## **Tensor programs**

Eugene Golikov

May 17, 2021

École Polytechnique Fédérale de Lausanne, Switzerland

### Tensor programs series:

- 1. Formalism:
  - Scaling Limits of Wide Neural Networks with Weight Sharing.
- 2. Formalism explained: ← today's talk
  - TP1: Wide Networks of any Architecture are Gaussian Processes.
  - TP2: Neural Tangent Kernel of any Architecture.
  - TP3: Neural Matrix Laws.
- 3. Applications: ← Greg's talk
  - Feature Learning in Infinite-Width Neural Networks.

Motivation: maximal-update

parameterization

Consider an L-hidden-layer MLP:

$$\underbrace{f = W^{L+1} x^L}_{\text{output}}, \quad \underbrace{x^l = \phi(h^l)}_{\text{activations}}, \quad \underbrace{h^l = W^l x^{l-1}}_{\text{pre-activations}} \quad \forall l \in [L], \tag{1}$$

where  $W^I \in \mathbb{R}^{n_I \times n_{I-1}}$  and suppose  $n_1 = \ldots = n_L = n$ .

Define a weight update:  $\Delta W_t^I = W_t^I - W_0^I$ .

This gives a hidden representation update:

$$\Delta h_t^{l} = \Delta W_t^{l} x_t^{l-1} + W_0^{l} \Delta x_t^{l-1}, \tag{2}$$

and an output update:

$$\Delta f_t = \Delta W_t^{L+1} x_t^L + W_0^{L+1} \Delta x_t^L. \tag{3}$$

#### Definition

For  $l \in [L+1]$ , we say  $W^l$  is updated maximally if  $\Delta W_t^l x_t^{l-1} = \Theta(1) \ \forall t \geq 1$  and input  $\xi$ :

$$\Delta h_t^l = \underbrace{\Delta W_t^l x_t^{l-1}}_{\text{finite as } n \to \infty} + W_0^l \Delta x_t^{l-1}, \tag{4}$$

#### Definition

We say  $W^{L+1}$  is initialized maximally if  $W_t^{L+1} \Delta x_t^L = \Theta(1) \ \forall t \geq 1$  and input  $\xi$ .

$$\Delta f_t = \underbrace{\Delta W_t^{L+1} x_t^L}_{\text{finite when updated maximally}} + \underbrace{W_0^{L+1} \Delta x_t^L}_{\text{finite as } n \to \infty}.$$
 (5)

- Standard parameterization:  $\Delta f_t = \omega(1)$  output blows up;
- NTK parameterization:  $W_0^{L+1} \Delta x_t^L = o(1)$  features are not learned;
- $\mu$ **P-paramaterization:** to be discussed below OK.

Suppose L = 2:

$$\underbrace{\bar{\chi} = \psi(\bar{h}), \ \bar{h} = Wx}_{\text{second hidden layer}}, \qquad \underbrace{\bar{\chi} = \phi(h), \ h = U\xi}_{\text{first hidden layer}},$$

where  $\xi \in \mathbb{R}$ ,  $V \in \mathbb{R}^{1 \times n}$ ,  $W \in \mathbb{R}^{n \times n}$ ,  $U \in \mathbb{R}^{n \times 1}$ .

Apply maximal update parameterization ( $\mu P$ ):

$$V = v/\sqrt{n}, \quad W = w, \quad U = \sqrt{n}u,$$

where v, w, and u are the trainable parameters initialized as  $v_{1\beta}$ ,  $w_{\alpha\beta}$ ,  $u_{\alpha1} \sim \mathcal{N}(0, 1/n)$ . Compare with other parameterizations:

- Standard: V = v, W = w, U = u initialized as  $v_{1\beta}$ ,  $w_{\alpha\beta} \sim \mathcal{N}(0, 1/n)$ ,  $u_{\alpha 1} \sim \mathcal{N}(0, 1)$ .
- NTK:  $V = v/\sqrt{n}$ ,  $W = w/\sqrt{n}$ , U = u initialized as  $v_{1\beta}$ ,  $w_{\alpha\beta}$ ,  $u_{\alpha1} \sim \mathcal{N}(0,1)$ .

Substitute V, W, and U with  $v/\sqrt{n}$ , w, and  $\sqrt{n}u$ :

$$\underbrace{f = v\bar{x}/\sqrt{n}}_{\text{output}}, \quad \underbrace{\bar{x} = \phi(\bar{h}), \ \bar{h} = wx}_{\text{second hidden layer}}, \quad \underbrace{x = \phi(h), \ h = \sqrt{n}u\xi}_{\text{first hidden layer}}, \quad (6)$$

Consider an SGD update with batch  $(x_t, y_t)$  and learning rate = 1:

$$v_{t+1} = v_t - \chi_t \bar{x}_t^{\top} / \sqrt{n}, \quad w_{t+1} = w_t - \chi_t d\bar{h}_t x_t^{\top} / n, \quad u_{t+1} = u_t - \chi_t dh_t \xi_t / \sqrt{n},$$
 (7)

where

- $\chi_t = \mathcal{L}'(f_t(\xi_t), y_t) \in \mathbb{R}$  gradient wrt output;
- $dh_t = n\nabla_h f_t(\xi_t)$  (scaled) gradient wrt pre-activations.

Recall w = W and  $W_{t+1} = W_0 + \Delta W_{t+1}$ ; we get then:

$$\Delta W_{t+1} = \Delta W_t - \chi_t \frac{d\bar{h}_t x_t^{\top}}{n} = \Delta W_t - \sum_{s=0}^t \chi_s \frac{d\bar{h}_s x_s^{\top}}{n}.$$
 (8)

#### Do we update maximally?

$$\bar{h}_{t+1} = W_{t+1} x_{t+1} = W_0 x_{t+1} + \underbrace{\Delta W_{t+1} x_{t+1}}_{\text{needs to be } \Theta(1)} = W_0 x_{t+1} - \sum_{s=0}^{t} \chi_s \underbrace{d\bar{h}_s}_{\text{a vector with}} \underbrace{x_s^\top x_{t+1}}_{\text{n}} . \tag{9}$$

### Do we update maximally?

$$d\bar{h}_s = \Theta_{n \to \infty}(1)$$
?  $\frac{x_s^\top x_{t+1}}{n} = \frac{1}{n} \sum_{\alpha=1}^n x_{s,\alpha} x_{t+1,\alpha} = \Theta_{n \to \infty}(1)$ ?

#### Yes! Moreover,

- $d\bar{h}_s o$  a Gaussian with iid components with computable mean and var;
- $ullet \ \frac{x_{\mathbf{s}}^{\top} x_{t+1}}{n} 
  ightarrow \mathbf{a}$  finite computable scalar.

**Tensor programs** is a general framework for expressing neural network computations (i.e. forward/backward pass).

The main theoretical result: for a set of "pre-activation-like" vectors  $g^1, \ldots, g^M$  of a tensor program satisfying certain initialization assumptions,

$$rac{1}{n}\sum_{lpha=1}^n \psi(g_lpha^1,\ldots,g_lpha^M) 
ightarrow$$
a finite computable scalar

for any "well-behaved"  $\psi$  a.s. as  $n \to \infty$ .

#### Goals of the talk:

- 1. Introduce a machinery of tensor programs;
- 2. Apply it to prove several well-known properties of neural nets as  $n \to \infty$ .

# Convergence to Gaussian

processes

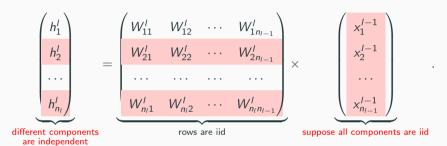
#### Consider a forward pass:

$$\underbrace{h^{l} = W^{l} x^{l-1}}_{\text{pre-activations, } \in \mathbb{R}^{n_{l}}}, \qquad \underbrace{x^{l-1} = \phi(h^{l-1})}_{\text{activations, } \in \mathbb{R}^{n_{l-1}}}; \qquad W^{l} \sim \mathcal{N}\left(0, \frac{\sigma_{W}^{2}}{n_{l-1}}\right). \tag{10}$$

In a matrix form:

$$\begin{pmatrix} h_{1}^{l} \\ h_{2}^{l} \\ \dots \\ h_{n_{l}}^{l} \end{pmatrix} = \begin{pmatrix} W_{11}^{l} & W_{12}^{l} & \cdots & W_{1n_{l-1}}^{l} \\ W_{21}^{l} & W_{22}^{l} & \cdots & W_{2n_{l-1}}^{l} \\ \dots & \dots & \dots & \dots \\ W_{n_{l}1}^{l} & W_{n_{l}2}^{l} & \cdots & W_{n_{l}n_{l-1}}^{l} \end{pmatrix} \times \begin{pmatrix} x_{1}^{l-1} \\ x_{2}^{l-1} \\ \dots \\ x_{n-1}^{l-1} \end{pmatrix}.$$
all iid  $\sim \mathcal{N}(0, \sigma_{Nl}^{2}/n_{l-1})$ 

$$\begin{pmatrix} h_1^l \\ h_2^l \\ \dots \\ h_{n_l}^l \end{pmatrix} = \begin{pmatrix} W_{11}^l & W_{12}^l & \cdots & W_{1n_{l-1}}^l \\ W_{21}^l & W_{22}^l & \cdots & W_{2n_{l-1}}^l \\ \dots & \dots & \dots & \dots \\ W_{n_l1}^l & W_{n_l2}^l & \cdots & W_{n_ln_{l-1}}^l \end{pmatrix} \times \begin{pmatrix} x_1^{l-1} \\ x_2^{l-1} \\ \dots \\ x_{l-1}^{l-1} \end{pmatrix}$$
 components tend to Gaussians as  $n_{l-1} \to \infty$  by CLT suppose all components are iid



$$\begin{pmatrix} h_1^l \\ h_2^l \\ \dots \\ h_{n_l}^l \end{pmatrix} = \begin{pmatrix} W_{11}^l & W_{12}^l & \cdots & W_{1n_{l-1}}^l \\ W_{21}^l & W_{22}^l & \cdots & W_{2n_{l-1}}^l \\ \dots & \dots & \dots \\ W_{n_l1}^l & W_{n_l2}^l & \cdots & W_{n_ln_{l-1}}^l \end{pmatrix}$$
 with iid components as  $n_{l-1} \to \infty$  by CLT

suppose all components are iid

$$\begin{pmatrix}
h'_1 & \bar{h}'_1 \\
h'_2 & \bar{h}'_2 \\
\cdots & \cdots \\
h'_{n_l} & \bar{h}'_{n_l}
\end{pmatrix}$$

each row converges to a multivariate Gaussian vector as  $n_{l-1} \to \infty$  by the vector CLT

$$= \underbrace{\begin{pmatrix} W_{11}^{I} & W_{12}^{I} & \cdots & W_{1n_{l-1}}^{I} \\ W_{21}^{I} & W_{22}^{I} & \cdots & W_{2n_{l-1}}^{I} \\ \cdots & \cdots & \cdots & \cdots \\ W_{n_{l}1}^{I} & W_{n_{l}2}^{I} & \cdots & W_{n_{l}n_{l-1}}^{I} \end{pmatrix}}_{\text{all iid}} \sim \mathcal{N}(0, \sigma_{W}^{2}/n_{l-1})$$

$$\begin{pmatrix}
x_1^{l-1} & \bar{x}_1^{l-1} \\
x_2^{l-1} & \bar{x}_2^{l-1} \\
\dots & \dots \\
x_{n_{l-1}}^{l-1} & \bar{x}_{n_{l-1}}^{l-1}
\end{pmatrix}$$

suppose all components of each column are iid

Let  $\xi_{1:M}$  be a batch of M inputs.

$$\begin{pmatrix} h'_{1}(\xi_{1}) & h'_{1}(\xi_{2}) & \dots & h'_{1}(\xi_{M}) \\ h'_{2}(\xi_{1}) & h'_{2}(\xi_{2}) & \dots & h'_{2}(\xi_{M}) \\ \dots & \dots & \dots & \dots \\ h'_{n_{l}}(\xi_{1}) & h'_{n_{l}}(\xi_{2}) & \dots & h'_{n_{l}}(\xi_{M}) \end{pmatrix}$$

- Batch dimension tends to a multivariate zero-mean Gaussian as  $n_{l-1} \to \infty$ ;
- Neuron dimension components tend to iid Gaussians.

# Theorem ([Matthews et al., 2018]) Given a model of the form

$$h^{l+1}(\xi) = W^{l+1} x^{l}(\xi), \quad x^{l}(\xi) = \phi(h^{l}(\xi)), \quad h^{1}(\xi) = W^{1} \xi,$$
 (11)

where  $W^{l+1} \in \mathbb{R}^{n_{l+1} \times n_l}$ , suppose  $W_{ij}^{l+1} \sim \mathcal{N}(0, \sigma_w^2/n_l)$  iid.

Then,  $\forall I$  as  $n_{1:I} \rightarrow \infty$  sequentially,

- 1. all components of  $h^{l+1}(\xi)$  become iid  $\forall \xi$ , and
- 2.  $\forall \alpha \in [n_{l+1}] \ \forall M \in \mathbb{N} \ \forall \xi_{1:M} \ \{h_{\alpha}^{l+1}(\xi_1), \dots, h_{\alpha}^{l+1}(\xi_M)\}$  converges weakly to  $\mathcal{N}(0, \Sigma^{l+1})$ , where

$$\Sigma_{ij}^{l+1} = \sigma_W^2 \mathbb{E}_{z_{1:M} \sim \mathcal{N}(0, \Sigma^l)} \phi(z_i) \phi(z_j), \tag{12}$$

and 
$$\Sigma_{ij}^1 = \sigma_W^2 \xi_i^T \xi_j$$
.

Does the previous result hold if some weights are shared?

Suppose we want to compute the limit distribution of WWx:

We can directly apply CLT if WW has iid components.

Let us compute the limit distribution of  $(WW)_{\alpha}$ :

$$\underbrace{\begin{pmatrix} W_{\alpha 1} & W_{\alpha \alpha} & \cdots & W_{\alpha n} \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

Fortunately, since  $W_{\alpha\alpha} \sim \mathcal{N}(0, \sigma_W^2/n)$ ,  $W_{\alpha\alpha}^2 x_{\alpha} \propto 1/n \rightarrow 0$ .

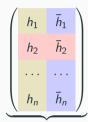
#### **Conclusion:**

- 1. **CLT** is still applicable even if the same matrix W is used several times;
- 2.  $(WWx)_{\alpha}$  and  $(W\tilde{W}x)_{\alpha}$  with  $\tilde{W} \stackrel{d}{=} W$  have the same distribution in the limit.

However, we cannot substitute W with its iid copy  $\tilde{W}$ :

- WWx and Wx are correlated in the limit;
- $W\tilde{W}x$  and  $\tilde{W}x$  are not.

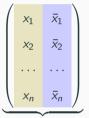
Consider h = Wx and  $\bar{h} = W\bar{x}$  where x and  $\bar{x}$  can depend on W.



each row converges to a zero-mean Gaussian with covariance  $\sigma_W^2 \mathbb{E}(x^\top \bar{x})/n$ as  $n \to \infty$  by the vector CLT



all iid  $\sim \mathcal{N}(0, \sigma_W^2/n)$ 



suppose all components of each column are iid

A Netsor program = (a set of input vars, a sequence of commands),

where variables are of three different types:

- 1. A-vars: matrices with iid Gaussian entries;
- 2. G-vars: vectors with asymptotically iid Gaussian entries;
- 3. H-vars: images of G-vars by coordinatewise nonlinearities.

Each command generates a new variable from the previous ones using one of the following ops:

- 1. MatMul:  $(W : A, x : H) \rightarrow Wx : G$ ;
- 2. LinComb:  $(\{x_i : \mathsf{G}, \ a_i \in \mathbb{R}\}_{i=1}^k) \to \sum_{i=1}^k a_i x_i : \mathsf{G};$
- 3. Nonlin:  $(\{x_i : \mathsf{G}\}_{i=1}^k, \ \phi : \mathbb{R}^k \to \mathbb{R}) \to \phi(x_{1:k}) : \mathsf{H}.$

### Algorithm 1 Example: MLP with two hidden layers

```
Input: W^1x : G(n^1) {layer 1 embedding of input}
Input: b^1 : G(n^1) {laver 1 bias}
Input: W^2: A(n^2, n^1) {layer 2 weights}
Input: b^2 : G(n^2) {layer 2 bias}
Input: v : G(n^2) {readout layer weights}
  h^1 := W^1 x + b^1 : \mathsf{G}(n^1) \{ \text{LinComb} \}
  x^1 := \phi(h^1) : H(n^1) {layer 1 activation: Nonlin}
  \tilde{h}^2 := W^2 x^1 : G(n^2) \{ MatMul \}
  h^2 := \tilde{h}^2 + b^2 : \mathsf{G}(n^2) {layer 2 preactivation; LinComb}
  x^2 := \phi(h^2) : H(n^2) {layer 2 activation: Nonlin}
Output: v^{\top}x^2/\sqrt{n^2}
```

We can absorb  $\operatorname{LinComb} + \operatorname{Nonlin}$  into a single  $\operatorname{Nonlin}$ :  $x^2 = \phi(h^2) = \phi(\tilde{h}^2 + b^2) = \bar{\phi}(h^2, b^2)$ .

### Algorithm 2 Example: MLP with two hidden layers and a batch-norm

```
Input: \{W^1x_k: G(n^1)\}_{k=1}^B {layer 1 embeddings of inputs in a batch}
Input: b^1 : G(n^1) {layer 1 bias}
Input: W^2 : A(n^2, n^1) {laver 2 weights}
Input: b^2 : G(n^2) {laver 2 bias}
Input: v : G(n^2) {readout layer weights}
   \{h_k^1 := W^1 x_k + b^1 : \mathsf{G}(n^1)\}_{k=1}^B \{\text{LinComb}\}
   \{x_k^1 := \tilde{\phi}_k(h_{1:R}^1) : \mathsf{H}(n^1)\}_{k=1}^B \{\mathsf{BN} + \mathsf{activation for layer 1 (see below); Nonlin}\}
   \{\tilde{h}_{t}^{2} := W^{2}x_{t}^{1} : \mathsf{G}(n^{2})\}_{t=1}^{B} \{\text{MatMul}\}\
   \{h_k^2 := \tilde{h}_k^2 + b^2 : \mathsf{G}(n^2)\}_{k=1}^B {layer 2 preactivation; LinComb}
   \{x_k^2 := \tilde{\phi}_k(h_{1:R}^2) : \mathsf{H}(n^2)\}_{k=1}^B \{\mathsf{BN} + \mathsf{activation for layer 2}; \mathsf{Nonlin}\}
Output: \{v^{\top}x_{k}^{2}/\sqrt{n^{2}}\}_{k=1}^{B}
```

Here  $\tilde{\phi}: \mathbb{R}^B \to \mathbb{R}^B$  is defined as

$$\tilde{\phi}(h^{1:B}) = \phi\left(\frac{h^{1:B} - \mu(h^{1:B})}{\sigma(h^{1:B})}\right), \quad \mu(h^{1:B}) = \frac{1}{B} \sum_{k=1}^{B} h^{k}, \quad \sigma(h^{1:B}) = \sqrt{\frac{1}{B} \sum_{k=1}^{B} (h^{k} - \mu(h^{1:B})_{k})^{2}}.$$

#### Initialization assumption:

- 1. All hidden dimensions are equal to n;
- 2.  $\forall W$ : A we sample  $W_{\alpha\beta} \sim \mathcal{N}(0, \sigma_W^2/n)$  iid;

**Our goal:** compute the distributions of all G-vars in the program in the limit of  $n \to \infty$ .

#### Claim:

Let  $g^{1:M}$  be a set of all G-vars in the program.

- "Batch" dimension converges to  $\mathcal{N}(\mu, \Sigma)$  with  $\mu = \{\mu(g^i)\}_{i=1}^M$  and  $\Sigma = \{\Sigma(g^i, g^j)\}_{i,j=1}^M$  defined below;
- Neuron dimension components tend to iid Gaussians.

 $(g^1_{\alpha},\ldots,g^M_{\alpha})$  becomes jointly Gaussian with mean and covariance **defined by CLT**<sup>1</sup>:

$$\mu(g) = \begin{cases} 0 & \text{if } g = Wy. \end{cases} \tag{13}$$

$$\Sigma(g,\bar{g}) = \begin{cases} \sigma_W^2 \mathbb{E}_Z \phi(Z) \bar{\phi}(Z) & \text{if } g = W \phi(Z) \text{ and } \bar{g} = W \bar{\phi}(Z); \\ 0 & \text{else.} \end{cases}$$
(14)

Here  $Z \sim \mathcal{N}(\mu, \Sigma)$  is a set of all previous G-vars.

 $<sup>^{1}</sup>$ we have suppressed the  $\operatorname{LinComb}$  op for brevity.

#### **Definition**

We say  $\phi: \mathbb{R}^k \to \mathbb{R}$  is controlled if  $\exists C, c, \epsilon > 0 : \forall x \in \mathbb{R}^k \ |\phi(x)| < e^{C||x||_2^{2-\epsilon} + c}$ .

Theorem (Netsor Master Theorem, [Yang, 2019]) Let the  ${
m NETSOR}$  program satisfy the initialization assumption and let all nonlinearities be controlled. Let  $g^{1:M}$  be a set of all G-vars in the program. Then, for any controlled  $\psi$ ,

$$\frac{1}{n} \sum_{\alpha=1}^{n} \psi(g_{\alpha}^{1}, \dots, g_{\alpha}^{M}) \to \underbrace{\mathbb{E}_{Z \sim \mathcal{N}(\mu, \Sigma)} \psi(Z)}_{\text{expectation}}$$

$$\underbrace{\mathbb{E}_{Z \sim \mathcal{N}(\mu, \Sigma)} \psi(Z)}_{\text{expectation over rows}}$$
over the corresponding Gaussian

a.s. as 
$$n \to \infty$$
, where  $\mu = \{\mu(g^i)\}_{i=1}^M$  and  $\Sigma = \{\Sigma(g^i, g^j)\}_{i,j=1}^M$ .

#### A NETSOR program

- is able to express the **first forward pass** of a wide class of neural nets (i.e. with shared/structured weights, with BNs etc.);
- reveals its limiting Gaussian process behavior.

#### Questions:

- 1. Can we express a  $backward\ pass$  as a  $\operatorname{NETSOR}$  program?
- 2. What is its limiting behavior?

Intermedia: a Neural Tangent

Kernel

Let  $f(\cdot; \theta)$  be a parametric model.

Define a neural tangent kernel as

$$\Theta_t(\xi,\bar{\xi}) = \underbrace{\nabla_{\theta}^T f(\xi;\theta_t) \nabla_{\theta} f(\bar{\xi};\theta_t)}_{\text{"gradient similarity"}}.$$
 (16)

It drives evolution of model predictions; e.g. for square loss:

$$\dot{f}(\bar{\xi}; \theta_t) = (\vec{y} - f(\vec{\xi}; \theta_t))^{\top} \Theta_t(\vec{\xi}, \bar{\xi}), \text{ where } (\vec{\xi}, \vec{y}) \text{ is a train dataset.}$$

Assuming  $\Theta_t(\cdot,\cdot) \approx \Theta_0(\cdot,\cdot)$  makes the dynamics analytically tractable.

**Theorem ([Jacot et al., 2018], informal)**Suppose we have a feedforward neural net of width n parameterized in a certain way. Then, as  $n\to\infty$ ,

- 1.  $\Theta_0(\xi,\bar{\xi})$  converges to a deterministic  $\mathring{\Theta}(\xi,\bar{\xi})$ ;
- 2. Moreover,  $\Theta_t(\xi,\bar{\xi})$  converges to the same  $\mathring{\Theta}(\xi,\bar{\xi})$ .

Parameterize  $W^I$  as  $\omega^I/\sqrt{n_{I-1}}$ :

$$\underbrace{f = \frac{1}{\sqrt{n_L}} \omega^{L+1} x^L}_{\text{the network output}}, \quad \underbrace{x^l = \phi(h^l)}_{\text{activations}}, \quad \underbrace{h^l = \frac{1}{\sqrt{n_{l-1}}} \omega^l x^{l-1}}_{\text{preactivations}}, \quad I \leq L; \quad \omega^l_{ij} \sim \mathcal{N}(0, \sigma_W^2) \text{ iid.}$$

NTK is defined as

$$\Theta(\xi,\bar{\xi}) = \nabla_{\theta}^{T} f(\xi;\theta) \nabla_{\theta} f(\bar{\xi};\theta) = \sum_{l=1}^{L+1} \underbrace{\operatorname{tr}(\nabla_{\omega^{l}}^{T} f(\xi) \nabla_{\omega^{l}} f(\bar{\xi}))}_{\text{layer-wise gradient similarity"}}.$$
 (17)

$$\Theta(\xi,\bar{\xi}) = \nabla_{\theta}^{T} f(\xi;\theta) \nabla_{\theta} f(\bar{\xi};\theta) = \sum_{l=1}^{L+1} \operatorname{tr}(\nabla_{\omega^{l}}^{T} f(\xi) \nabla_{\omega^{l}} f(\bar{\xi})) . \tag{18}$$

Weight gradient can be expressed as

$$\nabla_{\omega^{l}} f = \frac{1}{\sqrt{n_{l-1}n_{l}}} \underbrace{dh^{l}}_{\substack{\text{backward pass} \\ \text{up to the layer } l}} \times \underbrace{\chi^{l-1,\top}}_{\substack{\text{forward pass} \\ \text{up to the layer } l-1}}, \quad \text{where } dh^{l} \propto \nabla_{h_{l}} f. \tag{19}$$

Plug (19) into (18):

$$\Theta(\xi,\bar{\xi}) = \sum_{l=1}^{L+1} \underbrace{\left(\frac{dh^{l,\top}d\bar{h}^{l}}{n_{l}}\right)}_{\text{"backward pass similarity"}} \times \underbrace{\left(\frac{x^{l-1,\top}\bar{x}^{l-1}}{n_{l-1}}\right)}_{\text{"forward pass similarity"}}.$$
 (20)

Consider the second multiplier:

$$\frac{x^{l-1,\top}\bar{x}^{l-1}}{n_{l-1}} = \frac{1}{n_{l-1}} \sum_{\alpha=1}^{n_{l-1}} \phi(h_{\alpha}^{l-1}) \phi(\bar{h}_{\alpha}^{l-1}) = \underbrace{\frac{1}{n_{l-1}} \sum_{\alpha=1}^{n_{l-1}} \psi(h_{\alpha}^{l-1}, \bar{h}_{\alpha}^{l-1})}_{\text{the limit is given by the Master theorem!}} \text{for } \psi(x, y) = \phi(x) \phi(y).$$

Can we compute the limit of the first multiplier in the same way?

For simplicity, assume  $n_1 = \ldots = n_L = n$ . Recall  $W^I = \omega^I / \sqrt{n}$ .

## Relations between forward and backward passes:

Forward pass:	Backward pass:
$x' = \phi(h')$ : Nonlin	$dh^{\prime} = dx^{\prime} \odot \phi^{\prime}(h^{\prime})$ : Nonlin
$h' = W' x^{l-1} : MatMul$	$dx^{l-1} = W^{l,\top}dh^l : MatMul?$

### **Problems:**

- 1. W and  $W^{\top}$  cannot be both input variables since they are dependent;
- $2.\ A\ \mathrm{NETSOR}$  program does not allow for multiplying by a transposed A-var.

## A Netsor program cannot express the backward pass!

A NETSORT program = (a set of input vars, a sequence of commands),

where variables are of three different types:

- 1. A-vars: matrices with iid Gaussian entries;
- 2. G-vars: vectors with asymptotically iid Gaussian entries;
- 3. H-vars: images of G-vars by coordinatewise nonlinearities.

Each command generates a new variable from the previous ones using one of the following ops:

- 1. Trsp:  $W : A \rightarrow W^{\top} : A$ ;
- 2. MatMul:  $(W : A, x : H) \rightarrow Wx : G$ ;
- 3. LinComb:  $(\{x_i : \mathsf{G}, \ a_i \in \mathbb{R}\}_{i=1}^k) \to \sum_{i=1}^k a_i x_i : \mathsf{G};$
- 4. Nonlin:  $(\{x_i : G\}_{i=1}^k, \phi : \mathbb{R}^k \to \mathbb{R}) \to \phi(x_{1:k}) : H$ .

## Can we keep the same symbolic rules for mean and covariance of G-vars?

$$\mu(g) = \begin{cases} 0 & \text{if } g = Wy; \\ \mathbf{0?} & \text{if } g = \mathbf{W}^{\mathsf{T}} y. \end{cases}$$
 (21)

$$\Sigma(g,\bar{g}) = \begin{cases} \sigma_W^2 \mathbb{E}_Z \phi(Z) \bar{\phi}(Z) & \text{if } g = W \phi(Z) \text{ and } \bar{g} = W \bar{\phi}(Z);\\ \text{some other rule?} & \text{if } g = W \phi(Z) \text{ and } \bar{g} = W^\top \bar{\phi}(Z);\\ 0 & \text{else.} \end{cases}$$
 (22)

Here  $Z \sim \mathcal{N}(\mu, \Sigma)$  is a set of all previous G-vars.

Let us check that  $\mu(WWx) = 0$ :

$$\underbrace{ \begin{pmatrix} W_{\alpha 1} & W_{\alpha \alpha} & \cdots & W_{\alpha n} \\ & & & & \\ & &$$

$$\mu(WWx) = \mathbb{E}\left((WWx)_{\alpha}\right) = \mathbb{E}\left(\sum_{\beta \neq \alpha} \sum_{\gamma} W_{\alpha\beta} W_{\beta\gamma} x_{\gamma}\right) + \mathbb{E}\left(\sum_{\gamma} W_{\alpha\alpha} W_{\alpha\gamma} x_{\gamma}\right). \tag{23}$$

$$\mathbb{E}\left(\sum_{\beta \neq \alpha} \operatorname{iid} w. \operatorname{mean}=0\right)=0$$

Do we have  $\mu(WW^Tx) = 0$ ?

Let us compute  $\mu(WW^Tx)$ :

$$\underbrace{\begin{pmatrix} W_{\alpha 1} & W_{\alpha \alpha} & \cdots & W_{\alpha n} \end{pmatrix}}_{\text{all iid}} \underbrace{\begin{pmatrix} W_{11} & W_{\alpha 1} & \cdots & W_{n1} \\ W_{1\alpha} & W_{\alpha \alpha} & \cdots & W_{n\alpha} \\ \cdots & \cdots & \cdots & \cdots \\ W_{1n} & W_{\alpha n} & \cdots & W_{nn} \end{pmatrix}}_{\text{all iid}} = \underbrace{\begin{pmatrix} \sum (\text{iid w. mean} = 0) \\ \sum_{\beta} W_{\alpha \beta}^{2} \\ \cdots \\ \sum (\text{iid w. mean} = 0) \end{pmatrix}}_{\text{all iid except for } \alpha' \text{s term}}$$

$$\mu(WW^{\top}x) = \mathbb{E}\left((WW^{\top}x)_{\alpha}\right) = \mathbb{E}\left(\sum_{\beta}\sum_{\gamma\neq\alpha}W_{\alpha\beta}W_{\gamma\beta}x_{\gamma}\right) + \mathbb{E}\left(\sum_{\beta}W_{\alpha\beta}^{2}x_{\beta}\right). \tag{24}$$

$$\mathbb{E}\left(\sum_{\beta}\operatorname{iid} w. \operatorname{mean}=0\right)=0 \qquad \operatorname{converges to } \sigma_{W}^{2}\mu(x)\neq0$$

The previous symbolic rules are not applicable for  $\textbf{general}\ \mathrm{Netsor}\top$  programs,

## but

they are applicable to  $\operatorname{Netsor}\top$  programs expressing backpropagation.

Claim: the rule

$$\mu(g) = 0 \quad \text{if } g = Wy. \tag{25}$$

works for Netsor T programs expressing backpropagation.

**Evidence:** consider  $dx^{l-1} = W^{l,T}(dx^l \odot \phi'(h^l))$ . Let  $\phi(z) = z^2/2$ :

$$\mu(dx^{l-1}) = \mathbb{E}\left(dx_{\alpha}^{l-1}\right) = \underbrace{\mathbb{E}\left(\sum_{\beta} W_{\beta\alpha}^{l} dx_{\beta}^{l} \sum_{\gamma \neq \beta} W_{\beta\gamma}^{l} x_{\gamma}^{l-1}\right)}_{\mathbb{E}\left(\sum \text{iid w. mean} = 0\right) = 0} + \underbrace{\mathbb{E}\left(x_{\alpha}^{l-1} \sum_{\beta} (W_{\beta\alpha}^{l})^{2} dx_{\beta}^{l}\right)}_{\text{converges to } \mu(x^{l-1}) \sigma_{W}^{2} \mu(dx^{l})}. \quad (26)$$

Hence  $\mu(dx^{l-1}) \propto \mu(dx^l)$  which by induction implies  $\mu(dx^{l-1}) \propto \mu(dx^L)$ .

But 
$$dx^{L} = \omega^{L+1}!$$
 Hence  $\mu(dx^{l-1}) = \mu(\omega^{L+1}) = 0$ .

# Proposition (2)

Consider a neural network and a Netsor⊤ program expressing its backward pass.

The symbolic rules for  $\mu$  and  $\Sigma$  are valid, if

- 1. The output layer has zero mean;
- 2. It is sampled independently from other parameters;
- 3. It is not used anywhere else in the program.

<sup>&</sup>lt;sup>2</sup>There is a more general condition called "BP-likeness" which we do not show here.

### Definition

We say  $\phi: \mathbb{R}^k \to \mathbb{R}$  is polynomially bounded if  $\exists C, c, p > 0: |\phi(x)| \leq C ||x||_2^p + c$ .

Theorem (Netsor T Master Theorem, [Yang, 2020a])

Let a Netsort program be **BP-like** in a neural network, satisfy the initialization assumption, and let all nonlinearities be polynomially bounded. Let  $g^{1:M}$  be a set of all G-vars in the program. Then, for any polynomially bounded  $\psi: \mathbb{R}^M \to \mathbb{R}$ ,

$$\frac{1}{n}\sum_{\alpha=1}^n\psi(g_\alpha^1,\ldots,g_\alpha^M)\to\mathbb{E}_{Z\sim\mathcal{N}(\mu,\Sigma)}\psi(Z)$$

a.s. as 
$$n \to \infty$$
, where  $\mu = \{\mu(g^i)\}_{i=1}^M$  and  $\Sigma = \{\Sigma(g^i, g^j)\}_{i,j=1}^M$ .

Back to NTK computation:

$$\Theta(\xi,\bar{\xi}) = \sum_{l=1}^{L+1} \nabla_{\omega^l}^T f(\xi) \nabla_{\omega^l} f(\bar{\xi}) = \sum_{l=1}^{L+1} \left( \frac{dh^{l,\top} d\bar{h}^l}{n_l} \right) \left( \frac{x^{l-1,\top} \bar{x}^{l-1}}{n_{l-1}} \right). \tag{27}$$

Consider the first multiplier:

$$\frac{dh^{l,\top}\bar{d}h^{l}}{n_{l}} = \frac{1}{n_{l}}\sum_{\alpha=1}^{n_{l}}dx_{\alpha}^{l}d\bar{x}_{\alpha}^{l}\phi^{\prime}(h_{\alpha}^{l})\phi^{\prime}(\bar{h}_{\alpha}^{l}) = \frac{1}{n_{l}}\sum_{\alpha=1}^{n_{l}}\psi(dx_{\alpha}^{l},d\bar{x}_{\alpha}^{l},h_{\alpha}^{l},\bar{h}_{\alpha}^{l})$$

the limit is given by the Master theorem!

for 
$$\psi(x, y, z, w) = xy\phi'(z)\phi'(w)$$
. (28)

## A BP-like NETSOR<sup>⊤</sup> program

- is able to express the **first forward and backward passes** of a wide class of neural nets (i.e. with shared/structured weights, with BNs etc.);
- reveals their limiting Gaussian process behavior;
- can be applied to initial NTK computation.

Intermedia 2: the limiting

jacobian spectrum

Consider a forward pass:

$$\underbrace{h^{l} = W^{l} x^{l-1}}_{\text{pre-activations, } \in \mathbb{R}^{n_{l}}}, \qquad \underbrace{x^{l-1} = \phi(h^{l-1})}_{\text{activations, } \in \mathbb{R}^{n_{l-1}}}.$$
(29)

Define an **input-output jacobian**:

$$J = \frac{\partial h^L}{\partial h^1} = W^L D^{L-1} \dots W^2 D^1 \in \mathbb{R}^{n_L \times n_1}, \quad D^I = \operatorname{diag}(\phi'(h^I)).$$

We are interested in singular values of J, or, equivalently, **eigenvalues of**  $J^{\top}J$ .

Assume  $n_L = \ldots = n_1 = n$ .

Define the empirical spectral distribution:

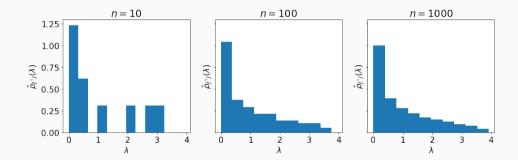
$$\hat{\rho}_{J^{\top}J} = \frac{1}{n} \sum_{k=1}^{n} \delta_{\lambda_k}, \quad \text{where } \lambda_{1:n} \text{ are eigenvalues of } J^{\top}J.$$

**Claim:** if  $\mathbb{E} W^I = 0$  and  $\mathbb{V}\mathrm{ar} W^I \propto n^{-1}$  then  $\exists \lim_{n \to \infty} \hat{\rho}_{J^\top J} =: \rho_{J^\top J}$ .

$$J = \frac{\partial h^L}{\partial h^1} = W^L D^{L-1} \dots W^2 D^1 \in \mathbb{R}^{n_L \times n_1}, \quad D^I = \operatorname{diag}(\phi'(h^I)).$$

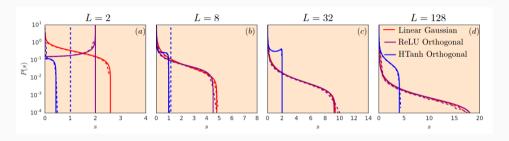
For L=2 and  $\phi=\mathrm{id}$ , J=W.

Given  $W_{ij} \sim \mathcal{N}(0, n^{-1})$ ,  $J^{\top}J = W^{\top}W$  is known as a **Wishart ensemble.** 



**Figure 1:**  $\hat{\rho}_{J^{\top}J}(\lambda)$  for a Wishart ensemble: J = W,  $W_{ij} \sim \mathcal{N}(0, n^{-1})$ .

$$J = \frac{\partial h^L}{\partial h^1} = W^L D^{L-1} \dots W^2 D^1 \in \mathbb{R}^{n_L \times n_1}, \quad D^I = \operatorname{diag}(\phi'(h^I)).$$



**Figure 2:** The limiting spectrum  $\rho_{I^{\top}I}$  depends on  $L!^3$ 

<sup>&</sup>lt;sup>3</sup>The figure is borrowed from [Pennington et al., 2017].

**Good situation:**  $\rho_{J^{\top}J}$  neither diffuses nor squeezes to zero as  $L \to \infty$ .

## Why is it good?

• It allows for training very deep nets! [Pennington et al., 2017, Xiao et al., 2018]

For **linear nets**, this can be achieved with orthogonal weight initialization:

$$J^{\top}J = I \text{ when } J = W^{L} \dots W^{2} \text{ and } W^{I} \in \mathcal{O}_{n \times n} \ \forall I \qquad \Rightarrow \qquad \rho_{J^{\top}J} = \delta_{1}.$$

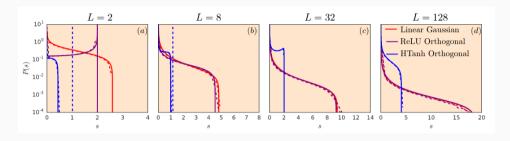


Figure 3: Linear nets with iid Gaussian initialization  $(W_{ij}^{l} \sim \mathcal{N}(0, 1/n))$  give  $\lambda_{\max} = (L+1)^{L+1}/L^{L} \sim eL$  — diffuses with L!

## How to compute $\rho_{J^{\top}J}$ ?

• Claim: it suffices to compute the moments:

$$\tau((J^{\top}J)^{k}) = \frac{1}{n}\mathbb{E} \operatorname{tr}((J^{\top}J)^{k}). \tag{30}$$

• Analogy: probability density  $p_X(x)$  of a scalar random variable X is expressible in terms of its moments  $\mathbb{E} X^k$ :

$$M_X(t) = \mathbb{E}_X e^{tX} = \sum_{k=0}^{\infty} \frac{t^k \mathbb{E}_X^k}{k!}; \qquad p_X(x) = \int_{-\infty}^{\infty} M_X(it) e^{itx} dt.$$
 (31)

How to compute  $tr((J^T J)^k)/n$ ? Use the identity:

$$\operatorname{tr}(X) = \mathbb{E}_{v \sim \mathcal{N}(0, I)}(v^{\top} X v). \tag{32}$$

This gives:

$$\frac{1}{n}\operatorname{tr}((J^{\top}J)^{k}) = \mathbb{E}_{v \sim \mathcal{N}(0,I)} \qquad \underbrace{\left(\frac{1}{n}\sum_{\alpha=1}^{n}v_{\alpha}((J^{\top}J)^{k}v)_{\alpha}\right)} \qquad . \tag{33}$$

the limit is given by the Master theorem?

Indeed,  $(J^{\top}J)^k v$  is expressible as a G-var in some  $\text{Netsor} \top \text{ program}^4$ .

But does the Master theorem work?

 $<sup>^4</sup>D^1v=\phi'(h^1)\odot v$  is given by Nonlin,  $W^2D^1v$  is given by MatMul, and so on.

Consider a Wishart ensemble: J = W.

Let us compute  $\mathbb{E} v_{\alpha}(WW^{\top}v)_{\alpha}$ .

We have the following symbolic rule:

$$\Sigma(g,\bar{g}) = \begin{cases} \sigma_W^2 \mathbb{E}_Z \phi(Z) \bar{\phi}(Z) & \text{if } g = W \phi(Z) \text{ and } \bar{g} = W \bar{\phi}(Z); \\ 0 & \text{else.} \end{cases}$$
(34)

According to this rule,

$$\mathbb{E} v_{\alpha}(WW^{\top}v)_{\alpha} = \Sigma(v, WW^{\top}v) = 0.$$

We expect to have  $\mathbb{E} v_{\alpha}(WW^{\top}v)_{\alpha} = 0$ .

$$\underbrace{\begin{pmatrix} W_{\alpha 1} & W_{\alpha \alpha} & \cdots & W_{\alpha n} \end{pmatrix}}_{\text{all iid}} \underbrace{\begin{pmatrix} W_{11} & W_{\alpha 1} & \cdots & W_{n1} \\ W_{1\alpha} & W_{\alpha \alpha} & \cdots & W_{n\alpha} \\ \cdots & \cdots & \cdots & \cdots \\ W_{1n} & W_{\alpha n} & \cdots & W_{nn} \end{pmatrix}}_{\text{all iid}} = \underbrace{\begin{pmatrix} \sum (\text{iid w. mean} = 0) \\ \sum_{\beta} W_{\alpha \beta}^{2} \\ \cdots \\ \sum (\text{iid w. mean} = 0) \end{pmatrix}}_{\text{all iid except for } \alpha' \text{s term}}^{\top}$$

$$v_{\alpha}(WW^{\top}v)_{\alpha} = v_{\alpha} \sum_{\beta,\gamma} W_{\alpha\beta} W_{\gamma\beta} v_{\gamma} = v_{\alpha} \underbrace{\sum_{\beta} W_{\alpha\beta} \sum_{\gamma \neq \alpha} W_{\gamma\beta} v_{\gamma}}_{\text{converges to a Gaussian indep. of } v_{\alpha} + \underbrace{\sum_{\beta} (W_{\alpha\beta})^{2} v_{\alpha}^{2}}_{\text{converges to } \sigma_{W}^{2} v_{\alpha}^{2}}.$$

Hence  $\mathbb{E} v_{\alpha}(WW^{\top}v)_{\alpha} = \sigma_{W}^{2}!$ 

### The previous rule:

 $g = W\phi(Z)$  tends to a Gaussian with iid components that is correlated **only** with G-vars of the form  $W\bar{\phi}(Z)$ :

$$\Sigma(g,\bar{g}) = \begin{cases} \sigma_W^2 \mathbb{E}_Z \phi(Z) \bar{\phi}(Z) & \text{if } g = W \phi(Z) \text{ and } \bar{g} = W \bar{\phi}(Z); \\ 0 & \text{else.} \end{cases}$$
(35)

### The corrected rule:

 $g = W\phi(Z)$  tends to a sum of **two terms**:

- 1. A **Gaussian** with iid components that is correlated only with G-vars of the form  $W\bar{\phi}(Z)$ ;
- 2. A linear combination of previously-generated vectors.

## **Example:**

$$(WW^\top v)_\alpha = \sum_\beta W_{\alpha\beta} \sum_{\gamma \neq \alpha} W_{\gamma\beta} v_\gamma + \sum_\beta (W_{\alpha\beta})^2 \textcolor{red}{v_\alpha} \rightarrow \underbrace{g_\alpha}_{\substack{\text{Gaussian;} \\ \text{does not correlate with } v_\alpha}} + \underbrace{\sigma_W^2 \textcolor{red}{v_\alpha}}_{\substack{\text{correlates with } v_\alpha}}$$

Back to learning a 2-layer perceptron!

An illustration for  $W_0 - W_0^{\top}$  interaction:

Suppose  $\phi(z) = z$ :

$$\bar{h}_1 = W_0 x_1 - \chi_0 d\bar{h}_0 \frac{x_0^\top x_1}{n},$$

$$x_1 = h_1 = \sqrt{n} u_1 \xi_1 = u_0 \xi_1 - \chi_0 dh_0 \xi_0 \xi_1 = u_0 \xi_1 - \chi_0 \xi_0 \xi_1 W_0^\top d\bar{h}_0.$$

$$W_0 x_1 = W_0 u_0 \xi_1 - \chi_0 \xi_0 \xi_1 W_0 W_0^\top d\bar{h}_0.$$

Hence for  $t \ge 1$  a Netsor $\top$  program is not BP-like!

# Theorem (Netsor⊤ Master Theorem, [Yang, 2020b])

Let a general Netsort program satisfy the initialization assumption, and let all nonlinearities be polynomially bounded. Let  $g^{1:M}$  be a set of all G-vars in the program. Then, for any polynomially bounded  $\psi: \mathbb{R}^M \to \mathbb{R}$ ,

$$\frac{1}{n}\sum_{\alpha=1}^n \psi(\mathbf{g}_{\alpha}^1,\ldots,\mathbf{g}_{\alpha}^M) \to \mathbb{E}_{Z \sim \mathcal{N}(\mu,\Sigma)} \psi(Z)$$

a.s. as  $n \to \infty$ , where  $\mu = \{\mu(g^i)\}_{i=1}^M$  and  $\Sigma = \{\Sigma(g^i, g^j)\}_{i,j=1}^M$ , and  $\mu(g)$  and  $\Sigma(g, \bar{g})$  are computed according to the **corrected rules** (which we do not write here).



Neural tangent kernel: Convergence and generalization in neural networks.

In Advances in neural information processing systems, pages 8571-8580.

Matthews, A. G. d. G., Hron, J., Rowland, M., Turner, R. E., and Ghahramani, Z. (2018). Gaussian process behaviour in wide deep neural networks.

In International Conference on Learning Representations.

Pennington, J., Schoenholz, S., and Ganguli, S. (2017).

Resurrecting the sigmoid in deep learning through dynamical isometry: theory and practice.

In Advances in neural information processing systems, pages 4785–4795.

Xiao, L., Bahri, Y., Sohl-Dickstein, J., Schoenholz, S., and Pennington, J. (2018).
Dynamical isometry and a mean field theory of cross: How to train 10 000-law

Dynamical isometry and a mean field theory of cnns: How to train 10,000-layer vanilla convolutional neural networks.

In International Conference on Machine Learning, pages 5393-5402. PMLR.

Yang, G. (2019).

Tensor programs i: Wide feedforward or recurrent neural networks of any architecture are gaussian processes.

arXiv preprint arXiv:1910.12478.



Yang, G. (2020a).

Tensor programs ii: Neural tangent kernel for any architecture.

arXiv preprint arXiv:2006.14548.



Yang, G. (2020b).

Tensor programs iii: Neural matrix laws.

arXiv preprint arXiv:2009.10685.