Fantastic neural networks and how to train them

Nikolai Hartmann

LMU Munich

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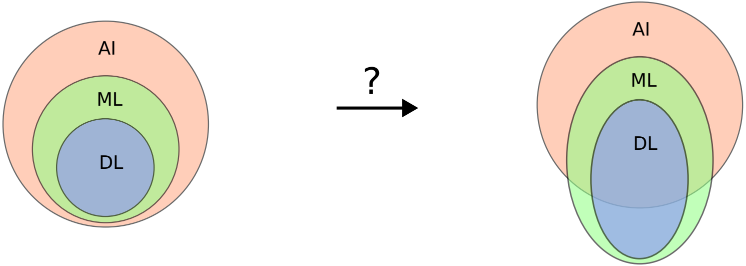
Buzzword definitions for this talk

The great thing about buzzwords - i can choose my own definition



- **Machine Learning:** Fitting, but we don't really care what exactly the model is (in classical fitting we usually have an interpretation for the parameters)
- **Deep learning:** Solving problems with neural networks i can't solve with BDTs (usually involving larger datasets and multiple layers)
- **A**rtificial **I**ntelligence: Emulating human intelligence/behavior (i want to draw a blurry boundary to the stuff we never did by hand before)

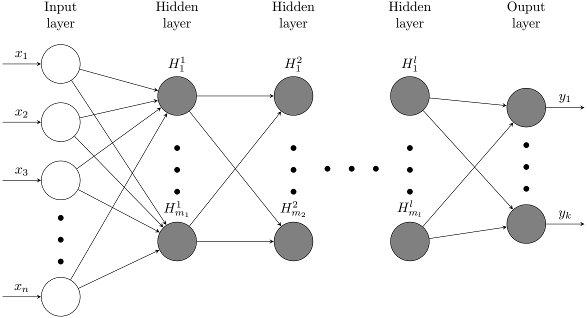
Supervised learning

Focussing on supervised learning in this talk
$\rightarrow$ visit talk by David Gisegh (26.06.) to learn more about unsupervised learning!

- Want to find a function that maps a set of input features $\mathbf{x} = [x_1, x_2, \ldots, x_n]$ to a set of output features $\mathbf{y} = [y_1, y_2, \ldots, y_n]$
- We only have (typically simulated) **training examples**
- Want to find (multidimensional) parametrisation of something that we can only simulate $\rightarrow$ **inverse problem**
- Two main goals:
  - **Classification:** map inputs to labels $y_i \in 0, 1$ (or a probability $p_i \in [0, 1]$)
  - **Regression:** predict continuous values $y_i \in \mathbb{R}$

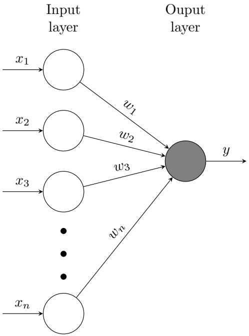
The fully-connected, feedforward neural network

Aka multilayer perceptron (MLP)

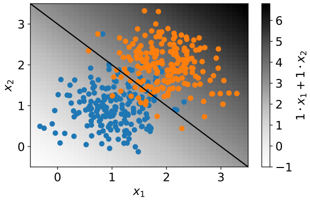


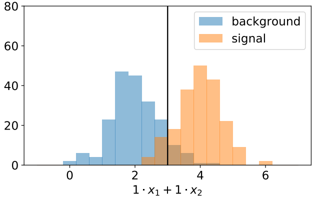
- Propagate information through the network by taking the weighted sum of inputs at each neuron and applying an activation function $\sigma(\sum_i w_i x_i + b)$
- Activation function adds non-linearity
  $\rightarrow$ can approximate any function with sufficient number of neurons!
- Each connection corresponds to one weight w
- Each neuron has one bias b
- Classification: one output neuron per possible label

The simplemost “neural network”



Example: 2D $w_1 = w_2 = 1$





- A single neuron (no hidden layer) corresponds to linear discriminant
  $\rightarrow$ Output $= \sum w_i x_i$
- Idea goes back to 1957 - the “Perceptron” (in Hardware!) by Frank Rosenblatt

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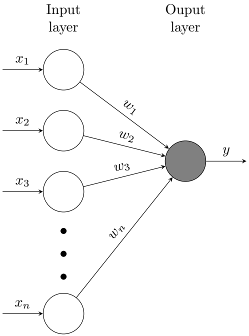

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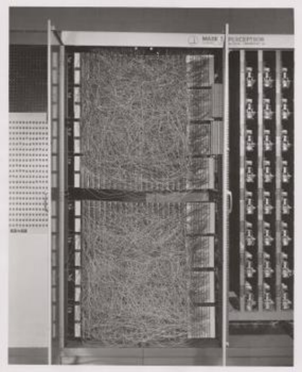

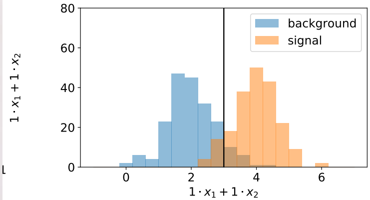

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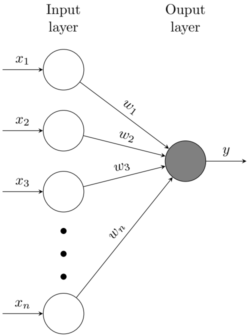

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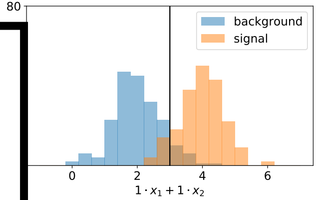

New York Times, July 7, 1958:

"The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, reproduce itself and be conscious of its existence."

- A single neuron (no hi ... nant
  $\rightarrow$ Output $= \sum w_i x_i$
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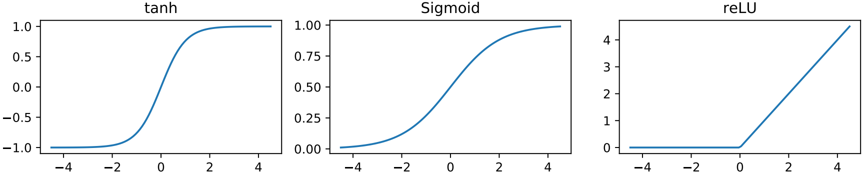
The power of hidden layers

- Hidden layers without activation functions don't help
  $\rightarrow$ linear combination of linear combinations is still a linear combination
- Non-linear activation function at each neuron in the hidden layer(s) allows to approximate **any** function! (given enough neurons)
  $\rightarrow$ proven for sigmoid in 1989 by George Cybenko
  $\rightarrow$ more generally proven in 1991 by Kurt Hornik
- One hidden layer is in principle enough
- Experience: multi-hidden-layer networks work better
  $\rightarrow$ "**Deep neural networks**"

Activation functions



- Derivatives:

tanh:

$$f'(x) = 1 - f(x)^2$$

sigmoid:

$$f'(x) = f(x)(1 - f(x))$$

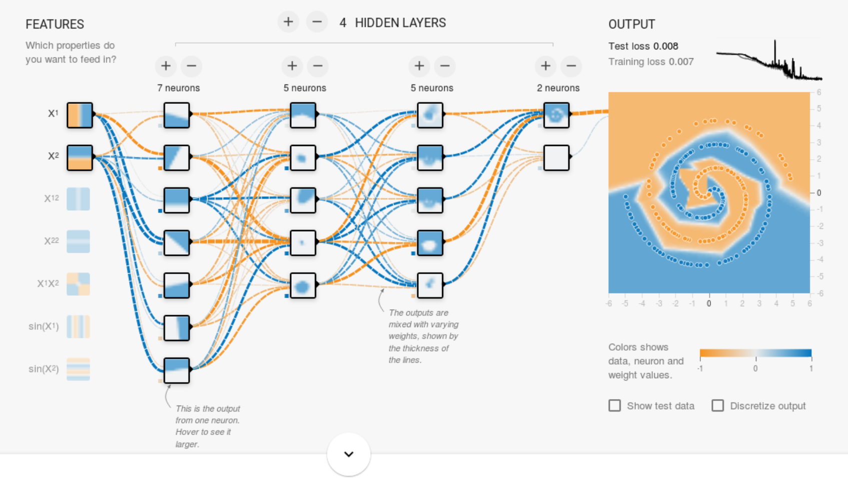
reLU:

$$f'(x) = \begin{cases} 0 & \text{for } x \leq 0 \\ 1 & \text{for } x > 0 \end{cases}$$

- tanh function in the hidden layers was popular for a long time
- Problem: gradient vanishes for large input values
  $\rightarrow$ especially problematic in multi-layer networks
- most popular nowadays: reLU and variants of it
- sigmoid is used wherever output should be in $[0, 1]$

Example

https://playground.tensorflow.org



Loss function

To solve the optimisation problem we need a measure for the distance between the current (pred) output and the desired (true) output

Mean squared error (MSE):

$L_{\mathrm{MSE}} = \frac{1}{N} \sum_i (y_i^{\mathrm{pred}} - y_i^{\mathrm{true}})^2$

$\rightarrow$ good for Regression, mean absolute error also popular

Cross entropy (CE):

$L_{\mathrm{CE}} = -\sum_{i=1}^{N_{\mathrm{classes}}} y_i \log \hat{y}_i$

$\rightarrow$ good for Classification, same as **maximum Likelihood**

Binary cross entropy (BCE) - for 2 classes, 1 output:

$L_{\mathrm{BCE}} = -\frac{1}{N} \sum_i \left[y_i^{\mathrm{true}} \ln y_i^{\mathrm{pred}} + (1 - y_i^{\mathrm{true}}) \ln(1 - y_i^{\mathrm{pred}}) \right]$

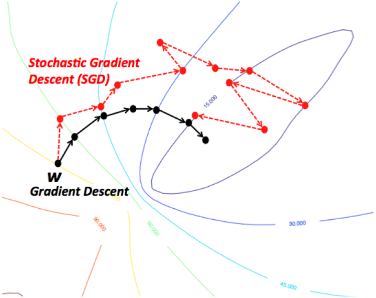
Backpropagation

The algorithm that makes neural networks work

- Know all operations and their derivatives the computation graphs
  $\rightarrow$ can use **chain rule**
  $\rightarrow$ compute once **forward**, store intermediate values, then **backward** to get gradient
- Single variable: $\frac{\partial f(g(x))}{\partial x} = \frac{\partial f}{\partial g} \frac{\partial g}{\partial x}$
- Multivariable: $\mathbf{J}_f(g(x)) = \mathbf{J}_f(g)\mathbf{J}_g(x)$, in components $\frac{\partial f_i}{\partial x_j} = \frac{\partial f_i}{\partial g_k} \frac{\partial g_k}{\partial x_j}$
- For derivative of **scalar** (loss): $\frac{\partial f}{\partial x_j} = \underbrace{\frac{\partial f}{\partial g_k}}_{\text{vector}} \underbrace{\frac{\partial g_k}{\partial x_j}}_{\text{Jacobian}}$
  $\rightarrow$ matrix multiply gradient (row) **vector** with the **Jacobian** in each step
  $\rightarrow$ referred to as vector-Jacobian-product (**VJP**)
- The cool thing: Usually not required to fully compute the Jacobian to get the VJP! (e.g. a single matrix multiplication to get VJP for matrix output w.r.t matrix input)

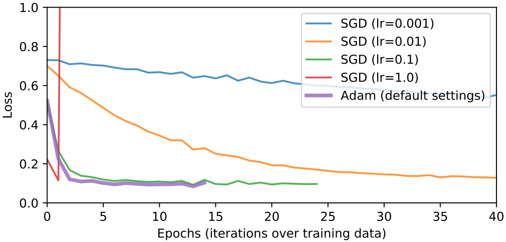
Stochastic Gradient Descent (SGD)

- Loss function is usually averaged over all training examples
  $L_{\text{tot}} = \frac{1}{n} \sum_i L_i$
- Need to propagate all training examples through the network for each gradient update
  $\rightarrow$ computationally intense for large training sets



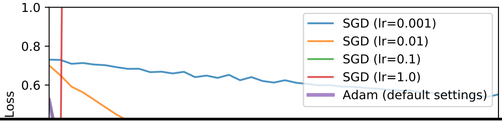
- Solution: Gradient updates on random subsets ("batches") of training data
- batch size gives a handle for tradeoff:
  number of gradient steps $\leftrightarrow$ iterations over dataset ("**epochs**")

Extensions to SGD



- Need to adjust the step size (“**learning rate**”) for good convergence
- Many approaches
  - schedule learning rate during training (start high, decrease, warmup, cosine schedule, ...)
  - use information on previous changes (“**momentum**”)
  - do this parameter wise
  - use second order moments of the gradients
  - ...
- Lots of research happening - keep an eye on it!
- Current (~~2018~~ 2024) best default choice: “**Adam**” and variants of it
  $\rightarrow$ works very well in default settings in most cases

Extensions to SGD



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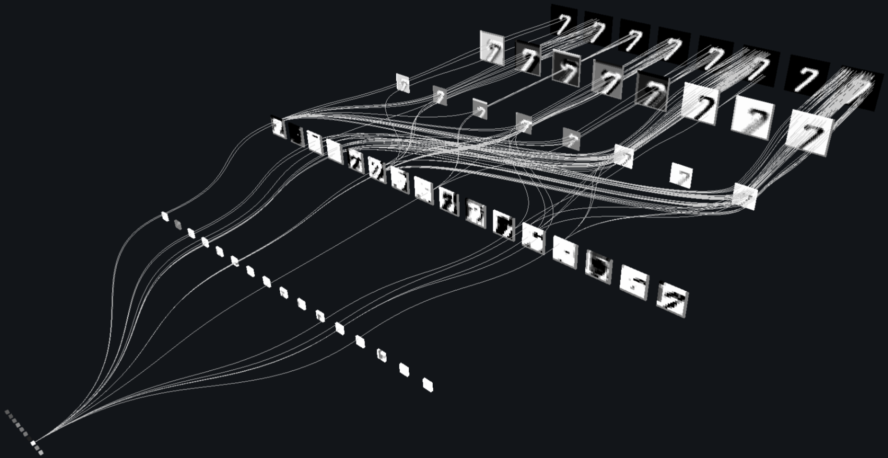
NN Architectures

Most architectures make use of symmetries in the data

- Translation invariance: **Convolutional neural networks (CNNs)**
  $\rightarrow$ "slide" a neural network over neighboring inputs (e.g. pixels)
- Sequential data: **Recurrent neural networks (RNNs)**
  $\rightarrow$ Stateful neurons, feed output back in, together with input of next time step
- Permutation invariance (and/or equivariance):
  - Sets without predefined relations: **Deep Sets**
    $\rightarrow$ process each element individually
    $\rightarrow$ aggregate globally over hidden states in permutation invariant way (e.g. sum)
  - Graphs: **Graph (convolutional) networks (GNNs)**
    $\rightarrow$ aggregate over neighbors in graph
  - **Transformers**: can be seen as graph networks with fully connected graph
    $\rightarrow$ now also standard for sequential data (see LLMs)

Moving more and more towards the permutation invariant architectures
(both in AI research and HEP ML)

Convolutional neural networks (CNNs)

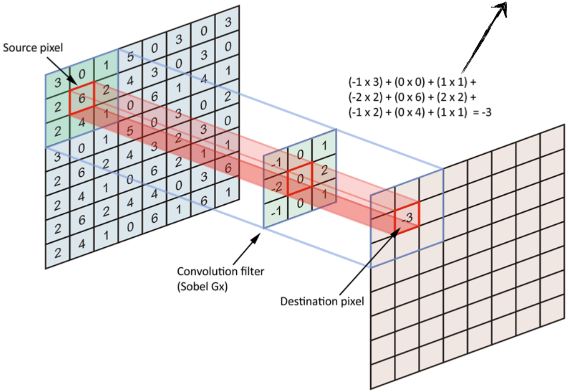


http://terencebroad.com/nnvis.html

Slide from Gregor Kasieczka's lecture at Terascale ML school 2018

Convolutional Layer

That's the weights we want to train



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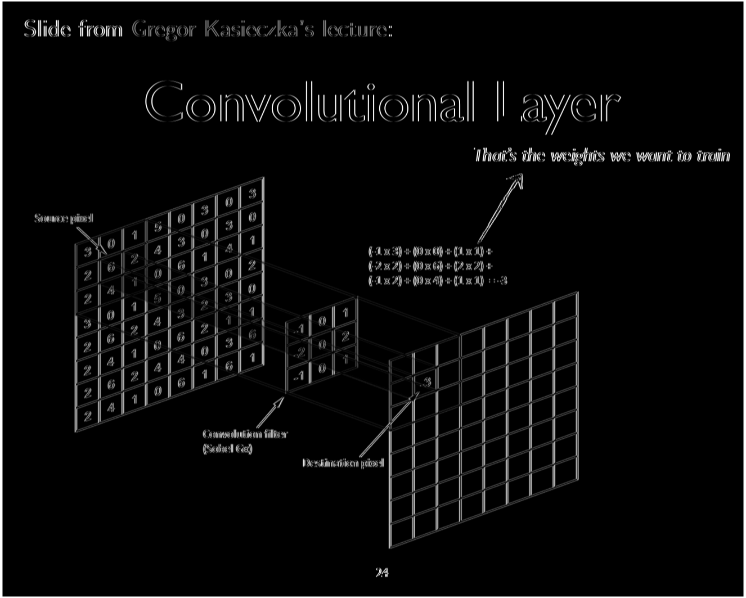

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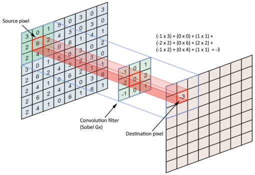
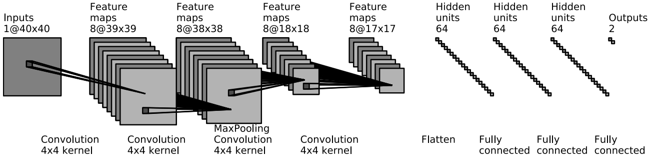
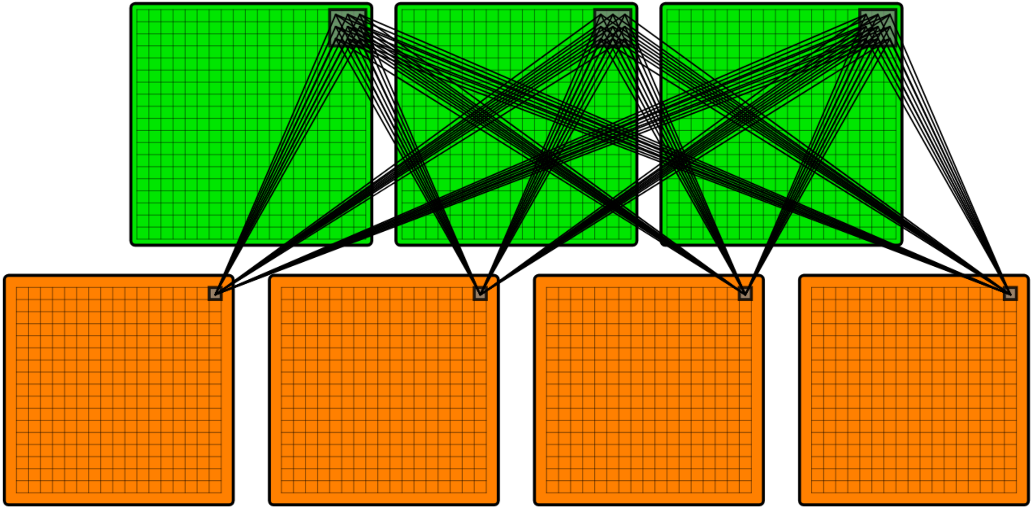
Convolutional Network



- ***How to build a convolutional network***
  - Chain multiple conv layers
  - Use multiple masks per layer
  - Pooling
    - Max Pooling
    - Average Pooling
  - Add a fully connected network in the end

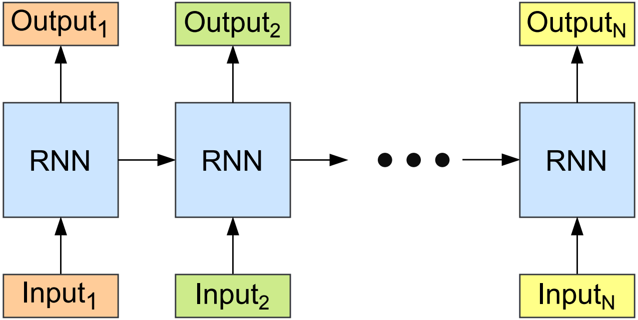


How $N_{\text{input}} \to M_{\text{output}}$ channels work:



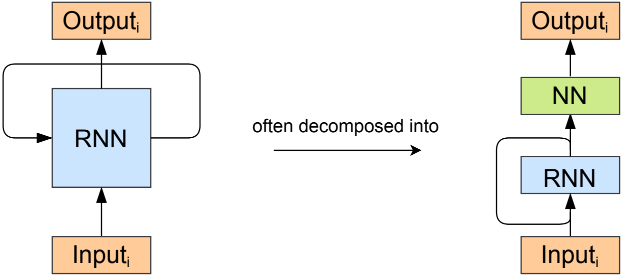
$\to$ animation

RNNs



- Operate on a sequence, passing-on a hidden **state**
- **Shared weights** across the sequence
- Usually thought of as a sequence **in-time**, but can be any **ordered sequence**

RNNs



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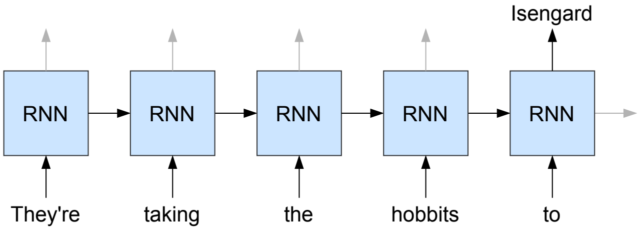
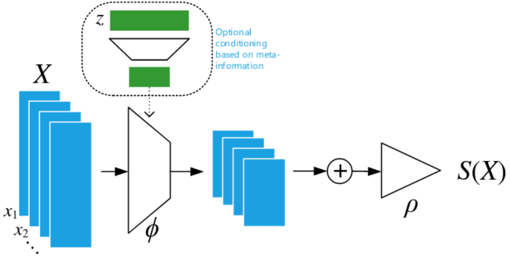
RNNs



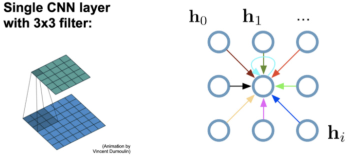
- Operate on a sequence, passing-on a hidden **state**
- **Shared weights** across the sequence
- Usually thought of as a sequence **in-time**, but can be any **ordered sequence**
- Used to be the standard for language models, but not anymore (Transformers took over)
  $\rightarrow$ also in particle physics it seems their time is mostly over ...

Deep Sets



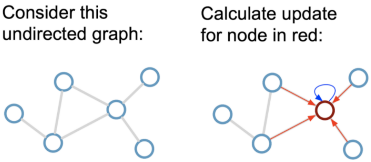
- **Per-item transformation** ϕ (e.g. MLP - shared weights!) followed by
- **Permutation invariant aggregation** (e.g. sum)
- Every **permutation-equivariant** ($f(\pi(x)) = \pi(f(x))$) transformation allowed for per-item step
  $\rightarrow$ e.g. add/concatenate global sum to each item
- Output is now fixed-length vector, can be transformed by another MLP
- Very simple to implement, give it a try!
  $\rightarrow$ Popularized in HEP by "Energy flow networks" paper (also soft/collinear safe variant)

Graph networks



Full update:

$$\mathbf{h}_4^{(l+1)} = \sigma\left(\mathbf{W}_0^{(l)}\mathbf{h}_0^{(l)} + \mathbf{W}_1^{(l)}\mathbf{h}_1^{(l)} + \cdots + \mathbf{W}_8^{(l)}\mathbf{h}_8^{(l)}\right)$$

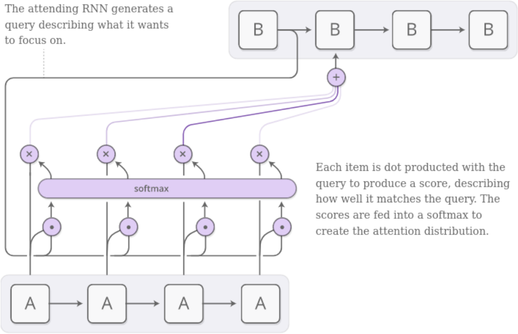


Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}^{(l)}\right)$$

- Update node featuers by **sum over neighbors in graph**
  $\rightarrow$ similar to sum over neighboring pixels in CNN
- Can't have fixed weight (no meaningful ordering of neighbors, number not constant)
- Simplest option: sum without weights (Graph convolutional network, GCN)
- More advanced: work with features on edges, features of neigboring nodes (e.g. attention)
  - in general can pass information from nodes to edges, edges to nodes ...
  - ... and to and from global features

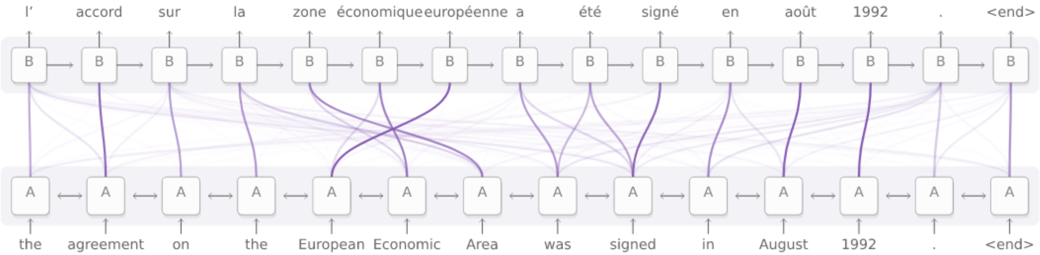
Attention



- Started as an attempt to improve translation tasks with RNNs
- Have each element of one sequence *attend* to elements of another sequence
- Possible implementation: score from dot product of each encoder, decoder step pair
- Precursor of transformers - *Attention is all you need*

[1] https://distill.pub/2016/augmented-rnns

Example for machine translation

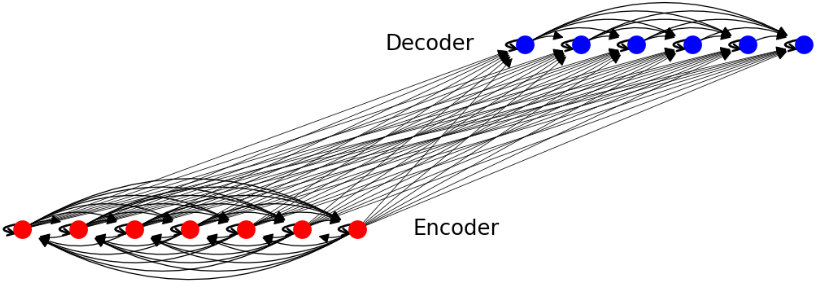


Input and target sequence can also be the same - **Self Attention**

[1] https://distill.pub/2016/augmented-rnns

Transformers as a Graph Network

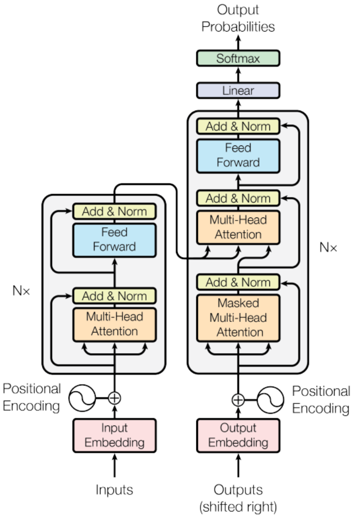
from https://docs.dgl.ai/en/latest/tutorials/models/4_old_wines/7_transformer.html



- Lines represent attention weights - inferred from features of nodes they connect
- **Decoder:** only connections to previous tokens (*causal mask*)
- **Encoder:** fully connected graph for attention
- Encoder-only: BERT, ParT
- Decoder-only: GPT(1,2,3)

Transformer details

Attention is all you need (2017) (arXiv:1706.03762)



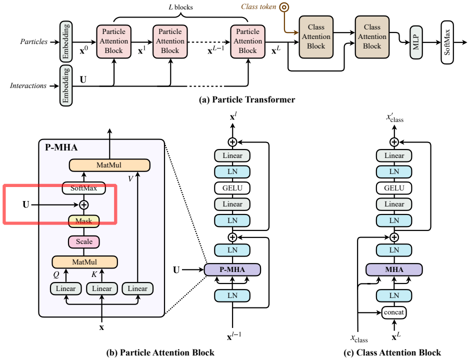
- Uses Multi-Head-Attention (MHA)
- MLP (with one hidden layer) after each MHA block
- Skip connections and normalization layers make deep models possible

Public data sets

- Public data sets help exchange and development of common models
- Nice example: **Top tagging dataset** (arXiv:1902.09914, 10.5281/zenodo.2603255)
  $\rightarrow$ Leading 200 jet constituents for $\approx$ 1M pythia (boosted) jets with Delphes detectors sim
  $\rightarrow$ Task: find out if the jet is normal QCD jet or comes from a top quark
  $\rightarrow$ Huge amount of architectures has been tested, often generally applicable

ParT

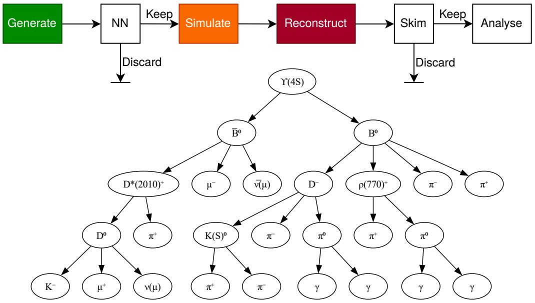
Particle Transformer for Jet Tagging arXiv:2202.03772



Modifications w.r.t. standard transformer:

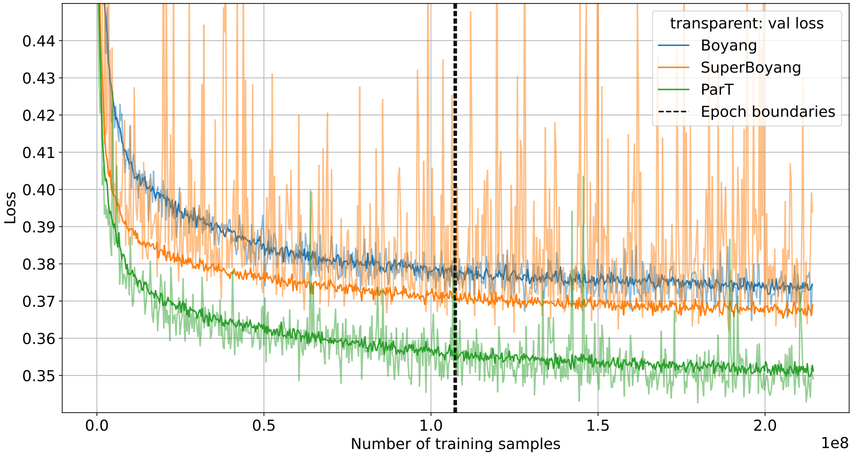
- Add embedded interaction features (e.g. invariant mass) as bias term to attention score $\rightarrow$ very similar to attention mechanism with edge features in graph networks
- Attention to class token to produce global classification result
- State-of-the-art for jet tagging if trained on large enough datasets (100M events)

Preliminary results on Belle II Smart Background project



- Use a NN as a MC filter
  $\rightarrow$ predict after event generation which events we will throw out later
- Graph neural networks, using the generator-level decay tree work well
- But maybe we have been fooled and it's mainly about the correlation between particles?
  $\rightarrow$ try ParT, can still feed in adjacency matrix as pair feature

Preliminary results on Belle II SmartBackground project



→ almost out-of-box better performance than our prevously optimized models!

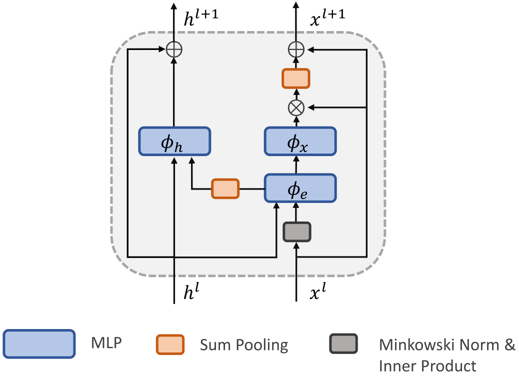
Working with Lorentz vectors

Working with 4-momentum vectors we can make use of Lorentz symmetry!

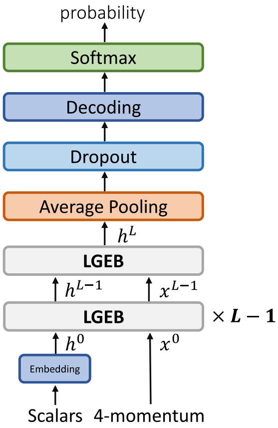
- Lorentz covariant quantities of a set of 4-momentum vectors can be constructed as functions of pairwise Minkowski inner products $f(p_1, p_2, ..., p_n) = f(\{p_i p_j\}_{i,j})$
- Two architectures with state-of-the art (2024) performance on jet-tagging tasks:
  - **LorentzNet** (arXiv:2201.08187): build a *Minkowski dot product attention* based on this
    $\rightarrow$ transform a set of 4-vectors into a new set of 4-vectors across layers
  - **PELICAN** (arXiv:2211.00454): run rank $2 \rightarrow 2$ permutation equivariant transformations
    $\rightarrow$ run transformation on the whole matrix of pairwise Minkowski products
    $\rightarrow$ needs fewer parameters than other models (but maybe more computation?)

LorentzNet

arXiv:2201.08187



Lorentz Group Equivariant Block (LGEB)



LorentzNet

$\rightarrow$ Caspar is applying this for background suppression in the $B \rightarrow K^* \nu\nu$ analysis!

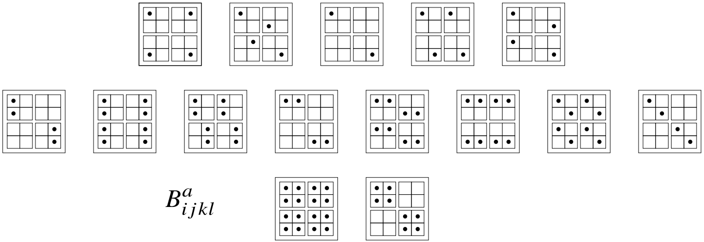
PELICAN

arXiv:2307.16506

Equivariant Layer: $T^{(\ell+1)} = \textsc{Agg} \circ \textsc{Msg}\left(T^{(\ell)}\right).$

$\textsc{Agg}$

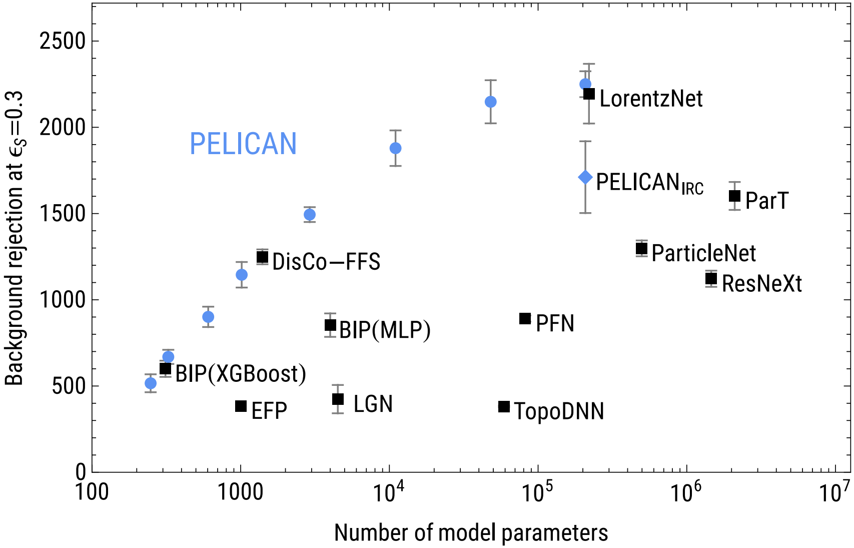
$$T'^{a}_{ij} = \sum_{k,l=1}^{N} B^{a}_{ijkl} T_{kl}.$$



B^{a}_{ijkl}

15 possible permutation equivariant matrix $\rightarrow$ matrix aggregators run in each layer

Performance on Top tagging



How to train on a large dataset

Preparing the data input pipline often requires a significant fraction of the work

Some recommendations:

- Do all preprocessing that doesn't blow up the amount of data much before
- Store in parquet or feather files (use pandas for flat tables, awkward array for the rest)
- Stuff that blows up data (padding with 0s, features for all pairs ...) better on-the-fly
- If data fits into memory, load it into memory
    - estimate memory usage before - one float takes 4 bytes
      $\rightarrow$ 8 GiB memory: 2.6M events, 100 particles each, 8 features per particle
    - in practice will need factor 2-3 more due to copies (not always easy to avoid)
- If not, load in large chunks (100k - 1M events per chunk)
    - typically 1 chunk = 1 file
    - generate randomized batches from the chunk
    - load random chunks
    - useful pattern: subprocess loads next chunk while training on previous chunk runs

Summary

- Neural networks most useful when we process lower level data
  → for high-level observables in tabular form, use BDTs! MLPs rarely beat them
- Processing lower level data usually requires making use of symmetries
  → CNNs, RNNs, Deep Sets, GNNs, Transformers
- Following developments on public datasets can be very useful
  → jet tagging is very active and the methods often generalizable
- Typical particle physics data format: List of 4-momentum vectors (+extra features)
  → ideal use case for Transformers (work well with small modifications, see ParT)
  → ... but also need large datasets (10-100M events)
- Smaller datasets can profit from imposing Lorentz symmetry
  → the most interesting approaches to date: LorentzNet, PELICAN
- Or having pre-trained models that can be fine-tuned to the samller datasets
  → ParT shows promising results for jet tagging
  → "Predict-the-next-particle" approaches getting more popular as well
  → e.g. arXiv:2305.10475, 2403.05618, 2401.13537

Outlook

- Let's talk more about the "boring" topic how we actually train these networks
  $\rightarrow$ usually large fraction of work in data preparation, setting up the input pipeline
  $\rightarrow$ we will likely see larger models and run our stuff on multiple GPUs soon
- Access to resources is not very uniform, for example here in Munich:
  - 3 local GPUs in the AG-Kuhr
  - 4 GPUs in C2PAP, need to apply for project - setup via VM (lrz cloud) or slurm queue
  - several multi-GPU nodes in lrz AI system, more to come
    $\rightarrow$ access can be requested by everyone with linux cluster account

If you want to learn more

- Machine learning schools by the ErUM-Data-Hub
  https://erumdatahub.de/veranstaltungen
- ODSL block courses, one currently going on (until today)
  https://indico.ph.tum.de/event/7606
  $\rightarrow$ slides and recordings online!
- Nice video tutorials by Andrej Karpathy (*Neural Networks: Zero to Hero*)
  https://www.youtube.com/playlist?list=PLAqhIrjkxbuWI23v9cThsA9GvCAUhRvKZ