Why is AI hard and Physics simple?

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September 21, 2021

Based on "Why is AI hard and Physics simple?" 2104.00008 &

The Principles of Deep Learning Theory w/ Yaida and Hanin, 2106.10165, to be published by Cambridge University Press in 2022.

Initialization

The simulation is such that [one] generally perceives the sum of many billions of elementary processes simultaneously, so that the leveling law of large numbers completely obscures the real nature of the individual processes.

John von Neumann

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Thanks to substantial investments into computer technology, modern **artificial intelligence** (AI) systems can now come equipped with many billions of elementary components.

Behind much of this success is deep learning: deep learning uses artificial neural networks as an underlying model for AI.

$$f(x) = x$$

$$f(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

Some functions are easily described in terms of elementary operations $\{+,-,\times,\div\}$:

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- ► Although there's an ∞ of terms, for many purposes it only takes a few terms to get a useful approximation.
- The description of the function only takes 1 in on the screen.*
- * depending on the size of your monitor.

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$$f(x) = \begin{cases} 1, & x = \left\{ \bigotimes, \bigotimes, \dots \right\}, \\ 0, & x \neq \left\{ \bigotimes, \bigotimes, \dots \right\}. \end{cases}$$

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$$f(x) = \begin{cases} 1, & x = \left\{ \textcircled{B}, & \swarrow, \dots \right\}, \\ 0, & x \neq \left\{ \textcircled{B}, & \swarrow, \dots \right\}. \end{cases}$$

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- It's clear that such a function can exist humans do it! but unclear how to represent in terms of elementary operations.
- ► AI is about functions of this sort easy for humans to compute, but hard for humans to describe by {+, -, ×, ÷}.

Initialization: Neural Networks

= A **neural network** is a recipe for computing a function built out of many computational units called **neurons**:



Neurons are then organized in parallel into **layers**, and *deep* neural networks are those composed of multiple layers in sequence.

For a moment, let's ignore all that structure and simply think of a neural network as a parameterized function,

 $f(x;\theta),$

where x is the input to the function and θ is a vector of a large number of **parameters** controlling the shape of the function.

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Second, we adjust the parameter vector as θ → θ^{*}, such that the resulting *network function* f(x; θ^{*}) is as close as possible to a desired *target function* f(x):

 $f(x; \theta^{\star}) \approx f(x).$

This is called **function approximation**.

Neural Networks Abstracted: Training

To find these tunings θ^* , we fit the network function $f(x; \theta)$ to **training data**, consisting of many pairs of the form (x, f(x)) observed from the desired – but only partially observable – target function f(x).

- Making these adjustments is called **training**.
- The particular procedure used to tune them is called a learning algorithm.

The goal of this talk is to explain a set of **principles** that enable us to theoretically analyze *deep* neural networks of *actual relevance*. To initialize you to this task, we'll try to explain

(i) why such a goal is even attainable in theory, and(ii) how we are able to get there in practice.

The Theoretical Minimum

Our goal is to understand this *trained* network function:

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One way to see the kinds of technical problems that we'll encounter in pursuit of this goal is to *Taylor expand* our trained network function $f(x; \theta^*)$ around the initialized value of the parameters θ

$$f(x; \theta^{\star}) = f(x; \theta) + (\theta^{\star} - \theta) \frac{df}{d\theta} + \frac{1}{2} (\theta^{\star} - \theta)^2 \frac{d^2 f}{d\theta^2} + \dots,$$

where $f(x; \theta)$ and its derivatives on the right-hand side are all evaluated at initialized value of the parameters.

The Theoretical Minimum: Problem 1

In general, the Taylor series contains an infinite number of terms

$$f$$
, $\frac{df}{d\theta}$, $\frac{d^2f}{d\theta^2}$, $\frac{d^3f}{d\theta^3}$, $\frac{d^4f}{d\theta^4}$, ...,

and in principle we need to compute them all.

The Theoretical Minimum: Problem 2

Since the parameters θ are randomly sampled from $p(\theta)$, each time we initialize our network we get a different function $f(x; \theta)$, and we need to determine the mapping:

$$p(\theta) \rightarrow p\left(f, \frac{df}{d\theta}, \frac{d^2f}{d\theta^2}, \ldots\right)$$

This means that each term f, $df/d\theta$, $d^2f/d\theta^2$, ..., in the Taylor expansion is really a *random function* of the input x, and this joint distribution will have intricate statistical dependencies.

The Theoretical Minimum: Problem 3

The learned value of the parameters, θ^{\star} , is the result of a complicated training process. In general, θ^{\star} is not unique and can depend on *everything*:

$$\theta^{\star} \equiv [\theta^{\star}] \left(\theta, f, \frac{df}{d\theta}, \frac{d^2f}{d\theta^2}, \ldots; \text{ learning algorithm; training data} \right)$$
.

Determining an *analytical* expression for θ^* must take "*everything*" into account.

Goal, restated

If we could solve all three of these problems, then we'd have a *distribution* over trained network functions

$$p(f^{\star}) \equiv p(f(x; \theta^{\star}) | \text{ learning algorithm; training data}),$$

now conditioned in a simple way on the learning algorithm and the data we used for training.

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If we could solve all three of these problems, then we'd have a *distribution* over trained network functions

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The development of a method for the analytical computation of $p(f^*)$ would let us *understand* AI systems and then let us use that knowledge to *improve* them.



"There ain't no such thing as a free lunch." (TANSTaaFL)

[Heinlein, Wolpert/Macready]

Why is AI (naively) hard?

- No "best" AI system when you average over all possible training examples and tasks.
- No matter how much we improve our tools for understanding, these improvements can do no better than random.

Some "examples"



Some "examples"



5 = ?

5 = 5





What don't humans do...



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... but Neural Networks can!

 $[{\sf Zhang}/{\sf Bengio}/{\sf Hardt}/{\sf Recht}/{\sf Vinyals}]$
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This is why (understanding how) AI (works) is hard.

The reason the laws of physics are even learnable at all is because the models we used to describe the universe are particularly simple models within the frameworks we used to enumerate the possible theories of physics.

$$\mathcal{L}_{SM} = \mathcal{L}_{Dirac} + \mathcal{L}_{mass} + \mathcal{L}_{gauge} + \mathcal{L}_{gf} + \mathcal{L}_{Higgs}$$

$$\begin{split} \mathcal{L}_{Dirac} &= i\bar{e}_{l}^{i} de_{l}^{i} + i\bar{\nu}_{L}^{i} dv_{L}^{i} + i\bar{e}_{h}^{i} de_{k}^{i} + i\bar{u}_{L}^{i} dv_{L}^{i} + h.c. \right) - M_{W}^{2} W_{\mu}^{+} W^{-\mu} - \frac{M_{W}^{2}}{2 \cos^{2} \theta_{W}} Z_{\mu} Z^{\mu} \\ \mathcal{L}_{gauge} &= -\frac{1}{4} (G_{\mu\nu}^{a})^{2} - \frac{1}{2} W_{\mu\nu}^{+} W^{-\mu\nu} - \frac{1}{4} Z_{\mu\nu} Z^{\mu\nu} - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \mathcal{L}_{WZA} \\ \mathcal{L}_{gf} &= -g_{3} A_{\mu}^{a} J_{(3)}^{\mu a} - g_{2} \left(W_{\mu}^{+} J_{W^{+}}^{\mu} + W_{\mu}^{-} J_{W^{-}}^{\mu} + Z_{\mu} J_{L}^{\mu} - eA_{\mu} J_{A}^{\mu} \right) \\ \mathcal{L}_{Higgs} &= \frac{1}{2} \partial_{\mu} h \partial^{\mu} h - \mu^{2} h^{2} - 6\lambda v h^{3} - 6\lambda h^{4} \\ &+ g_{2} M_{W} h W_{\mu}^{+} W^{-\mu} + \sqrt{g_{1}^{2} + g_{2}^{2}} M_{Z} h Z_{\mu} Z^{\mu} + \frac{1}{2} g_{2}^{2} h^{2} W_{\mu}^{+} W^{-\mu} + \frac{1}{2} (g_{1}^{2} + g_{2}^{2}) h^{2} Z_{\mu} Z^{\mu} \\ &- h \left(\lambda_{e}^{i} \bar{e}_{L}^{i} e_{R}^{i} + \lambda_{u}^{i} \bar{u}_{L}^{i} u_{R}^{i} + \lambda_{d}^{i} \bar{d}_{L}^{i} dr_{R}^{i} + h.c. \right) \\ \mathcal{L}_{WZA} &= ig_{2} \cos \theta_{W} \left[\left(W_{\mu}^{-} W_{\nu}^{+} - W_{\nu}^{-} W_{\mu}^{+} \right) \partial^{\mu} A^{\nu} + W_{\mu\nu}^{+} W^{-\mu} A^{\nu} - W_{\mu\nu}^{-} W^{+\mu} Z^{\nu} \right] \\ &+ ie \left[\left(W_{\mu}^{-} W_{\nu}^{+} - W_{\nu}^{-} W_{\mu}^{+} \right) \partial^{\mu} A^{\nu} + W_{\mu\nu}^{+} W^{-\mu} A^{\nu} - W_{\mu\nu}^{-} W^{+\mu} A^{\nu} \right] \\ &+ g_{2}^{2} \cos^{2} \theta_{W} \left(W_{\mu}^{+} W_{\nu}^{-} Z^{\mu} Z^{\nu} - W_{\mu}^{+} W^{-\mu} Z_{\nu} Z^{\nu} \right) \\ &+ g_{2}^{2} \left(W_{\mu}^{+} W_{\nu}^{-} A^{\mu} A^{\nu} - W_{\mu}^{+} W^{-\mu} A_{\nu} A^{\nu} \right) \\ &+ g_{2}^{2} \left(W_{\mu}^{+} W_{\nu}^{-} Z^{\mu} A^{\nu} - W_{\mu}^{+} W^{-\mu} A_{\nu} A^{\mu} \right) \\ &+ g_{2}^{2} \left(W_{\mu}^{+} W_{\nu}^{-} \right) \left(W^{+\mu} W^{-\nu} - W^{+\nu} W^{-\mu} \right) \\ G_{\mu\nu\nu}^{a} &= \partial_{\mu} A_{\nu}^{a} - \partial_{\nu} A_{\mu}^{a} A_{\nu}^{b} \phi_{\mu}^{b} h_{\nu}^{b}, \quad M_{\mu\nu}^{\pm} &= \partial_{\mu} W_{\nu}^{\pm} - \partial_{\nu} W_{\mu}^{\pm} , \quad Z_{\mu\nu} &\equiv \partial_{\mu} Z_{\nu} - \partial_{\nu} Z_{\mu}, \quad F_{\mu\nu} &\equiv \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu$$

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Physics is simple?

Actually quite simple considering it has the ability to describe almost every *experiment* that we could perform.



Thus, *useful* physical theories are **sparse**: we can organize according to a *local* action, where interactions happen between an O(1) number of particles at a point in spacetime.

Problems in Understanding Deep Learning

Problem 1, we need to compute an infinite number of terms:

$$f, \quad \frac{df}{d\theta}, \quad \frac{d^2f}{d\theta^2}, \quad \frac{d^3f}{d\theta^3}, \quad \frac{d^4f}{d\theta^4}, \quad \dots$$

Problem 2, each time we initialize our network we get a different function f(x; θ), and we need to determine the map:

$$p(\theta) \rightarrow p\left(f, \frac{df}{d\theta}, \frac{d^2f}{d\theta^2}, \ldots\right)$$

Problem 3, The learned value of the parameters, θ*, is the result of a complicated training process:

$$\theta^{\star} \equiv [\theta^{\star}] \left(\theta, f, \frac{df}{d\theta}, \frac{d^2f}{d\theta^2}, \dots; \text{ learning algorithm; training data}\right)$$

Fine, Structure

Solving our three problems for a general parameterized function $f(x; \theta)$ is not tractable. However, we only care about the functions that are deep neural networks:



To make progress we will have to make use of the particular **structure** of neural-network function.

Fine, Structure

Two essential aspects of a neural network *architecture* are its **width**, *n*, and its **depth**, *L*.



There are often simplifications to be found in the limit of a large number of components.



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It's not enough to consider any massive macroscopic system, and taking the right limit often requires some care.

In this case, the $n = \infty$ will make everything really simple, while the $L = \infty$ will be hopelessly complicated and useless in practice.



The Infinite-Width Limit

Let's begin by formally taking the limit

 $\lim_{n\to\infty}p(f^{\star}),$

and studying an *idealized* neural network in this limit.

[Neal, Lee/Bahri/..., Matthews/..., Jacot/..., ...]

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This is known as the infinite-width limit of the network, and as a strict limit it's rather unphysical for a network: obviously you cannot directly program a function to have an infinite number of components on a finite computer.

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- However, this extreme limit does massively simplify the distribution over trained networks p(f*), rendering each of our three problems completely benign.

[Neal, Lee/Bahri/..., Matthews/..., Jacot/..., ...]

Simplicity at Infinite Width

Addressing Problem 1, higher derivative terms will effectively vanish, and we only need to keep track of two terms:

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Addressing Problem 2, the distributions of these random functions will be independent,

$$\lim_{n\to\infty} p\left(f,\frac{df}{d\theta},\frac{d^2f}{d\theta^2},\ldots\right) = p(f) p\left(\frac{df}{d\theta}\right) \,,$$

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with each marginal distribution factor taking a simple form.

Addressing Problem 3, the training dynamics become linear and independent of the details of the learning algorithm, giving θ* in a closed form analytical solution:

$$\lim_{n\to\infty} \theta^{\star} = [\theta^{\star}] \Big(\theta, f, \frac{df}{d\theta}; \text{ training data} \Big)$$

These simplifications are the consequence of a **principle of sparsity**, and the fully-trained distribution,

 $\lim_{n\to\infty}p(f^{\star})\,,$

is a simple Gaussian distribution with a nonzero mean.

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- The distribution over *real* trained networks *does* depend on the properties of the learning algorithm used to train them.
- Infinite-width networks don't have representation learning: for any input x, its transformations in the hidden layers, z⁽¹⁾, z⁽²⁾, ..., z^(L-1), will remain unchanged from initialization.

Aside: Representation Learning

In the typical discussion of representation learning, we start with the fine-grained representation of an input such as an image in terms of its pixels:

$$x = oxtimes$$
.

For a classification task, a network might output a *coarse-grained* description of that image:

$$f(x) = \operatorname{cat}$$
.

In between, the signals at the hidden-layer neurons form intermediate **representations**.

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The *central limiting* problem is that the input of an infinite number of signals is such that the leveling law of large numbers completely obscures the subtle correlations between neurons that get amplified over the course of training for representation learning. We'll need to find a way to restore and then study the **interactions** between neurons that are present in realistic *finite-width* networks.

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To do so, we can use **perturbation theory** and study deep learning using a 1/n expansion, treating the inverse layer width, $\epsilon \equiv 1/n$, as our small parameter of expansion:

$$p(f^*) \equiv \left\{\lim_{n\to\infty} p(f^*)\right\} + \frac{p^{\{1\}}(f^*)}{n} + \frac{p^{\{2\}}(f^*)}{n^2} + \dots,$$

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Near-Simplicity at Finite Width

Addressing Problem 1, most derivatives will contribute as O(1/n²) or smaller, so we only need to keep track of 4 terms:

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Addressing Problem 2, the distribution of these random functions at initialization will be *nearly* simple at order 1/n:

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,

Addressing **Problem 3**, the *nonlinear* training dynamics can be tamed with *dynamical perturbation theory*, giving θ^* in a *closed form* analytical solution:

$$\theta^{\star} = [\theta^{\star}] \left(\theta, f, \frac{df}{d\theta}, \frac{d^2f}{d\theta^2} \frac{d^3f}{d\theta^3}; \text{ learning algorithm; training data} \right)$$

These near-simplifications are a further consequence of the **principle of sparsity**, and our *dual* **effective theory** description of the fully-trained distribution at order 1/n,

$$p(f^*) \equiv \left\{ \lim_{n \to \infty} p(f^*) \right\} + \frac{p^{\{1\}}(f^*)}{n} + O\left(\frac{1}{n^2}\right) \,,$$

will be a nearly-Gaussian distribution.

An important byproduct of the analysis is a careful understanding of the *deep* in deep learning. Defining the **aspect ratio**

$$r \equiv L/n$$
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we can recast our understanding of *infinite-width vs. finite-width* and *shallow vs. deep*:

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we can recast our understanding of *infinite-width vs. finite-width* and *shallow vs. deep*:

In the strict limit r → 0, the interactions between neurons turn off: the infinite-width limit is actually a decent description, but these networks are **not really deep**, as their relative depth is zero: L/n = 0.

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In the regime 0 < r ≪ 1, there are nontrivial interactions between neurons: the finite-width effective theory truncated at order 1/n gives an accurate accounting p(f*). These networks are effectively deep.

An important byproduct of the analysis is a careful understanding of the *deep* in deep learning. Defining the **aspect ratio**

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we can recast our understanding of *infinite-width vs. finite-width* and *shallow vs. deep*:

In the regime r ≫ 1, the neurons are strongly coupled: networks will behave chaotically, and there is no effective description due to large fluctuations from instantiation to instantiation. These networks are **overly deep**.
The Role of Depth as the Effective Theory Cutoff

An important byproduct of the analysis is a careful understanding of the *deep* in deep learning. Defining the **aspect ratio**

$$r \equiv L/n$$
,

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Networks of *practical use* have small aspect ratios: $r \sim r^* \ll 1$.

Consider a fixed combined training and test dataset of size N_D :

For the *infinite-width* Gaussian distribution, we only need

$$n_{\text{out}}N_{\mathcal{A}} + \left[\frac{N_{\mathcal{D}}(N_{\mathcal{D}}+1)}{2}\right] + \left[\frac{N_{\mathcal{D}}(N_{\mathcal{D}}+1)}{2}\right] = O(N_{\mathcal{D}}^2)$$

numbers in order to completely specify the distribution.

Consider a fixed combined training and test dataset of size N_D :

For the *finite-width* **nearly-Gaussian distribution** with $0 < r \ll 1$, we will instead need $O(N_D^4)$ numbers, with the counting dominated by the finite-width tensors.

Consider a fixed combined training and test dataset of size N_D :

For an accuracy $O(L^k/n^k)$, a macroscopic description

$$p(z(\infty)) = \sum_{m=0}^{k} \frac{p^{\{m\}}(z(\infty))}{n^m} + O\left(\frac{L^{k+1}}{n^{k+1}}\right),$$

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The 1/n expansion gives a sequence of effective theories with increasing accuracy at the cost of increasing complexity.

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- ► For larger r, a more generic O(N_D^{2k}) non-Gaussian description would in principle be necessary.

Conclusion

The practical success of deep learning in with large numbers of parameters is really telling us that useful theories of neural networks should be **sparse** – but not too sparse – so that they are also **deep**.

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Thank You!