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A new kind of science

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We discuss whether science is in the process of being transformed from a quest for causality to a quest for correlation in light of the recent development in artificial intelligence. We observe that while a blind trust in the most seductive promises of AI is surely to be avoided, a judicious combination of computer simulation based on physical insight and the machine learning ability to explore ultra-dimensional spaces, holds potential for transformative progress in the way science is going to be pursued in the years to come.

KEYWORDS

artificial intelligence, causality, correlation, large language models, machine learning (ML)

1 Introduction

On 8 October 2024 the Nobel Prize in Physics was awarded to John J. Hopfield and Geoffrey E. Hinton with the following motivation "for foundational discoveries and inventions that enable machine learning with artificial neural networks" [1].

The day after the Chemistry Nobel was awarded to David Baker (Washington University) for "for computational protein design," and to Demis Hassabis and John M. Jumper of DeepMind for "for protein structure prediction" [2].

John Hopfield was saluted with great satisfaction by the (statistical) physics community as a champion of that kind of interdisciplinary statistical physics that decisively impacts on different fields, in this case biology and neuroscience. Geoffrey Hinton came as a bit of a surprise, as he is a highly distinguished authority but rather in computer science than physics, as witnessed by his recent award of the Turing Prize, along with Yan LeCun and Joshua Bengio, for their groundbreaking work on neural networks. Yet, Hinton's work certainly related to physics, especially his celebrated recursive Boltzmann machines.

The Nobel Prize in Chemistry, on the other hand, came as a direct hommage to Artificial Intelligence (AI), a statement which is particularly true for the DeepMind winners.

In short, the main critique is that, at variance with most bombastic headlines, AlfaFold is a monumental and extremely impressive *tour de force* of computer science and engineering, but does not really "solve" the protein folding problem.

Many scientists think it does not, mainly because it did not deliver any real insight into the phenomenon of protein folding, namely the dynamics taking from primary structures to their native form. The point may seem far-fetched and kind of artificial, but it is not. Protein folding is a dynamical process and if we are to gain useful insights to cure neurological diseases, we need not just the end points but the entire trajectory, i.e., the dynamics. Maybe in five or 10 years from now AlfaFold will bridge this gap, but till then the claim that the protein folding problem is cracked, is simply overstated.

The reactions are hot and split: for some this is the end of Galilean science, as provocatively announced in C. Anderson's 2008 Wire Magazine article [3], namely the triumph of Correlation over Causation (for quick and direct counter-arguments see [4, 5]). For others, it is a mere fact of life that Machine Learning (ML) algorithms, no matter how empirical, manage to capture levels of complexity unattainable by any other method, including our most powerful theories and computer simulations. One may find a weak echo of this debate in that which surrounded the proof of the four color theorem in the seventies, which involved the use of computers doing parts of the proof that would be beyond human capability [6]. This time around, however, the questions raised need answers. Be as it may, some large pinch of caution is needed.

2 The power of insight

One of the main criticism to most intensive ML applications, such as AlfaFold and even more so latest chatGPT Large Language Model (LLM) algorithms, is the astronomical number of weights used, rapidly moving into the hundred billion regime. This is problematic in many respects, both fundamental and practical.

The fundamental aspect is that in theoretical physics, parameters are traditionally held as fudge factors, i.e., temporary fixes for our holes of understanding. Hence, the fewer parameters the better. Newton's law of gravitation epitomizes the beauty and universality of a good theory. Once you understand that two material bodies attract with a force F proportional to the product of their masses m_1 and m_2 inversely proportional to the square of their distance r, all you need to fix by experiment is the ratio

$$G = \frac{Fr^2}{m_1 m_2}. \quad (1)$$

The beauty of this expression rests with its universality: *any* experiment, whether you are using apples, billiard balls or the moon orbiting around planet Earth, will return the *same* value for this ratio, $G \approx 6.67 \times 10^{-11}\ Nm^2/kg^2$. All data, big or small, are captured within a single parameter (as long as gravitation is weak enough and non-quantum)! This is the power of Insight and explains why physicists place so much value in it. To this regard, it is worth recalling the famous Fermi's anecdote reported by Freeman Dyson, when he approach Fermi to discuss with him his pseudo-scalar theory for pions. Fermi asks "how many parameters do you have in your model?" "Five" replies Dyson. "My friend John von Neumann told me that with four parameters he can fit an elephant, and with five he can wriggle his trunk." And with that the conversation was over [7].

The practical aspect has to do with sustainability: it is estimated that training next-generation chatbots with some hundreds billion parameter may easily move into the GWatt power demand, corresponding to the output from a substantial nuclear power plant. The comparison with the 10 W of our brain is embarrassing, but that is another story [8].

One could observe that present-day top-end supercomputers are also pretty energy-thirsty with a power request in the order of ten MWatts, a million times more than human brain. The point though is that there a return for this: exascale computers compute some twenty orders of magnitude faster than our brain (a tiny fraction of Flops/s). So, the question becomes social and ethical: is it worth exhausting a substantial fraction of the worldwide energy budget to feed the insatiable appetite of chat-bots?

Science-wise, the astronomical disparity between the LLM's power request and that of our brain provide a strong pointer towards the need for a much better theory of machine learning [9]. This may spawn a genuinely new way of doing science but to achieve this goal it is important to keep an open mind. Here comes the point.

As noted above, centuries of physics (since Galileo) have taught us that the least number of parameters the best. So, let us call P the number of parameters required to produce a satisfactory fit to an ensemble consisting of D data. We may define a fitting efficiency as the ratio

$$f = \frac{D}{P}. \quad (2)$$

Clearly, the scientific method aims at large values of f, the zero-parameter limit $f \to \infty$ denoting the "Perfect Theory", one with no free-parameters at all. The Standard Model, still our most accurate description of fundamental interactions, is regarded by some as "ugly" because it demands 19 free parameters.

Machine learning, and most notably LLM's, work instead in the opposite limit $f \ll 1$, $f < 1$ denoting the infamous "over-fitting" regime: more parameters than data. Over-fitting is a notorious problem for ML, as it hinders the capability of extrapolate to capture unseen data, the whole purpose of the ML ordeal. Fact remains, though, that ML practitioners have proven capable of turning around it under circumstances where it was supposed to hit hard, the famous google transformer paper being an adamant example in point [10]: No systematic theory, a mathematical framework based on billions of free parameters, augmented with a set of semi-empirical hunches and recipes. Yet, in the end, it often works and sometimes big time so. Hence, while it is entirely healthy to remain skeptical of occasional success stories, no matter how spectacular, one should also be open to the possibility of making the most of this "unsuspected" capability of machine learning to bypass overfitting.

3 Fermi's belt in Los Alamos

This said, the Nobel Prize for Chemistry raises a point which goes beyond science. Let us assume that from now on that we have passed the Singularity and live in a world where radical Empiricism takes the lead in science: Correlation does supersede Causation and science can advance with just a little ancillary help of theory and simulation. Let us say that this is the ugly but effective winning route.

Our point here that at a deeper level, this is no longer about Correlation versus Causation, but rather Control versus Insight.

Current chat-bots can write pretty decent code in seconds, in the face of the hours or days for a skilled programmer. You could hail at this as to a major time-saver and for sure it is. But if you dig just a bit deeper, a poisoned apple pops out in plain sight.

Let's go back to Fermi again. There is little question that Fermi was one of the most versatile physicist of all time, with several achievements under his belt each worth a Nobel prize (fission, Fermi-Dirac statistics, beta decay, Thomas-Fermi theory of nuclei etc.).

Amazingly, once interviewed about what he regarded as his most impressive achievement, none of these were to come up in his reply. Instead, he quoted an episode from the Los Alamos period, when his Jeep got stuck in the desert because the transmission belt went bust. Not your best cup of tea if you are left alone in the Los Alamos desert …Fermi being Fermi, he managed to get out of the hook by replacing the transmission belt with …his own belt!

That means being able to face tough problems and adversity, something that the relentless promise to relieve us, in fact our brain, from any burden, is rapidly grinding to a halt. A few high-tech companies will take care of writing codes for you, that is where Control of a few over the rest of us, shows up beyond any reasonable doubt: chat-bots write codes in seconds, no need of programming for the new generations, Google brains will take care of this for you.

Now, leaving aside Fermi, even on our modest personal scale, we can quote many instances in which we were sure we had it all sorted out, but when it was time to finally code it up, we actually realized that we did not really know how to do it exactly. So we had to pedal our way back and figure out where the loophole was, a process of immense value for our scientific growth.

One may see a concrete example of this in comparing Refs. [11, 12]. The first paper, based entirely on theory, missed a crucial ingredient—the co-moving velocity—which is of increasing importance in the field of two-phase flow in porous media. It was only through computations that we discovered it, and with it in hand, we realized that Ref. [11] was not correct, replacing it with [12].

So, the question is: is it worth saving our time to code it up? Our answer is yes, but only to a point; We surely welcome automatic help, but not to the point where it would kick us completely out of the show.

We all speculate about the Singularity as the day when AI supersedes Natural Intelligence, (NI) where the latter is typically thought of a constant in time. It is not, at least on average, some of the most aggressive AI applications do lower NI levels, thereby accelerating the Singularity. Hence, the Singularity itself is probably not as much of a problem as the degradation of NI. This is not to say that AI is should be rejected, but rather to stand for a cooperative pattern whereby the ultimate control is left to NI.

4 The bright side of machine learning

In the previous sections we have raised a number of warnings against the backsides of AI, and particularly to its most aggressive claims. The "grumpy old men" part of the paper ends here.

Indeed, it would be poor-sighted to deny that machine-learning has brought a new dimension to scientific investigation along the three standard pillars of Theory, Simulation and Experiment. AI is contributing in many respects to the scientific endeavour but here we focus on one that appears to be particularly relevant across many scientific and societal applications: the infamous Curse of Dimensionality (CoD) [13].

Our brain, as well as much of our math, is notoriously at odds with handling high-dimensional information, the main reason being the exponential growth of the volume with dimensions $V_D = V_1^D$. Assuming a uniform density of information, ρ, the total information $I(V) = \rho V$ stored in a given volume of state space also scales exponentially with the number of dimensions. Take standard four-dimensional spacetime, with $N = 10^3$ degrees of freedom per dimension and unit density everywhere, we obtain $I_4 = 10^{12}$, which is basically as much as we can accomodate on present-day Exascale computers. Many problems in science and engineering live in much higher dimensional state spaces with thousands, millions or even billions of dimensions, spelling complete doom for most of our mathematical methods. Fortunately, Nature is usually merciful and the amount of information does not grow accordingly because most of these ultra-dimensional spaces are empty and the relevant (active) degrees of freedom use to populate a much smaller manifold of dimension $d \ll D$ (d is usually known as Intrinsic Dimension). Finding such manifolds is a highly non-trivial task, not only because they occupy an extremely tiny portion of state-space but also because their topology is often highly irregular and scattered out. This is a central issue in modern computational statistical physics and many other fields of modern science. Machine learning in general and transformers in particular can be viewed as highly non-ergodic discrete dynamical systems, targeted to locate the solution manifold as efficiently as possible, without wasting resources to visit empty regions of state-space. Let us spell the idea out in some more detail. Transformer operation (see Figure 1) can be paralleled to a discrete dynamical system of the form [14]:

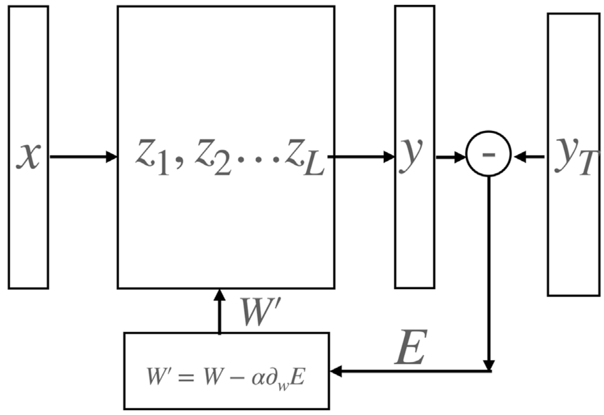

FIGURE 1
A schematic representation of the transformer architecture. Note that each layer carries the same number of neurons.

$$y = f^L[Wx - b], \tag{3}$$

where x is the input state in D-dimensional feature space, y is the corresponding output, the pair (W, b) indicates the set of weights and biases connecting the hidden layers $\{z_1, z_2 \ldots z_L\}$ and f is the activation function applied across each of the L hidden layers. The above "forward-step" is complemented by a backward-error propagation step in which the weights are adjusted in such a way as to minimize the departure from the desired target ("truth") y_T, also known as Loss Function

$$\mathcal{L} = \|y - y_T\|, \tag{4}$$

where $\|.\|$ indicates a suitable metric in feature space. Such minimization is usually performed with steepest-descent-like techniques

$$W' = W - \alpha \frac{\partial \mathcal{L}}{\partial W}, \tag{5}$$

where α is a relaxation parameter known as "learning rate". The above backward-forward loop is repeated over a huge set of data (x, y) until the optimal weight configuration is found.

By paralleling the layers to discrete time steps, the above procedure amounts to a discrete dynamical system starting at $z_0 = x$ and ending at $z_{L+1} = y$, evolving under the feed-back control of the backward error propagation step.

The analogy has been discussed in detail in [14] and here we only point out that such trajectories appear to be efficient in catching the desired target y_T in ultra-dimensional space. For instance leading-edge LLM's with near trillions weights can find solutions in manifolds with $d \sim 40$. Leaving aside all reservations about computational and energetic parsimony as well as lack of physical insight and explainability, this is unquestionably a remarkable deed.

The magic is probably less arcane than it may seem at first sight. The transformer loop discussed above typically lands on random matrix solutions for the weights, even in the case where the problem has a definite structure, say a sparse matrix using standard discretization techniques. This may seem weird at first glance, but it actually reflects the fact that the ensemble of random matrices is astronomically larger than the ensemble of ordered (structured) matrices arising from grid discretization methods. It is therefore no surprise that machine-learning search ends up in this huge ensemble rather than on the incommensurably smaller ensemble of structured matrices. In the end, the usual entropic argument. The price, of course, is a vastly larger number of parameters and training costs, aggravated by the lack of a systematic convergence theory. Ignoring the latter dark-sides, as it is typical of the most aggressive AI claims, is to be highly deprecated and must be countered: the Fermi's belt anedocte should not go forgotten. Yet, the fact remains that developing suitable strategies combining the conceptual transparency of the scientific method with the ability of transformers to chase "golden nuggets" in ultra-dimensional spaces, holds major potential to transformative progress in the way scientific investigation will be pursued in the years to come.

5 Outlook

Machine Learning is often hyped as a universal panacea, which is most certainly not. Hence it is crucial to keep a critical attitude towards the most bombastic and aggressive AI claims. However a judicious and clever combination of computer simulation based on physical insight and the machine learning power to explore active regioins of ultra-dimensional spaces, may lead to transformative progress in the future of science.

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AH: Conceptualization, Writing – original draft, Writing – review and editing. SS: Conceptualization, Writing – original draft, Writing – review and editing.

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