

Lecture II: Introduction to Deep Learning

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SLAC

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Modern Neural Networks

People are now building a **new kind of software** by assembling networks of **parameterized functional blocks** and by **training them from examples using some form of gradient-based optimization**.

- Yann LeCun, 2018



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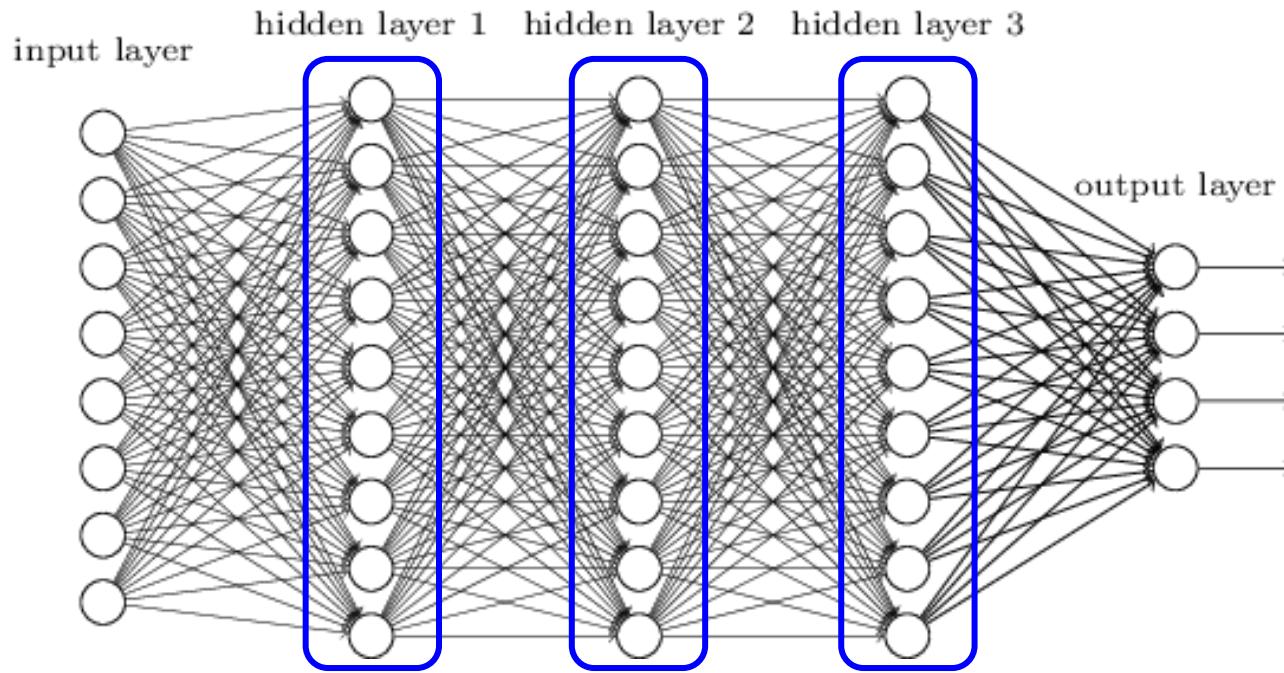
- Non-linear operations of data with parameters
- Layers (set of operations) designed to perform specific mathematical operations
- Chain together layers to perform desired computation
- Train system (with examples) for desired computation using gradient descent

The Plan

- Deep Learning is a **HUGE** field
 - O(10,000) papers submitted to conferences
- I'm will condense *some* parts of what you would find in *some lectures* of a Deep Learning course
- Highly recommend taking the time to go more slowly through lectures from a class. Online-available Recommendations:
 - [Francois Fleuret course at University of Geneva](#)
 - [Gilles Louppe course at University of Liege](#)
 - [Yann LeCun & Alfredo Canziani course at NYU](#)

Deep Neural Networks

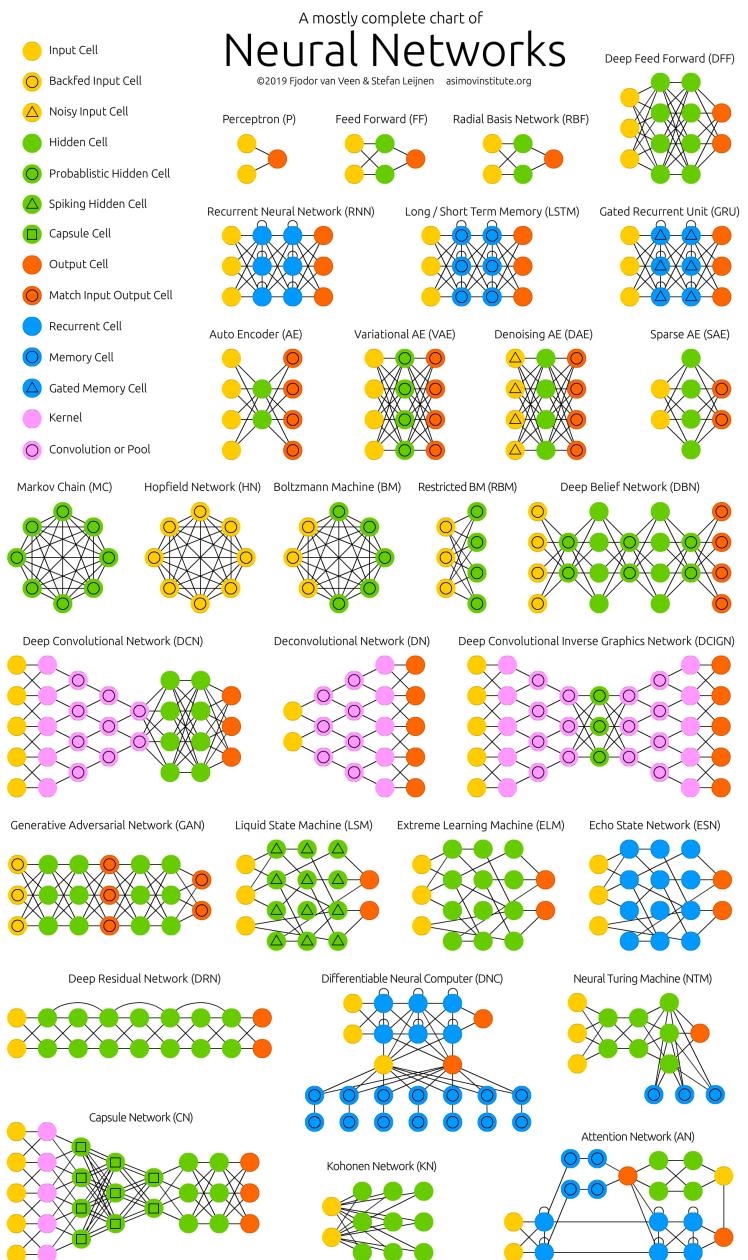
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- As data complexity grows, need exponentially large number of neurons in a single-hidden-layer network to capture all structure in data
- Deep networks *factorize learning* of structure in data across layers
- Large datasets, fast computing (GPU / TPU) and new training procedures / network structures made training possible

Neural Network Zoo

- Structure of the networks, and the node connectivity can be adapted for problem at hand
- Moving inductive bias from feature engineering to model design
 - *Inductive bias:*
Knowledge about the problem
 - *Feature engineering:*
Hand crafted variables
 - *Model design:*
The data representation and the structure of the machine learning model / network



Neural Network Zoo – “Optimization” Perspective

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- A single layer network may need a width exponential in D to approximate a depth-D network's output
 - Simplified version of Telgarsky ([2015](#), [2016](#))

Neural Network Zoo – “Optimization” Perspective

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- A single layer network may need a width exponential in D to approximate a depth- D network’s output
 - Simplified version of Telgarsky ([2015](#), [2016](#))
- Over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction

[Belkin et. al. 2018](#)

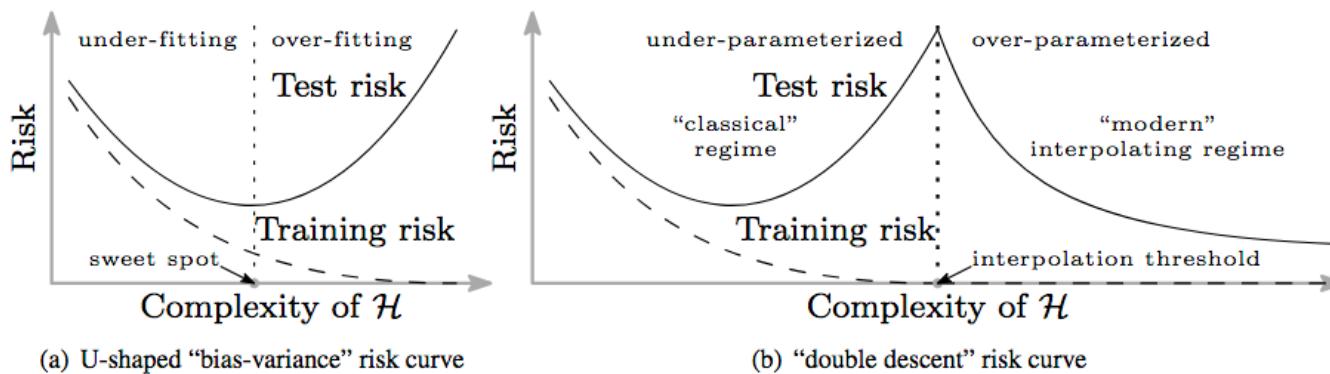


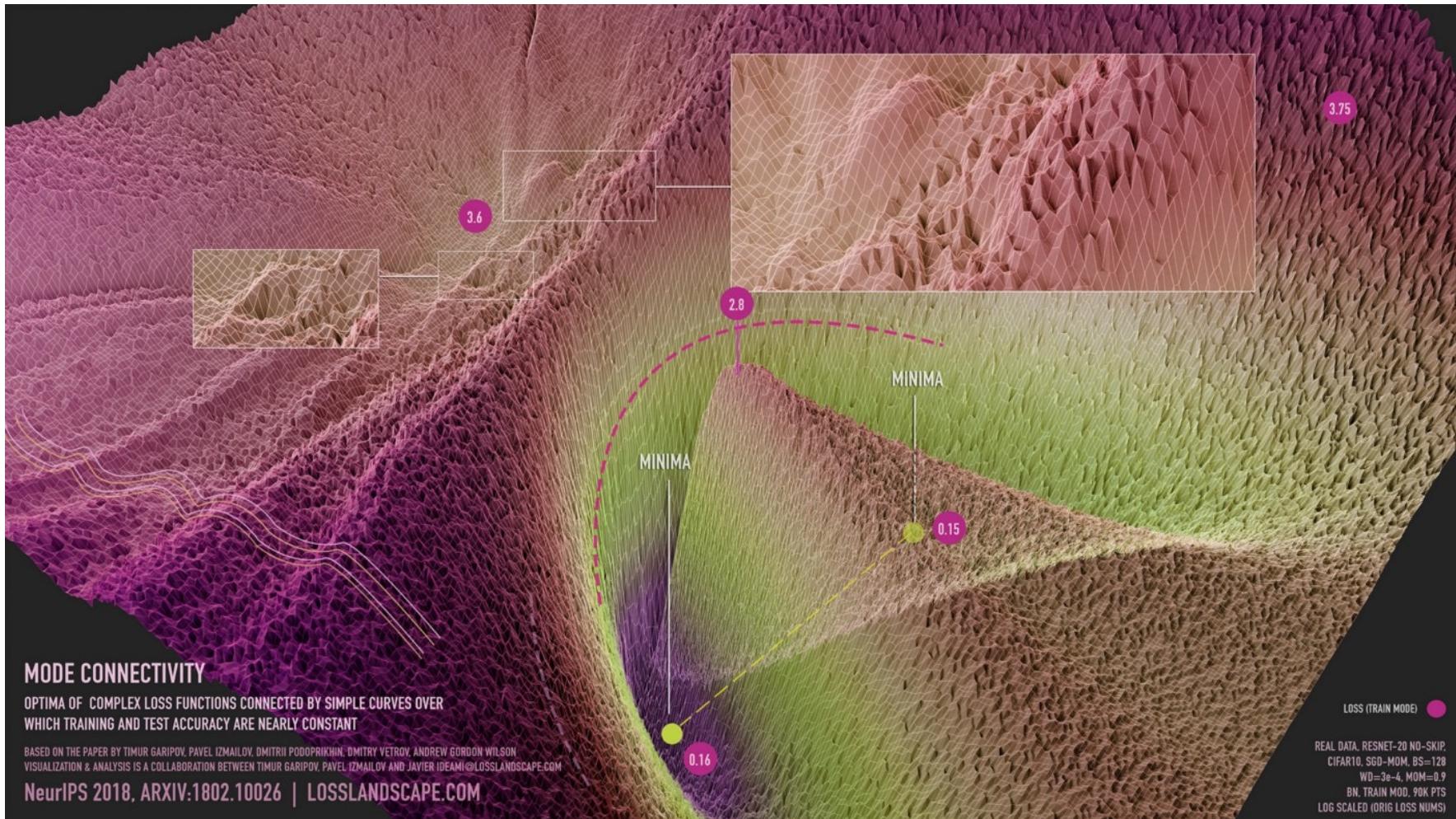
Figure 1: Curves for training risk (dashed line) and test risk (solid line). (a) The classical *U-shaped risk curve* arising from the bias-variance trade-off. (b) The *double descent risk curve*, which incorporates the U-shaped risk curve (i.e., the “classical” regime) together with the observed behavior from using high complexity function classes (i.e., the “modern” interpolating regime), separated by the interpolation threshold. The predictors to the right of the interpolation threshold have zero training risk.

- A single layer network may need a width exponential in D to approximate a depth- D network's output
 - Simplified version of Telgarsky ([2015](#), [2016](#))
- Over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction
 - But we must control that:
 - Gradients don't vanish
 - Gradient amplitude is homogeneous across network
 - Gradients are under control when weights change

- A single layer network may need a width exponential in D to approximate a depth- D network's output
 - Simplified version of Telgarsky ([2015](#), [2016](#))
- Over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction
- Major part of deep learning is choosing the right function
 - Need to make gradient descent work, even if substantial engineering required

Deep Neural Networks Loss Landscape

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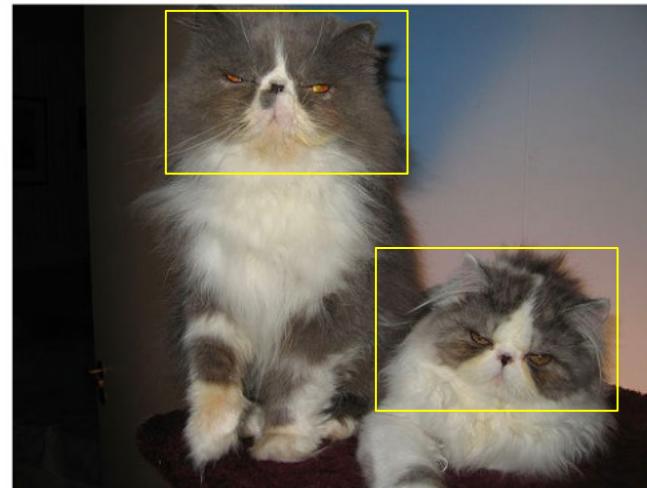
<https://arxiv.org/abs/1802.10026>

Convolutional Neural Networks

Convolutional Neural Networks

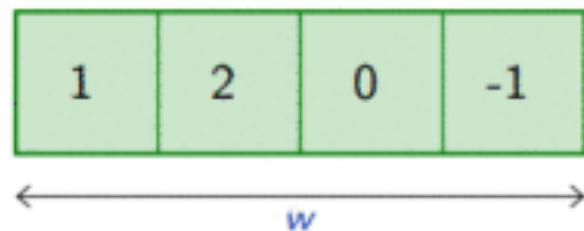
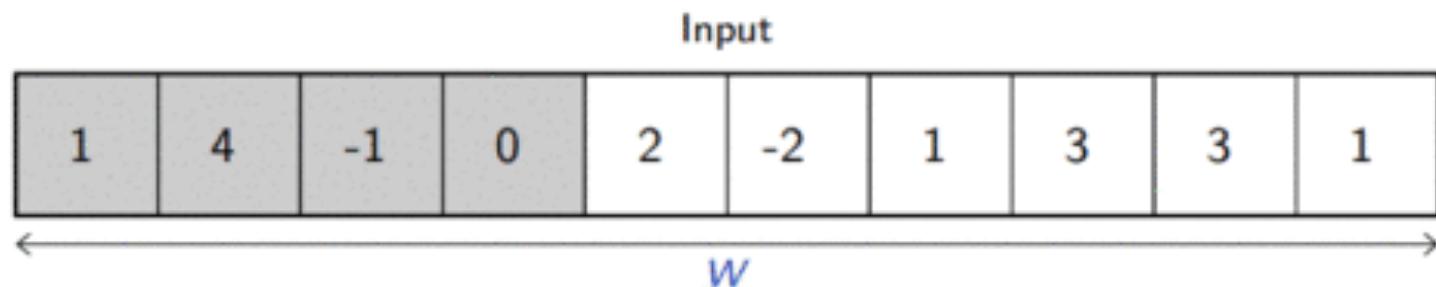
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- When the structure of data includes “invariance to translation”, a representation meaningful at a certain location can / should be used everywhere

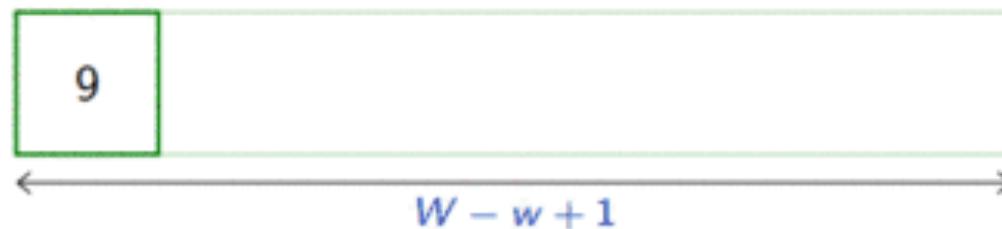


- Convolutional layers build on this idea, that the same “local” transformation is applied everywhere and preserves the signal structure

1D Convolutional Layer Example



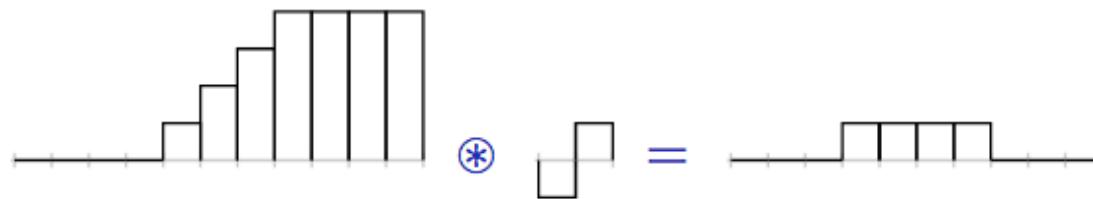
Output



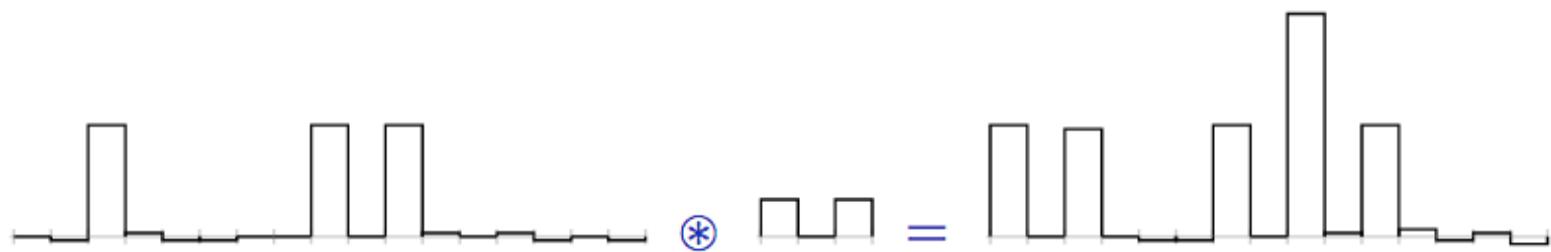
Convolutional Filters

Convolution can implement particular differential operators, e.g.

$$(0, 0, 0, 0, 1, 2, 3, 4, 4, 4, 4) \circledast (-1, 1) = (0, 0, 0, 1, 1, 1, 1, 0, 0, 0).$$

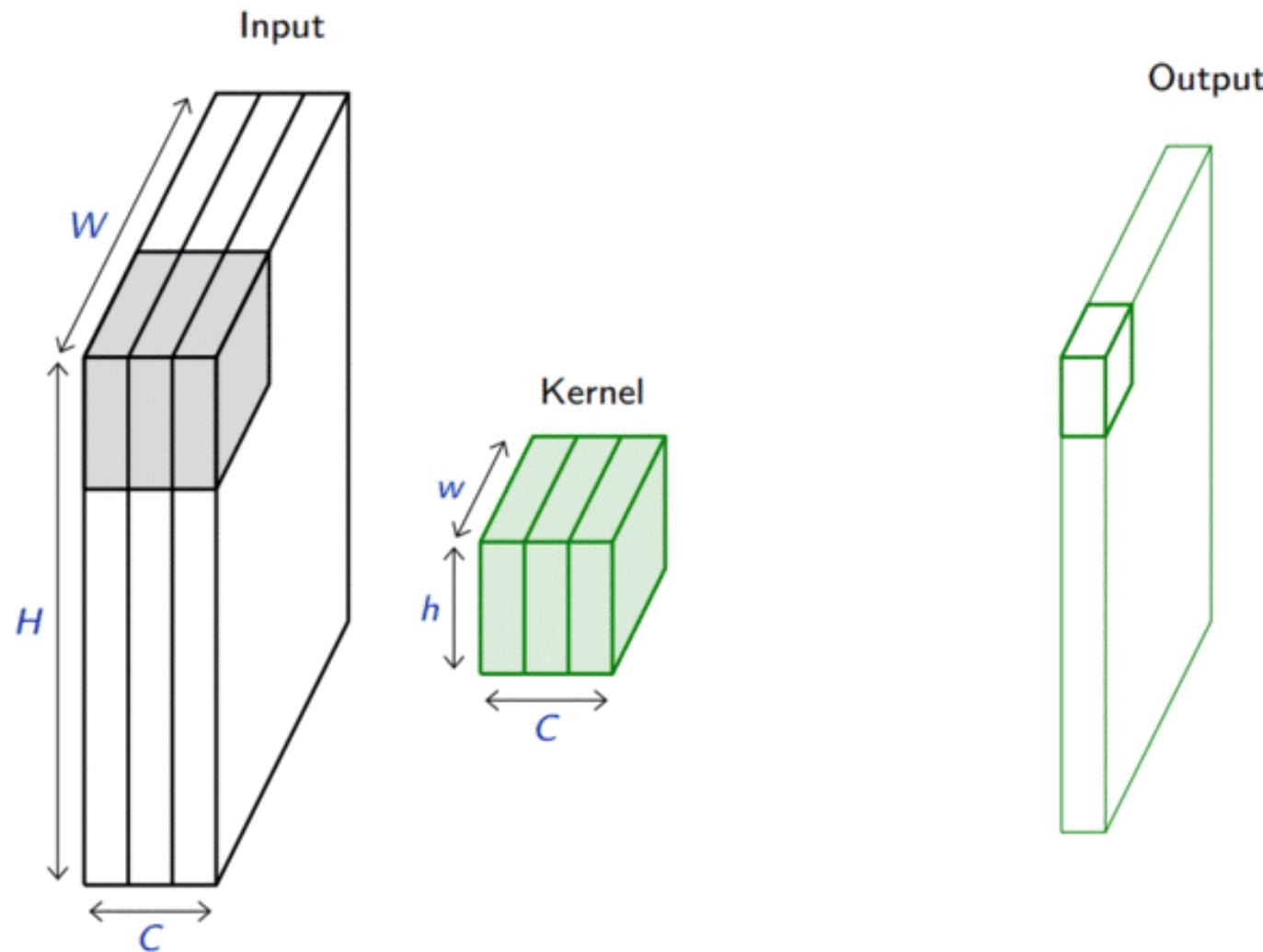


or crude “template matcher”, e.g.



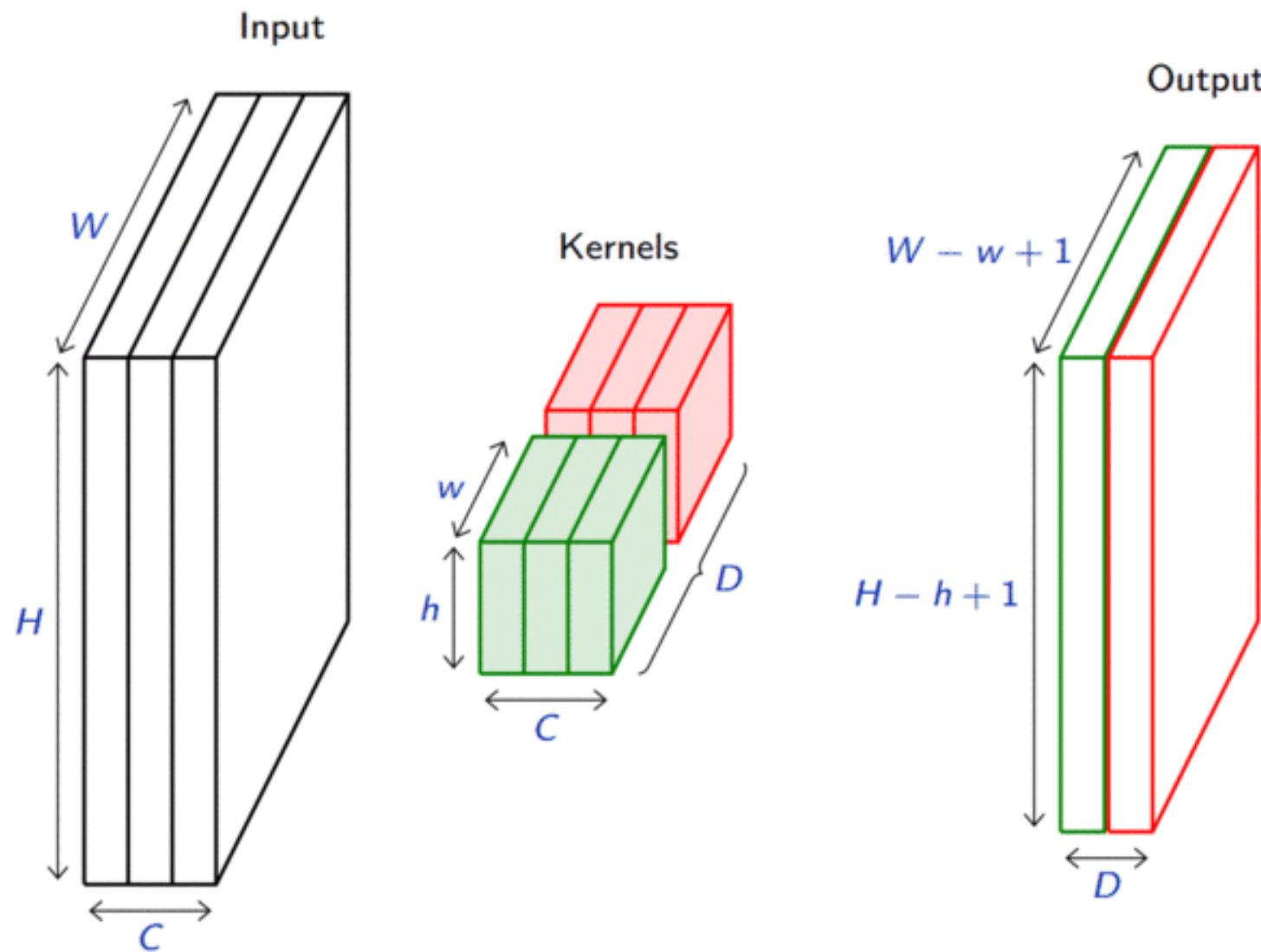
2D Convolution Over Multiple Channels

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2D Convolution Over Multiple Channels

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2D Convolutional Layer

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- Input data (tensor) \mathbf{x} of size $C \times H \times W$
 - C channels (e.g. RGB in images)
- Learnable Kernel \mathbf{u} of size $C \times h \times w$
 - The size $h \times w$ is the *receptive field*

$$(\mathbf{x} \circledast \mathbf{u})_{i,j} = \sum_{c=0}^{C-1} (\mathbf{x}_c \circledast \mathbf{u}_c)_{i,j} = \sum_{c=0}^{C-1} \sum_{n=0}^{h-1} \sum_{m=0}^{w-1} \mathbf{x}_{c,n+i,m+j} \mathbf{u}_{c,n,m}$$

- Output size $(H - h + 1) \times (W - w + 1)$ for each kernel
 - Often called *Activation Map* or *Output Feature Map*

Shared Weights: Economic and Equivariant

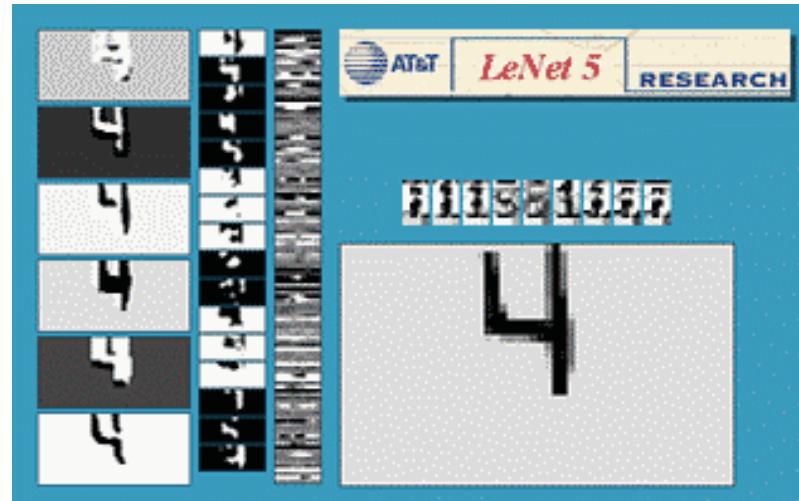
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- Parameters are *shared* by each neuron producing an output in the activation map
- Dramatically reduces number of weights needed to produce an activation map
 - Data: $256 \times 256 \times 3$ RGB image
 - Kernel: $3 \times 3 \times 3 \rightarrow 27$ weights
 - Fully connected layer:
 - $256 \times 256 \times 3$ inputs $\rightarrow 256 \times 256 \times 3$ outputs $\rightarrow O(10^{10})$ weights

Shared Weights: Economic and Equivariant

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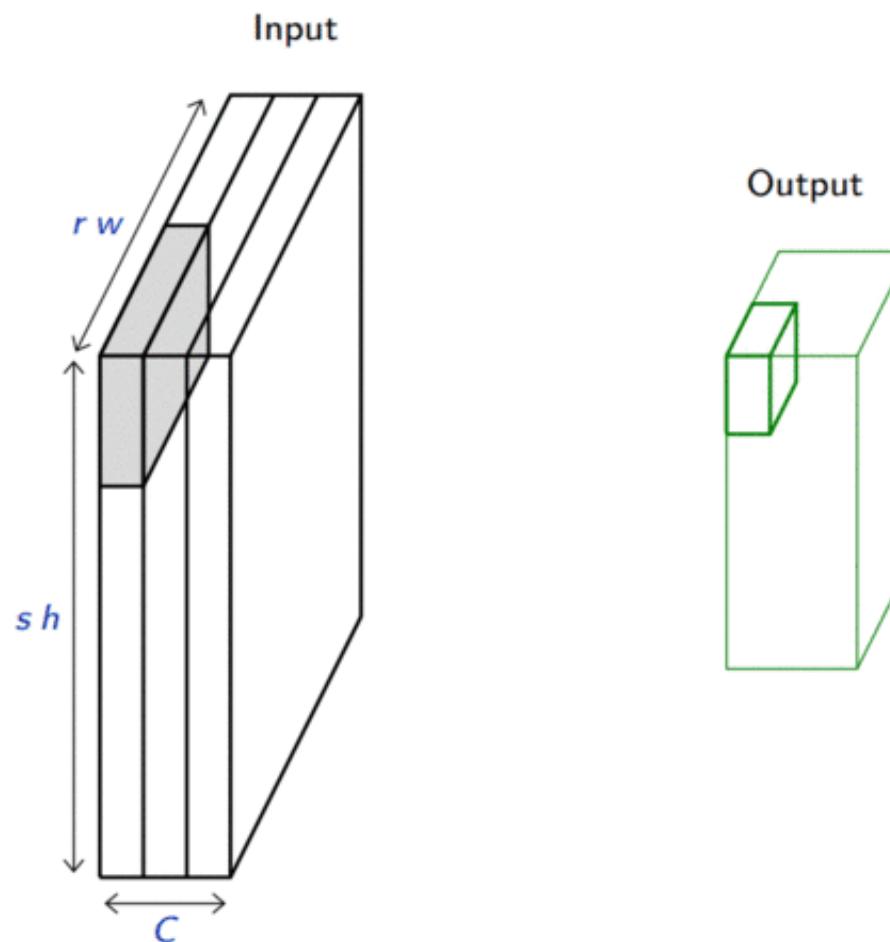
- Parameters are *shared* by each neuron producing an output in the activation map
- Dramatically reduces number of weights needed to produce an activation map
- Convolutional layer does pattern matching at any location → Equivariant to translation



Pooling

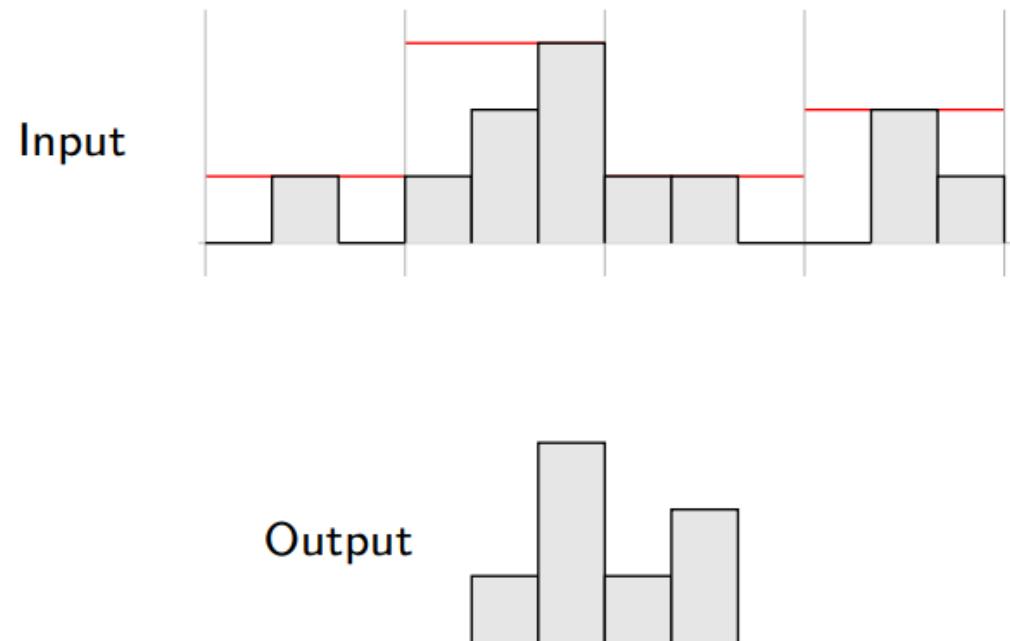
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- In each channel, find *max* or *average* value of pixels in a pooling area of size $h \times w$



Pooling

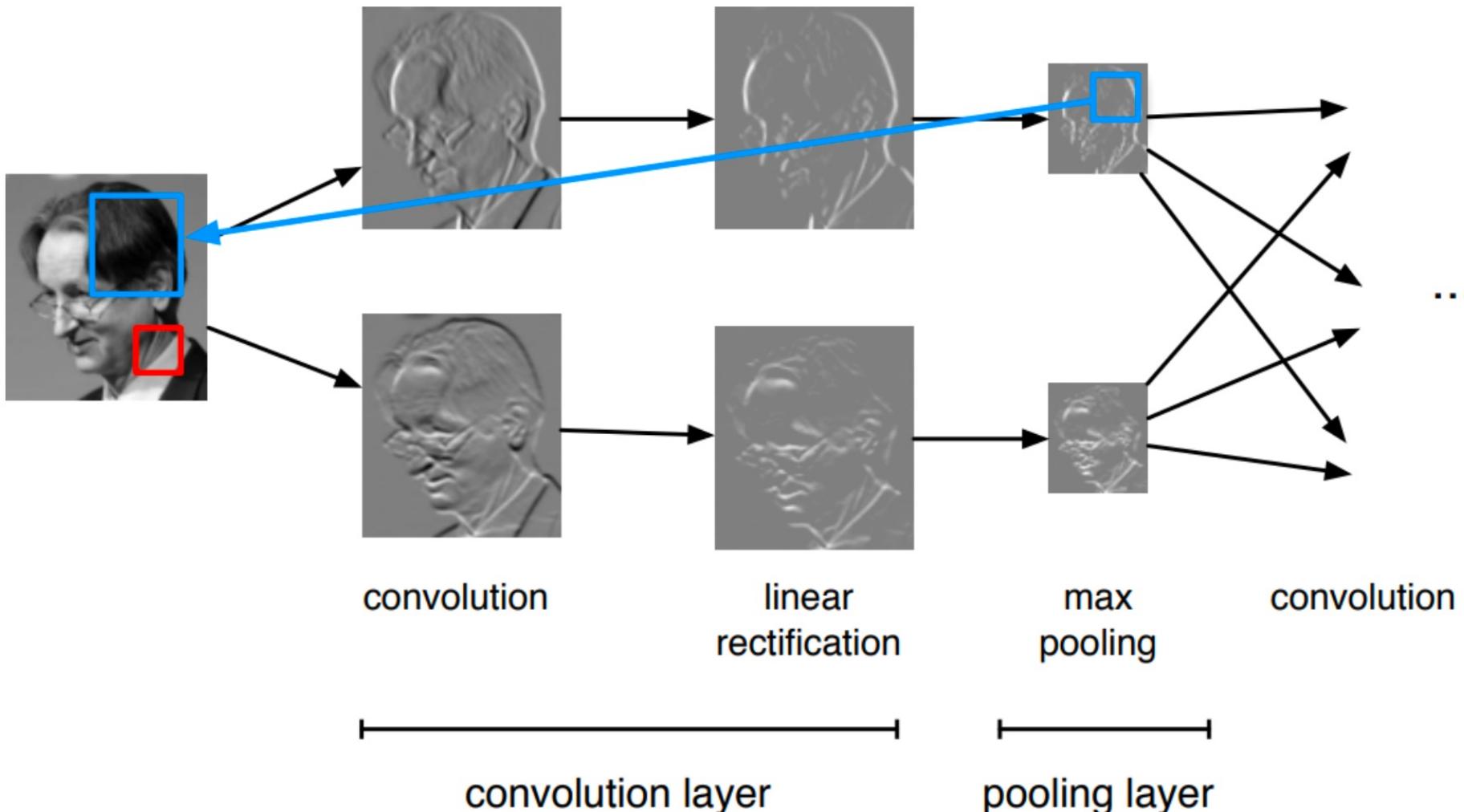
- In each channel, find *max* or *average* value of pixels in a pooling area of size $h \times w$
- Invariance to permutation within pooling area
- Invariance to local perturbations



Convolutional Network

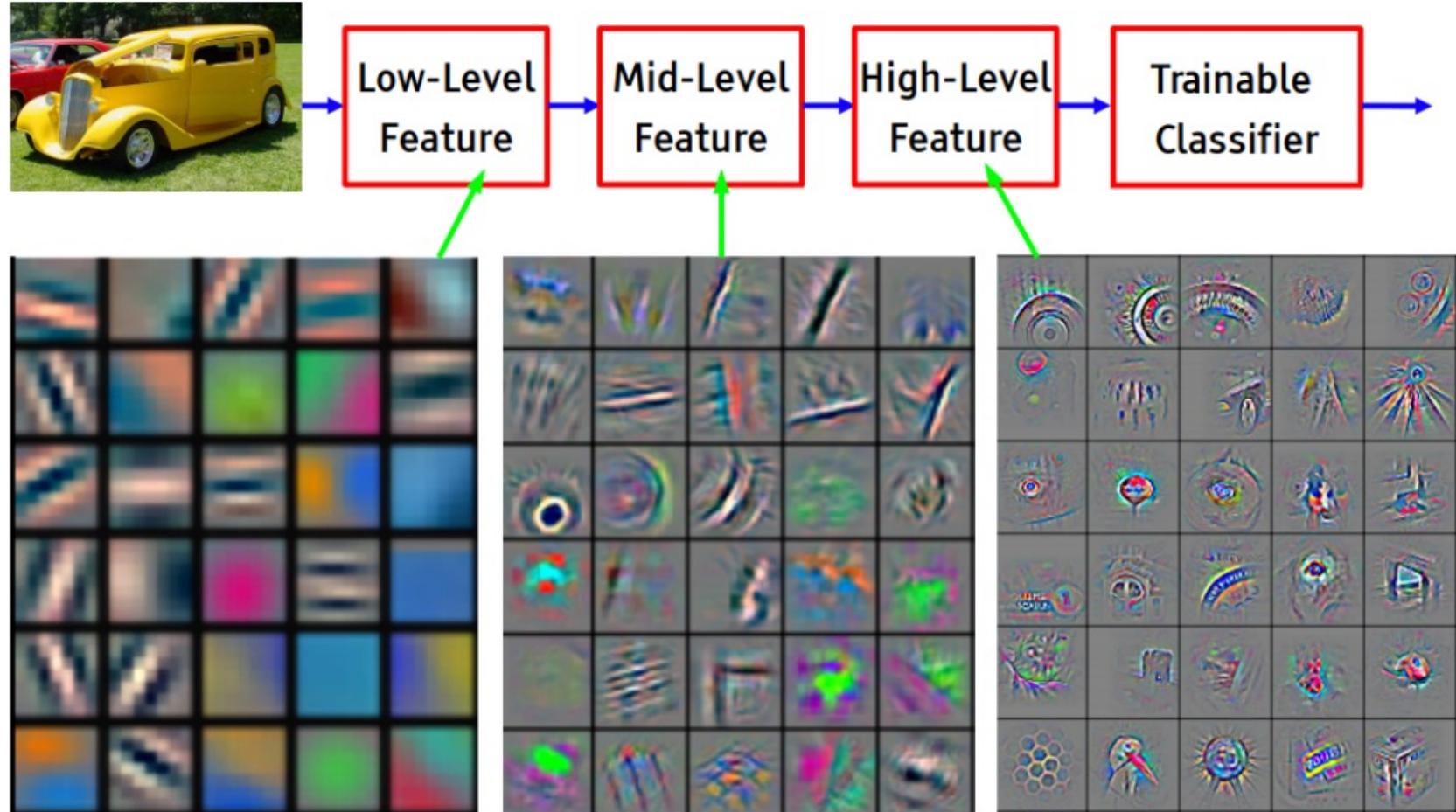
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- A combination of convolution, pooling, ReLU, and fully connected layers



Hierarchical Composition of Features

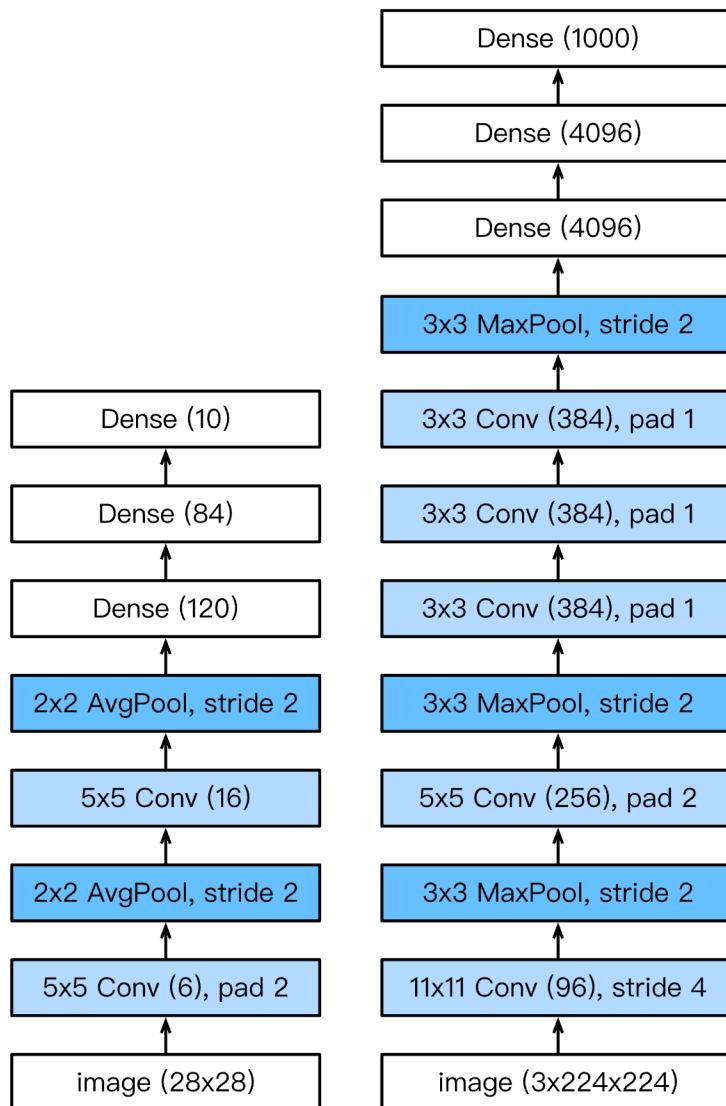
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Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

Convolutional Networks

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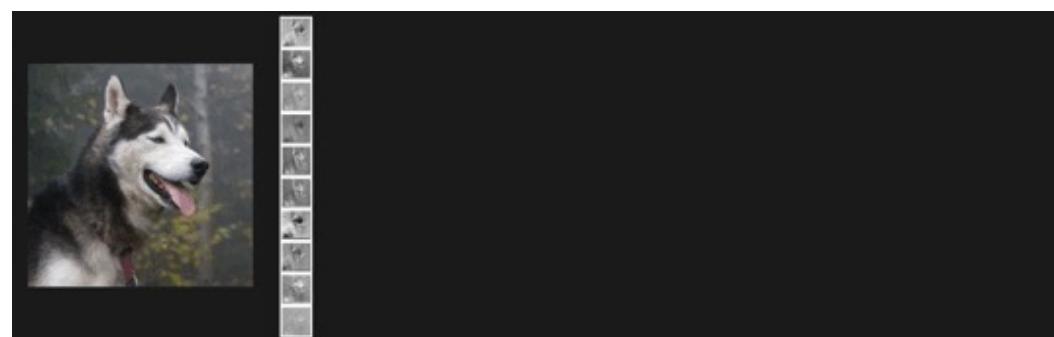


LeNet

(LeCun et al, 1998)

AlexNet

(Krizhevsky et al, 2012)

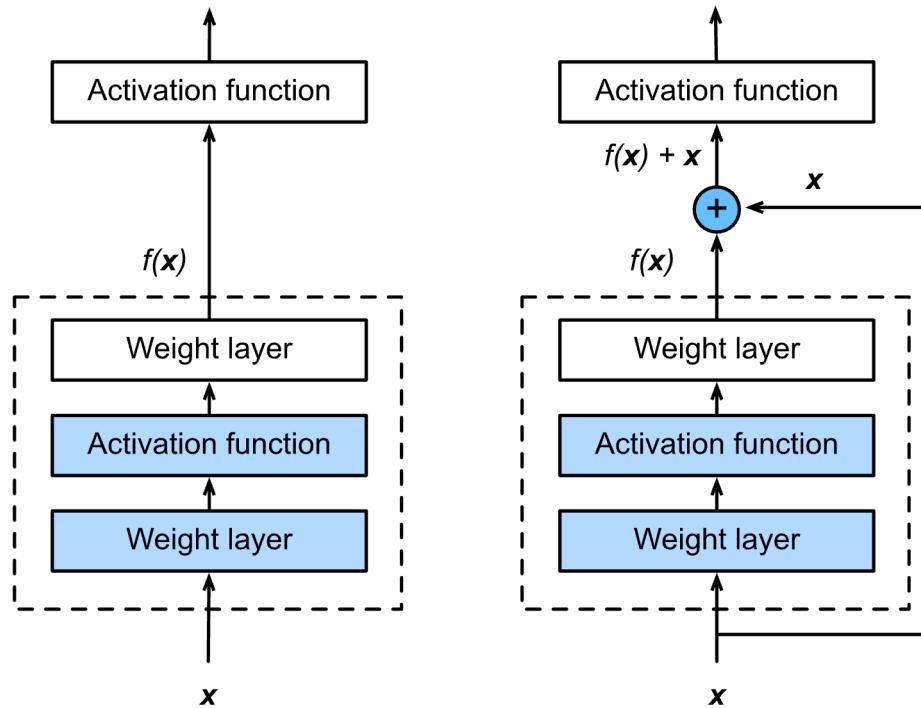


ImageNet Classification

Residual Connections

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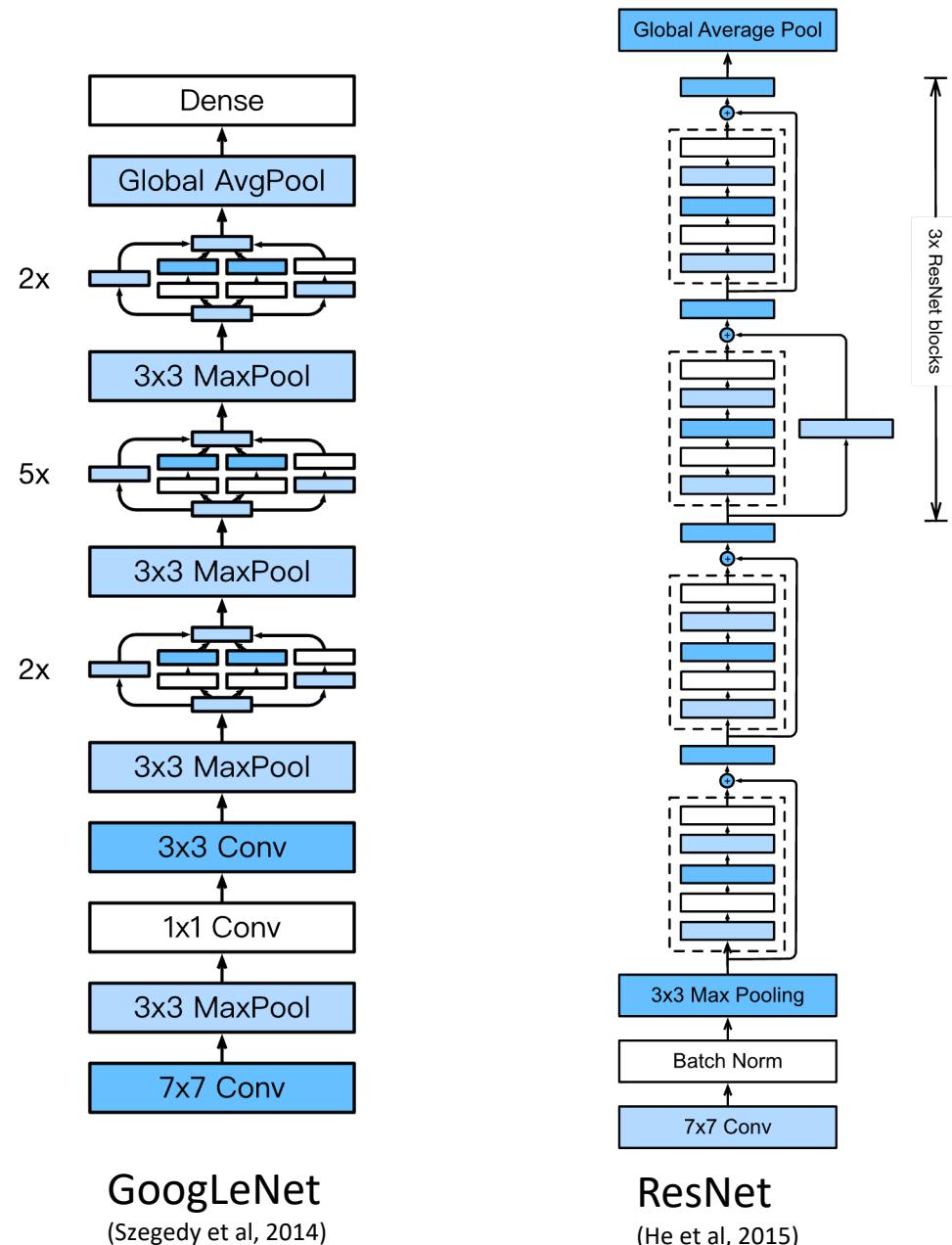
- Training very deep networks is made possible because of the **skip connections** in the residual blocks. Gradients can shortcut the layers and pass through without vanishing.



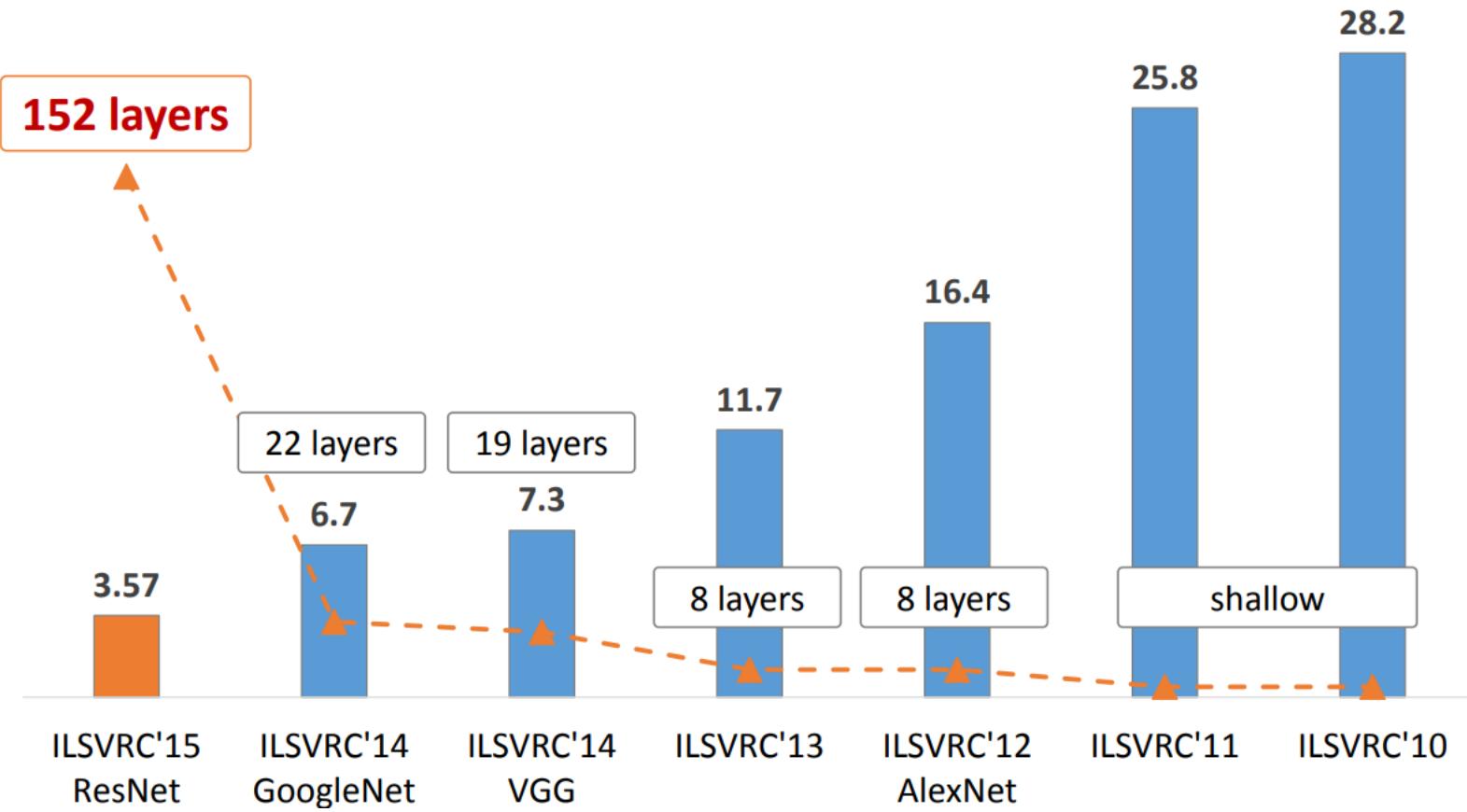
Deep CNNs

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- To go deeper, architectures become much more complex
 - Multiple convolutions in parallel and recombined
 - Skip connections
- Recent ResNet-152 has 152 layers!



Benefits of Depth



Recurrent Neural Networks

- Many types of data are not fixed in size
- Many types of data have a temporal or sequence-like structure
 - Text
 - Video
 - Speech
 - DNA
 - ...
- MLP expects fixed size data
- How to deal with sequences?

Sequential Data

- Given a set \mathcal{X} , let $S(\mathcal{X})$ be the set of sequences, where each element of the sequence $x_i \in \mathcal{X}$
 - \mathcal{X} could be reals \mathbb{R}^M , integers \mathbb{Z}^M , etc.
 - Sample sequence $x = \{x_1, x_2, \dots, x_T\}$
- Tasks related to sequences:
 - Classification $f: S(\mathcal{X}) \rightarrow \{p \mid \sum_{c=1}^N p_i = 1\}$
 - Generation $f: \mathbb{R}^d \rightarrow S(\mathcal{X})$
 - Seq.-to-seq. translation $f: S(\mathcal{X}) \rightarrow S(\mathcal{Y})$

- Input sequence $x \in S(\mathbb{R}^m)$ of *variable* length $T(x)$
- Standard approach: use recurrent model that maintains a **recurrent state** $\mathbf{h}_t \in \mathbb{R}^q$ updated at each time step t .
For $t = 1, \dots, T(x)$:

$$\mathbf{h}_{t+1} = \phi(\mathbf{x}_t, \mathbf{h}_t; \theta)$$

- Simplest model:
- $$\phi(\mathbf{x}_t, \mathbf{h}_t; W, U) = \sigma(W\mathbf{x}_t + U\mathbf{h}_t)$$
- Predictions can be made at any time t from the recurrent state

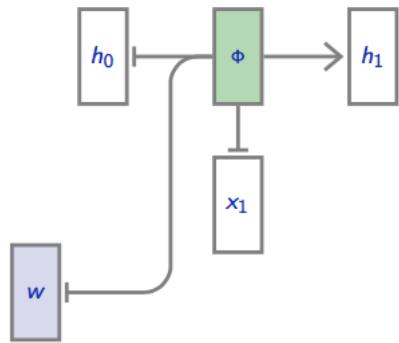
$$\mathbf{y}_t = \psi(\mathbf{h}_t; \theta)$$

Recurrent Neural Networks

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Recurrent Model

$$\mathbf{h}_{t+1} = \phi(\mathbf{x}_t, \mathbf{h}_t; \theta)$$

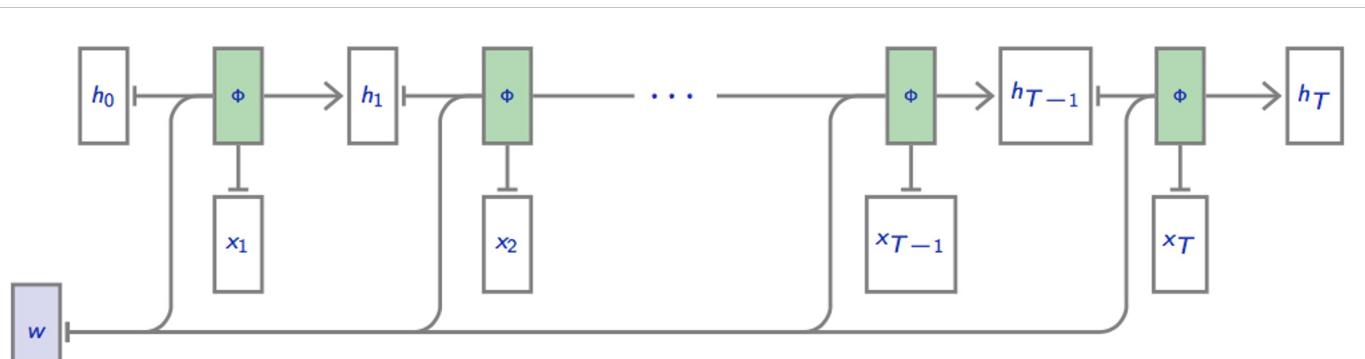


Recurrent Neural Networks

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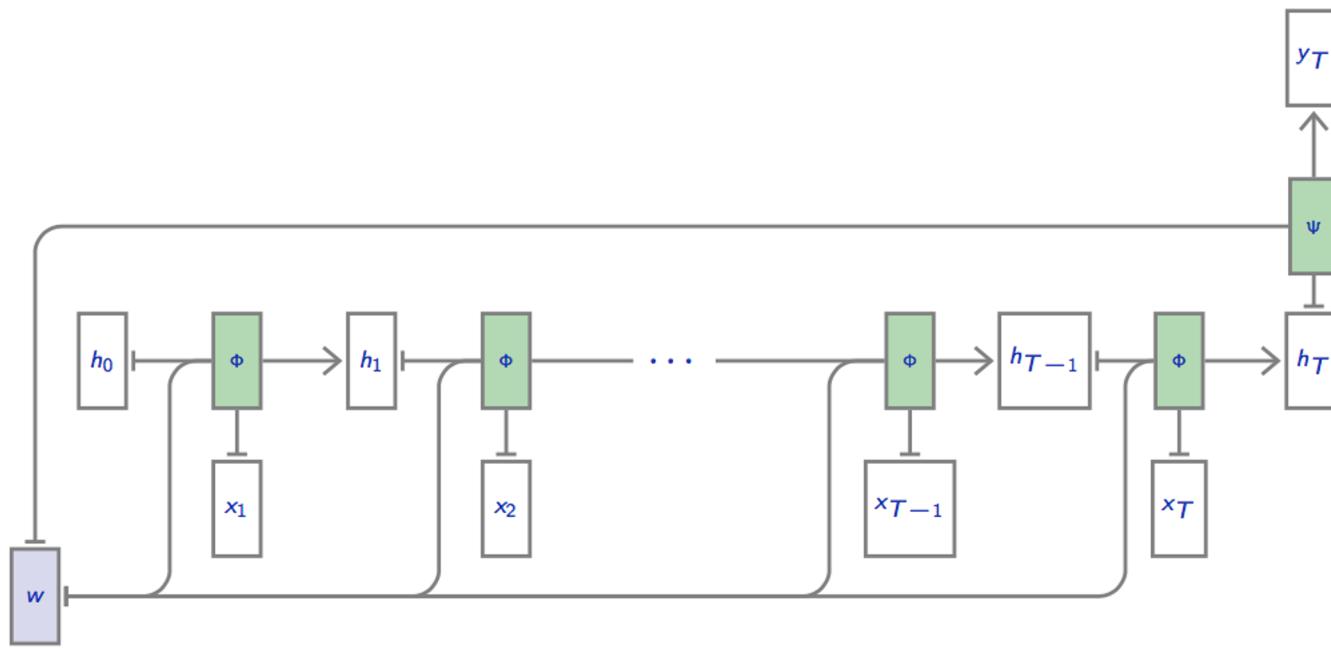
Recurrent Model

$$\mathbf{h}_{t+1} = \phi(\mathbf{x}_t, \mathbf{h}_t; \theta)$$

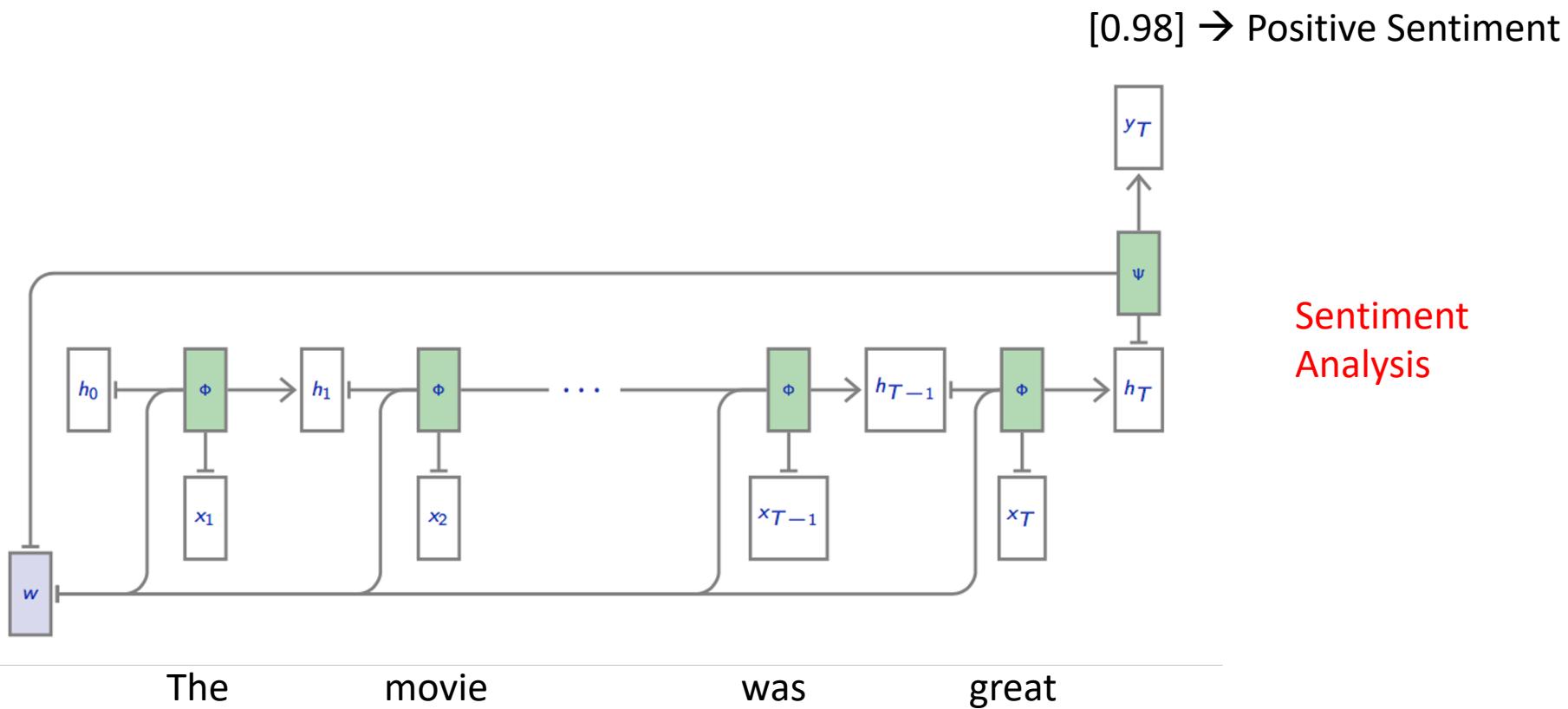


Recurrent Neural Networks

Prediction
 $y_t = \psi(h_t; \theta)$

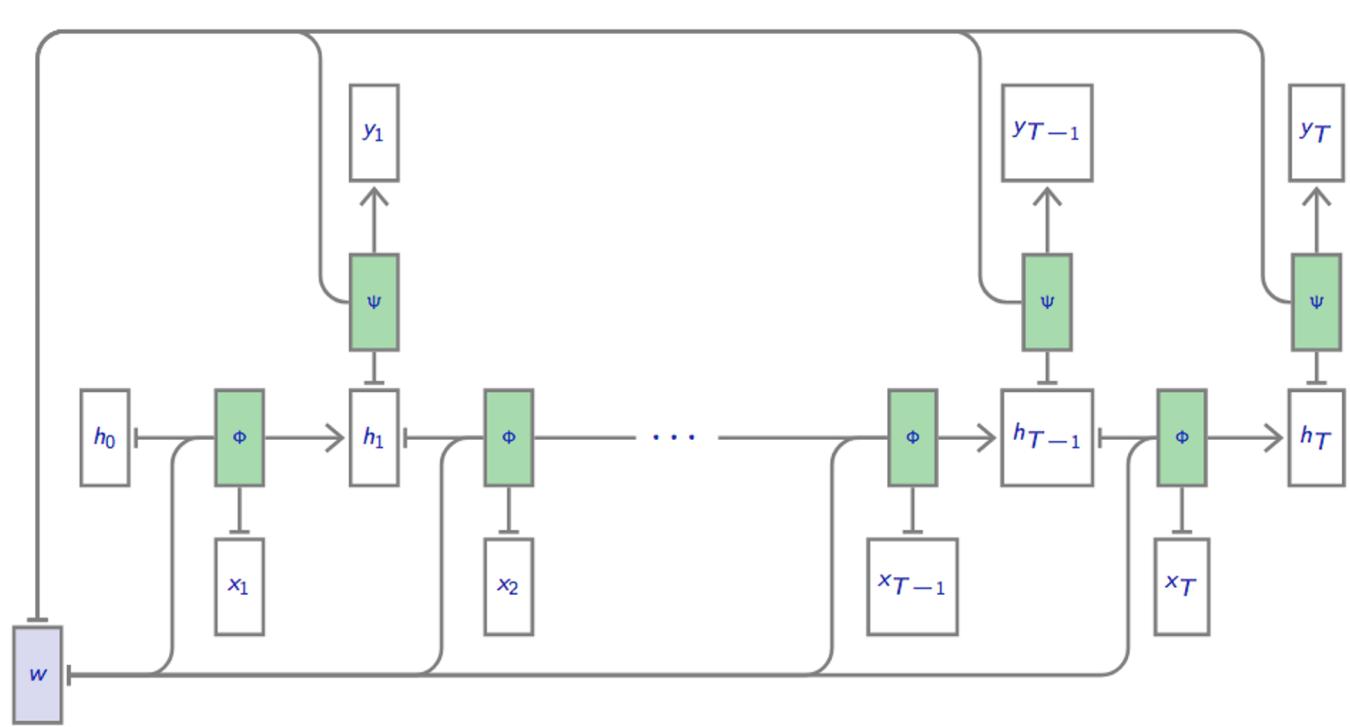


Recurrent Neural Networks



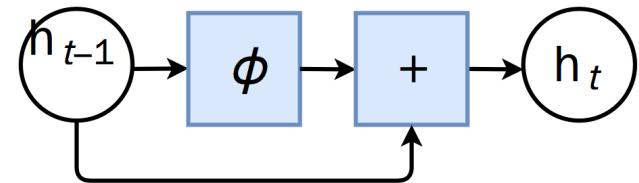
Recurrent Neural Networks

Prediction per sequence element



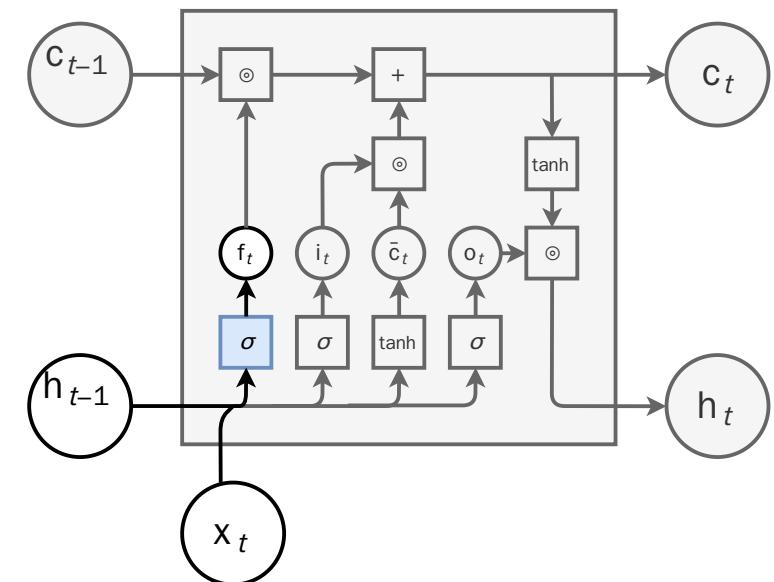
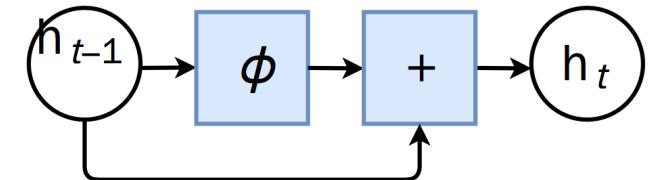
Although the number of steps $T(x)$ depends on x , this is a standard computational graph and automatic differentiation can deal with it as usual. This is known as “backpropagation through time” (Werbos, [1988](#))

- Gating:
 - network can grow very deep, in time → vanishing gradients.
 - *Critical component*: add pass-through (additive paths) so recurrent state does not go repeatedly through squashing non-linearity.



Long Short Term Memory (LSTM)

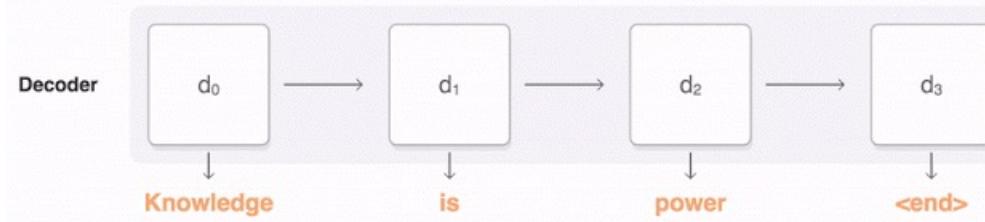
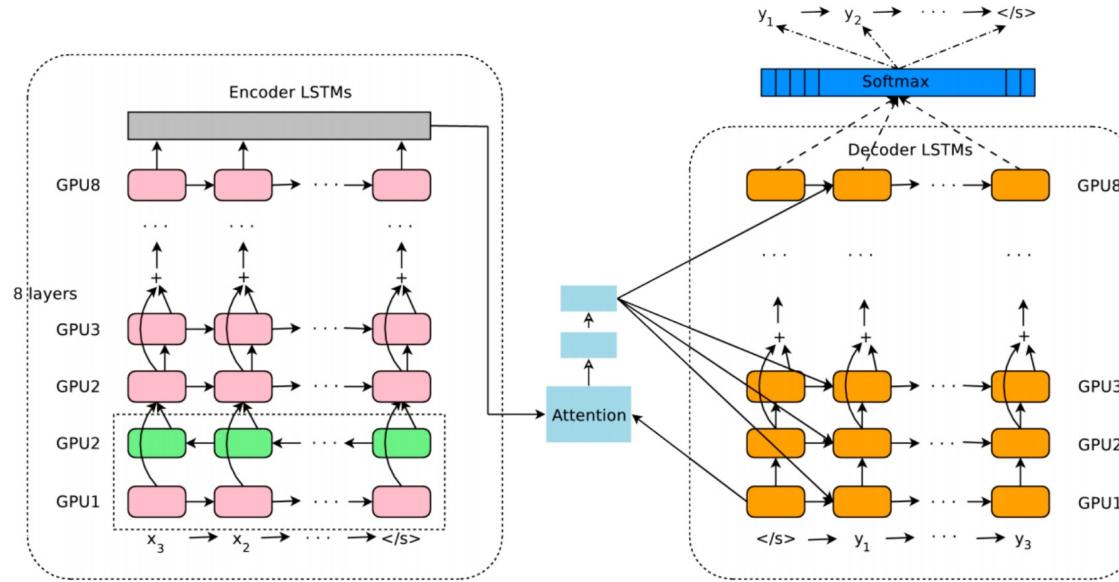
- Gating:
 - network can grow very deep, in time → vanishing gradients.
 - *Critical component*: add pass-through (additive paths) so recurrent state does not go repeatedly through squashing non-linearity.
- LSTM:
 - Add internal state separate from output state
 - Add input, output, and forget gating



Examples

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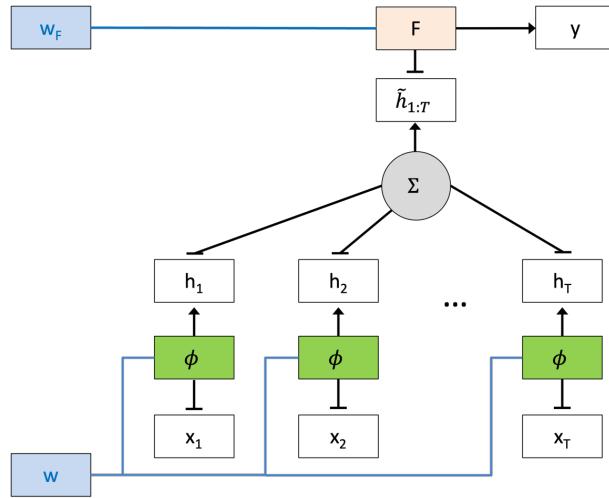
Neural machine translation



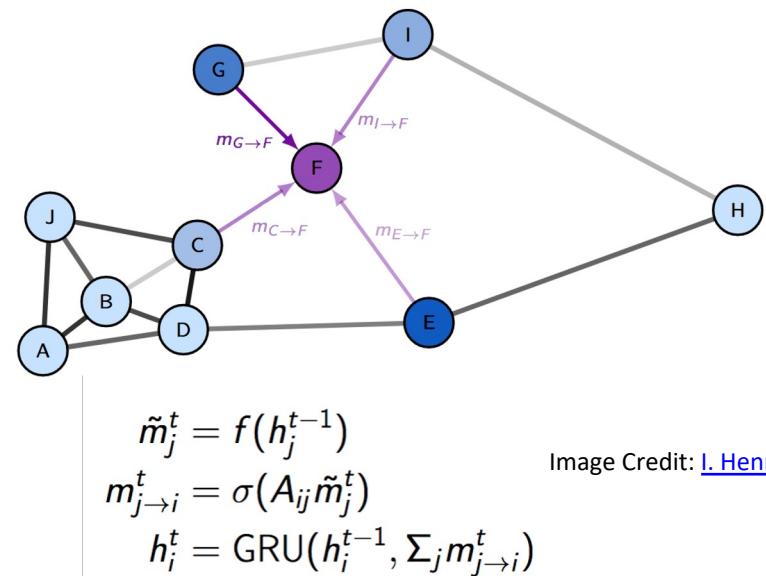
Many Other Architecture Choices

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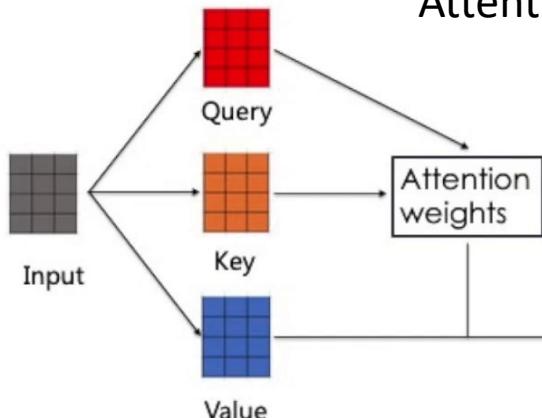
Deep Sets



Graph Neural Networks

Image Credit: [I. Henrion](#)

Attention and Transformers



$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

+ More...

Beyond Regression and Classification

Beyond Regression and Classification

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- Not all tasks are predicting a label from features, as in classification and regression
- May want to explicitly model a high-dim. signal
 - Data synthesis / simulation
 - Density estimation, Anomaly detection
 - Denoising, Super Resolution, Data compression
 - ...
- Often don't have labels → *Unsupervised Learning*
- **Generative models** aim to:
 - Learn a density $p(x)$ that explains the data
 - Draw samples of plausible data points

Generative Models Are Everywhere These Days

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Prompt:

*street style photo of a woman
selling pho at a Vietnamese
street market, sunset,
shot on fujifilm*



Deep Generative Model Examples in Science

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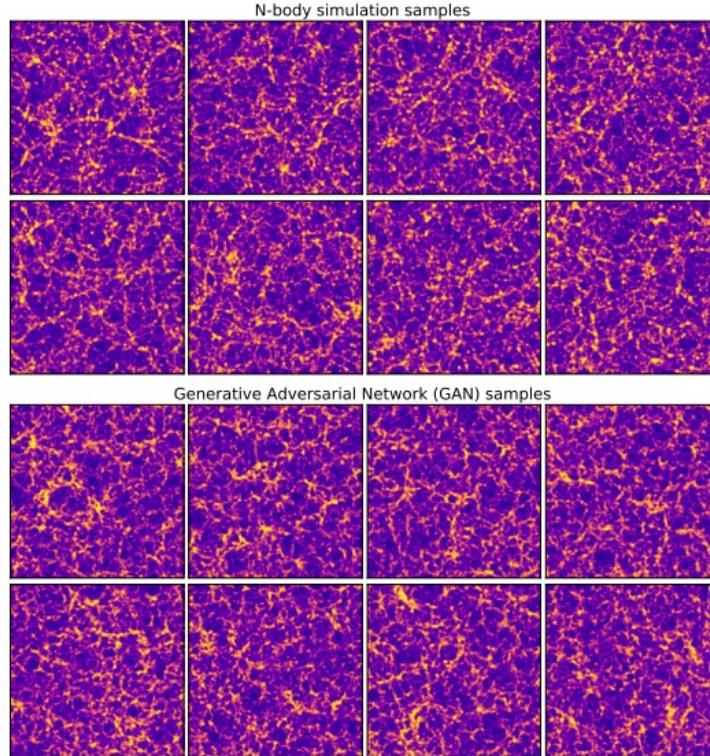
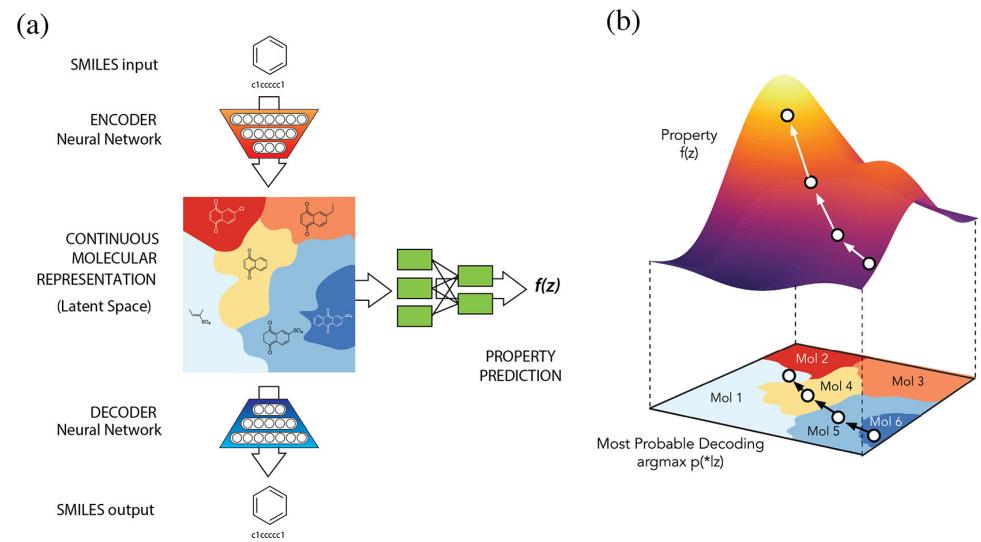
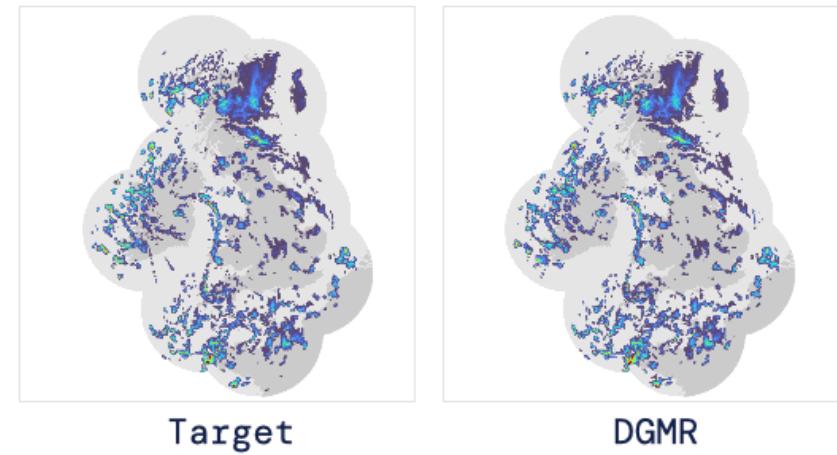


Figure 1: Samples from N-body simulation and from GAN for the box size of 500 Mpc. Note that the transformation in Equation 3.1 with $a = 20$ was applied to the images shown above for better clarity.

Learning cosmological models (Rodriguez et al, 2018)



Design of new molecules with desired chemical properties.
(Gomez-Bombarelli et al, 2016)



Deep Generative Model of Rainfall (Ravuri et. al. 2021)

Generative Models Goal

A **generative model** is a probabilistic model q that can be used as a simulator of the data.

Goal: generate synthetic, realistic high-dimensional data

$$x \sim q(x; \theta)$$

that is as close as possible to the unknown data distribution $p(x)$ for which we have empirical samples.

i.e. want to recreate the raw data distribution (such as the distribution of natural images).

Generative Models Goal

A **generative model** is a probabilistic model q that can be used as a simulator of the data.

Goal: generate synthetic, realistic high-dimensional data

$$x \sim q(x; \theta)$$

x is a random variable sampled from the distribution $q(x; \theta)$

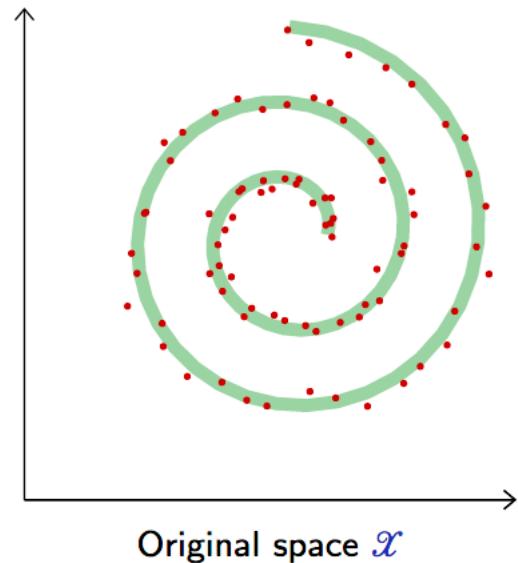
Goal: Learn θ

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i.e. want to recreate the raw data distribution (such as the distribution of natural images).

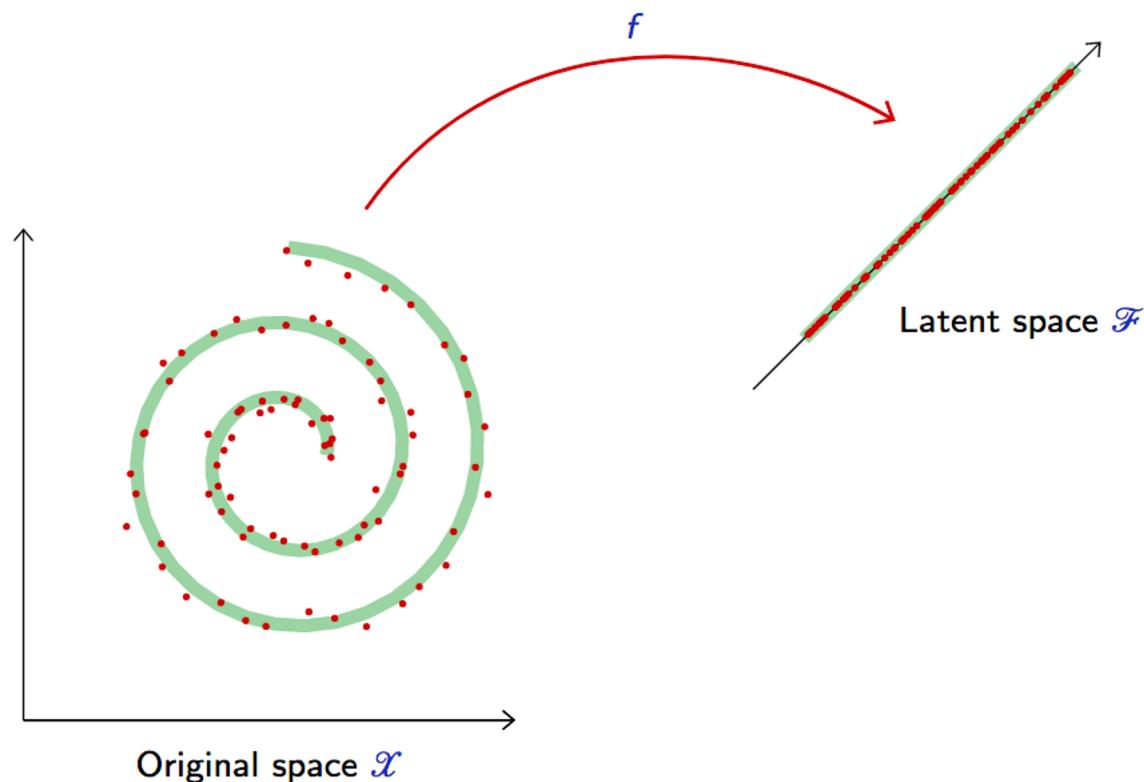
Modeling Data and Meaningful Degrees of Freedom

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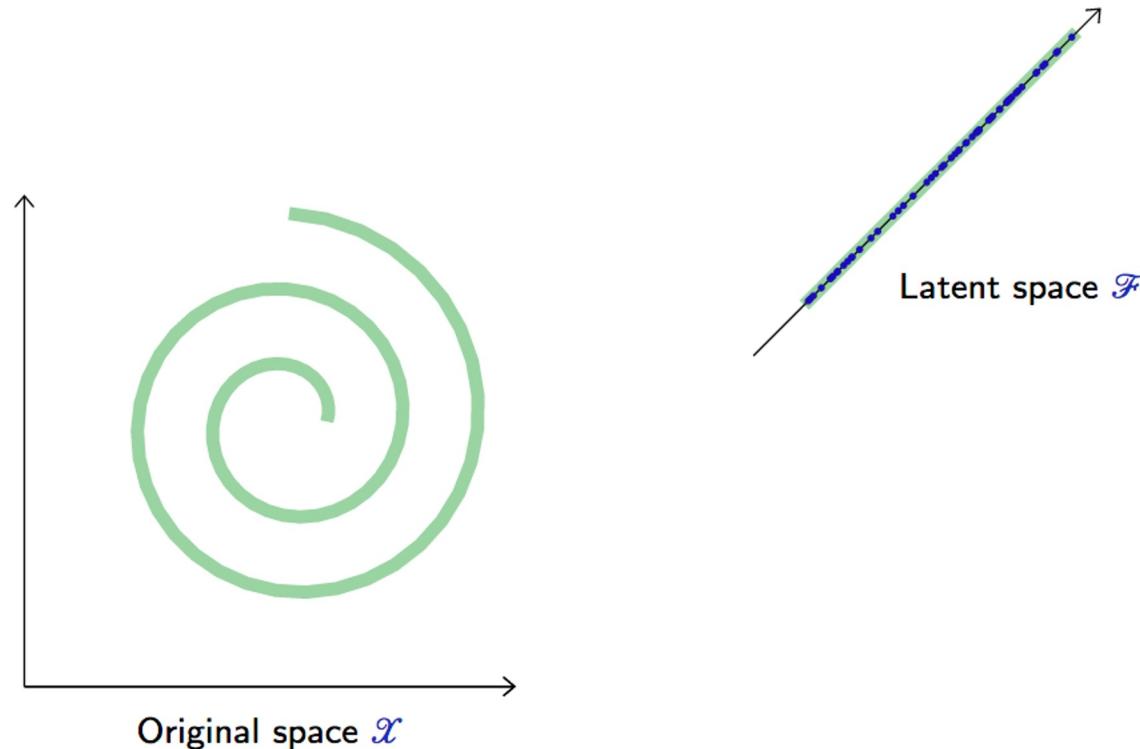
Modeling Data and Meaningful Degrees of Freedom

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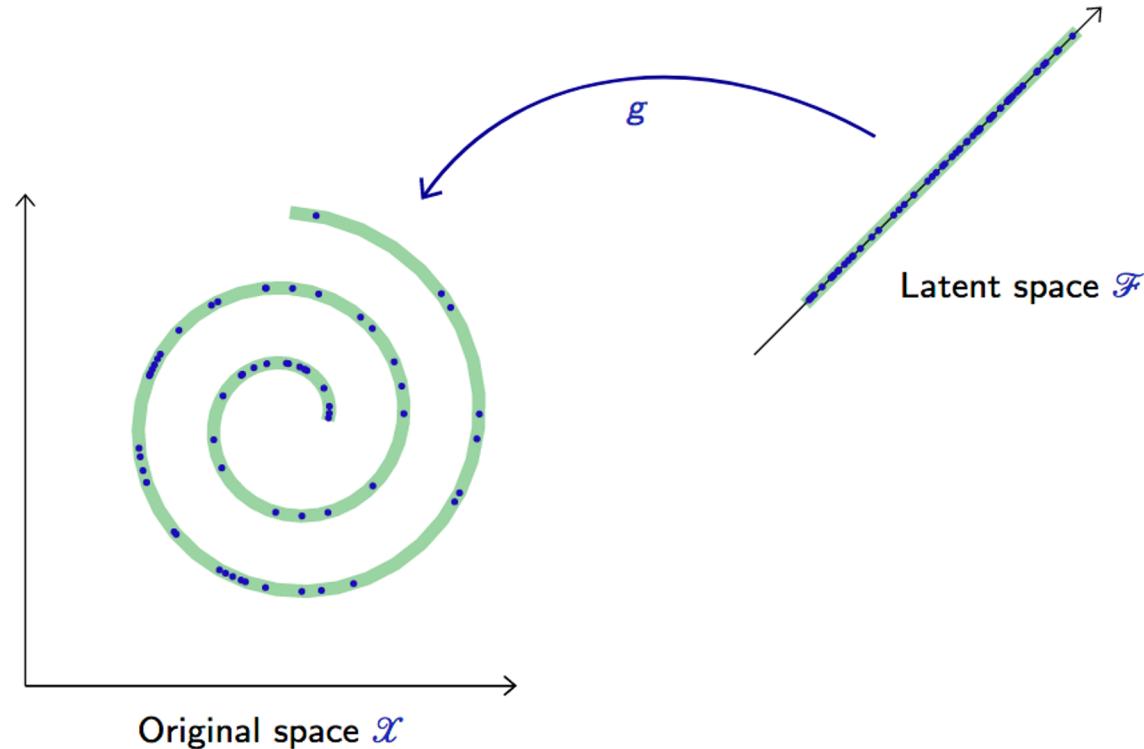
Modeling Data and Meaningful Degrees of Freedom

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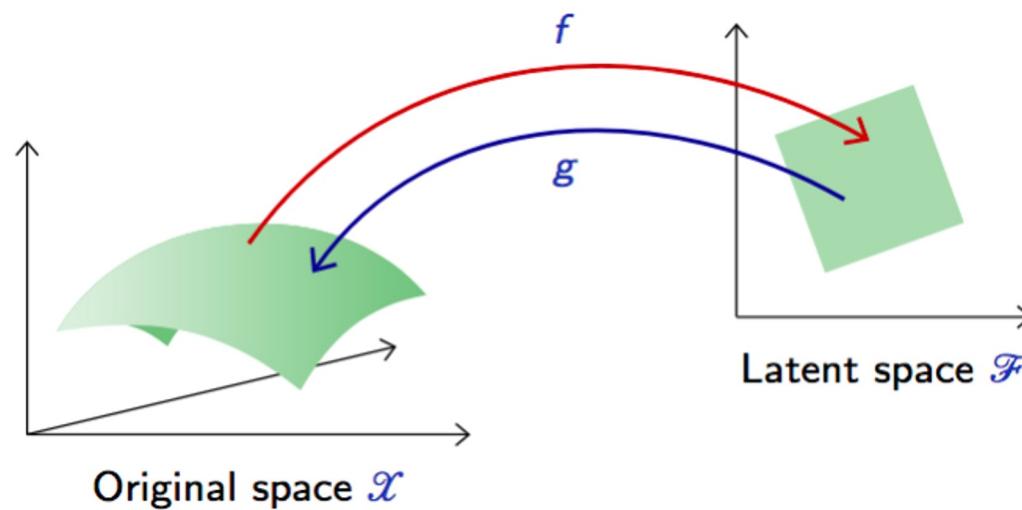
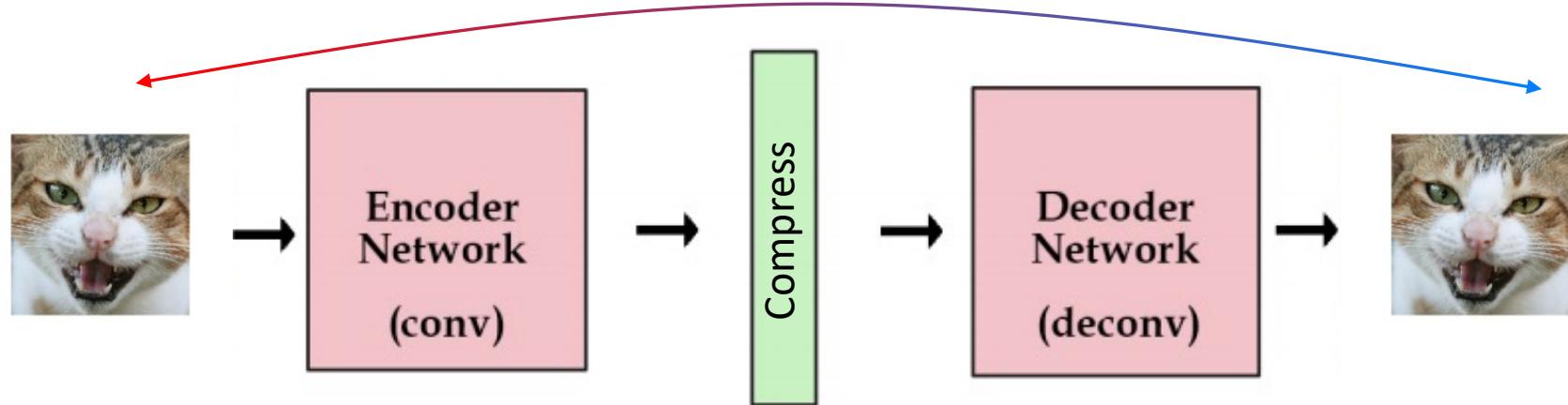
Modeling Data and Meaningful Degrees of Freedom

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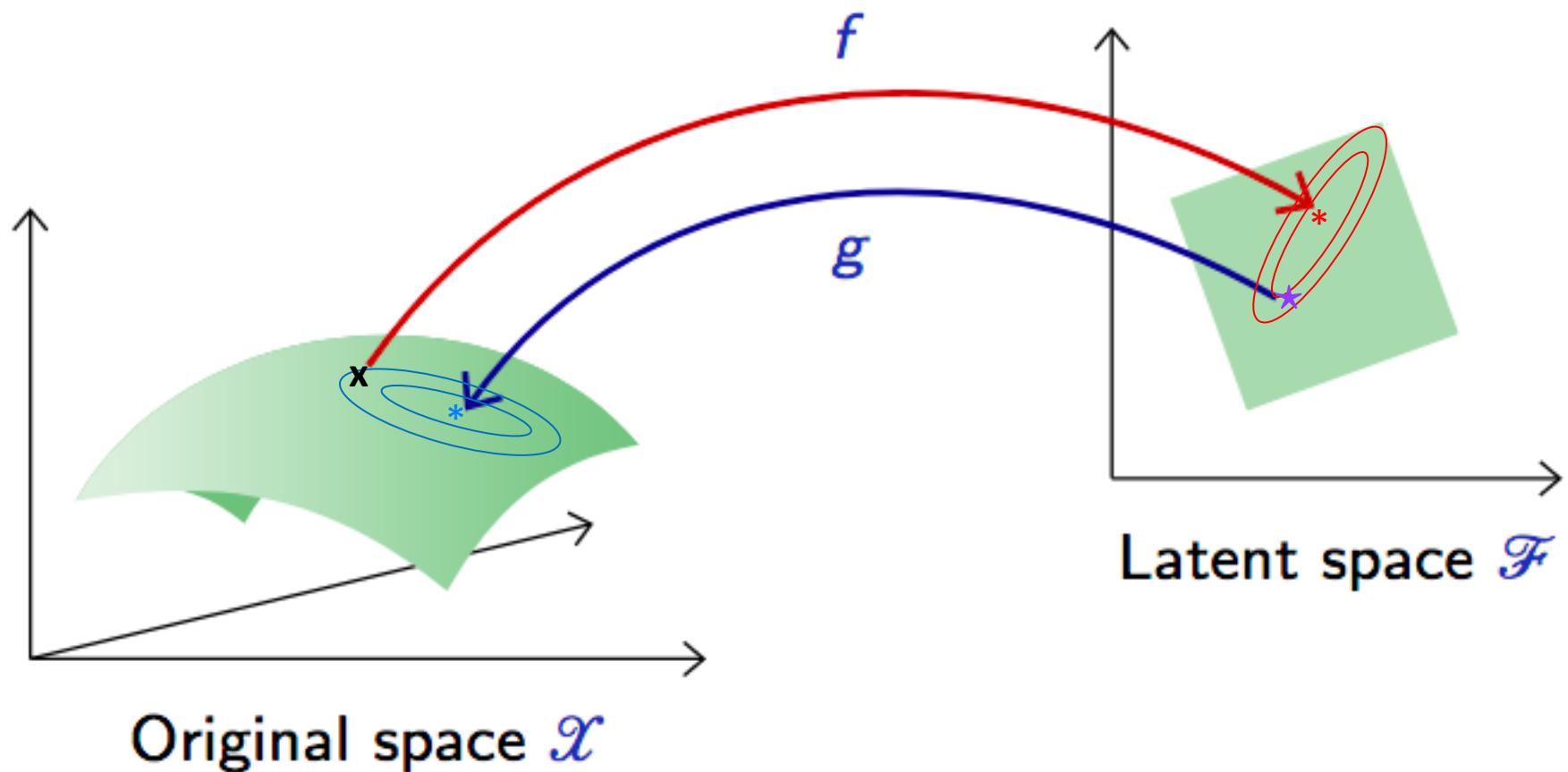
AutoEncoders

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Modeling Data and Meaningful Degrees of Freedom

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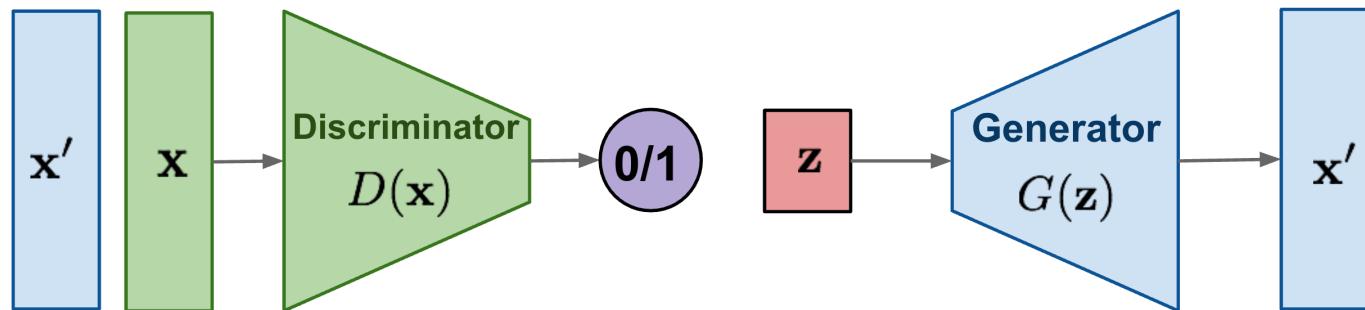


Common Approach to Deep Generative Modeling:
Choose **known distribution** for latent space and **learn map** to data space

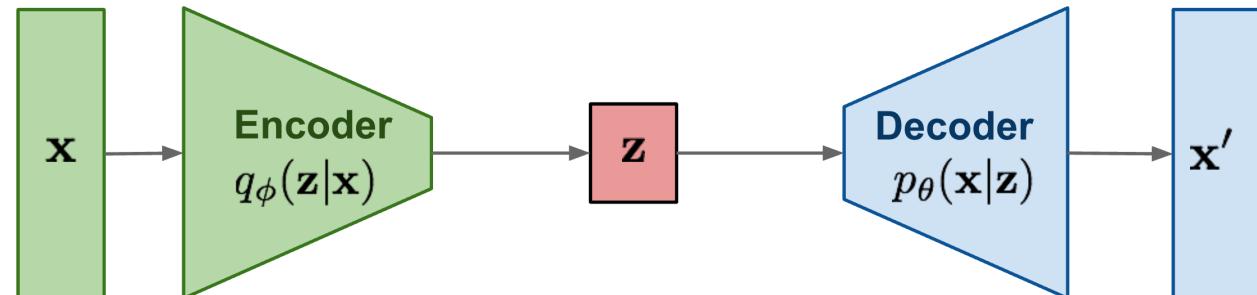
What Deep Generative Models Are There?

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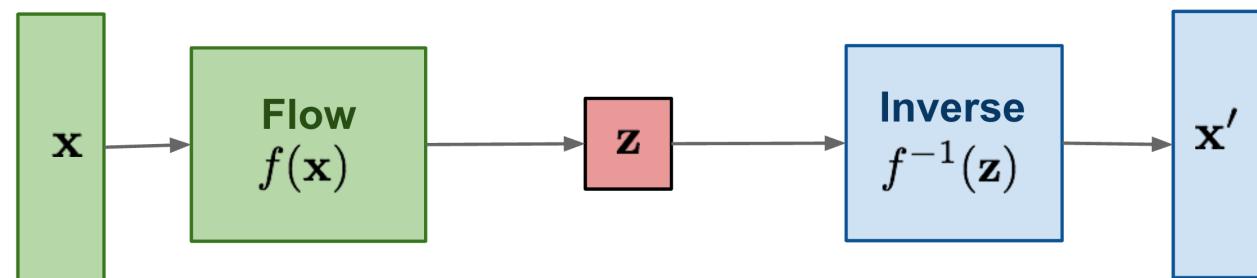
GAN: Adversarial training



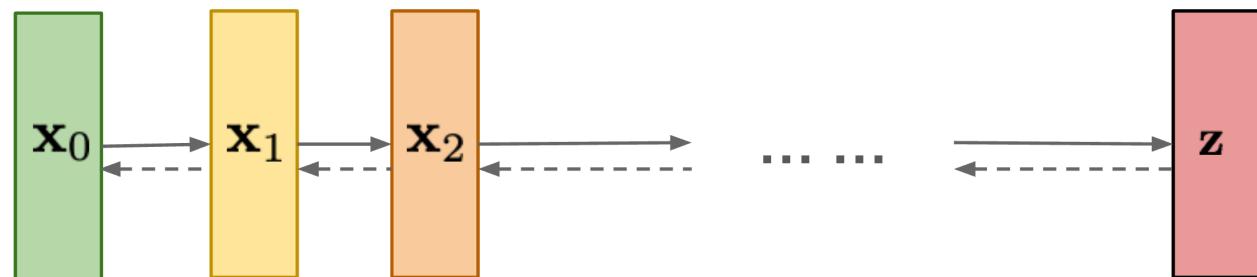
VAE: maximize variational lower bound



Flow-based models:
Invertible transform of distributions

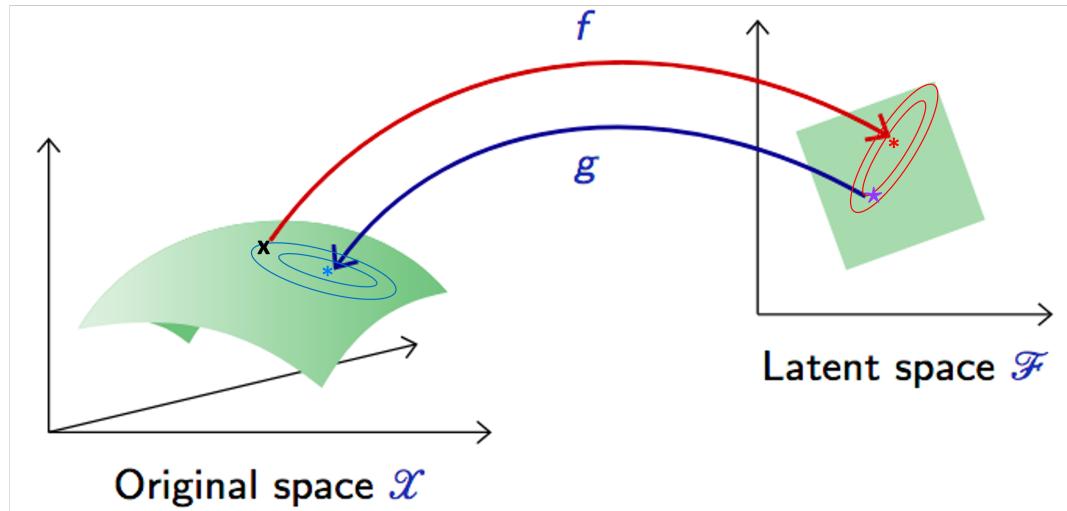
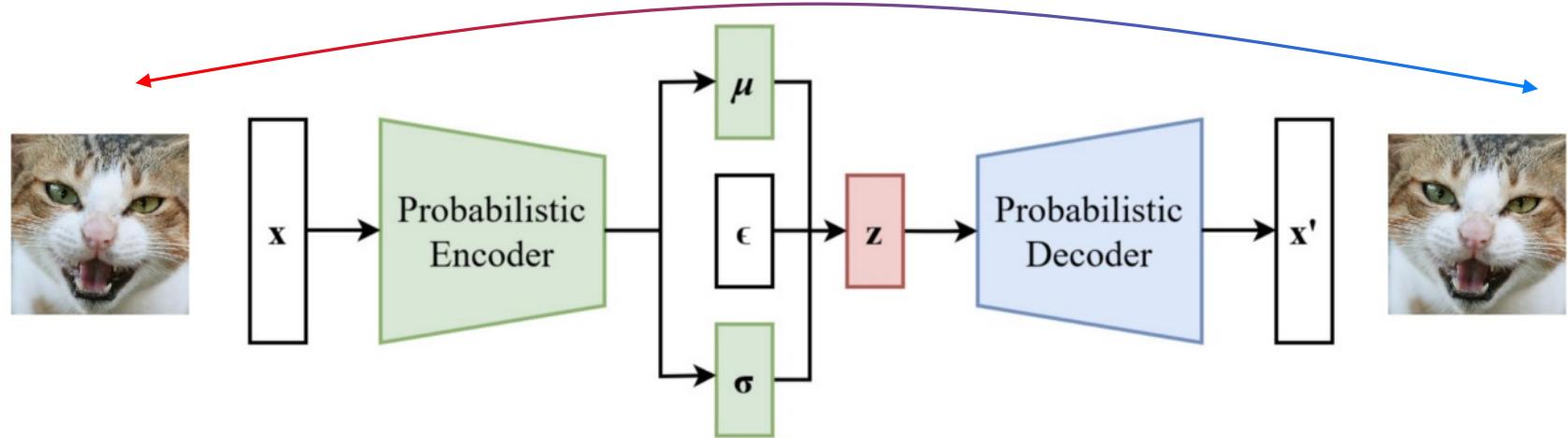


Diffusion models:
Gradually add Gaussian noise and then reverse



Variational AutoEncoders

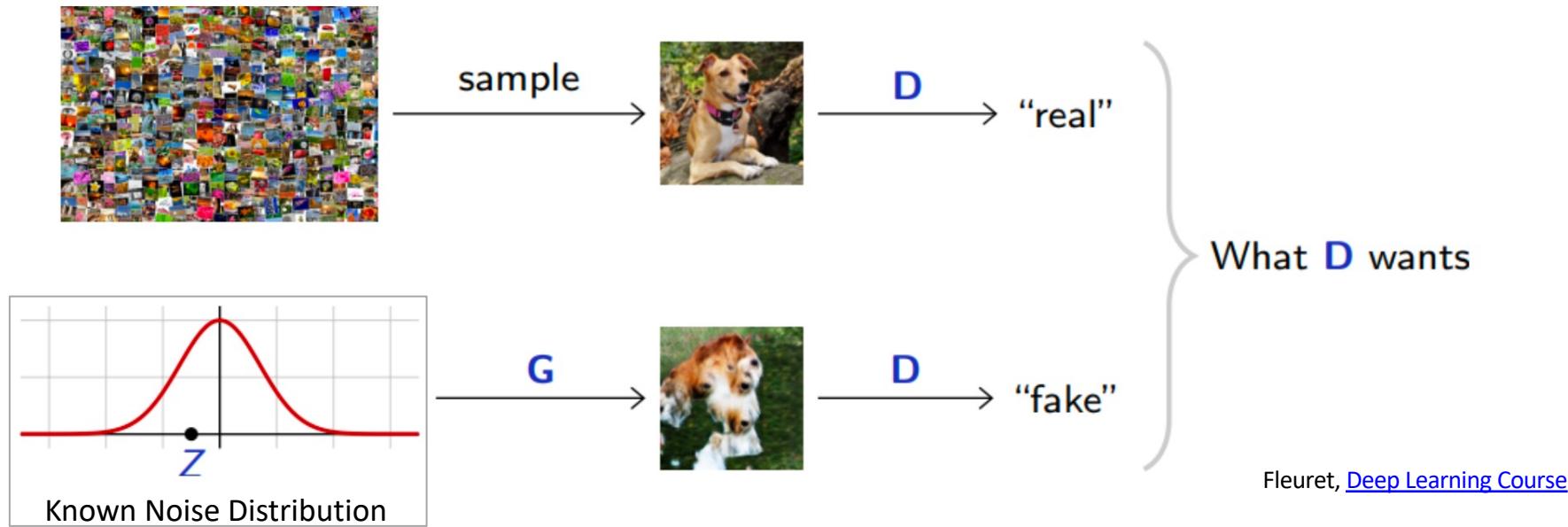
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Generative Adversarial Networks (GAN)

Goodfellow et. al., [2014](#)

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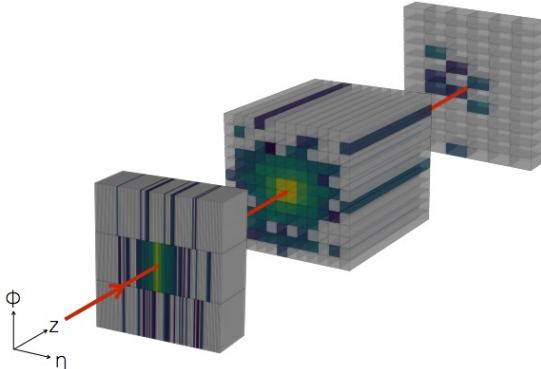
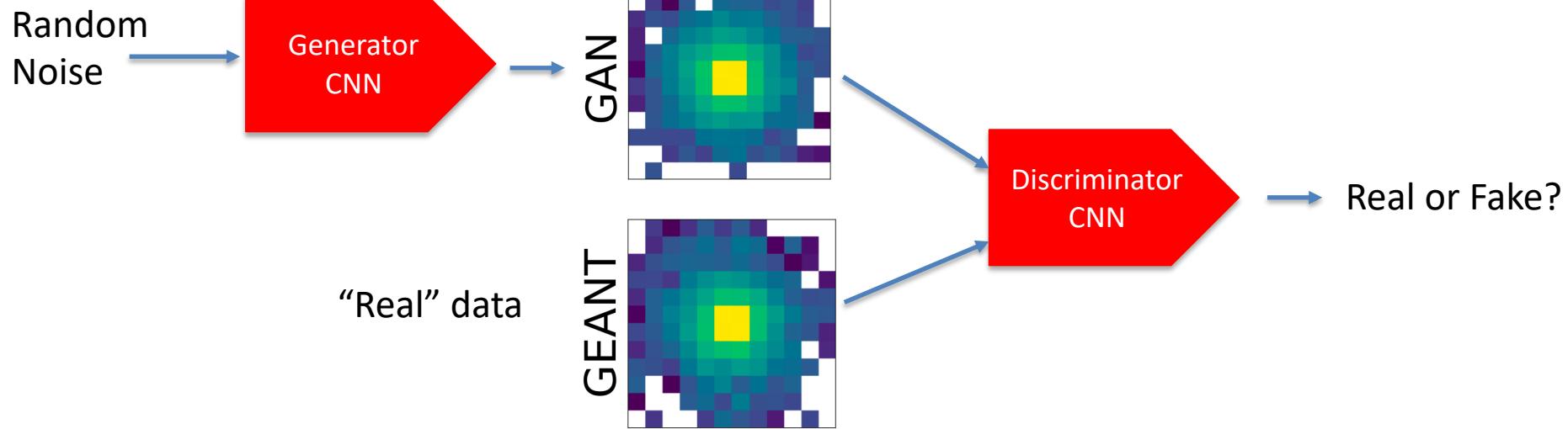


Fleuret, [Deep Learning Course](#)

- **Generator goal:**
 - Produce *fake* data to trick discriminator to classify as *real*
- **Discriminator goal:**
 - Classify data as *real* or *fake*, as well as possible
- **Adversarial setup**
 - Two-player game with two networks w/ opposing objectives

GANs for Calorimeter Energy Depositions

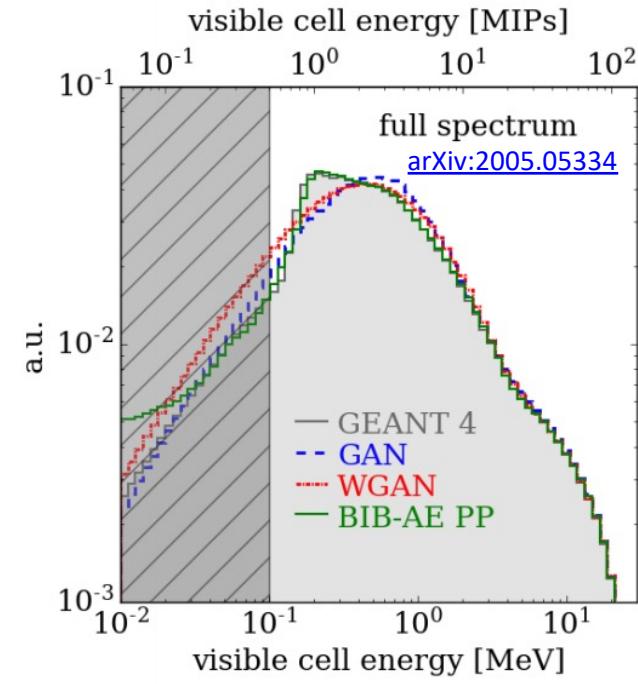
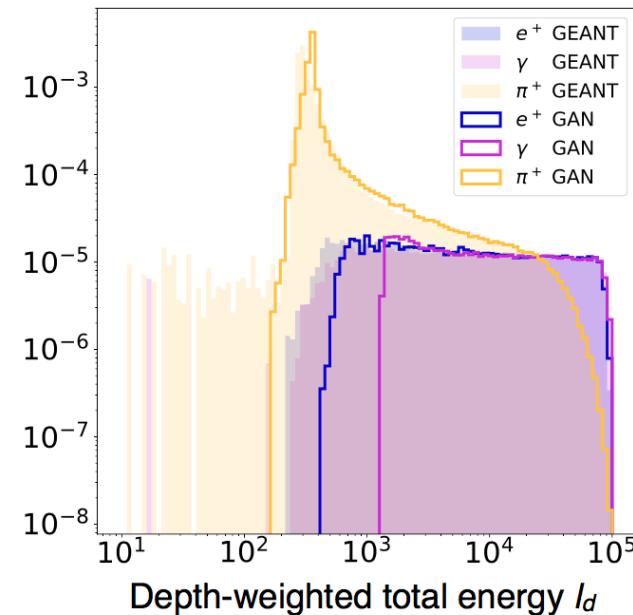
57



PRD97, 014021 (2018)

arXiv:1705.02355

arXiv:1701.05927



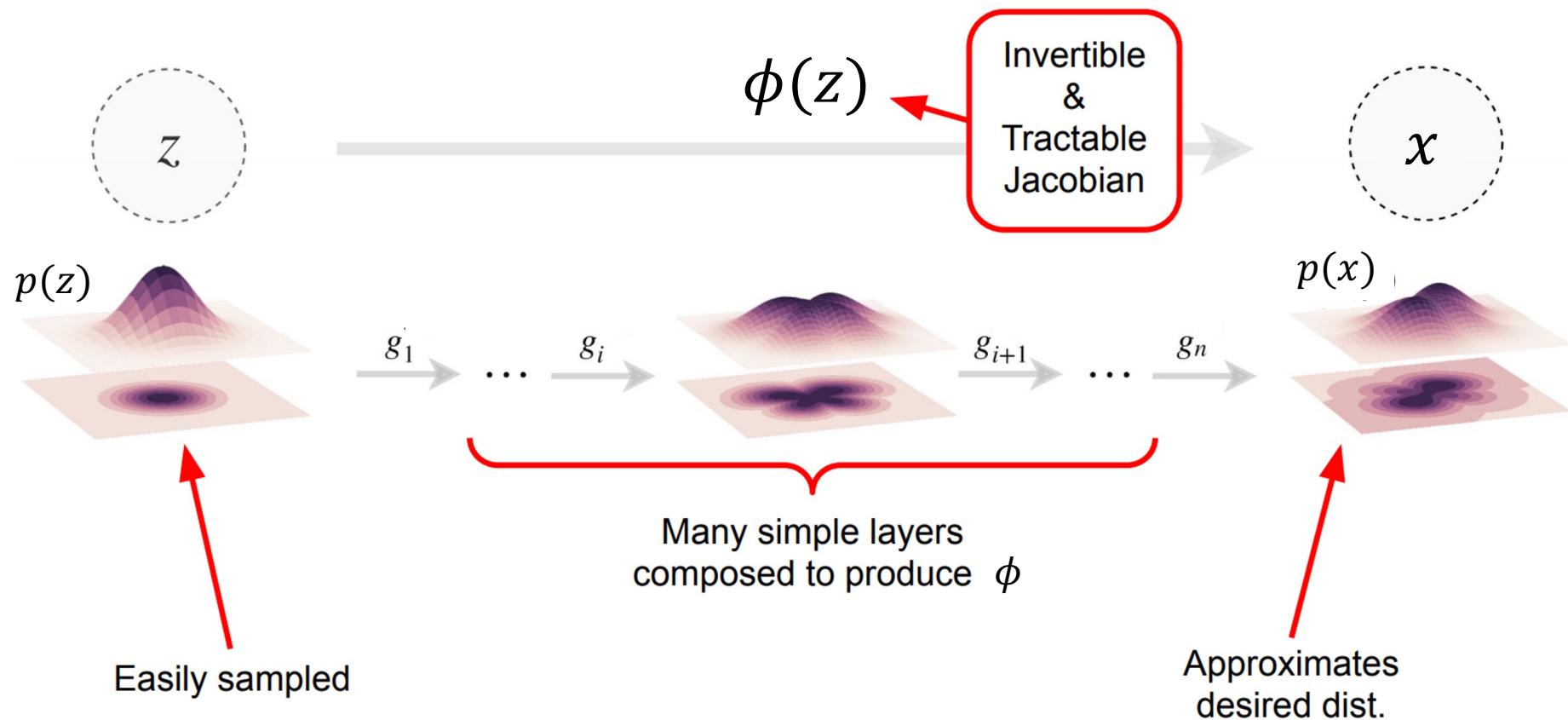
Normalizing Flows

58

Normalizing flows allows *explicit density estimation*

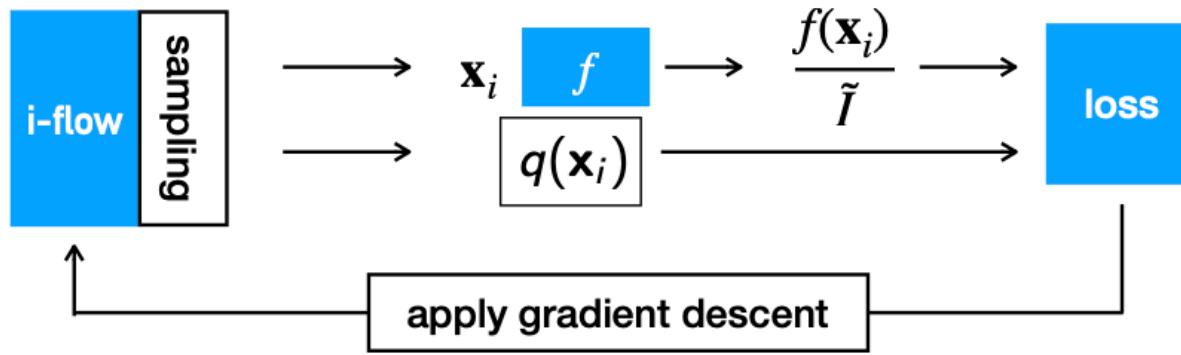
We can evaluate density $p(x)$

$$p_x(\mathbf{x}) = p_z(\mathbf{z}) \left| \det \left(\frac{\partial \phi(\mathbf{z})}{d\mathbf{z}} \right)^{-1} \right|$$



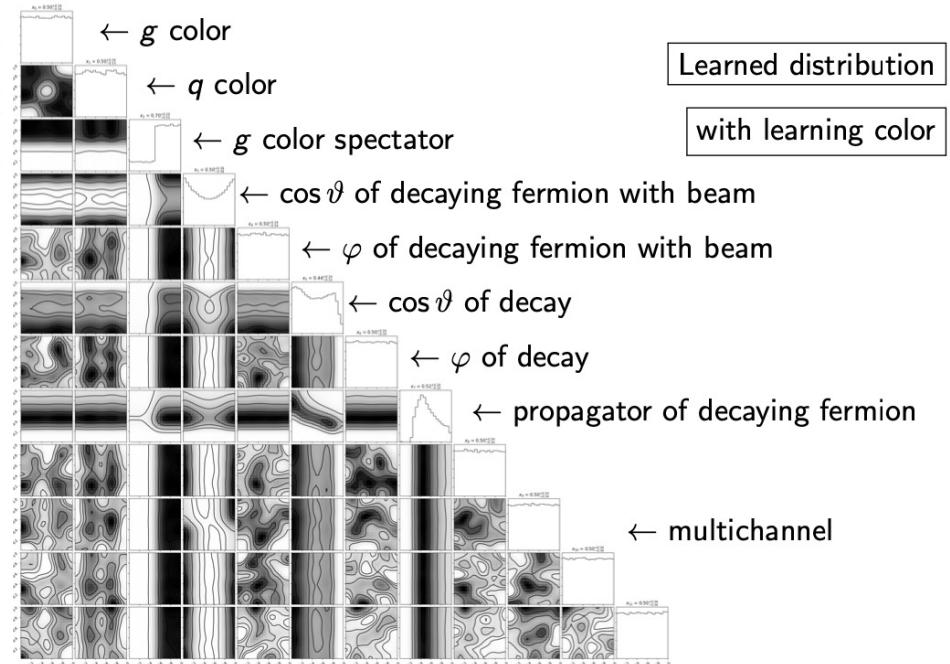
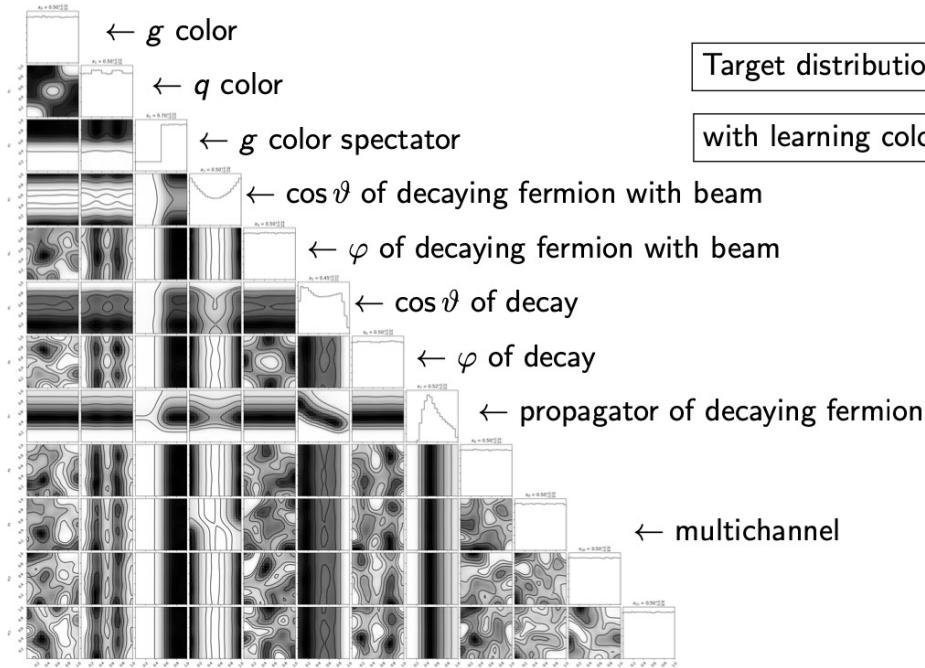
Event Generation with Normalizing Flows

59



arXiv: 2001.05486, ML:ST
 arXiv: 2001.10028, PRD
 Slide credit: [C. Krause](#)

Example: Learning $e^+e^- \rightarrow 3j$



- Deep neural networks allow us to learn complex function by hierarchically structuring the feature learning
- We can express our inductive bias about a system in terms of model design, and can be adapted to a many types of data
- Many neural networks structures are available for training models on a wide array of data types.
- Beyond classification and regression, deep neural networks allow for powerful generative models to enable us to model and generate data

Backup

People are now building a **new kind of software** by assembling networks of **parameterized functional blocks** and by **training them from examples using some form of gradient-based optimization**.

- Yann LeCun, 2018

An increasingly large number of people are **defining the networks procedurally in a data-dependent way** (with loops and conditionals), allowing them **to change dynamically as a function of the input data** fed to them. It's really very much **like a regular program, except it's parameterized**

- Yann LeCun, 2018

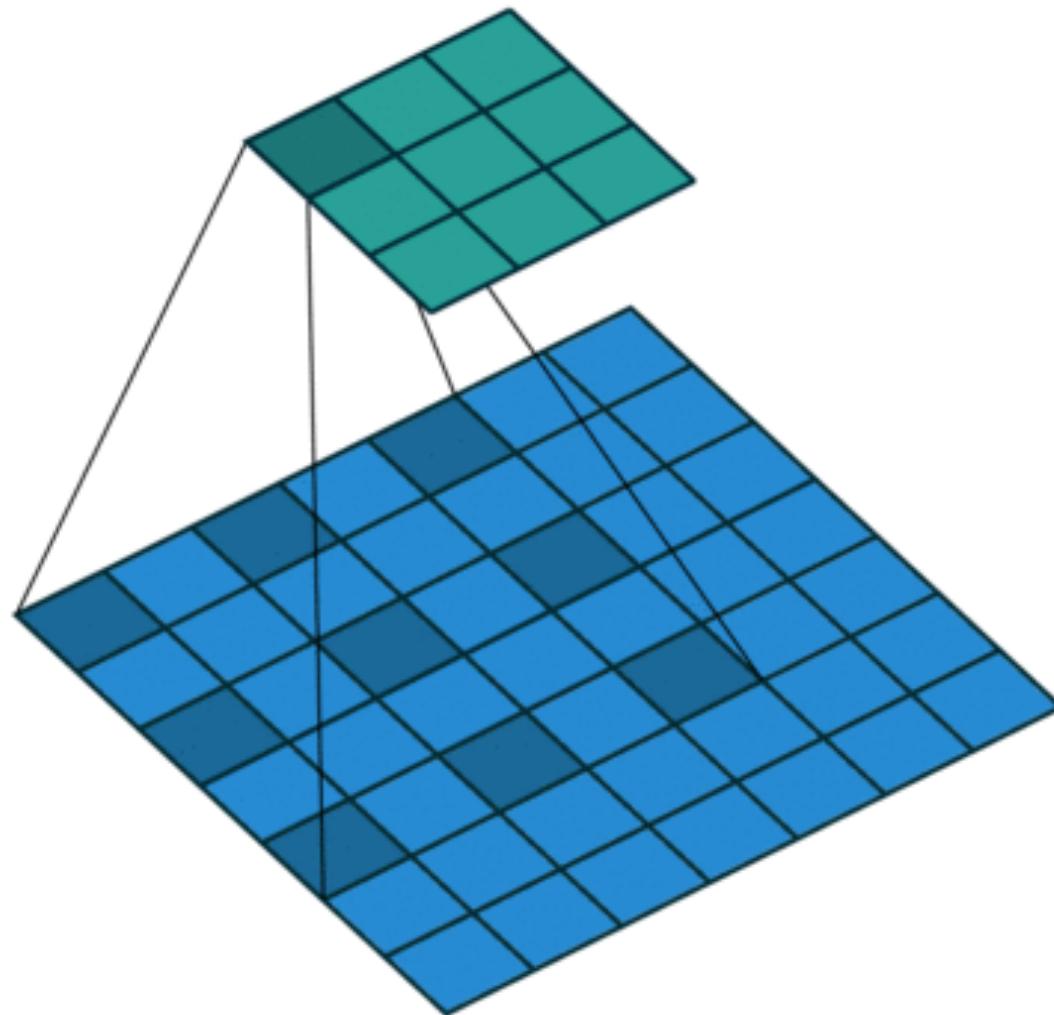
CNN

1D Convolutional Layers

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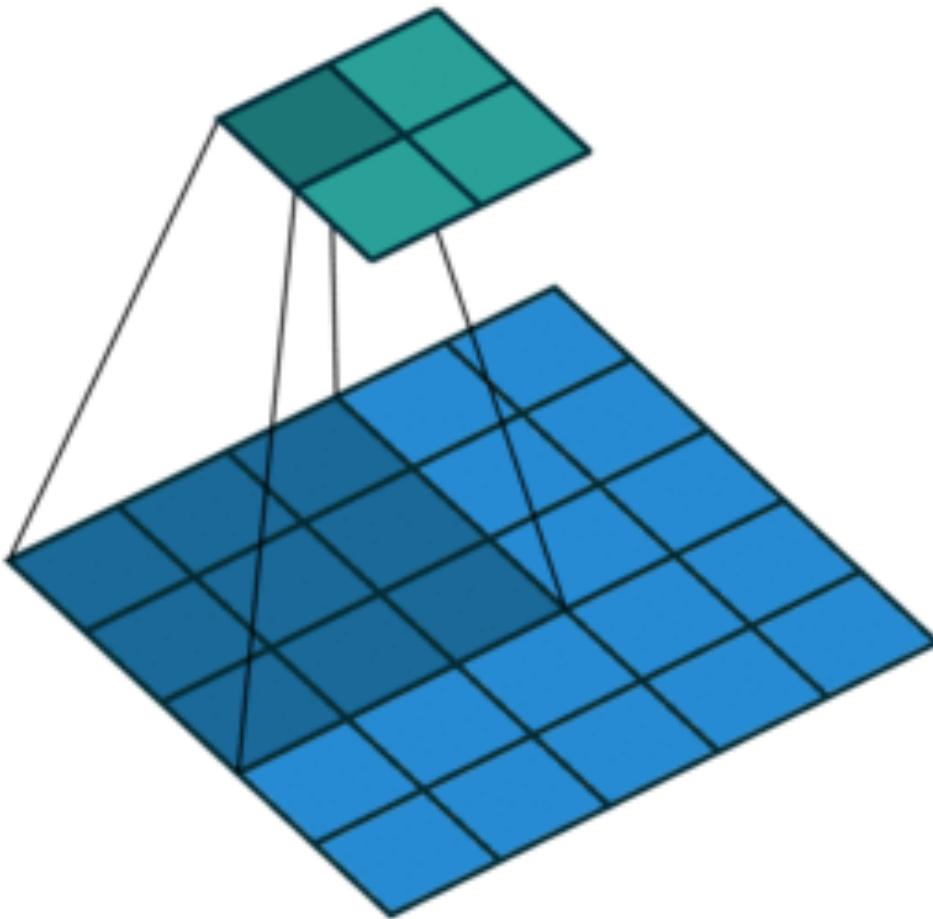
- **Data:** $x \in \mathbb{R}^M$
- **Convolutional kernel of width k:** $u \in \mathbb{R}^k$
- Convolution $x \odot u$ is vector of size $M-k+1$
$$(x \odot u)_i = \sum_{b=0}^{k-1} x_{i+b} u_b$$
- Scan across data and multiply by kernel elements

Dilation



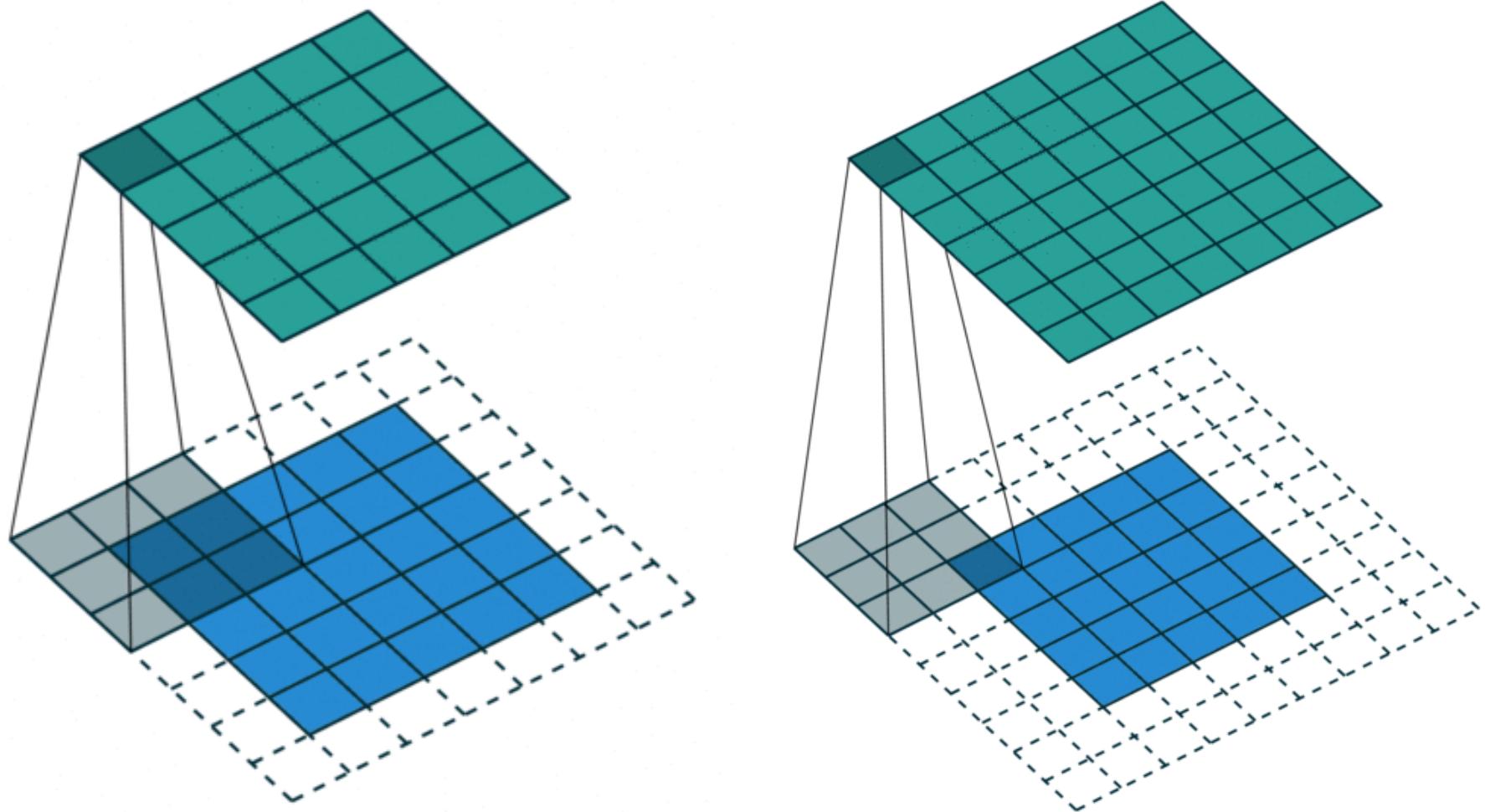
Stride – Step Size When Moving Kernel Across Input

66



Padding – Size of Zero Frame Around Input

67

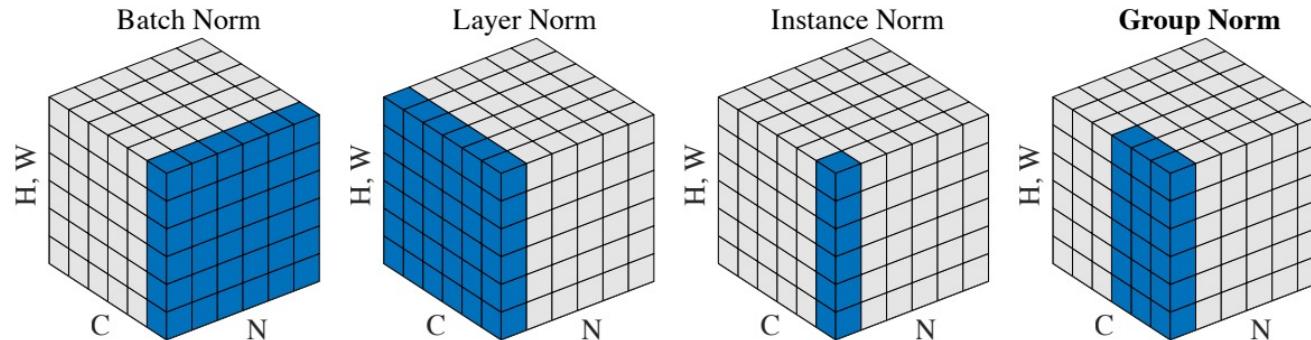


Normalization

- Maintaining proper statistics of the activations and derivatives is a critical issue to allow the training of deep architectures

“Training Deep Neural Networks is complicated by the fact that **the distribution of each layer’s inputs changes during training, as the parameters of the previous layers change**. This slows down the training by requiring lower learning rates and careful parameter initialization ...”

Ioffe, Szegedy,
Batch Normalization, ICML 2015



Batch Normalization

- During training batch normalization shifts and rescales according to the mean and variance estimated on the batch.
 - During test, use empirical moments estimated during training
- Per-component mean and variance on the batch

$$m_{batch} = \frac{1}{B} \sum_{b=1}^B x_b$$

$$\sigma_{batch}^2 = \frac{1}{B} \sum_1^B (x_b - m_{batch})^2$$

- Normalize and compute output $\forall b = 1 \dots B$

$$z_b = \frac{x_b - m_{batch}}{\sqrt{\sigma_{batch}^2 + \epsilon}}$$

$$y_b = \gamma \odot z_b + \beta$$

- γ and β are parameters to optimize

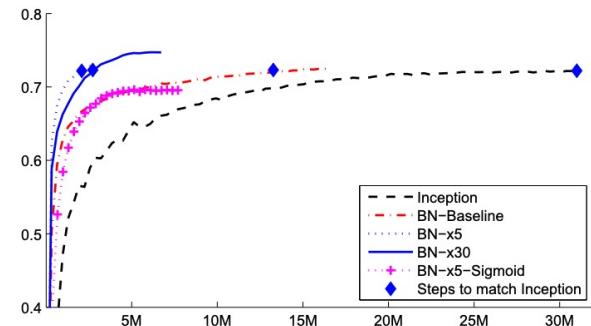
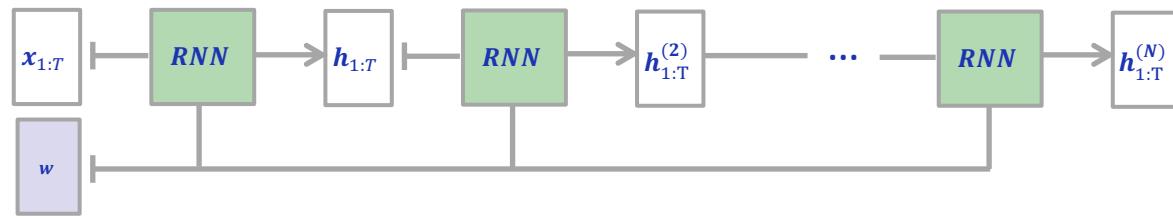


Figure 2: Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.

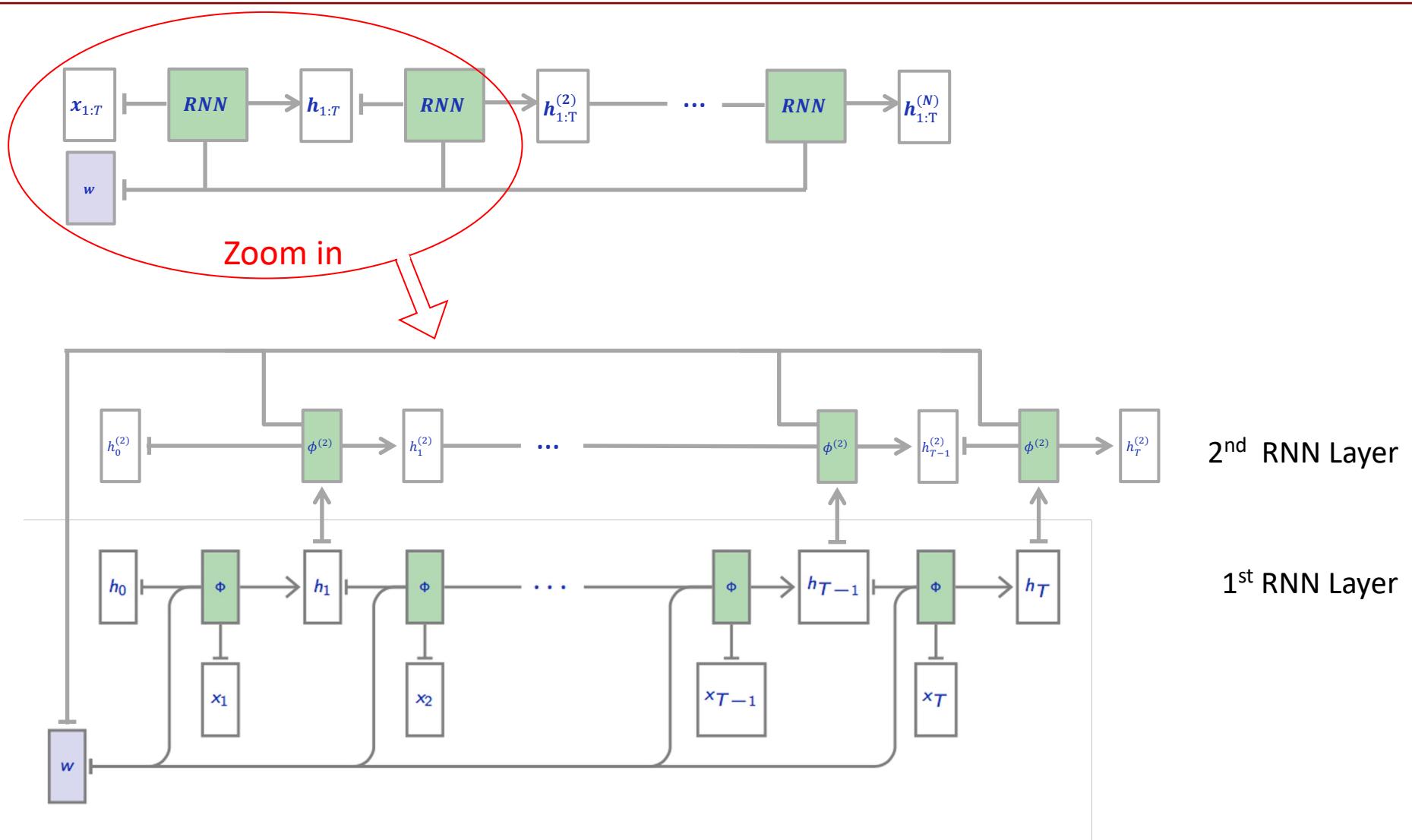
RNN

Stacked RNN



Stacked RNN

72

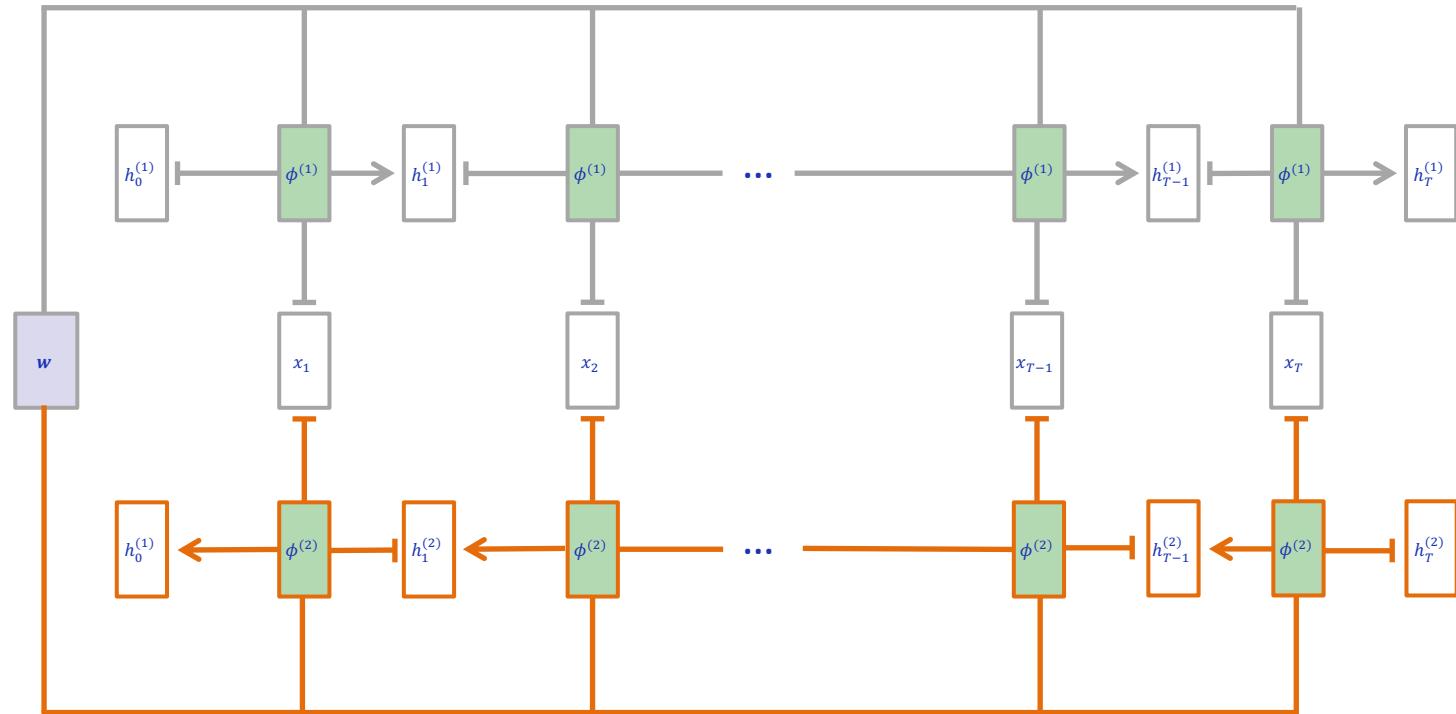


Two Stacked LSTM Layers

Bi-Directional RNN

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Forward in time RNN Layer
→



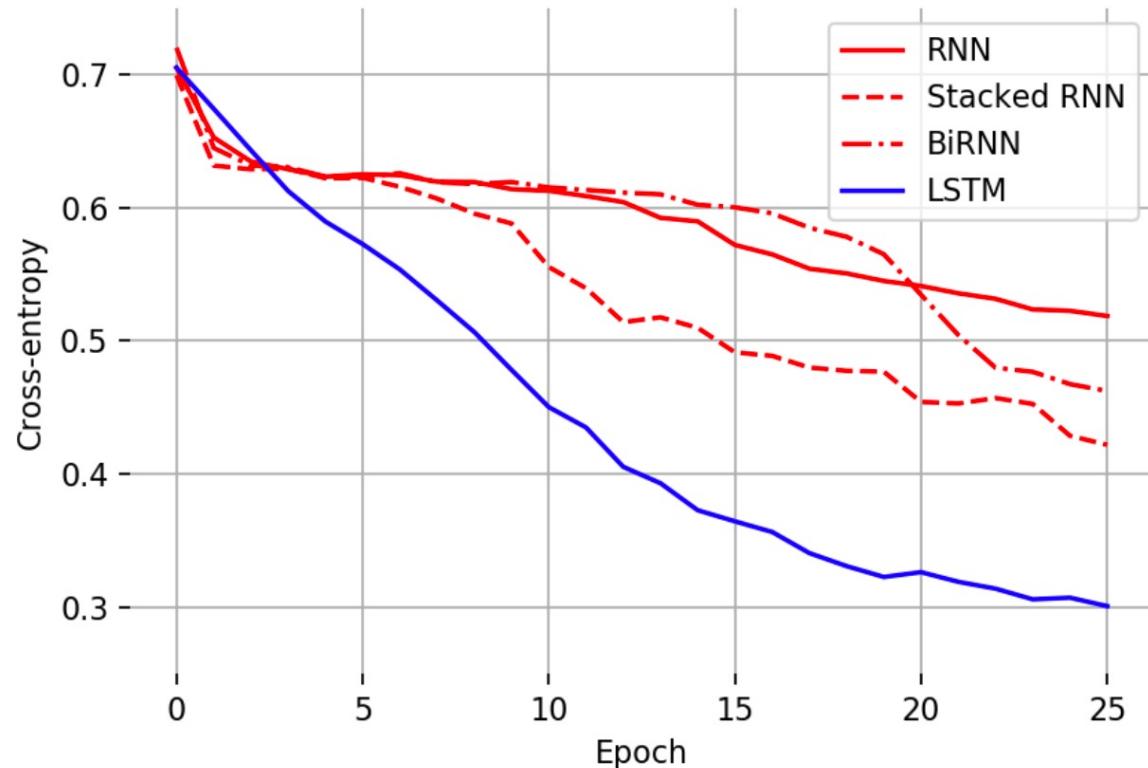
Backward in time RNN Layer
←

Comparison on Toy Problem

74

Learn to recognize palindrome
Sequence size between 1 to 10

x	y
(1, 2, 3, 2, 1)	1
(2, 1, 2)	1
(3, 4, 1, 2)	0
(0)	1
(1, 4)	0



Examples

This is a screenshot from a Mario Kart race, specifically on the Toad HQ track. The main view shows Mario driving his kart towards the finish line. The top right corner displays the race time as 01' 00" 67. Below the track, a small window shows the neural network's internal state, which consists of several grayscale images representing different sensor inputs or internal states. A text overlay explains that this is a recurrent neural network trained to play Mario Kart like the user, with its goal being to predict controller inputs rather than winning. It also mentions that the bottom display shows what the neural network sees and its internal state and controller predictions. Another text overlay below states that the AI is currently trying every cup in 50cc on repeat to see if it can get medals in each cup, noting that the user is not actually present.

T MarioFlow - Self-Driving Mario Kart w/ Recurrent Neural Network

Watch later Share

This is a recurrent neural network that I've trained to play Mario Kart like me. This NN is very different from Mari/O, because its goal is not to win, but rather to predict what controller inputs I would use in any given situation. The display on the bottom shows what the neural network sees, and its internal state and controller predictions.

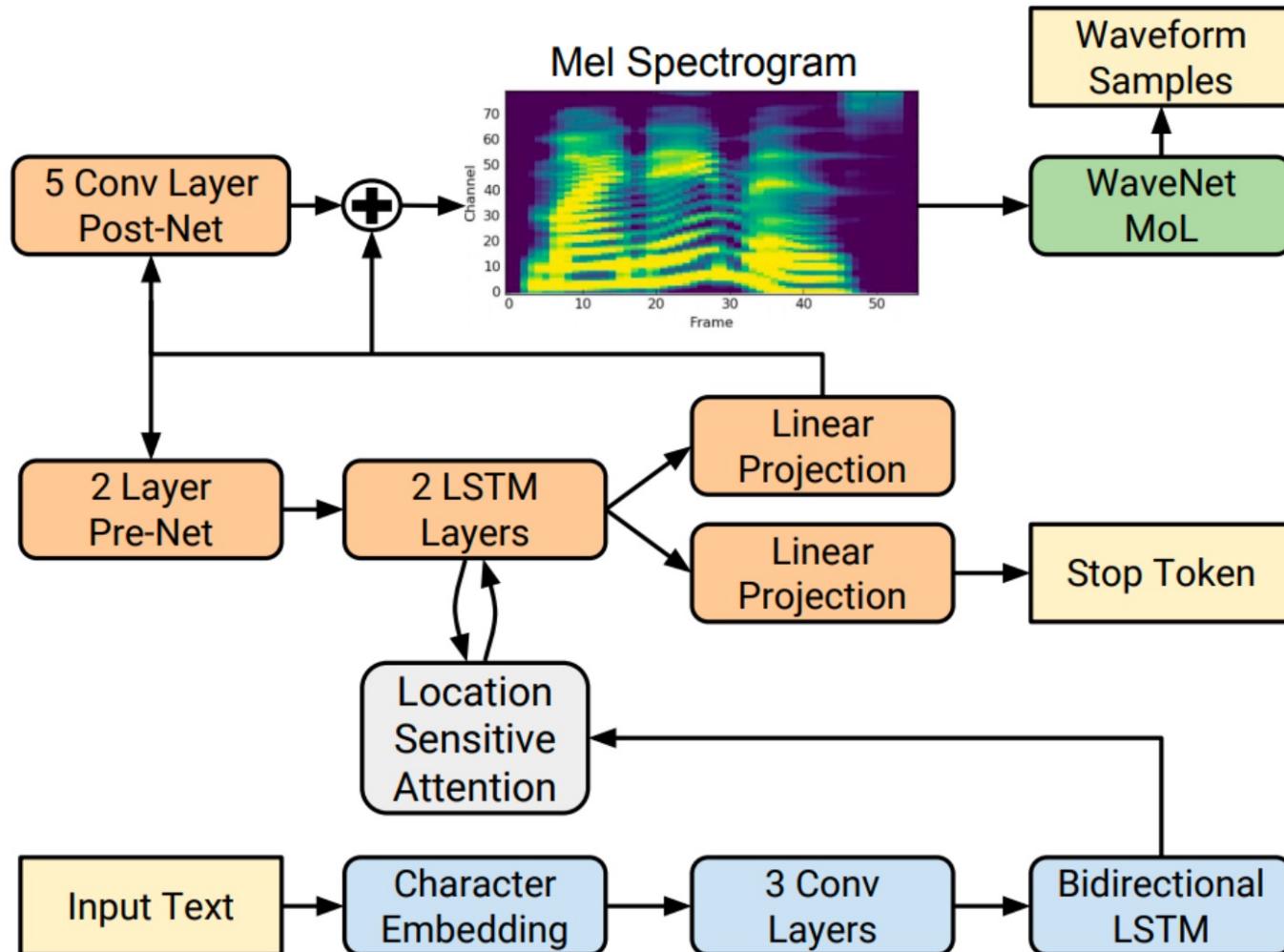
It's currently trying every cup in 50cc on repeat. The goal is to see if it can get medals in each cup. I'm not actually present. If you see something interesting clip it so I can see it later and potentially include it in my video!

MORE VIDEOS

01:34:58

CC YouTube

Text-to-speech synthesis



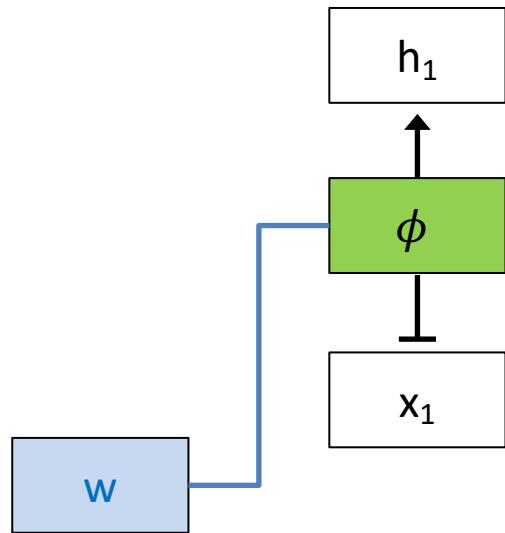
Deep Sets

What if our data has no time structure?

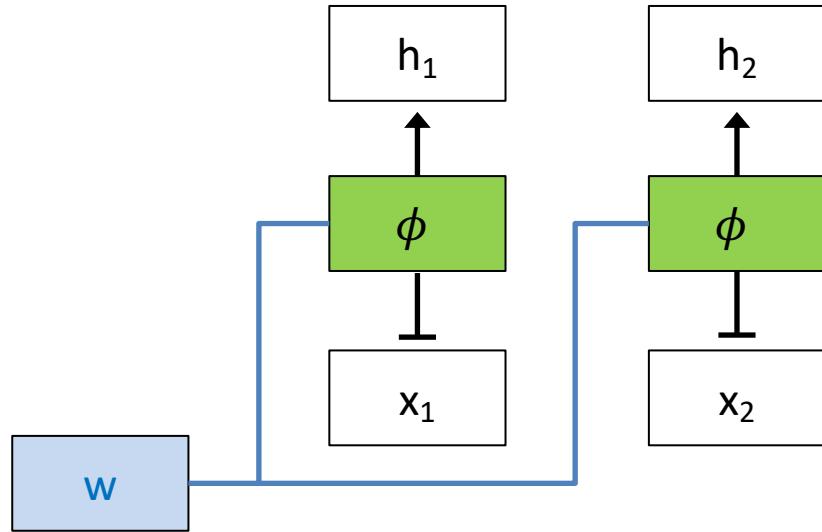
78

- Data may be variable in length but have no temporal structure → *Data are sets of values*
- *One option:* If we know about the data domain, could try to impose an ordering, then use RNN
- *Better option:* use system that can operate on variable length sets in permutation invariant way
 - Why permutation invariant → so order doesn't matter

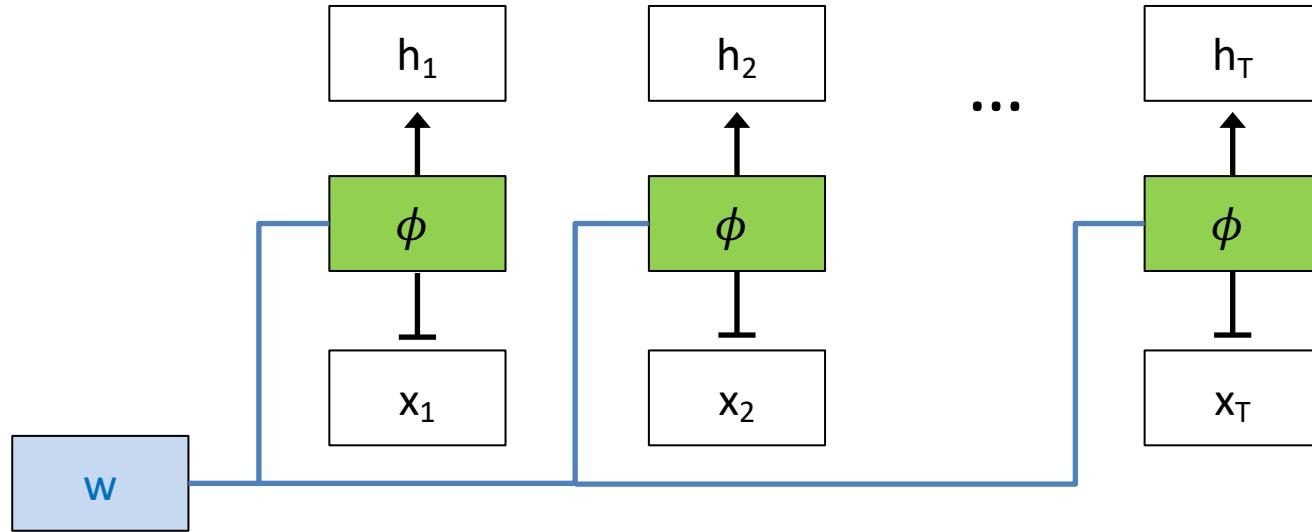
Deep Sets



Deep Sets

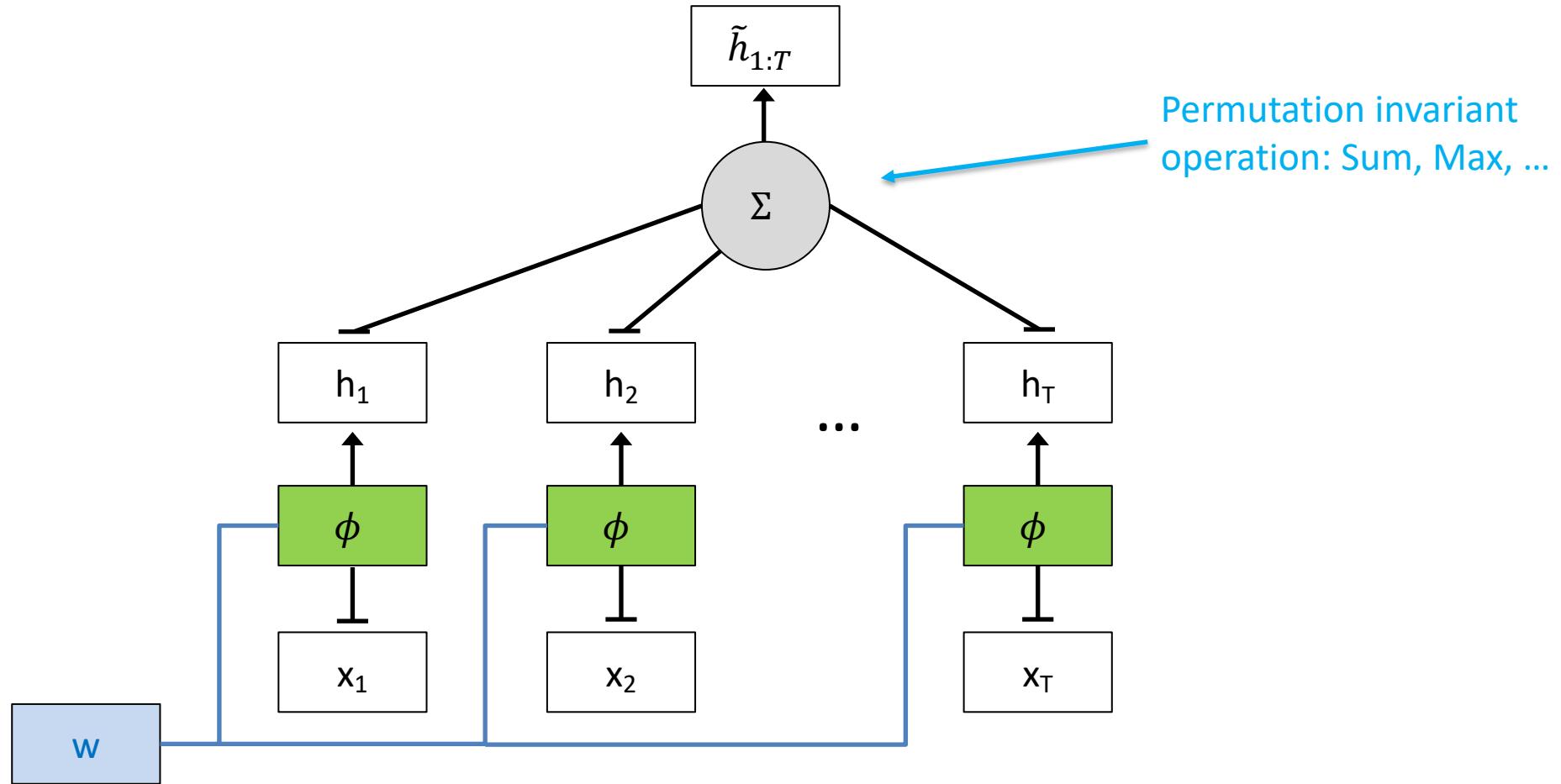


Deep Sets

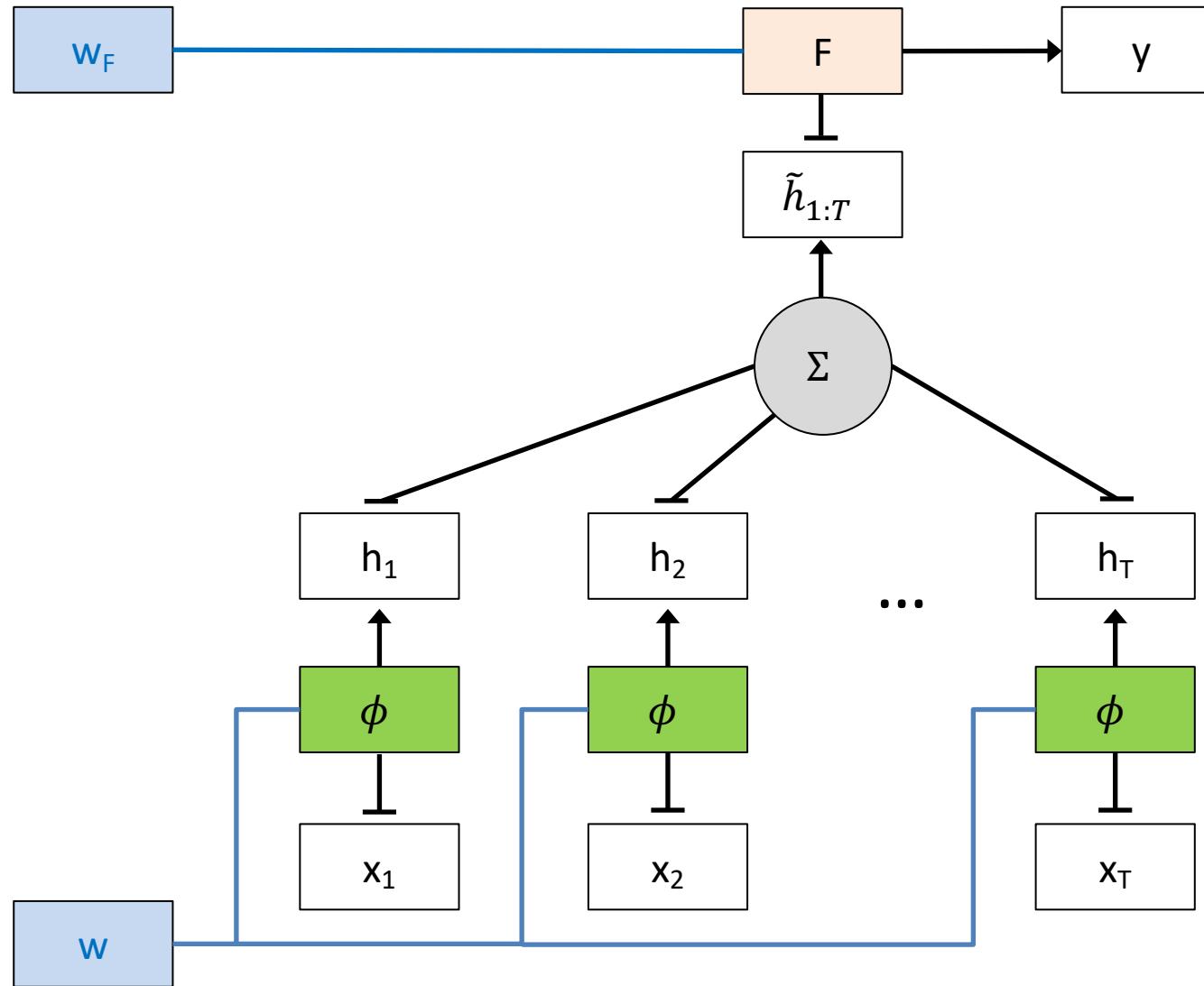


Deep Sets

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Deep Sets



Examples

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Outlier detection



M. Zaheer et. al [2017](#)

Medical Imaging

With more complex architecture

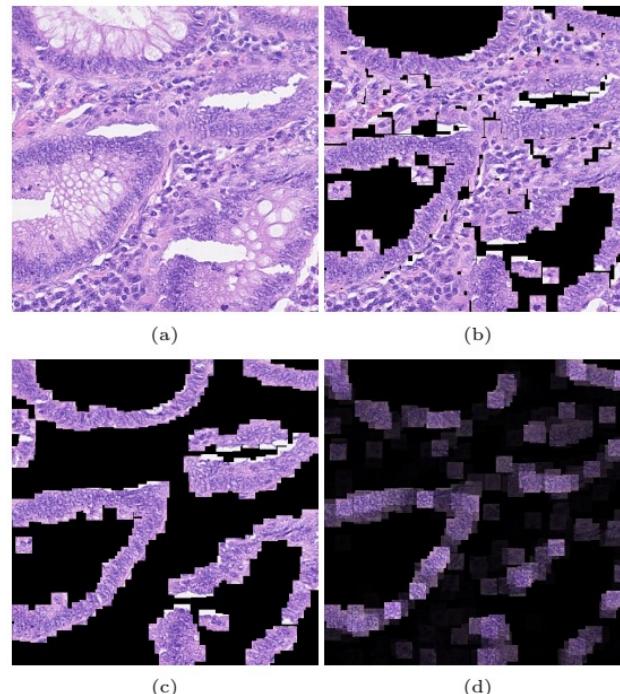


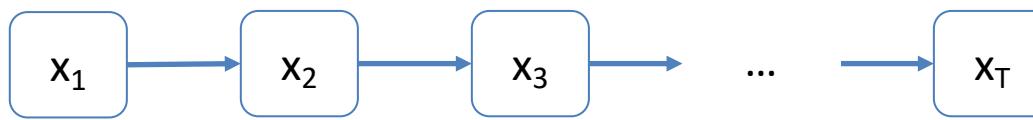
Figure 5. (a) H&E stained histology image. (b) 27×27 patches centered around all marked nuclei. (c) Ground truth: Patches that belong to the class epithelial. (d) Heatmap: Every patch from (b) multiplied by its corresponding attention weight, we rescaled the attention weights using $a'_k = (a_k - \min(\mathbf{a})) / (\max(\mathbf{a}) - \min(\mathbf{a}))$.

M. Ilse et al., [2018](#)

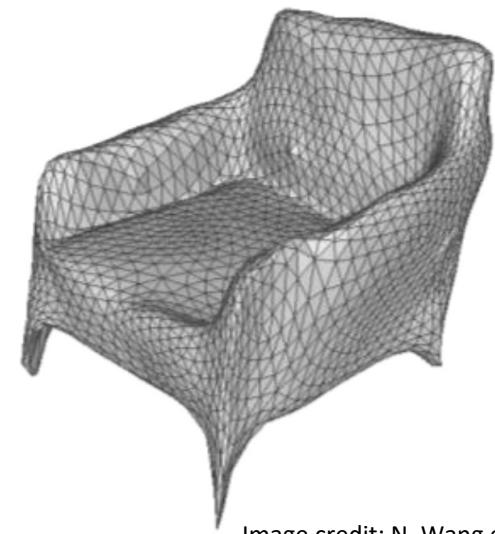
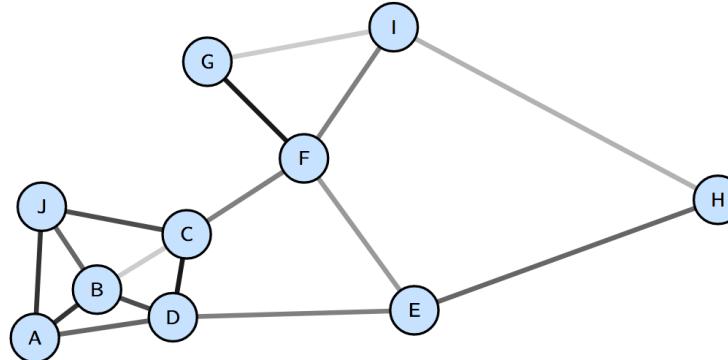
Graph Data

Graph Data

86

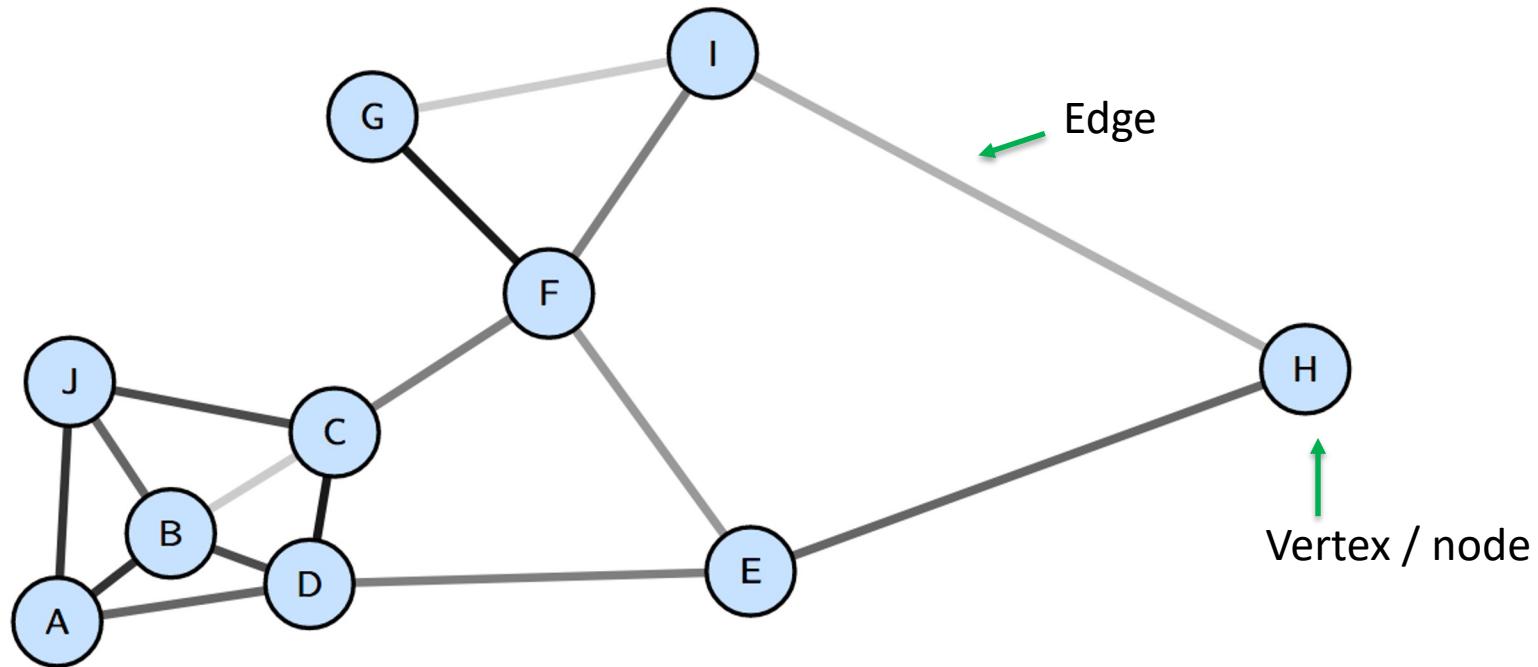


- Sequential data has single (directed) connections from data at current time to data at next time
- What about data with more complex dependencies



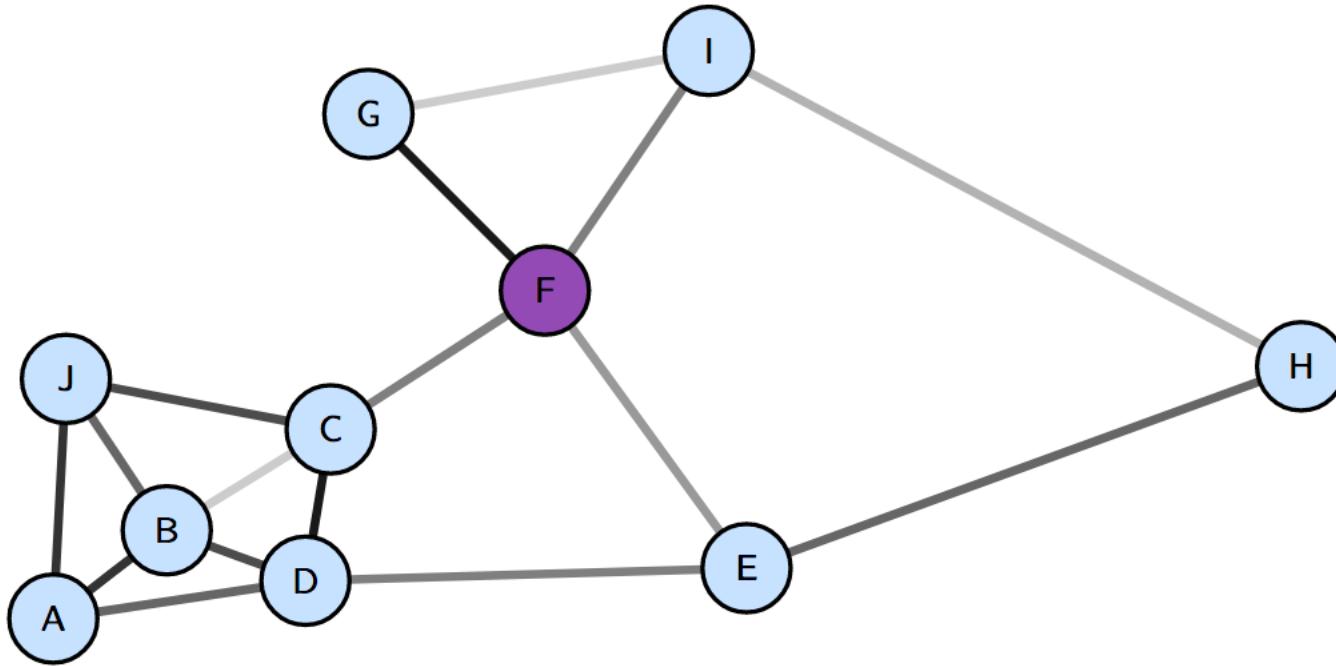
Graphs

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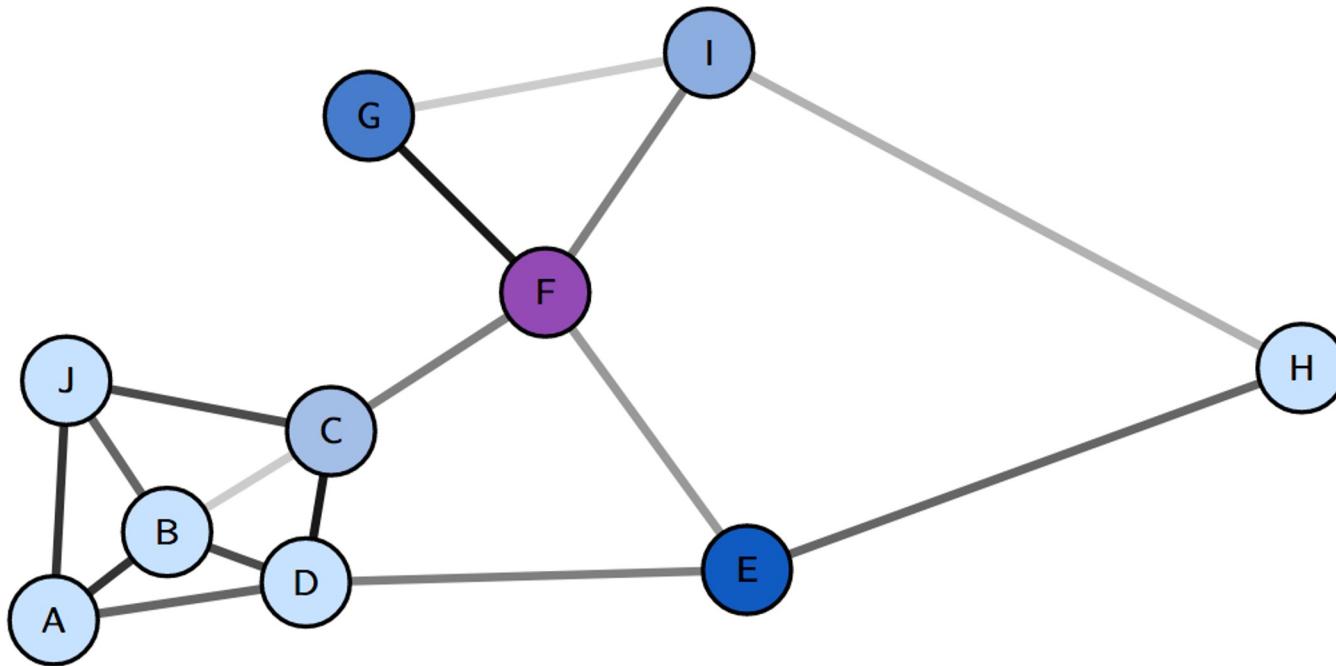


- Adjacency matrix: $A_{ij} = \delta(\text{edge between vertex } i \text{ and } j)$
- Each node can have features
- Each edge can have features, e.g. distance between nodes

Neural Message Passing

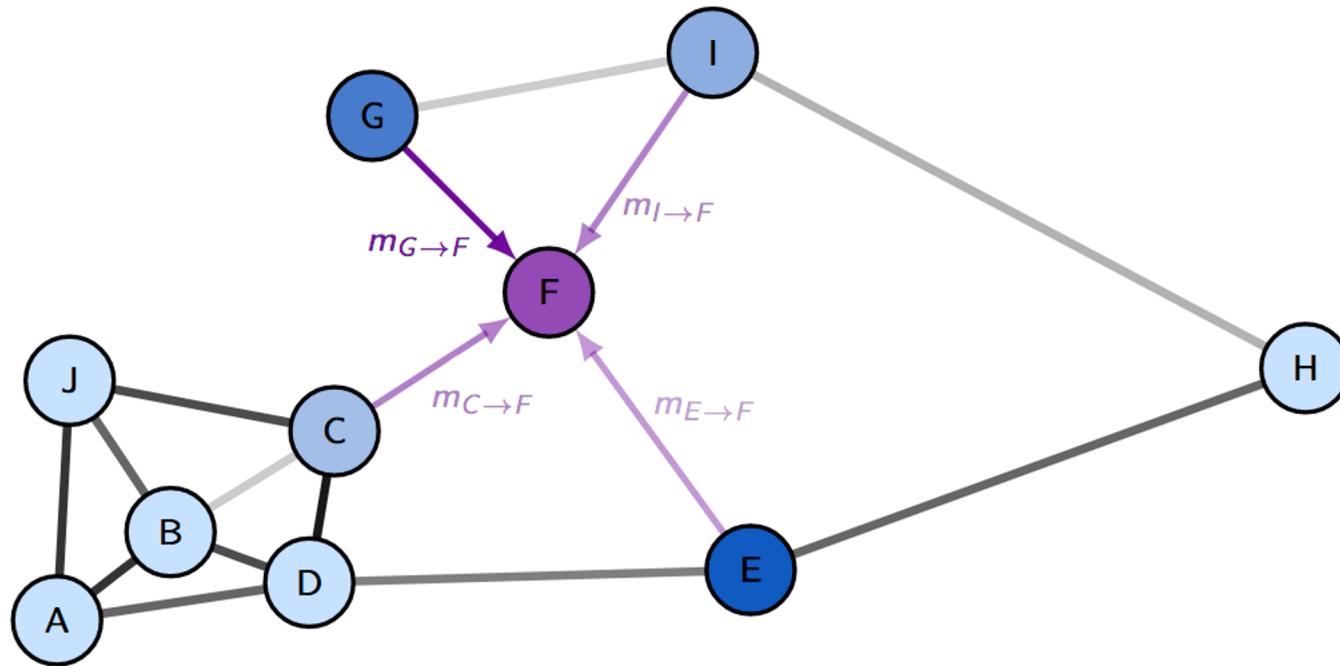


Neural Message Passing



$$\tilde{m}_j^t = f(h_j^{t-1})$$

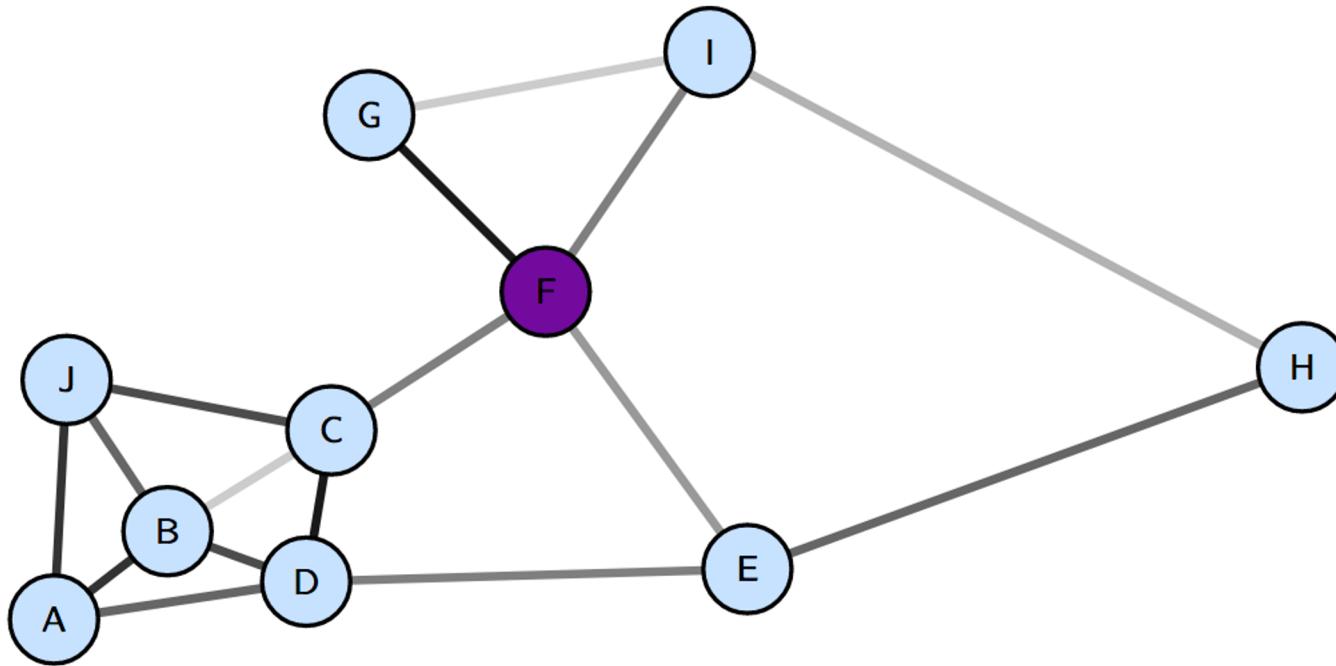
Neural Message Passing



$$\tilde{m}_j^t = f(h_j^{t-1})$$

$$m_{j \rightarrow i}^t = \sigma(A_{ij}\tilde{m}_j^t)$$

Neural Message Passing



$$\tilde{m}_j^t = f(h_j^{t-1})$$

$$m_{j \rightarrow i}^t = \sigma(A_{ij} \tilde{m}_j^t)$$

$$h_i^t = \text{GRU}(h_i^{t-1}, \sum_j m_{j \rightarrow i}^t)$$

Algorithm 1 Message passing neural network

Require: $N \times D$ nodes \mathbf{x} , adjacency matrix A

$\mathbf{h} \leftarrow \text{Embed}(\mathbf{x})$

for $t = 1, \dots, T$ **do**

$\mathbf{m} \leftarrow \text{Message}(A, \mathbf{h})$

$\mathbf{h} \leftarrow \text{VertexUpdate}(\mathbf{h}, \mathbf{m})$

end for

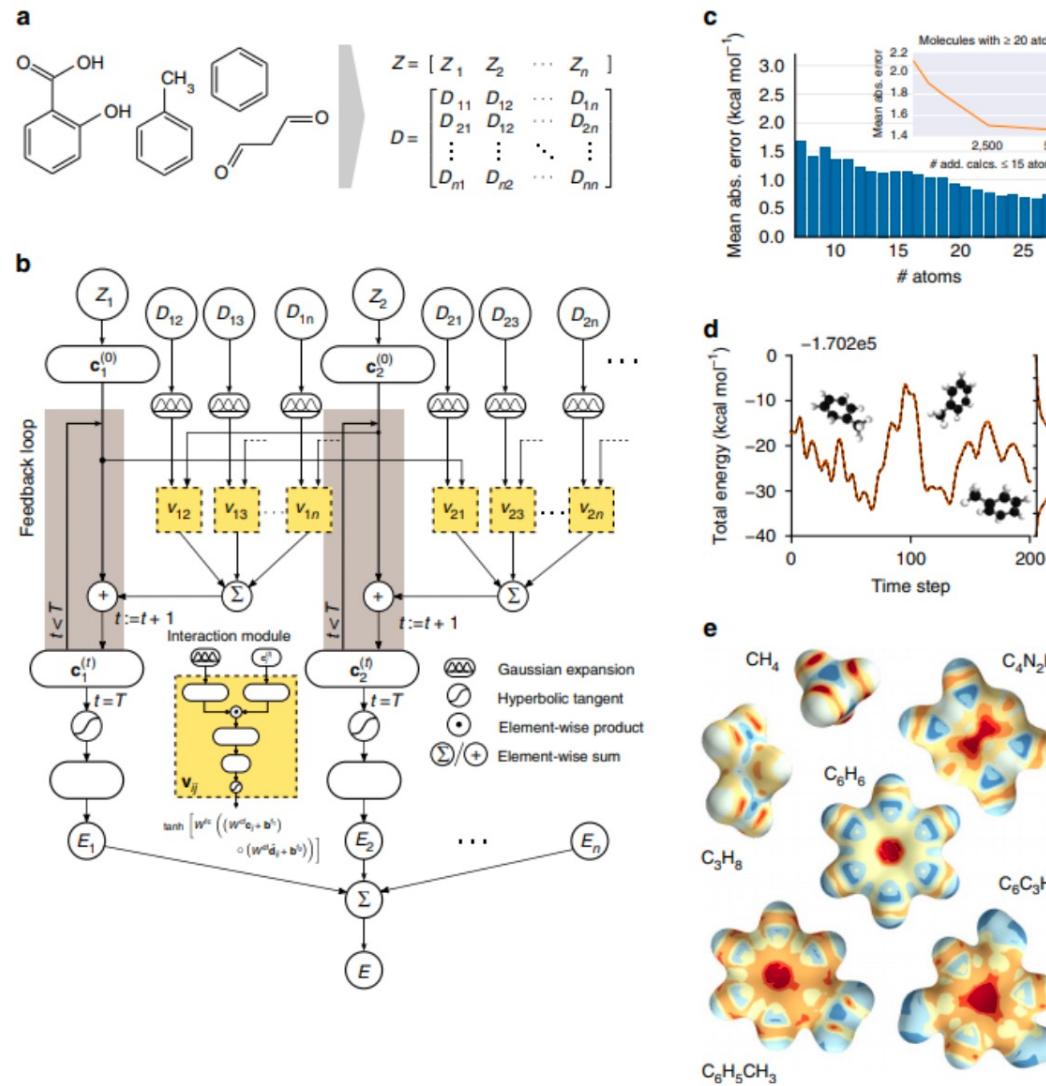
$\mathbf{r} = \text{Readout}(\mathbf{h})$

return $\text{Classify}(\mathbf{r})$

Examples

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Quantum chemistry with graph networks



Examples

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Learning to simulate physics with graph networks

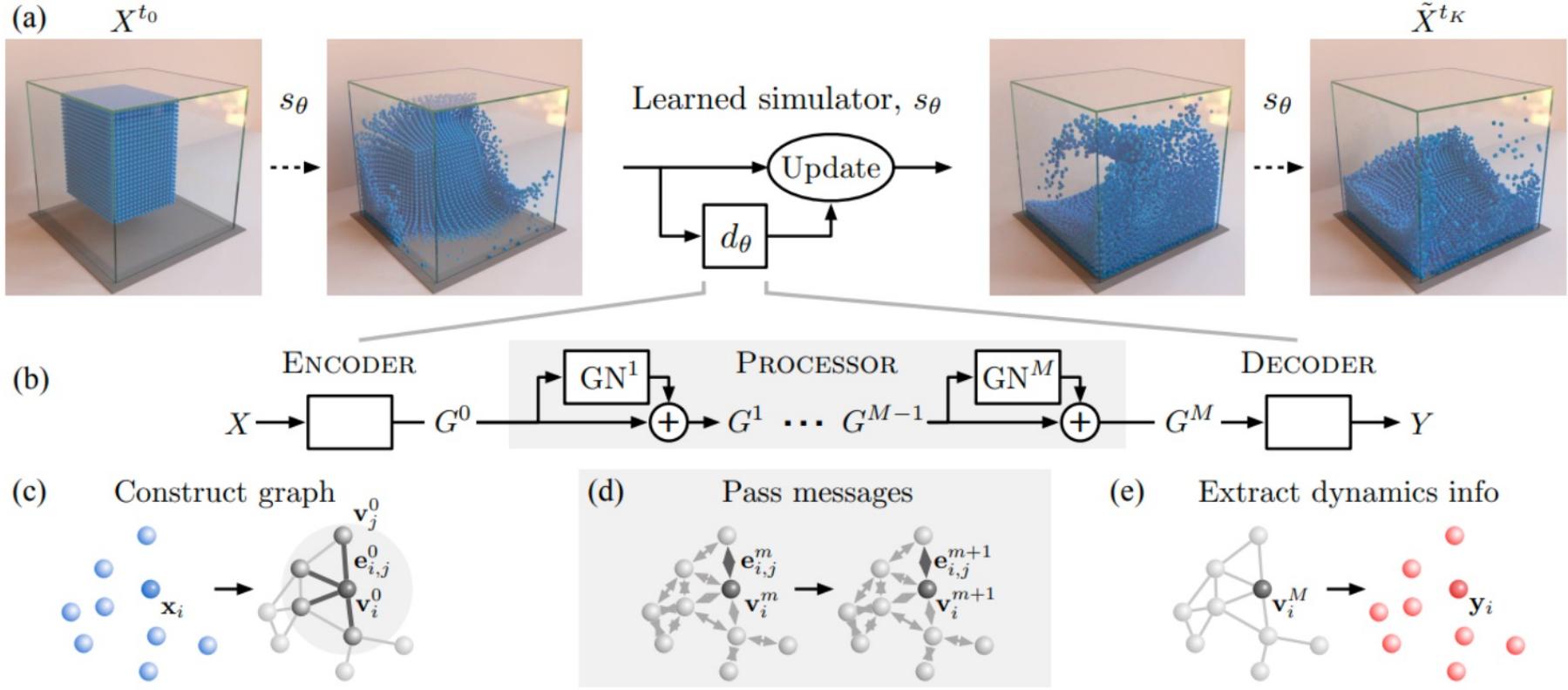


Figure 2. (a) Our GNS predicts future states represented as particles using its learned dynamics model, d_θ , and a fixed update procedure. (b) The d_θ uses an “encode-process-decode” scheme, which computes dynamics information, Y , from input state, X . (c) The ENCODER constructs latent graph, G^0 , from the input state, X . (d) The PROCESSOR performs M rounds of learned message-passing over the latent graphs, G^0, \dots, G^M . (e) The DECODER extracts dynamics information, Y , from the final latent graph, G^M .

Deep Generative Model Examples

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BigGan



(Brock et al, 2018)



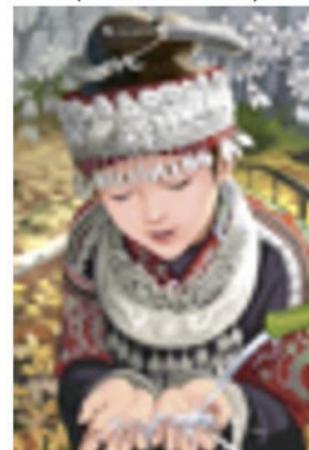
Image-to-Image Translation with CycleGAN

[Zhu et. al. 2017](#)

Simulate future
trajectories of
environments
based on actions
for planning.
(Finn et al,
2016)

Single Image Super-Resolution (Ledig et al, 2016)

original

bicubic
(21.59dB/0.6423)SRGAN
(20.34dB/0.6562)Text
description

This bird is red
and brown in
color, with a
stubby beak

64x64
GAN-INT-CLS

Text-to-Image Synthesis
with StackGAN
(Zhang et. al. 2017)

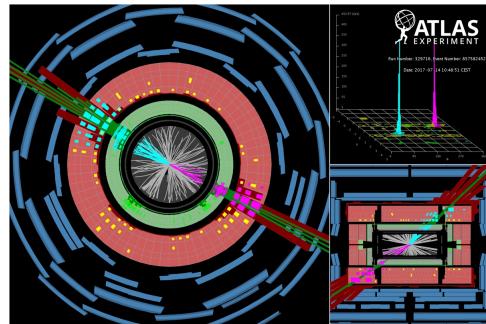
128x128
GAWWN256x256
StackGAN-v1

Generative Models

Different Kinds of Generative Models

97

Generative Models approximate and simulate the data generation process

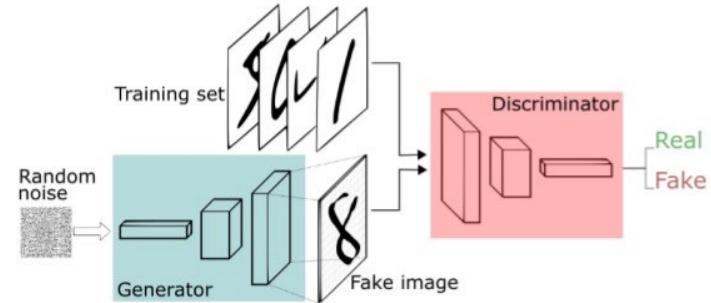


Scientific Simulators

- Built from science knowledge
- Relatively few parameters, often interpretable
- High Fidelity, often computationally costly

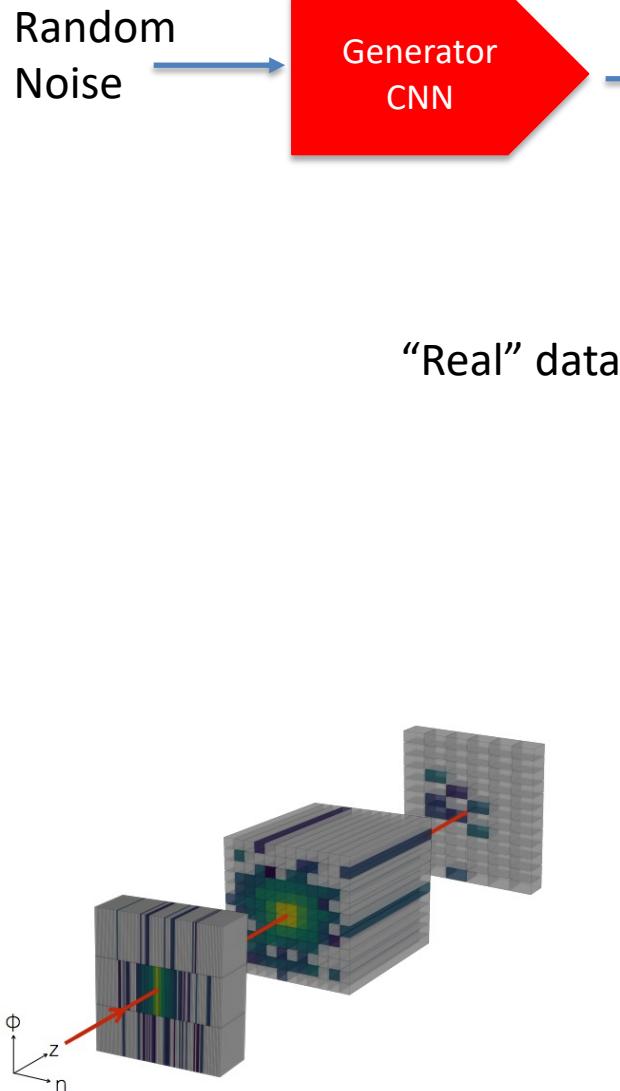
Machine Learning

- Fit to data, inductive bias in model design / optimization
- Can have $>10^6$ parameters, often not interpretable
- Often slow to train, fast to evaluate

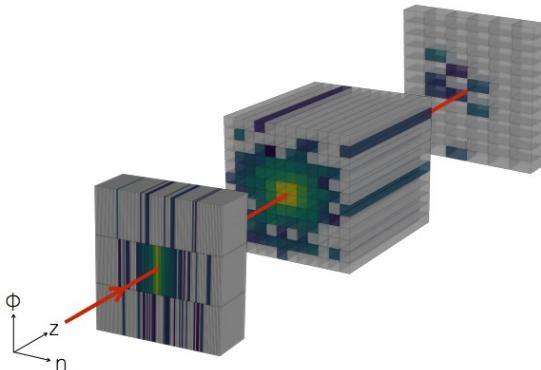


GANs for Calorimeter Energy Depositions

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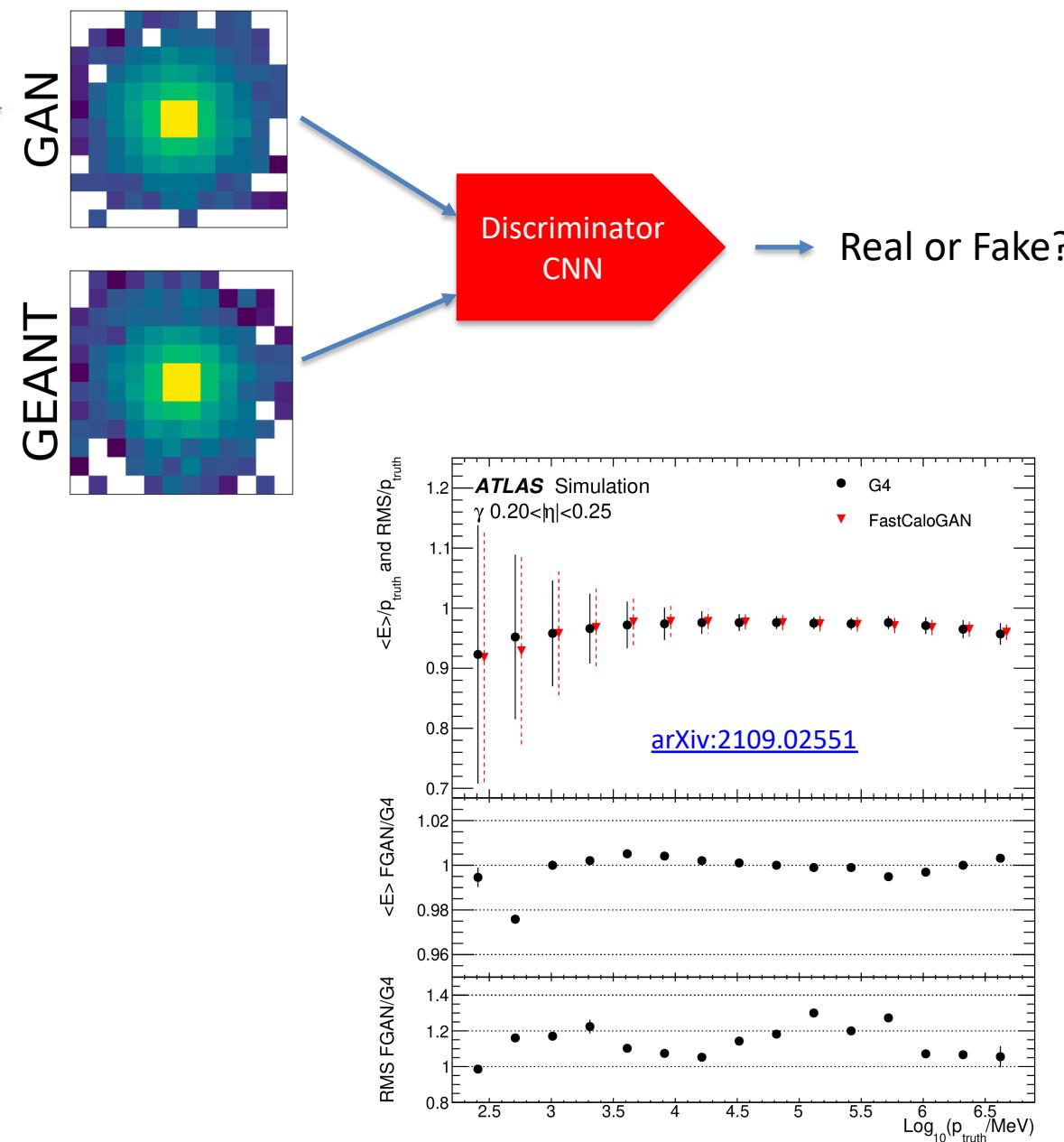
"Real" data



[PRD97, 014021 \(2018\)](#)

[arXiv:1705.02355](#)

[arXiv:1701.05927](#)

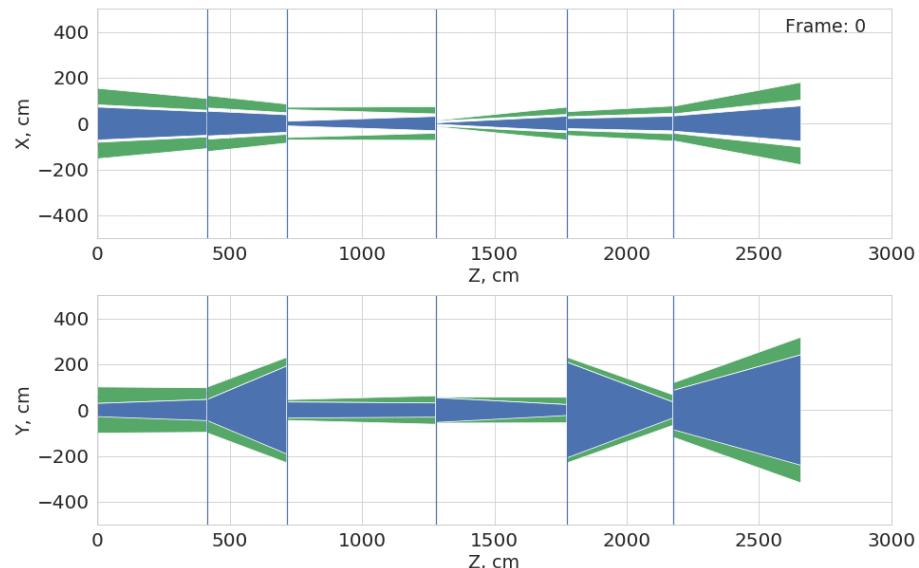
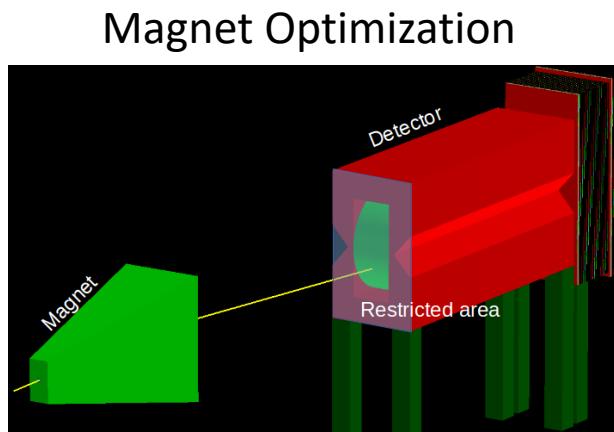


[arXiv:2109.02551](#)

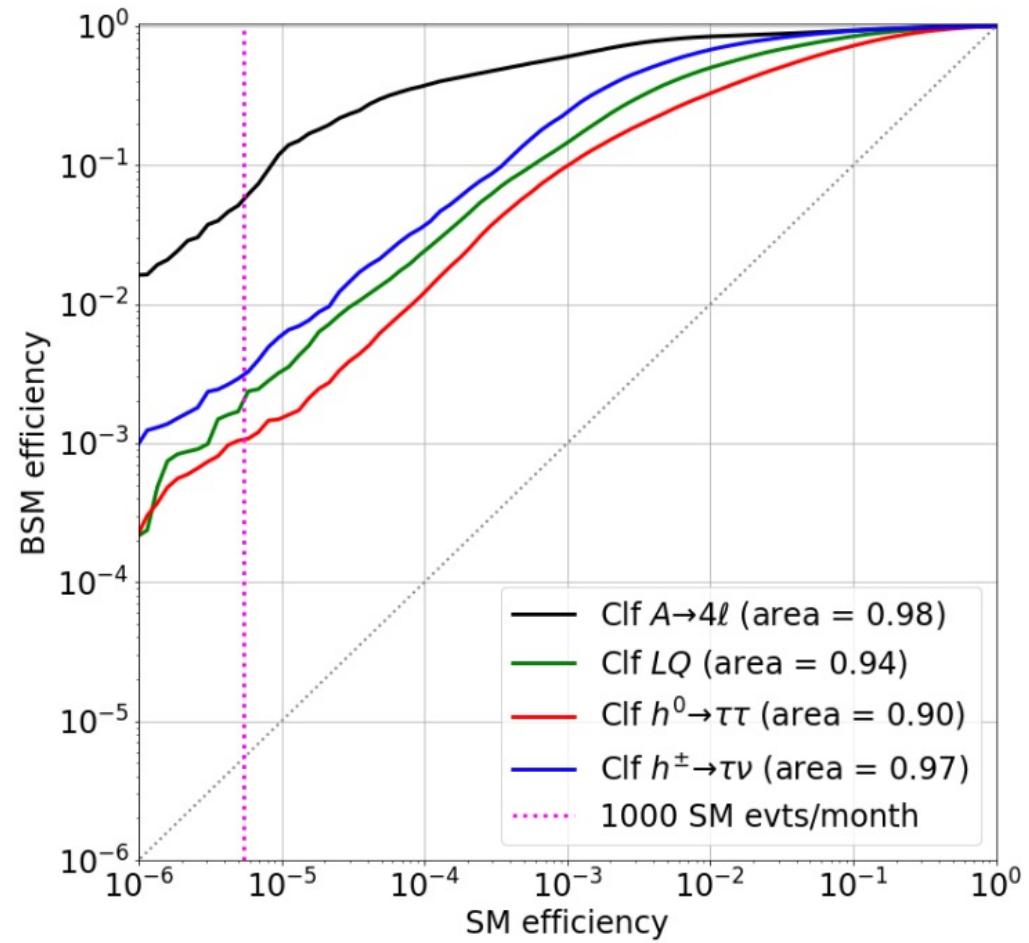
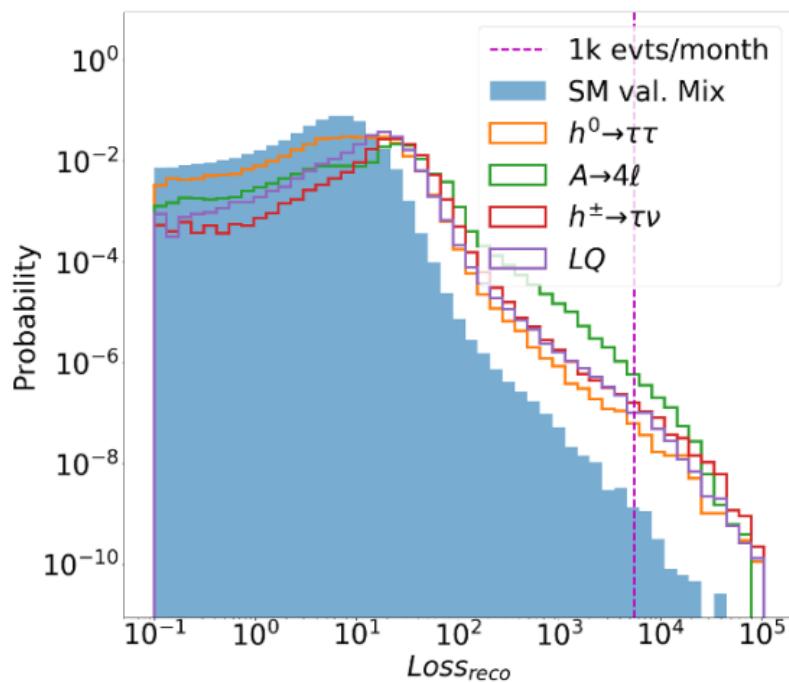
GANs for Detector Design

99

- GAN to emulate detector simulation $\tilde{x} = g(z|\psi)$ given detector parameters ψ (e.g. magnet shape below)
- Design objective C to minimize: $\min_{\psi} \mathbb{E}_{\tilde{x}}[C(\tilde{x} = g(z|\psi))]$
- GAN is differentiable → Minimize with gradient descent



Anomaly Detection with VAE

10
0

- Train on SM
- Test if New Physics is poorly reconstructed