Non-Perturbative Non-Lagrangian Neural Network Field Theories

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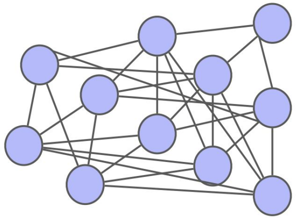

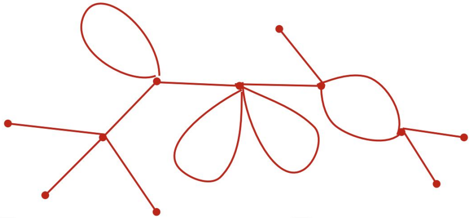

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Based on arxiv: 2008.08601, 2106.00694 &
220x.xxxxx (w/ Jim Halverson, Matt Schwartz,
Mehmet Demirtas & Keegan Stoner)

Punchlines

- Ensembles of Neural Network outputs behave as Euclidean Field Theories.
- Neural Network Gaussian Processes (NNGP) corresponds to Free Field Theories. Deviations from NNGP turn on interaction terms.
- Small & large deviations leads to weakly coupled & non-perturbative Neural Network Field Theories, respectively.
- NNs also have a dual “parameters + architecture” description.
- Symmetries, correlators, partition function of NN Field Theories can be studied in this dual framework; knowledge of action isn’t necessary.

References & Related Works

Based on:

1. arXiv:2008.08601
2. arXiv:2106.00694
3. arXiv:220x.xxxxx (to appear soon)

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

What are Neural Networks?

Backbones of Deep Learning.

Outputs are functions of inputs, with continuous learnable parameters θ and discrete hyperparameter N.

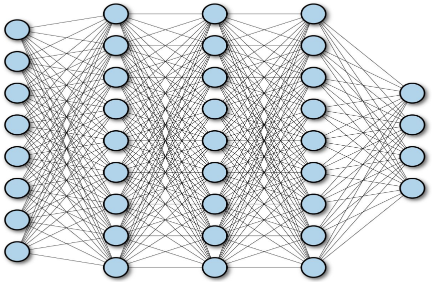
$$f_{\theta,N} : \mathbb{R}^{d_{\text{in}}} \to \mathbb{R}^{d_{out}}$$

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

Fully Connected NN :

$\longrightarrow$ "depth"

$\longrightarrow$ Width N



input $\longrightarrow$ hidden $\longrightarrow$ …
$\longrightarrow$ hidden$\longrightarrow$ output

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

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

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

Action S[ϕ] is the 'log-likelihood'

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

Outline

1. Free Field Theories in Neural Networks
2. Weakly Coupled Field Theories in Neural Networks
3. Non-Perturbative Neural Network Field Theories
4. Symmetry, Partition Function, Cumulants via Duality

Free Field Theories in Neural Networks

Free Neural Network Field Theories

Limit N $\longrightarrow \infty$: NN output is a sum over infinite independently and identically distributed (iid) random variables, drawn from a Gaussian distribution.

NNGP references (ML): [Neal], [Williams] 1990's , [Lee et al., 2017], [Matthews et al., 2018] , [Yang, 2019], [Yang, 2020]

Neural Network Gaussian Process

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

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

log-likelihood: $S = \frac{1}{2}\int d^{d_{\rm in}}x\, d^{d_{\rm in}}x'\; f(x)\Xi(x,x')f(x')$

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

Free Field Theory:

"free" := Gaussian distributions on field space, given by Feynman path integral:

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

e.g., free scalar field theory.

$$S[\phi] = \int d^dx\, \phi(x)(\Box + m^2)\phi(x)$$

Free Neural Network Field Theories

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}

$$G^{(2)}_{\mathrm{GP}}(x_1, x_2) = K(x_1, x_2)$$

$=$ 

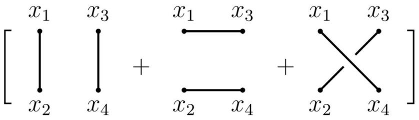
Physics analogy: NN Gaussian Process $\Longleftrightarrow$ Free Field Theory, on Euclidean metric (without particle interactions).

Test on 3 different architectures at various widths; 100 expt, each with 10^5 Nets.

Feynman diagrams for NN correlators.

$$\Delta G^{(n)}(x_1, \ldots, x_n) = G^{(n)}(x_1, \ldots x_n) - G^{(n)}_{\mathrm{GP}}(x_1, \ldots, x_n)$$

$$\Delta G^{(4)} = \frac{1}{n_{\mathrm{nets}}} \sum_{\alpha}^{n_{\mathrm{nets}}} f_\alpha(x_1) f_\alpha(x_2) f_\alpha(x_3) f_\alpha(x_4) - \Big[\cdots + \cdots + \cdots \Big]$$

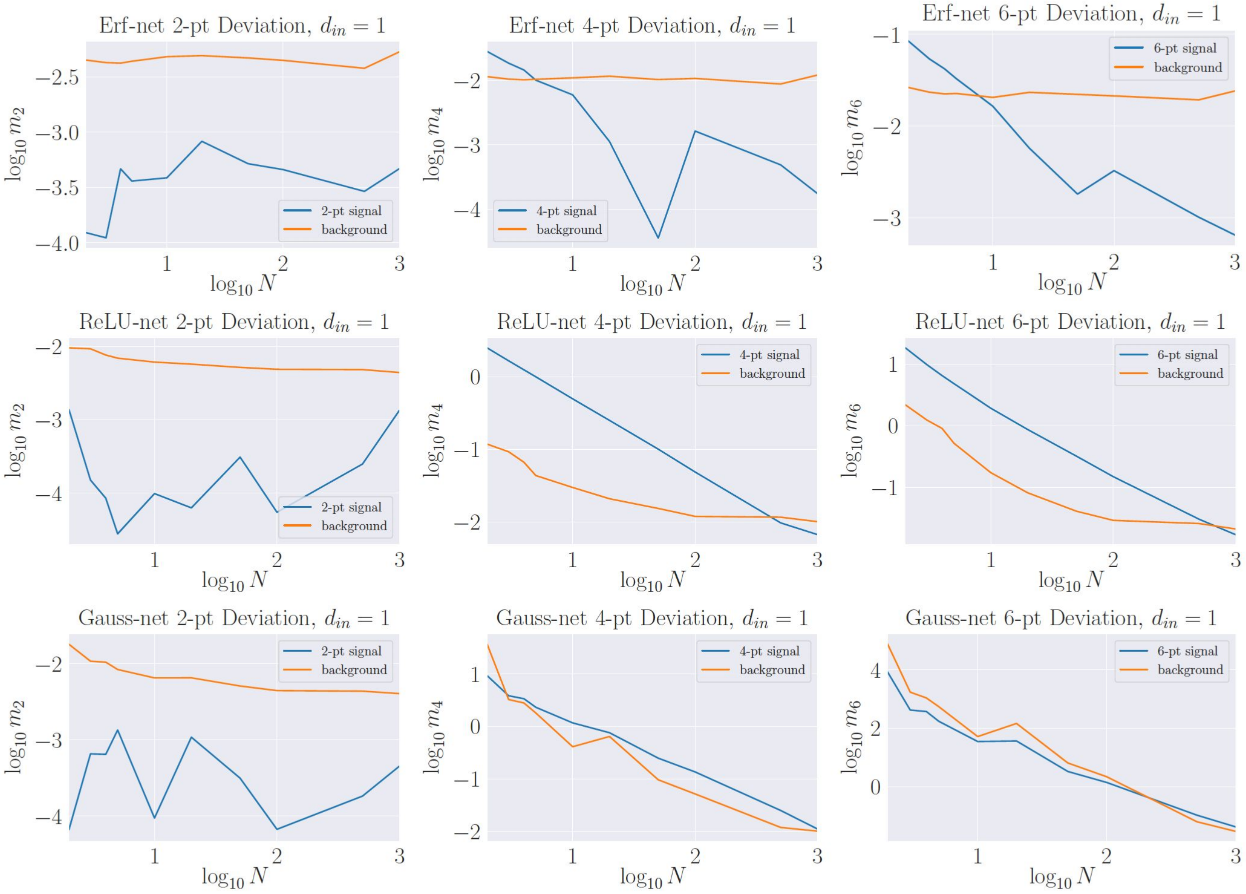


Erf-net: $\sigma(z) = \mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z dt\, e^{-t^2}$

Gauss-net: $\sigma(x) = \frac{\exp(W x + b)}{\sqrt{\exp[2(\sigma_b^2 + \frac{\sigma_W^2}{d_{\mathrm{in}}} x^2)]}}$

ReLU-net: $\sigma(z) = \begin{cases} 0 & z < 0 \\ z & z \geq 0 \end{cases}$

Some Results



$$m_n = \Delta G^{(n)} / G^{(n)}_{\text{GP}}$$

For n>2 , experimentally determined scaling

$$\Delta G^{(n)} \propto N^{-1}$$

NN distributions must receive 1/N suppressed non-Gaussian corrections, close to NNGP.

Weakly Coupled Field Theories in Neural Networks

Weakly Coupled Neural Network Field theories

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

More NN parameters → simpler NN Field Theory actions.

Closeness to NNGP → "irrelevance" of non-Gaussian terms in Field Theory.

Field Theory: κ more irrelevant than λ, can be ignored. Further, κ is 1/N suppressed relative to λ.

Close to the GP, introduce EFT interaction terms to describe NN Field Theory action.

$$S = S_{\mathrm{GP}} + \Delta S$$

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

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

$$= \frac{\int df \;\, f(x_1) \dots f(x_n) \left[1 - \int d^{d_{\mathrm{in}}}x\, g_k f(x)^k + O(g_k^2)\right] \; e^{-S_{\mathrm{GP}}}/Z_{\mathrm{GP},0}}{\int df \;\, \left[1 - \int d^{d_{\mathrm{in}}}x\, g_k f(x)^k + O(g_k^2)\right] e^{-S_{\mathrm{GP}}}/Z_{\mathrm{GP},0}}$$

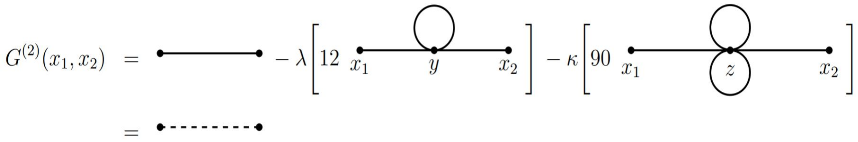
Mean-free NN distributions: $S = S_{\mathrm{GP}} + \int d^{d_{\mathrm{in}}}x \;\, \left[\lambda\, f(x)^4 + \kappa\, f(x)^6\right]$

Predict NN correlators by Feynman diagram.

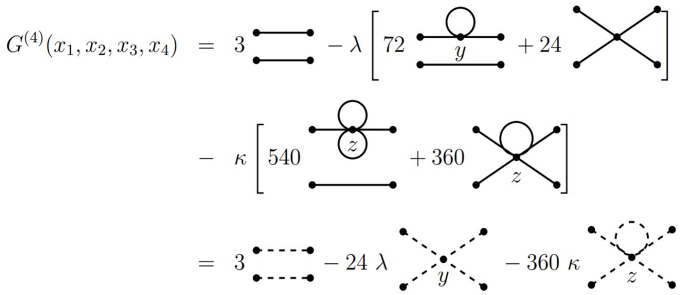
Weakly Coupled Neural Network Field Theories

Estimate λ from 4-pt function expts

Fully connected feedforward NNs have an exact
2-pt function at all non-Gaussianities.



$$= K(x_1, x_2),$$

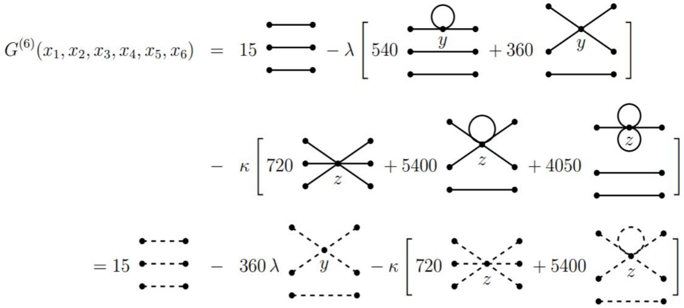


$$\begin{aligned} &= K(x_1, x_2)K(x_3, x_4) + K(x_1, x_3)K(x_2, x_4) + K(x_1, x_4)K(x_2, x_3) \\ &- 24 \int d^{d_{\text{in}}}y \, \lambda \, K(x_1, y)K(x_2, y)K(x_3, y)K(x_4, y) \\ &- 360 \int d^{d_{\text{in}}}z \, \kappa \, K(x_1, z)K(x_2, z)K(x_3, z)K(x_4, z)K(z, z) \end{aligned}$$

$$\lambda = \frac{K(x_1, x_2)K(x_3, x_4) + K(x_1, x_3)K(x_2, x_4) + K(x_1, x_4)K(x_2, x_3) - G^{(4)}(x_1, x_2, x_3, x_4)}{24 \int d^{d_{\text{in}}}y \, K(x_1, y)K(x_2, y)K(x_3, y)K(x_4, y)}$$

λ is a rank-4 tensor, we average over all its elements

Weakly Coupled Neural Network Field Theories

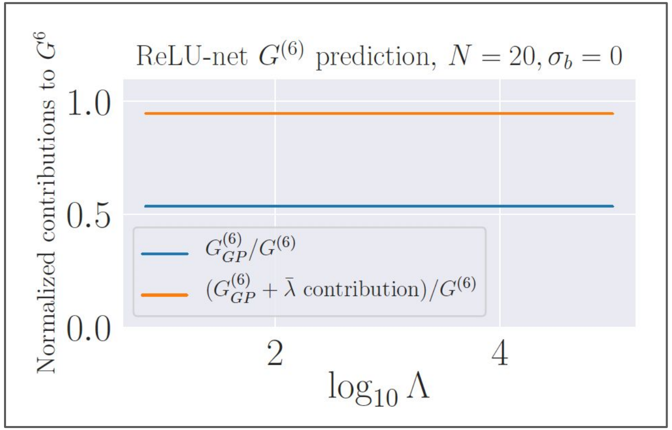


$$
\begin{aligned}
= & \Big[K_{12}K_{34}K_{56} + K_{12}K_{35}K_{46} + K_{12}K_{36}K_{45} + K_{13}K_{24}K_{56} + K_{13}K_{25}K_{46} + K_{13}K_{26}K_{45} + K_{14}K_{23}K_{56} \\
+ & K_{14}K_{25}K_{36} + K_{14}K_{26}K_{35} + K_{15}K_{23}K_{46} + K_{15}K_{24}K_{36} + K_{15}K_{26}K_{34} + K_{16}K_{23}K_{45} + K_{16}K_{24}K_{35} \\
+ & K_{16}K_{25}K_{34}\Big] - 24 \int d^{d_{\text{in}}}y\, \lambda \Big[K_{1y}K_{2y}K_{3y}K_{4y}K_{56} + K_{1y}K_{2y}K_{3y}K_{5y}K_{46} + K_{1y}K_{2y}K_{4y}K_{5y}K_{36} \\
+ & K_{1y}K_{3y}K_{4y}K_{5y}K_{26} + K_{2y}K_{3y}K_{4y}K_{5y}K_{16} + K_{1y}K_{2y}K_{3y}K_{6y}K_{45} + K_{1y}K_{2y}K_{4y}K_{6y}K_{35} \\
+ & K_{1y}K_{3y}K_{4y}K_{6y}K_{25} + K_{2y}K_{3y}K_{4y}K_{6y}K_{15} + K_{1y}K_{2y}K_{5y}K_{6y}K_{34} + K_{1y}K_{3y}K_{5y}K_{6y}K_{24} \\
+ & K_{2y}K_{3y}K_{5y}K_{6y}K_{14} + K_{1y}K_{4y}K_{5y}K_{6y}K_{23} + K_{2y}K_{4y}K_{5y}K_{6y}K_{13} + K_{3y}K_{4y}K_{5y}K_{6y}K_{12}\Big] \\
- & 720 \int d^{d_{\text{in}}}z\, \kappa\, K_{1z}K_{2z}K_{3z}K_{4z}K_{5z}K_{6z} - 360 \int d^{d_{\text{in}}}z\, \kappa \Big[K_{zz}K_{1z}K_{2z}K_{3z}K_{4z}K_{56} \\
+ & K_{zz}K_{1z}K_{2z}K_{3z}K_{5z}K_{46} + K_{zz}K_{1z}K_{2z}K_{4z}K_{5z}K_{36} + K_{zz}K_{1z}K_{3z}K_{4z}K_{5z}K_{26} \\
+ & K_{zz}K_{2z}K_{3z}K_{4z}K_{5z}K_{16} + K_{zz}K_{1z}K_{2z}K_{3z}K_{6z}K_{45} + K_{zz}K_{1z}K_{2z}K_{4z}K_{6z}K_{35} \\
+ & K_{zz}K_{1z}K_{3z}K_{4z}K_{6z}K_{25} + K_{zz}K_{2z}K_{3z}K_{4z}K_{6z}K_{15} + K_{zz}K_{1z}K_{2z}K_{5z}K_{6z}K_{34} \\
+ & K_{zz}K_{1z}K_{3z}K_{5z}K_{6z}K_{24} + K_{zz}K_{2z}K_{3z}K_{5z}K_{6z}K_{14} + K_{zz}K_{1z}K_{4z}K_{5z}K_{6z}K_{23} \\
+ & K_{zz}K_{2z}K_{4z}K_{5z}K_{6z}K_{13} + K_{zz}K_{3z}K_{4z}K_{5z}K_{6z}K_{12}\Big],
\end{aligned}
$$

Use λ to predict 6-pt function.

Expt. 6-pt - GP predictions = NGP correction

$$
\begin{aligned}
\delta'(x_1,\dots,x_6) \;:=\; & G^{(6)}(x_1,\dots,x_6) - \sum_{\text{15 combinations}} \Big[K(x_i,x_j)K(x_k,x_l)K(x_m,x_n) \\
& - 24 \int d^{d_{\text{in}}}y\; \lambda\; K(x_i,y)K(x_j,y)K(x_k,y)K(x_l,y)K(x_m,x_n)\Big]
\end{aligned}
$$



Non-Perturbative Neural Network Field Theories

Non-Perturbative Neural Network Field Theories

Small width and/or large parameter correlations violate i.i.d. assumption and CLT by large extent.

Large non-Gaussianities lead to non-perturbative NN field theories, with the action often unknown.

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

NN processes can be studied using parameter distributions, too.

Field Space

$$G^{(n)}(x_1, \cdots, x_n) = \frac{1}{Z} \int D\phi \, e^{-S[\phi]} \, \phi(x_1) \cdots \phi(x_n)$$

Parameter Space

$$G^{(n)}(x_1, \cdots, x_n) = \frac{1}{N^{n/2}} \sum_{i_1, \cdots, i_n} \int Dh \, P(h) \, h_{i_1}(x_1) \cdots h_{i_n}(x_n)$$

Same observables can be studied without knowledge of actions.

Deduce symmetries, cumulants, PDF etc.

Symmetry, Cumulants, Partition Function via Duality

Symmetry via Duality

NNGP: symmetries of 2-pt function determine symmetries of NN distribution.

$$G^{(2)}_{i_1 i_2}(x_1, x_2) = \delta_{i_1 i_2} K(x_1, x_2)$$

Mean-free SO(D) invariant parameter distributions lead to SO(D) invariant NNGP action. D := output dim.

$$G^{(2n)}_{i_1,\ldots,i_{2n}}(x_1,\ldots,x_{2n}) = \sum_{P\in\text{Wick}(2n)} \delta_{i_{a_1} i_{b_1}} \ldots \delta_{i_{a_n} i_{b_n}} K(x_{a_1}, x_{b_1}) \ldots K(x_{a_n}, x_{b_n})$$

R ∈ SO(D), output transforms as $f_i \mapsto R_{ij} f_j$.

$$\delta_{ik} \mapsto R_{ij} R_{kl} \delta_{jl} = (R\,R^T)_{ik} = \delta_{ik}$$

Break i.i.d. assumptions: n>2 correlators receive Field Theoretic non-Gaussian corrections.

NN action unknown: symmetries can't be deduced in field space.

Study NN correlators in parameter space.

NN action is invariant

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

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

Symmetry via Duality

Absorb transformations of correlators into transformations of parameters $\theta_T \subset \theta$.

Invariance of P_{θ_T} leads to invariance of NN action S[f].

$$\mathbb{E}[f(x_1)\dots f(x_n)] = \frac{1}{Z_f}\int Df\, e^{-S[f]}\, f(x_1)\dots f(x_n)$$

$$= \frac{1}{Z_f}\int Df'\, e^{-S[f']}\, f'(x_1)\dots f'(x_n) = \frac{1}{Z_f}\int D[\Phi f]\, e^{-S[\Phi f]}\, \Phi(f(x_1'))\dots \Phi(f(x_n'))$$

$$= \frac{1}{Z_f}\int Df\, e^{-S[f]}\, \Phi(f(x_1'))\dots \Phi(f(x_n')) = \mathbb{E}[\Phi(f(x_1'))\dots \Phi(f(x_n'))]$$

Symmetries of NN input and output layers → symmetries of space-time and internal symmetries of fields respectively.

Examples:

(a) SO(D) Output Symmetry: Final linear layer parameters drawn from mean-free SO(D) invariant distributions.

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

$$P_W = P_{R^{-1}\tilde{W}} = P_{\tilde{W}} \qquad P_b = P_{R^{-1}\tilde{b}} = P_{\tilde{b}}$$

$$R \in SO(D) \qquad f_i \mapsto R_{ij} f_j$$

(a) SO(d) Input Symmetry: First linear layer parameters drawn from mean-free SO(d) invariant distributions.

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

$$R \in SO(d) \qquad x_i \mapsto x_i' = R_{ij} x_j$$

Cumulants via Duality

Cumulant Generating Functional (CGF) of NN field theory in terms of cumulants of neurons in parameter space.

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

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

Correlated parameter distributions.

$$P(h|\vec{a} = \vec{0}) = \prod_{i=1}^{N} P_i(h_i) \qquad \vec{\alpha} = \{\alpha_1, \cdots, \alpha_q\}$$

$$W[J] = \sum_{r=0}^{\infty} \Big(\prod_{i=1}^{r} \int dx_i \Big) \frac{G^{(r)}_{\mathrm{con},\phi}(x_1,\cdots,x_r) J(x_1) \cdots J(x_r)}{r!}$$

$$= \log \left[\int Dh\, P(h|\vec{\alpha})\, e^{\frac{1}{\sqrt{N}} \sum_{i=1}^{N} \int dx\, h_i(x) J(x)} \right]$$

Finite width, no parameter correlations:

$$G^{(r)}_{\mathrm{con},\phi}(x_1, \cdots, x_r) = \frac{G^{(r)}_{\mathrm{con},h_i}(x_1,\cdots,x_r)}{N^{r/2}}$$

Finite width, parameters correlated: NN field theory cumulants receive contributions from multiple cumulants of all neurons.

Partition Function via Duality

Edgeworth Expansion: Inverse Fourier transform of NN Field Theory CGF to obtain the PDF, and the partition function.

$$Z_\phi[J] = \int D\phi P_\phi \, e^{i\int dx\, J(x)\phi(x)}$$

$$W_\phi[J] = \log Z_\phi[J]$$

PDF of Non-Perturbative NNFT $\longrightarrow$ perturbative expansions around PDF of Free NNFT.

$$P_\phi = \int DJ \exp\Big(\sum_{r=3}^{\infty} \frac{(-i)^r}{r!} \int \prod_{i=1}^{r} d^d x_i G^{(r)}_{\text{con},\phi}(x_1, \cdots, x_r) \frac{\partial}{\partial\phi(x_1)} \cdots \frac{\partial}{\partial\phi(x_r)}\Big)$$

$$\times \exp\Big(-i\int dx\, J(x)\phi(x) - \frac{1}{2}\int dx_1 dx_2\, J(x_1) G^{(2)}_{\text{con},\phi}(x_1,x_2) J(x_2)\Big).$$

Cumulants are expressed via parameter space.

$N \to \infty, \vec{\alpha} \to \vec{0}$: Free NNFT PDF

$$P_\phi = \exp\Big(-\frac{1}{2}\int dx_1 dx_2\, \phi(x_1)\Xi(x_1,x_2)\phi(x_2)\Big)$$

$$\int dx'\, \Xi(x_1, x') G^{(2)}_{\text{con},\phi}(x', x_2) = \delta(x_1 - x_2)$$

Partition Function for NN Field Theory.

$$Z_{\phi,\alpha}[J=0] = Z_{\phi,\vec{\alpha}=0}[J=0] + \prod_{i=1}^{N} \sum_{r=1}^{\infty} \sum_{j_1,\cdots,j_r=1}^{q} \frac{\alpha_{j_1}\cdots\alpha_{j_r}}{r!} \times$$

$$\int D\phi\, Dt\, e^{i\int dx\, t(x)\phi(x)} \mathbb{E}_{p_i(h_i)}\Big[\mathcal{P}_{r,\{j_1,\cdots,j_r\}}\big|_{\vec{\alpha}=0} e^{-\frac{i}{\sqrt{N}}\int dx\, t(x) h_i(x)}\Big]$$

where $\mathcal{P}_{r,\{s_1,\cdots,s_r\}} := \frac{1}{P(h|\vec{\alpha})} \partial_{\alpha_{s_1}} \cdots \partial_{\alpha_{s_r}} P(h|\vec{\alpha})$

Conclusions

- NN output distributions have a field space and a parameter space description.
- Field space description leads to Free Field theories, Weakly Coupled Field Theories and Non-Perturbative Non-Lagrangian Field Theories respectively for NNGP, small and large violations of CLT.
- When NN output correlators satisfy Osterwalder-Schrader axioms, NNs define Quantum Field Theories.
- More parameters in NN towards GP limit, lesser non-Gaussian coefficients in NN Field Theory.
- Less parameters, or parameter correlations in NN, non-perturbative field theory with unknown action, but observables can be studied in parameter space to deduce properties of NN Field Theory action.
- Learning symmetries, cumulants, and expression for partition function for non-perturbative non-Lagrangian NN Field Theories can be helpful for Physics.

Thank You!

Questions?

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