Title: Scalar and Grassmann Neural Network Field Theory

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Abstract: Neural Network Field Theories (NNFTs) are field theories defined via output ensembles of initialized Neural Network (NN) architectures, the backbones of current state-of-the-art Deep Learning techniques. Different limits of NN architectures correspond to free, weakly interacting, and non-perturbative regimes of NNFTs, via central limit theorem and its violations. Nature of field interactions in NNFTs can be controlled by tuning architecture parameters and hyperparameters, systematically, at initialization. I will present a systematic construction of scalar NNFT actions, using various attributes of NN architectures, via a new set of Feynman rules and techniques from statistical physics. Conversely, I will present the construction of a class of NN architectures exactly corresponding to some interacting scalar field theories, via a systematic deformation of NN parameter distributions. As an example of the latter method, I will present the construction of an architecture for $\lambda \phi^4$ scalar NNFT. Lastly, I will introduce Grassmann NNFTs, their free and interacting regimes via central limit theorem for Grassmanns, and construction of an architecture corresponding to free Dirac NNFT. This approach provides us a way to initialize NN architectures exactly representing certain field configurations, and are useful for computing attributes, e.g. correlators, of field theories on lattice.

Zoom link

Scalar and Grassmann Neural Network Field Theory

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Perimeter ML Initiative Seminar, 16 Feb 2024

PERIMETER INSTITUTE **Postdoctoral Fellow**

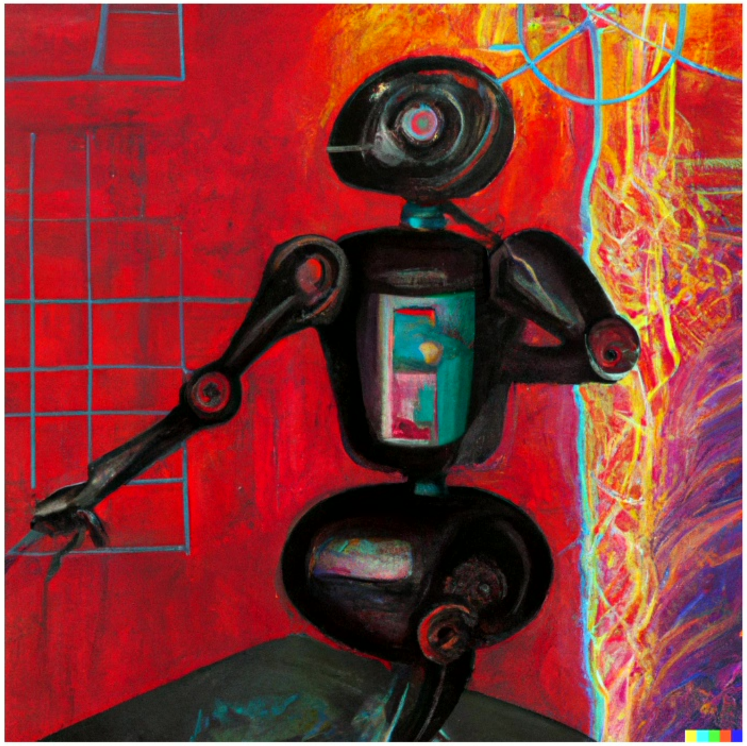
Based on [24xx.xxxxx], [2307.03223], [2106.00694], [2008.08601] w/ Halverson, Schwartz, Demirtas, Ruehle, Stoner, Frank

What is a Neural Network Field Theory?

Field theory defined by output ensembles of an initialized NN architecture.

Introduction

- Neural Networks are universal approximators.
- ML for QFT: powerful approach to represent target field theories, up to numerical precisions.
- Simply put, ML-for-QFT engineers QFTs via optimization algorithms.
- A step to improve uncertainty quantification — start where initialized Neural Networks are.



Introduction

- How to make 'engineering QFTs via ML' more robust and interpretable?
- Simple answer: show how NN architectures represent field theories, at initialization.
- Discover constrains on NN architectures to engineer symmetries, interactions, ...
- Start at 'NN architectures for QFTs' before involving optimization algorithms.

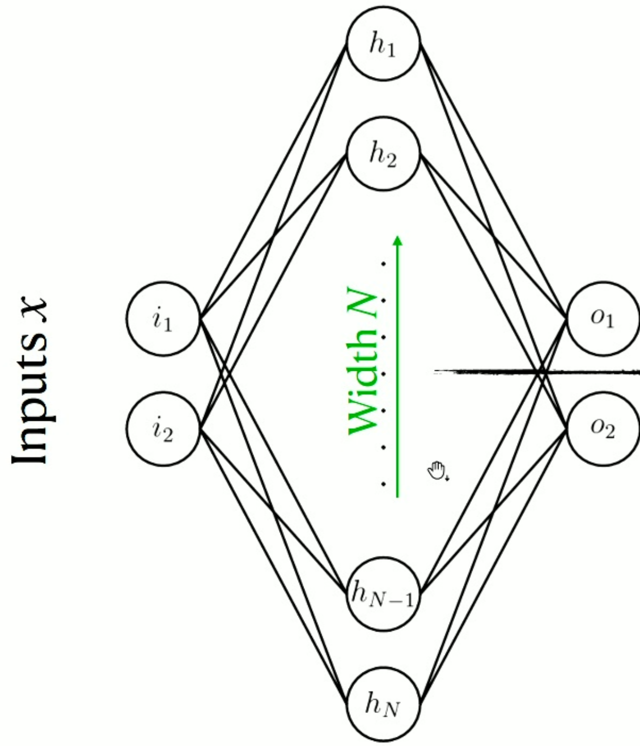
How to get NN Field Theory?

Open NN blackboxes and identify knobs that gives rise to field theoretic properties.

Talk Outline

- Intro to NN field theory.
- Scalar NN field theory: Construct action $S[\phi]$ given an architecture.
- Scalar NN field theory: Construct NN architecture given $S[\phi]$.
- Grassmann NN field theory: introduction and free Dirac example.

Intro to NNFT



$h_1(x)$

$h_2(x)$

.

.

.

N neurons

.

.

.

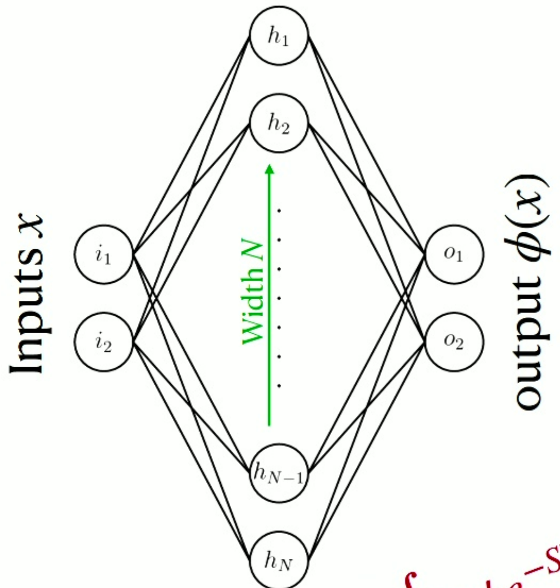
$h_{N-1}(x)$

$h_N(x)$

output $\phi(x)$

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

Intro to NNFT



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

NN inputs	Space or space-time
NN outputs	Field

An ensemble of initialized NN outputs is a statistical distribution over functions $\phi(x)$.

↕

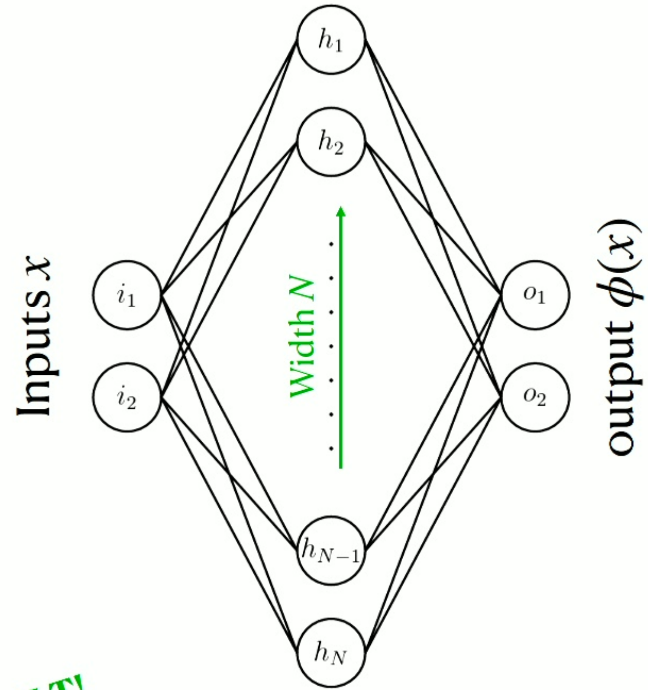
In path integral formalism, field theories are functional distributions.

NN field theory := field theory defined by NN architecture

Intro to NNFT

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

- Origin of field interactions in $S[\phi]$ is due to violations of Central Limit Theorem (CLT).
- When NN parameters are identically, independently distributed (i.i.d.), all $h_i(x)$ are i.i.d.
- At $N \to \infty$, sum $\phi(x)$ is a draw from a Gaussian distribution, or a free NN field theory. ⟵ from CLT!

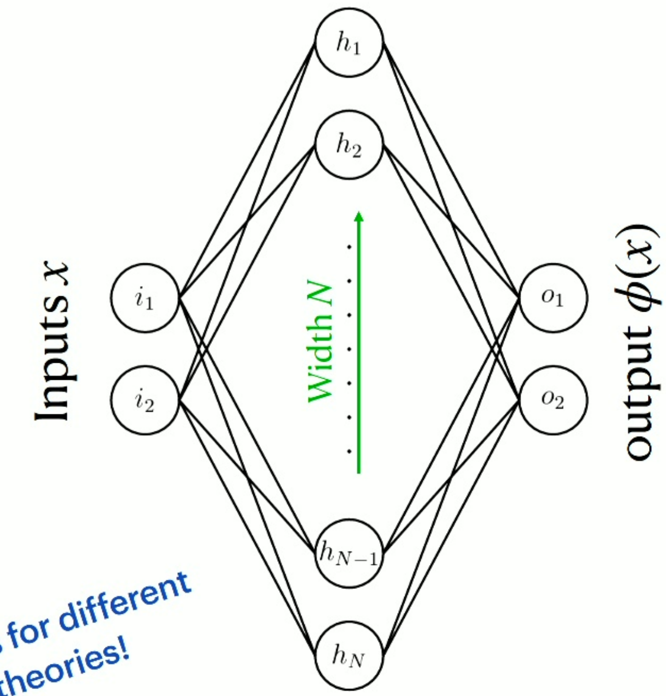


Intro to NNFT

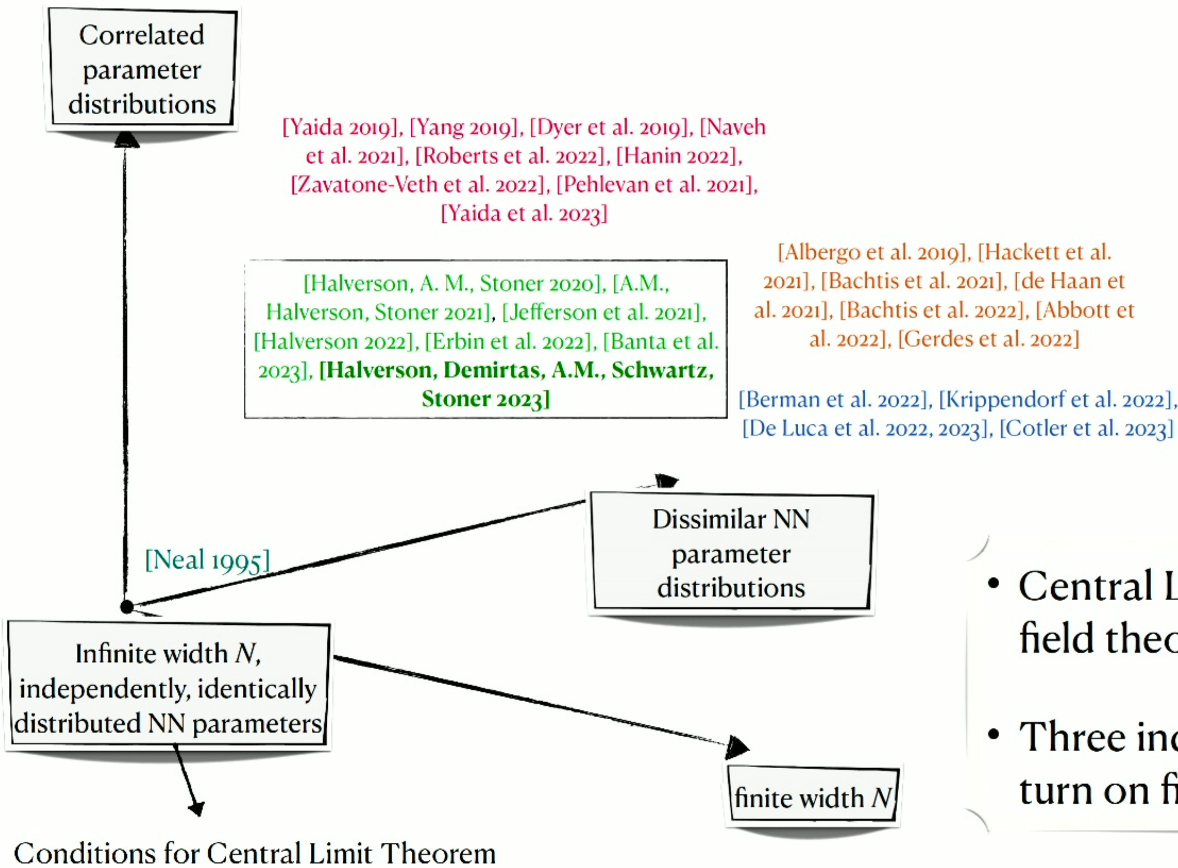
$$\phi(x) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} h_i(x)$$

- Violate CLT: 1. Finite N, 2. Dissimilar NN parameters, 3. Correlated NN parameters.
- Parametric tunings at NN initializations, that violate CLT, control field interactions in $S[\phi]$.

Different initializations for different interacting field theories!



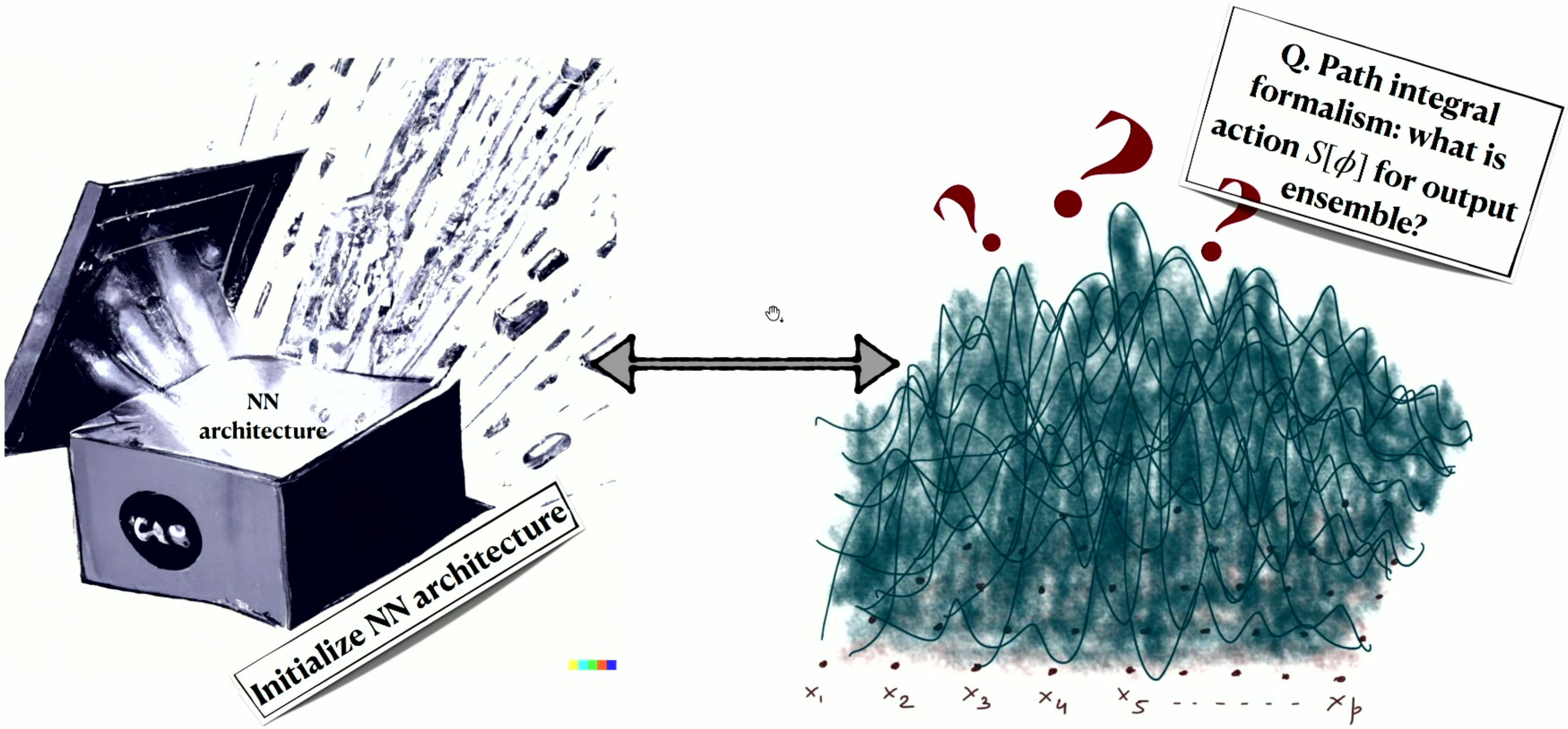
Related works



- ML for field theories on lattice
- Correspondences between learning dynamics and high energy physics
- Correspondences between initialized NNs and field theory
- Field theory & theoretical physics for deep learning
- Theory of NN at asymptotically large width

- Central Limit Theorem (CLT) constrains NN field theories as free ones.
- Three independent ways to violate CLT, i.e. turn on field interactions.

Summarize NNFT



Are NNFTs Quantum?

- NNFTs are Euclidean or statistical field theories.

- However, if **all** NNFT correlation functions satisfy **Osterwalder-Schrader axioms**, this field theory has analytic continuation to Lorentzian background. [Halverson 2021]

- Such NN architectures correspond to ***quantum*** field theories.

Deduce NNFT action $S[\phi]$

- NN field action $S[\phi]$ for generic architectures.

$$Z[J] = \int D\phi \, e^{-S_{\text{free}}[\phi] - S_{\text{int}} + \int d^d x J(x)\phi(x)}$$

- Free field action can be derived exactly.

$$S_{\text{free}}[\phi] = \frac{1}{2} \int d^d x_1 \, d^d x_2 \, \phi(x_1) \, G_c^{(2)}(x_1, x_2)^{-1} \phi(x_2)$$

Scalar NNFT:

Construct $S[\phi]$ given NN Architecture

[Halverson, A.M., Schwartz, Demirtas, Stoner 2023]

Deduce NNFT action $S[\phi]$

Start with a duality

NN 'parameter space'

$$G^{(n)}(x_1, \cdots, x_n) := \mathbb{E}[\phi(x_1)\cdots\phi(x_n)] = \int dh P(h)\phi(x_1)\cdots\phi(x_n)$$

Observables, e.g. NN Correlators

NN 'field space'

$$G^{(n)}(x_1, \ldots, x_n) = \int D\phi\, e^{-S[\phi]}\, \phi(x_1)\ldots\phi(x_n)$$

Deduce NNFT action $S[\phi]$

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Deduce NNFT action $S[\phi]$

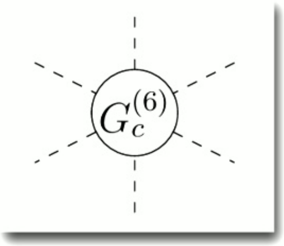
How do we get leading order NN field interactions?

$$S_{\text{int}} = \sum_{r=3}^{\infty} \int \prod_{i=1}^{r} d^d x_i \, g_r(x_1, \ldots, x_r) \, \phi(x_1) \ldots \phi(x_r)$$

Introduce a new set of Feynman rules, to construct NNFT couplings $g_r(x_1, \cdots, x_r)$, using connected correlators from **dual** parameter space.

Deduce NNFT action $S[\phi]$

New Feynman rules: connected correlators are internal vertices.



$$G^{(n)}(x_1, \cdots, x_n) := \mathbb{E}[\phi(x_1)\cdots\phi(x_n)] = \int dh P(h)\phi(x_1)\cdots\phi(x_n)$$

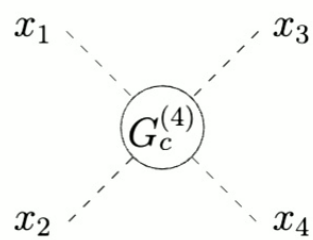
- CLT-violation at finite width, i.i.d. NN parameters $\quad G_c^{(r)} \propto \dfrac{1}{N^{r/2-1}}$.
- CLT-violation at finite width, non-i.i.d. NN parameters $G_c^{(r)} \to$ mixed N-scalings.

Eg: NNFT @ Finite N, i.i.d. parameters

- **Quartic coupling**

$$g_4(x_1,\ldots,x_4) = \frac{1}{4!}\left[\int dy_1 dy_2 dy_3 dy_4\, G_c^{(4)}(y_1,y_2,y_3,y_4)\, G_c^{(2)}(y_1,x_1)^{-1} G_c^{(2)}(y_2,x_2)^{-1} G_c^{(2)}(y_3,x_3)^{-1} G_c^{(2)}(y_4,x_4)^{-1} + \text{Comb.}\right] + O\left(\frac{1}{N^2}\right),$$

$$= \quad \text{[diagram]} \quad + O\left(\frac{1}{N^2}\right).$$

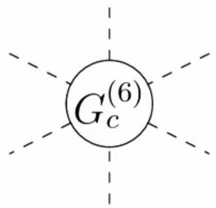


- **Perturbative NNFT action**

$$S[\phi] = S_{\text{free}}[\phi] - \int d^d x_1 \cdots d^d x_4\, g_4(x_1,\cdots,x_4)\,\phi(x_1)\cdots\phi(x_4) + O\left(\frac{1}{N^2}\right)$$

Deduce NNFT action $S[\phi]$

New Feynman rules: connected correlators are internal vertices.



$$G^{(n)}(x_1, \cdots, x_n) := \mathbb{E}[\phi(x_1)\cdots\phi(x_n)] = \int dh P(h)\phi(x_1)\cdots\phi(x_n)$$

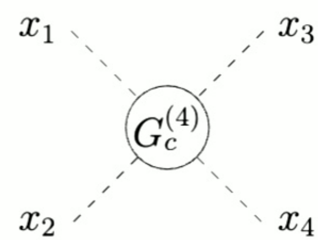
- CLT-violation at finite width, i.i.d. NN parameters $G_c^{(r)} \propto \frac{1}{N^{r/2-1}}$.
- CLT-violation at finite width, non-i.i.d. NN parameters $G_c^{(r)} \to$ mixed N-scalings.

Eg: NNFT @ Finite *N*, i.i.d. parameters

- **Quartic coupling**

$$g_4(x_1,\ldots,x_4) = \frac{1}{4!}\bigg[\int dy_1 dy_2 dy_3 dy_4\, G_c^{(4)}(y_1,y_2,y_3,y_4)\, G_c^{(2)}(y_1,x_1)^{-1} G_c^{(2)}(y_2,x_2)^{-1} G_c^{(2)}(y_3,x_3)^{-1} G_c^{(2)}(y_4,x_4)^{-1} + \text{Comb.}\bigg] + O\left(\frac{1}{N^2}\right),$$

$=$



$$+\, O\left(\frac{1}{N^2}\right).$$

- **Perturbative NNFT action**

$$S[\phi] = S_{\text{free}}[\phi] - \int d^d x_1 \cdots d^d x_4\, g_4(x_1,\cdots,x_4)\,\phi(x_1)\cdots\phi(x_4) + O\Big(\frac{1}{N^2}\Big)$$

Eg. $S[\phi]$ for Real-Life NN architecture

Network output $\phi(x) = W_i^1 \cos(W_{ij}^0 x_j + b_i^0)$

i.i.d. parameter distributions

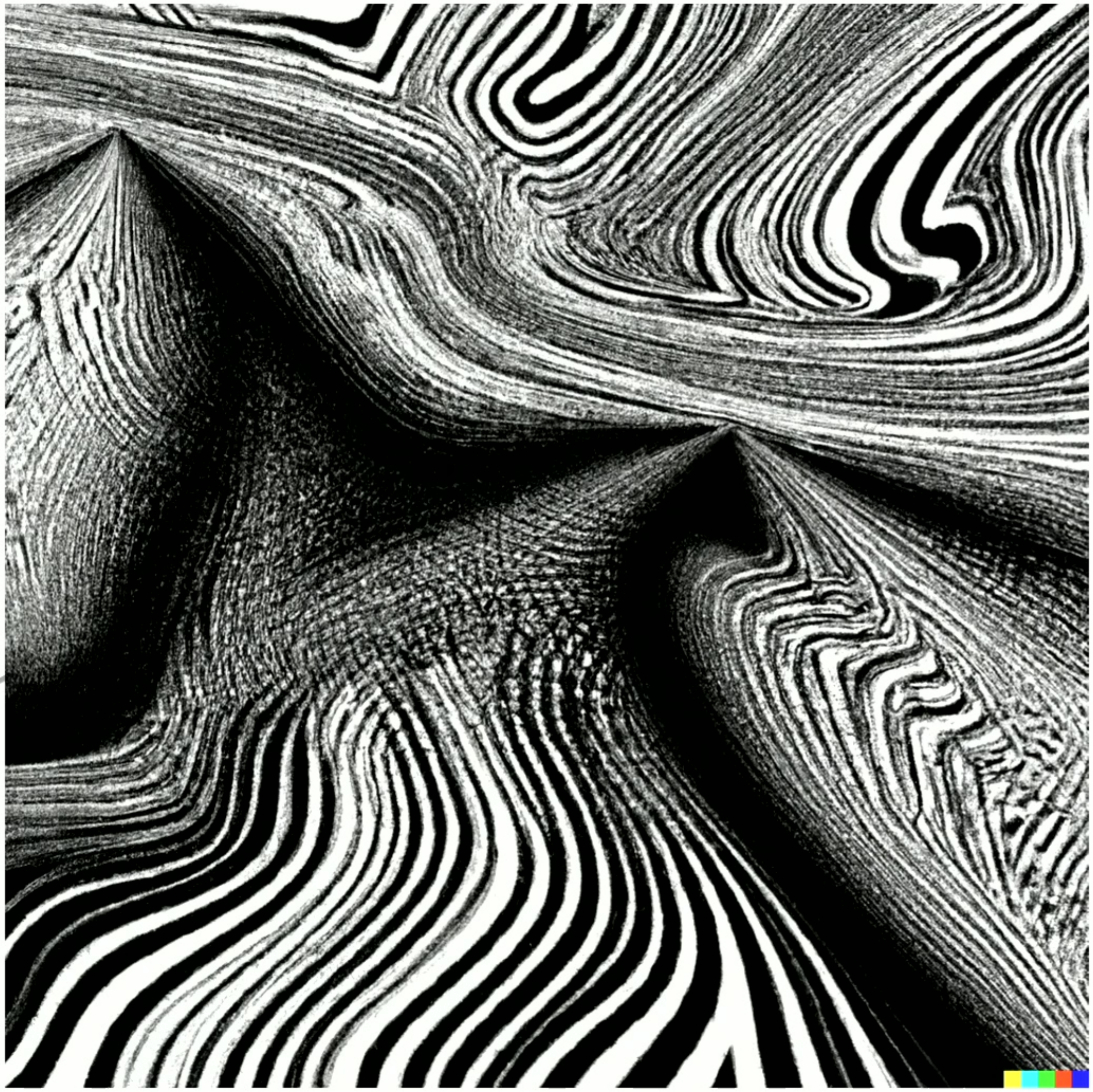
$$W^0 \sim \mathcal{N}(0, \sigma_{W_0}^2/d)$$
$$W^1 \sim \mathcal{N}(0, \sigma_{W_1}^2/N)$$
$$b^0 \sim \mathrm{Unif}[-\pi, \pi]$$

Interacting NNFT action (due to finite N), at leading order

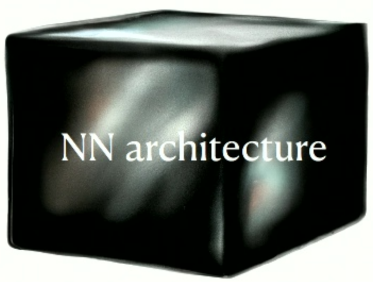
$$S_{\mathrm{Cos}}[\phi] = \frac{2\sigma_{W_0}^2}{\sigma_{W_1}^2 d} \int d^d x\, \phi(x)\, e^{-\frac{\sigma_{W_0}^2 \nabla_x^2}{2d}} \phi(x) \;-\; \int d^d x_1 \cdots d^d x_4 \left[\frac{4\sqrt{6}\pi^{3/2}\sigma_{W_0}^4}{N d^2 \sigma_{W_1}^4} \sum_{\mathcal{P}(abcd)} e^{-\frac{\sigma_{W_0}^2 \nabla_{r_{abcd}}^2}{6d}} \right.$$
$$\left. - \frac{8\pi\sigma_{W_0}^4}{N d^2 \sigma_{W_1}^4} \sum_{\mathcal{P}(ab,cd)} e^{-\frac{\sigma_{W_0}^2 (\nabla_{r_{ab}}^2 + \nabla_{r_{cd}}^2)}{2d}} \right] \phi(x_1) \cdots \phi(x_4) + O(1/N^2).$$

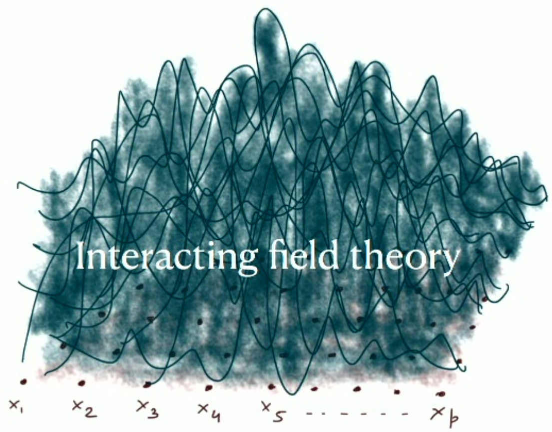
Scalar NNFT: Construct NN Architecture given $S[\phi]$

[Halverson, AM, Schwartz, Demirtas, Stoner 2023]



NN Architectures for $S[\phi]$





What are the rules to fix the architecture?

If target field action is

$$Z[J] = \int D\phi \, e^{-S[\phi] + \int d^d x J(x)\phi(x)}$$

$$S[\phi] = S_{\text{free}}[\phi] + \lambda \int d^d x_1 \cdots d^d x_r \, \mathcal{O}_\phi(x_1, \cdots, x_r)$$

NN Architectures for $S[\phi]$

NN architecture for exact free action $S_{\text{free}}[\phi]$ is easy.

Start with that network.

- $\lim N \to \infty$
- i.i.d. parameters $P(h) := P_G(h)$
- Intelligently guess other architecture details

NN Architectures for $S[\phi]$

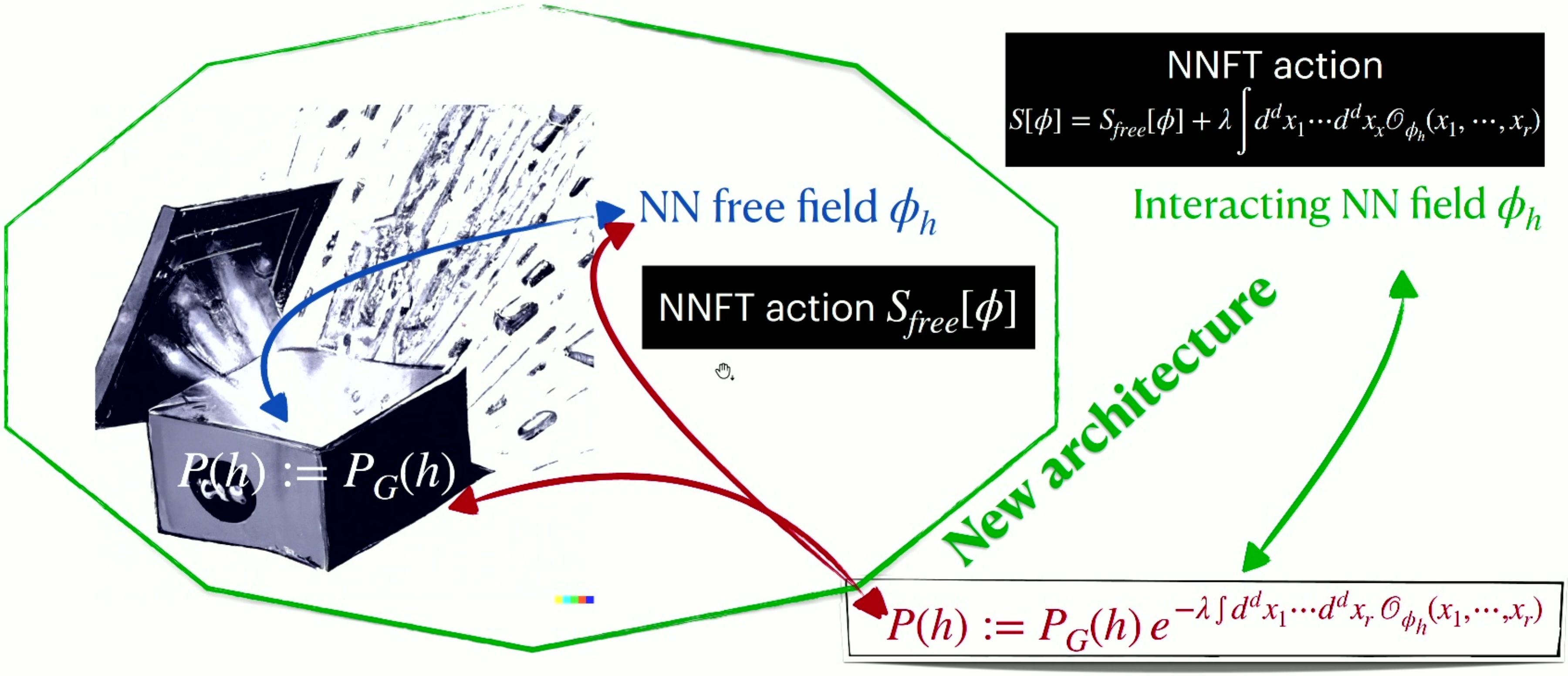
Take the architecture for free NNFT.

Next, deform NN parameters at infinite N.

- Redefine $P(h) := P_G(h)\, e^{-\lambda \int d^d x_1 \cdots d^d x_r\, \mathcal{O}_{\phi_h}(x_1, \cdots, x_r)}$

This inserts $S_{\text{int}}[\phi] = \lambda \int d^d x_1 \cdots d^d x_r \mathcal{O}_\phi(x_1, \cdots, x_r)$ in NNFT action.

Summarize NN Architectures for $S[\phi]$



Eg: Scalar $\lambda\phi^4$ theory

Target NNFT action $$S[\phi] = \int d^d x \left[\phi(x)(\nabla^2 + m^2)\phi(x) + \frac{\lambda}{4!}\phi(x)^4\right]$$

$$\nabla^2 := \frac{\partial^2}{\partial x^2}$$

Solution **Step A) architecture for free action**

$\lim N \to \infty$

$$\phi_{a,b,c}(x) = \sqrt{\frac{2\,\mathrm{vol}(B^d_\Lambda)}{\sigma_a^2 (2\pi)^d}} \sum_{i,j} \frac{a_i \cos(b_{ij} x_j + c_i)}{\sqrt{\mathbf{b}_i^2 + m^2}}$$

$$P_G(a) = \prod_i e^{-\frac{N}{2\sigma_a^2} a_i a_i}$$

$$P_G(b) = \prod_i P_G(\mathbf{b}_i) \text{ with } P_G(\mathbf{b}_i) = \mathrm{Unif}(B^d_\Lambda)$$

$$P_G(c) = \prod_i P_G(c_i) \text{ with } P_G(c_i) = \mathrm{Unif}([-\pi, \pi])$$

$$\boxed{G^{(2)}(p) = \frac{1}{p^2 + m^2}}$$

Eg: Scalar $\lambda\phi^4$ theory

Step B) architecture for full action $P(a,b,c) = P_G(a)P_G(b)P_G(c)\; e^{-\frac{\lambda}{4!}\int d^dx\,\phi_{a,b,c}(x)^4}$

Inserts $e^{-\frac{\lambda}{4!}\int d^dx\,\phi_{a,b,c}(x)^4}$ in free partition function.

$$Z[J] = \int da\,db\,dc\;\; P(a,b,c)\; e^{\int d^dx J(x)\,\phi_{a,b,c}(x)}$$

- NN parameters are Euclidean invariant, so is $S[\phi]$. ← Symmetry-via-duality theorem
- Correlators satisfy OS axioms. Analytic continuation to Lorentzian.

[Halverson, AM, Stoner 2021]

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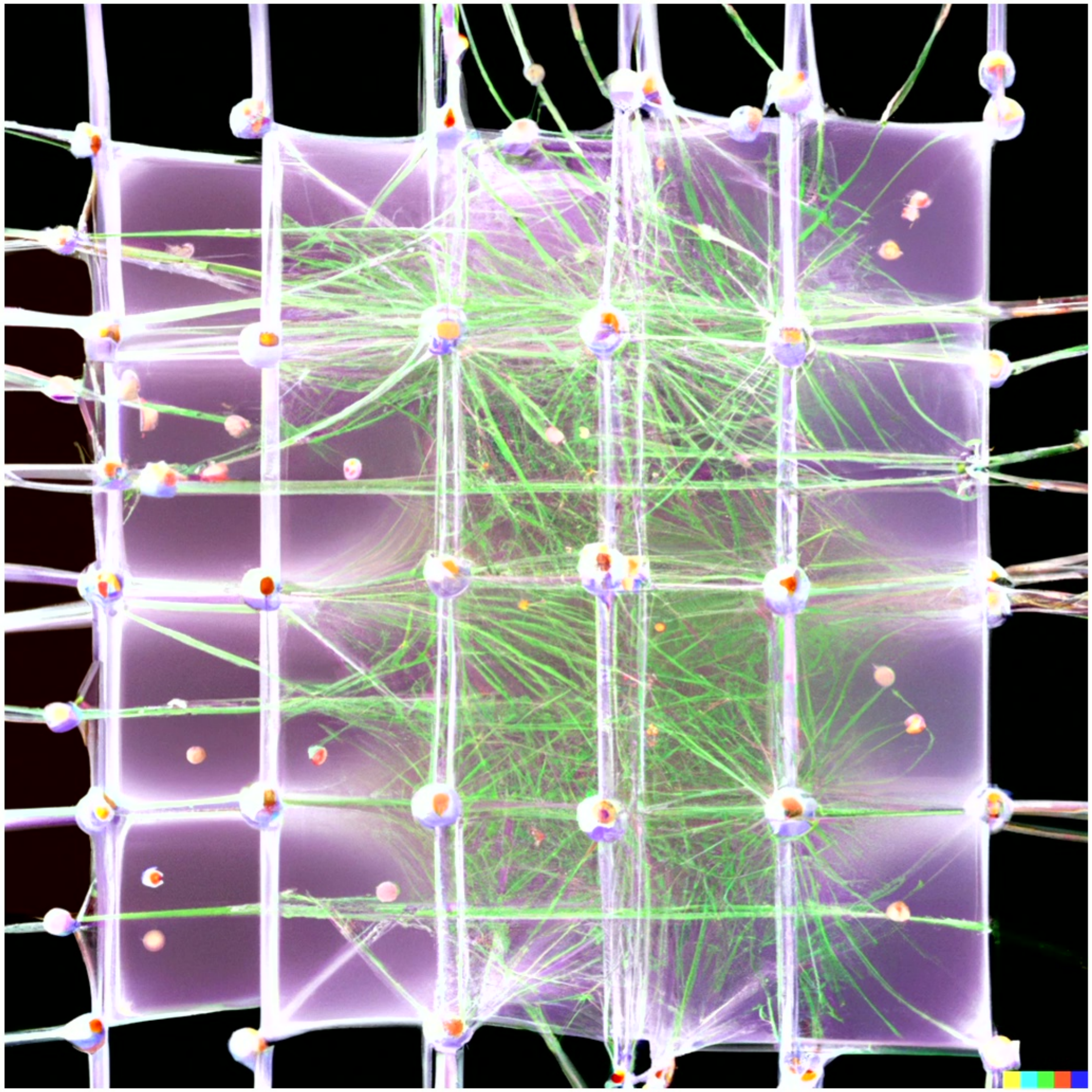
Grassmann NNFT: intro and free Dirac example

[work in progress, Halverson, AM, Frank, Ruehle 2024]



Intro to Grassmann NNFT

Grassmann CLT: a sum over N i.i.d. Grassmann random variables is Gaussian distributed as $N \to \infty$.

Consider $$\psi_j = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} X_{ij}, \quad j = 1, \cdots, d$$

i : statistical index
j : Grassmann index

Anticommutation relation $\{X_{ij}, X_{kl}\} = 0 \;\; \forall\ i, j, k, l$

Intro to Grassmann NNFT

Impose mean-free i.i.d. constraints on Grassmann variables

$$P(X) = \prod_{i=1}^{N} P(X_{i1}, \cdots, X_{id})$$

$$\mathbb{E}[X_{ij}] = 0 \ \forall \ i, j$$

$$P(X_{11}, \cdots, X_{1d}) \equiv \cdots\cdots \equiv P(X_{N1}, \cdots, X_{Nd})$$

$$P(X_{i1}, \cdots, X_{id}) \neq \prod_{j=1}^{d} P(X_{ij})$$

i : statistical index

j : Grassmann index

Intro to Grassmann NNFT

Grassmann CLT: a sum over N i.i.d. Grassmann random variables is Gaussian distributed as $N \to \infty$.

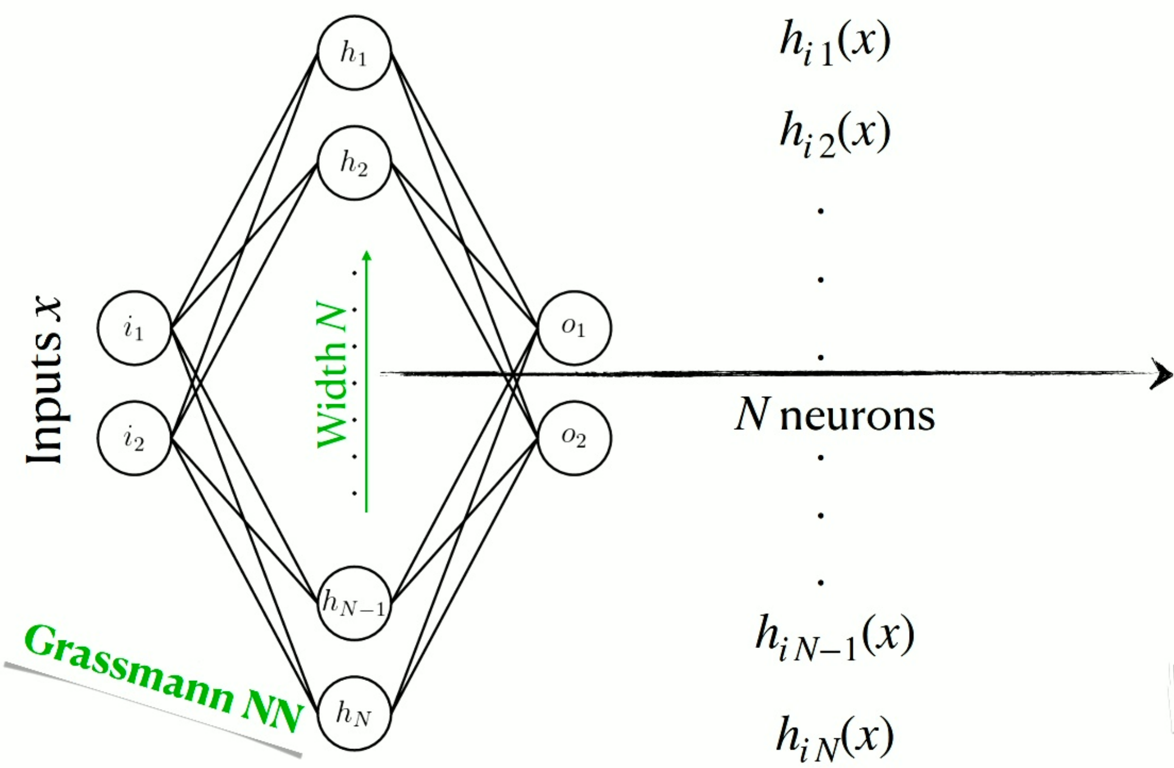
$$\kappa^{\psi}_{j_1 \cdots j_r} = \frac{\kappa^{X_{ij}}_{j_1 \cdots j_r}}{N^{r/2-1}}$$

i : statistical index
j : Grassmann index

When $N \to \infty$, all cumulants $r > 2$ vanish.

$$\kappa^{X_{ij}}_{j_1 \cdots j_r} := \mathbb{E}^{(c)}_{P(X_{i1}, \cdots, X_{id})}[X_{ij_1} \cdots X_{ij_r}]$$

Intro to Grassmann NNFT



Grassmann outputs $\psi_i(x)$

$$\psi_i(x) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} h_{ij}(x)$$

j : statistical index.

$i = 1, \cdots, D$ for different Grassmann fields.

Intro to Grassmann NNFT

Grassmann NNFT

$$\psi_i(x) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} a_{ij} \rho_j(x)$$

Case 1: a_{ij} Grassmanns, $\rho_j(x)$ c-numbers.

Case 2: a_{ij} c-numbers, $\rho_j(x)$ Grassmanns.

Intro to Grassmann NNFT

Case 1: a_{ij} Grassmanns, $\rho_j(x)$ c-numbers.

$$\psi_i(x) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} h_{ij}(x)$$

lim $N \to \infty$, cumulants $r > 2$ vanish: free Grassmann NNFT.

$$G^{(r)}_{c,\psi}(x_1, \cdots, x_r)\Big|_{i_1,\cdots,i_r} = \frac{G^{(r)}_{c,(h_{i_1},\cdots,h_{i_r})}(x_1, \cdots, x_r)}{N^{r/2-1}}$$

(a) Finite N, (b) Non-identical a_{ij} and other network parameters, (c) Statistical correlations in a_{ij} along axis j : turns on interactions in $S[\psi]$.

Intro to Grassmann NNFT

Case 1: a_{ij} Grassmanns, $\rho_j(x)$ c-numbers.

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(a) Finite N, (b) Non-identical a_{ij} and other network parameters, (c) Statistical correlations in a_{ij} along axis j : turns on interactions in $S[\psi]$.

Grassmann NNFT: free Dirac

Free Dirac NNFT: requires 8 degrees of freedom on Euclidean space, instead of 4.

Free Dirac propagator on Minkowski space:

$$\Delta^{(2)}(x,y) = \langle 0|T\psi(x)\bar{\psi}(y)|0\rangle$$

$$\Delta^{(2)}_{ij}(p) = \left(\frac{-i}{\gamma^\mu p_\mu + m}\right)_{ij}$$

↓

Wick rotate to Euclidean space space:

$$\langle 0|\psi(x)\psi^*(y)|0\rangle$$

Not Hermitian!

Intro to Grassmann NNFT

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$$\psi_i(x) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} h_{ij}(x)$$

lim $N \to \infty$, cumulants $r > 2$ vanish: free Grassmann NNFT.

$$G^{(r)}_{c,\psi}(x_1, \cdots, x_r)\Big|_{i_1,\cdots,i_r} = \frac{G^{(r)}_{c,(h_{i_1},\cdots,h_{i_r})}(x_1, \cdots, x_r)}{N^{r/2-1}}$$

(a) Finite N, (b) Non-identical a_{ij} and other network parameters, (c) Statistical correlations in a_{ij} along axis j : turns on interactions in $S[\psi]$.

Grassmann NNFT: free Dirac

Free Dirac NNFT: requires 8 degrees of freedom on Euclidean space, instead of 4.

Resolution by Osterwalder and Schrader:

Introduce auxiliary field χ: fills the role of $\bar{\psi}$, but not related to ψ through Hermitian conjugation.

$$G^{(2)}(x,y) = \langle 0|\psi(x)\chi(y)|0\rangle$$

$$G^{(2)}_{ij}(p) = \left(\frac{-1}{\gamma^\mu p_\mu + m}\right)_{ij}$$

Wick rotation $\gamma^0 \to -i\gamma^0 \qquad \gamma^k \to \gamma^k$

Grassmann NNFT: free Dirac

What is the architecture?

Free Dirac NNFT action

$$S_{\text{free}}[\Psi] = \int d^d x\, \chi(x)(-\gamma^\mu \partial_\mu - m)\psi(x).$$

w/ propagator

$$G^{(2)}_{ij}(p) = \left(\frac{-1}{\gamma^\mu p_\mu + m}\right)_{ij}$$

Grassmann NNFT: free Dirac

NN architecture solution

$$\Psi(x) = \begin{Bmatrix} \psi_i(x) \\ \chi_i(x) \end{Bmatrix}, \qquad i = 1, \cdots, D.$$

$\lim N \to \infty$

$$\psi_i(x) = \sqrt{\frac{2\text{vol}(B^d_\Lambda)}{N\sigma_a^2(2\pi)^d}} \sum_{j=1}^{N} (R_j)_{i\alpha} a^{(0)}_{\alpha,j} \cos(b_{j\mu}x^\mu + e_j)$$

$$\chi_i(x) = \sqrt{\frac{2\text{vol}(B^d_\Lambda)}{N\sigma_a^2(2\pi)^d}} \sum_{j=1}^{N} (R_j^T)_{i\alpha} a^{(1)}_{\alpha,j} \cos(b_{j\mu}x^\mu + e_j)$$

Grassmann NNFT: free Dirac

NN architecture solution

$$R_j = \Big(\sum_{\mu=1}^{d} \gamma^{\mu}_{D\times D} b_{j\mu} + m\mathbf{1}_{D\times D}\Big)^{-1/2}$$

$$P(a,b,e) = P_G(a)P_G(b)P_G(e)$$

$\lim N \to \infty$ and i.i.d. parameters along statistical axis:

$$P_G(a) = \prod_{i=1}^{N} P_G(\mathbf{a}_i), \quad \text{with} \quad P_G(\mathbf{a}_i) = e^{-\frac{1}{\sigma_a^2} a^{(0)}_{\alpha,i} a^{(1)}_{\alpha,i}}, \quad \alpha = 1, \cdots, D,$$

$$P_G(b) = \prod_{i=1}^{N} P_G(\mathbf{b}_i), \quad \text{with} \quad P_G(\mathbf{b}_i) = \text{Unif}(B^d_\Lambda) \quad \text{and} \quad \mathbf{b}_i = (b_{i1}, \cdots, b_{id}),$$

$$P_G(e) = \prod_{i=1}^{N} P(e_i), \quad \text{with} \quad P(e_i) = \text{Unif}([-\pi, \pi]),$$

NN hyperparameters: m, Λ