Deep Learning as Model Independence Work in Progress, MCMP June 15, 2023

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"No, there is no crisis in particle physics. Except maybe in some people's minds. But the thing is that we are living in times that we don't know yet. We are at a real crossroads, if you want, and we can't disentangle yet where the arrows pointing or which ones we should be following."

(De Roeck, 03.07.19)

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No indications in favour of predictions from BSM models
No statistically significant deviations in SM precision measurements

No indications in favour of predictions from BSM models
No statistically significant deviations in SM precision measurements

Sounds good.

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1 SM research programme is (in a sense) complete

 $\hfill\square$ SM as a theory is not

2 No new high-energy particle accelerator

 $\hfill\square$ theorists and experimentalists have to get clever

So, where will new physics come from?

- $\hfill\square$ well, we don't know, but discoveries
 - \Box won't be done in the same way
 - $\hfill\square$ won't be easy

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- \Box it will require an openness
 - $\hfill\square$ an independence from traditional modelling assumptions

The rise of "model-independent" methods

- **1** SM precision measurements
 - $\hfill\square$ to search for any deviations whatever
- 2 SMEFT

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 $\hfill\square$ to parametrise deviations given some assumptions

3 Deep Learning

 $\hfill\square$ to analyse low-level data with fewer high-level physics assumptions

1 Introduction

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- State of the Art
- Crossroads

2 Deep Learning

- Basics
- Deep Learning in HEP

3 Epistemic Issues

- In General
- Issues in HEP

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1 Identify, examine, and minimise the role of biases

- $\hfill\square$ explore new alternatives
- □ re-evaluation of principles (e.g., naturalness)
- $\Box \ \mbox{model-based} \rightarrow \mbox{model-independent} \ (\mbox{top-down} \rightarrow \mbox{bottom-up})$
- 2 Shift in cognitive division of labour

"So just before the Higgs discovery, I was just doing model building for model building's sake. And I don't do that at all any more. I'm much more connected to experiment and I think that's true for most people."

Matthew McCullogh

Shifting Approaches

Sunthere https://doi.org/10.1007/s11229-019-02216-7

S.I.: REASONING IN PHYSICS

From a boson to the standard model Higgs: a case study in confirmation and model dynamics

Cristin Chall¹ , Martin King¹ , Peter Mättig¹ , Michael Stöltzner²

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Our paper studies th Collider and its influ tigate the phases of landscape of elemer dard model (SM). A breaking (EWSB) s own understanding allowed us an empl draw two main phili a complex experim standpoint, some SI Higgs discovery the accepted account of tion and expose son discovery as a victor natives in the face of a research program other aspects adapt landscape of EWSE model-group, and w



programmes - Higg



Fig. 2 Overview of model-groups (HEP-PH) from Jan 2010-Dec 2017

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are, quite surprisingly, fairly steady over the eight year period, though showing a recent decline. Theoretical studies on the SM Higgs remained fairly constant, primarily focusing on improving the precision of the calculations.

There are two interesting messages that the search data conveys. First, even though

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Bottoms up: The Standard Model Effective Field Theory from a model perspective



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R T I C L E I N F O

ABSTRACT

Krywords: Scientific modelling Beyond standard model Particle physics Effective field theory Models and theories Representation Topoteness in particle physics have latters finded to produce any application existence for the many exploring and/or of physics physics the introduce biddi (GM) that has the proposed one way from plot donks. As even about the physics physics was an even of the physics of the physics of the physics of the physics physics in the research physics of the physics physics or nonline, we gray the fits new real physics of the physics of the physics of the physics physics or nonlines, we gray the fits the new real of the physics of the physics of the physics physics or nonlines are physical distanciant descence of the physics of the physics physics or nonlines are physical distances on physical distances on physical distances on physical physics or nonlines are physical distances on physical distances on physical distances on physical physics or nonlines are physical distances on physical distances on physical distances on physical physics or nonlines are physical distances on physical distances on physical distances on physical distances on physical distances of the physical distances on physical distances are physical distances on physical distances on physical distances on physical distances on physical distances are physical distances on physical d

1. Introduction

To date, the Large Hadron Collider (LHC) has produced no significant evidence in favour of the many models beyond the Standard Model (BSM) that have been previously proposed. The data gathered since has increasingly reduced the parameter space in which these existing models dualt, while not indication acone which those new models downd he. aspects of the use of the SM-EFT at the LHC. We want to ask: what is the SM-EFT and the bottom-up research strategy, what is model-independent about it, and how should we understand it in the context of the philosophical literature on models and effective field theories?

An EFT efficiently describes phenomena on a specific energy scale by availing itself of a separation of scales and absorbing the physics at higher energies only, into the narameters of lower scale obvios, that are deterII M



Shifting Approaches

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BSM models are underdetermined by data

- **1** theory assessment; non-empirical theory confirmation (Dawid, 2019, 2022)
- 2 novel ways of looking at empirical evidence; model-independent methods and DL

Possible theoretical avenues:

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- 1 big, beautiful theories
- 2 small, low-energy models connected to current experiments
- **3** reevaluating assumptions/questioning foundations
- 4 accept fine-tuning, ad hocness

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Forget a theory of everything,

"I'd be happy with a theory of anything,"

John Ellis

Possible experimental avenues:

1 higher energy collider

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- 2 astro-particle physics/cosmology
- 3 neutrino observatories
- 4 SM precision tests at HL-LHC, elsewhere
 - \Box Higgs physics
 - \Box b-quarks
 - □ muon g-2
- 5 low energy frontier
 - $\hfill\square$ long-lived particles (FASER), axion experiments, etc.
- 6 DL on existing and new data

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D model-dependent: full BSM models

- \square search for processes and signatures in the context of a particular, well-defined BSM model
 - charged Higgs of Type-II 2HDM with mSUSY
- $\hfill\square$ Very specific, narrow focus



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 - charged Higgs of Type-II 2HDM with mSUSY
- □ Very specific, narrow focus
- □ partially model-dependent: simplified models
 - $\hfill\square$ search for particles common to many BSM models
 - leptoquark, vector triplet, stop
 - □ specific, broadly applicable searches

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 - $\hfill\square$ specific, broadly applicable searches
- D model-independent: precision measurements, using SMEFT, e.g.
 - $\hfill\square$ not to search for predictions of a model but search for deviations against the background

Model Independence is characterised by:

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 $\hfill\square$ a strong reduction of the influence of modelling biases

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For BSM searches:

I WL

- **1** a lack of a well-defined *target model* or *target phenomenon*
- 2 where there is a well-defined background theory (SM) against which deviations can be observed

 $\hfill\square$ this can be relaxed

Deep Learning

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- provides the tools to make analyses based on 'low-level' data with minimal preprocessing and input from physicists
- □ can be *unsupervised*
- \square aim of finding patterns in data, without being told what patterns to look for \square anomaly detection

Model Independence

- $\hfill\square$ doesn't have to stem from deep networks
- $\hfill\square$ not qualitative difference, but significant quantitative

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Deep Learning in HEP

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Neural Network

- $\hfill\square$ automated decision algorithm of nodes and links, thought to resemble neurons in a brain
 - $\hfill\square$ nodes are organized in layers from input through hidden layers to output
 - □ the outputs are *weighted* with free parameters (matrix)
 - $\hfill\square$ through tuning the parameters to data, the model 'learns' to optimize the weights
- □ shallow or deep
 - $\hfill\square$ hidden layers





$$y_{out} = F_w(y_{in}) \tag{1}$$

16/56

Steps

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- 1 an input signal sent to some array of nodes
- 2 the nodes compute their **activation functions** and pass an output signal to the next layer along their links
- $\ensuremath{\underline{3}}$ these links have different weights w which modify outputs at every stage
- 4 the activation of the nodes propagates until it reaches the output layer of nodes
- 5 this is then decoded and taken as the network's decision for that input
- **6** typically there is a teaching or training goal, such that the network adjusts its weights to best achieve the goal

(Buckner, 2019)

1 Convolution

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- \Box linear operation passes a $\mathit{kernal/filter}$ over the data to amplify desired features
- $\hfill\square$ exploits 'translational' symmetry, reducing the number of parameters

2 Rectification (ReLU)

- $\hfill\square$ threshold activation unit
- 3 Max Pooling
 - □ downsampling function, combining many kernals(filters), pooling only maximum values

The main practical goal is generalisation

1 learn a set of data

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- $\hfill\square$ avoid underfitting
- $\hfill\square$ divide data into training set and test set
- 2 have it apply to new data
 - $\hfill\square$ avoid overfitting
 - $\hfill\square$ various methods of *regularization*
 - dropping out nodes, penalty terms, modifying input data, etc.



Reward is rare

- **1** conduct a bunch of trajectories
- 2 sum over rewards for each
- 3 apply gradient training

Backpropagation

- $\Box \, \rightarrow \mathsf{true} \; \mathsf{gradient}$
- approximate with stochastic gradient descent

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"In the relatively few years that modern machine learning has existed, it has already made traditional collider physics obsolete. In the past, physicists, including me, would devote their efforts to understanding signatures of particular particles or processes from first-principles: why should a stream of pions coming from a W boson decay look different than a stream coming from an energetic gluon? Now we simply simulate the events, and let neural network learn to tell the two samples apart."

(Schwartz, 2021)
The difficulty that deep learning can deal with is not the sheer amount of data, but the *high-dimensionality* of LHC data

Task in HEP

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- \square estimate probability function $p(x|\theta)$ of observing some data x, given the model's parameters θ
- \square estimating is possible for low-dimensional data (d<5)
- \square number of samples to estimate the function grows with the power of the dimensionality of data N^d

Must reduce the dimensionality of the data, $d={\cal O}10^8$

(Guest et al., 2018)

Strategy

□ Construct higher-level, lower-dimensional objects and analyse those

Steps

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- reconstruction algorithms are used to process raw data into objects (clusters and tracks)
- 2 use this to estimate the energy and momentum of particles
- 3 identify particles
- 4 build event-level summaries
- **5** perform event selection for further analysis

The reconstruction and selection are traditionally based on *physicist-identified* features of the data (shape of the shower in the calorimeter)

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- □ works pretty well, but not *optimal*
- \Box DL helps optimize this process

I ML

Most tasks can be formulated in terms of the optimization of a loss function L[y, f(x)]

- \square search f(x) that optimizes move from high-dimensional space of observed data \rightarrow low-dimension space
- \Box the (reduced) space of functions searched is given by a series of transformations mapping inputs x onto hidden states h_i and then to the output y

$$h_{i+1} = g_i(W_i h_i + b_i)$$
 (2)

where g_i is the activation function and a particular h_i is the *i*th transformation, called the embedding and the W's are matrices and the *b*'s are biases

- $\hfill\square$ the model is trained by optimizing the values of the weights
- \Box training examples are used to calculate the gradient of the loss function with respect to the model parameters $\nabla_{\phi} L[f_{\phi}(x), y]$, often via backpropagation

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- 1 Outperforms traditional methods in many areas
- 2 More computationally efficient

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3 Offers model-independent ways of analyzing data

All Along Data Pipeline

1 Simulation

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- 2 Improving trigger timing
- 3 Low-level: hit and track reconstruction
- 4 Mid-level: object identification
- 5 High-level: event classification

The Need for Speed

At HL-LHC, there will be $7 \times$ luminosity (20x run-2 data set), not enough more computing resources

- □ ML has been used for decades (multivariate analysis, boosted decision trees)
- $\hfill\square$ DL solutions are needed

1 Detector

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- $\hfill\square$ discovery requires comparing the detector response with SM and BSM expectations
- $\hfill\square$ detector response cannot be analytically computed

2 Events

- □ Trillions of collisions need to be simulated in order to make accurate comparisons
- $\hfill\square$ DL can learn the physics and generate new events

3 Background

- □ background can be learned more accurately (can be in situ)
- $\hfill\square$ aid in anomaly detection

CMS/ATLAS have ${\sim}100$ million channels sampled every ${\sim}25 \text{ns}$

 \Box 60Tb/s raw data

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40 million events/s must be searched in real time

1 L1 hardware trigger ightarrow 100k/s

□ calorimeter + muon spectrometer energy threshold (+topo)

 $\hfill\square$ decision in 200 nano secs

2 L2 software (high-level) trigger ightarrow 1000/s

 \Box jets, missing p_T

3 ATLAS has L3 trigger \rightarrow 200 events

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DL offers the possibility of triggering on events that cannot currently be stored

- \square acceptance 1 in 40,000 events
 - \Box can write 15Pb/y for offline analysis
- \square try to keep low-energy DM signatures, b and c quark physics, etc.
- $\hfill\square$ event selection based on cuts may miss a lot of events of interest

(ATLAS Collaboration, 2021; CMS, 2018)

I MU



 \square may only be one event of interest in a bunch of 150-200 interactions \square the rest is called *pile up*

 $\hfill\square$ it can be removed by having the algorithm remove noise

DNN can more faithfully and more quickly build tracks from hits

Process

I MU

- **1** clusters hits in innermost chamber (pixel sensors)
- **2** 10^8 pixel channels give 10^3 tracks
- 3 almost 100% efficient, but computationally very intensive
 - $\hfill\square$ at HL-LHC increase in events/s leads to combinatorial increase in false seeds for tracks

1 flavour tagging

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 \Box top tagging: high mass, decays to 3 lighter quarks (jets), displaced vertex

 $\hfill\square$ ignore the physics, let the DNN decide which features to care about

2 substructure tagging

- □ structure of calorimeters makes for a cylindrical projective surface on which the detectors can serve like pixels of image
- $\hfill\square$ leverage DL image recognition
- $\hfill\square$ typically requires preprocessing, but DL works better without

(Guest et al., 2018; Schwartz, 2021)

Traditionally

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- $\hfill\square$ analyses use reconstructed invariant masses of particles
- □ high-level physicist-processed data

DL end-to-end

- can use 4-momenta
- $\hfill\square$ low-level raw data with minimal input and processing
- outperforms traditional classification

(Guest et al., 2018; Baldi, 2014)

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Task: distinguish signal from background



A signal is often a peak due to resonance

 $\hfill\square$ in that region the background is negligible

 $\hfill\square$ elsewhere the signal is negligible

Probability distribution

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$$P_{data} = \alpha_S P_S + \alpha_B P_B \tag{3}$$

and then determine the coefficients and see if α_S is zero

- \square it takes many, many events to be able to constrain α_S
- □ analyses typically done on *one* variable at a time (histogram)

Deep Learning

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- $\hfill\square$ run through the entire data with minimal assumptions
- $\hfill\square$ make decisions based on more than one variable at the same time
- $\hfill\square$ identify background without knowing the SM
- $\hfill\square$ identify anomalous events
 - $\hfill\square$ rank by typicality

LML

If you want to tag a top quark ($t\bar{t}$ pair production)

- □ don't tell the model that the top is heavy, that it decays to three other jets, that it has a slightly displaced vertex, etc.
- $\hfill\square$ feed it tons of simulated data and it will have a higher success rate

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1 lack of theory

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- $\hfill\square$ no help in design
- 2 lack of opacity
 - \Box which features is it latching onto?
- 3 lack of explainability
 - $\hfill\square$ how are decisions justified?
- 4 predictions without explanation
 - \Box getting an answer is nice, but will it give us satisfying explanations?



Given any decision, we don't know along what lines it was made

- □ model decision output with understandable model (xAI)
 - $\hfill\square$ need to show over which domain the net is reliable and accurate, where it breaks down, and where its behaviour is uncertain
 - $\hfill\square$ can't always be done
 - $\hfill\square$ no guarantee that it is picking up on the same features
 - $\hfill\square$ means more computation
- vary input

I MT

 \Box are we varying it in the right way?

(Boge, 2021; Mittelstadt et al., 2019)

I MT

- **1** explaining the model's decisions
 - $\hfill\square$ in many contexts one may be asked to justify to decision
 - $\hfill\square$ all one can point to is the reliability of the outcome
- **2** using the input-output in explanation
 - $\hfill\square$ like a black-box or complex simulation
 - \Box limited use
 - no view of the process/components
 - no causal or mechanical information
- **3** Not an ordinary black box
 - $\hfill\square$ there is an in-principle opacity

(Boge, 2021; Schubbach, 2019; Sullivan, 2019)

There are two broad aims in xAI

1 transparency—how a model functions internally

 \Box simulatability

I MT

- □ decomposability
- □ algorithmic transparency
- 2 post hoc interpretation—how the model behaves
 - □ input-output relations
 - $\hfill\square$ relative influence of components
 - $\hfill\square$ local explanations by retrofitting a simplified model, or assessing its robustness
 - $\hfill\square$ identifying most similar training data

(Mittelstadt et al., 2019)

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No theory of DL

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- 2 Reliance on Simulated Data
- 3 Mismodelling
- Interpretability and Understanding

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The mathematical theory of statistical learning lags far behind the success of DL models

- $\hfill\square$ little to offer in terms of design and refinement of algorithms and new techniques
- □ matter of heuristics and trial and error
- $\hfill\square$ No theoretical guarantee of reliability or optimality

(Bahri et al., 2020; Belkin, 2021)

Simulations and simulated data is used everywhere in HEP

(Morrison, 2015)

Quantum data The quantum nature of the real event means that simulated data is different

- \Box there are no ground truths
- □ for a given event, you cannot say 'Higgs' or 'no Higgs' decisively
- \square all one can do is collect statistics and try to reject the background only hypothesis

(Schwartz, 2021)

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Trusted simulations work in low-dimensional spaces with high-level physics features

□ correlations in a high-dimensional space may not be faithful

Just because a model has a better false-positive rate doesn't mean it will perform better in particle identification

- □ e.g. if it works better on simulated data than real
- □ performance will be up to systematic uncertainties, signal-to-background ratio, etc.

 \square things that are traditionally accounted for, but ignored in DL

I MU

Progress on computation is often a trade off with understanding the model's decisions "Generically, we should anticipate a trade-off between performance and interpretability"

(Guest et al., 2018, p. 175)

It is not a like an analytic function, where the structure of the solution can be analysed

reverse engineering the classification strategy is impossible due to the high-dimensional nature of the data

The decisions may be faster, more accurate, more computationally tractable, but as long as we don't understand the decisions, they will be of limited benefit

 $\hfill\square$ maybe the features being picked up on could be insightful, but we won't know

Specificity

- Perhaps something learned in a network trained on top tagging could be useful in bottom tagging, but we won't know
- □ Sharing with other experiments may not be possible, since they often run different software

Non-traditional

□ not a cut-based analysis given in histograms and natural language description

- **1** No theory is kind of okay, as long as it works
- 2 Sufficient data for reliability

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3 Post hoc interpretation—the model's don't do everything

Justification is not explanation

- □ justification comes from success
- $\hfill\square$ its decisions can be easily justified, but not easily explained

The proof is in the pudding

□ theoretical guarantees still rely on statistical arguments that are essentially about reliability of results

No need In principle, one can proceed in HEP entirely without simulations.

- $\hfill\square$ if it can be simulated, it can be done with pen and paper
- \Box it would be slow

Use real data

□ DL can also be run on real data (without ground truths), or mix of real and sim □ there is roughly the same amount of sim and real data at LHC (trillion events)

Sufficient data

 $\hfill\square$ in HEP there is too much data and computing resources

- $\hfill\square$ train and test until the cows come home
- □ statistical errors are small, systematics become the issue
 - **DL** can help with this too! $(error_{sys} \rightarrow \nu)$

Varied approaches

- $\hfill\square$ data is public and there are open competitions
- new approaches and architectures are tried across the globe

Maybe its just not for that

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- $\hfill\square$ it is not already a model of new physics
- □ if an anomaly is discovered, the deep CNN (or whatever it is) will provide no understandable model in terms of intuitive physics

Maybe its just not for that

IMU

- $\hfill\square$ it is not already a model of new physics
- □ if an anomaly is discovered, the deep CNN (or whatever it is) will provide no understandable model in terms of intuitive physics

But it will indicate where new physics is

- □ then traditional model-building will turn on
- □ similar to EFT approach
- □ similar to xAI

It is can be tool to identify correlations, but it will not likely help in interpreting the data
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"statistical algorithms find patterns where science cannot"

"We usually don't know about causation, and we often don't necessarily care... the objective is more to predict than it is to understand the world... It just needs to work; prediction trumps explanation."

(Kitchin, 2014)



□ three important feature of DL: performance, efficiency, and model independence

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□ three important feature of DL: performance, efficiency, and model independence
□ has many practical and epistemic difficulties to overcome

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three important feature of DL: performance, efficiency, and model independence
has many practical and epistemic difficulties to overcome
but these are *issues* not *problems*

Thank you

Closing

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