)$: output of i^{th} neuron in final hidden layer.

NN output ensembles can be studied using NN architecture and parameter distributions, too.

Field Space

$$G^{(n)}(x_1, \ldots, x_n) = \frac{\int df \; f(x_1) \ldots f(x_n)\, e^{-S}}{Z_0}$$

Parameter Space

$$\mathbb{E}[f(x_1) \cdots f(x_n)]$$
$$= \frac{1}{N^{h/2}} \sum_{i_1, \cdots, i_n = 1}^{N} \int DhP(h) h_{i_1}(x_1) \cdots h_{i_n}(x_n)$$

Properties and observables, e.g. locality, symmetries, partition functions etc. can be studied without knowledge of actions.

Study of NN Field Theories via Dual Parameter Space

Symmetry in NN Field Theories

Non-perturbative regime: field theory action is unknown – symmetries can't be deduced in field space.

NN action remains invariant

$$D[\Phi f]\, e^{-S[\Phi f]} = Df\, e^{-S[f]}$$

if transformations $f'(x) = \Phi(f(x'))$ leave correlators invariant.

Absorb transformations of correlators into transformations of parameters.

Invariance of parameter distributions leads to invariance of NN action S[f].

Symmetries of NN input and output layers → spatial symmetries and internal symmetries of the field, respectively.

Examples:

(a) **Rotational Symmetry of the fields:** NN final layer parameter distributions are invariant under rotations.

$$f_i(x) = W_{ij} g_j(x) + b_i$$

(b) **Spatial Rotational Symmetry:** NN first layer parameter distributions are rotationally invariant.

$$f_i(x) = g_{ij}(W_{jk} x_k)$$

Connected Correlators in Field Theories

Cumulant Generating Functional (CGF) of NN field theories can be expressed in terms of cumulants / connected correlators in NN architecture framework.

NN output as a field or as a sum over neuron contributions.

$$f_{\theta,N}(x) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} h_i(x)$$

Correlated NN parameter distributions.

$$P(h|\vec{\alpha}) \neq \prod_i P_i(h_i) \quad \vec{\alpha} = \{\alpha_1, \cdots, \alpha_q\}$$

CGF of NN field theory:

$$W_f[J] = \sum_{r=1}^{\infty} \int \prod_{i=1}^{r} d^{d_{\text{in}}} x_i \frac{J(x_1)\dots J(x_r)}{r!} G^{(r)}_{\text{con},f}(x_1,\dots,x_r)$$
$$= \log\left[\int Dh\, P(h|\vec{\alpha})\, e^{\frac{1}{\sqrt{N}} \sum_{i=1}^{N} \int dx\, h_i(x) J(x)}\right]$$

Finite width, no parameter correlations:

$$G^{(r)}_{\text{con},f}(x_1,\cdots,x_r) = \frac{G^{(r)}_{\text{con},h_i}(x_1,\cdots,x_r)}{N^{r/2-1}}$$

Finite width, parameters correlated: each cumulant in NN field theory receives contributions from cumulants of all neurons.

Locality via Cluster Decomposition

We can study locality via cluster decomposition, even in the absence of action, using cumulants / connected correlators of field theories, expressed in terms of variables in NN parameter space.

$$\sum_{r=1}^{\infty} \int \prod_{i=1}^{r} d^{d_{\rm in}} x_i \frac{J(x_1)\dots J(x_r)}{r!} G^{(r)}_{{\rm con},f}(x_1,\dots,x_r) = \log\left[\int \left(\prod_{i=1}^{N} Dh_i\right) P(h|\vec{\alpha}) e^{\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\int d^{d_{\rm in}}x\, h_i(x) J(x)}\right]$$

Take any two subsets of input points (x_1, …, x_r) infinitely apart.

If all connected correlators (r>1) decay to 0 exponentially or faster, then the field theory action is local.

Correlated parameter distributions.

$$P(h|\vec{\alpha}) \neq \prod_i P_i(h_i) \qquad \vec{\alpha} = \{\alpha_1, \cdots, \alpha_q\}$$

$h_i(x)$: output of i[th] neuron in final hidden layer.

Conclusions

- NN output ensembles have dual descriptions by field space and NN parameter space.
- Free Field theories, Wilsonian EFTs and Non-Perturbative Non-Lagrangian Field Theories arise in NNs at GP limit, small, and large deviations from GP limit, respectively.
- More parameters in NN towards GP limit, fewer relevant interaction terms in field theory action. Useful for Machine Learning community.
- Small width and / or large parameter correlations lead to non-perturbative NN field theories.
- Symmetry, connected correlators, locality via cluster decomposition, and partition functions can be studied without necessitating the field action, using NN parameter space.

Thank You!

Questions?

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