

Machine Learning in Particle Physics

going beyond classification and regression

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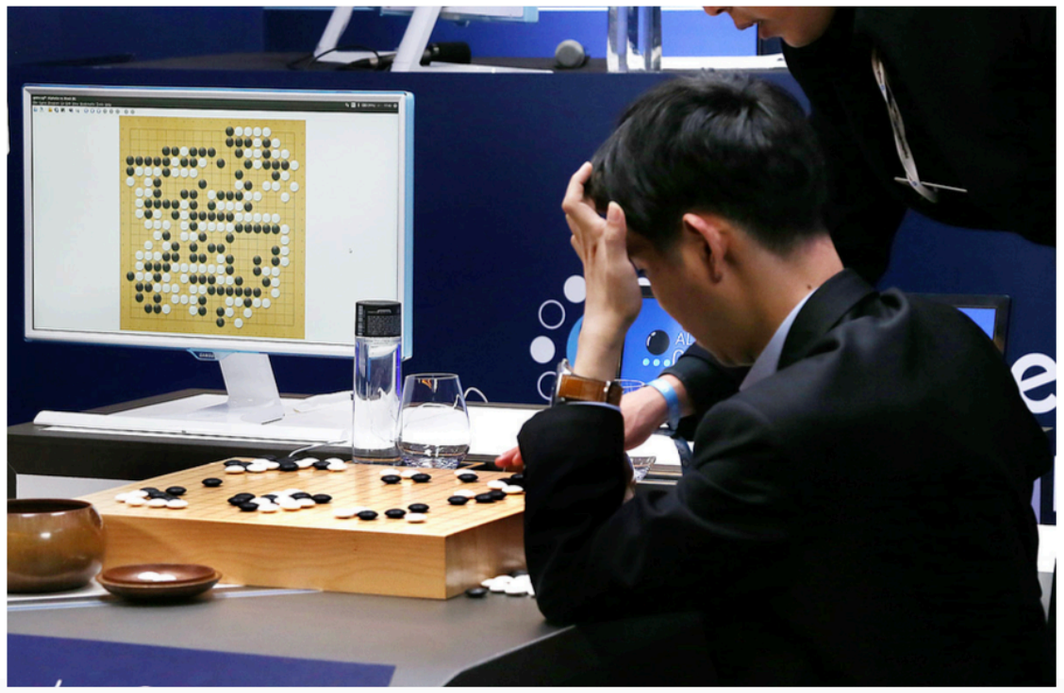
THE DAWN OF BIG DATA
Share of market activity
25%
75%
Passive market share
Changes in the activity of the active and passive market is uncertain. Established positive trends in various market segments.
Projected sales of main products in 2013
Distribution of market share among the major industry players: IT & C and BN & T was 74% and 26% percent respectively. A further change in the economic situation in the market will be characterized by a more equal distribution of market share major players
26% BN&T
74% IT&C
N FEB MAR APR MAY JUN JUL AUG SEP OCT NOV DEC
Big Data Analytics


ALSO
BIG
DATA
TOOLS
DISK
TARGET
APPLIED
SENSOR
SHARED
DEFINITION
MOVING
WITHIN
EXAMPLES
RECONSIDER
PRACTITIONERS
CAPTURE
INTERNET
BUSINESS
SETS
GENOMICS
DISTRIBUTED
MANAGEMENT
TERABYTES
CASE
PETABYTES
INCLUDE
ABILITY
SYSTEMS
TOLERABLE
STORAGE
SIZE
PARALLEL
SAN
MASSIVELY
GROW
ANALYTICS
COMPLEX
SOCIAL
RELATIONAL
CONNECTOMICS
ORGANIZATIONS
CONTINUES
LARGER
TENS
CITATION
INDEXING
HUNDREDS
BIOLOGICAL
PROCESSING
CAPACITY
NETWORKS
DATABASES
RECORDS
SEARCH
GARTNER
WORKING
EVERY
DIFFICULTY
SOLID
TYPES
CURRENTLY
OPPORTUNITIES
AMOUNT
ZETTABYTES
DESCRIBING
RADIO-FREQUENCY
THOUGHT
COMPLEXITY
ELAPSED
FORMS
SINCE
QUALITIES
MPP
DESKTOP
BURIED
WORLD'S
UBIQUITOUS
NOW

Humans vs Machines

- 2015 **Image Classification**:
  - K. He et al (Microsoft Research), *Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification,* 1502.01852
- 2016 **Go**:
  - Alpha Go (D. Silver et al, *Mastering the game of Go with deep neural networks and tree search*, Nature 529, pp484–489 and D. Silver et al *Mastering the game of Go without human knowledge,* Nature 550, pp354–359)
- 2016 **Speech recognition:**
  - W. Xiong et al (Microsoft Research) *Achieving Human Parity in Conversational Speech Recognition,* 1610.05256
- 2017 **Poker** (heads-up no-limits Texas Hold'em):
  - N Brown and T Sandholm, *Superhuman AI for heads-up no-limit poker: Libratus beats top professionals, Science 359, Issue 6374, pp418-424*
- 2018 ***Translation*** (Chinese-English)
  - H H Awadalla et al (Microsoft AI & Research) *Achieving Human Parity on Automatic Chinese to English News Translation*
- 20?? **Particle Physics**



Machine Learning

=

The scientific study of algorithms and statistical models that computer systems use in order to perform a specific task effectively without using explicit instructions, relying on patterns and inference instead. (Wikipedia)

In other words: Algorithm-based extraction of correlations between input and output

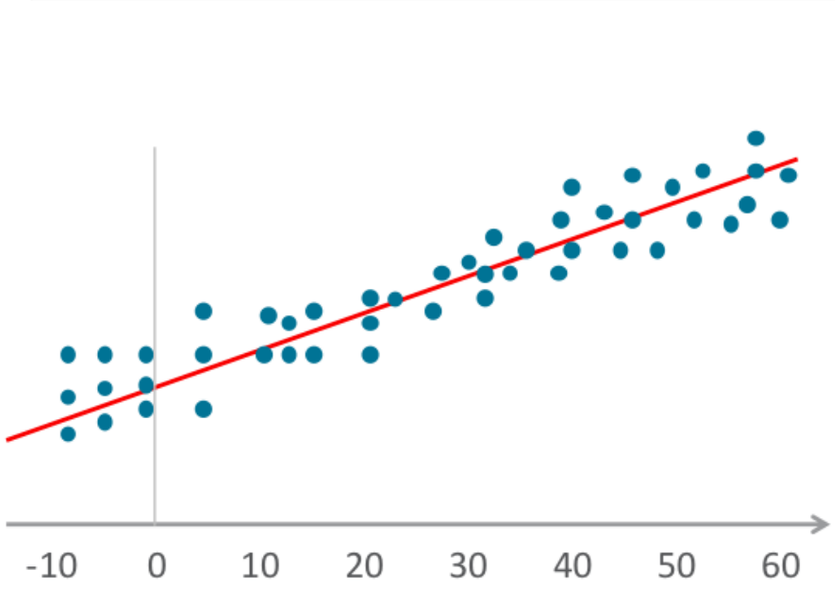
In particle physics, mostly used in context of

Regression and **Classification**

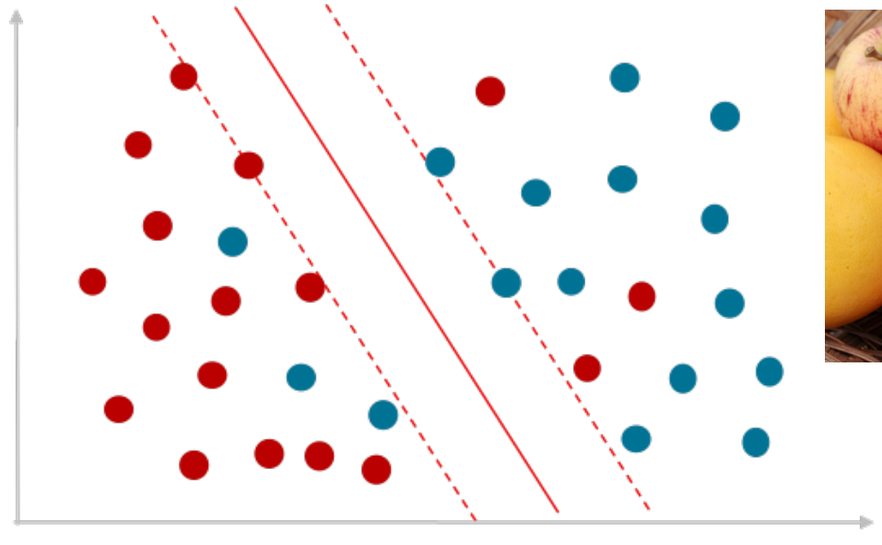
(upcoming clustering and anomaly detection)

Supervised

Regression

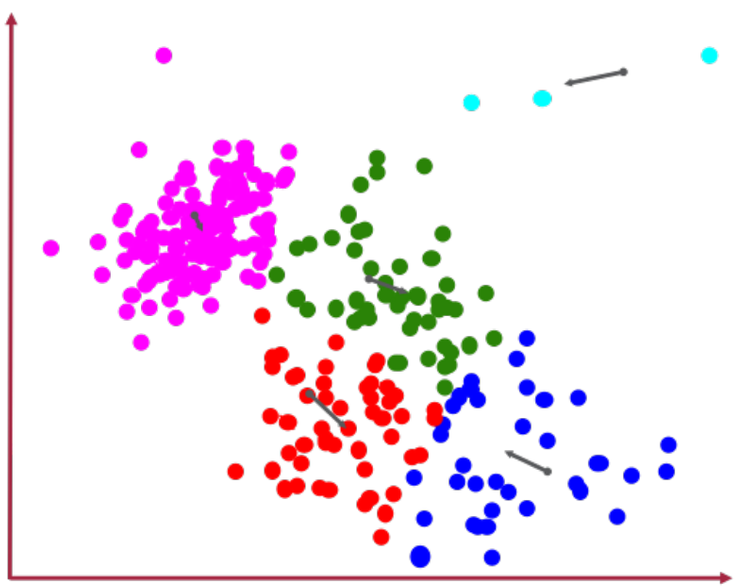


Classification



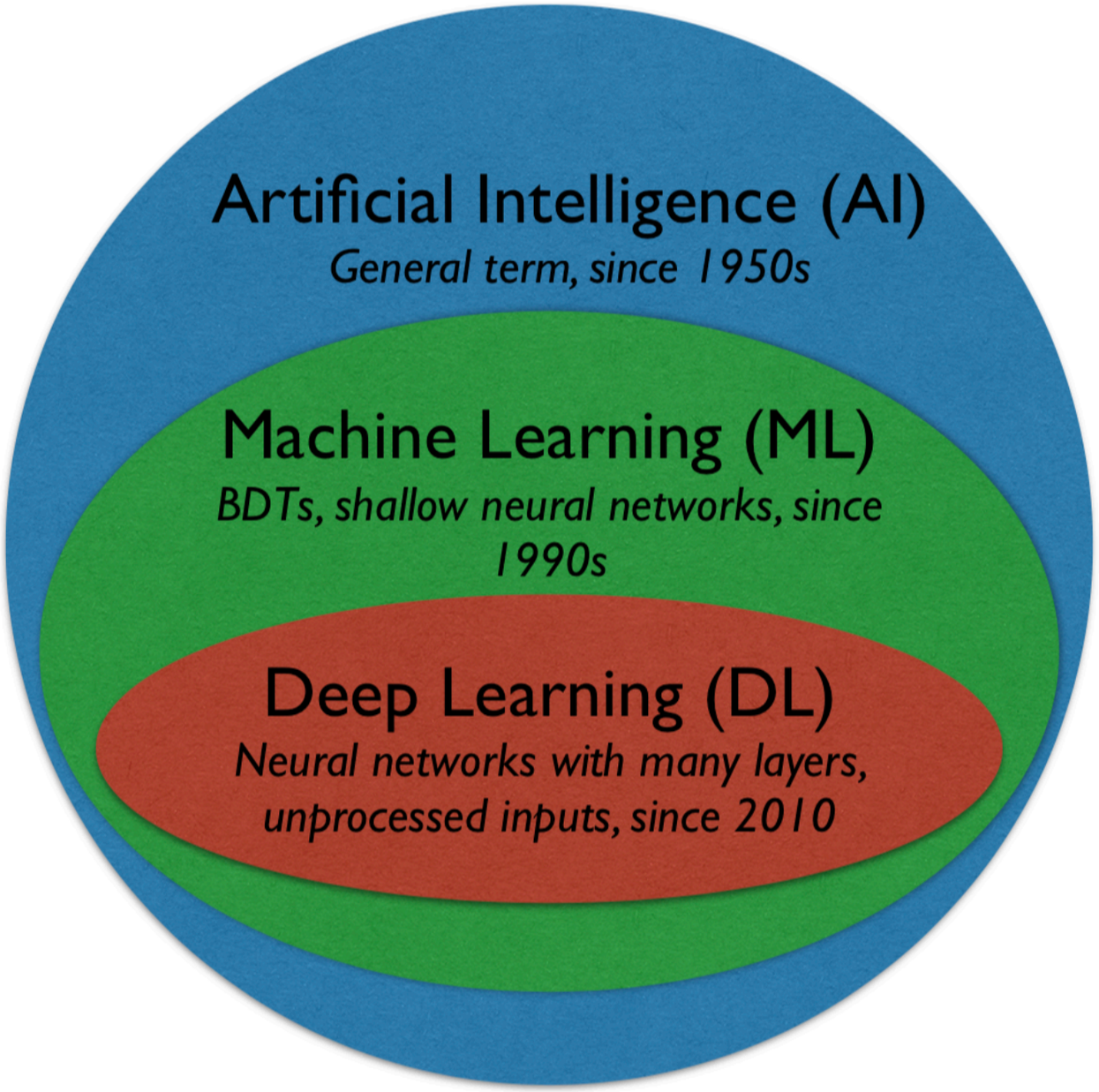
Unsupervised

Clustering



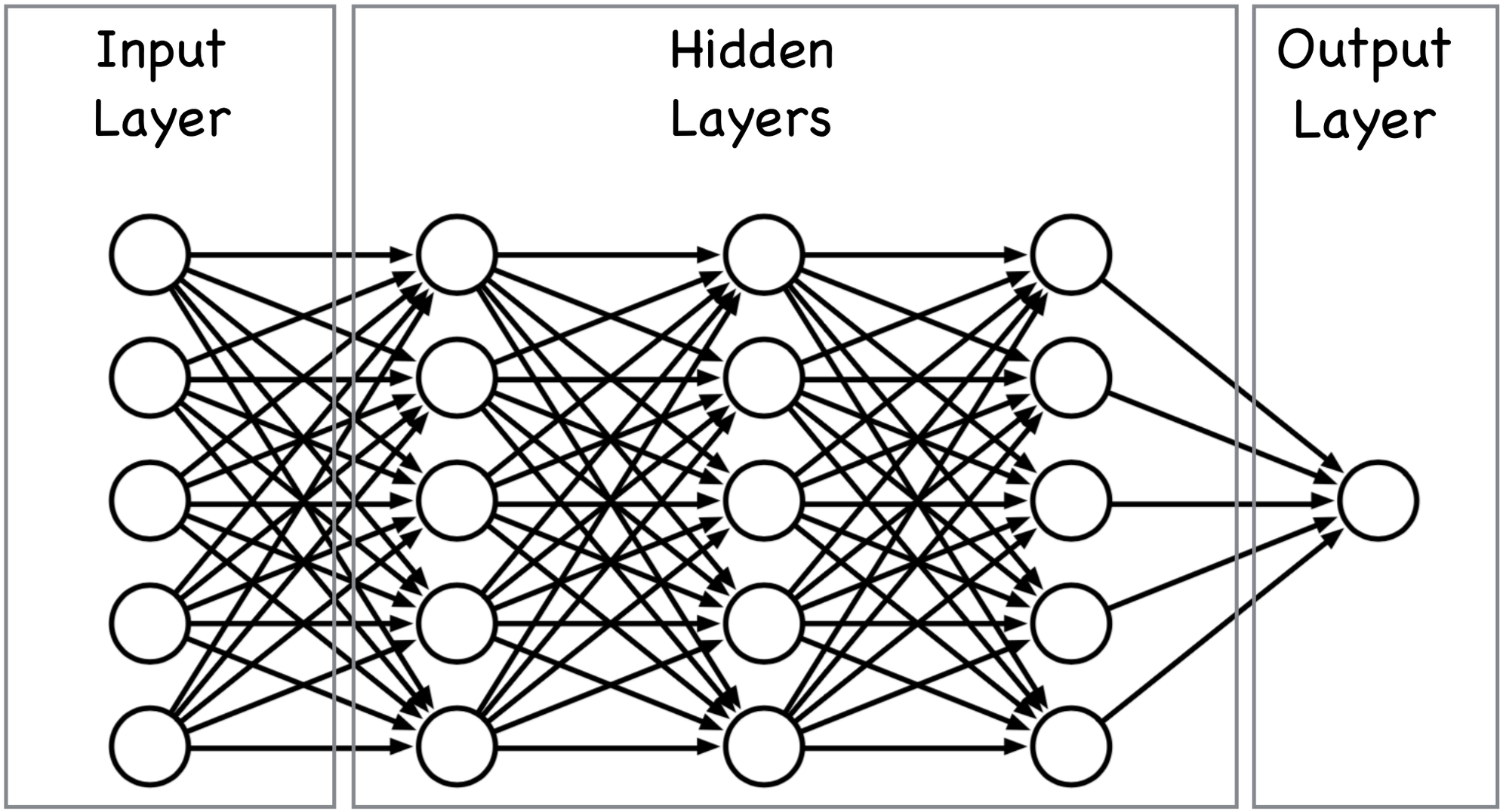
Anomaly Detection

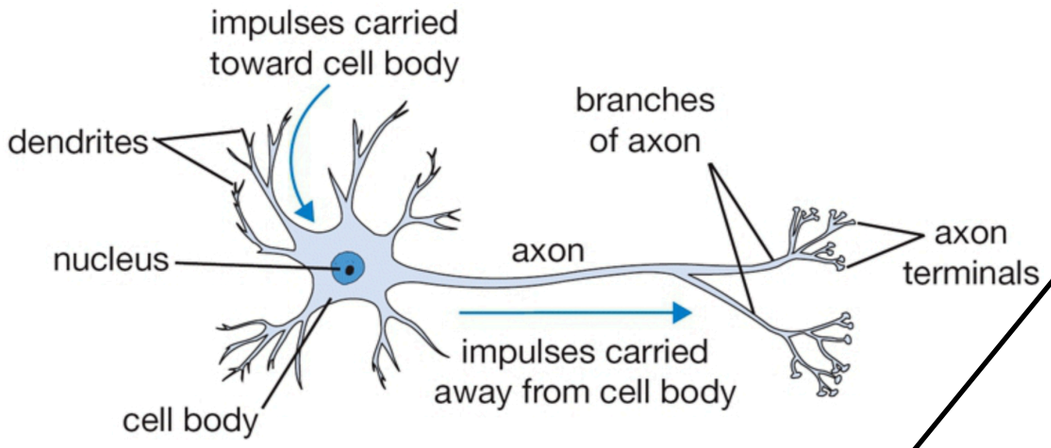
Not new, but HIP - even in particle physics

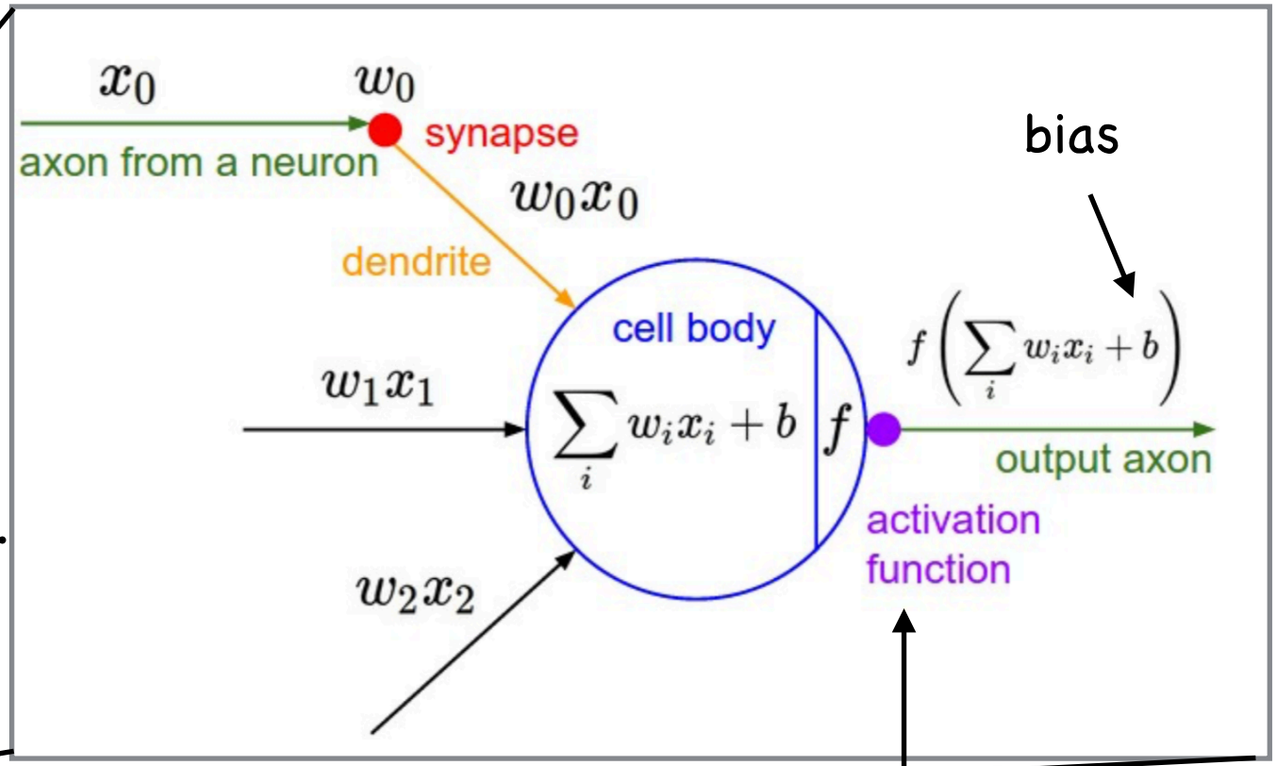


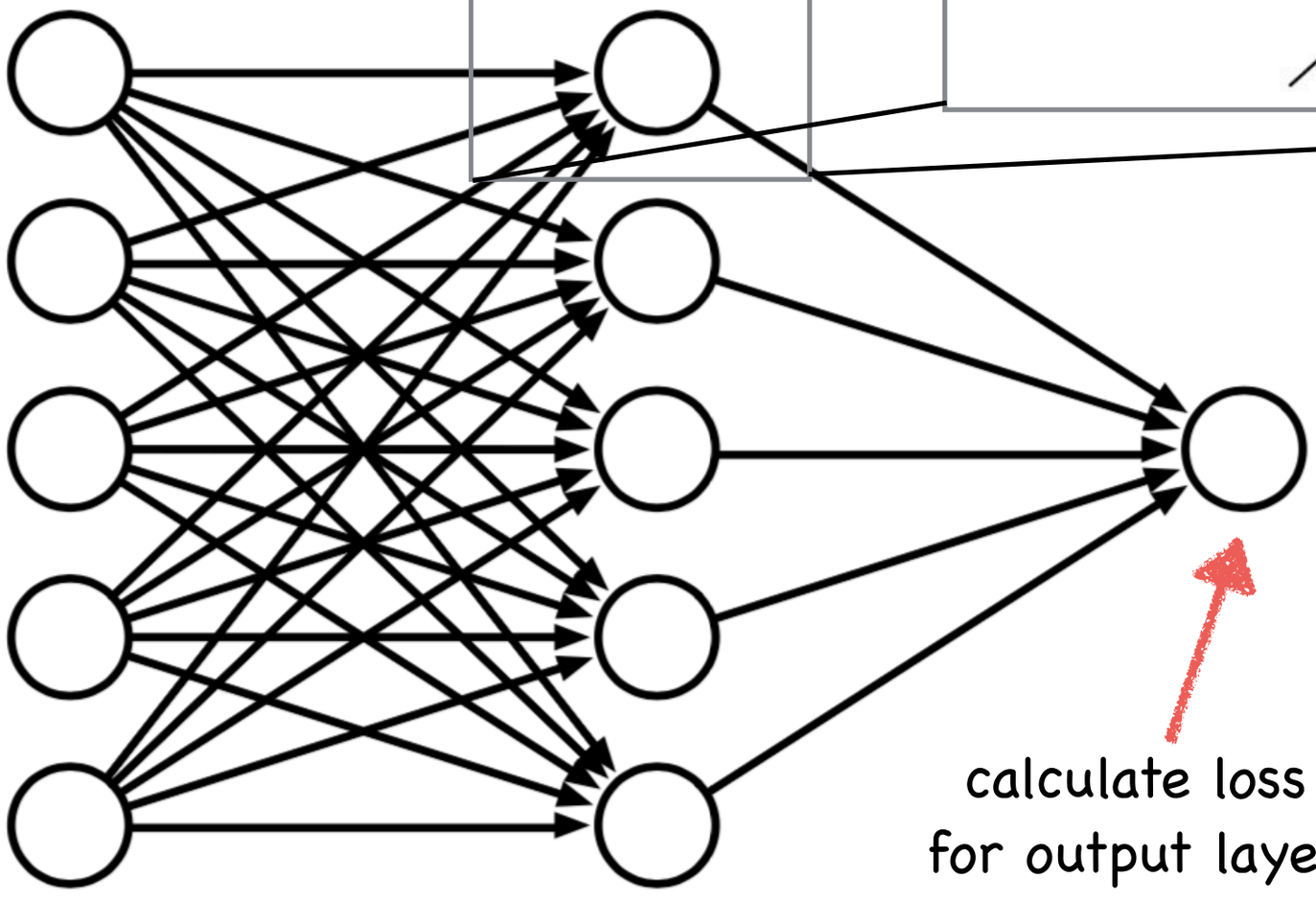
Machine-Learning with Deep Neural Networks

- Regression and Classification = correlating input and output
- Various applications in particle physics





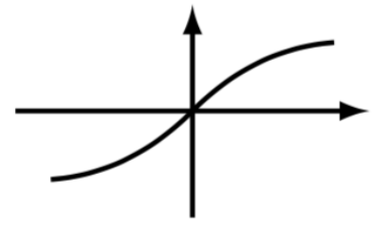




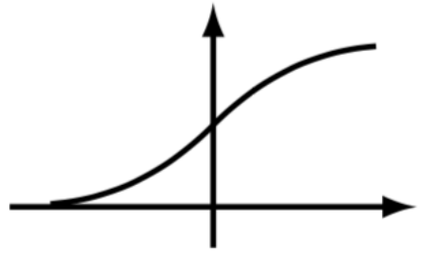
calculate loss
for output layer

Many options for
activation function f, e.g.

tanh



sigmoid



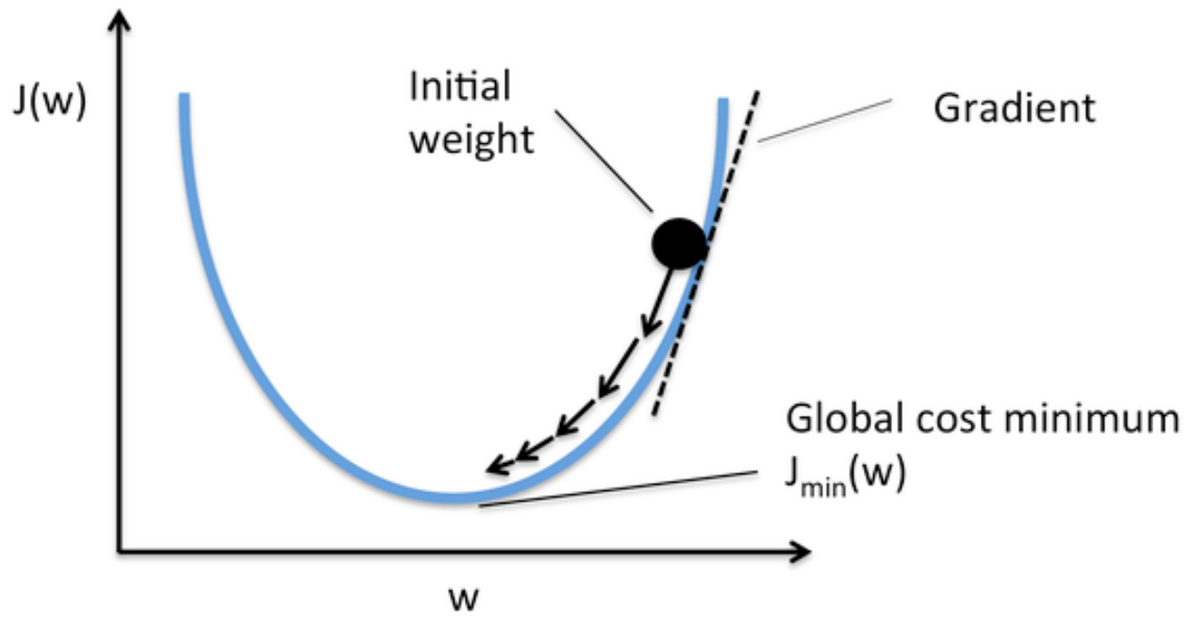
Gradient descent

- After forward propagation, ie. establishing the weights for all nodes (including the output node), we evaluate the **loss function**, to establish the error we are making.

  Loss function = difference between predicted and true function,

  e.g. $E(y, y') = \frac{1}{2}|y - y'|^2$

- Gradient descent: change network such, that you move towards the error minimum.
- Compute gradient -> get direction towards error minimum.



Learning via backpropagation

- Backpropagation is method to compute the partial derivative of the loss function E(y,y'). It is about determining how changing the weights impact the overall loss in the NN
  - variation of loss with respect to weight w_k of NN is

$$\frac{dE}{dw_k} = \frac{dE}{dy}\frac{dy}{ds}\frac{ds}{dw_k}$$ with

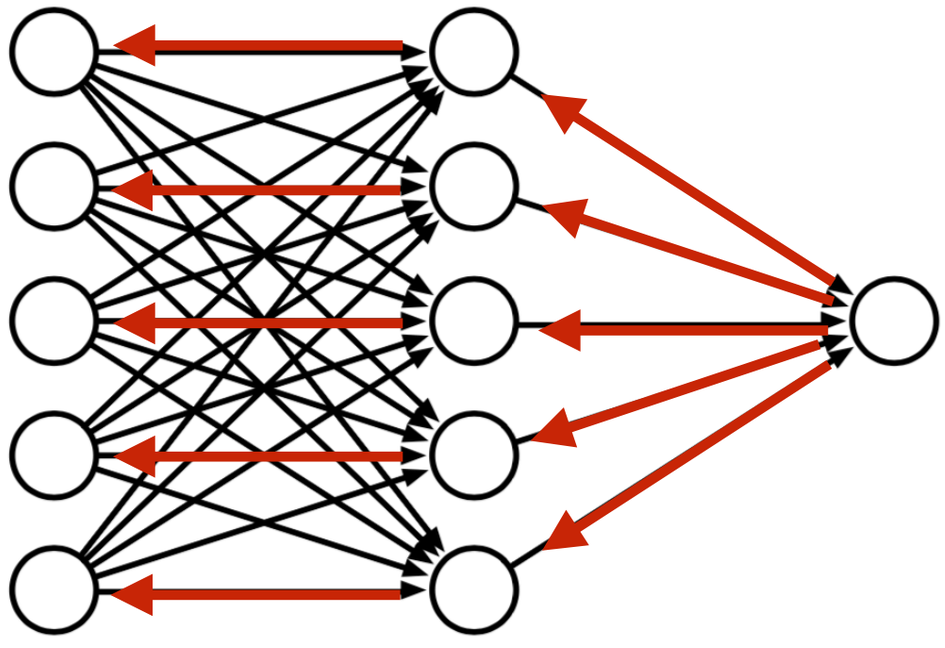
comb of weights $s = \sum_k w_k h_k$

activation function y

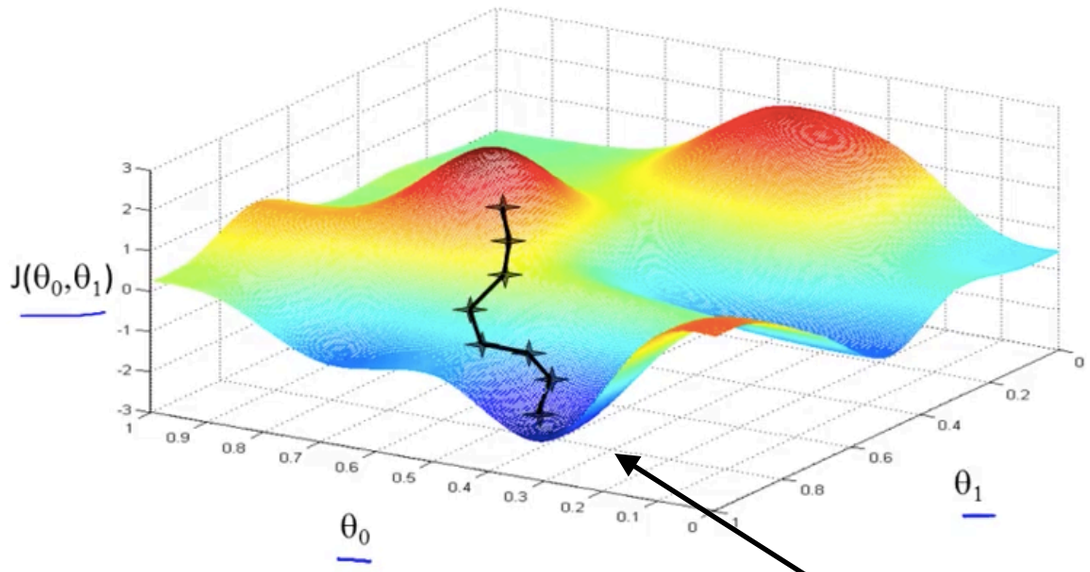
- weights of network adjusted by learning rate μ

$$\Delta w_k = -\mu \frac{dE}{dy}\frac{dy}{ds}\frac{ds}{dw_k}$$

- New network weights reduce value of loss function

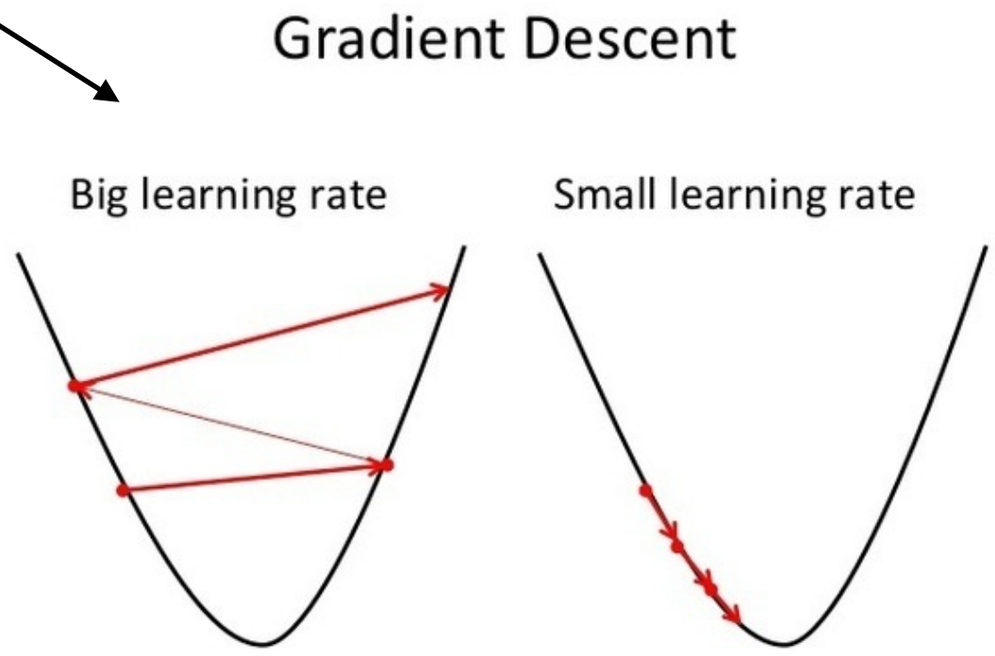


Neural Net



All a Neural Net does is give an analytic expression for the loss function, and then attempts to minimise the loss function using gradient descent and backpropagation

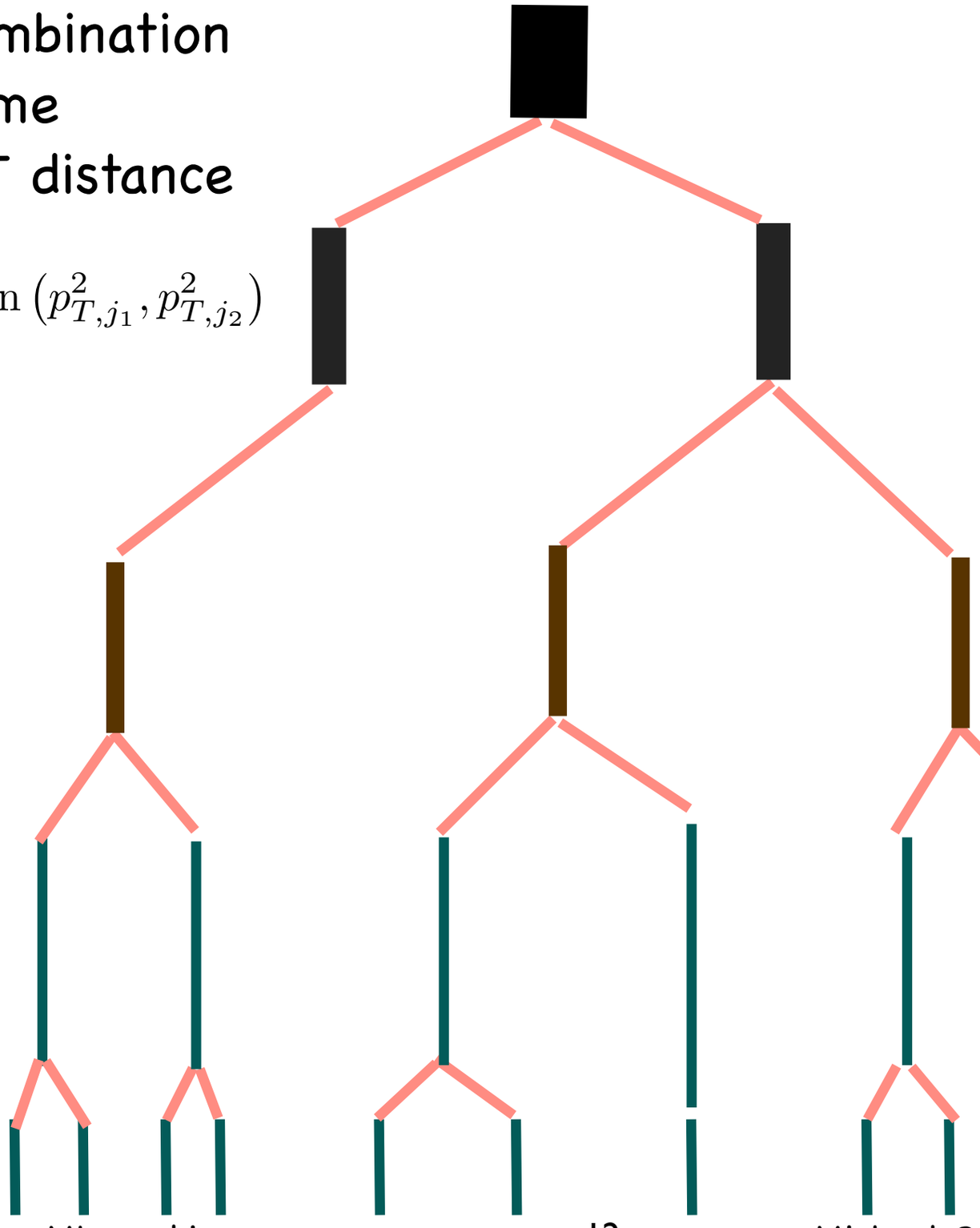
Overall, optimisation problem. Need to optimise hyperparameters to problem, e.g. learning rate …



Application often to jet physics, i.e. top, W, Z, H vs lf jets

order of recombination defined by some metric, e.g. kT distance

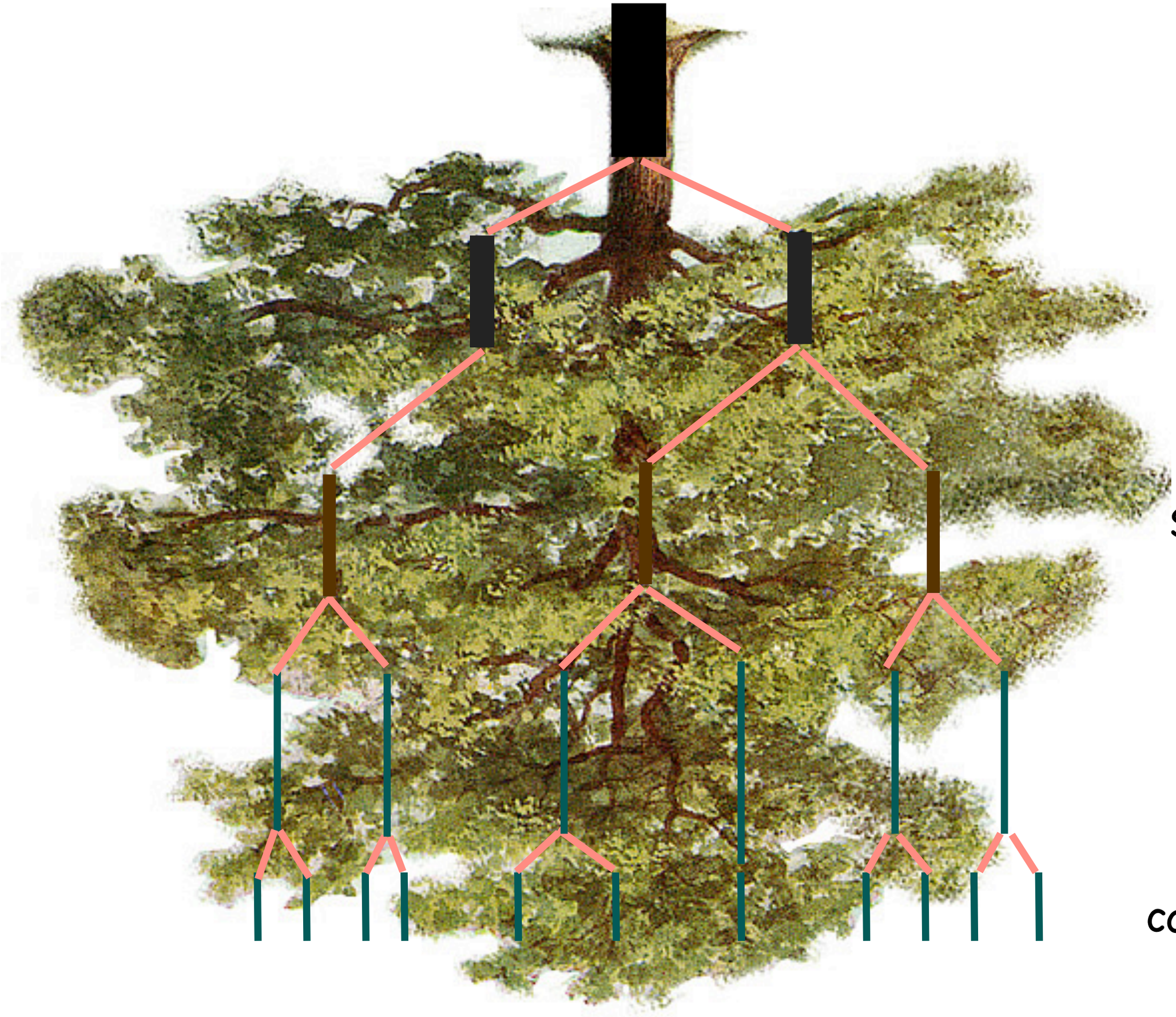
$$d_{j_1 j_2} = \frac{\Delta R^2_{j_1 j_2}}{D^2} \min\left(p^2_{T,j_1}, p^2_{T,j_2}\right)$$



Jet

Subjets

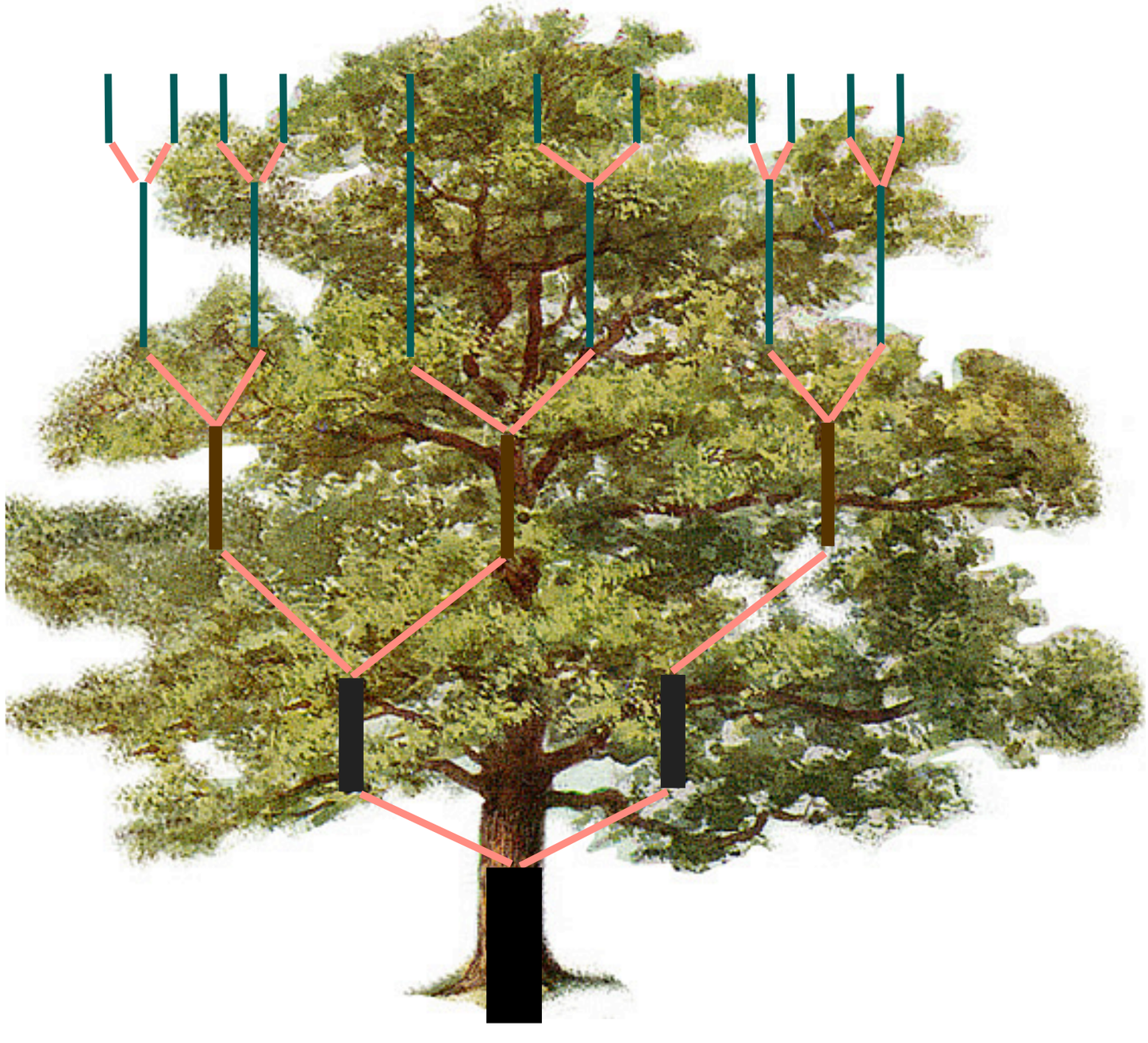
Jet constituents


Jet
Subjets
Jet
constituents

Intrinsic scales and energy sharing of jet substructure different

→ Can be used to discriminate QCD jet from resonance jet

W/Z/H-boson jet



QCD jet

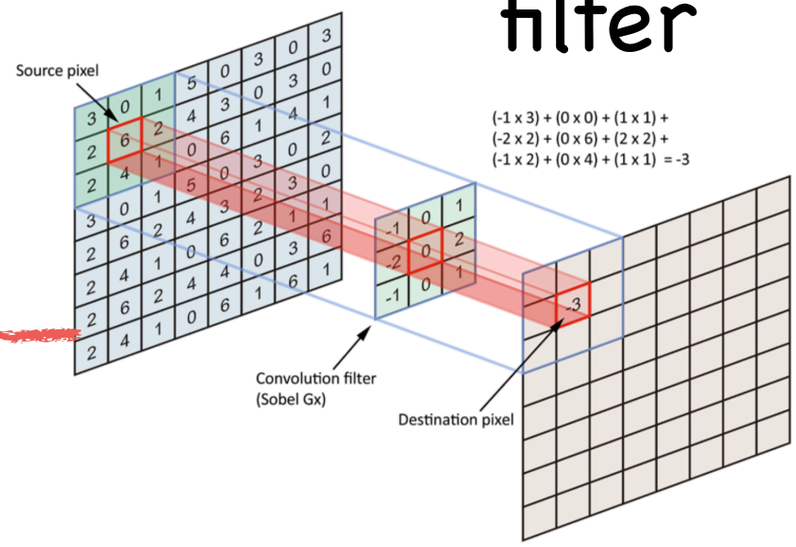
What are some of the common Neural Nets

Supervised

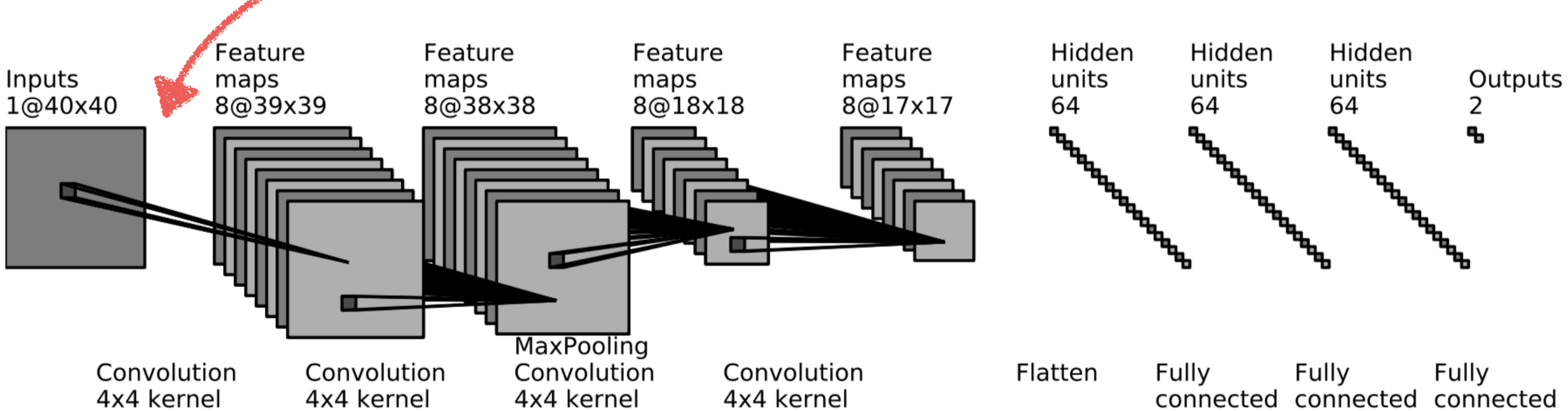
- (D)NN
- Convolutional NN

  Often used for image recognition

filter



Standard setup:

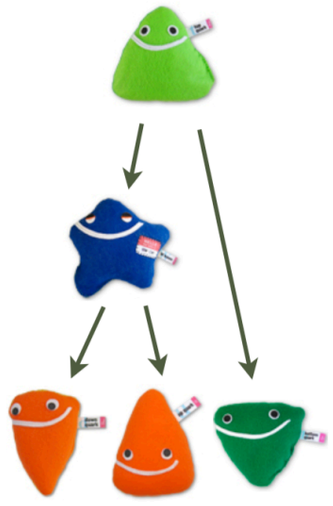


Allows to be sensitive on translationally invariant features

CNN has a sense of distance and orientation

Application to top tagging

Top Quark



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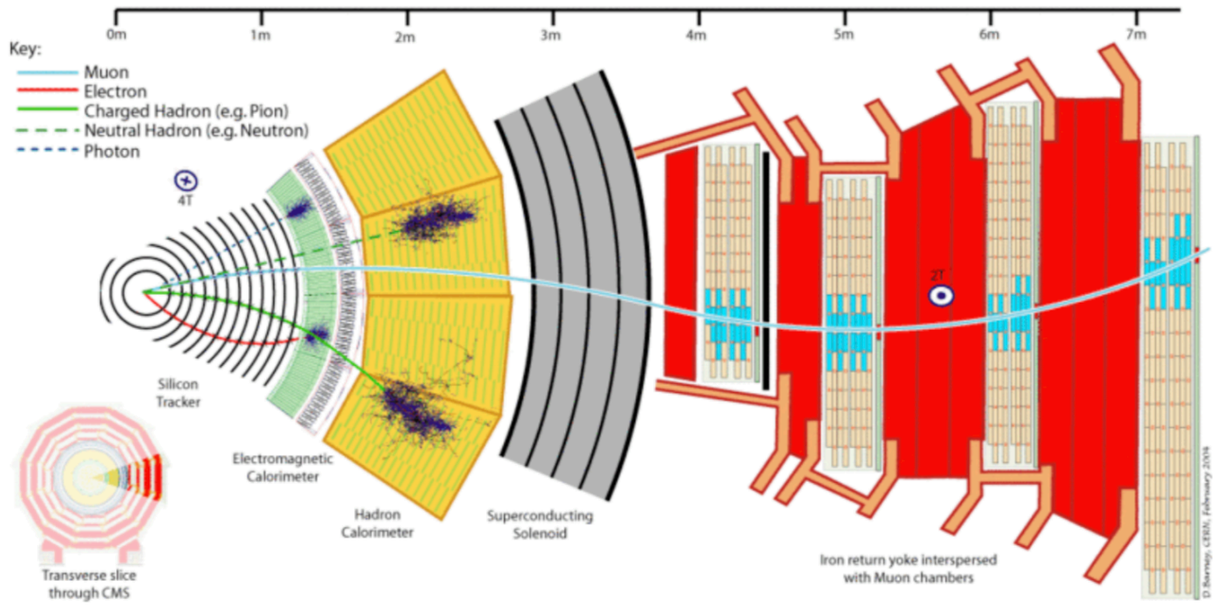
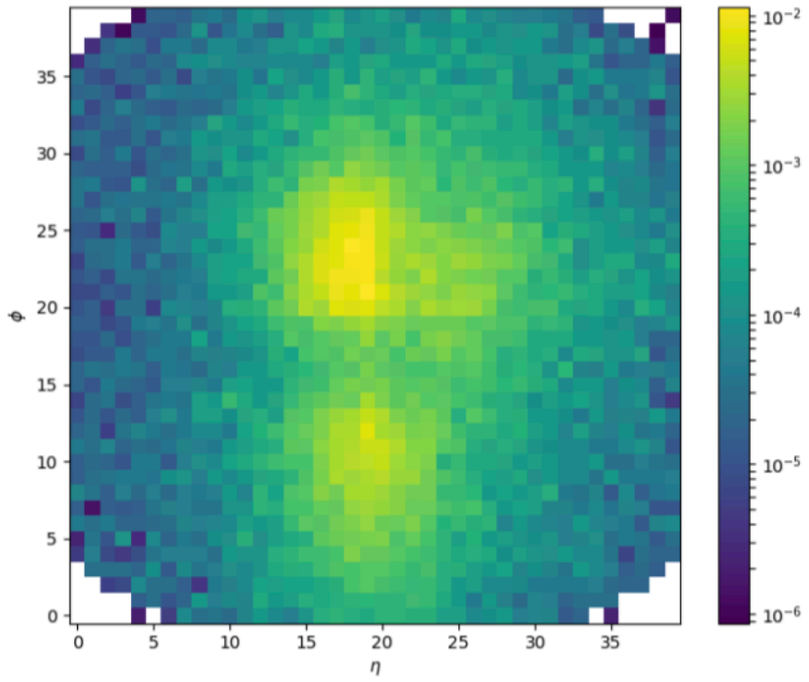
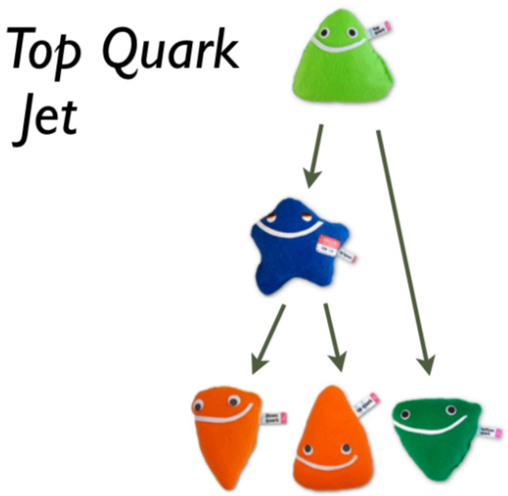


1. Measure particle energies in calorimeter
2. Reconstruct jet
3. Image preprocessing: center, rotate mirror, pixelate, trim, normalise



1000 image average

However, on event-by-event basis not so clear-cut...



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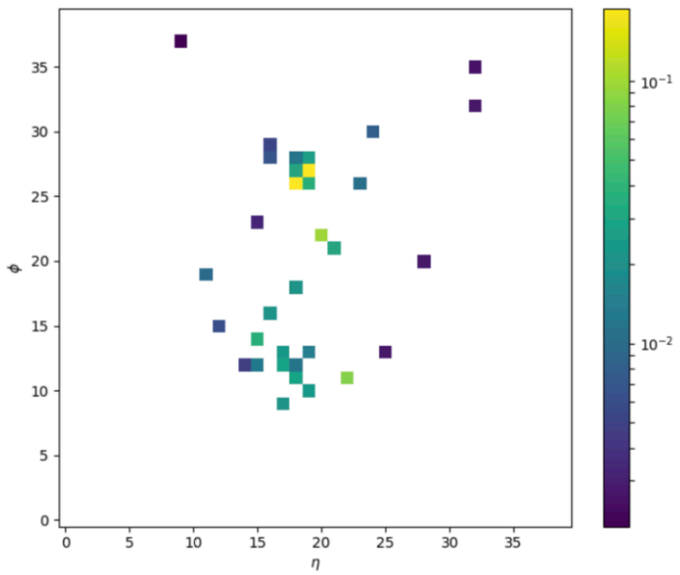

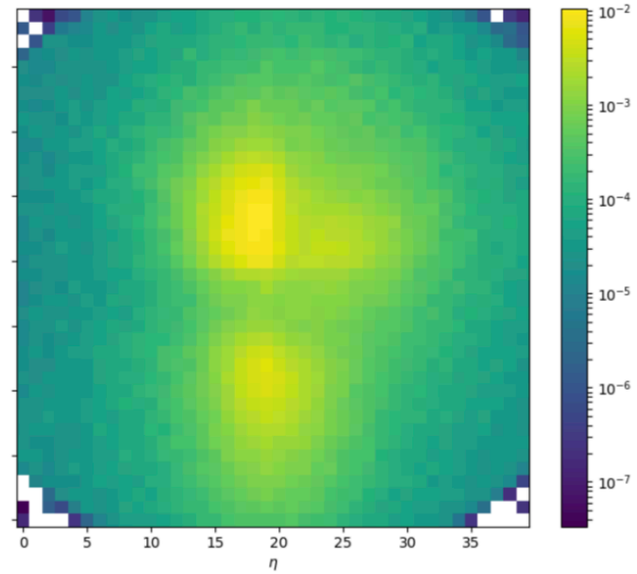

VS

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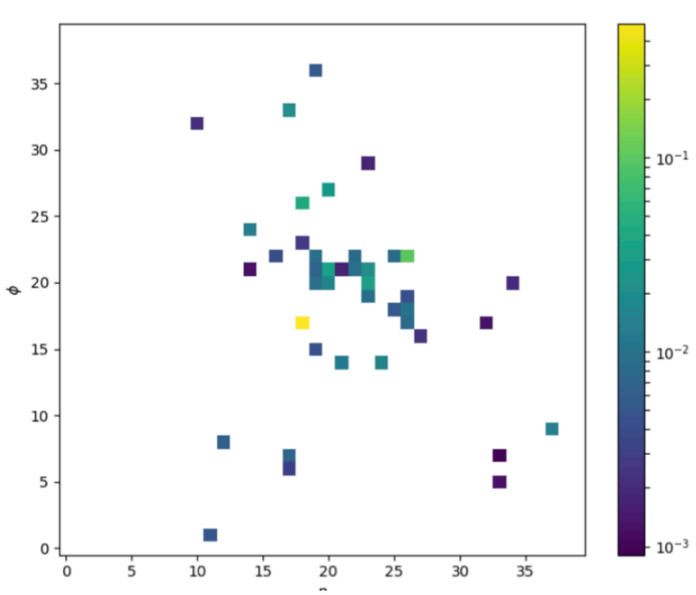
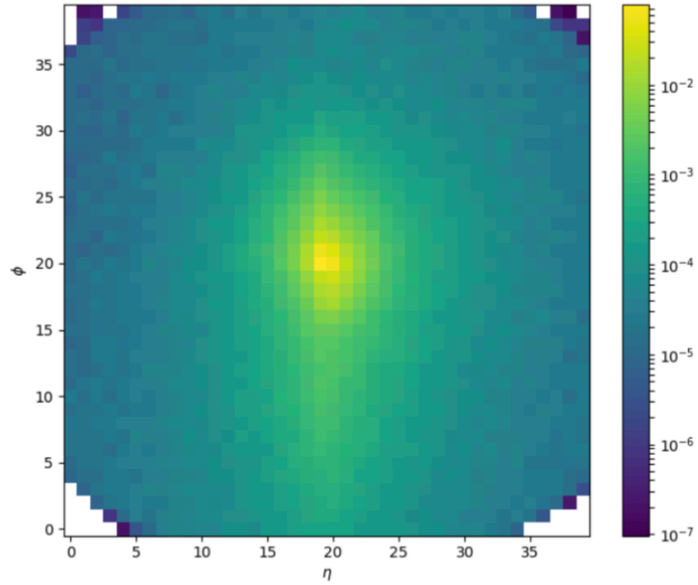
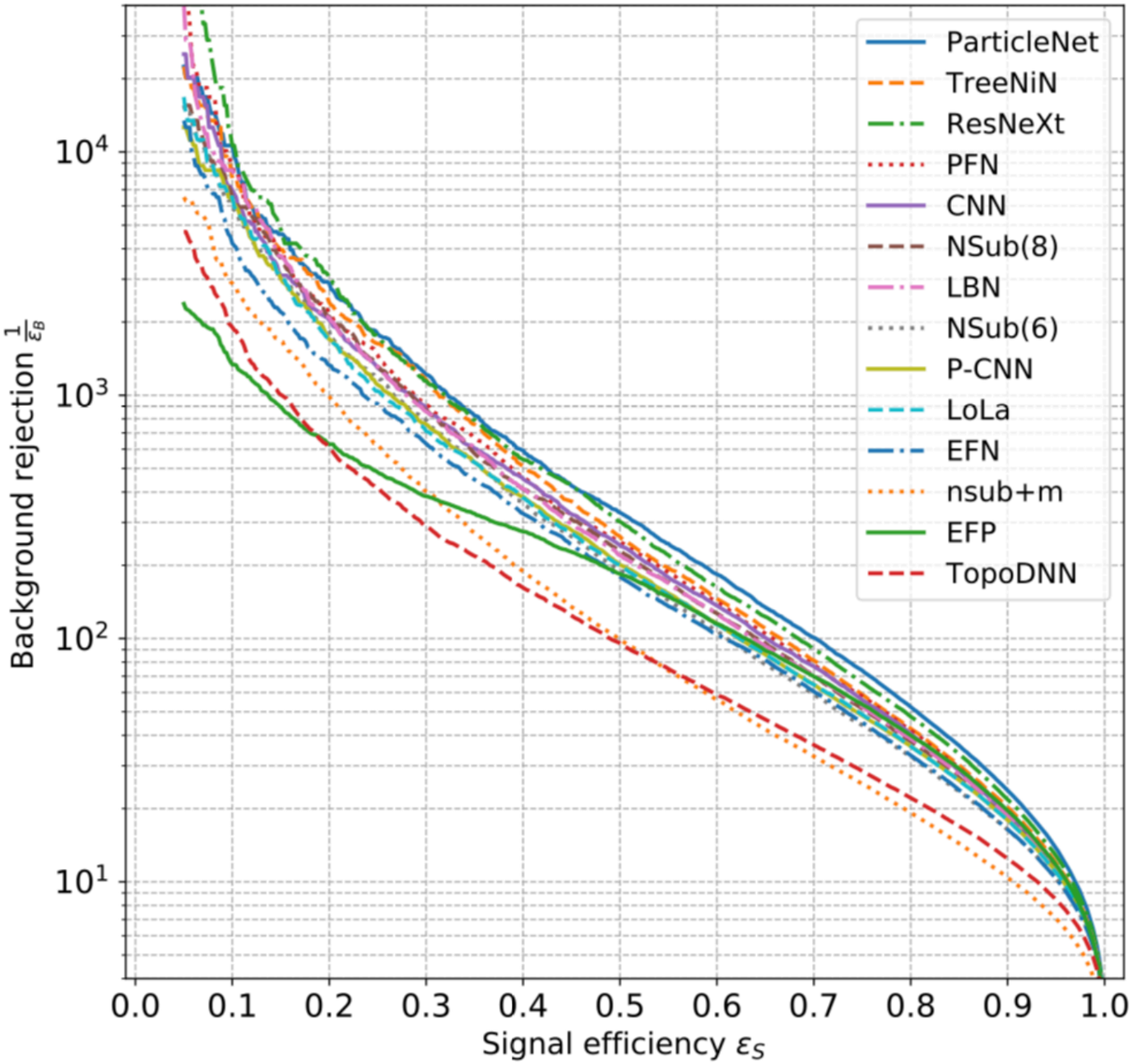




tough call... problems: sparsity of image

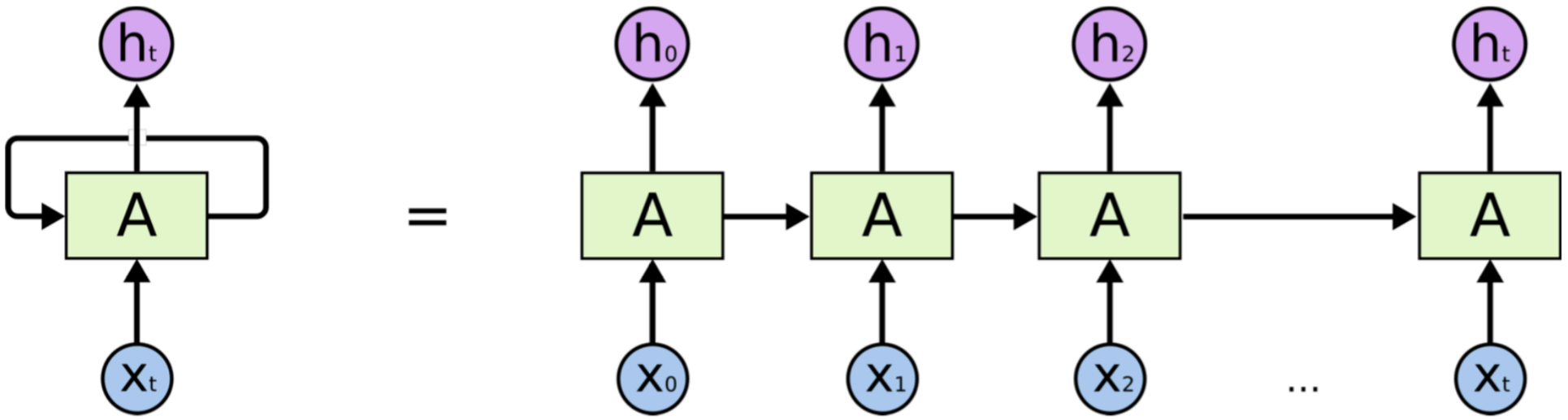
Top tagging performance comparison of various NN approaches



[1902.09914]

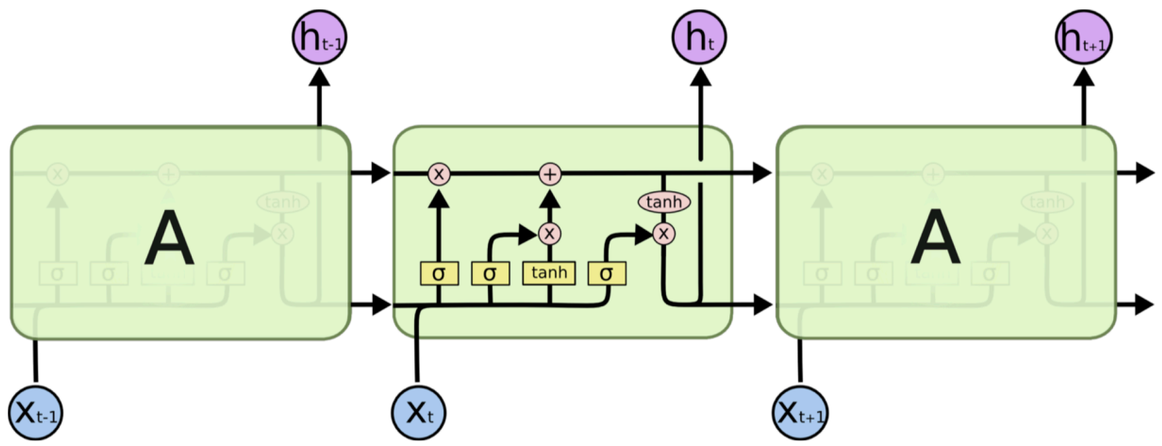
- Recurrent NN

for prediction only one output though



Long Short-Term Memory (LSTM)

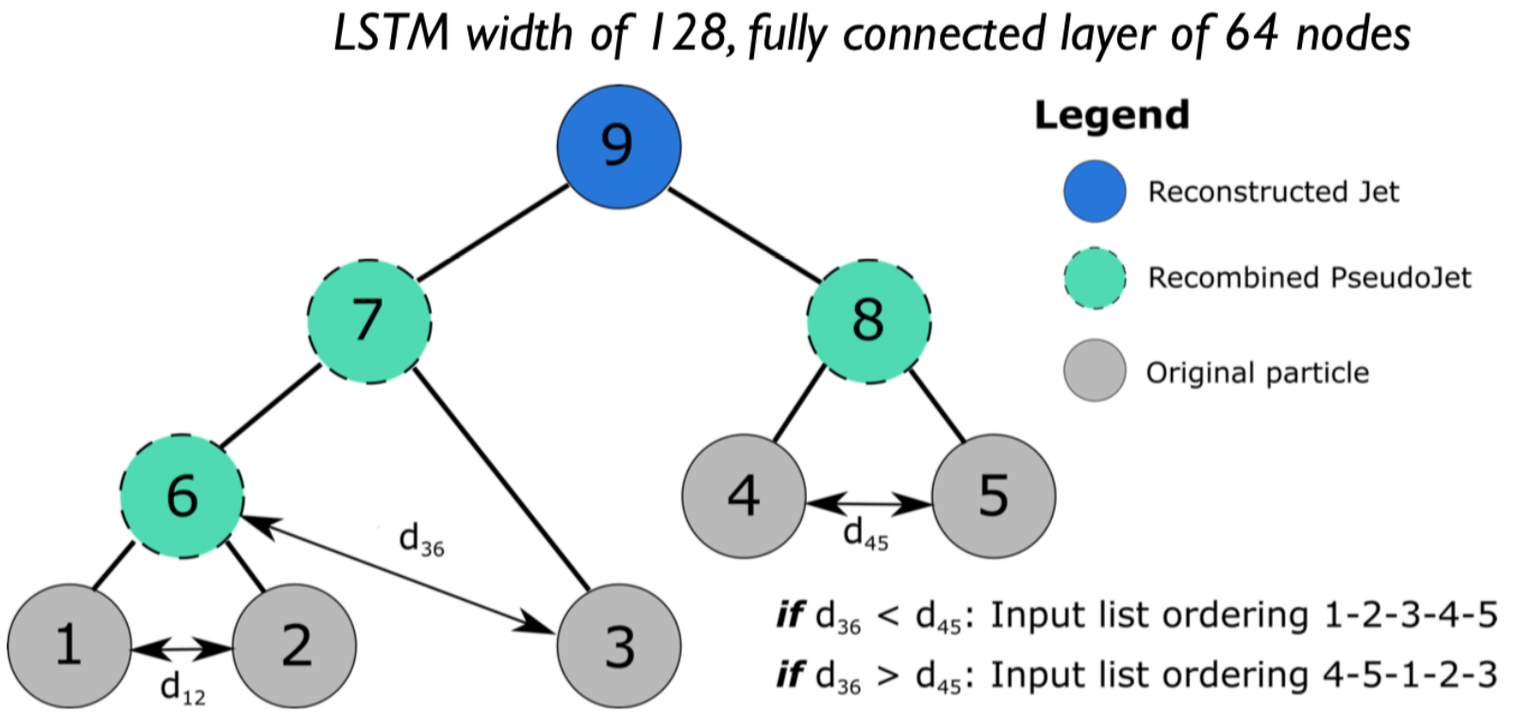
Often used for language processing

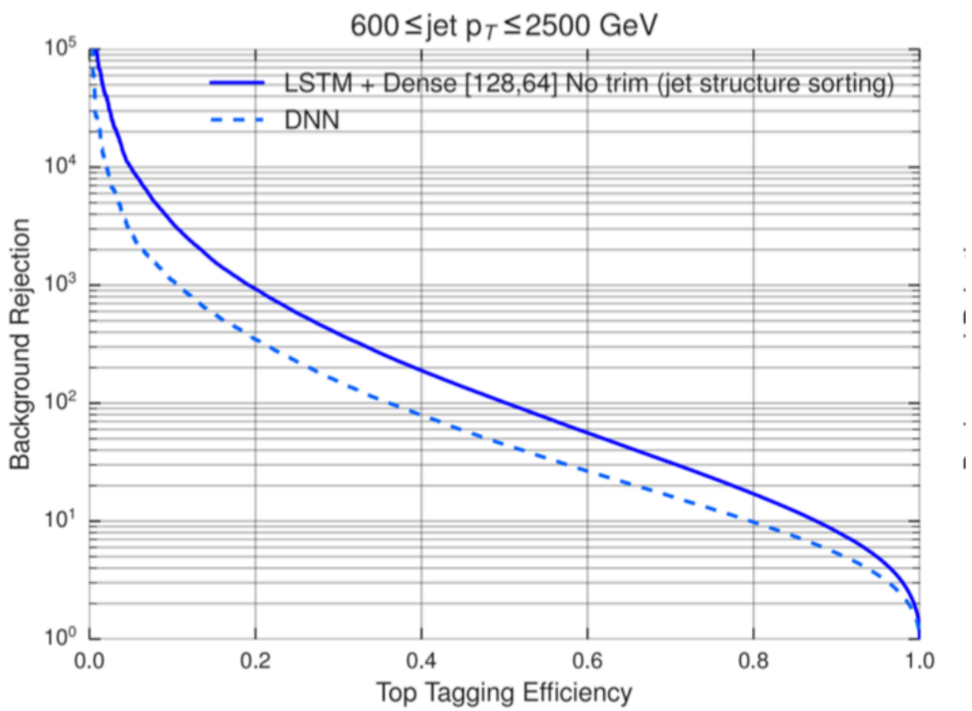


RNN (LSTM) has a sense of time and a memory

Good for variable-length inputs, as can be stopped after n iterations

Application to top tagging with RNN





[Egan, Fedorko, Lister, Pearkes, Gay '17]

Jet cluster algorithm defines ordered sequence (timing)

recombination history

<->

ordering of sentence

Shows good performance compared to DNN

see also [Louppe, Cho, Becot, Cranmer '17]

Unsupervised

- autoencoder

autoencoder used for anomaly detection

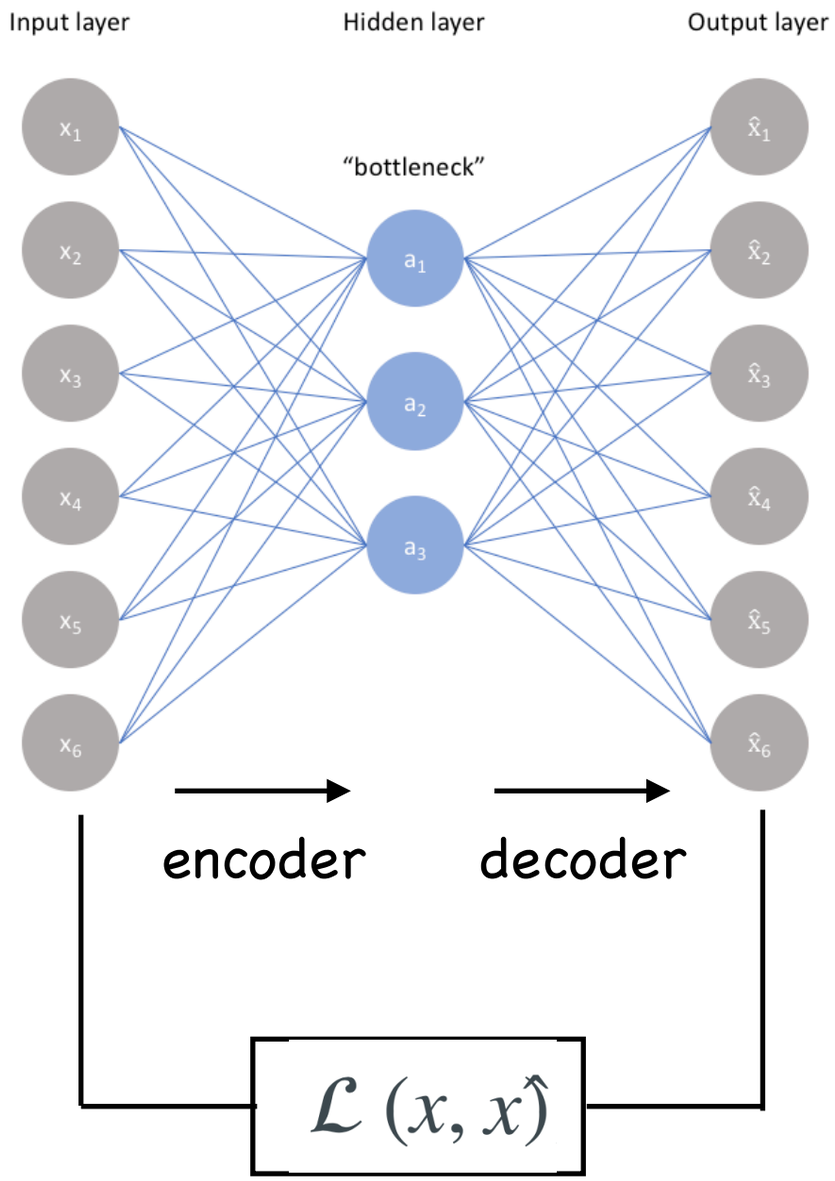
in first step input is encoded into information bottleneck

between input/output layer and bottleneck can be many hidden layers
-> highly non-linear

after bottleneck decoding step

Reconstructed output is then compared with input via loss-function (usually MSE)

NN is trained such that input and output high degree of similarity



usually MSE

"The strange death of theory"

Frankfurter Allgemeine Zeitung

23.01.2017

or is it?

Pros and Cons of ML in Particle Theory

- Particle theory in some sense **worst** and **best** place to use ML

- MVA well motivated to extract correlations without existing theory, i.e. **stock trade**

- In particle physics we established gauge theories, thus, we have existing theory to predict connection of 'input with output'

- Current pheno approach:

  We take first-principle QFT: $\mathcal{L} = \mathcal{L}_{\rm EW} + \mathcal{L}_{\rm QCD} + \mathcal{L}_{\rm Higgs}$

  Put it into an event generator to generate pseudo-data

  Then a smart physicist or MVA comes up with way to access the Lagrangian we put in in the first place

  → Seems like an unnecessary detour...
  More suitable: **All-order Matrix Element Method**

[Soper, MS '14]
[Ferreira de Lima, Mattelaer, MS '17]
[Prestel, MS '19]

Training ML on pseudo-data

- MVAs will optimise for - according to MC - most sensitive exclusive phase space regions

  ⟶ theory uncertainties difficult to control

- Full event generators are mashup of different parts that are partly tuned, i.e. hard interaction, UE, ISR,...

- Highly computationally intensive. If you want to template correlations of say 7 particles:

  - Time estimate:

    7 microjets, each 4-momentum components divided into only 10 bins

    -> $10^{28}/7! \sim 10^{24}$ configurations

    If MC takes 1 ms per event -> 10^{13} years to have 1 hit per config.

Training ML on data only

- Less plagued by theoretical uncertainties

- But only possible if objects to reconstruct or events to measure already in data.

  problem for new or rare physics:

  ➡ gluino-tag

  ➡ axion-tag

  ➡ pp -> HH

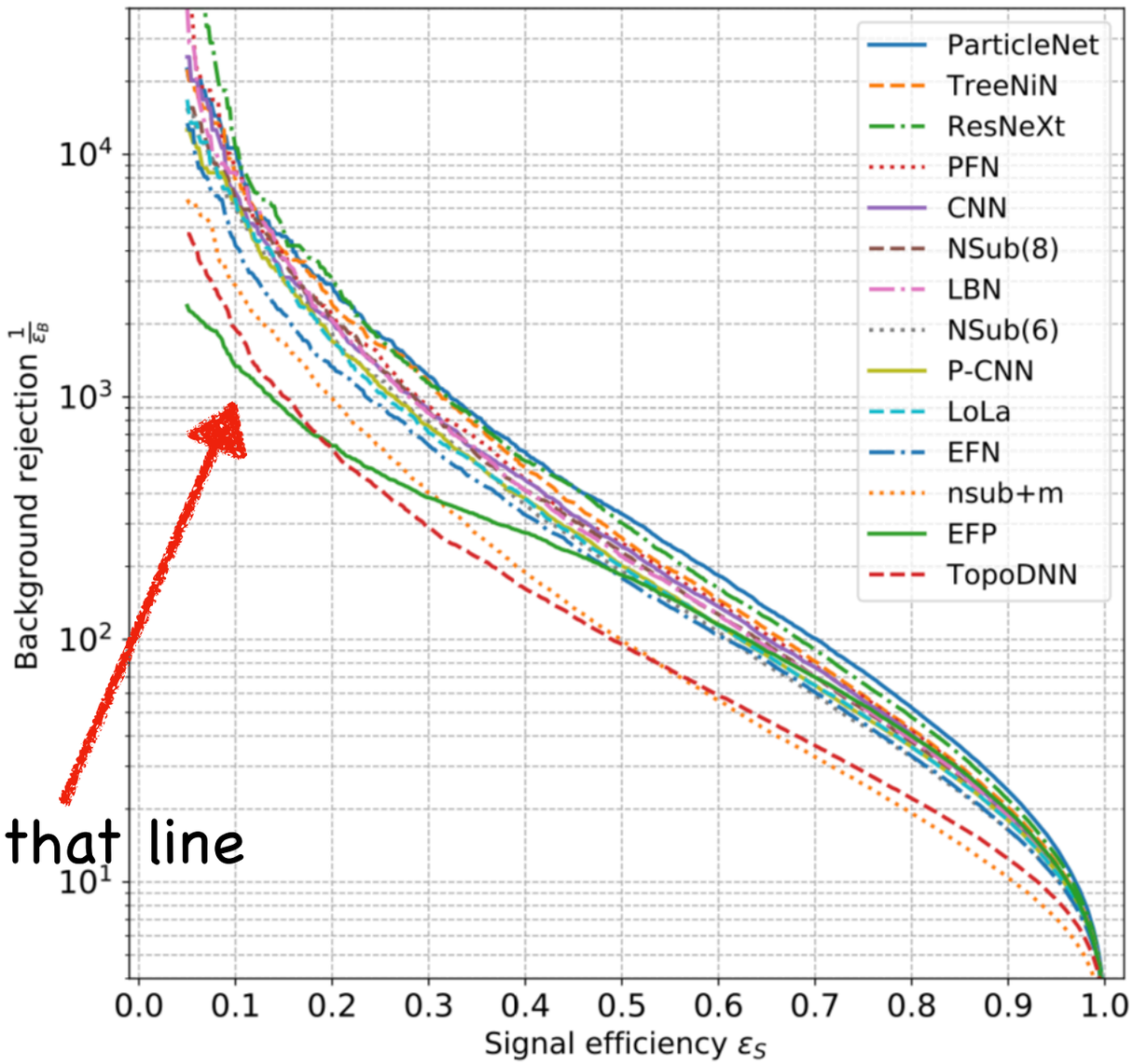
  ➡ ...

- Everything done purely on data without theory cross-check has 0 safety margins...

  ➡ now gone 2 TeV excess in ATLAS and CMS might be an example

  [Goncalves, Krauss, MS '15]

Top tagging performance comparison of various NN approaches



[1902.09914]

Attention to that line

High performance in tagging efficiencies can be achieved.
However, be careful in taking these efficiencies at face value

Current ROC curves do not come with uncertainty bands

Decorrelation of nuisance parameters

Solution: use a pivotal quantity as a classifier [DeGroot, Schervish '75]

Pivot =	quantity whose distribution is invariant with nuisance parameters

- training method for pivotal classifier using adversarial networks

[Louppe, Kagan, Cranmer '16]

- showed that it works for systematic uncertainties which affect classification on an event-by-event basis (e.g. event reconstruction uncertainties)

- use pivotal classifier in the context of theoretical scale uncertainties affecting the event sample as a whole

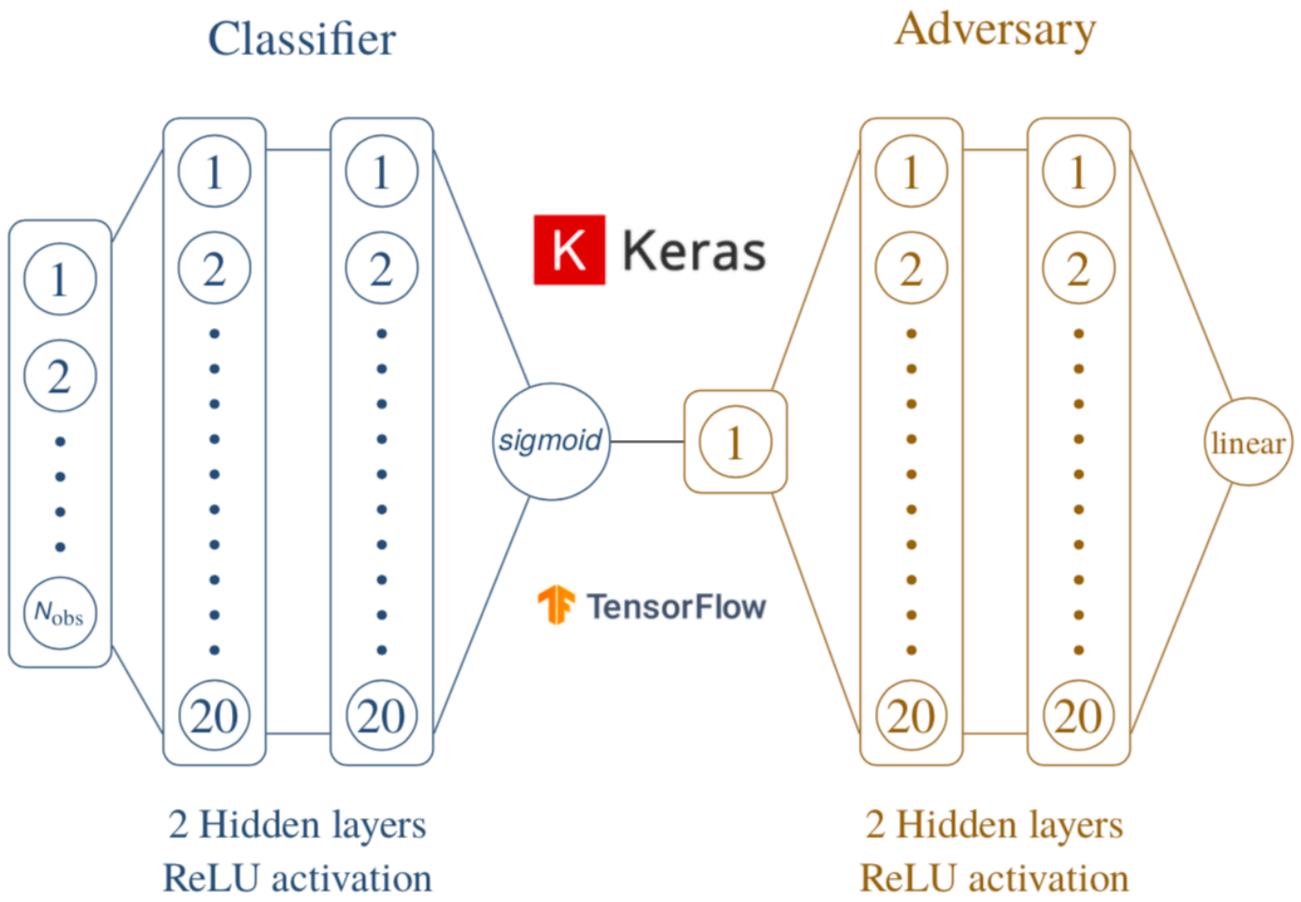
[Englert, Galler, Harris, MS '19]

implementation of adversarial

- Connect both networks through loss function

$$L = L_{\text{Class}} - \kappa L_{\text{Adv}}$$

- Adversarial will force the Classifier output to look the same for each 'smearing class'

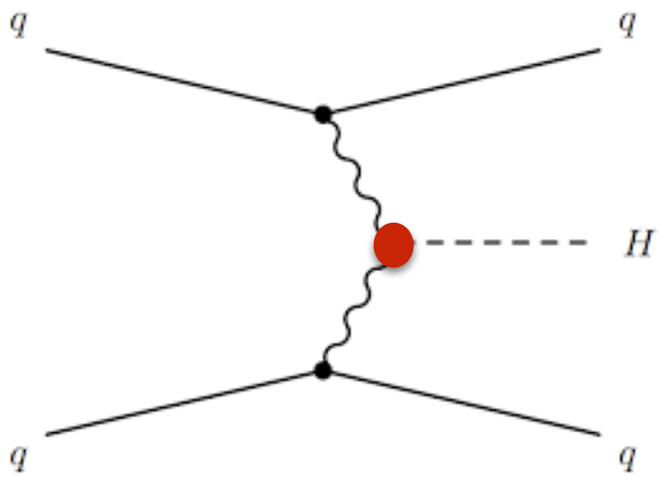


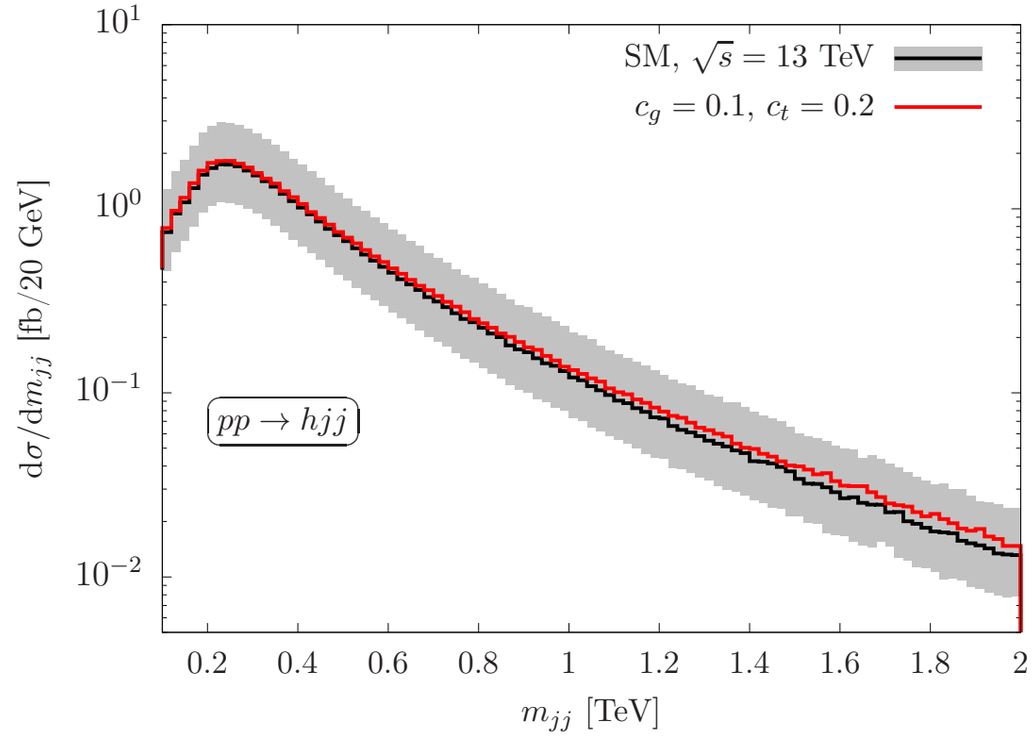
- Both networks have to be trained and improve simultaneously -> ping-pong training

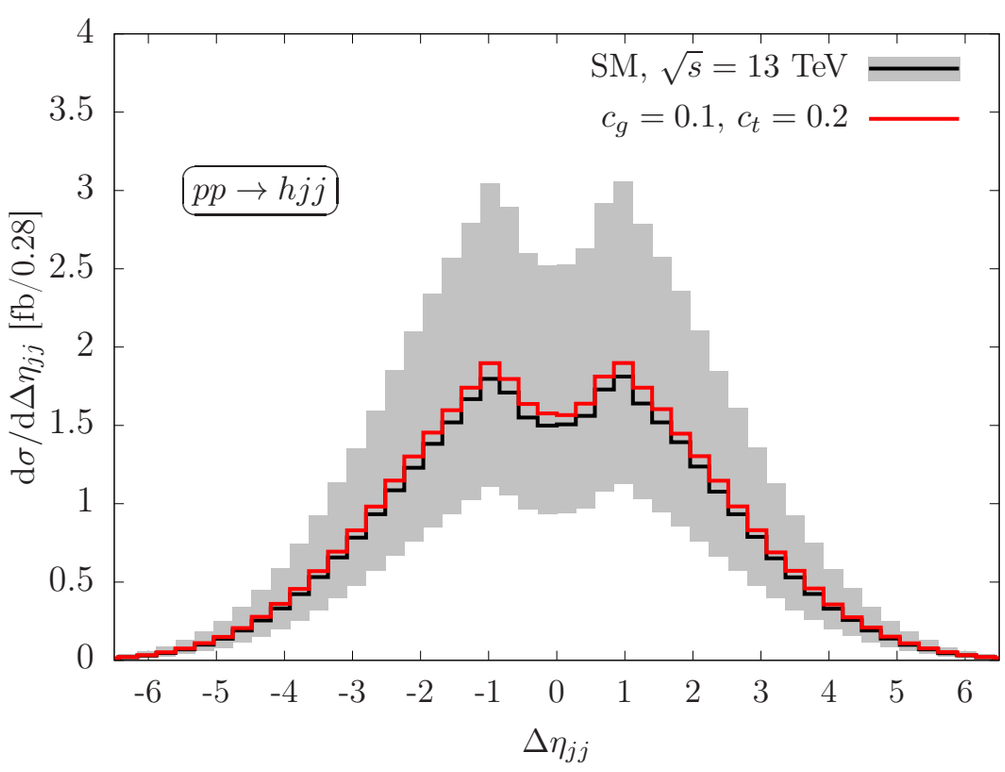
- Approach can be used for systematic and theoretical uncertainties

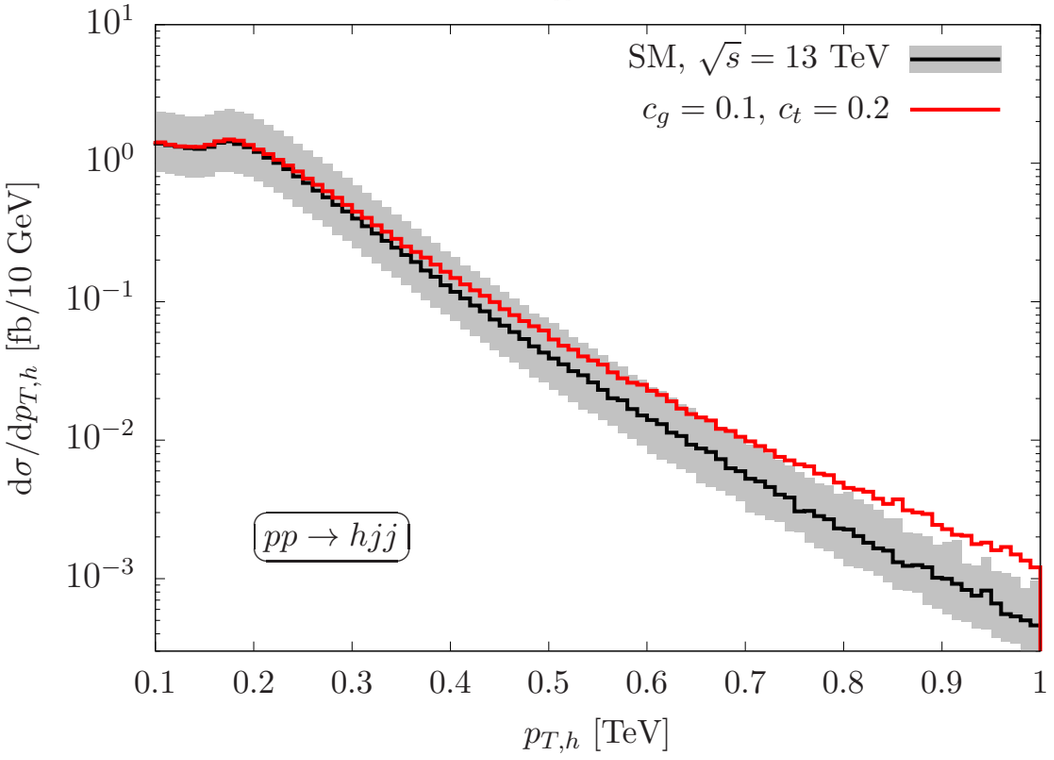
[Louppe, Kagan, Cranmer '16] [Englert, Galler, Harris, MS '19]

Example: EFT hypothesis test in H+jets

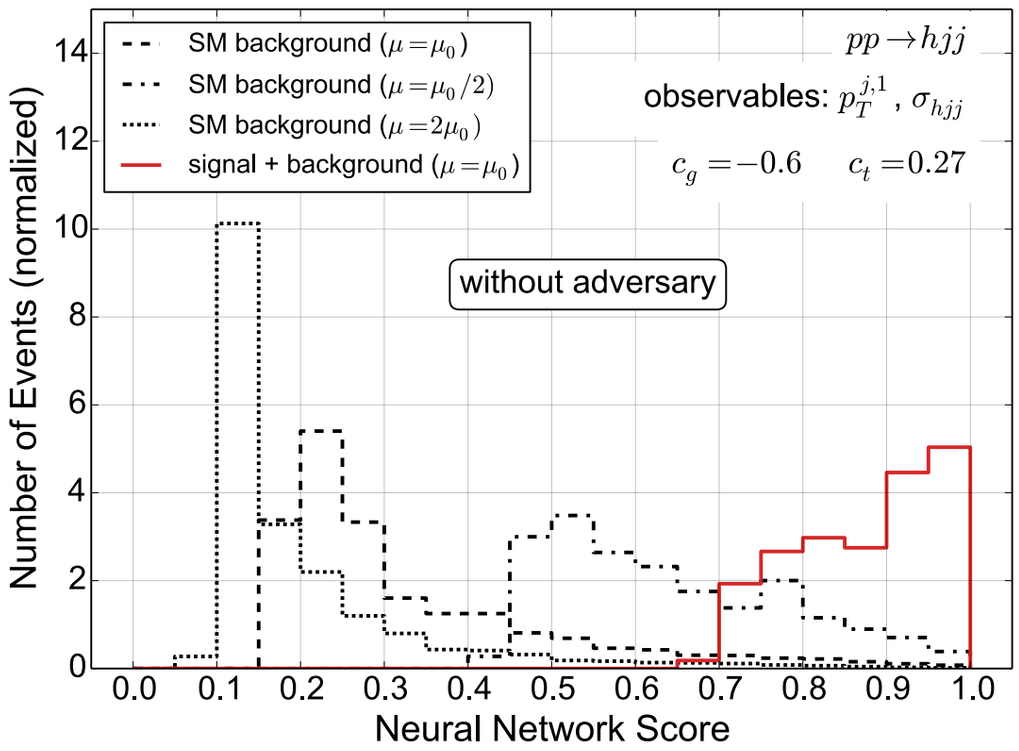


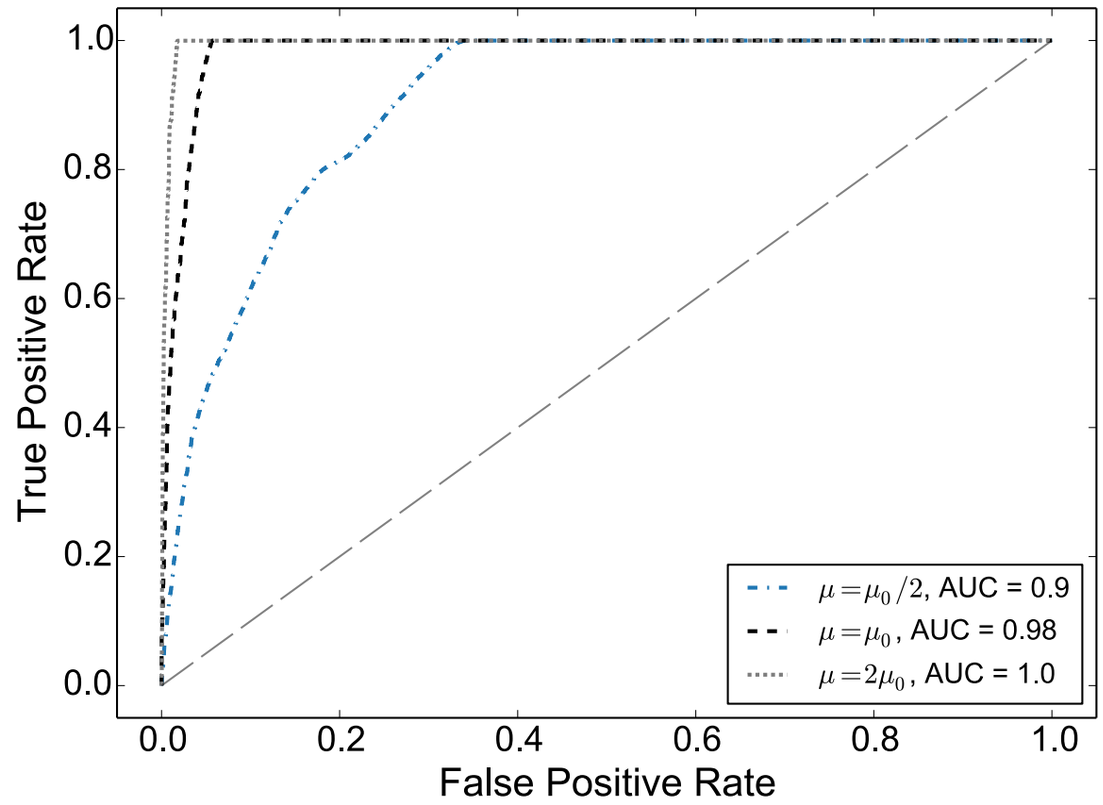




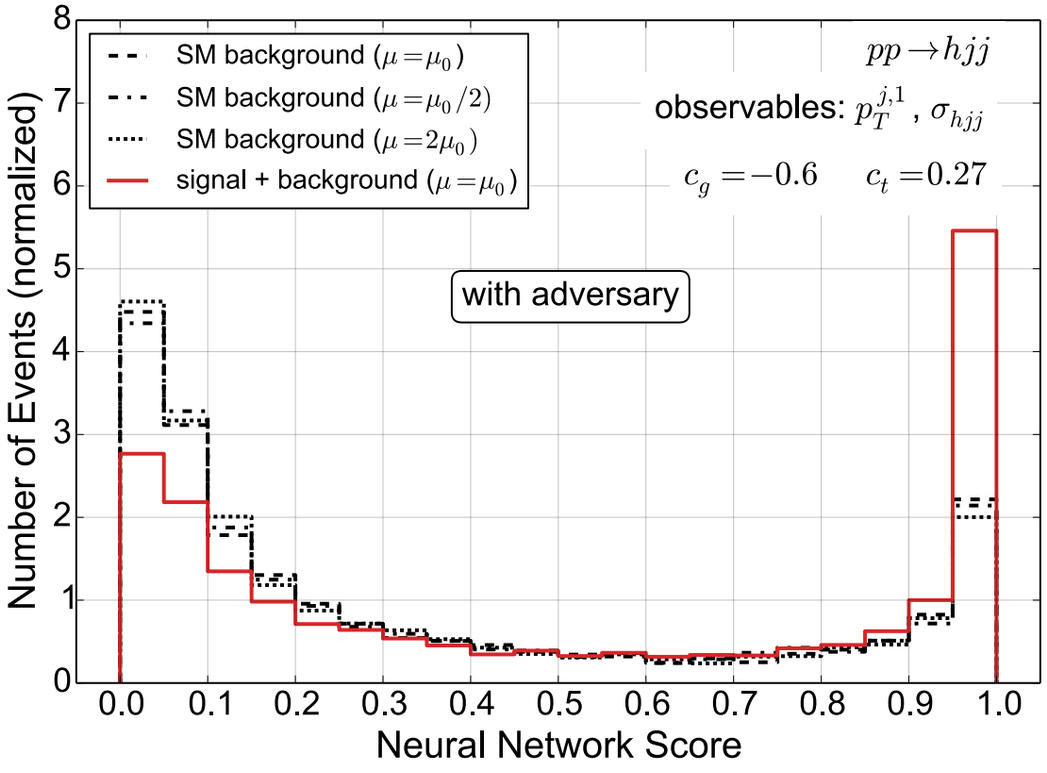


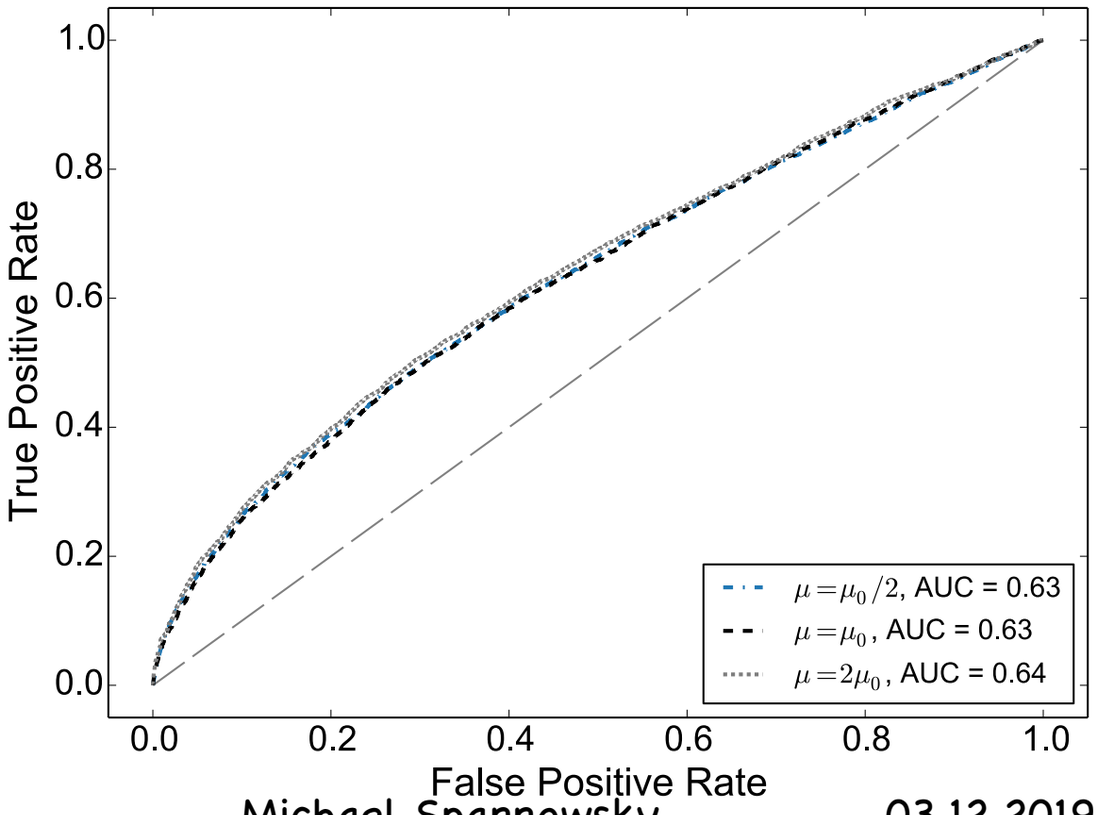
no adversarial





with adversarial



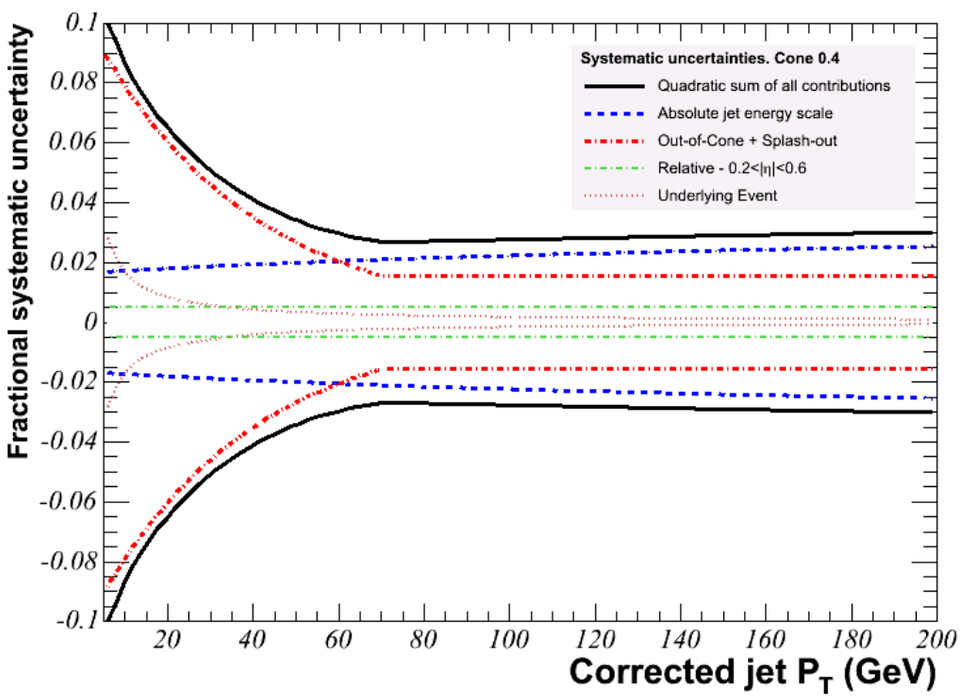


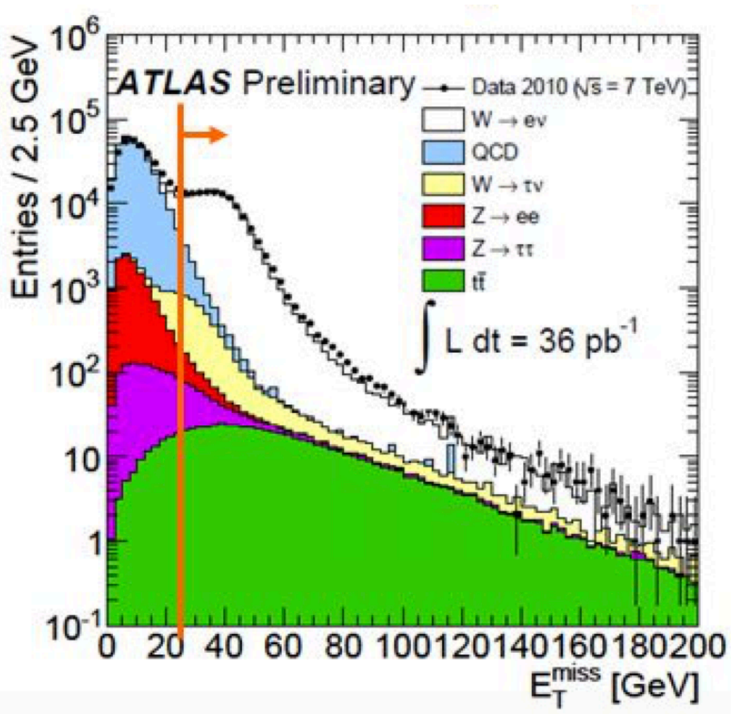
- Remember, we never wanted to train on MC

- We want to discover new physics without knowing what we are looking for

➡ Anomaly detection via unsupervised learning

→ systematic (experimental) uncertainties last remaining uncertainties, e.g. energy smearing of jets or MET

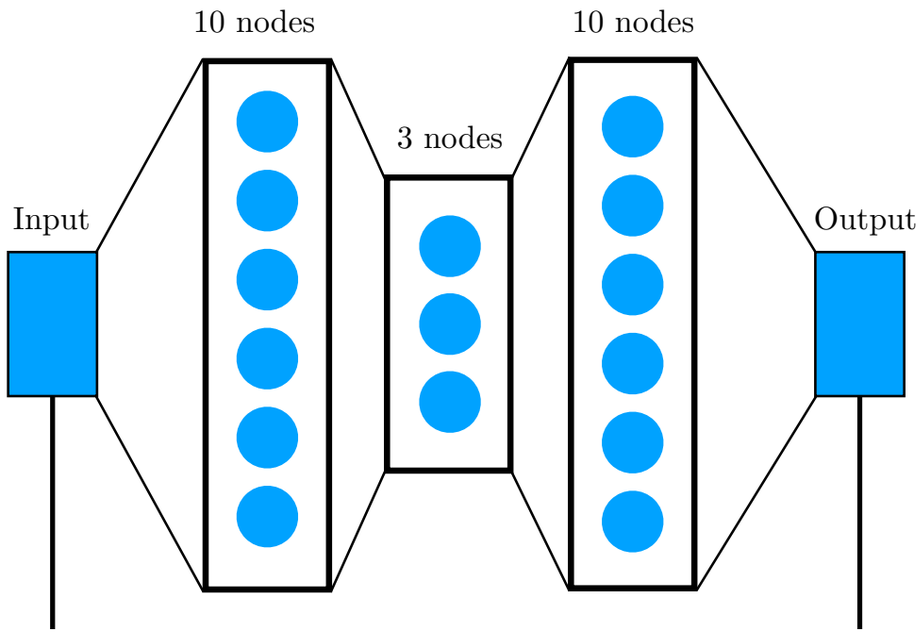




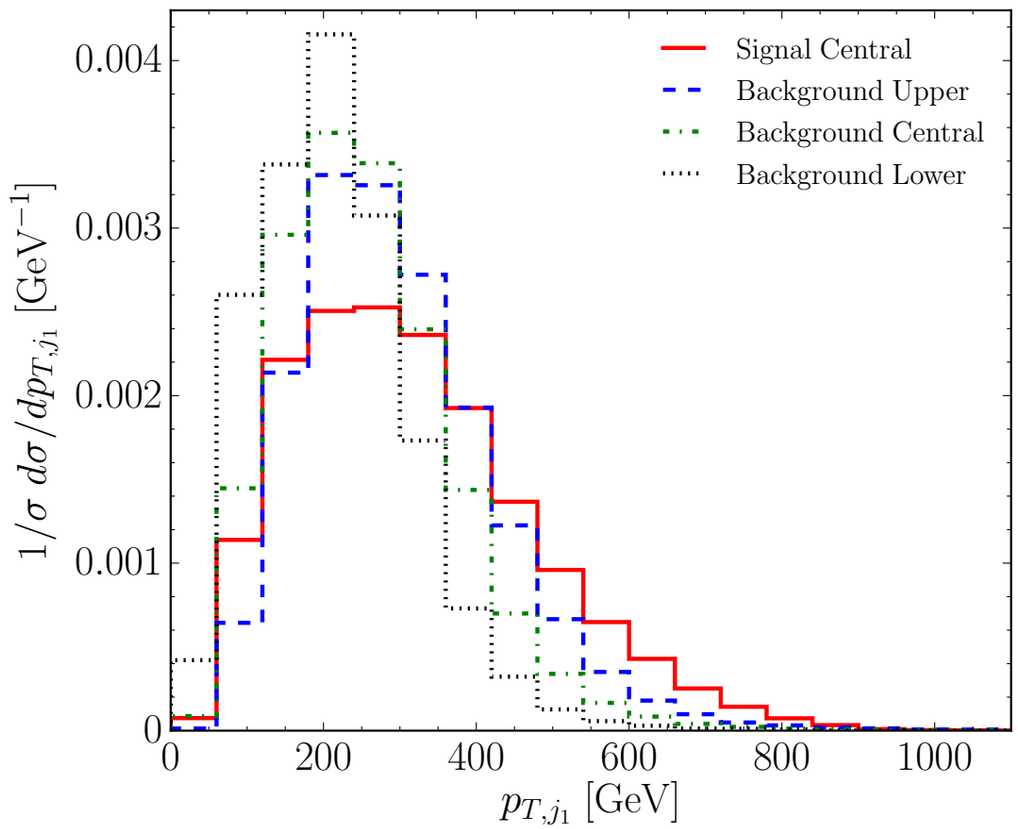
Uncertainties via adversarial for autoencoder (**unsupervised**)

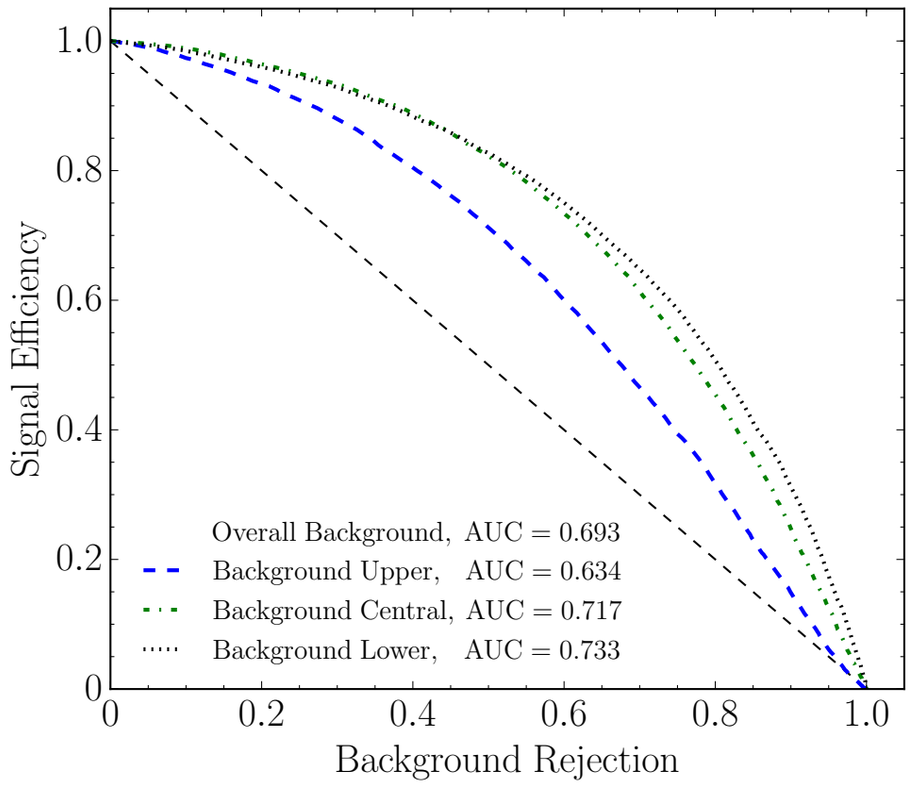
signal: pp->Z'->tt bkg: pp->tt

- to benchmark sensitivity first without adversarial
- only train on bkg (anomaly detection)
- syst. uncertainties via jet, MET smearing



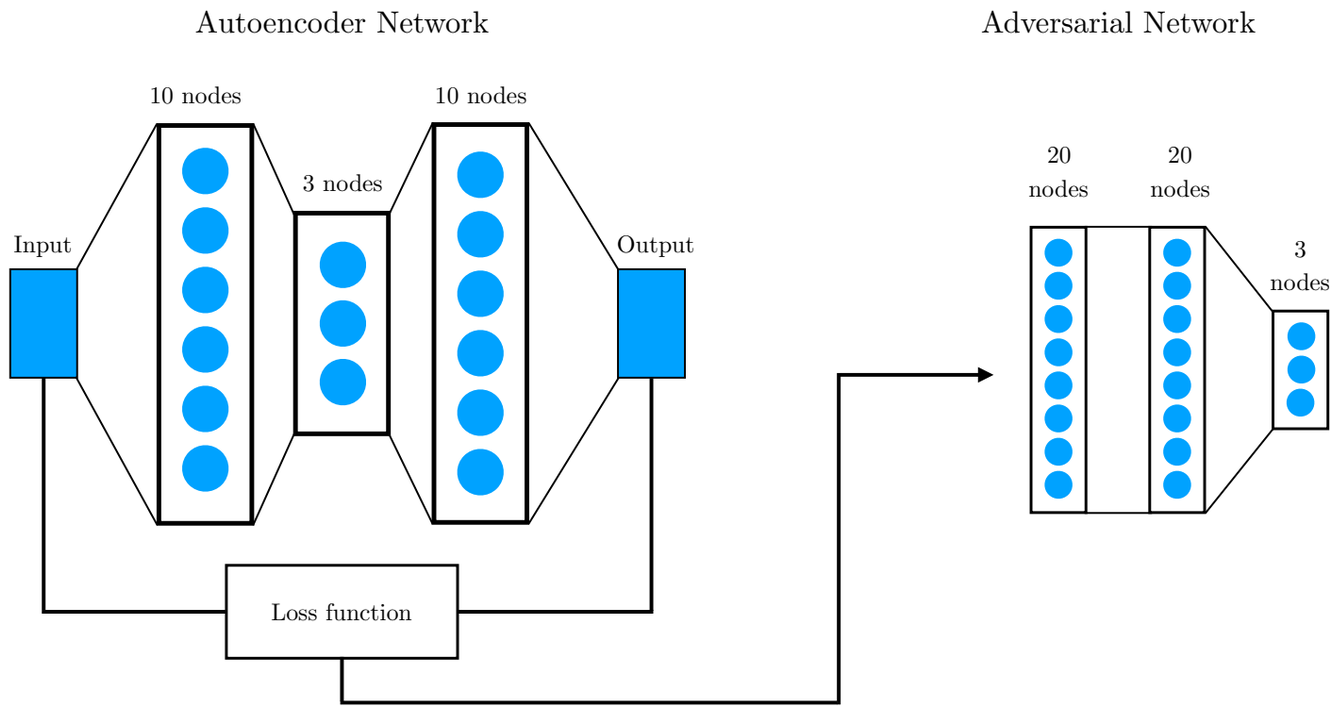
smeared jet distributions for bkg

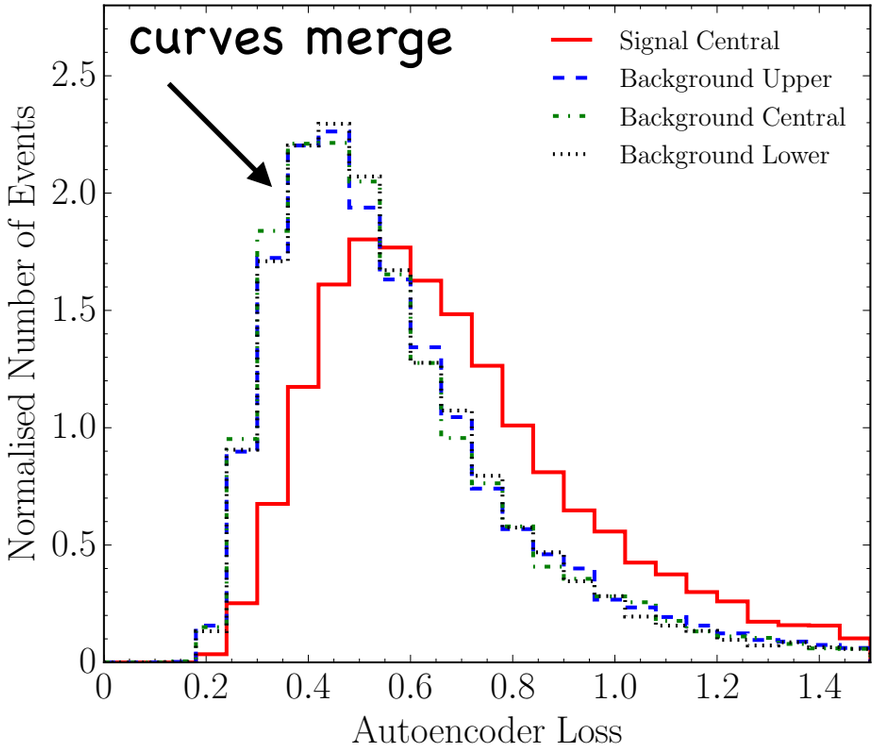


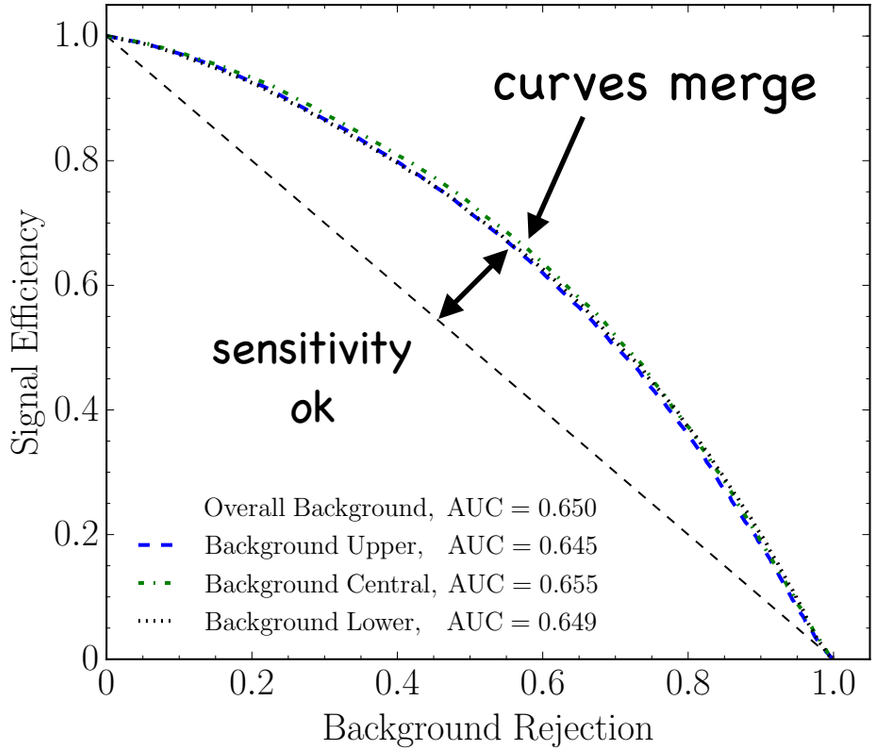


- We can remove dependance on smearing by applying an adversary that will try to classify the direction of smearing

- The two networks are in a zero-sum game - an increase in adversary performance will result in the autoencoder being penalised.







→ Robust, yet sensitive, anomaly detection with adversarial autoencoders

Going beyond classification and regression

- All previous examples and methods for classification and regression - either supervised or unsupervised

- If theorist should do that is up for debate... development of methods is done in data science (not particle theory)
  -> only track available is heavy user

- **Question**: Can we use ML (NN) such that we obtain new physics results - instead of extracting correlations we hide in pseudo data in the first place?

- **Answer**: Yes, neural nets are great numerical solvers!

[Piscopo, MS, Waite '19]

Universal approximation theorem: [Hornik et al '89] [Hornik '91]

feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of R^n, under mild assumptions on the activation function.

Expression of the output of a neural net:

$$N_m(\vec{x}, \{w, \vec{b}\}) = \sum_{k,n} w^f_{mk} g(w^h_{kn} x_n + b^h_k) + b^f_m$$

final

hidden

m outputs

single hidden layer with k units

n inputs

Our method can solve any equation that can be cast as an **optimisation problem**, i.e. can be brought into the form

$$\mathcal{F}_m(\vec{x}, \phi_m(\vec{x}), \nabla\phi_m(\vec{x}), \cdots, \nabla^j\phi_m(\vec{x})) = 0$$

Application to differential equations

(but tested also on integral equations)

Build the full function, here a DE into the loss function, incl boundary conditions

$$\mathcal{L}(\{w,\vec{b}\}) = \frac{1}{i_{\max}} \sum_{i,m} \hat{\mathcal{F}}_m(\vec{x}^i, \hat{\phi}_m(\vec{x}^i), \cdots, \nabla^j \hat{\phi}_m(\vec{x}^i))^2$$

$$+ \sum_{\text{B.C.}} (\nabla^p \hat{\phi}_m(\vec{x}_b) - K(\vec{x}_b))^2 \ ,$$

identify trial solution with network output $\hat{\phi}_m(\vec{x}) \equiv \breve{N}_m(\vec{x}, \{w,\vec{b}\})$

Build the full function, here a DE into the loss function, incl. boundary conditions

- Each part of the NN is differentiable (activation functions are chosen such)

  -> derivatives can be obtained analytically (no loss of precision)

- Hyperparameters can be optimised for speed of convergence and accuracy: activation function, nr hidden layers, width of NN, learning rate, epochs...

Example simple ODE

I first order: $\frac{d\phi}{dx} + \left(x + \frac{1+3x^2}{1+x+x^3}\right)\phi - x^3 - 2x - x^2\frac{1+3x^2}{1+x+x^3} = 0\,,$

with boundary condition $\phi(0) = 1$ in domain $x \in [0, 2]$

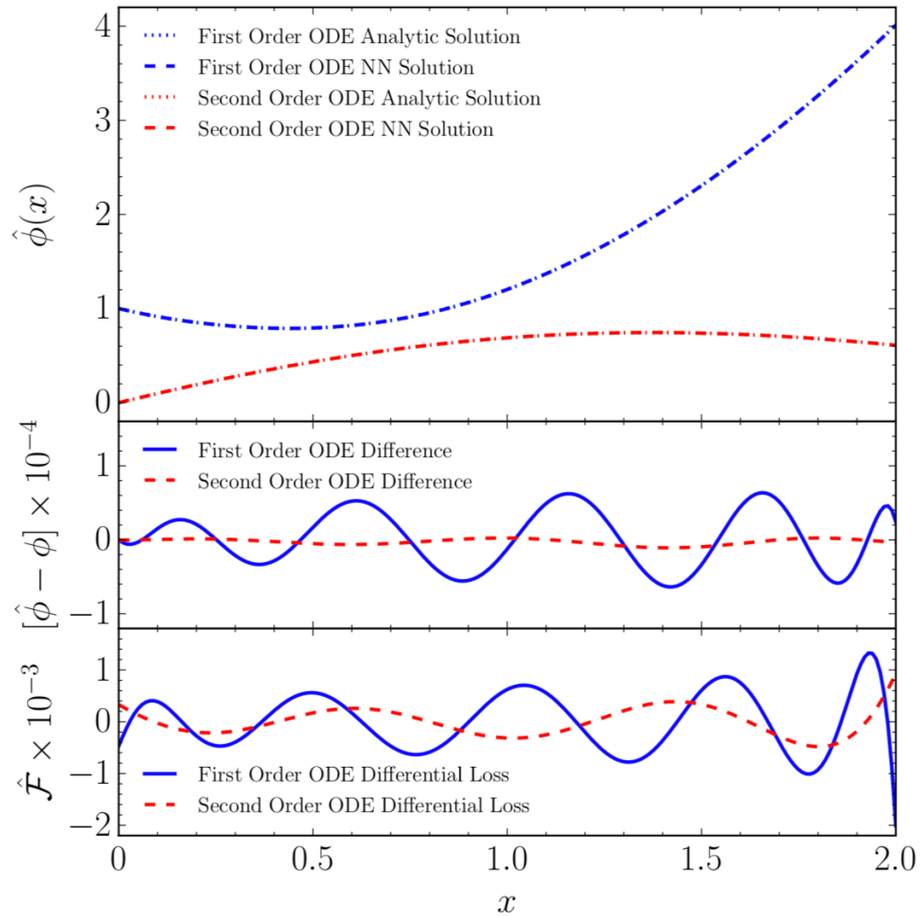
II second order: $\frac{d^2\phi}{dx^2} + \frac{1}{5}\frac{d\phi}{dx} + \phi + \frac{1}{5}e^{-\frac{x}{5}}\cos x = 0$

with boundary conditions $\phi(0) = 0$ and

$\frac{d}{dx}\phi(0) = 1$ in domain $x \in [0, 2]$

comparison between true and NN solution →

true solution independent measure how well functional is solved in each point of domain →



Second example PDE
(but tested many more)

Differential equation: $\nabla^2\phi - e^{-x}(x - 2 + y^3 + 6y) = 0$

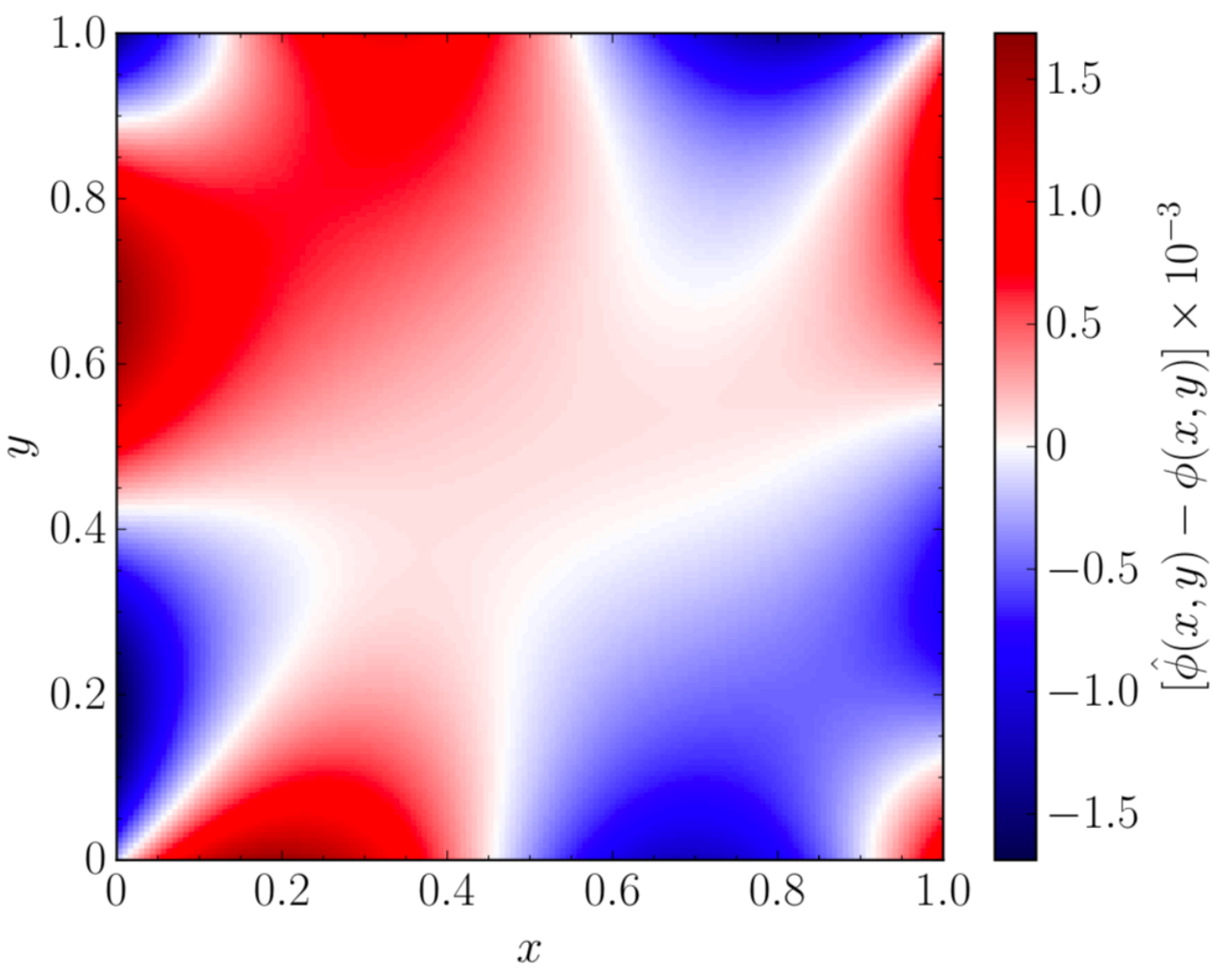
boundary conditions

$$\phi(0, y) = y^3 \ , \quad \phi(1, y) = (1 + y^3)e^{-1} \ ,$$
$$\phi(x, 0) = xe^{-x} \ , \quad \phi(x, 1) = e^{-x}(x + 1) \ ,$$

domain $(x, y) \in [0, 1] \times [0, 1]$

- Here deeper network pays off!
- Method also used for coupled PDE

difference between analytic and numeric solution



A true physics problem to solve:

Semiclassical calculations for bubbles and phase transitions

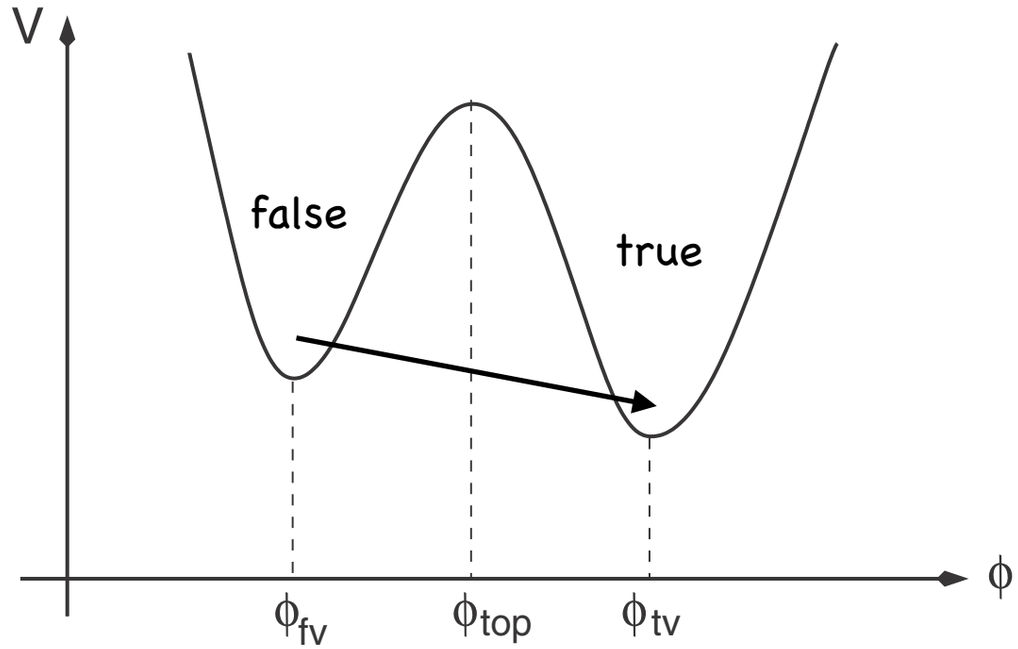
Need to find stationary points of Euclidean action:

Potential energy

$$S = \int d\tau\, d^3x \left[\frac{1}{2} \left(\frac{\partial \phi}{\partial \tau} \right)^2 + \frac{1}{2} (\boldsymbol{\nabla} \phi)^2 + V(\phi) \right]$$

Transition from false to true via tunnelling. Bubble can nucleate anywhere, with nucleation rate per unit volume:

$$\frac{\Gamma}{\mathcal{V}} = A e^{-B} \qquad B = S(\phi_b) - S(\phi_{\rm fv})$$

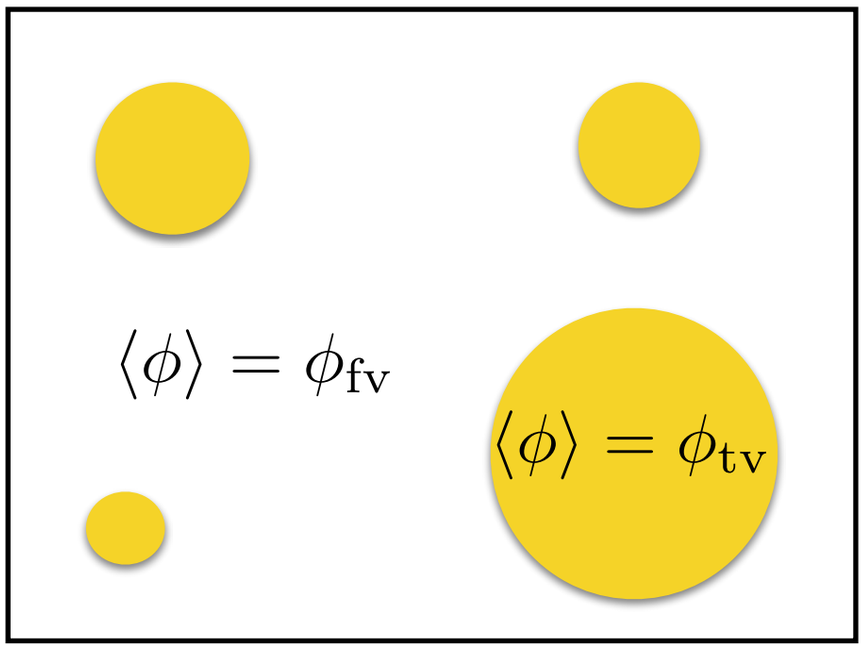


Growth of bubble via classical equation of motion

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 \right) \phi = \frac{\partial}{\partial \phi} V(\phi)$$

Methods to calculate bubble nucleation:

- Thin-wall approximation
- Polygon approximation [Guada, Maiezza, Nemevsek '18]
- over/undershoot method
- **Neural-Net approach** [Piscopo, MS, Waite '19]

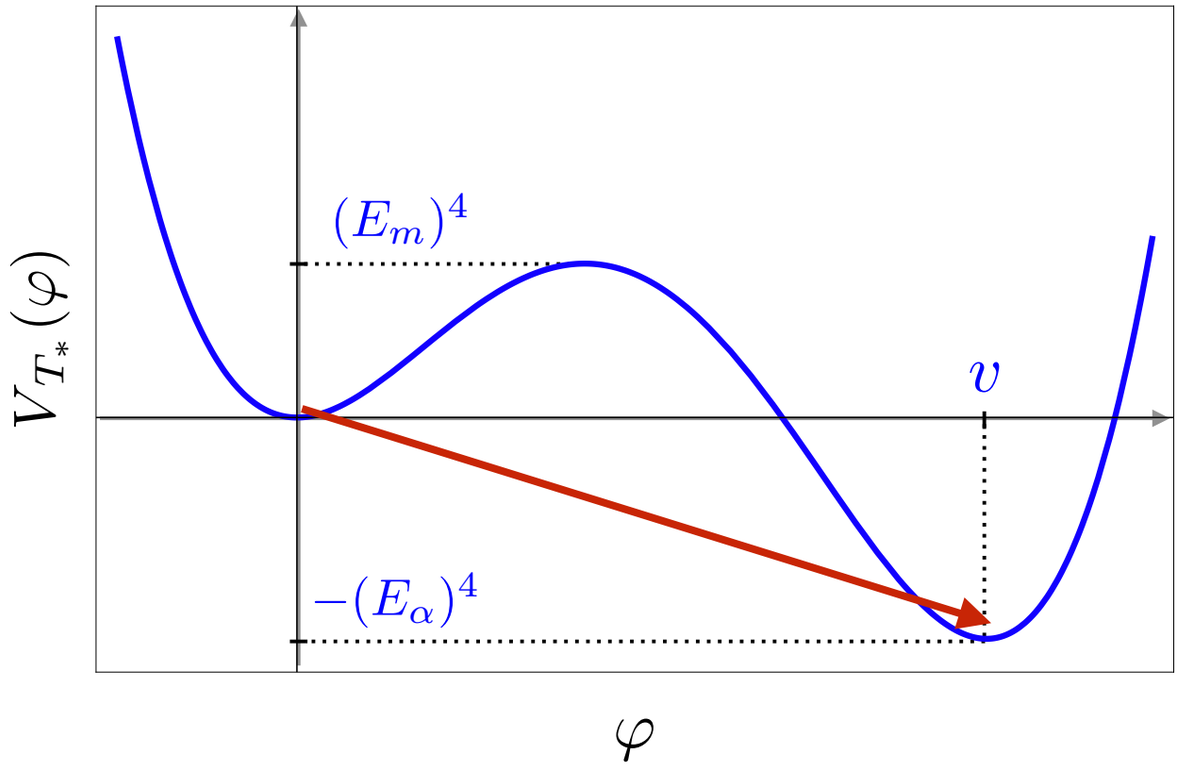


Bubble nucleation rate

$$\Gamma(T) = A(T) e^{-S_3(T)/T}$$

Duration of phase transition to Hubble rate

$$\frac{\beta}{H} = \left[T \frac{d}{dT} \left(\frac{S_3(T)}{T} \right) \right] \Bigg|_{T=T_*}$$



Probability for a single bubble to nucleate within the horizon volume

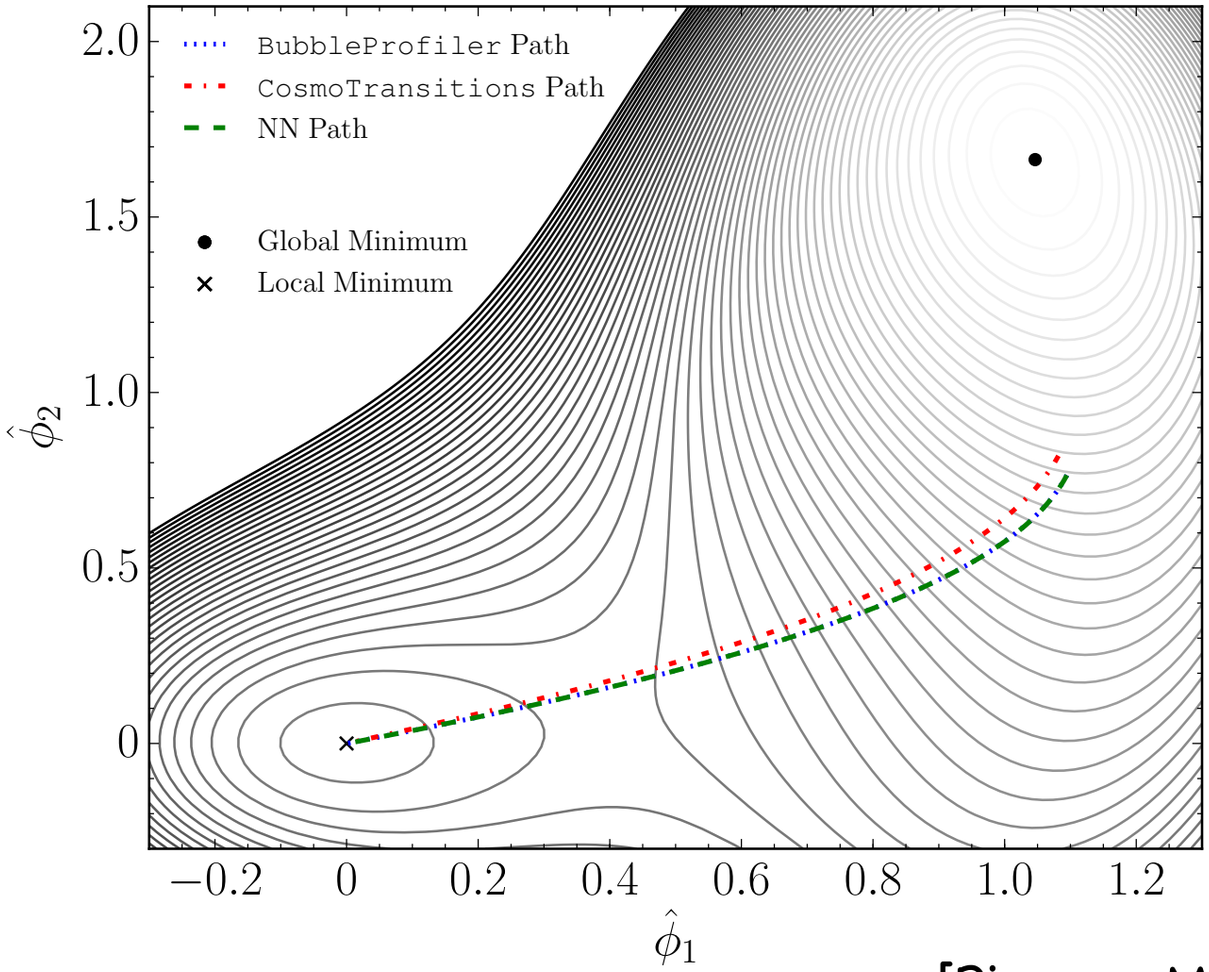
[Linde '83]

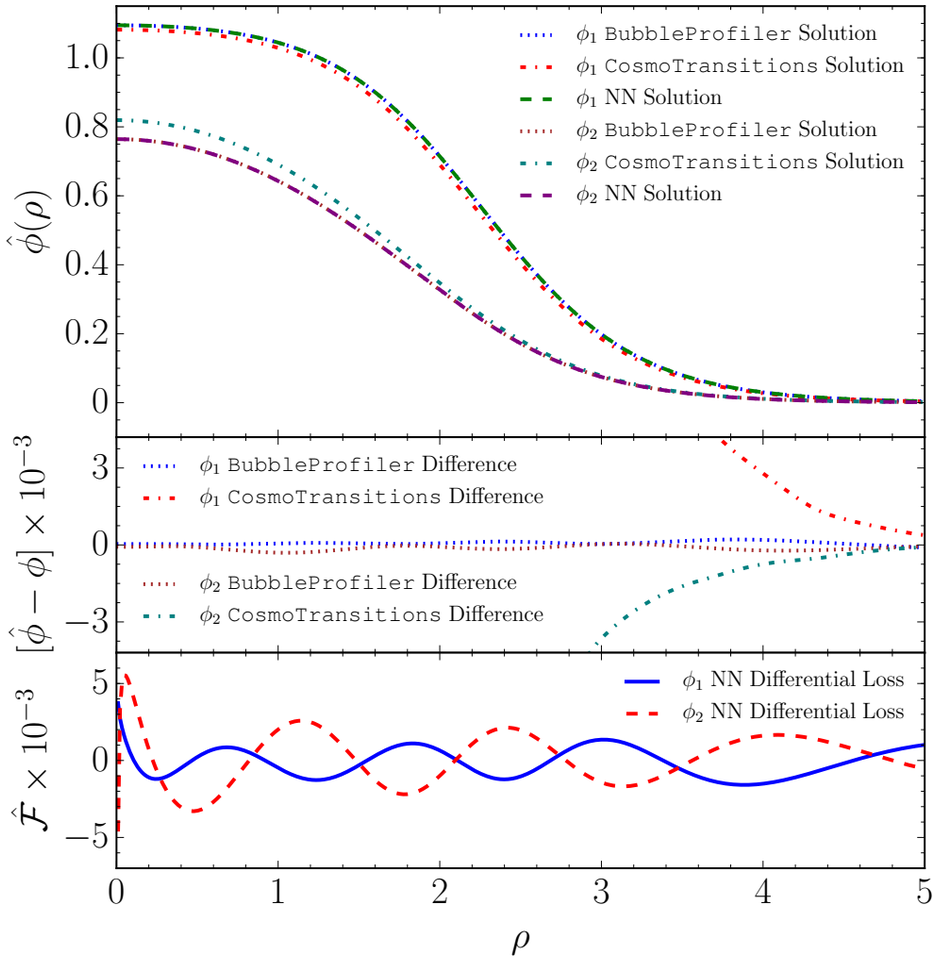
$$P(T_*) = \int_\infty^{T_*} \frac{dT}{T} \left(\frac{2\zeta M_{\rm Pl}}{T} \right)^4 \exp\left[-\frac{1}{T} S_3^{\rm cl}(T) \right] \quad \text{with} \quad \zeta^{-1} = 4\pi \sqrt{\pi g_*(T)/45}$$

To be of O(1) exponential factor should be compensated by prefactor

$$P(T_*) \simeq 1 \quad \Rightarrow \quad \frac{1}{T_*} S_3^{\rm cl}(T_*) \simeq 140 - 4 \log \frac{T_*}{100\,\text{GeV}} \simeq 100$$

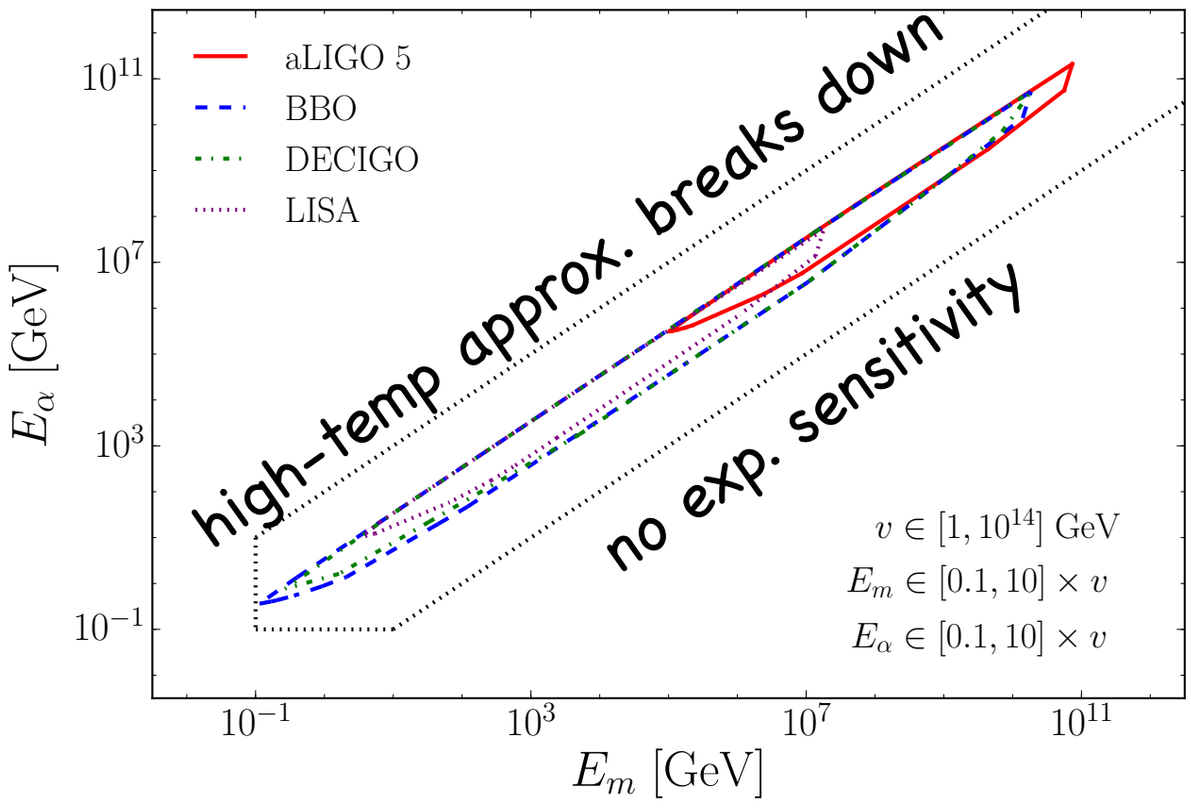
Field profiles and tunnelling path

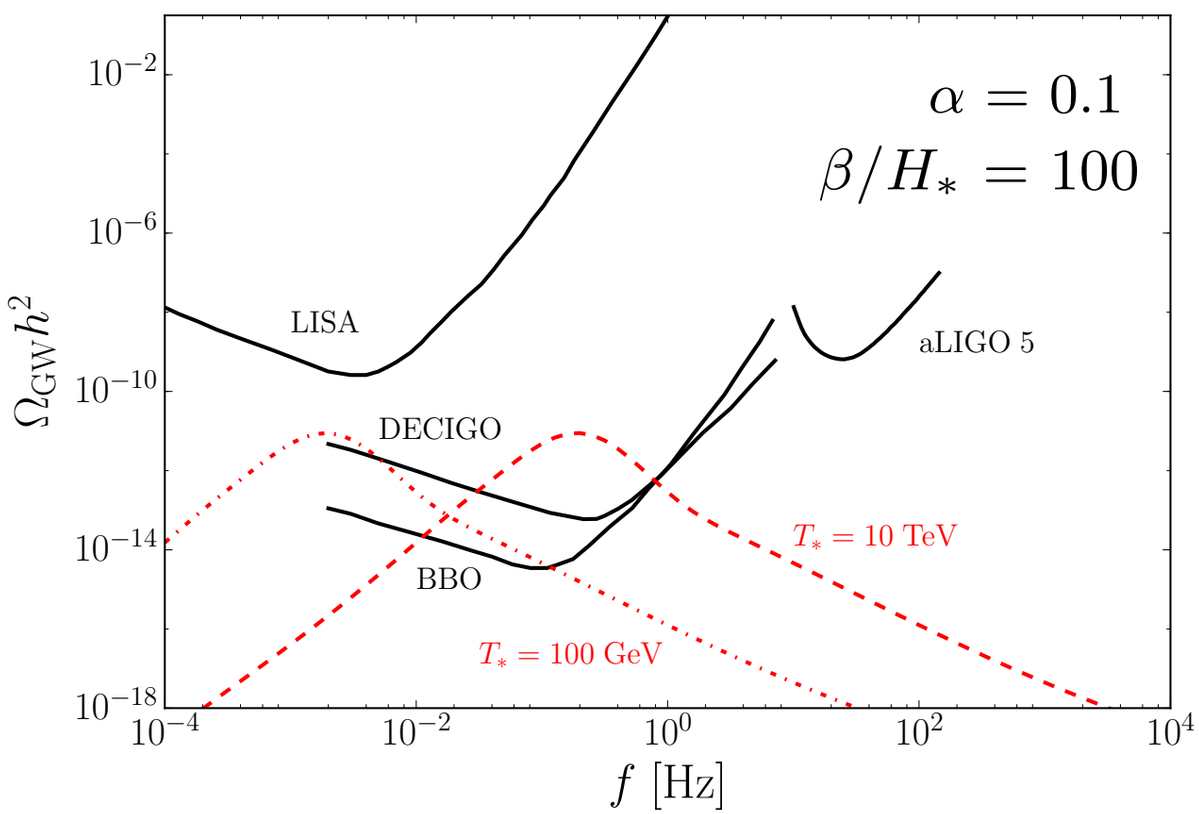




[Piscopo, MS, Waite '19]

- NN-approach often more reliable and more precise than dedicated PT solver, e.g. CosmoTransitions, BubbleProfiler
- $\hat{\mathcal{F}}$ is measure for quality of the solution
- Many applications beyond phase transitions



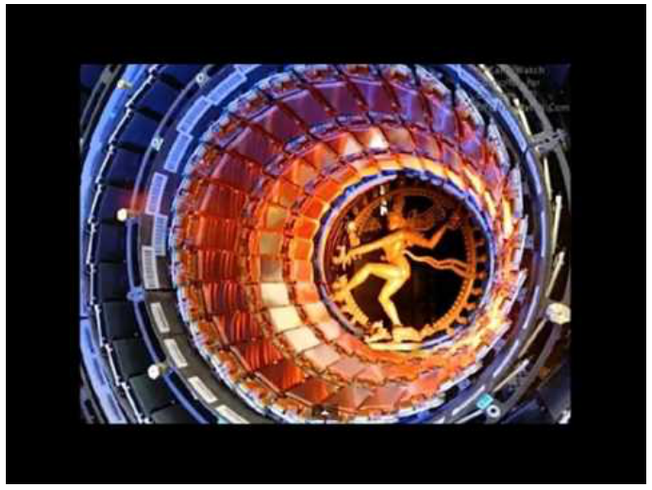


- All experiments (exisitng and future) are sensitive to the region $E_\alpha \sim (0.1 - 10) \times E_m$

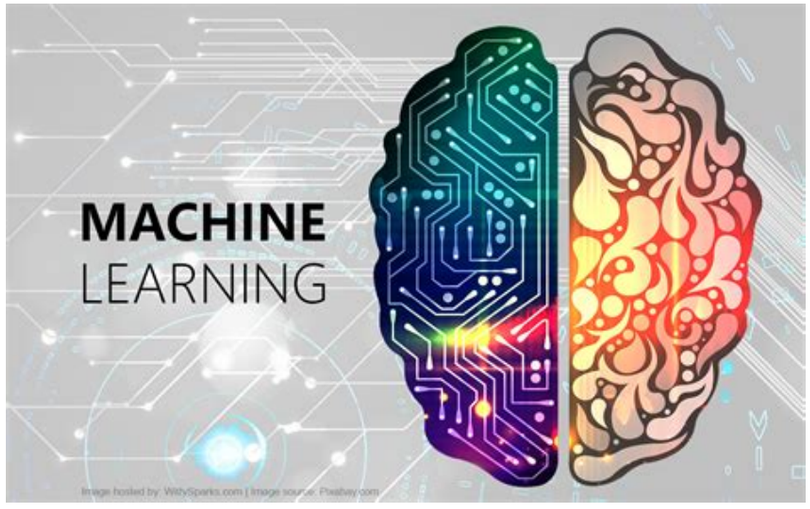
- aLIGO has sensitivity to high temperatures, LISA to ELW temperatures and large E_α

- Can check for generic models without using CosmoTransitions et. al. using approach and data from: [Chala, Khoze, MS, Waite '19]

https://www.ippp.dur.ac.uk/~mspannow/gravwaves.html



Summary



- Machine Learning methods are powerful tools to address relevant physics questions, i.e. finding correlations in multi-dim parameter spaces, regression, anomaly detection, but also as numerical solvers

- Particle Physicist: Working on ML == probably more like using ML

- For theorists ML can be powerful in providing solutions to numerical problems