Machine Learning for Jet Physics

RTG Student Lecture

Peter Sorrenson

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Lecture 1

ML history

- Main idea of ML: learn statistical patterns from data in order to perform tasks without explicit programming
    - Driving force: continually dropping cost of computation and data (*Two Centuries of Productivity Growth in Computing*, Nordhaus 2007)

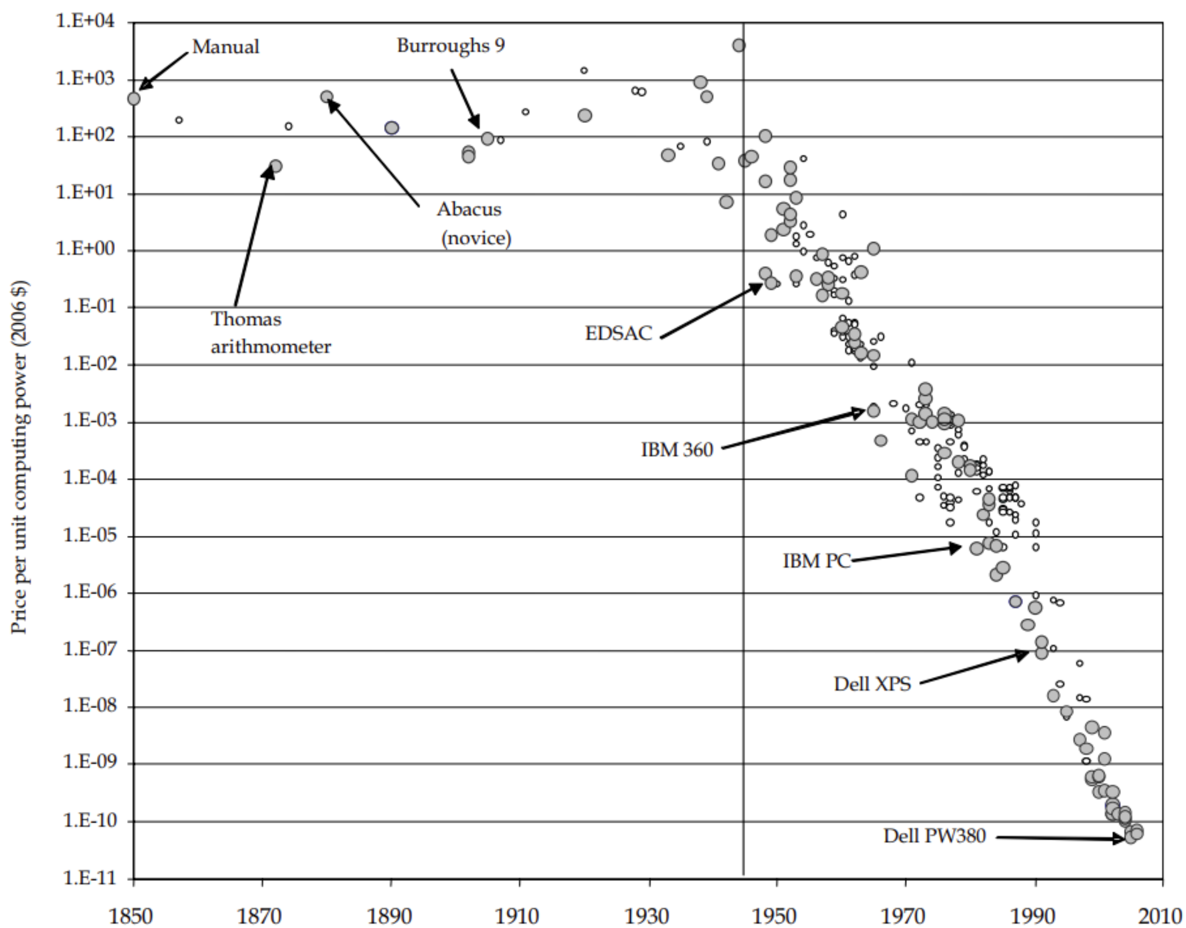
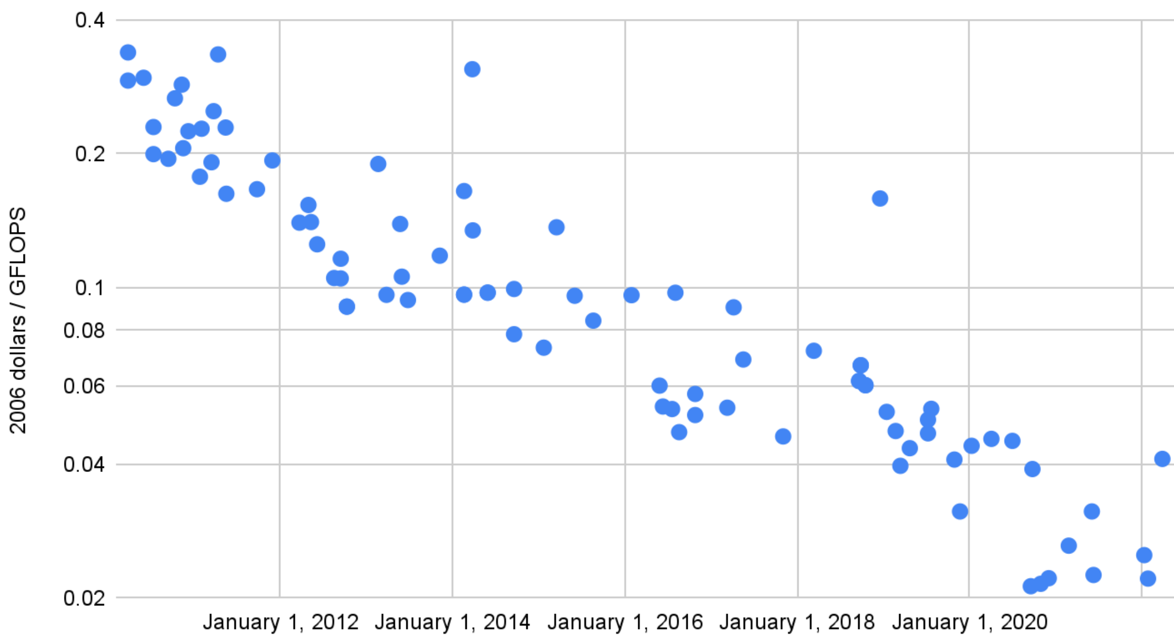
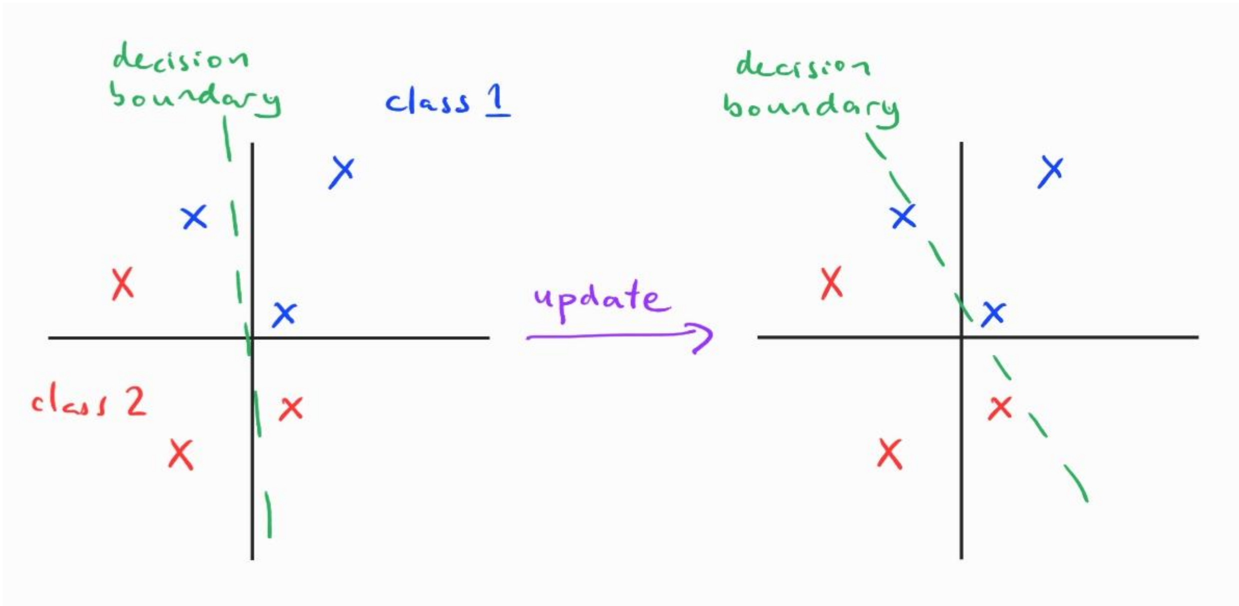


FIGURE 3
THE PROGRESS OF COMPUTING MEASURED IN COST PER COMPUTATION PER SECOND DEFLATED BY THE PRICE INDEX FOR GDP IN 2006 PRICES

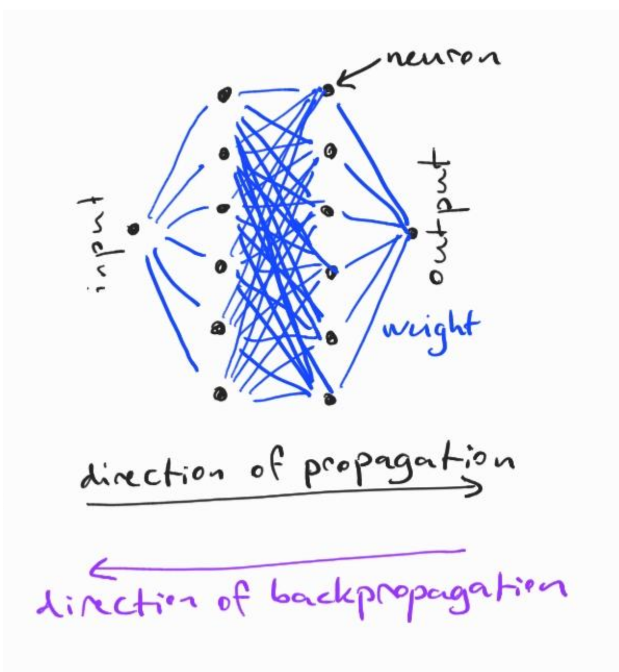
Nvidia GeForce price performance history

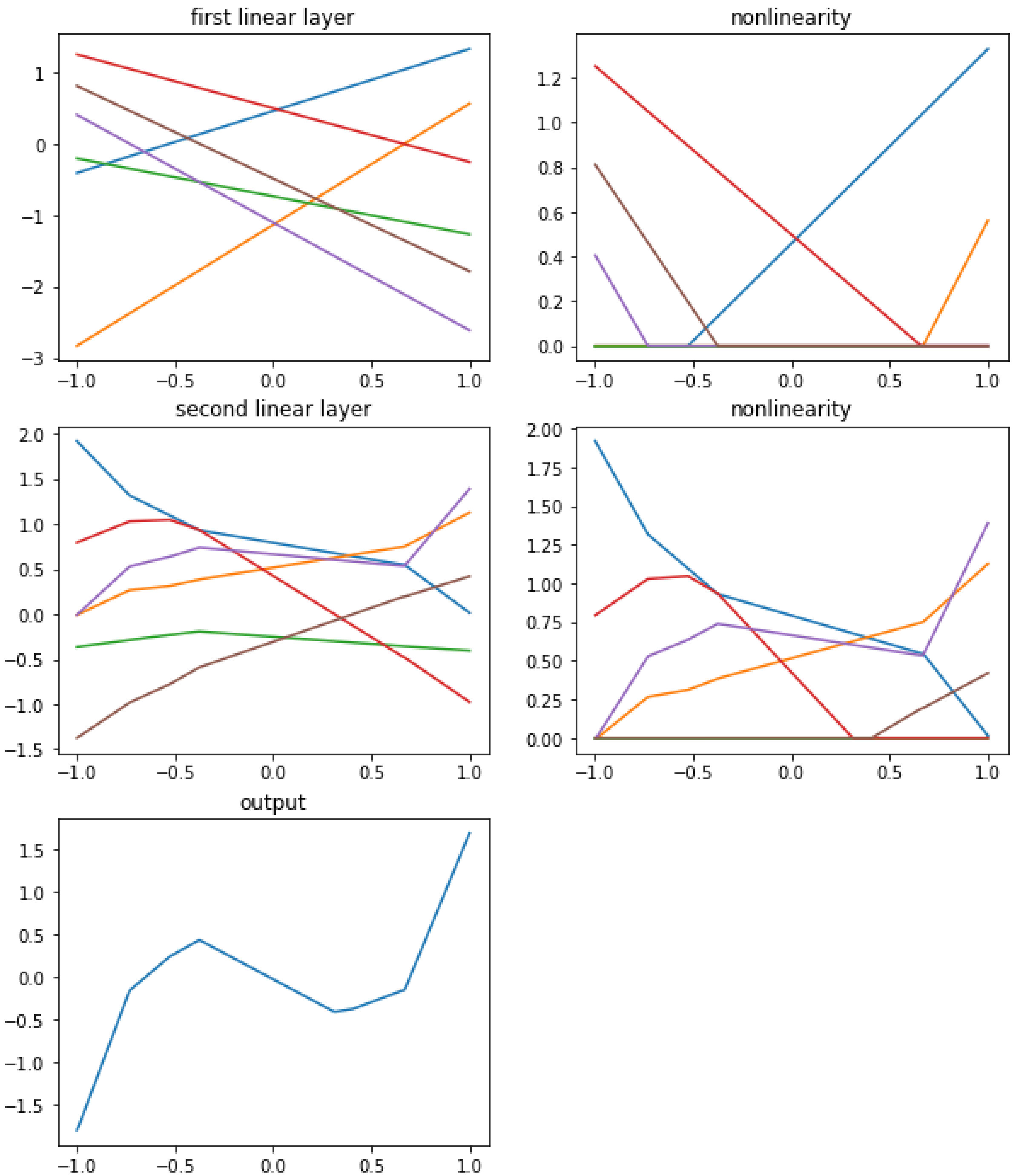


    - Especially good at hard-to-define tasks that work in high-dimensional spaces, e.g. classifying an image
    - Software 2.0: rather than programming a function (software 1.0), provide data that defines the input -> output pair
        - It turns out that for many interesting problems it's significantly easier to collect the data than to define the program
    - “Every time I fire a linguist, the performance of our speech recognition system goes up” (Fred Jelinek from 1985)
- Invention of transistor (1947) and Shannon’s theory of information (1948)
    - Events which kicked off the information age
- Perceptron (1957)
    - Linear model which is updated iteratively to find a decision boundary
    - Sketch of perceptron update:

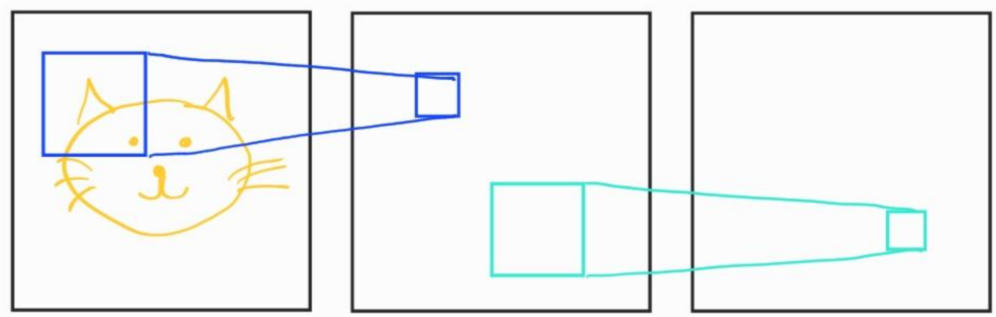


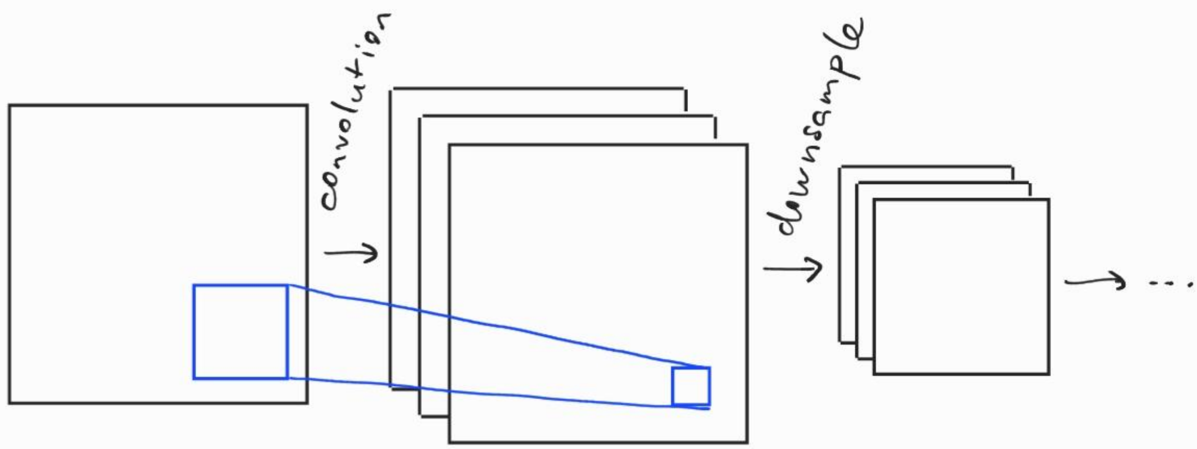
- Backpropagation (first described 1970, rediscovered 1986)
    - Allows training of multiple-layer neural networks
    - Example of three-layer network: 1D input to 1D output with 2 hidden layers of 6 neurons each



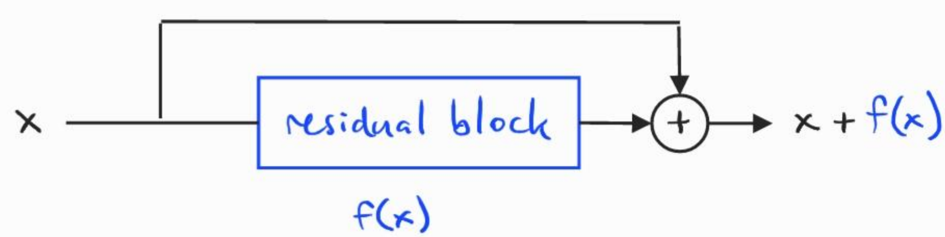


- Convolutional neural net (LeNet 1989)
  - Efficient image processing
  - Exploits translational symmetry of images
  - Sketch of stacked convolutional layers:

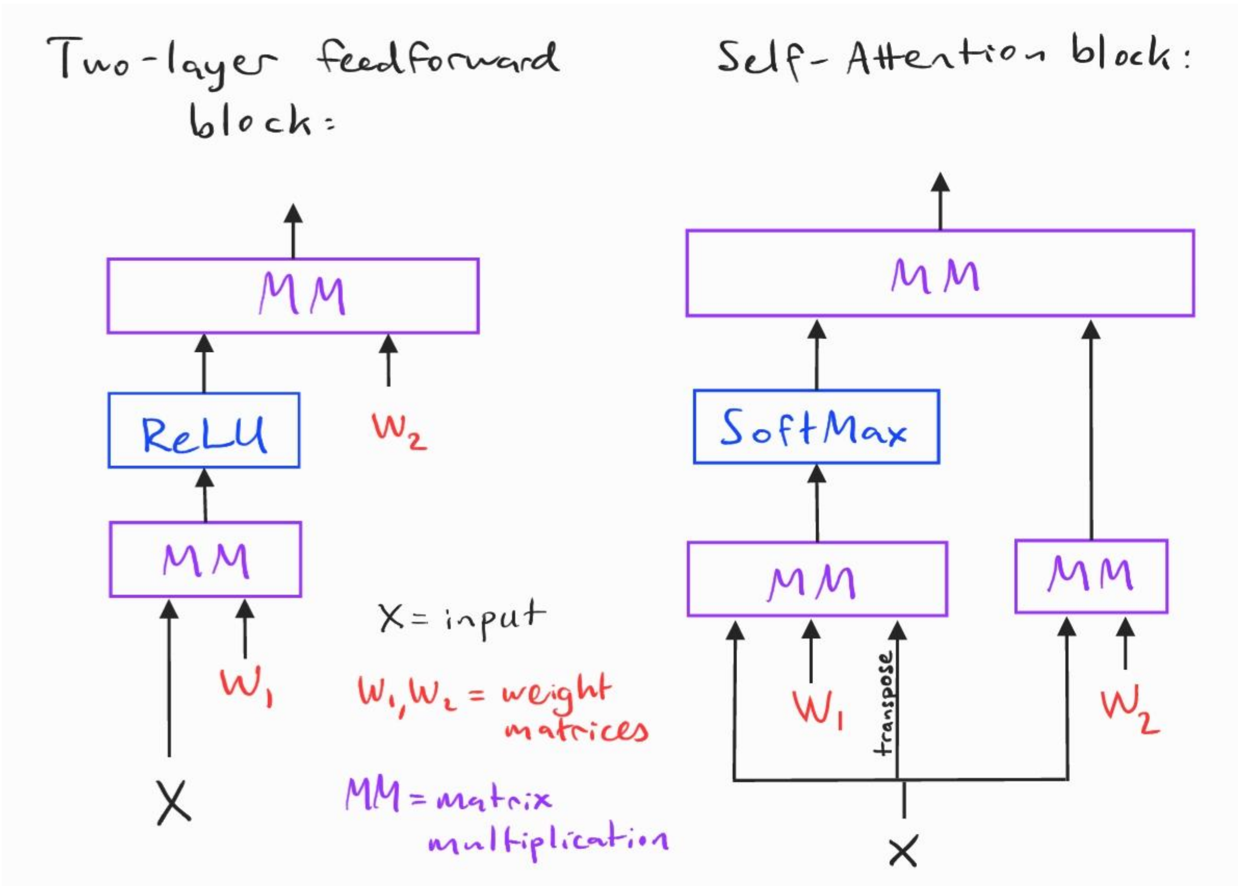




- Deep Blue beats Kasparov (1997)
- Development of GPUs (2000s)
- Deep neural nets (2010s)
  - ImageNet (2009)
    - Huge labeled dataset which kicked off deep learning
  - AlexNet (2012)
    - The model which made it clear that neural nets are the most powerful models around (at least for computer vision)
    - Used custom CUDA kernels to speed up convolutional nets
  - ResNet (2015)
    - Allowed very deep models, template for what followed
    - Sketch of residual blocks:

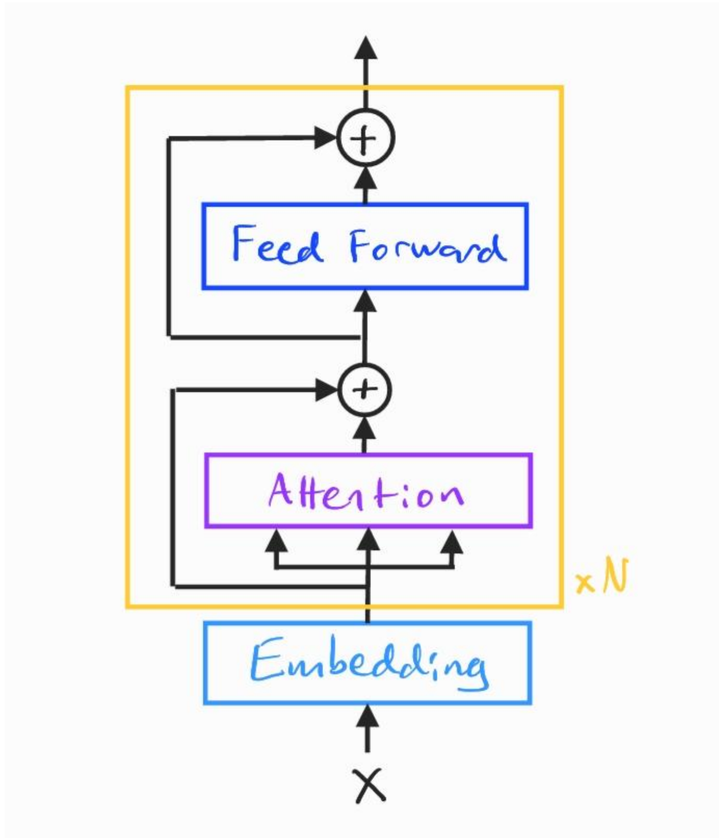


- AlphaGo (2016)
  - Maturation of reinforcement learning through self-play in discrete perfect-information games
  - AlphaZero a year later
- Transformer (2017)
  - General purpose model which can be applied to almost any type of data
  - Extensive use of attention mechanisms:



  - Attention is powerful because it allows for the expressive modeling of interactions within a sequence or set of data. Most data can be expressed as a sequence or a set (e.g. an image is a sequence of small patches)

- Sketch of transformer structure:



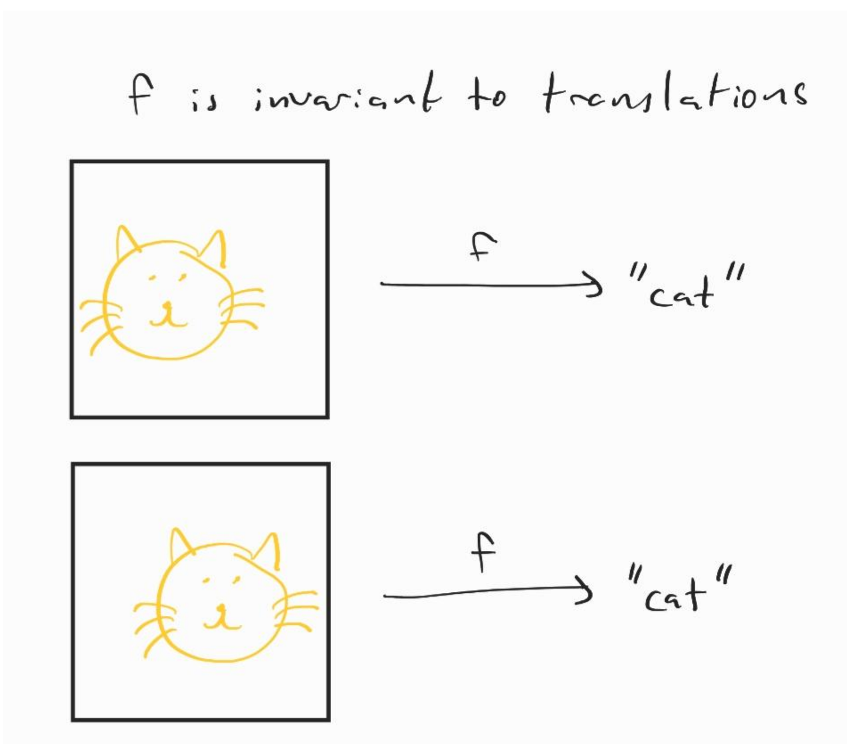
- GPT-3 (2020)
    - Large language model with surprisingly good fluency in natural language and ability to generalize and perform logical tasks
- AlphaFold 2 (2021)
    - Protein folding prediction to unprecedented accuracy
- The basics remain the same: sequential computations based on large matrix multiplications, trained via gradient descent on lots of data
- Interactive tool: see effect of NN layers and play around at https://playground.tensorflow.org/

Lecture 2

Applications to jet physics

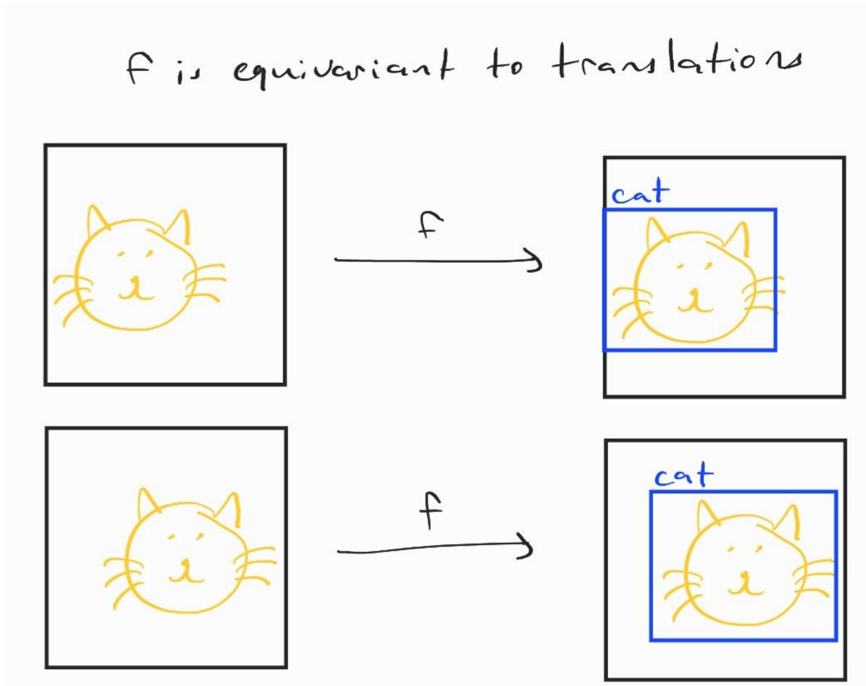
Symmetries

- Symmetry is ubiquitous in physics
- In ML it is known that respecting the symmetries of the system in question means you need less data and compute
  - Convolutional neural nets (translational symmetry in images)
  - Set and graph networks (permutation symmetry)
  - Molecular modeling (isometries: translations, rotations)
  - If you have enough data and compute you can actually learn the symmetries, often ends up with better performance than hard-coding symmetries (e.g. ViT, i-GPT). But you need a lot of data and compute…
  - Can also learn to be invariant to symmetries using data augmentation and contrastive learning
- Difference between invariance and equivariance under symmetry
  - Invariance: the output doesn't change under a given symmetry (e.g. image classification)
    - Sketch:



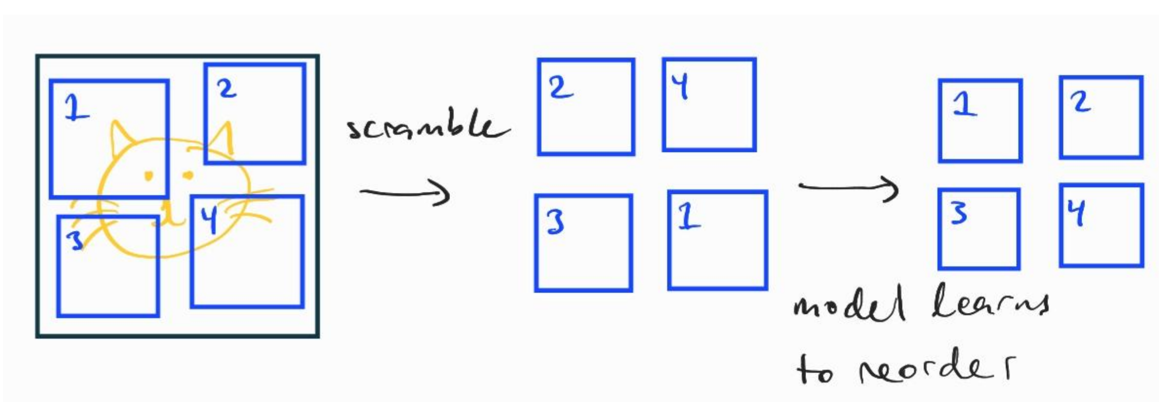
  - Equivariance: the output changes according to the same symmetry as the input (e.g. bounding boxes)

- Sketch:

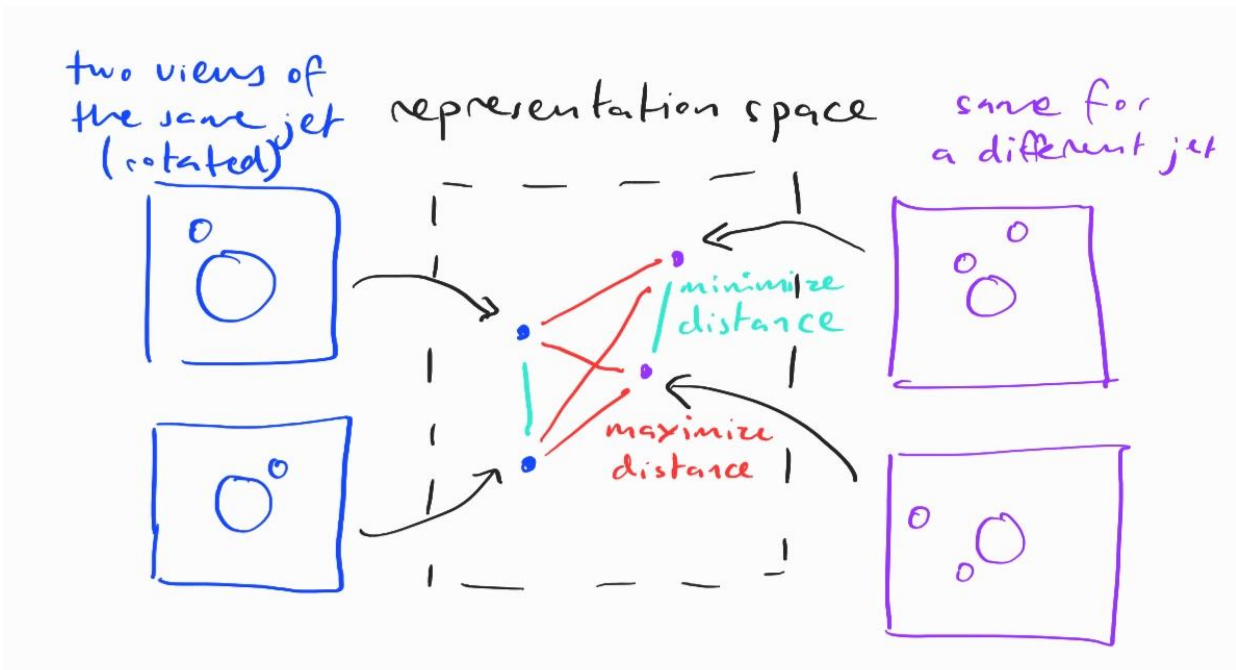


Representation learning

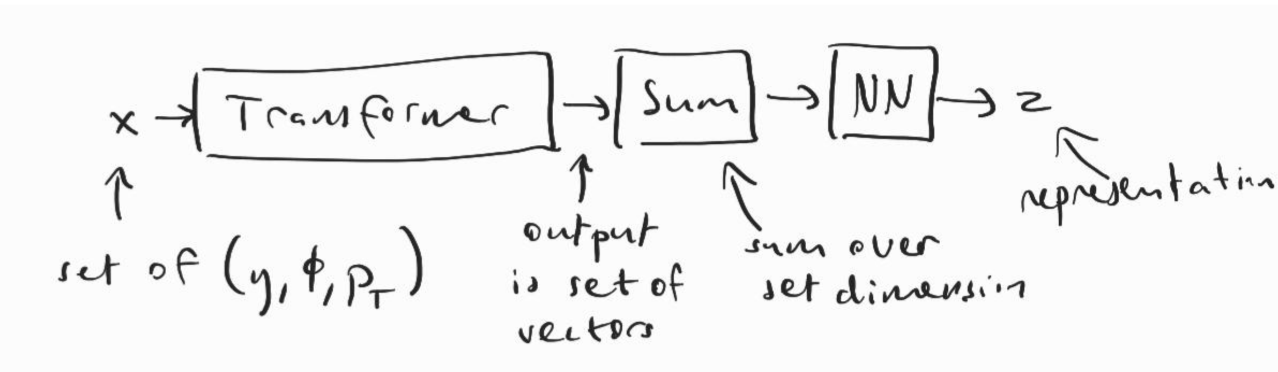
- You can take a classifier trained on a large labeled dataset, cut off the final layer and use it as a feature space to perform other tasks
- Is it possible to do the same thing without labeled training data? (labeled data is expensive to collect)
- Self-supervised learning (now one of the most important paradigms in deep learning due to the availability of unlabeled data)
- Create a task from data
    - Mask part of an image and predict the missing pixels
    - Predict the next word in a sequence of text
    - Jigsaw puzzle: cut an image into pieces, mix them up and learn how to reconstruct them. Sketch:



- Rotate an image and learn to predict the rotation
- In order to complete the task the model has to extract non-trivial features from the data. The hope is that these features are useful for other tasks
- Type of self-supervised learning: contrastive learning
  - Create pairs of data points (called augmentations) which represent the same underlying object
  - E.g. images in which rotations, blurring, noise and other distortions added
  - The model maps these pairs to a space (called the representation space) where they should be close together
  - At the same time any representation should be far away from other representations which do not correspond to the same object
  - Sketch:



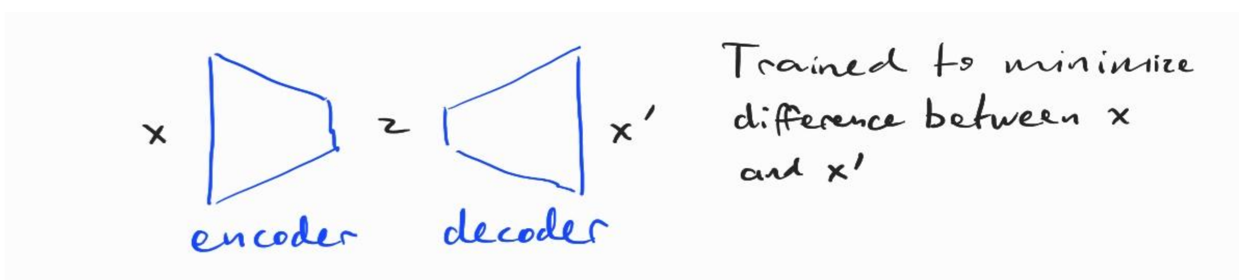
- JetCLR: contrastive learning for jets
  - Jets represented by sets of (eta, phi, pT) coordinates
  - Augmentations defined by translations and rotations in (eta, phi) plane, addition of soft radiation, collinear splitting of particles
  - Augmentations define the learned invariances. Permutation invariance is hard-coded
  - Use a transformer (permutation equivariant) followed by a sum (permutation invariant) and feedforward nets to map to representation space. Sketch:



- JetCLR representations allow for a simple linear classifier to perform well on a supervised classification task (tag top quark jets in a QCD background)
  - Better than a hand-crafted baseline (energy flow polynomials)
  - Hope is that representations can be used for other downstream tasks, e.g. anomaly detection

Anomaly detection

- At the LHC there is a huge stream of data. Rare events corresponding to new physics might be present in the data but haven't be found yet because the search space is too large
- Traditional methods are model based, e.g. testing a model hypothesis against the data, e.g. a bump hunt
- It would be useful to also have model-free methods, that can flag anomalies without making assumptions about the processes that generate them
- Proposal in jet physics: autoencoders
- Autoencoders try to reconstruct inputs while passing them through a bottleneck dimension. This forces the model to learn the most important features of the input and discard unneeded information. Sketch:



- If we train autoencoders on normal, background data, we might be able to detect anomalies by looking for events with a high reconstruction error
  - This would suggest the features of the input are not similar to those of the training data, something expected of anomalies
- However, this doesn't always work as expected
  - If we train on QCD background, top jets are tagged as anomalous

    - But if we train on a top jet background, QCD jets are not tagged as anomalous, even though they are not seen during the training
    - The main problem seems to be that the autoencoder is still able to reconstruct signals of lower complexity than those it was trained on
- Solution (tentative): normalize the autoencoder
    - Don’t just train the autoencoder to reconstruct inputs, but train it so that it fails to reconstruct inputs not in the training set
    - This training method is more expensive but more effective
    - We can improve the ability of the autoencoder to detect QCD jets as anomalous when trained on top background
    - Also shows promise in detecting dark matter jets which have lower complexity than normal QCD background