HISS Summer School

Intro and Overview

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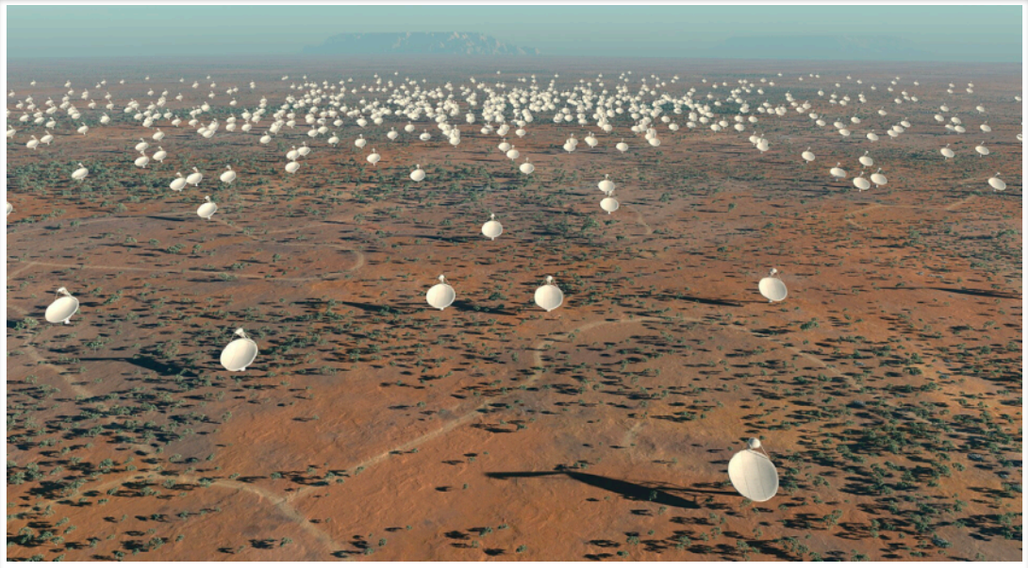
What's special about Physics?

Different fields, unified by **digitisation challenges:**

- **Immense data volumes** with high complexity
- Weak signals overshadowed by much larger background processes
- Large data-throughput requiring custom solutions



The planned Square Kilometre Array (SKA) telescope will produce one exabyte of raw data/day (~10 PB after compression)

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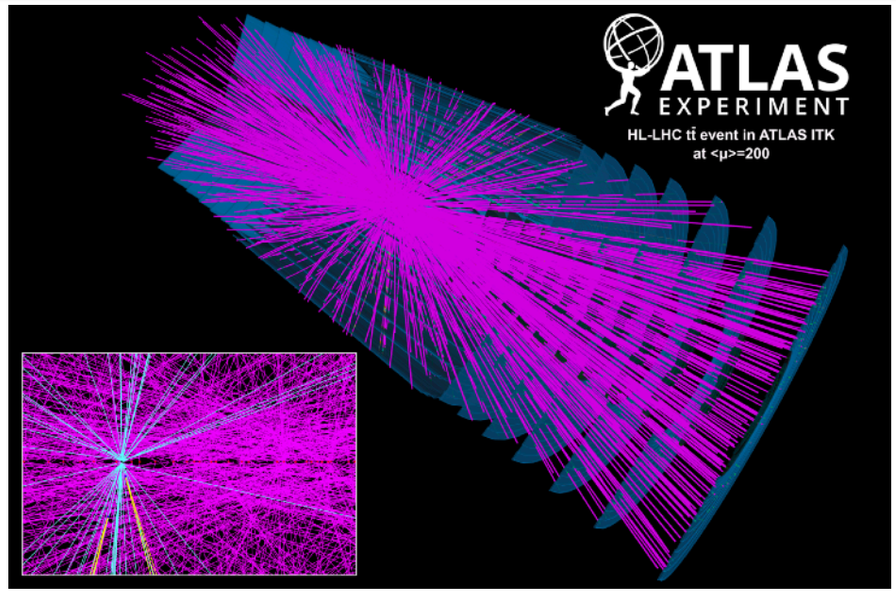

At the High Luminosity LHC, overlapping collisions mean that thousands of trajectories need to be reconstructed in parallel

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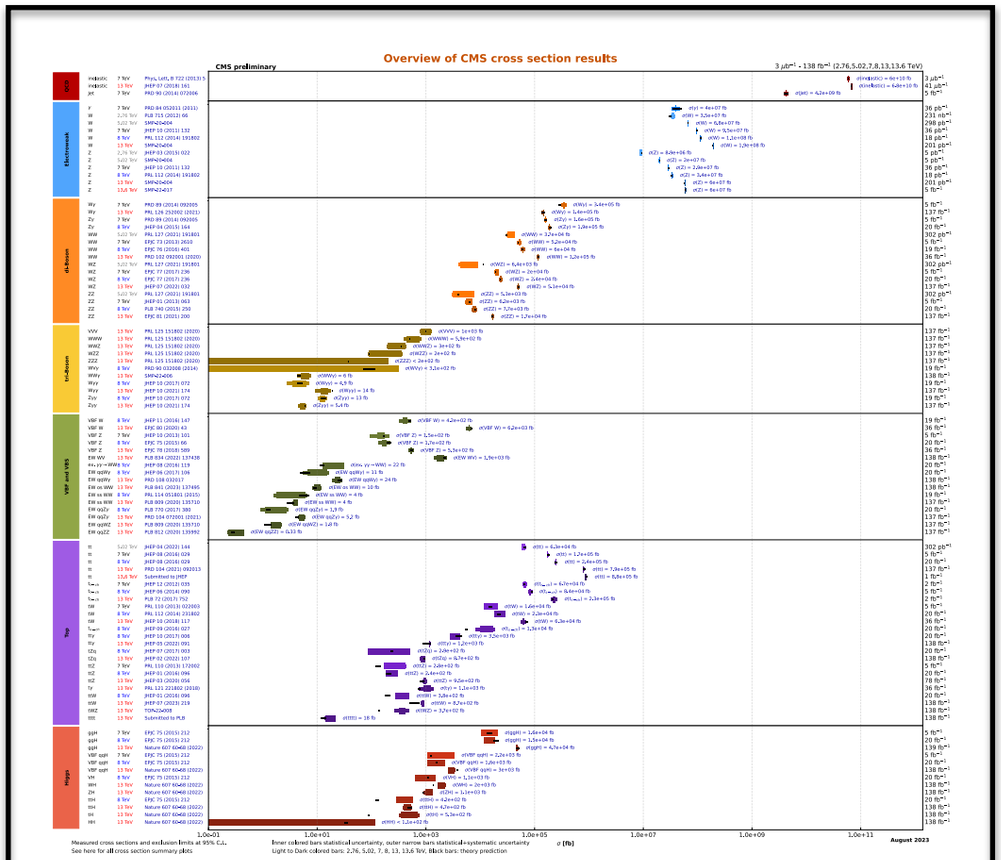

Rare interesting processes only occur in 1 of 10 billion events in particle physics experiments

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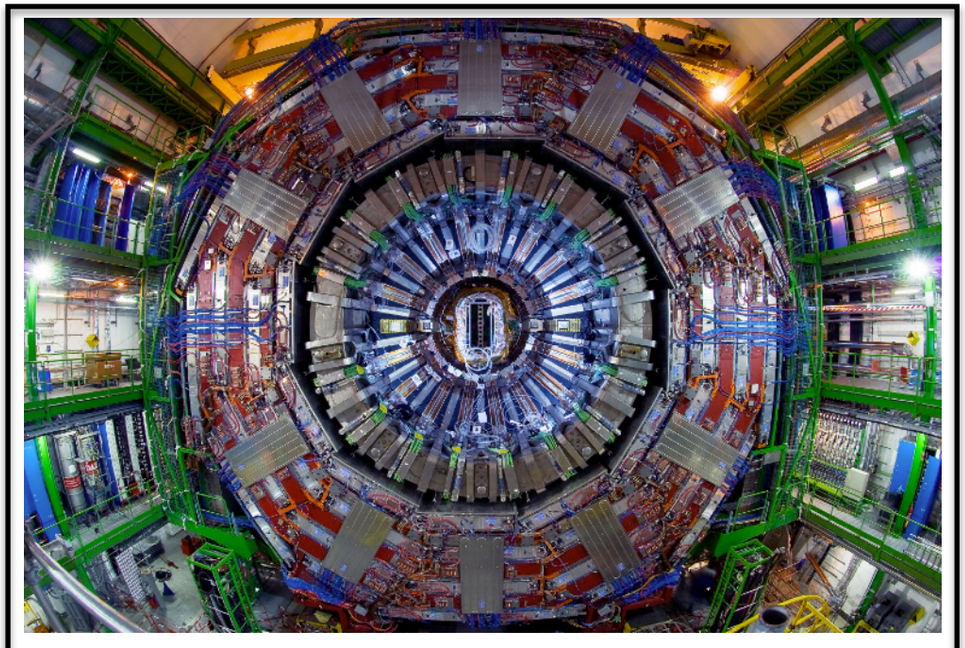
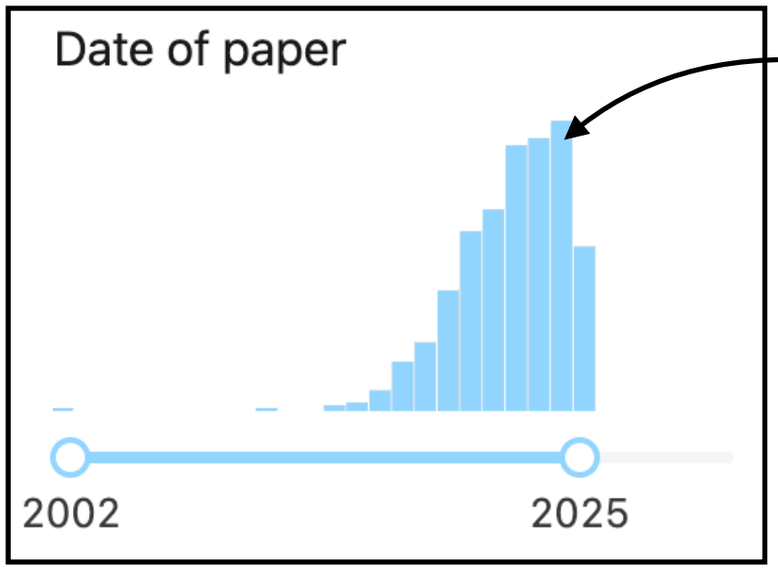


Trigger systems filter 40 million particle collisions/second at experiments at the Large Hadron Collider (LHC) at CERN

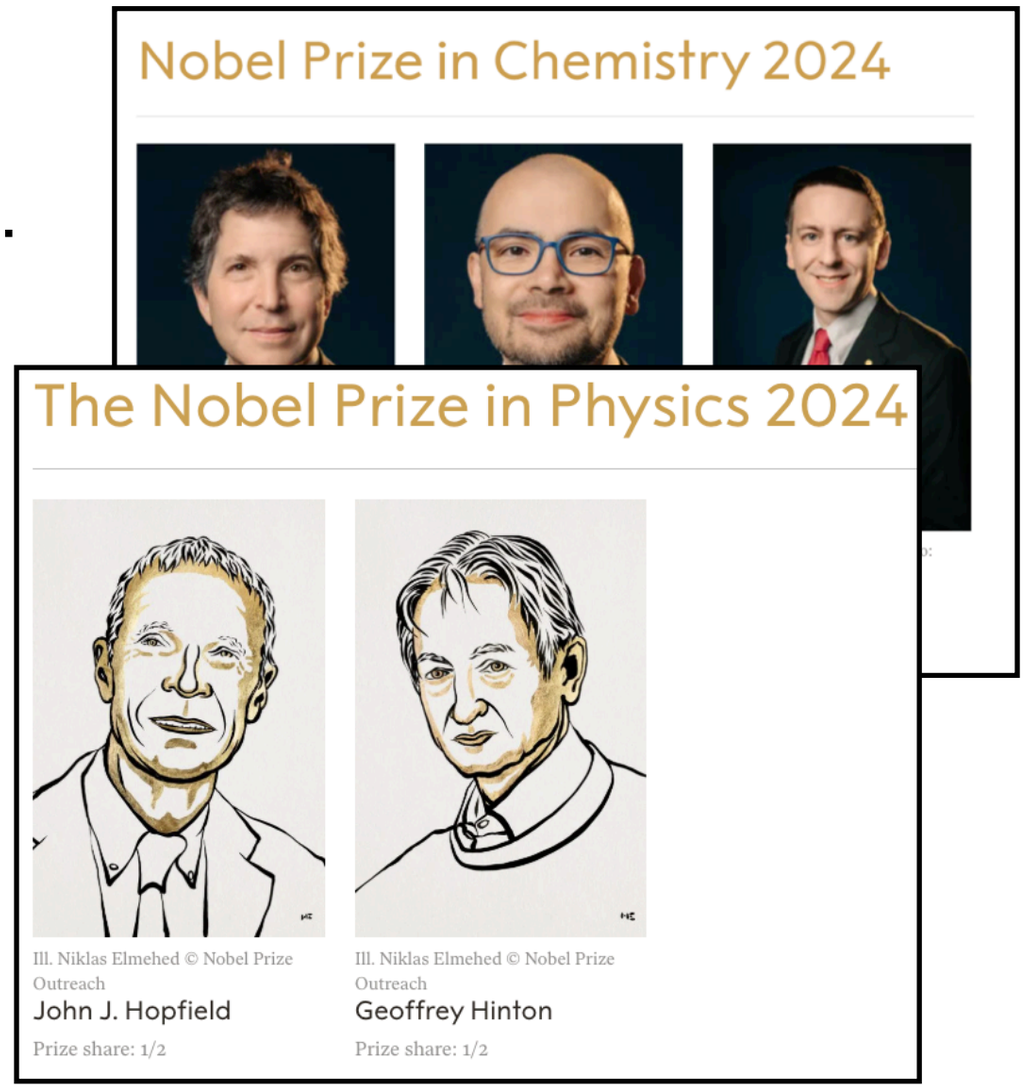
State of AI in Physics

literature ('machine learning' or 'deep learning') in hep-ex



200+ papers in 2024

Similar for nucl-ex, astro-ph, hep-ph, …



Rapid rise of AI in fundamental physics

Transition from concepts to applications

Recognition of AI work as Nobel-prize worthy

See also https://iml-wg.github.io/HEPML-LivingReview/

Plan

- Lecture 1:
  - Basics of Neural Networks
  - Classification example: Top Tagging
- Lecture 2:
  - Generative Models
  - Anomaly Detection

Resources

Free online: https://www.deeplearningbook.org/

Lecture Slides

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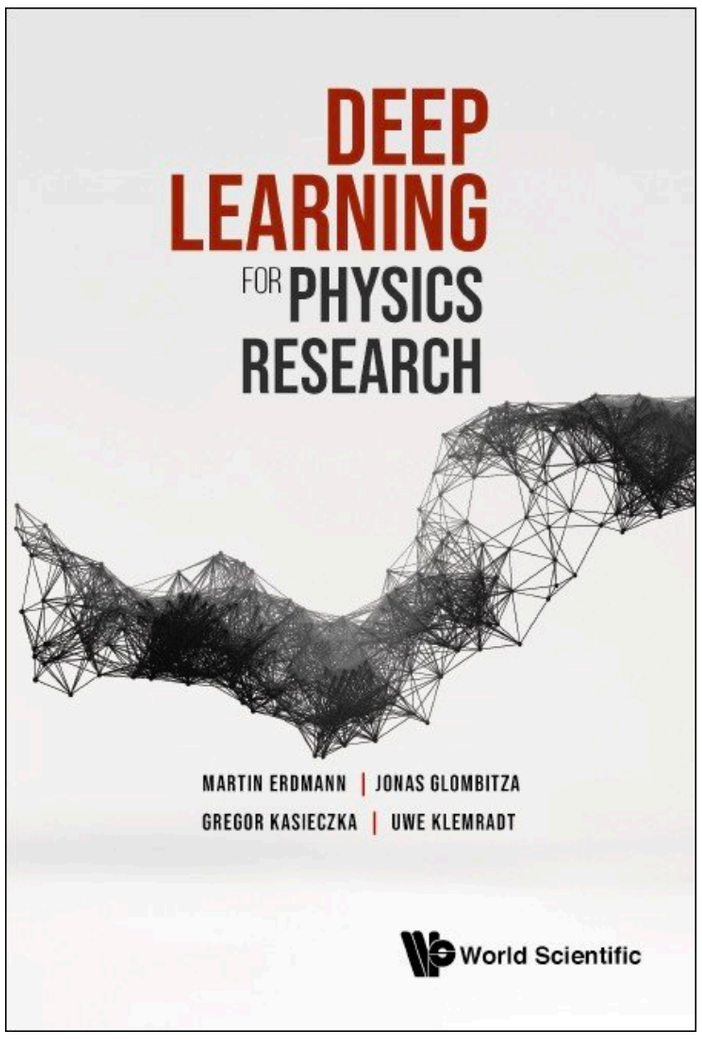
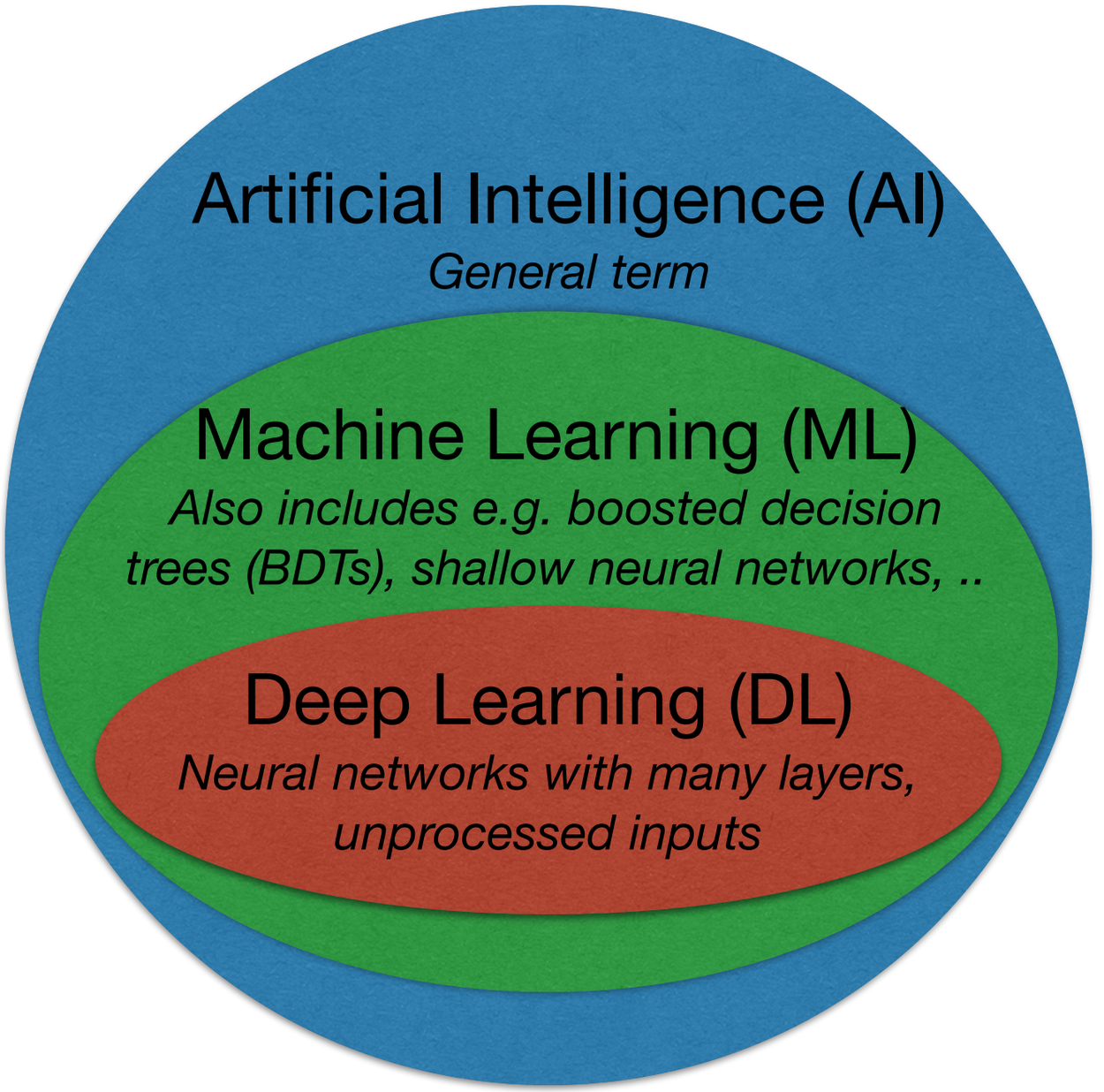


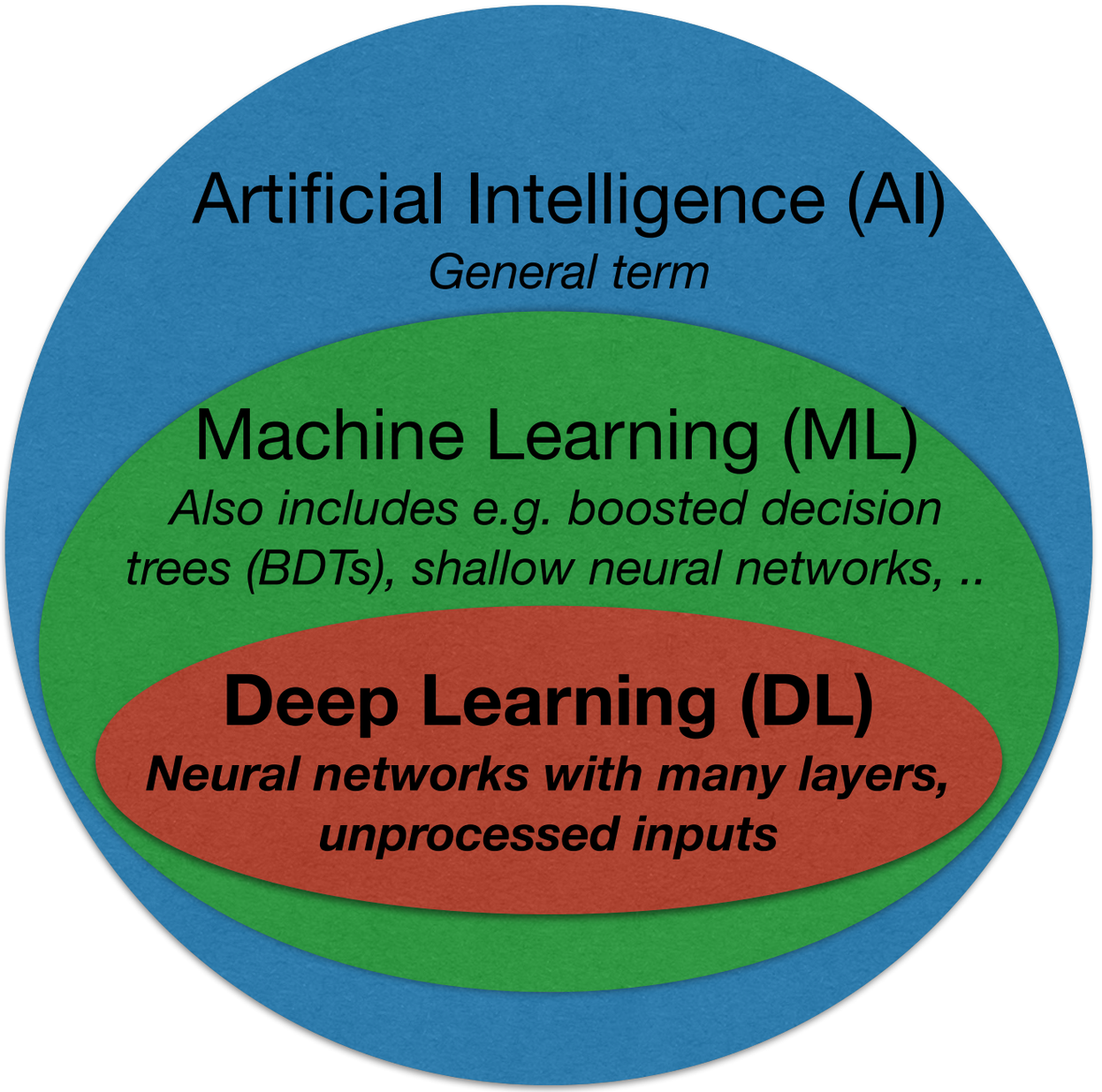
https://www.worldscientific.com/worldscibooks/10.1142/12294#t=aboutBook
(available in UHH library)

Learning like a machine

Terminology



Terminology



Basic idea

- Classical approach:
  - Write a sequence of instructions to solve a specific task
  - e.g.:
    - Tracking algorithm
    - Jet clustering
    - Calculation of physical observables

```
    if (trackerTopology.pxfSide(detId) == 1) {
      trackingLayer._side = TrackingLayer::Side::NEG_ENDCAP;
    } else if (trackerTopology.pxfSide(detId) == 2) {
      trackingLayer._side = TrackingLayer::Side::POS_ENDCAP;
    } else {
      throw cms::Exception("FastSimulation/Tracking")
          << "Tracker hit for seeding in FPix seems neither on positive nor on negative disk side: "
          << trackerTopology.print(detId).c_str();
    }
    trackingLayer._layerNumber = trackerTopology.pxfDisk(detId);
  }
  //TIB
  else if (subdet == StripSubdetector::TIB) {
    trackingLayer._subDet = TrackingLayer::Det::TIB;
    trackingLayer._side = TrackingLayer::Side::BARREL;
    trackingLayer._layerNumber = trackerTopology.tibLayer(detId);
  }
  //TID
  else if (subdet == StripSubdetector::TID) {
    trackingLayer._subDet = TrackingLayer::Det::TID;
    if (trackerTopology.tidSide(detId) == 1) {
      trackingLayer._side = TrackingLayer::Side::NEG_ENDCAP;
    } else if (trackerTopology.tidSide(detId) == 2) {
      trackingLayer._side = TrackingLayer::Side::POS_ENDCAP;
    } else {
      throw cms::Exception("FastSimulation/Tracking")
          << "Tracker hit for seeding in TID seems neither on positive nor on negative disk side: "
          << trackerTopology.print(detId).c_str();
    }
    trackingLayer._layerNumber = trackerTopology.tidWheel(detId);
  }
  //TOB
  else if (subdet == StripSubdetector::TOB) {
```

Basic idea

- Machine learning approach:
  - Rephrase task as a minimisation problem..
  - ..and “simply” solve:

$$\theta^* = \text{argmin}_\theta \, \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})} \left[\mathcal{L}\left(f_\theta(\mathbf{x}), \mathbf{x} \right) \right]$$

- Will now go step-by-step to understand the underlying ideas, focusing on neural networks.

General Strategy

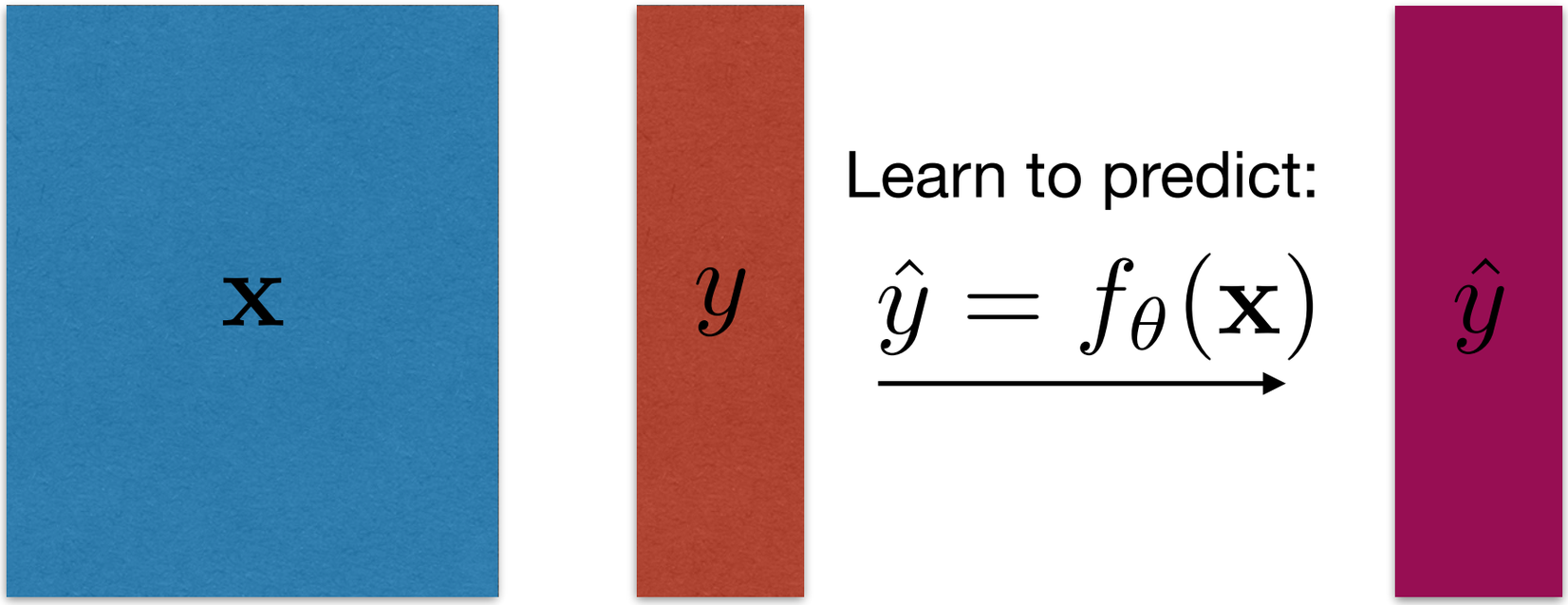
Loss function $\mathcal{L}$

- Define an optimisation target (loss function)

Loss function: Supervised

Supervised Learning:
Attempt to infer some target *(truth label)*:
classification, regression (often also clustering/inference)

Use training data with known labels
(often from Monte Carlo simulation)



observable features such as kinematics, tracks,…

truth label
(e.g. true energy)

predicted energy

Regression: Minimize mean squared error:

$$\mathcal{L} = (y - \hat{y})^2$$

Classification Tasks

Distinguish a pair of classes (binary) or several (multi-class).

Images

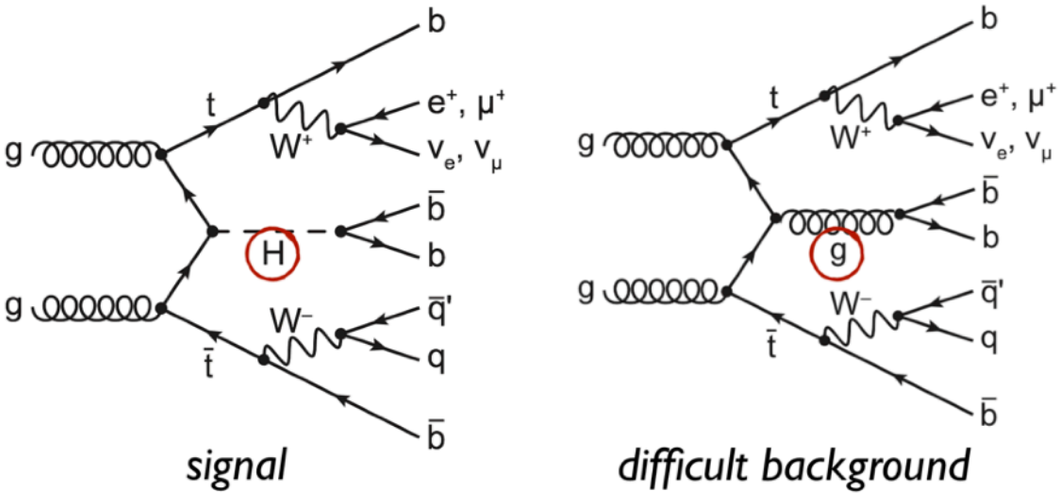
Loss function: Cross entropy

$$\mathcal{L} = -y \log(\hat{y}) - (1-y) \log(1-\hat{y})$$

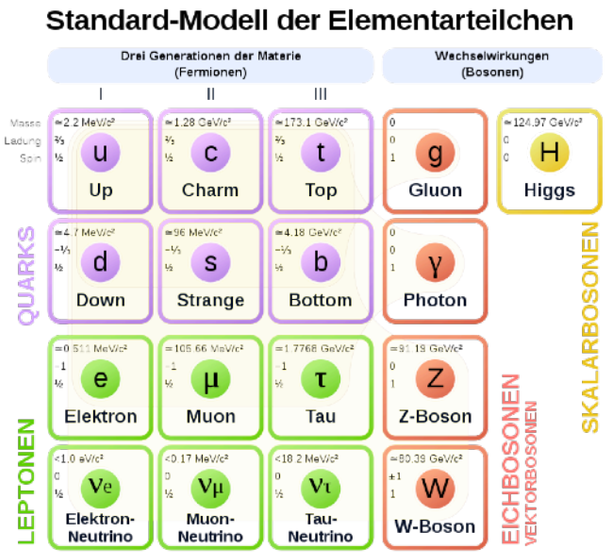
Classification Tasks

Distinguish a pair of classes (binary) or several (multi-class).

Event Topologies



Particles



Loss function: Cross entropy

$$\mathcal{L} = -y \log(\hat{y}) - (1-y) \log(1-\hat{y})$$

Cross Entropy

- Example: Binary classification
  - 2 Classes with labels: $y_k = 0, 1$
  - Build the NN such that we the output is a probability: $\hat{y}(x_k) \in [0,1]$
- -> Bernoulli Trial with probabilities p and $\mathrm{q} = 1 - \mathrm{p}$
- Likelihood:

$$L = \prod_{k}^{N} [\, y_k \cdot \hat{y}(x_k) + (1 - y_k) \cdot (1 - \hat{y}(x_k)) \,]$$

Jacob Bernoulli 1654-1705

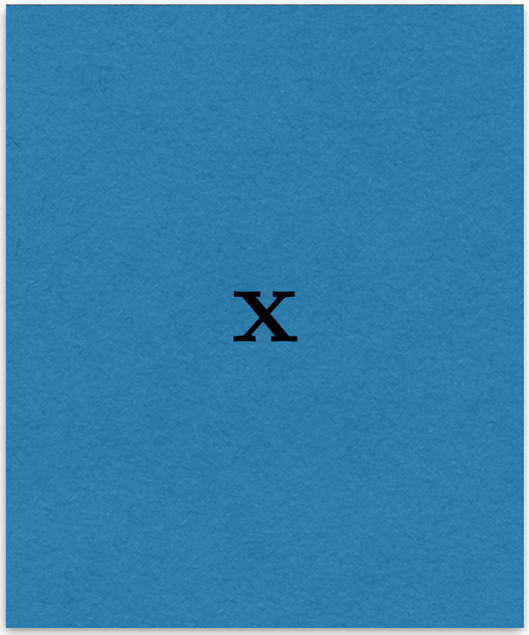
- We want to minimize the average negative log-likelihood:

$$-\frac{1}{N}\log(L) = -\frac{1}{N}\sum_{k}^{N}[y_k \cdot \log(\hat{y}(x_k)) + (1 - y_k) \cdot \log(1 - \hat{y}(x_k))]$$

Loss function: Unsupervised

Unsupervised Learning:
No target, learn the probability distribution (directly from data)

Can use for sampling, anomaly detection, unfolding, …



Learn to predict:

$$\hat{p}(\mathbf{x}) = f_\theta(\mathbf{x})$$

$$p(\mathbf{x})$$

True probablity density

There also exists a number of other less-than-supervised approaches (weakly supervised learning, semi-supervised learning, …) Not so important for now.

Distribution learning: Maximise likelihood (minimize log-likelihood):
(either directly or with approximations)

$$\mathcal{L} = -\log\left(\hat{p}(\mathbf{x})\right)$$

General Strategy

Loss function $\mathcal{L}$ ✓

Neural network f_θ

Parameters θ

Opt. Parameters θ^*

Data $\mathbf{x}$

Data distribution $p(\mathbf{x})$

$$\theta^* = \text{argmin}_\theta \, \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})} \left[\mathcal{L}(f_\theta(\mathbf{x}), \mathbf{x}) \right]$$

General Strategy

Loss function $\mathcal{L}$

Neural network f_θ

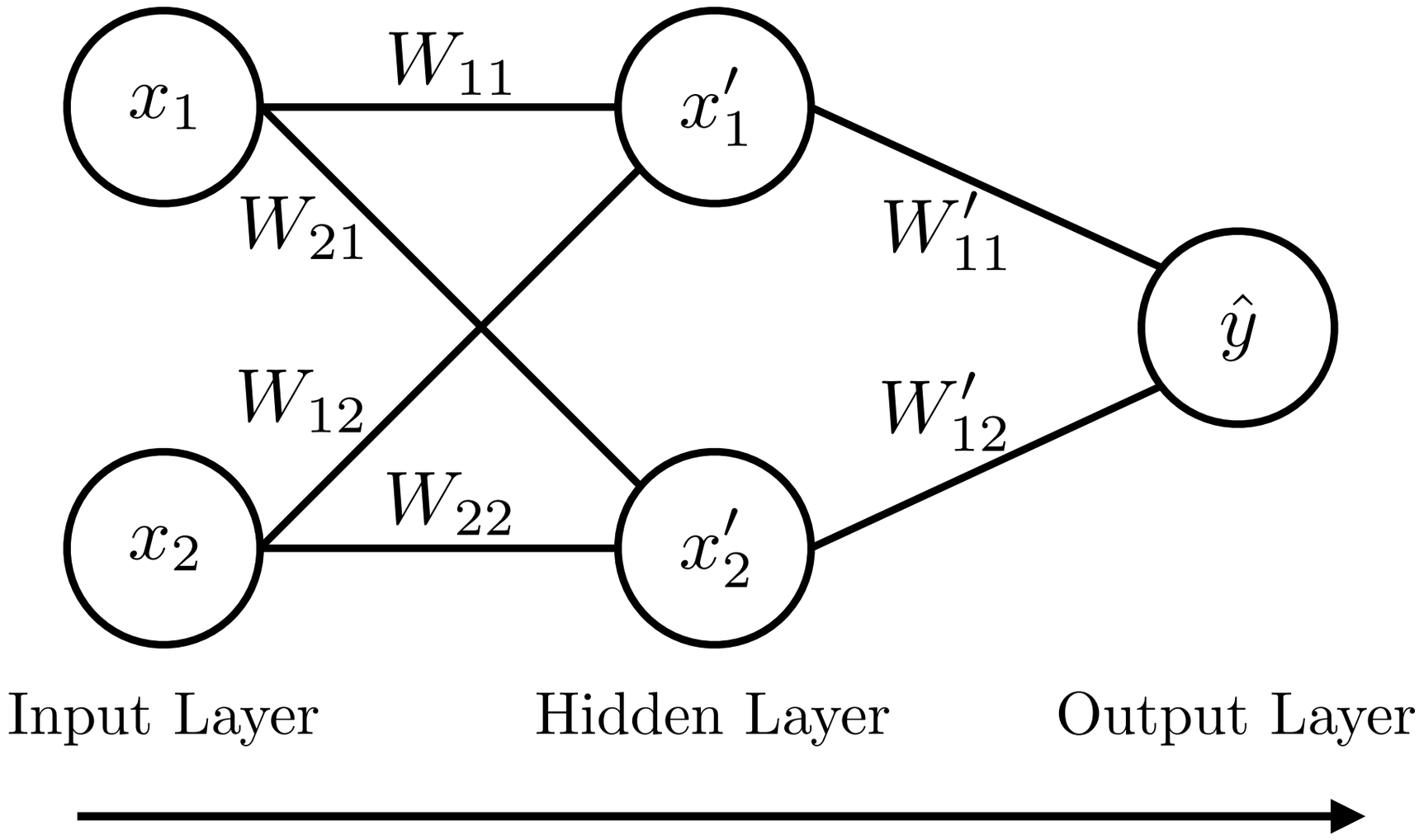
Parameters θ

- Define an optimisation target (loss function)
- Choose a non-linear, expressive, parametrised function (e.g. a neural network)

Neural networks

We need an expressive function
(universal approximator)
with tuneable parameters and useful
implicit biases

$$x'_1 = f(W_1 1 \cdot x_1 + W_1 2 \cdot x_2)$$



Neural Networks

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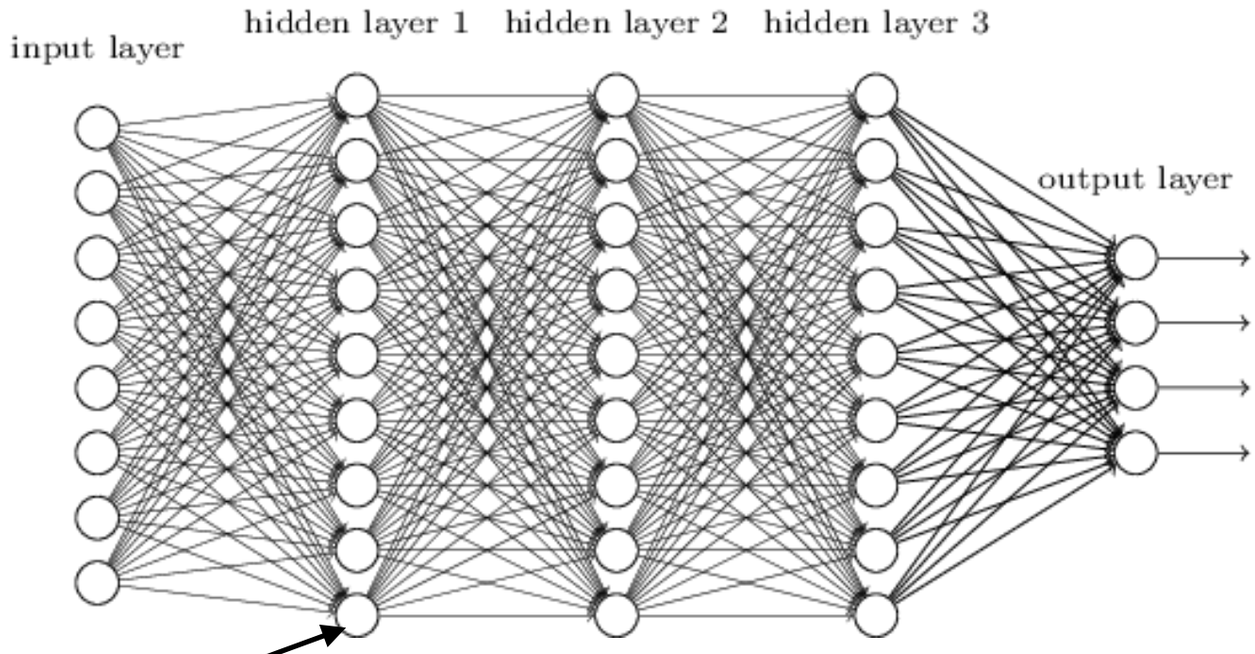
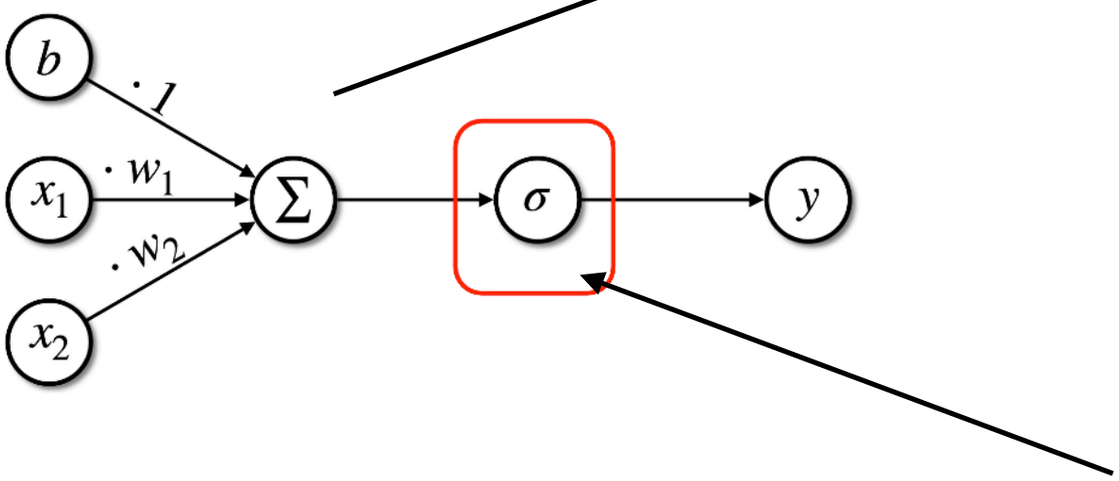
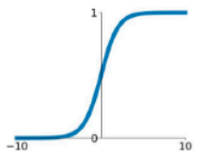
Neural networks



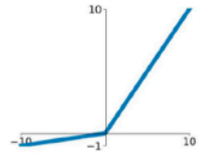


Activation Functions

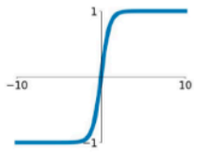
Sigmoid
$\sigma(x) = \frac{1}{1+e^{-x}}$



Leaky ReLU
$\max(0.1x, x)$

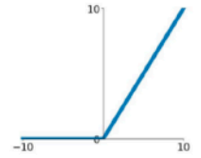


tanh
$\tanh(x)$

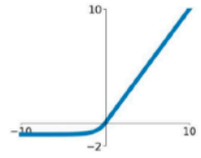


Maxout
$\max(w_1^T x + b_1, w_2^T x + b_2)$

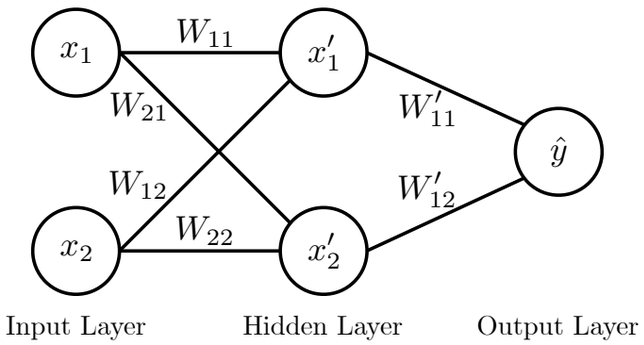
ReLU
$\max(0, x)$



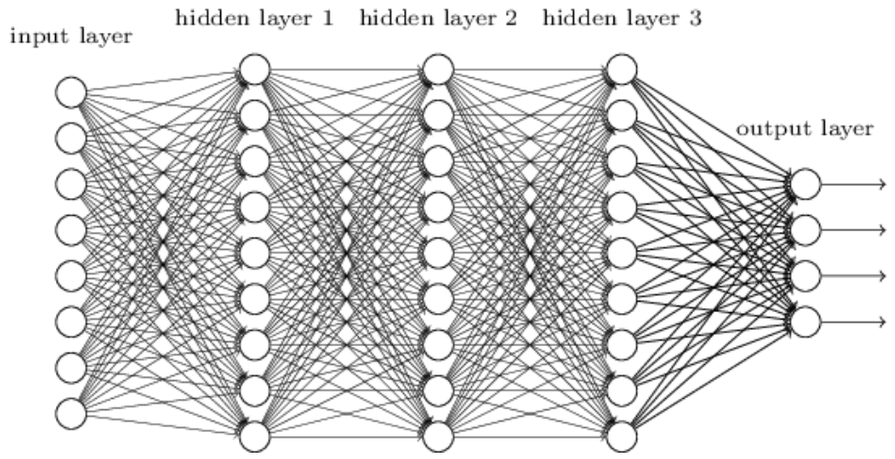
ELU
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Complexity



6 weights



300 weights

Deep Learning:
Complex network + low level inputs

25 million weights:
2016 state of the art for image classification

stage	output	ResNet-50	**ResNeXt-50 (32×4d)**
conv1	112×112	7×7, 64, stride 2	7×7, 64, stride 2
conv2	56×56	3×3 max pool, stride 2	3×3 max pool, stride 2
		$\begin{bmatrix} 1\times1, 64 \\ 3\times3, 64 \\ 1\times1, 256 \end{bmatrix} \times3$	$\begin{bmatrix} 1\times1, 128 \\ 3\times3, 128, C{=}32 \\ 1\times1, 256 \end{bmatrix} \times3$
conv3	28×28	$\begin{bmatrix} 1\times1, 128 \\ 3\times3, 128 \\ 1\times1, 512 \end{bmatrix} \times4$	$\begin{bmatrix} 1\times1, 256 \\ 3\times3, 256, C{=}32 \\ 1\times1, 512 \end{bmatrix} \times4$
conv4	14×14	$\begin{bmatrix} 1\times1, 256 \\ 3\times3, 256 \\ 1\times1, 1024 \end{bmatrix} \times6$	$\begin{bmatrix} 1\times1, 512 \\ 3\times3, 512, C{=}32 \\ 1\times1, 1024 \end{bmatrix} \times6$
conv5	7×7	$\begin{bmatrix} 1\times1, 512 \\ 3\times3, 512 \\ 1\times1, 2048 \end{bmatrix} \times3$	$\begin{bmatrix} 1\times1, 1024 \\ 3\times3, 1024, C{=}32 \\ 1\times1, 2048 \end{bmatrix} \times3$
	1×1	global average pool 1000-d fc, softmax	global average pool 1000-d fc, softmax
# params.		$\mathbf{25.5}\times10^6$	$\mathbf{25.0}\times10^6$
FLOPs		$\mathbf{4.1}\times10^9$	$\mathbf{4.2}\times10^9$

175 billion weights: *2020 GPT-3 text model (GPT-4 ~**1.8 trillion weights**)*

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

General Strategy

Loss function $\mathcal{L}$ ✓

Neural network f_θ ✓

Parameters θ ✓

Opt. Parameters θ^*

Data $\mathbf{x}$

Data distribution $p(\mathbf{x})$

- Define an optimisation target (loss function)
- Choose a non-linear, expressive, parametrised function (e.g. a neural network)
- Use training data to optimise parameters, then apply to new examples

$$\theta^* = \text{argmin}_\theta \, \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})} \left[\mathcal{L}(f_\theta(\mathbf{x}), \mathbf{x}) \right]$$

How do networks learn?

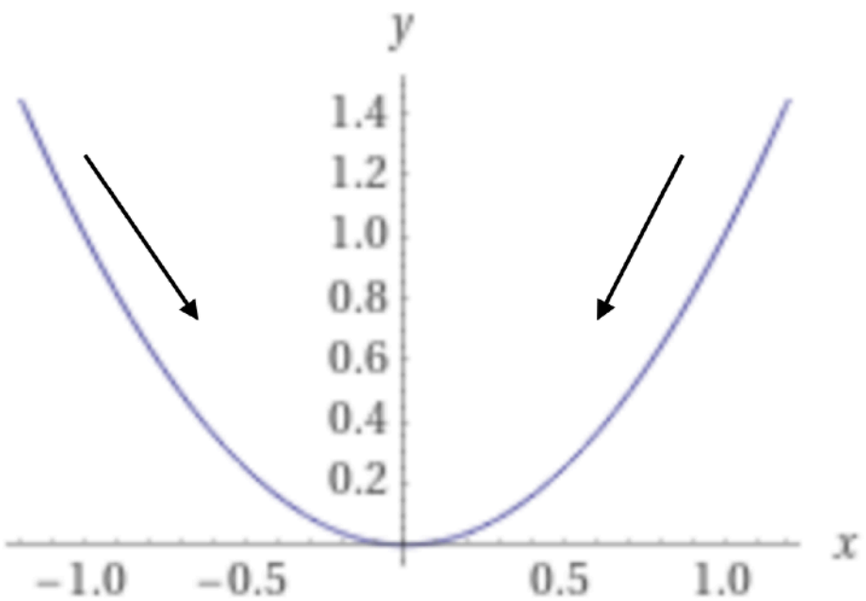
- *Backpropagation + Gradient descent*
- Important: Loss function needs to be differentiable
  - (Or find a differentiable approximation)
- Pass input (x_1, x_2, …) to networks
- From output calculate loss function
  Find gradient of loss function with respect to weights
- Use gradient to find new weights

$$\theta_{t+1} = \theta_t - \eta \frac{\partial \mathcal{L}}{\partial \theta_t} = \theta_t - \eta \nabla \mathcal{L}$$

Learning rate

- In practice, handled by optimise algorithm (e.g. Adam)

How do networks learn?



$$f(x) = x^2$$

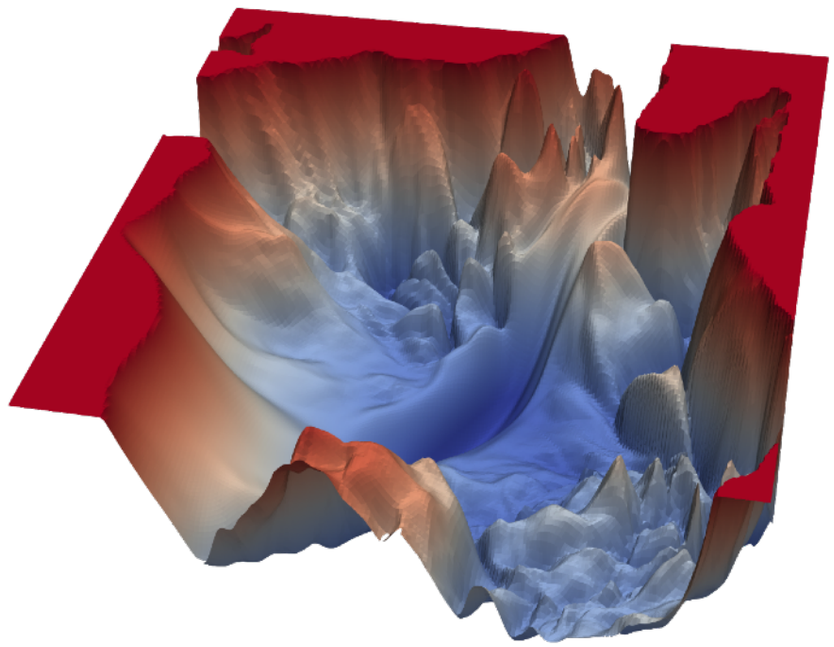
$$f'(x) = 2x$$

$x < 0 \implies -f'(x) > 0$ “Go right”

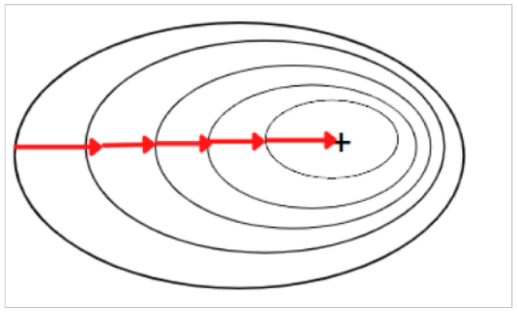
$x > 0 \implies -f'(x) < 0$ “Go left”

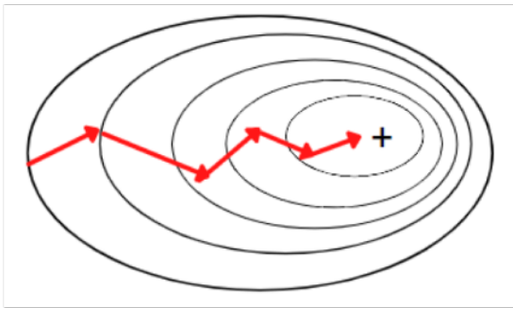
Batches and Epochs

- The loss depends on O(1k-1b) parameters
- To minimize it these parameters need to be adjusted
- For large networks the loss landscape can get very complicated with many local minima



- Better convergence
  - Multiple passes (epochs) over training data
  - Split training data in batches with a minimization call and model update after each batch

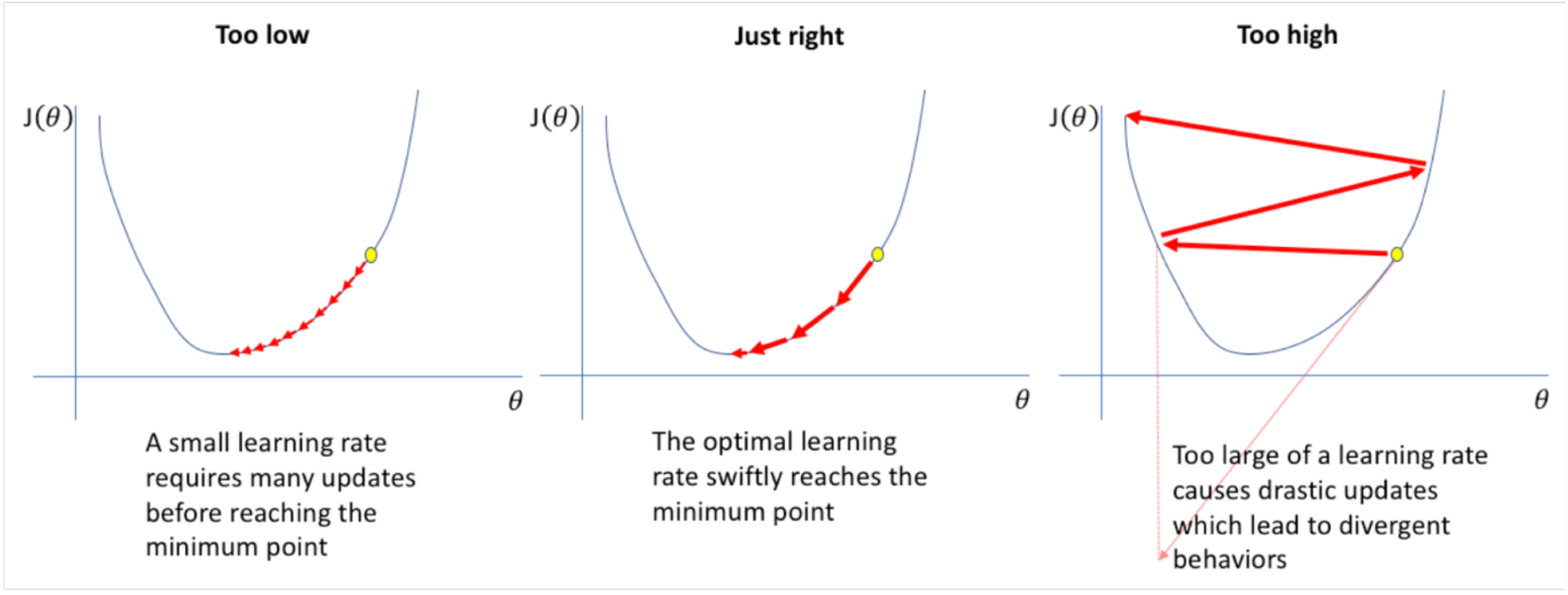




Learning Rate

- Many popular minimization algorithms have a tunable parameter called Learning rate α
- Should be chosen such that the training smoothly converges

$$\theta \to \theta - \alpha \frac{\partial L(\theta)}{\partial \theta}$$



https://www.jeremyjordan.me/nn-learning-rate/

Adam

$$m_w^{(t+1)} \leftarrow \beta_1 m_w^{(t)} + (1 - \beta_1) \nabla_w L^{(t)}$$

$$v_w^{(t+1)} \leftarrow \beta_2 v_w^{(t)} + (1 - \beta_2) \left(\nabla_w L^{(t)} \right)^2$$

$$\hat{m}_w = \frac{m_w^{(t+1)}}{1 - \beta_1^t}$$

$$\hat{v}_w = \frac{v_w^{(t+1)}}{1 - \beta_2^t}$$

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \frac{\hat{m}_w}{\sqrt{\hat{v}_w} + \epsilon}$$

Maintain history of previous changes: momentum

Exponential moving average of gradient and gradient squares

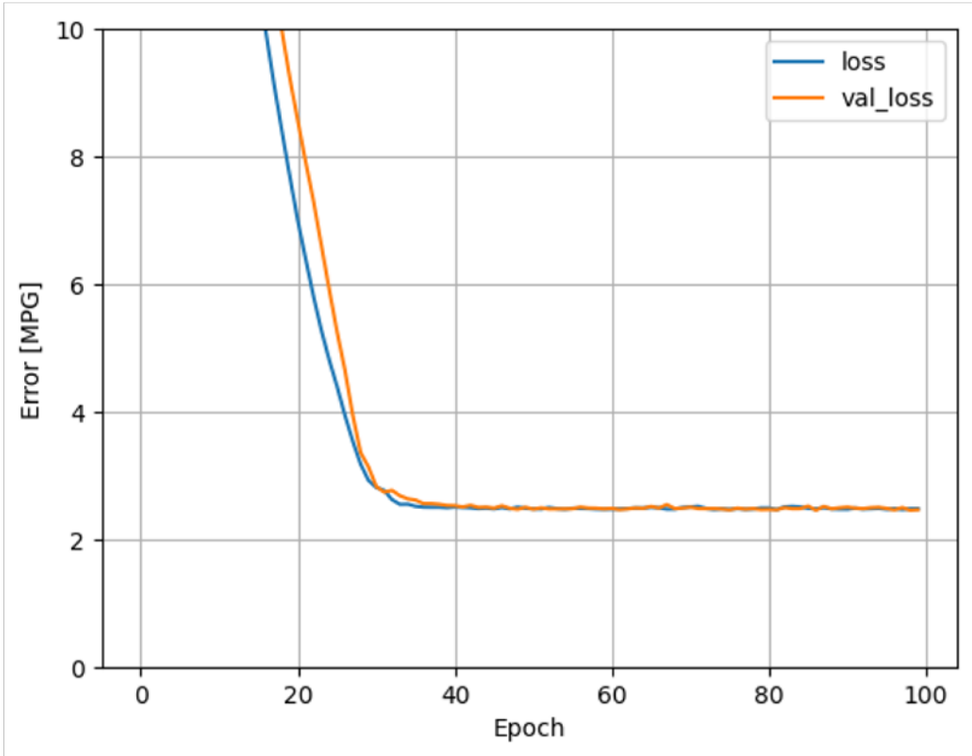
https://arxiv.org/abs/1412.6980

The loss curve

- Once the training is done it is time to analyze the training process and the performance of the model

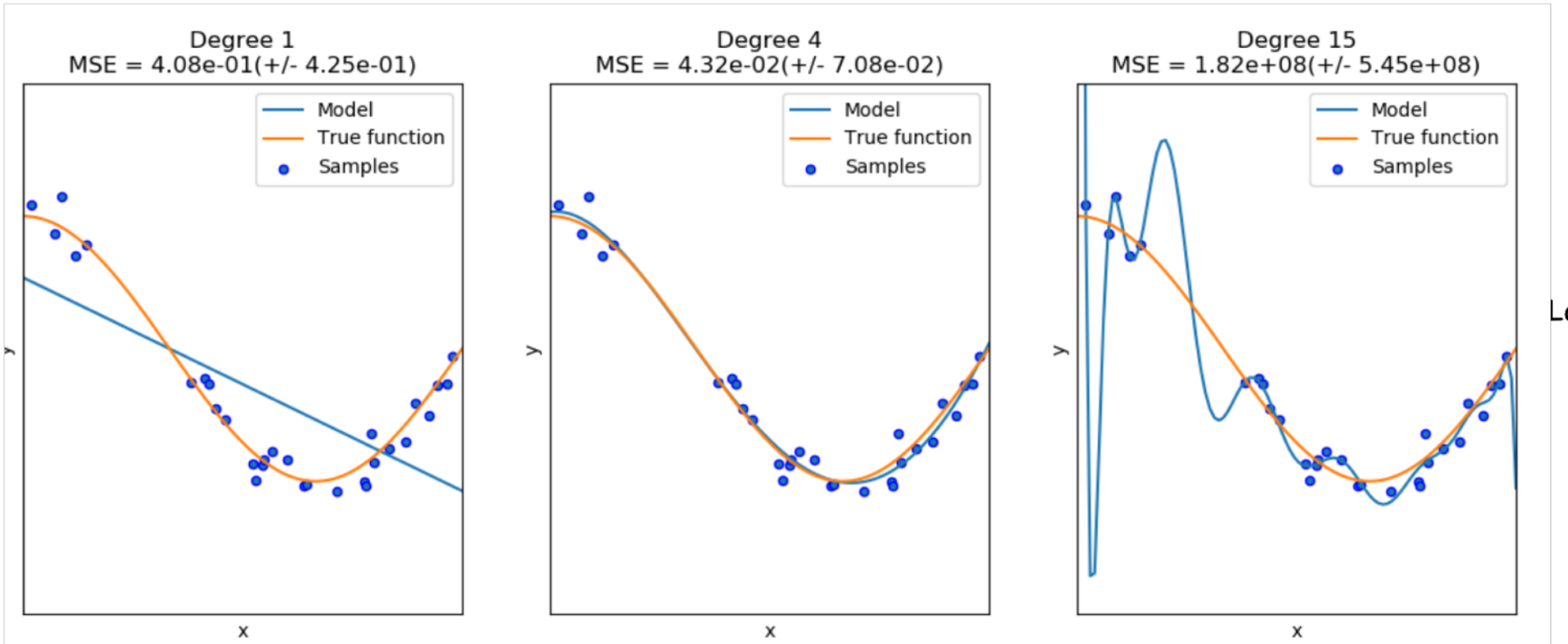
- For the training process it is a good idea to look at the loss as a function of the number of epochs – for the training data and validation data

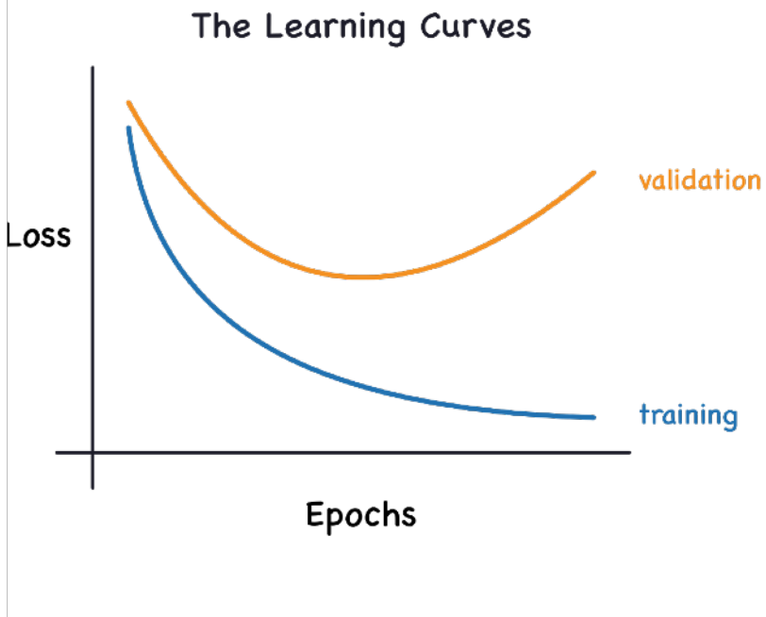
- Ideally the training converges with similar loss values for the validation and training data



Overfitting

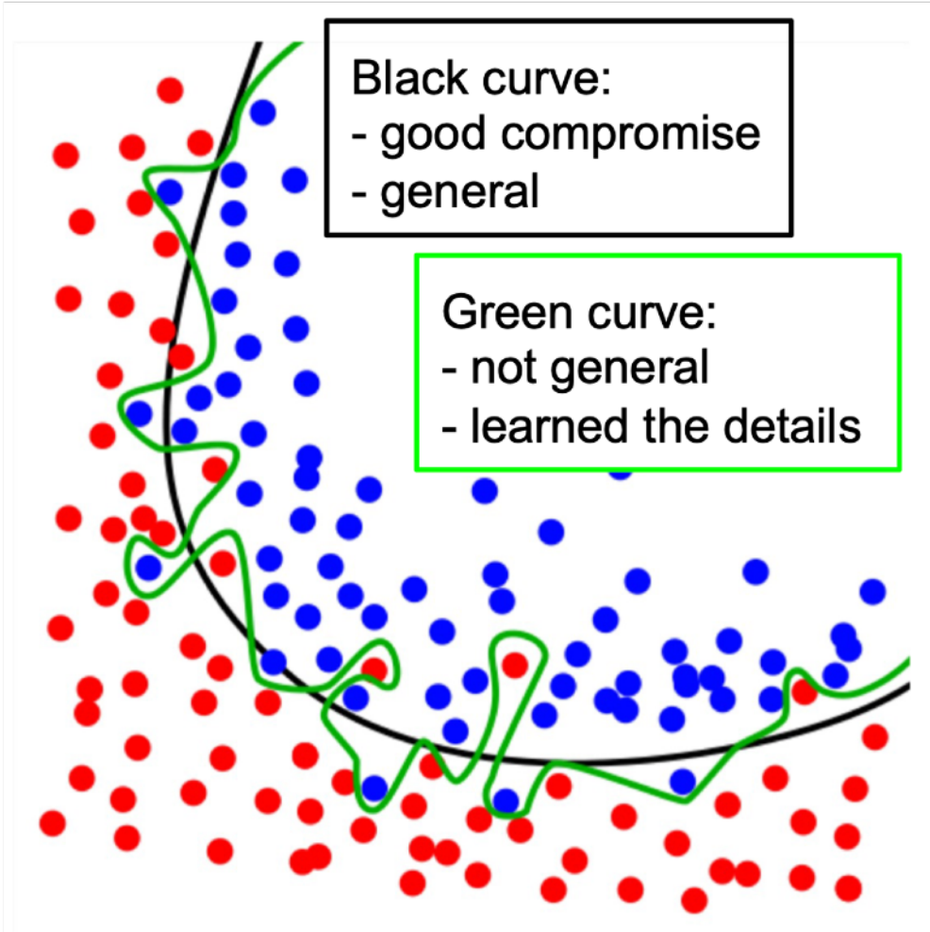
- If the model has too many parameters it can overfit the data
- This leads to a worse performance on data with different statistical fluctuations than the training data
- -> the training and validation losses diverge





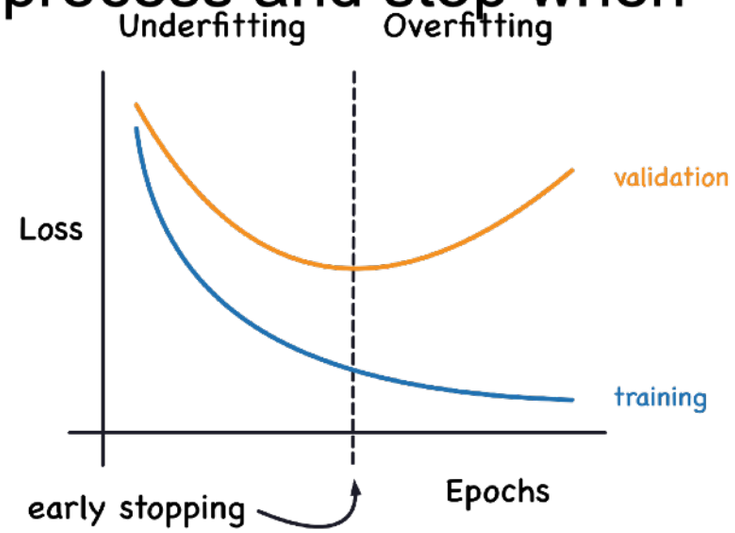
Overfitting

- Also an issue in classification tasks (which are after all a form of regression of discrete values)
- Overfitting can be interpreted as remembering the training samples
- We can see that the performance would change if the dots move around even a bit



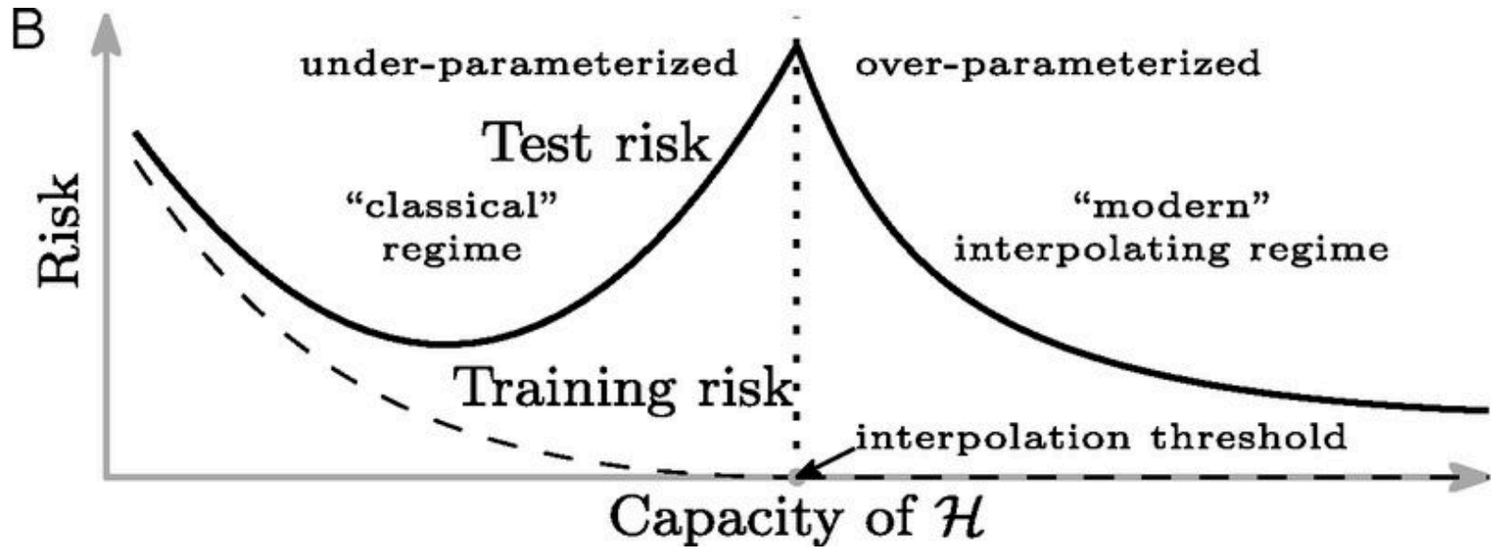
Overfitting - Mitigation

- There are multiple ways to mitigate overfitting such as dropout, regularization or early stopping
- Dropout:
  - Add layers that randomly discard a fraction of inputs in training phase
- Early stopping:
  - Monitor training and validation loss during the training process and stop when they diverge
- Regularisation:
  - Add penalty for large weight values in loss function



Side note: Overfitting

Reconciling modern machine-learning practice and the classical bias–variance trade-off (PNAS, Belkin et al)



- Recent observation in computer science
  - Extremely high capacity does not guarantee overfitting
- Even more recent:
  - Grokking: Sudden generalisation of a trained model
- Active research into foundations, does not stop us from using it

General Strategy

Loss function $\mathcal{L}$ ✓

Neural network f_θ ✓

Parameters θ ✓

Opt. Parameters θ^* ✓

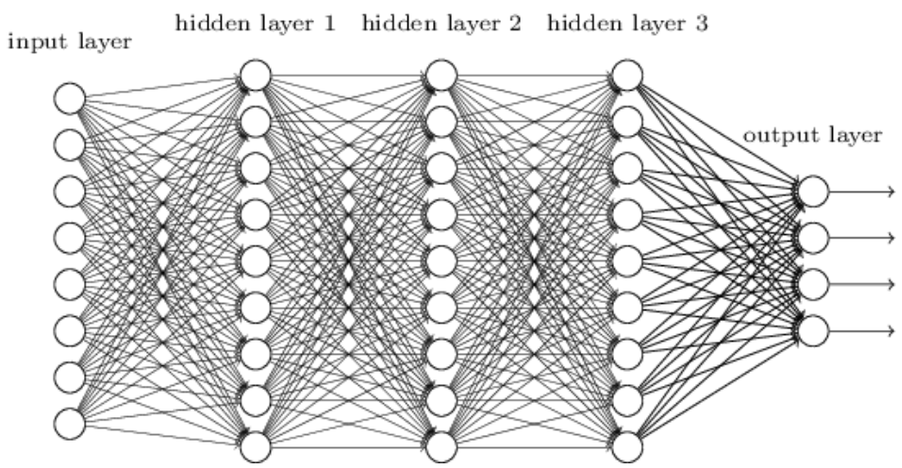
Data $\mathbf{x}$

Data distribution $p(\mathbf{x})$

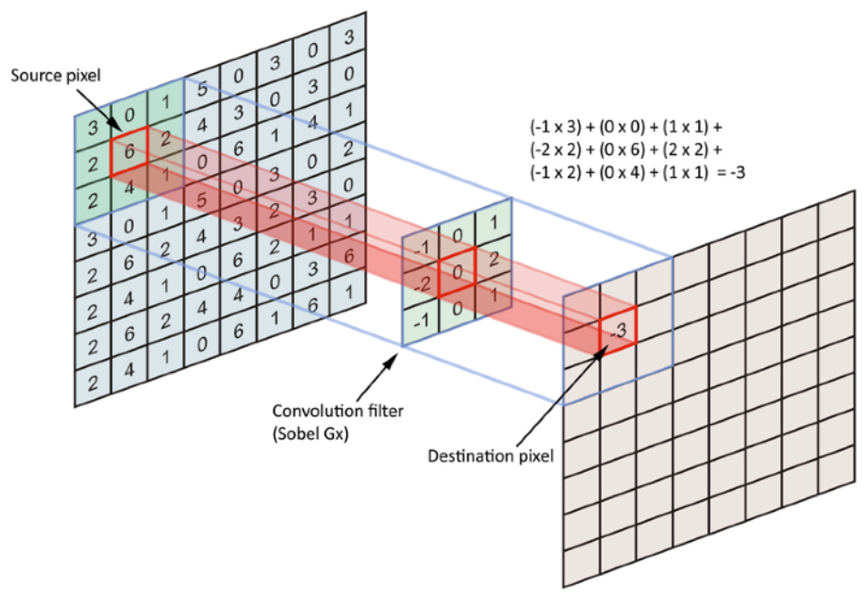
$$\theta^* = \text{argmin}_\theta \, \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})} \left[\mathcal{L}(f_\theta(\mathbf{x}), \mathbf{x}) \right]$$

Data Representation

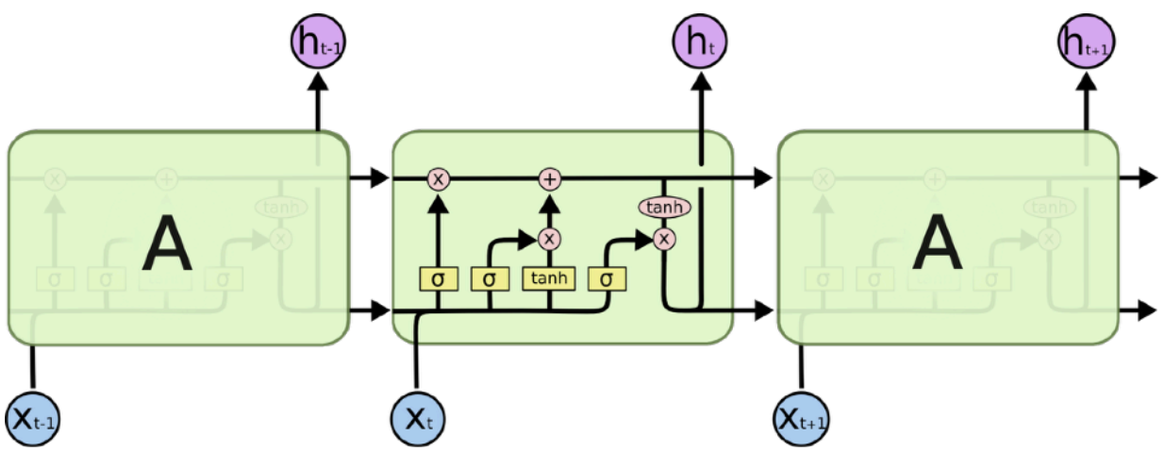
High-level/no structure: Fully Connected



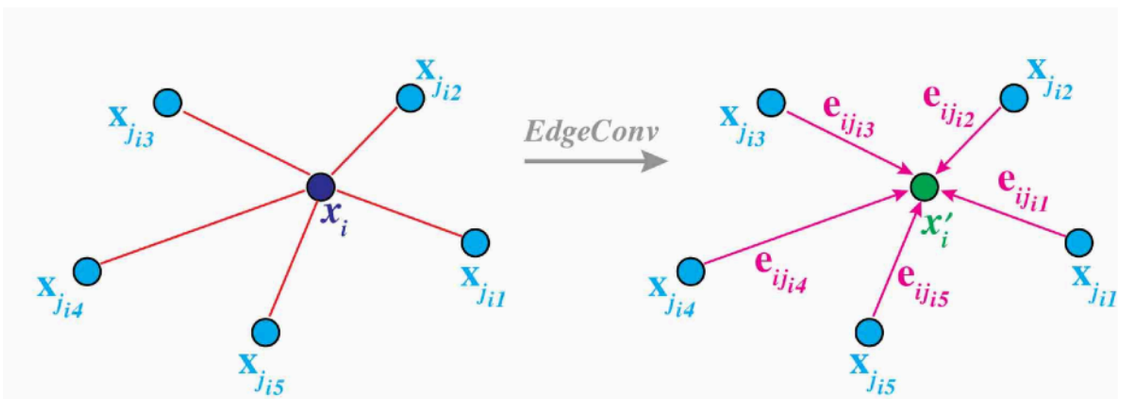
Regular grid: Convolution



Sequence/Time Series: Recurrent



Point cloud: Sets & Graphs



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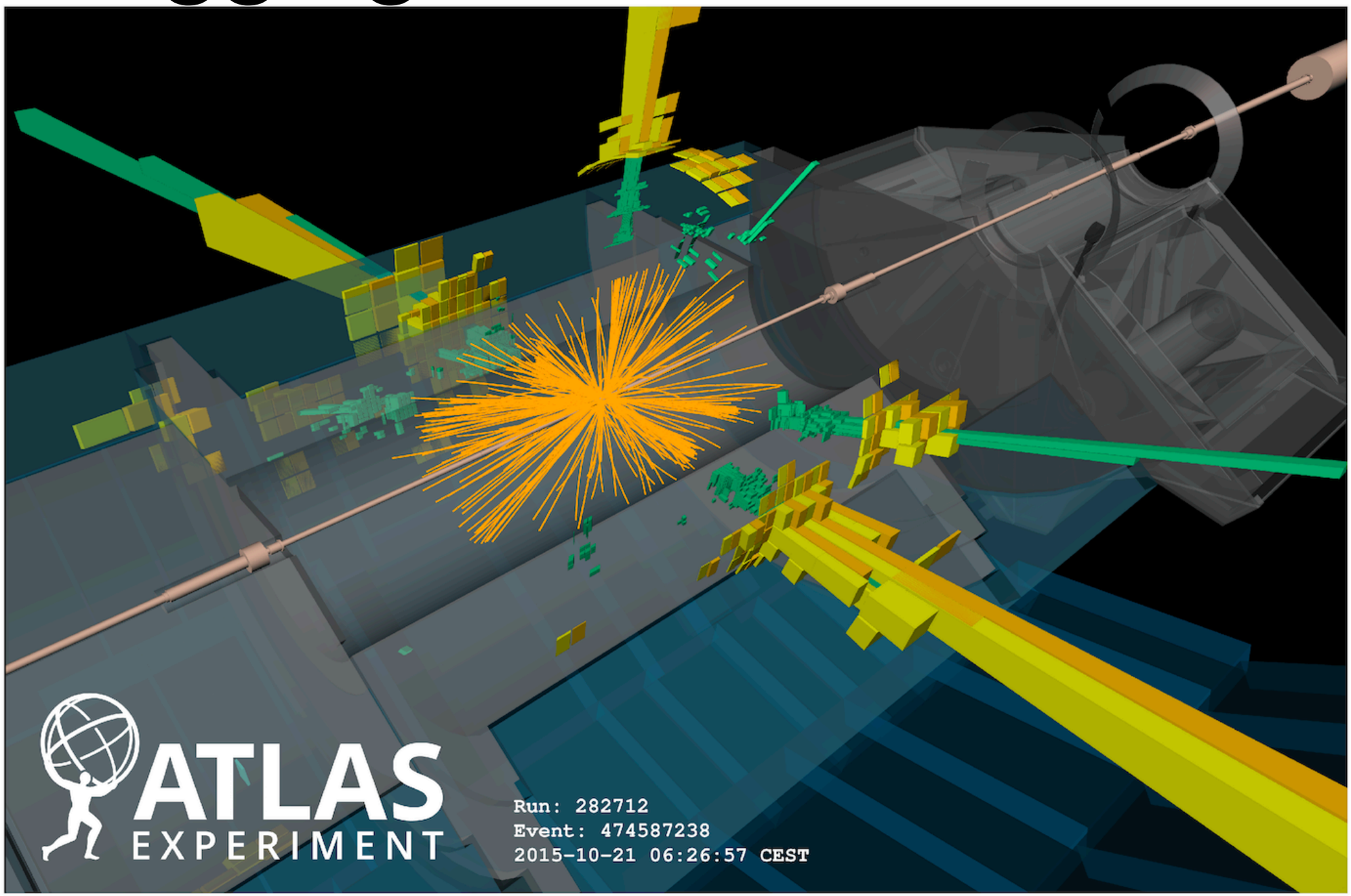
Summary so far

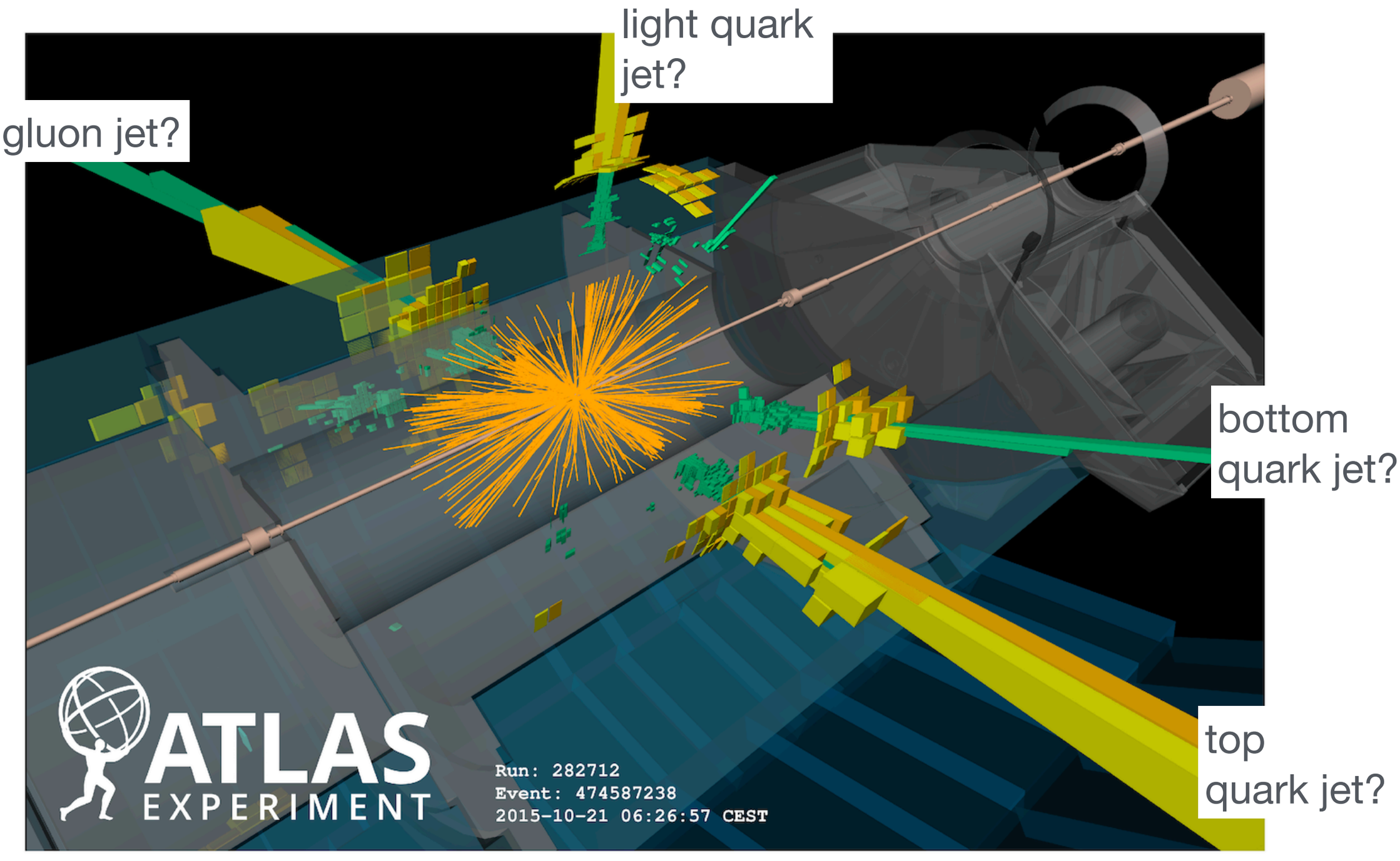
- Key idea of deep learning:
  - Define a optimisation target and use an expressive function (neural network) to minimise it using gradient descent

- Let’s look at a typical problem in particle physics…

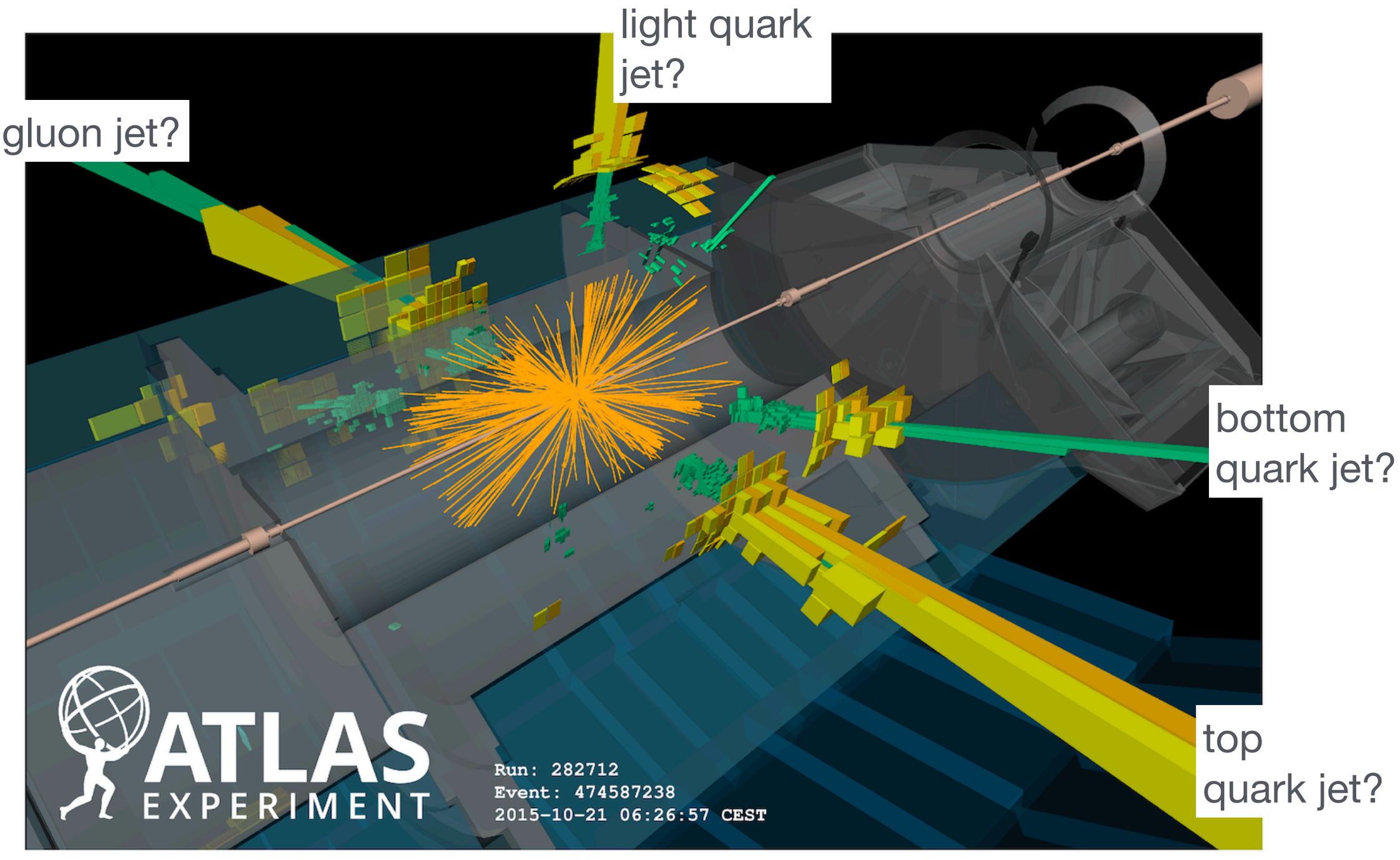
Jet Tagging



A jet is a
collimated shower of particles in the detector



We want to know
which particle produced a jet



How to build ML algorithms for complex, heterogenous data?

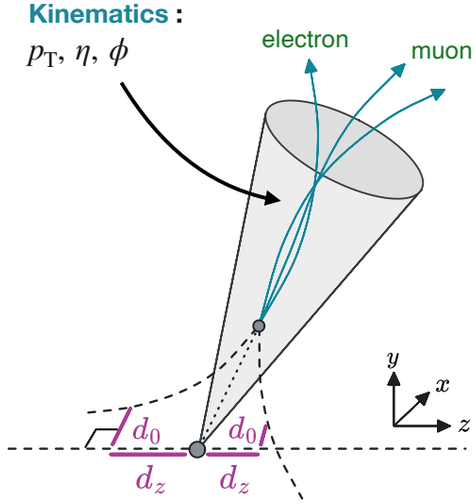
Data most naturally viewed as point cloud:

Each input (e.g. jet, event, ..) is a set of k-dimensional vectors (individual particles, hits, ..)

$$J_i = \{\vec{p_1}, \ldots, \vec{p_n}\}$$

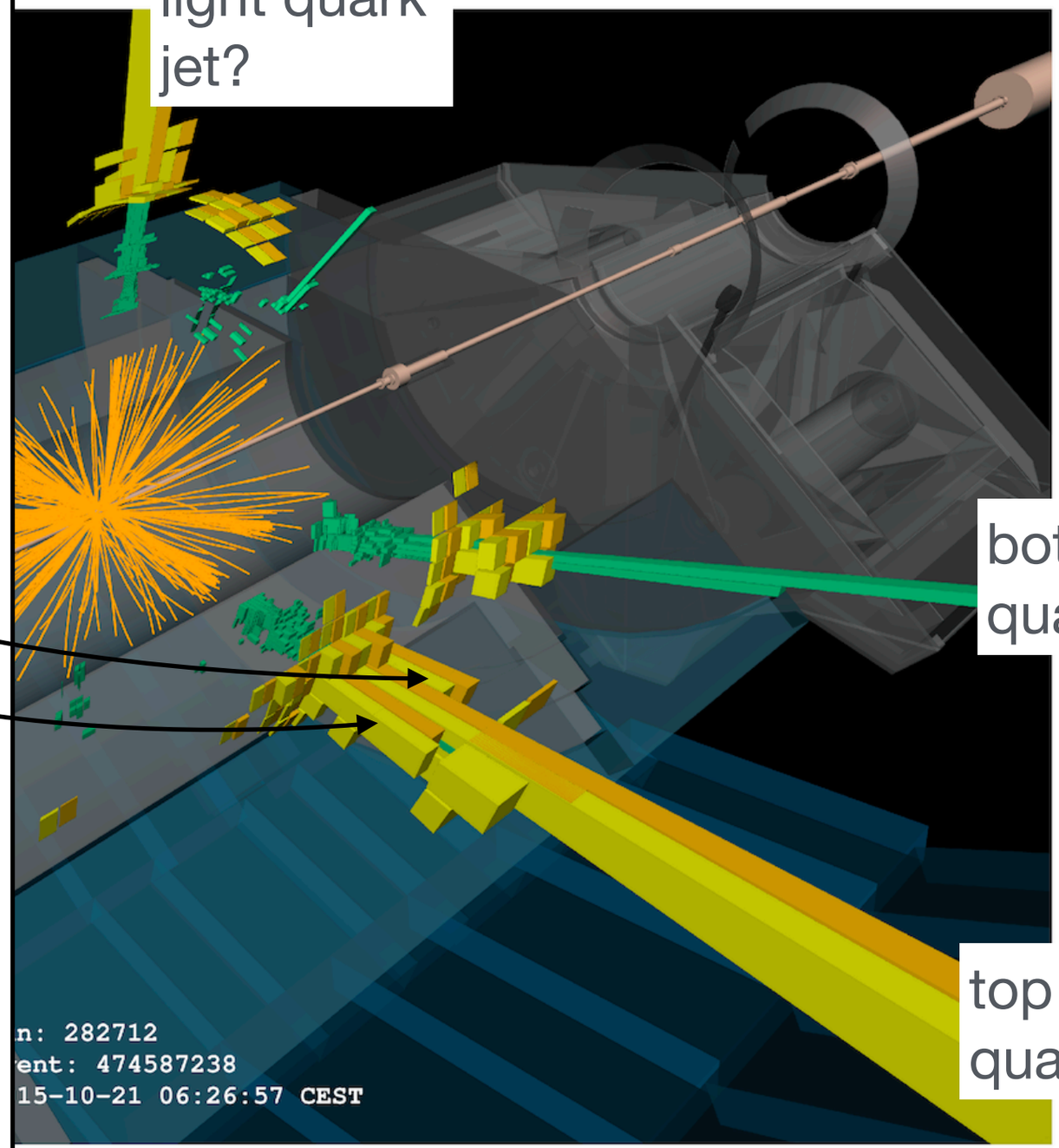
Particle-ID and charge :
`isElectron, isMuon, …`

Kinematics :
p_T, η, ϕ



Example per-particle features

Trajectory displacement :
d_0 : closest approach to PV in xy-plane
d_z : z position where d_0 is evaluated



light quark jet?

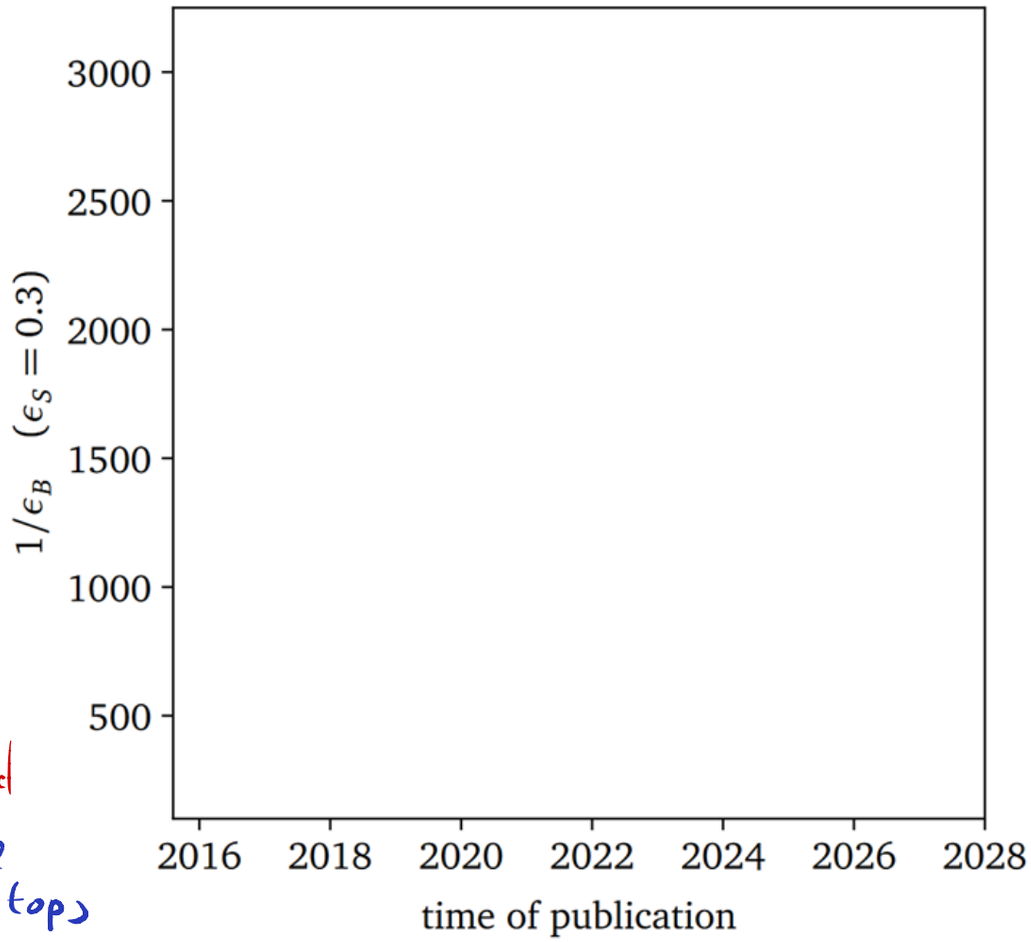
bottom quark jet?

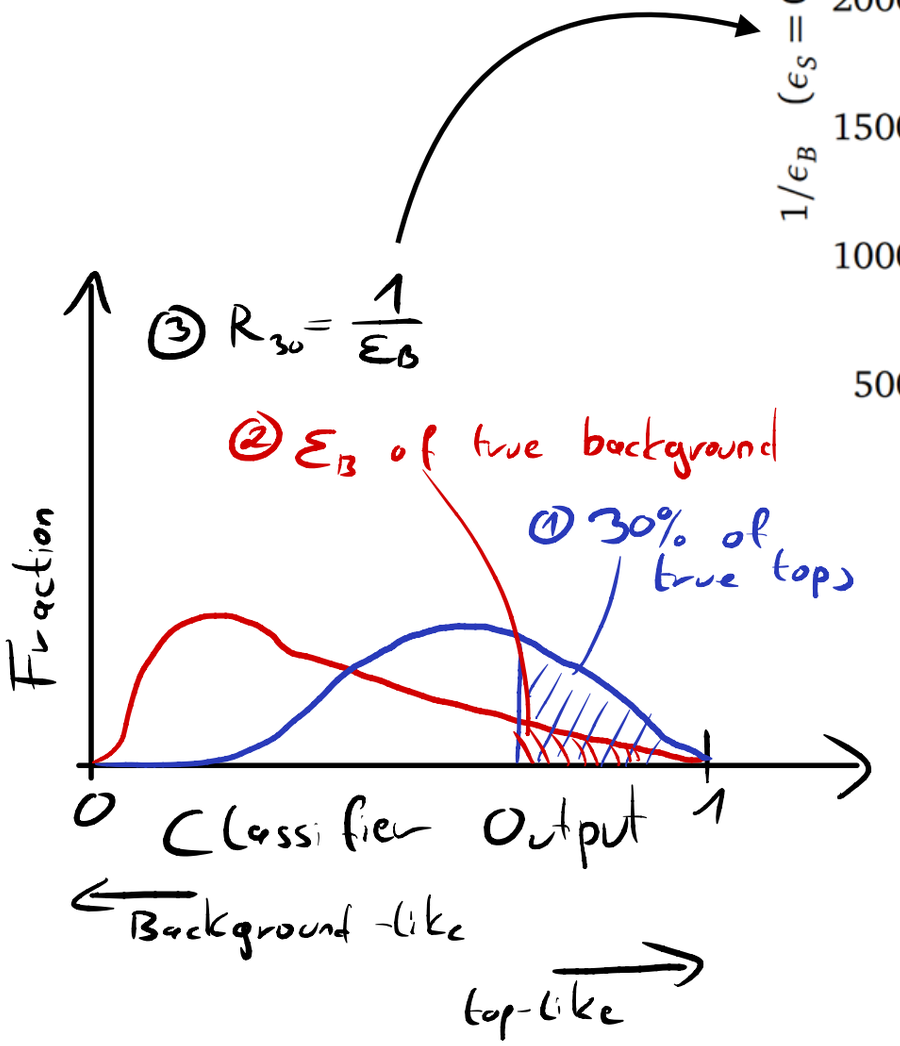
top quark jet?

1810.05165; **GK** et al 2312.00123

Top Quark Tagging

Public simulated*
benchmark dataset





GK, Plehn, et al 1902.09914

The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)[1], T. Plehn (ed)[2], A. Butter[2], K. Cranmer[3], D. Debnath[4], B. M. Dillon[5], M. Fairbairn[6], D. A. Faroughy[5], W. Fedorko[7], C. Gay[7], L. Gouskos[8], J. F. Kamenik[5,9], P. T. Komiske[10], S. Leiss[1], A. Lister[7], S. Macaluso[3,4], E. M. Metodiev[10], L. Moore[11], B. Nachman,[12,13], K. Nordström[14,15], J. Pearkes[7], H. Qu[8], Y. Rath[16], M. Rieger[16], D. Shih[4], J. M. Thompson[2], and S. Varma[6]

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15 LPTHE, CNRS & Sorbonne Université, Paris, France
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July 24, 2019

Abstract

Based on the established task of identifying boosted, hadronically decaying top quarks, we compare a wide range of modern machine learning approaches. Unlike most established methods they rely on low-level input, for instance calorimeter output. While their network architectures are vastly different, their performance is comparatively similar. In general, we find that these new approaches are extremely powerful and great fun.

* techniques are also applied to collider data

Landscape Dataset

- Open dataset for the development of better tagging algorithms for particle physics
- 2 million simulated examples
- Input: momentum sorted list of 200 particles/jet with 3 features/particle (p_X, p_Y, p_Z)
- Perfect class labels: top jet or light quark/gluon jet
- Supervised learning problem

SciPost Physics Submission

The Machine Learning Landscape of Top Taggers

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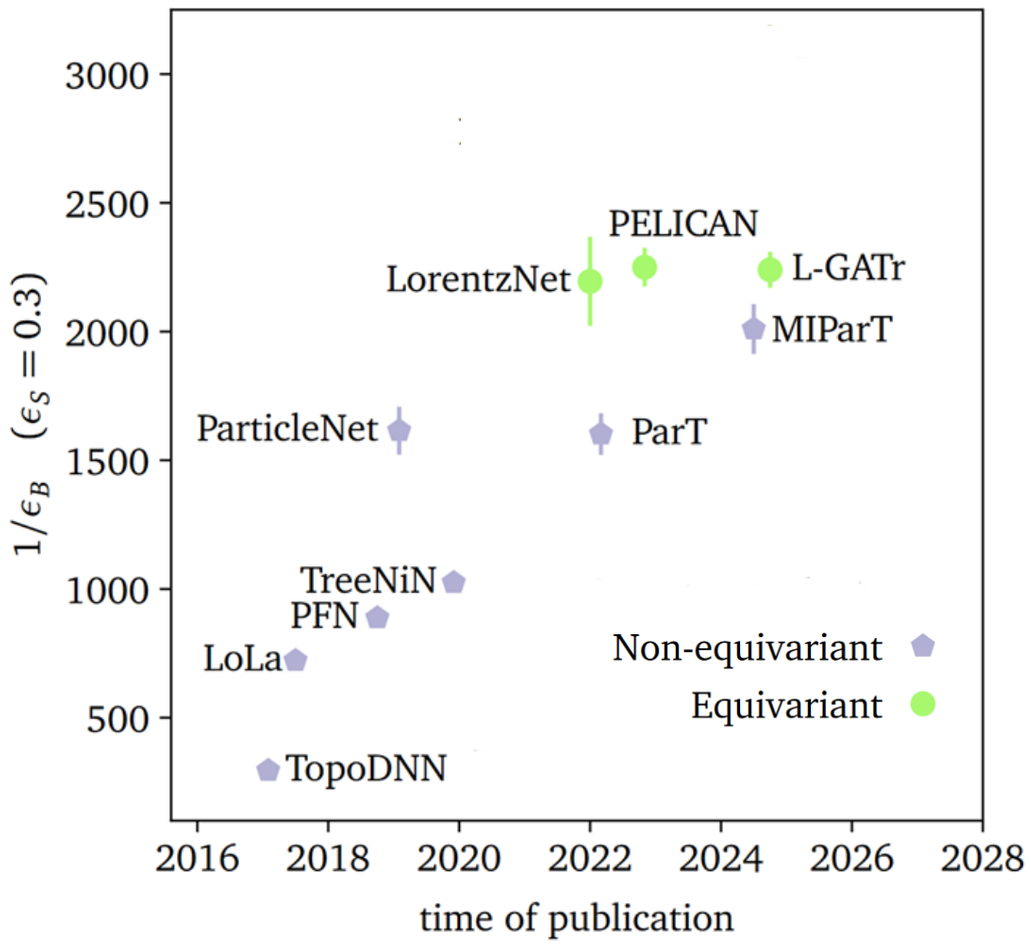
GK, Plehn, et al 1902.09914

Top Quark Tagging

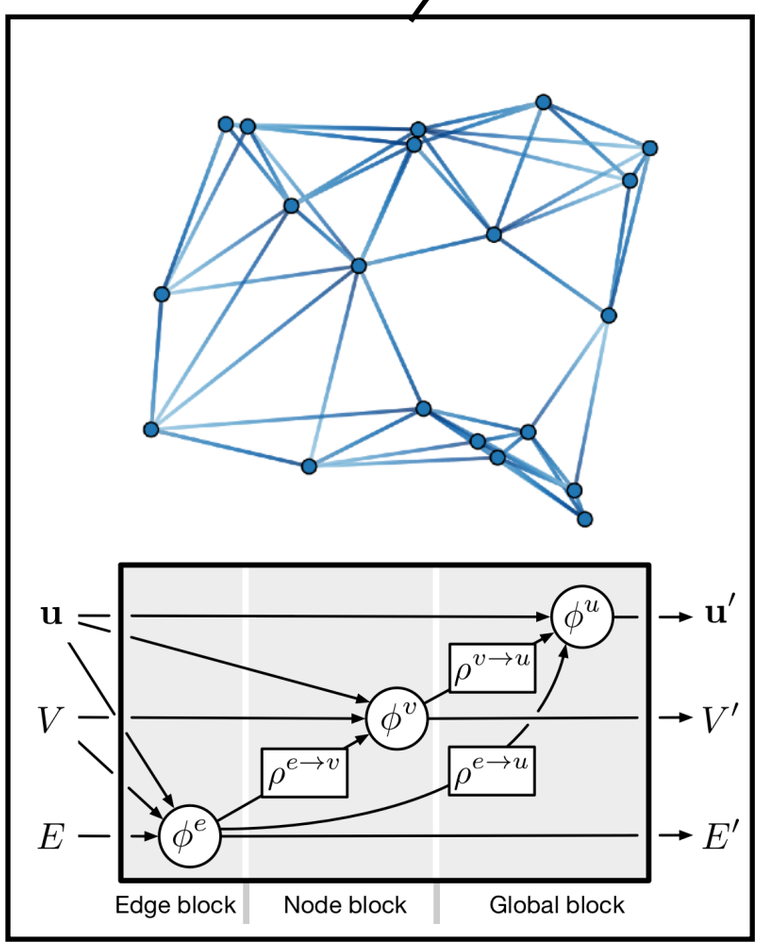


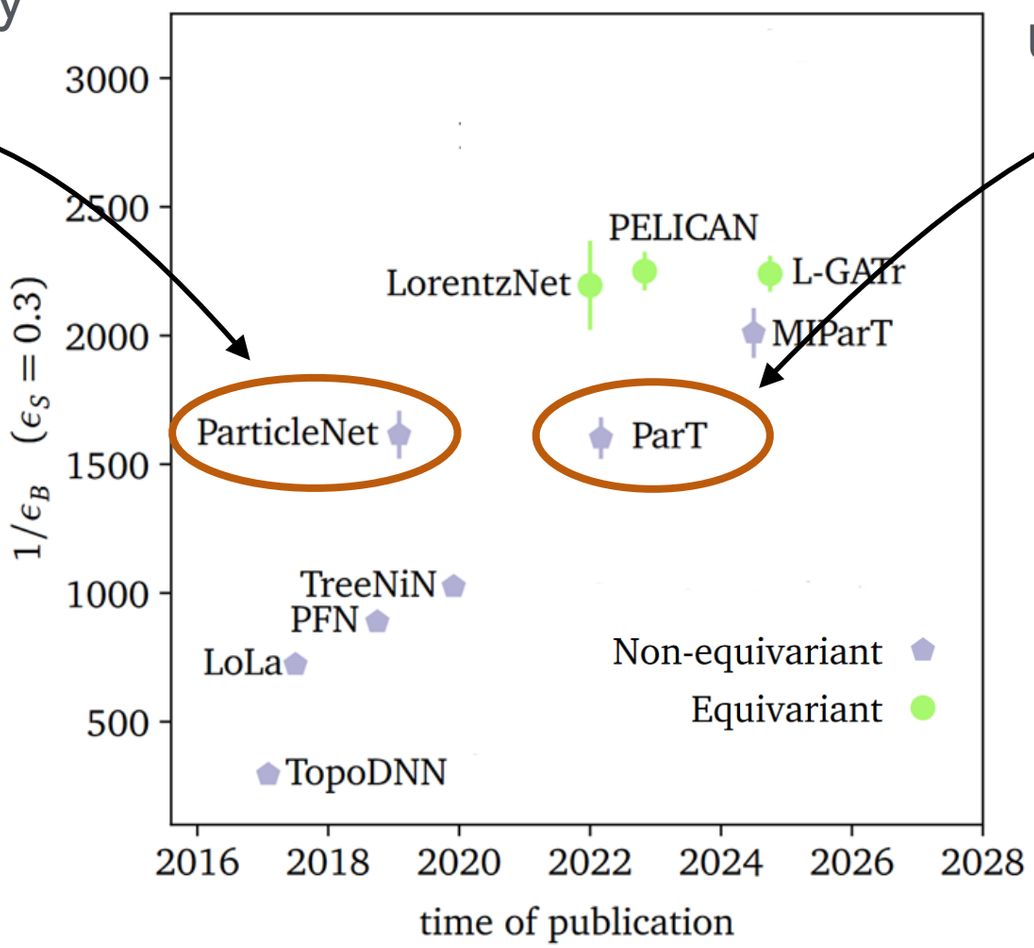
(*Subset of methods, graph from V Breso at ML4Jets)

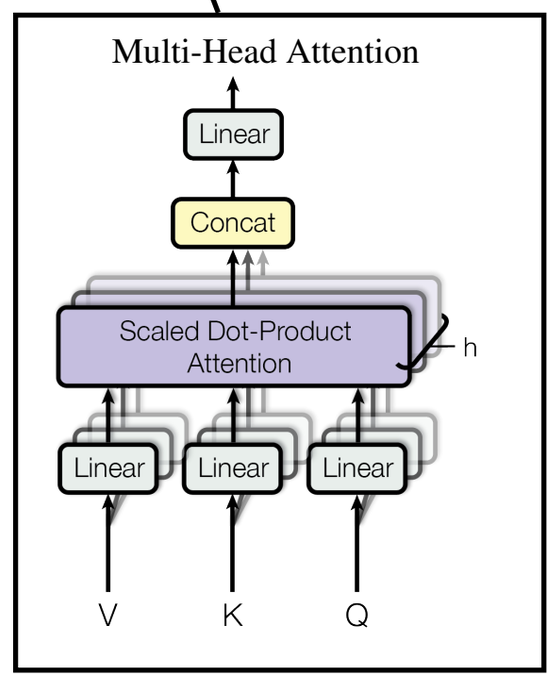
Top Quark Tagging

View data as
graph based on geometry
& use message passing

Learn relations from data
using attention



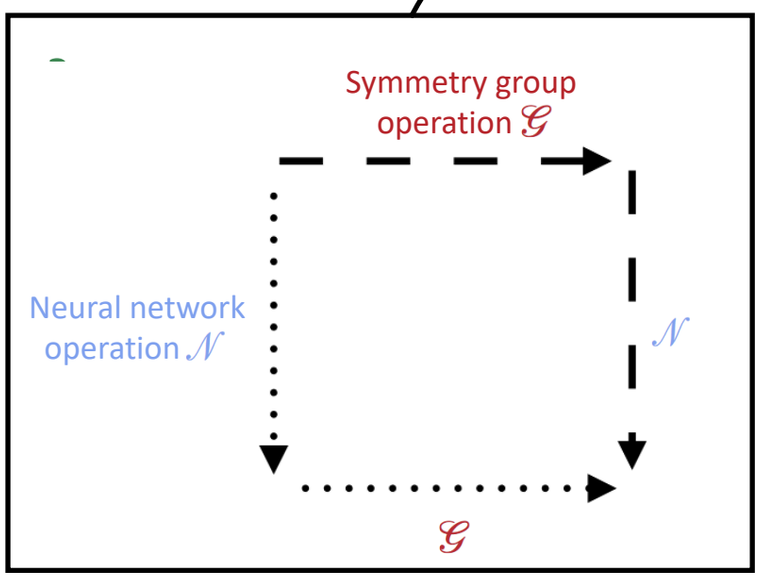


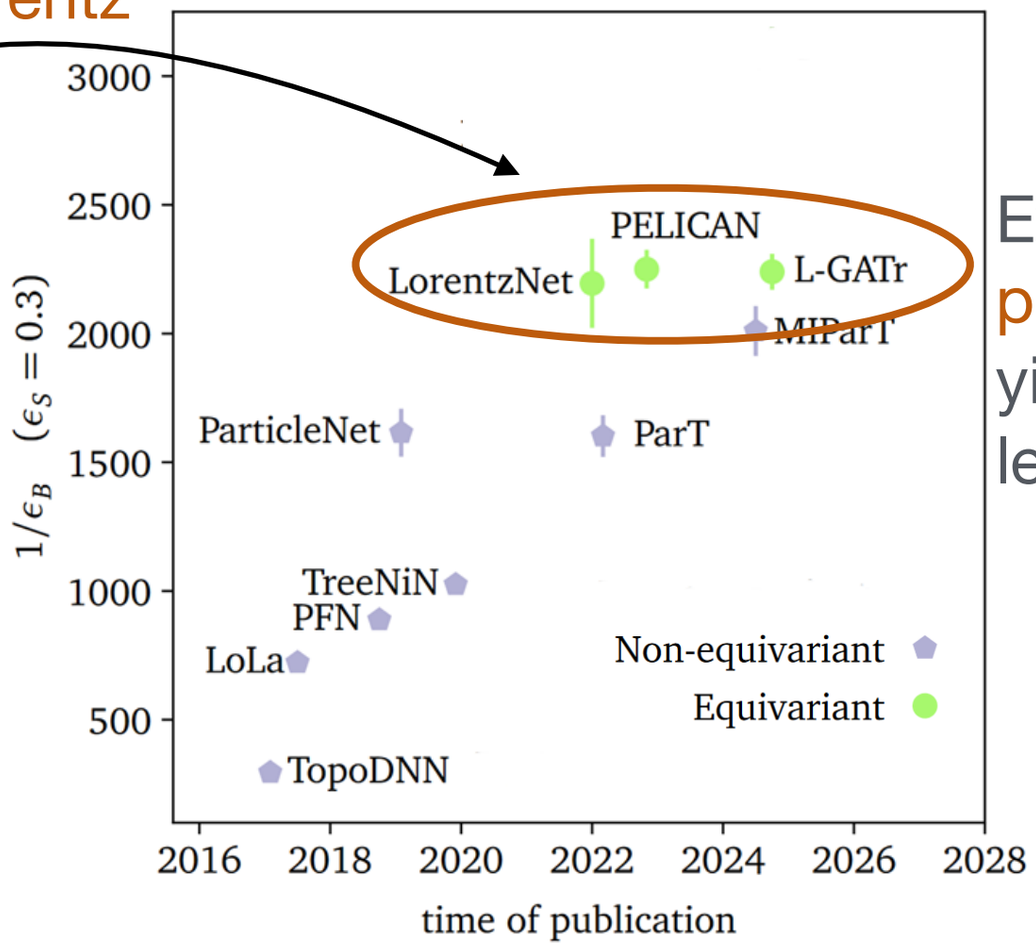


Qu, Gouskos 1902.08570; Qu et al 2202.03772; Gong et al 2201.08187; Shlomi et al 2007.13681;
Bogatskiy et al 2211.00454;

Top Quark Tagging

Constrain functions to be equivariant under the Lorentz group

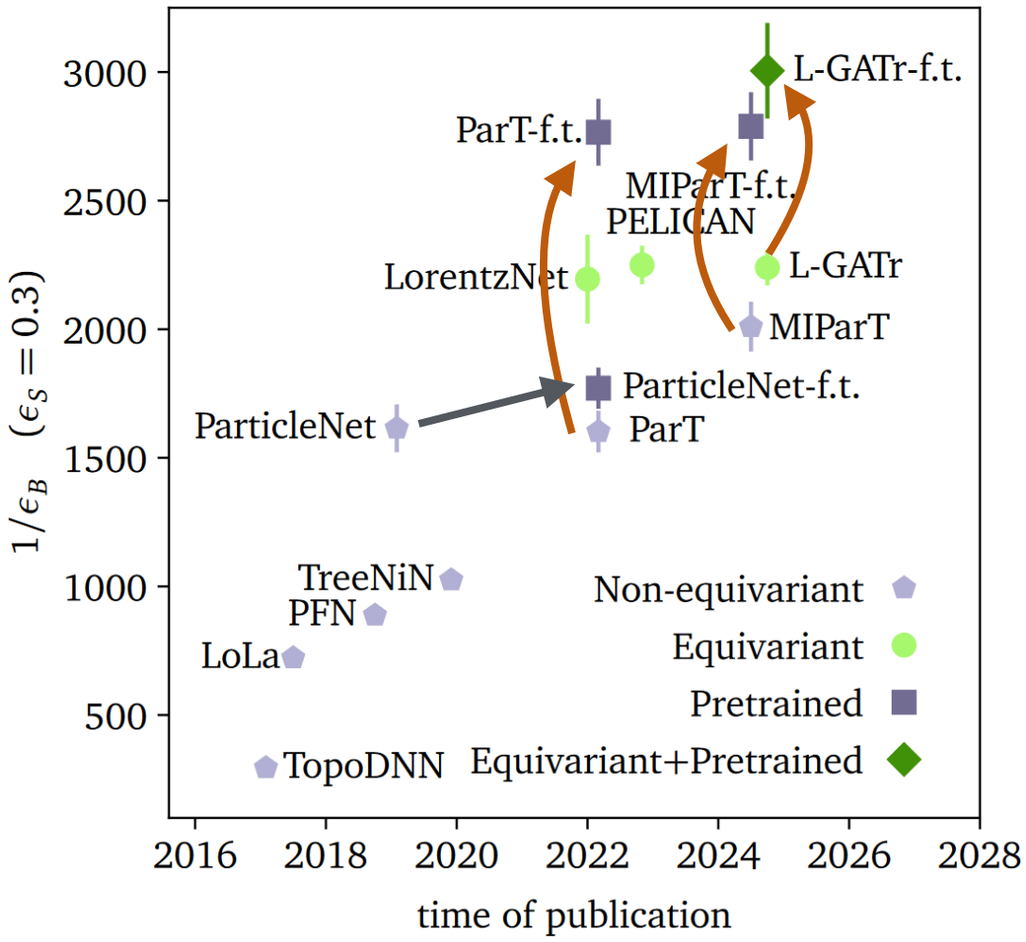




Explicitly injecting physics knowledge yields more efficient learning

Qu, Gouskos 1902.08570; Qu et al 2202.03772; Gong et al 2201.08187; Shlomi et al 2007.13681; Bogatskiy et al 2211.00454; Brehmer et al 2411.00446

Top Quark Tagging



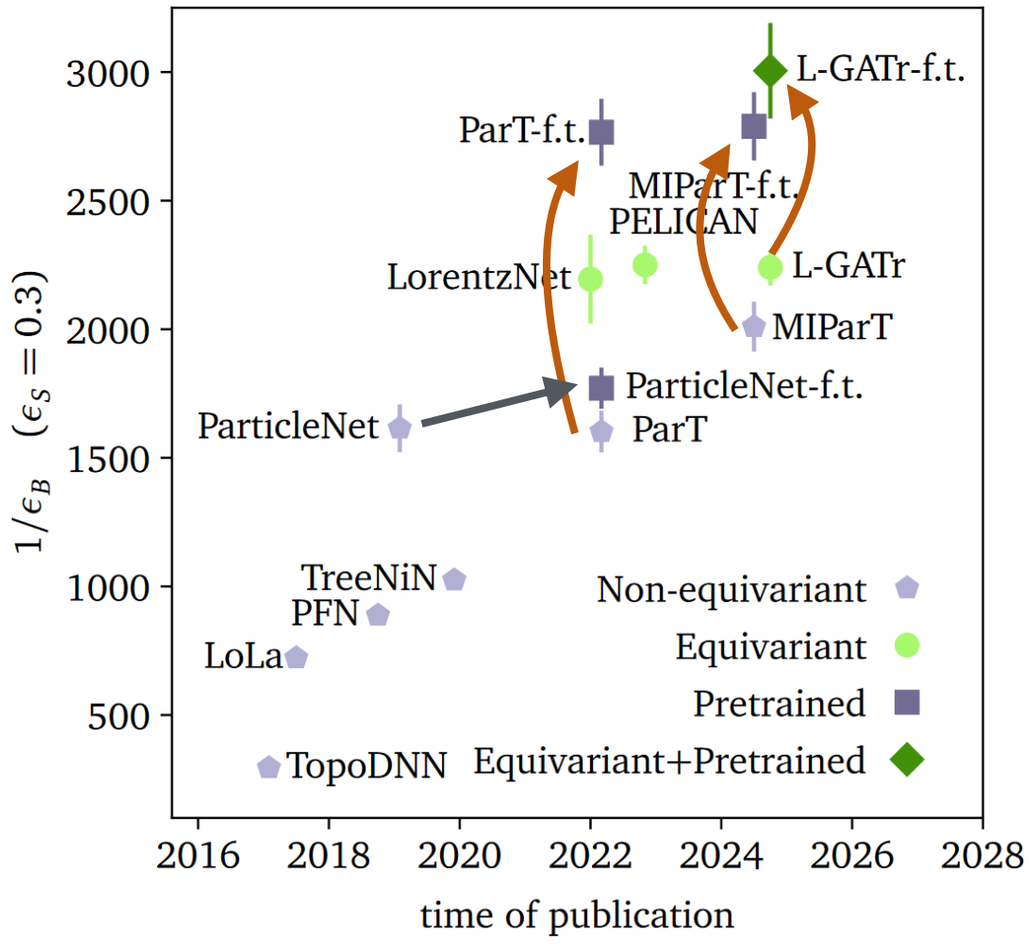
Fine tuning:
Pre-train on one dataset and recycle weights for training on new data

Yields substantial boost in performance (for transformer-based models)

Can combine with equivariance

Top Quark Tagging

- Usefulness of open benchmark data
- Good representation of data pays off
- Transformers + physics rules
- Boost by fine-tuning across datsets



Important issues on application side

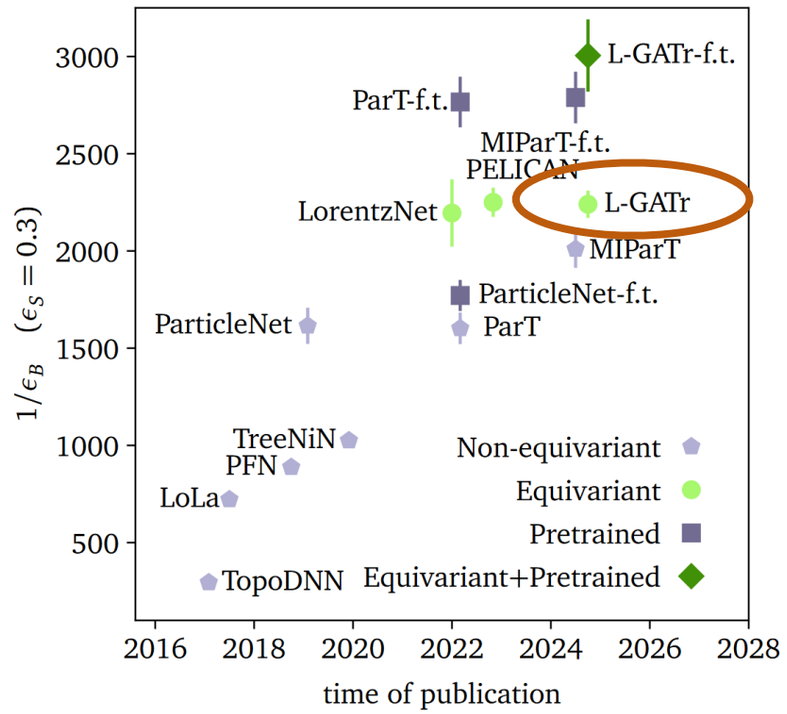
- Domain shift
- Calibrateable
- Compute cost

Modern tagging algorithms are widely used in searches for new particles

End of Part I.

Bonus Material

Symmetries



Reminder: Space-time described by Lorentz group (rotations, boosts)

$$(t, x, y, z) \mapsto t^2 - x^2 - y^2 - z^2$$

Equivariance:

$$\text{L-GATr}\Big(\Lambda(x)\Big) = \Lambda\Big(\text{L-GATr}(x)\Big)$$

Multivector:

$$x = x^S\, 1 + x^V_\mu\, \gamma^\mu + x^B_{\mu\nu}\, \sigma^{\mu\nu} + x^A_\mu\, \gamma^\mu\gamma^5 + x^P\, \gamma^5$$

Scalar

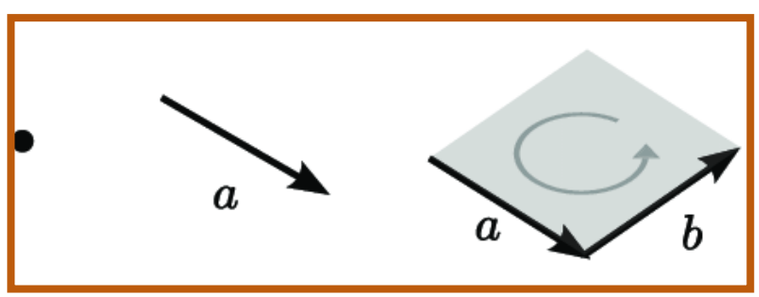
Vector

Bi-Vector

Axial-Vector

Pseudo-Scalar

"Grades" with well defined behaviour under Lorentz transformations



$$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$\gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \quad \gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

2411.00446

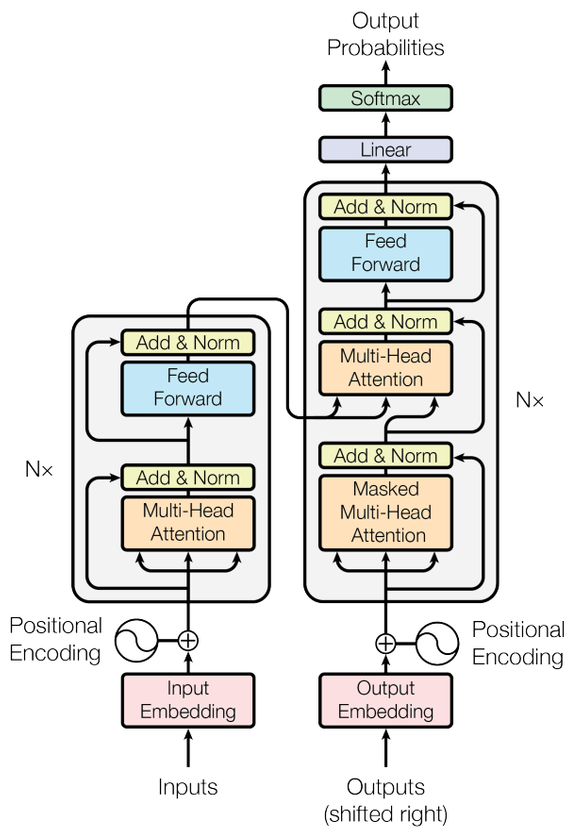
Symmetries

Sum over grades

Layer type	Transformer	L-GATr
Linear(x)	$vx + w$	$\sum_{k=0}^{4} v_k \langle x \rangle_k$
Attention$(q,k,v)_{ic}$	$\sum_{j=1}^{n_t} \mathrm{Softmax}_j \left(\sum_{c'=1}^{n_c} \frac{q_{ic'} k_{jc'}}{\sqrt{n_c}} \right) v_{jc}$	$\sum_{j=1}^{n_t} \mathrm{Softmax}_j \left(\sum_{c'=1}^{n_c} \frac{\langle q_{ic'}, k_{jc'} \rangle}{\sqrt{16 n_c}} \right) v_{jc}$
LayerNorm(x)	$x \left[\frac{1}{n_c} \sum_{c=1}^{n_c} x_c^2 + \epsilon \right]^{-1/2}$	$x \left[\frac{1}{n_c} \sum_{c=1}^{n_c} \sum_{k=0}^{4} \left\lvert \left\langle \langle x_c \rangle_k, \langle x_c \rangle_k \right\rangle \right\rvert + \epsilon \right]^{-1/2}$
Activation(x)	GELU(x)	GELU$(\langle x \rangle_0) x$
GP(x,y)	—	xy

Norm of inner product by grade

Inner product (requires some work but can compute Algebra-rules in advances)



$$x_\mu x^\mu = \eta_{\mu\nu} x^\mu x^\nu = (ct)^2 - \mathbf{x} \cdot \mathbf{x} \overset{\text{def}}{=} (c\tau)^2$$

$$\eta^{\mu\nu} = \eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

2411.00446

Classification

Cross Entropy?

$$-\frac{1}{N}\log(L) = -\frac{1}{N}\sum_{k}^{N}[y_k \cdot \log(\hat{y}(x_k)) + (1-y_k)\cdot\log(1-\hat{y}(x_k))]$$

- Note:

$$y_k \cdot \log\big(\hat{y}(x_k)\big) + (1-y_k)\cdot\log\big(1-\hat{y}(x_k)\big) = \sum_i q_i \log(p_i)$$

- Now remember entropy

$$\text{entropy} = \int p(x)\log\big(p(x)\big)dx$$

$$\text{cross-entropy} = \int q(x)\log\big(p(x)\big)dx$$

Gibbs inequality:
Cross entropy is minimal if
p=q

For multiple classes: Categorical cross entropy

Multiple classes

- For more than 2 classes it is usually a good idea to use **One-Hot-Encoding**

  -> For m classes the output is a m-dimensional vector with components

  $\hat{y}_c(x_k) \in [0,1]$

- One neuron per class in output layer
- All outputs should sum to one
- Loss function: Extension of cross entropy to multiple classes: **Categorical cross entropy**

Label Encoding

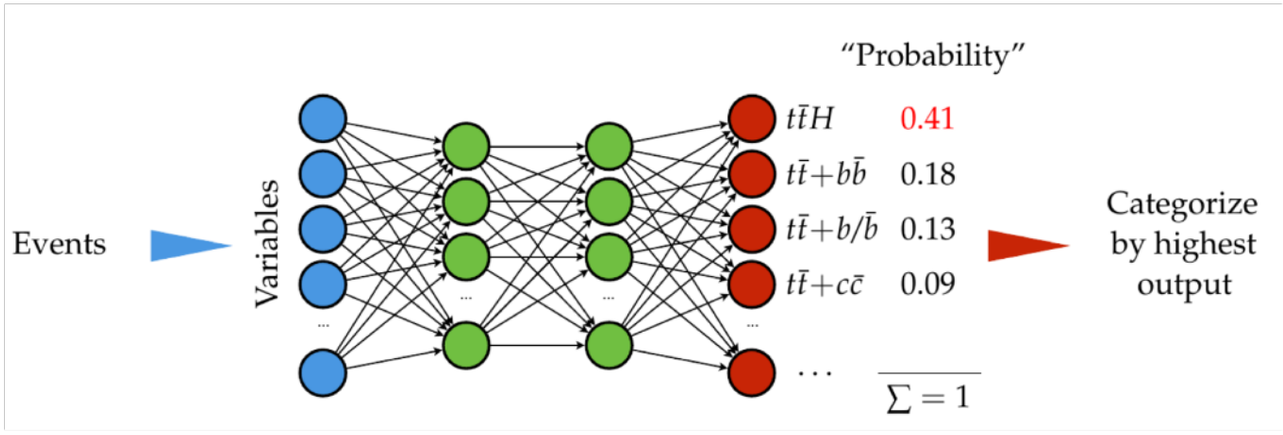
Food Name	Categorical #	Calories
Apple	1	95
Chicken	2	231
Broccoli	3	50

→

One Hot Encoding

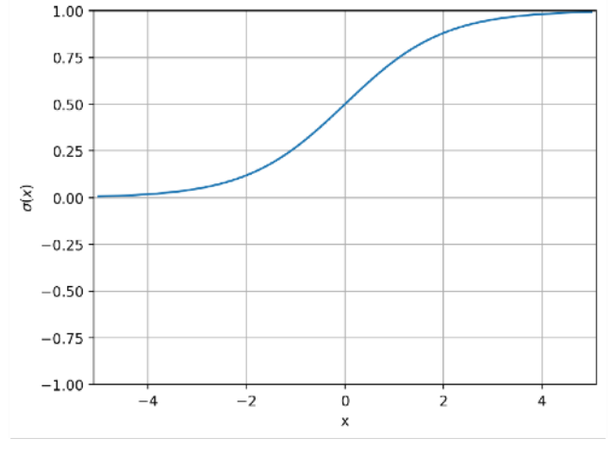
Apple	Chicken	Broccoli	Calories
1	0	0	95
0	1	0	231
0	0	1	50

https://medium.com/@michaeldelsole/



Activation functions for Classification

- Need activations in the output layer that allow probability interpretation:
  - $\hat{y}(x_k) \in [0,1]$
  - $\sum_{classes} \hat{y}(x_k) = 1$



- Binary classification:
  - Only 1 output node needed
  - Activation: Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

- Multiclassification:
  - One output node per class i
  - Softmax activation:

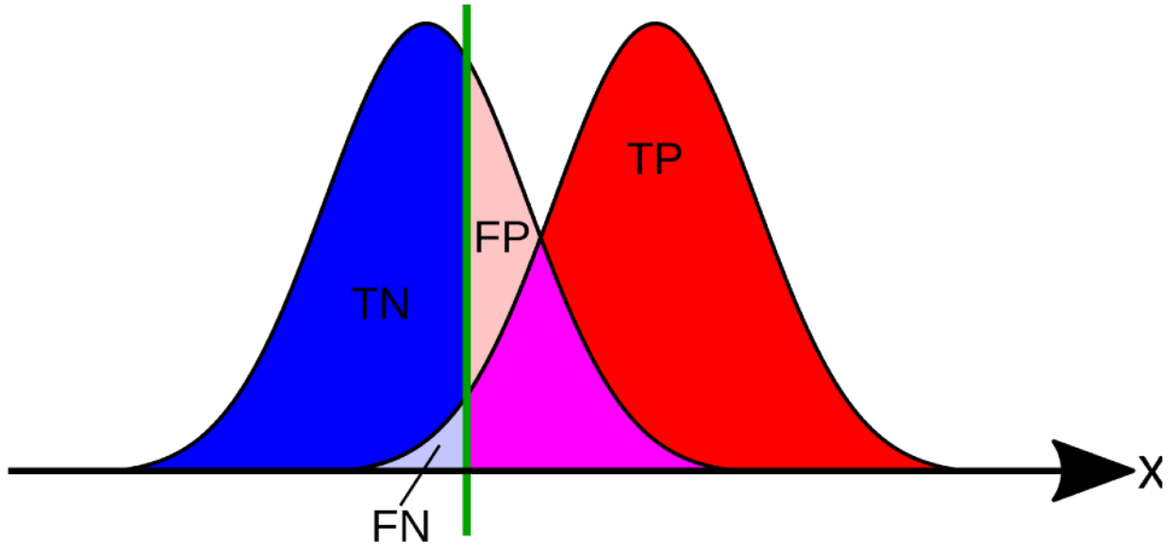
$$\sigma(x) = \frac{e^{x_i}}{\sum_j^{classes} e^{x_j}}$$

Binary Classification Outputs

- The NN outputs a score for belonging to class „signal“ (high value) or class „background“ (low value)

- Often you need to make a decision based on this score -> Choose a threshold

- Key quantities:
  - True Positives (TP)
  - False Positives (FP)
  - True Negatives (TN)
  - False Negatives (FN)



- Purity/Precision = TP/(TP+FP): How pure is the sample predicted as signal?

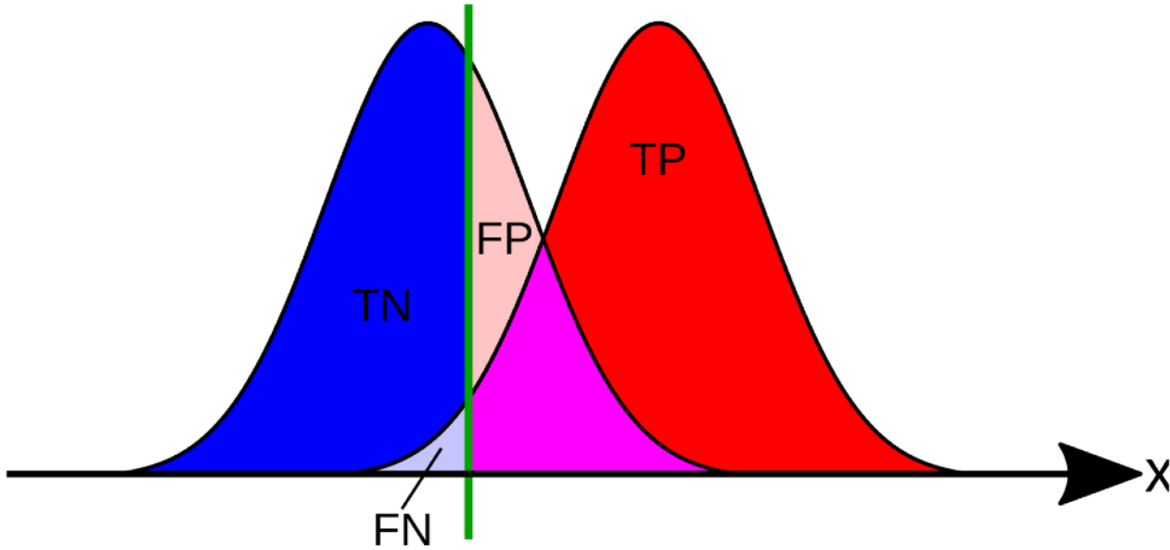
- True Positive Rate/Sensitivity/Efficiency/Recall = TP/(TP+FN): What fraction of the signal is classified correctly?

- False Positive Rate = FP/(FP +TN)

- Accuracy = (TP+TN)/(TP+FP+TN+FN): What fraction of all data is classified correctly?

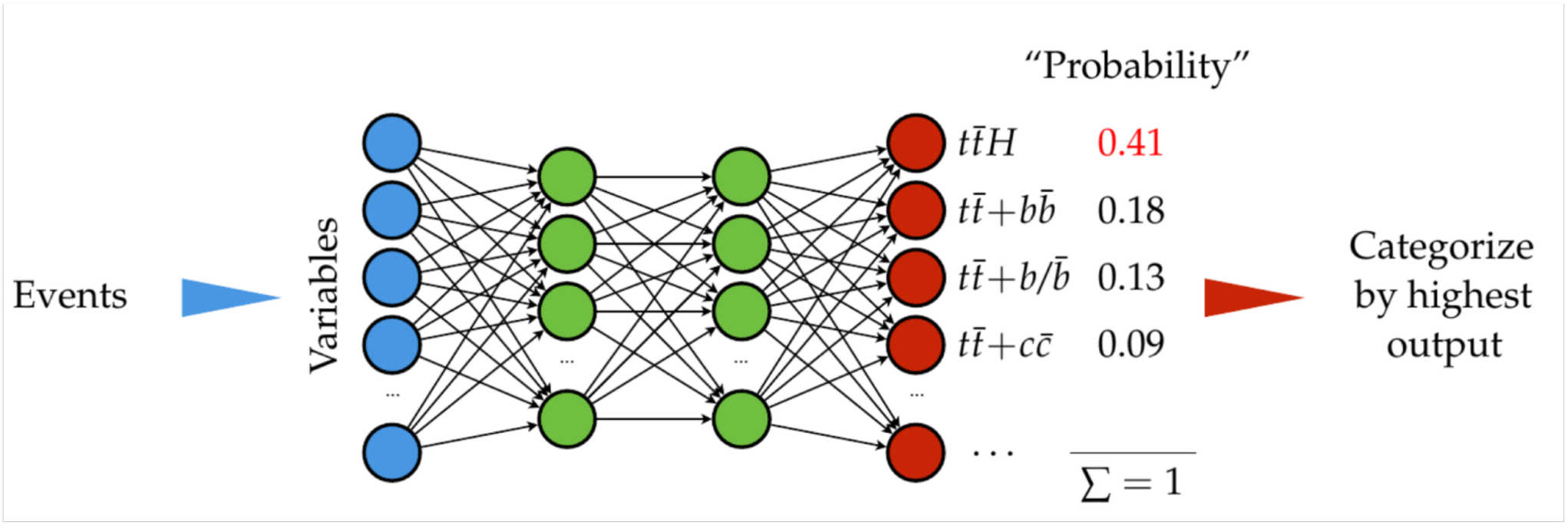
Choosing a threshold

- Which threshold to choose?
- Depends on your problem:
  - Think about what questions you want to answer
  - The cost of being wrong
- Do you need a high purity? (“We need to be sure that all animals we tag as harmless are actually harmless!“)
- Do you need a high Efficiency? („We need to detect as many positive Covid cases as possible“)



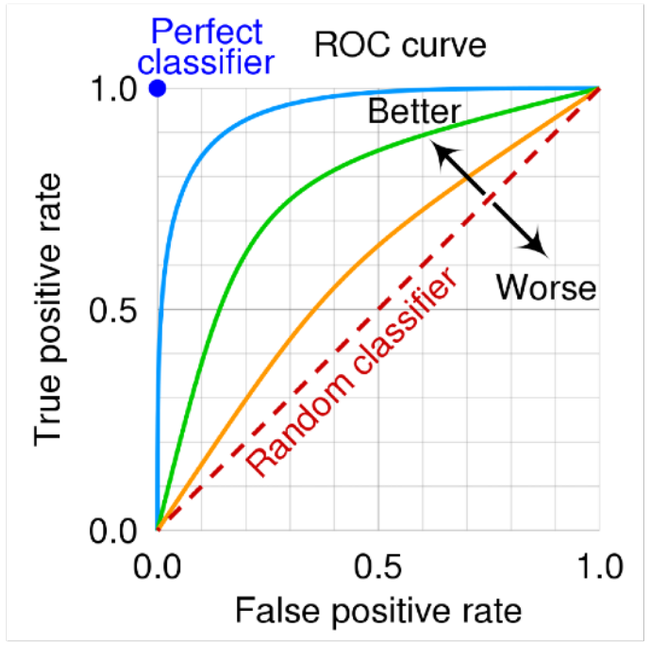
Multiclassification

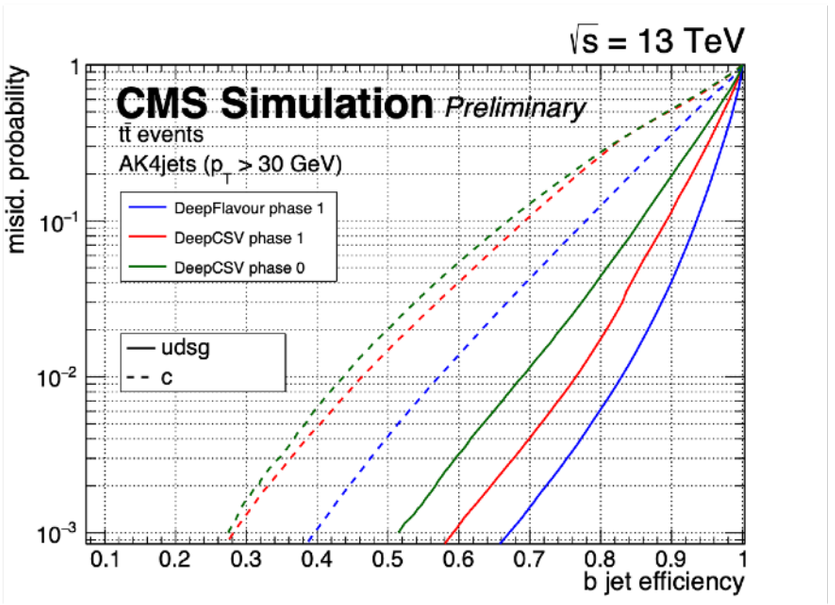
- In multiclassification we have one output neuron for each class
- If we use softmax as final activation function, the values of each output neuron sum to 1 and can be interpreted as probability
- Common approach: Classify a sample according to the neuron with the highest output value



Receiver Operator Characteristic (ROC)

- Overall performance of a classifier is usually visualized using the ROC curve:
  - Scan all possible thresholds and evaluate True Positive Rate and False Positive Rate
  - Plot one as a function of the other
- Area under the curve (AUC) often quoted as performance metric
- ROCs can aide in choosing a classifier and threshold
- Note: Sometimes ROCs of different classifiers cross each other -> they are better at different TPR regions





Confusion matrices

- With a chosen threshold we can plot confusion (migration) matrices
- Shows migration from one class to another
- Very usefull for multiclassification:
  - Which background class looks most signal like?
  - Which classes are difficult to separate?
- Can be normalized to:
  - True classes (efficiency matrix)
  - Predicted class (purity matrix)