Machine Learning:

A new toolbox for Theoretical Physics

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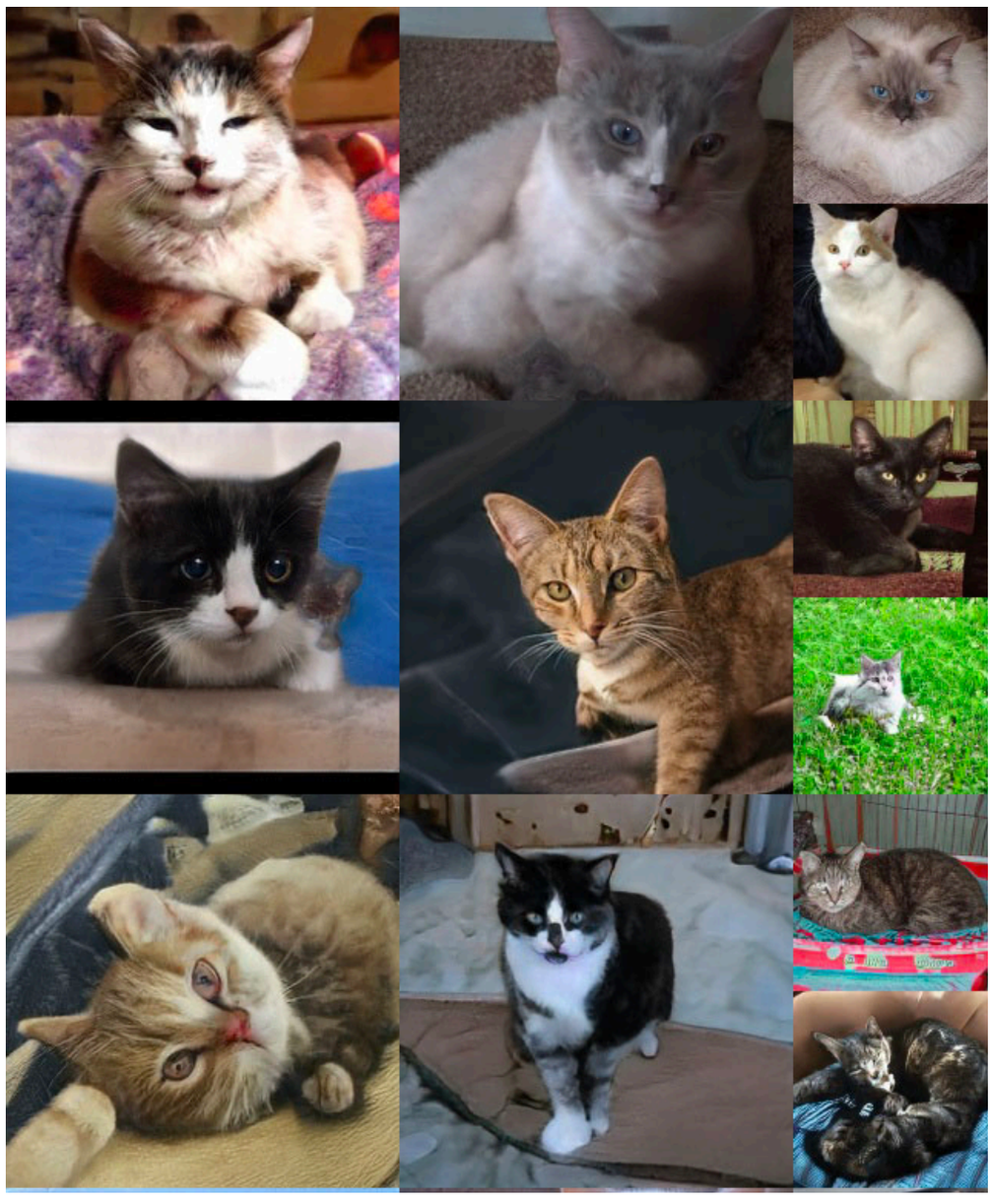
Today's lecture

- Convolutional Neural Networks
- Energy-based models and Boltzmann learning
- Generative Models and Adversarial Learning
- Applications of Machine Learning to Theoretical Physics

Convolutional Neural Networks

Convolutional Neural Networks

Like physical systems, many datasets and supervised learning tasks also possess additional **symmetries and structure** what can (and should) be exploited



e.g. we want to train a classifier to identify pictures of cats. What **high-level features** must one learn first?

Convolutional Neural Networks

Like physical systems, many datasets and supervised learning tasks also possess additional **symmetries and structure** what can (and should) be exploited

e.g. we want to train a classifier to identify pictures of cats. What **high-level features** must one learn first?

- *The features that define ``cat'' are local in the picture: whiskers, tail, paws …: **locality***

- *Cats can be anywhere in the image: **translational invariance***

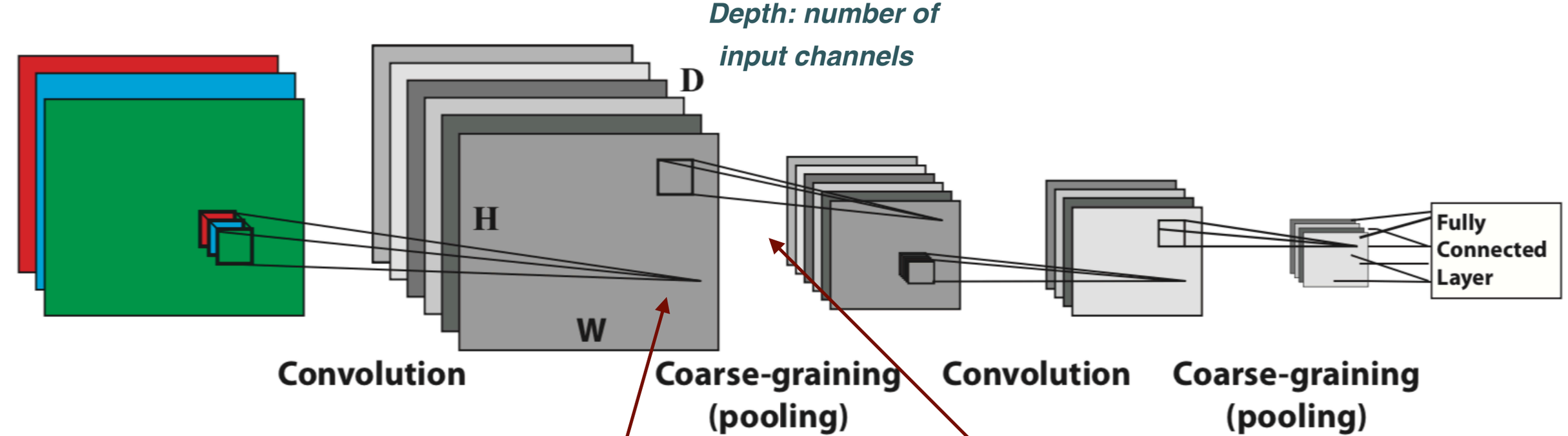
- *Relative position of features must be respected (eg whiskers and tail shoaled appear in opposite sides of ``cat''): **rotational invariance***

Our classifier should exhibit all these high-level features

Convolutional Neural Networks

Convolutional Neural Networks (CNNs) are architectures that take **advantage of this additional high-level structures** that all-to-all coupled networks fail to exploit

A CNN is a translationally invariant neural network that respects locality of the input data

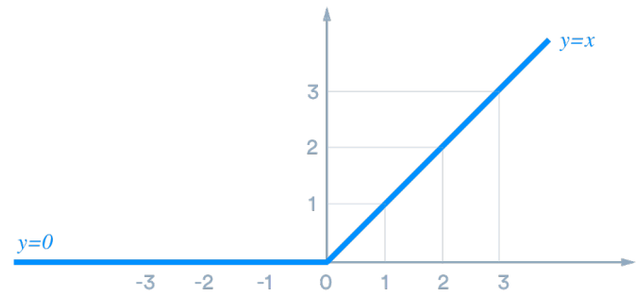


Convolutional Neural Networks

CNNs are composed by

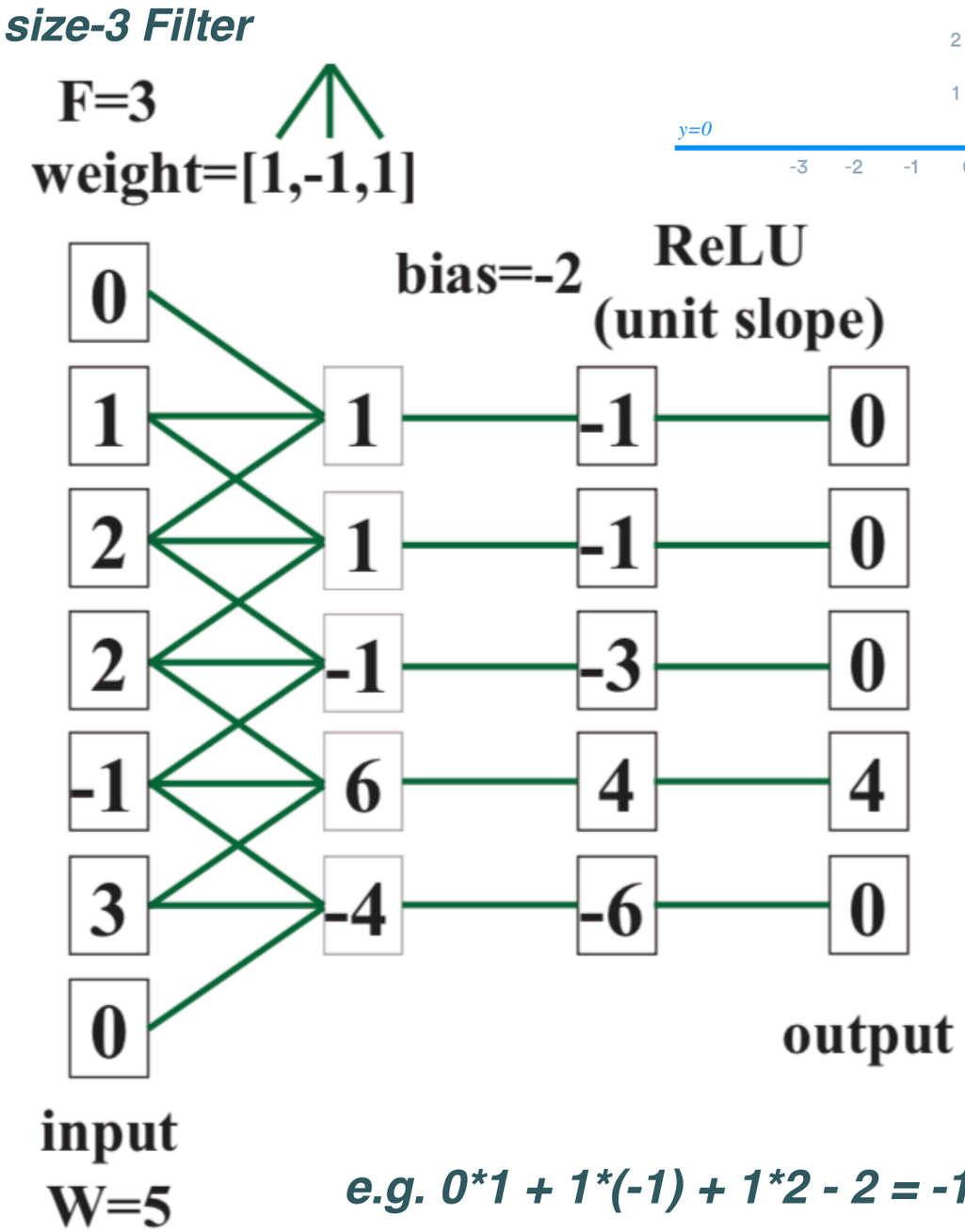
two kinds of layers

Convolution of input with **filters**



example of

convolutional layer



e.g. 0*1 + 1*(-1) + 1*2 - 2 = -1

note that convolution changes the depth,

but not the height and width of the network

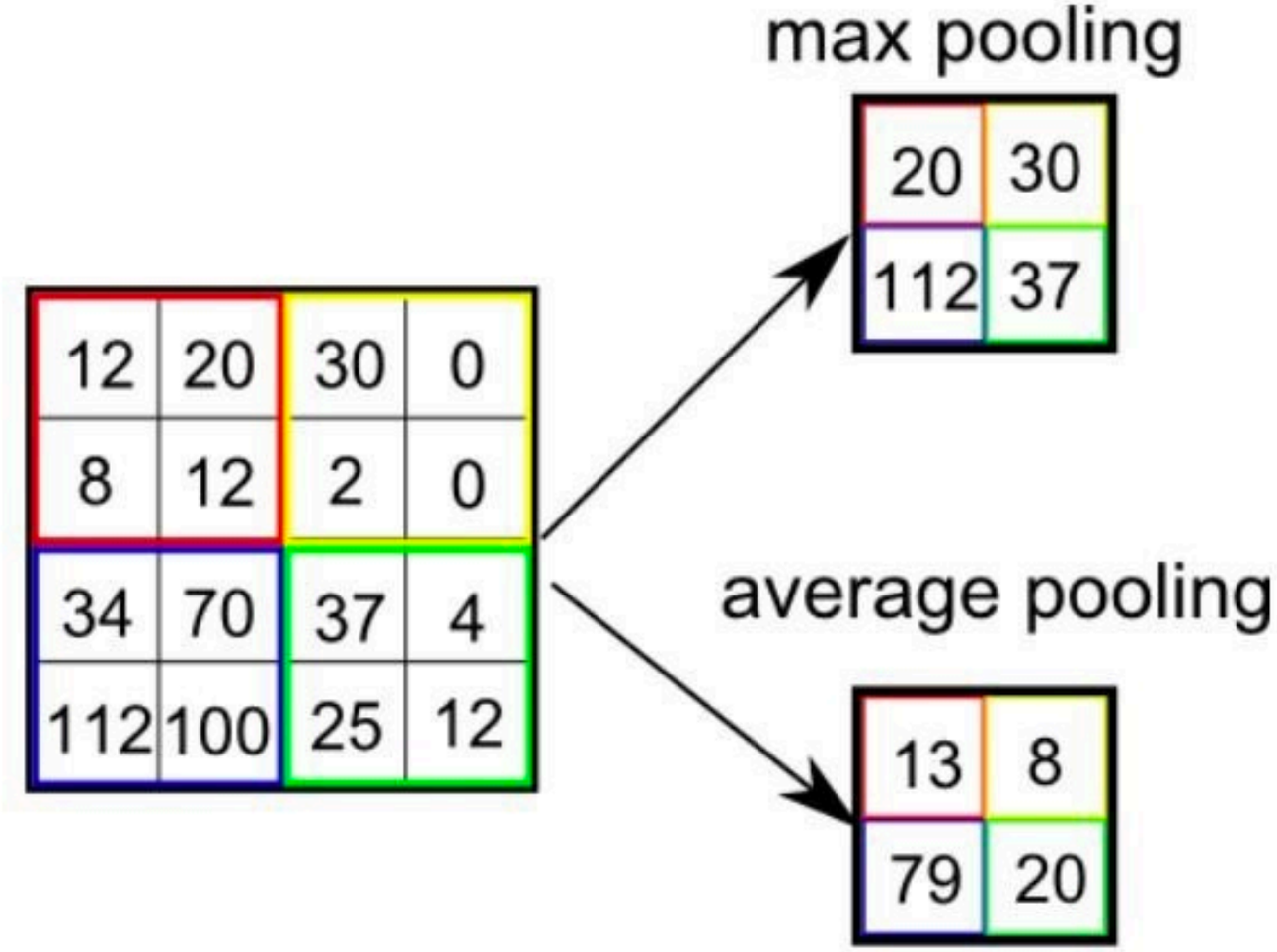
Convolutional Neural Networks

CNNs are composed by two kinds of layers

- Convolution layer of input with **filters**
- **Pooling** layer that coarse-grains the input while maintaining locality and spatial structure

e.g. **MaxPool**, the spatial dimensions are coarse-grained by replacing a small region by single neuron whose output is maximum value of the output in the region

in average pooling, one averages over output in region



Convolutional Neural Networks

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- Convolution layer of input with **filters**
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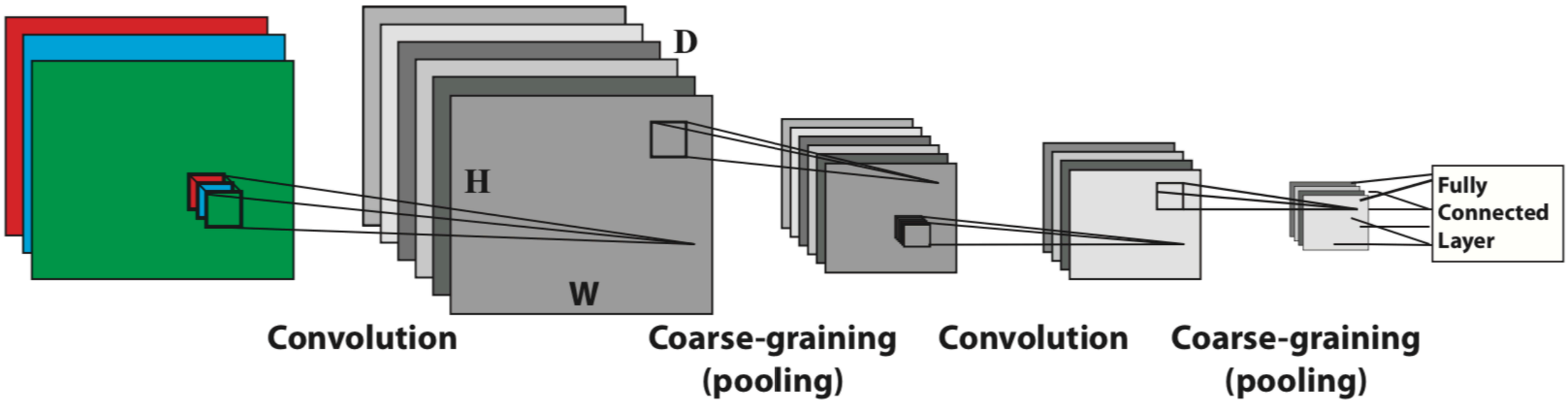
the convolution and max-pool layers are followed by an **all-to-all connected layer and a high-level classifier**, so that one can train CNNs using the standard backpropagation algorithm



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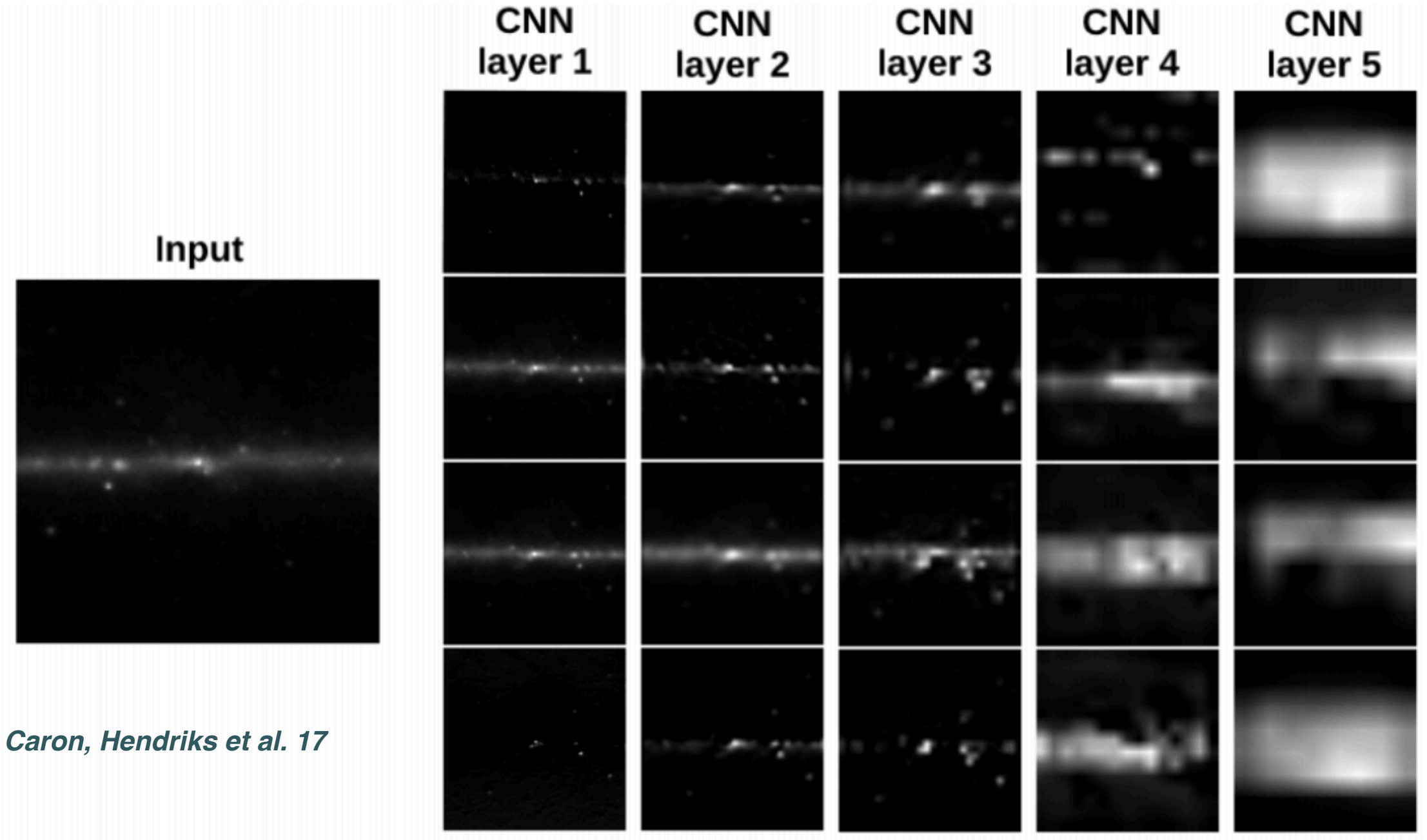
note that only problems characterised by a **spatial locality** are amenable to CNNs:
for example the 2D Ising dataset can be studied with CNNs, but not the SUSY dataset

Application to Dark Matter searches

Use CNNs to discriminate between **point sources** (astrophysical origin) and **diffuse flux** (dark matter) in galactic centre images, to compare with predictions of DM models



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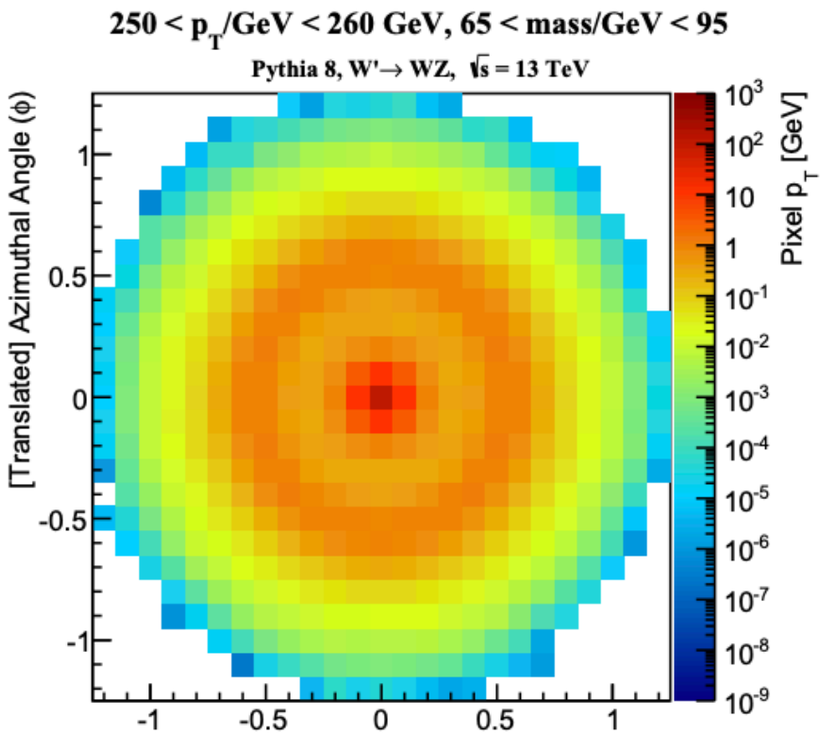
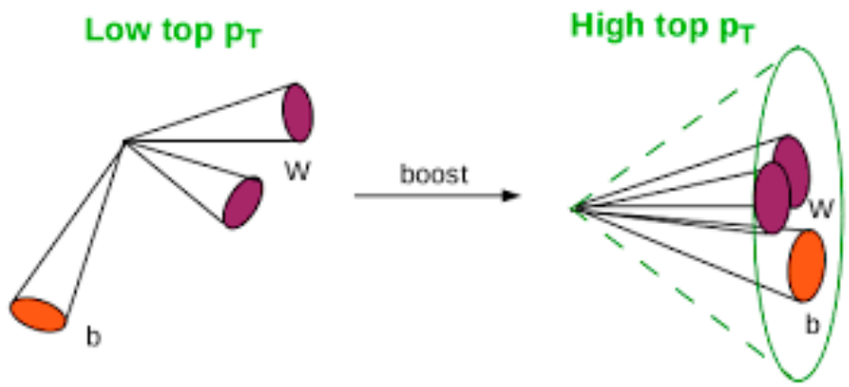
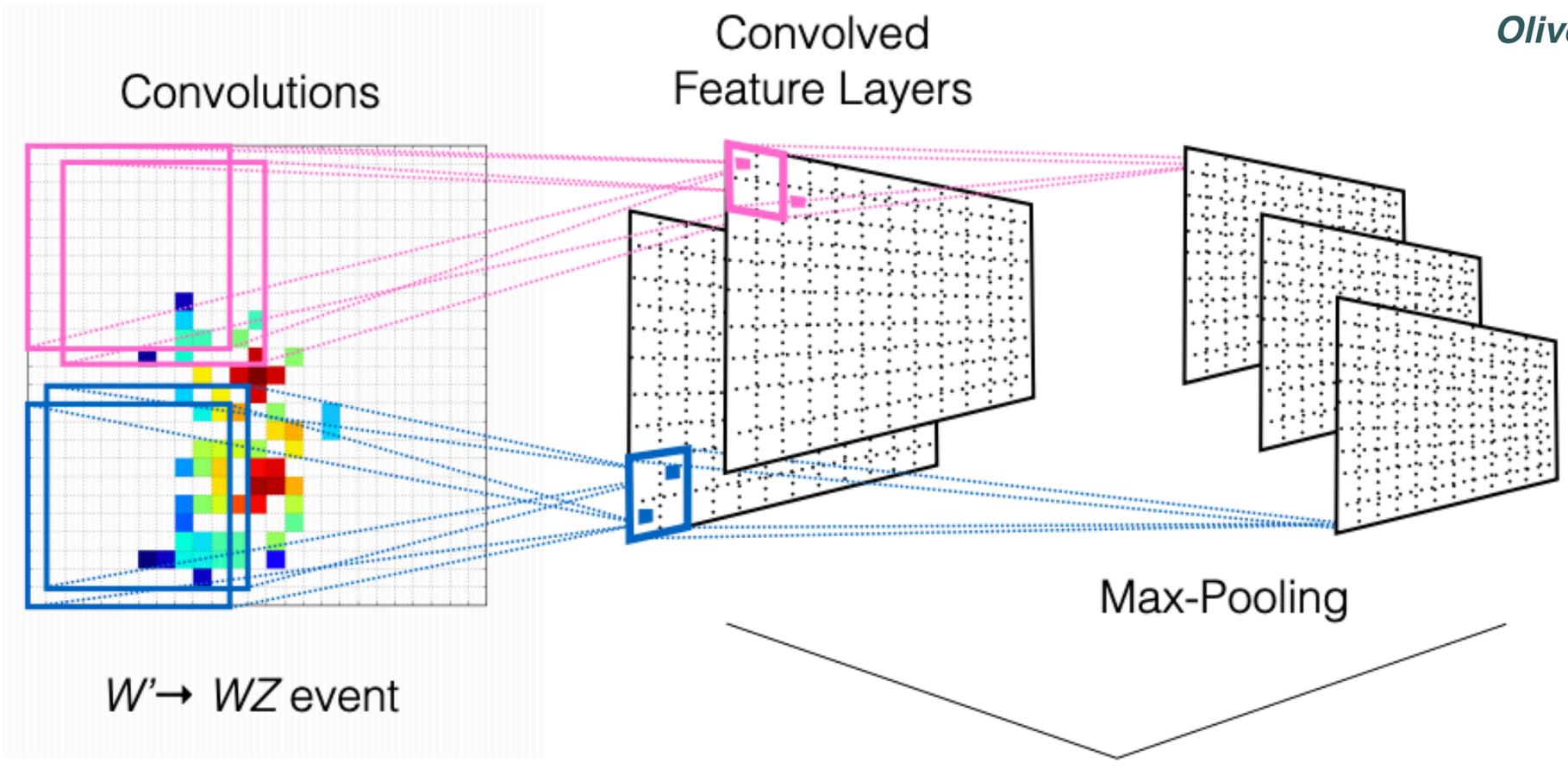
Application to LHC physics



Train CNNs on jet **images** (energy deposits in detector) to discriminate between signal and background events





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Energy-Based Models and Boltzmann Learning

Generative Models

Most ML models discussed here (Supervised NNs, logistic regression, ensemble models) are **discriminative:** designed to identify **differences between groups of data**

e.g. cats vs dogs discrimination

these models cannot carry some tasks such as **drawing new examples** from an unknown probability distribution: for this we need **generative models**

e.g. learn how to draw new examples of cat and dog images

e.g. generate new samples of a given phase of the Ising model

generative models are Machine Learning techniques that allows to learn **how to generate new examples** similar to those found in a training dataset

Here we consider **energy-based generative models**: close connection with statistical physics

hence the term Boltzmann Learning

Maximum Entropy Generative Models

basic concept is the **Shannon information-theoretic entropy**, which quantifies the statistical uncertainty one has about a random variable drawn from a probability distribution

$$S_p = \mathrm{Tr}_{\boldsymbol{x}} p(\boldsymbol{x}) \log \boldsymbol{x}$$

sum/integral over all possible values of variable

assume we have a **set of models**, functions of ***x,*** whose average should coincide with some observed values. What should be their **underlying prob dist**?

$$\{f_i(\boldsymbol{x})\} \qquad \langle f_i \rangle_{\mathrm{obs}}$$

models ***observations***

Principle of Maximum Entropy: choose the probability distribution with the largest uncertainty (Shannon entropy) subject to the observational constraints

$$\langle f_i \rangle_{\mathrm{model}} = \int d\mathbf{x} f_i(\mathbf{x}) p(\mathbf{x}) = \langle f_i \rangle_{\mathrm{obs}}$$

the selected distribution is the one that makes admits the most ignorance beyond the stated data

Maximum Entropy Generative Models

this condition can be expressed as a **Lagrange Multiplier problem** by minimising:

$$\mathscr{L}[p] = -S_p + \sum_i \lambda_i \left(\langle f_i \rangle_{\text{obs}} - \int d\boldsymbol{x}\, f_i(\boldsymbol{x}) p(\boldsymbol{x}) \right) + \gamma \left(1 - \int d\boldsymbol{x} p(\boldsymbol{x}) \right)$$

Shannon entropy ***observational constraints*** ***normalisation***

whose solution gives us the **Maximum Entropy distribution**

$$p(\boldsymbol{x}) = \frac{\exp\left(\sum_i \lambda_i f_i(\boldsymbol{x}) \right)}{\int d\boldsymbol{x}\, \exp\left(\sum_i \lambda_i f_i(\boldsymbol{x}) \right)} = \frac{\exp\left(\sum_i \lambda_i f_i(\boldsymbol{x}) \right)}{Z}$$

partition function $E = -\sum_i \lambda_i f_i(\boldsymbol{x})$

which is nothing but the **Boltzmann distribution in statistical mechanics,** and where the parameters of the distribution are fixed by the observations

$$\partial_{\lambda_i} \log Z = \langle f_i \rangle_{\text{data}}$$

Energy-based Generative Models

these MaxEnt models can be used to **infer the underlying probability distributions** from a finite set of observations, which subsequently can be used to generate new instances

training an energy-based generative model: using the data to infer the model parameters

$$E\left(\boldsymbol{x};\boldsymbol{\theta}\right) = -\sum_i \theta_i f_i(\boldsymbol{x})$$

as in Supervised Learning, we need to specify a **cost function,** which however in the case of generative models is much subtler: what defines a good model?

the most useful method is to **maximise the log-likelihood** of the training set

$$\hat{\boldsymbol{\theta}} = \arg\,\min_{\theta} \mathscr{L}(\{\boldsymbol{\theta}\})$$

$$\mathscr{L}(\{\boldsymbol{\theta}\}) = \left\langle \log p_{\theta}(\boldsymbol{x}) \right\rangle_{\text{data}} = -\left\langle E(\boldsymbol{x};\boldsymbol{\theta}) \right\rangle_{\text{data}} - \log Z(\{\boldsymbol{\theta}\})$$

where we have used that the **generative probability distribution** is of the Boltzmann form and that the partition function does not depend on the data

Boltzmann machines

The training of **energy-based generative models** proceeds usually via SGD

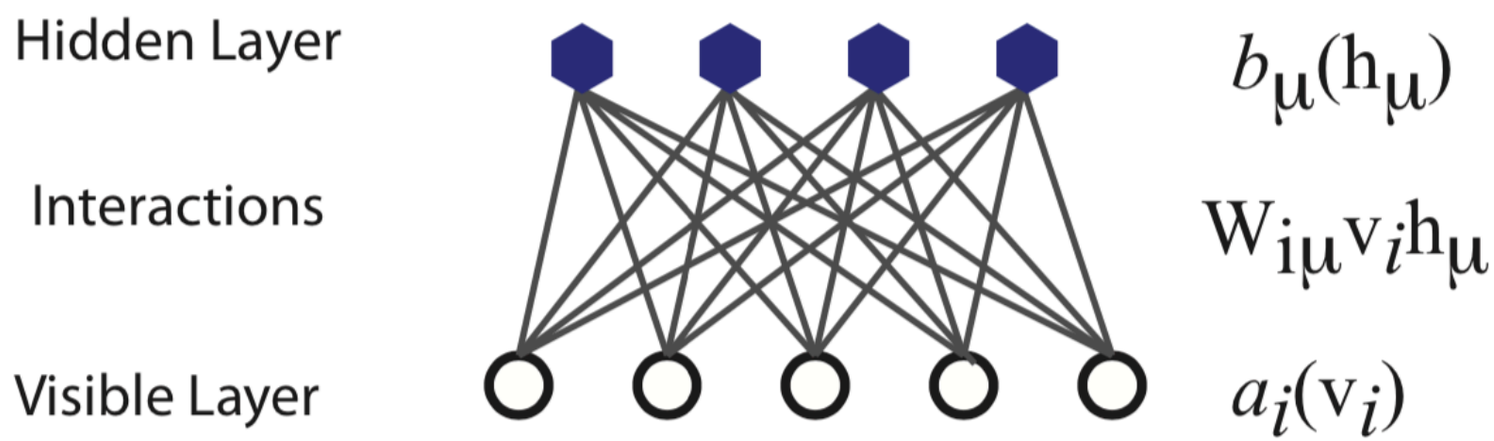
MaxEnt generative models are defined by the choice of the **energy**

$$p(\boldsymbol{x}) = \frac{\exp\left(\sum_i \lambda_i f_i(\boldsymbol{x})\right)}{\int d\boldsymbol{x}\, \exp\left(\sum_i \lambda_i f_i(\boldsymbol{x})\right)} = \frac{\exp\left(\sum_i \lambda_i f_i(\boldsymbol{x})\right)}{Z} = \frac{\exp\left(-E(\boldsymbol{x};\boldsymbol{\lambda})\right)}{Z}$$

one can construct various **other generative models** with different choices of the energy

e.g. Restricted Boltzmann machines

$$E(\boldsymbol{x};\boldsymbol{\theta}) = -\sum_i a_i(v_i) - \sum_\mu b_\mu(h_\mu) - \sum_{i\mu} W_{i\mu} v_i h_\mu$$



Generative Models & Adversarial Learning

The Kullback-Leibler divergence

The KL divergence, a measure of the similarity between two probability distributions *p(**x**)* and *q(**x**)* plays an important role in machine learning applications

$$D_{KL}\left(p\,||\,q\right) = \int d\boldsymbol{x}\, p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} \qquad D_{KL}\left(q\,||\,p\right) = \int d\boldsymbol{x}\, q(\boldsymbol{x}) \log \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}$$

which can be symmetrised to construct a **squared metric** (distance)

$$D_{JS}\left(p\,||\,q\right) = \frac{1}{2}\left(D_{KL}\left(p\,\middle|\middle|\,\frac{p+q}{2}\right) + D_{KL}\left(q\,\middle|\middle|\,\frac{p+q}{2}\right)\right)$$

Jensen-Shannon divergence

The KL-divergence is **positive-definite**, and only vanishes when *p(**x**)=* q*(**x**)*

$$D_{KL}\left(p\,||\,q\right) \geq 0$$

in general the integral cannot be computed and one needs to sample the two probability distributions by means of a suitable binning

The Kullback-Leibler divergence

In **generative models** one deals with two probability distributions (data and model), which we would like to have as similar as possible

$$p_\theta(\boldsymbol{x}) \qquad p_{\text{data}}(\boldsymbol{x})$$

from model *from training data*

however subtleties about how we define **similarity** have large implications for the model training

maximising the **log-likelihood of the data under the model** is the same as **minimising the KL divergence** between the data distribution and the model distribution

$$D_{KL}\left(p_{\text{data}}||p_\theta\right) = \int d\boldsymbol{x}\, p_{\text{data}}(\boldsymbol{x}) \log \frac{p_{\text{data}}(\boldsymbol{x})}{p_\theta(\boldsymbol{x})}$$

$$= \int d\boldsymbol{x}\, p_{\text{data}}(\boldsymbol{x}) \log p_{\text{data}}(\boldsymbol{x}) - \int d\boldsymbol{x}\, p_{\text{data}}(\boldsymbol{x}) \log p_\theta(\boldsymbol{x})$$

$$= S[p_{\text{data}}] - \left\langle \log p_\theta \right\rangle_{\text{data}}$$

The Kullback-Leibler divergence

maximising the **log-likelihood of the data under the model** is the same as **minimising the KL divergence** between the data distribution and the model distribution

$$\left\langle \log p_\theta(\boldsymbol{x}) \right\rangle_{\text{data}} = S[p_{\text{data}}] - D_{KL}\left(p_{\text{data}} \,||\, p_\theta\right)$$

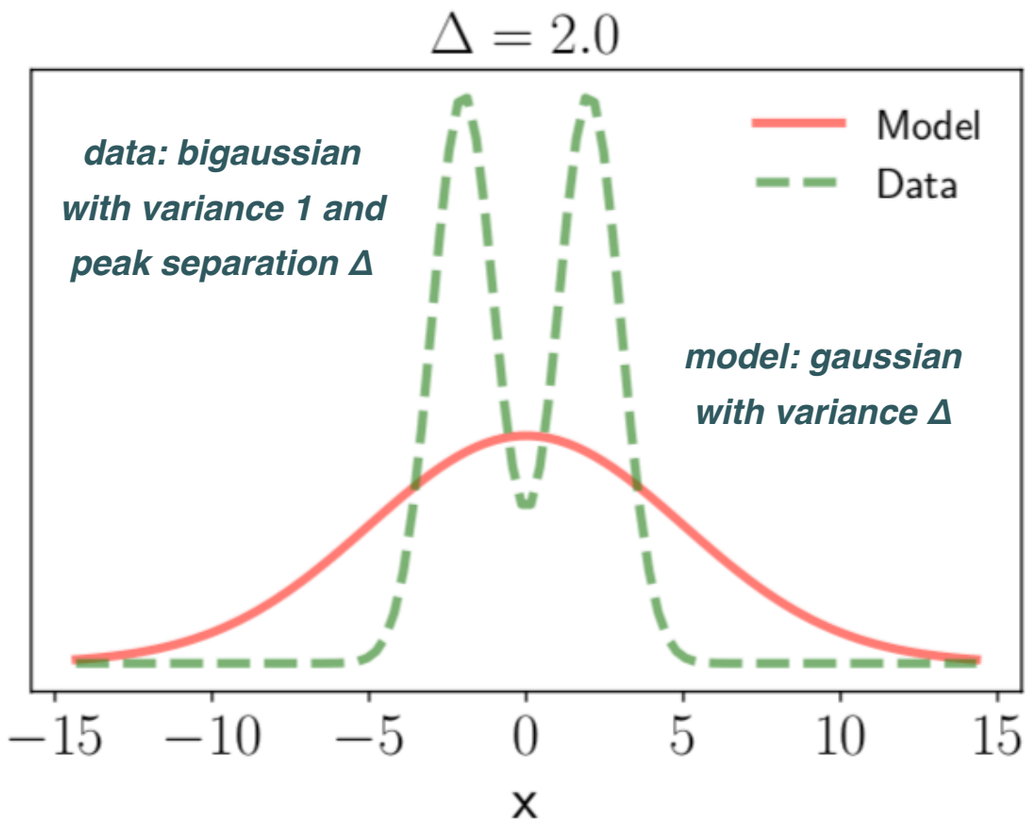
Log-likelihood of data under model

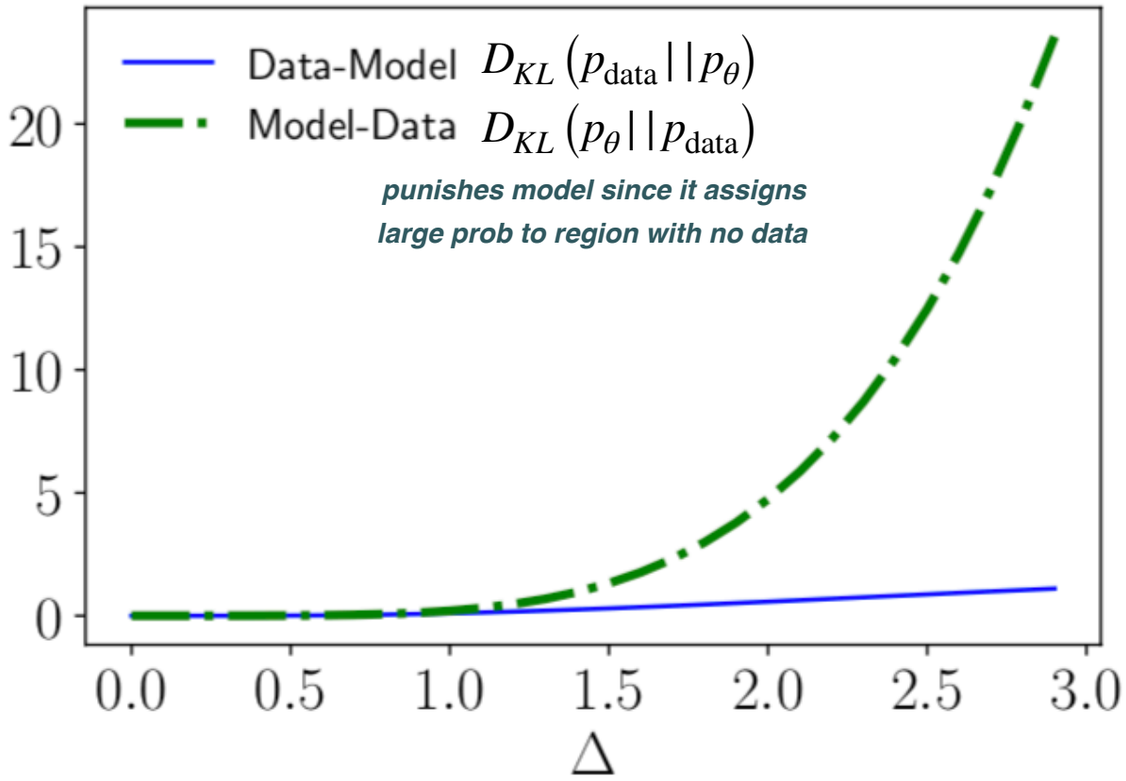
entropy of data: independent of model parameters

KL-divergence

Similarity

Similarity between probability distributions is a subtle concept





$D_{KL}\left(p_{\text{data}}||p_\theta\right)$ → misses important information when comparing the data and theory probability distributions

Adversarial Learning

(draw values of θ accordingly to p_θ and compare with data)

(1) $D_{KL}\left(p_{\text{data}} || p_\theta\right)$ → ***Calculable using sampling***

(2) $D_{KL}\left(p_\theta || p_{\text{data}}\right)$ → ***Large when model over-weights low-density regions near real peaks***

→ ***but not calculable since p_{data} unknown ….***

In **Adversarial Learning** we achieve a similar goal as that of minimising ***(2)*** by training a **discriminator** to distinguish between real data points and samples from the model

By punishing the model for generating points that can be easily discriminated from the data, Adversarial Learning decreases the **weight of regions in the model space that are far away from data points,** regions that inevitably arise when maximising the likelihood

Generative adversarial networks

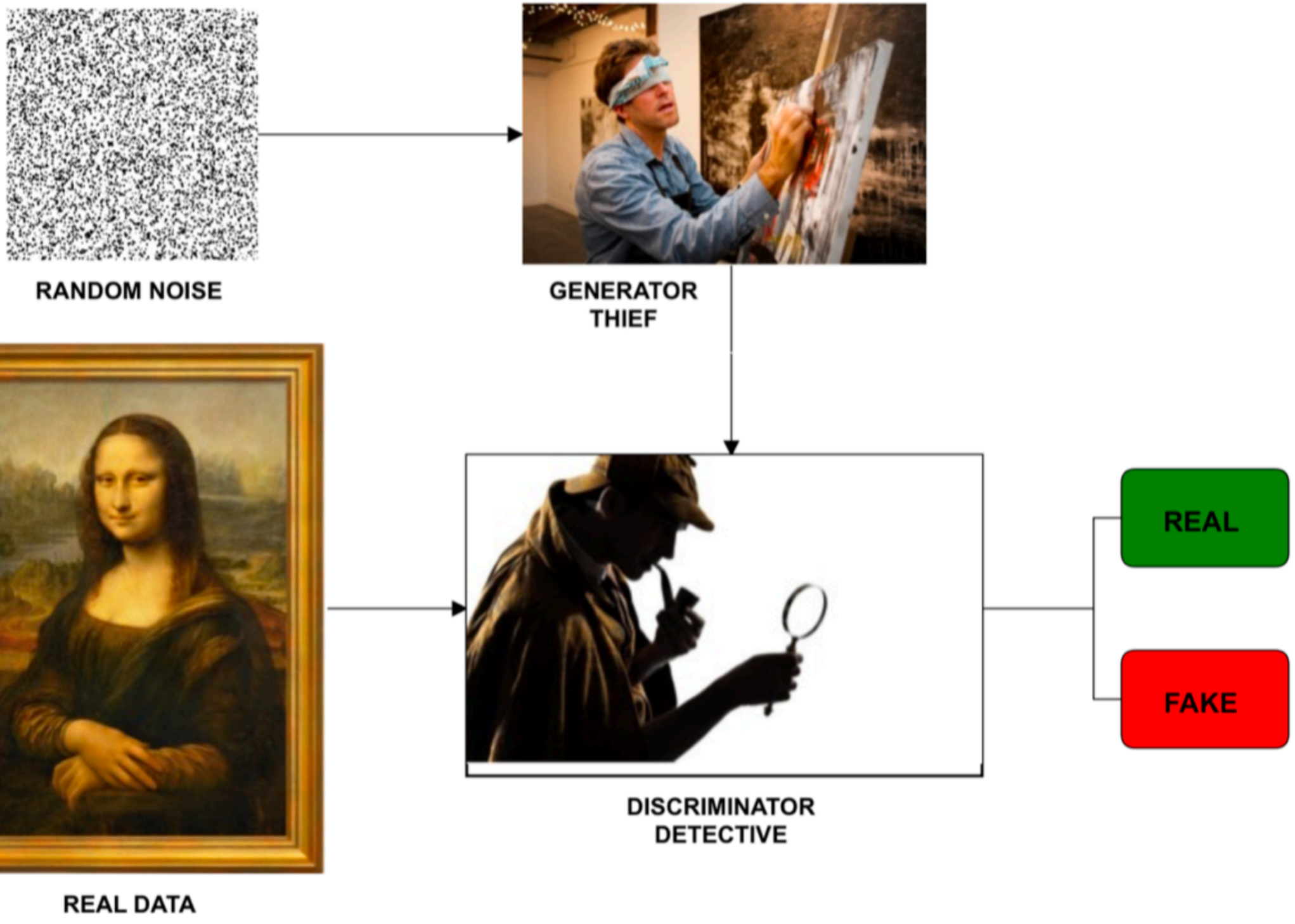
Generative Adversarial Networks (GANs) are deep neural network architectures, composed by two independent NNs which **compete against each other**

- ***(1)*** A **generator G** NN that creates (samples) pseudo-data by inferring the probability distribution associated to the training dataset

- ***(2)*** A **discriminator D** NN which determines the probability of a given sample arises from the actual training data rather than having been produced by **G**

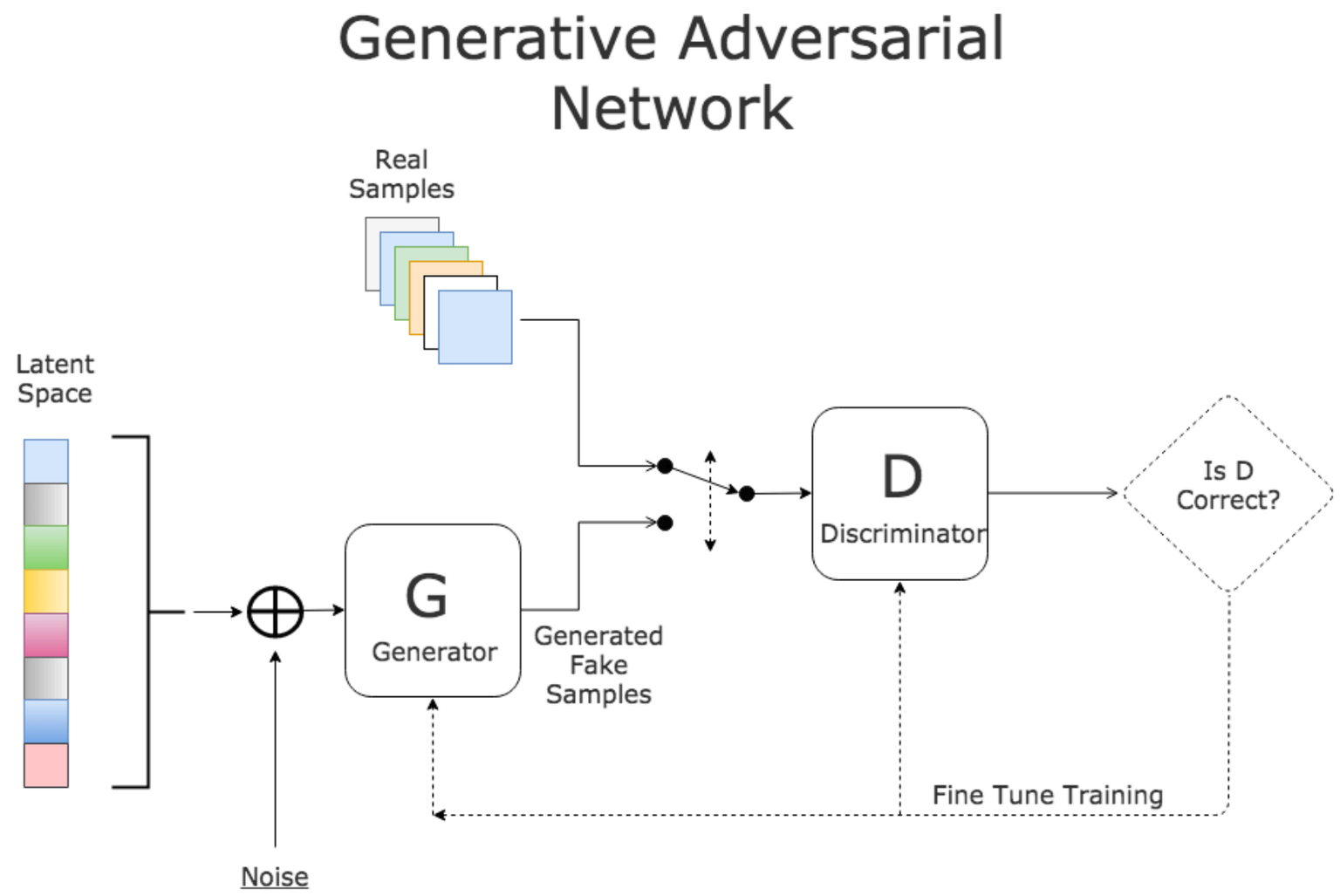
the generator network **G** should be trained to maximise the probability that the discriminator network **D** makes a mistake: that is, **G** should generate pseudo-data samples that are virtually **indistinguishable** from the actual data

Generative adversarial networks



Generative Adversarial Networks

- New architecture for an **unsupervised neural network training** (unlabelled samples)
- Based on two **independent nets** that work separately and act as **adversaries:**
  - the **Discriminator (D)** undergoes training and plays the role of classifier
  - the **Generator (G)** and is tasked to generate random samples that **resemble real samples** with a twist rendering them as fake samples.



GAN training

As with other NN architectures one uses GD to train GANs, but now one has to **update sequentially** the model parameters of both **G** and **D**

- Take a sample of *N* data points from the training set

$$\{\boldsymbol{x}_n\}_{n=1}^{N} \qquad \boldsymbol{x}_n = (x_{n,1}, x_{n,2}, \ldots, x_{n,p})$$

p = number of features per sample

- Produce a sample of *N* pseudo-data points from generator **G** (at ite$_0$ this is random noise)

$$\{\boldsymbol{z}_n\}_{n=1}^{N} \qquad \boldsymbol{z}_n = (z_{n,1}, z_{n,2}, \ldots, z_{n,p})$$

- Evaluate the cost function: since we are dealing with binary classification (true/false) the appropriate cost function is the **cross-entropy**

$$C\left(\boldsymbol{\theta}_D, \boldsymbol{\theta}_G\right) = \frac{1}{N}\sum_{n=1}^{N}\left(\log D(\boldsymbol{x}_i) + \log(1 - D(G(\boldsymbol{z}_i)))\right)$$

NN params of D ***NN params of G*** ***output of D when input a real data sample*** ***output of D when input a ``fake'' data sample produced by G***

- Train **D** using GD to maximise its discrimination capability

GAN training

- Evaluate the cost function: since we are dealing with binary classification (true/false) the appropriate cost function is the **cross-entropy**

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- Train **D** using GD to maximise its discrimination capability

$$\mathbf{v}_t = \eta_t \nabla_{\theta_D} C(\boldsymbol{\theta}_{D,t}, \boldsymbol{\theta}_G)\,, \qquad \boldsymbol{\theta}_{D,t+1} = \boldsymbol{\theta}_{D,} - \mathbf{v}_t$$

- At this point **D** can tell apart data from pseudo-data pretty well, so we need to train **G** to generate better (closer to the training set) pseudo-data samples
- Produce a sample of *N* pseudo-data points from the generator **G** $\{\boldsymbol{z}_n\}_{n=1}^{N}$

$$C\left(\boldsymbol{\theta}_D, \boldsymbol{\theta}_G\right) = \frac{1}{N}\sum_{n=1}^{N}\log(1 - D(G(\boldsymbol{z}_i)))$$

output of D (now with its parameters fixed)

$$\mathbf{v}_t = \eta_t \nabla_{\theta_G} C(\boldsymbol{\theta}_{D,t}, \boldsymbol{\theta}_G)\,, \qquad \boldsymbol{\theta}_{G,t+1} = \boldsymbol{\theta}_{G,t} - \mathbf{v}_t$$

GAN training

the generator and discriminator are sequentially trained and iterated until convergence is achieved, at this point **D** cannot tell apart the pseudo-data from **G** from the real data

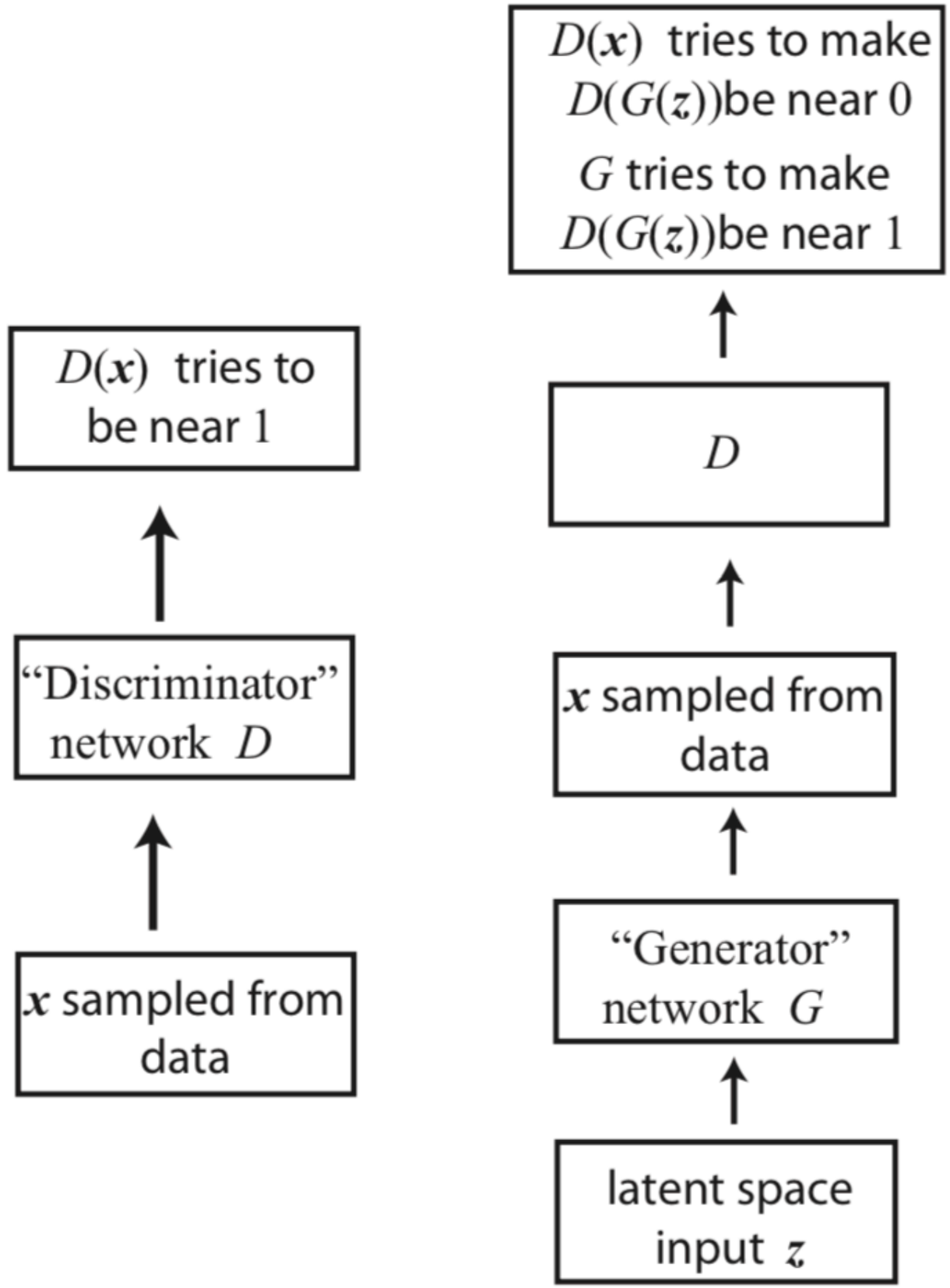


Image generation with GANs

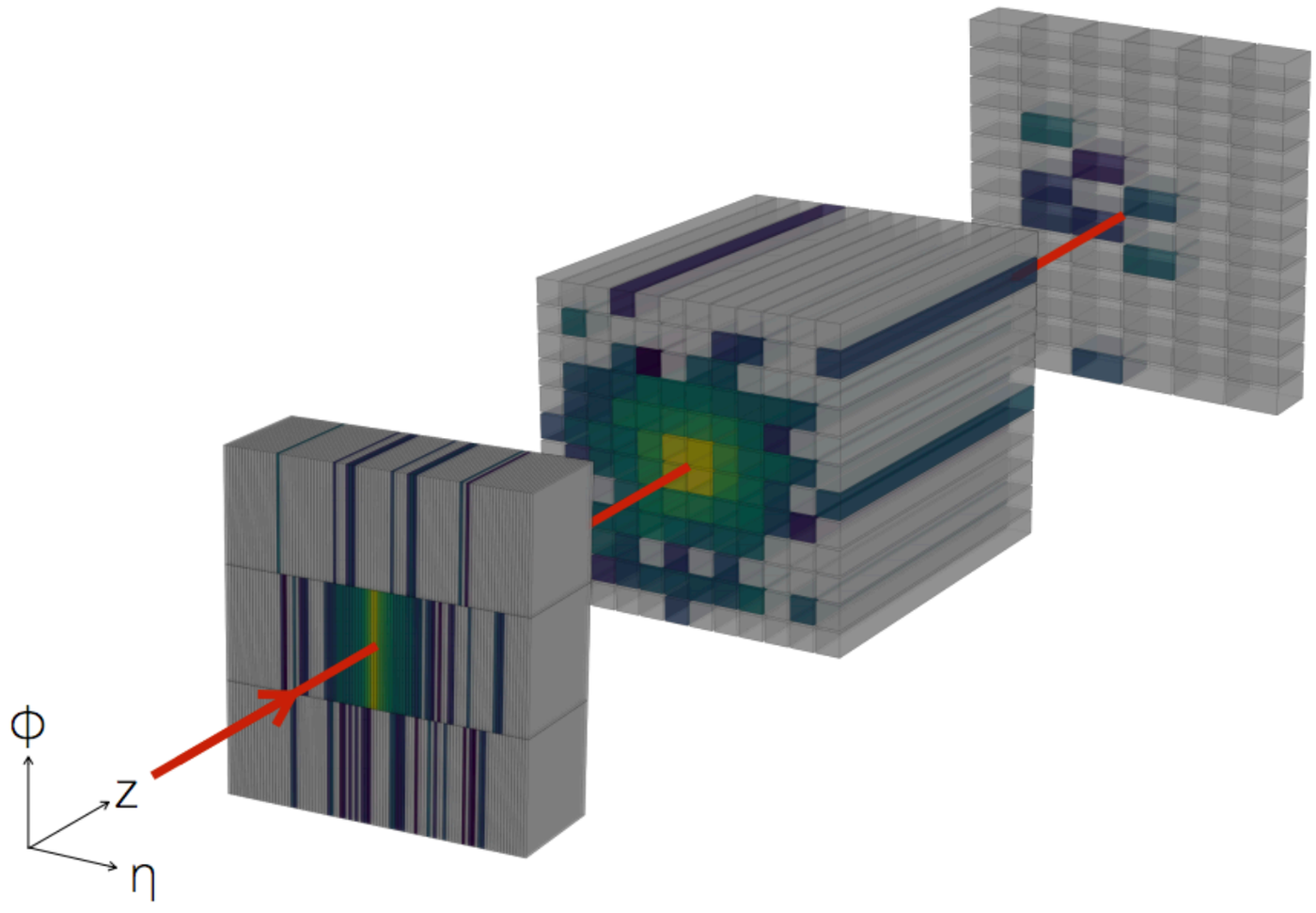
https://thispersondoesnotexist.com/

GANs for detector simulation in HEP

- Modelling accurately the response of detectors with the **propagation of high energy particles** is an essential task for present and future HEP experiment

- **Detector simulation at the LHC** is a very CPU-intensive task, dominated by modelling of particle showers inside calorimeters

- **Generative Adversarial Networks** can speed up detector simulation by orders of magnitude



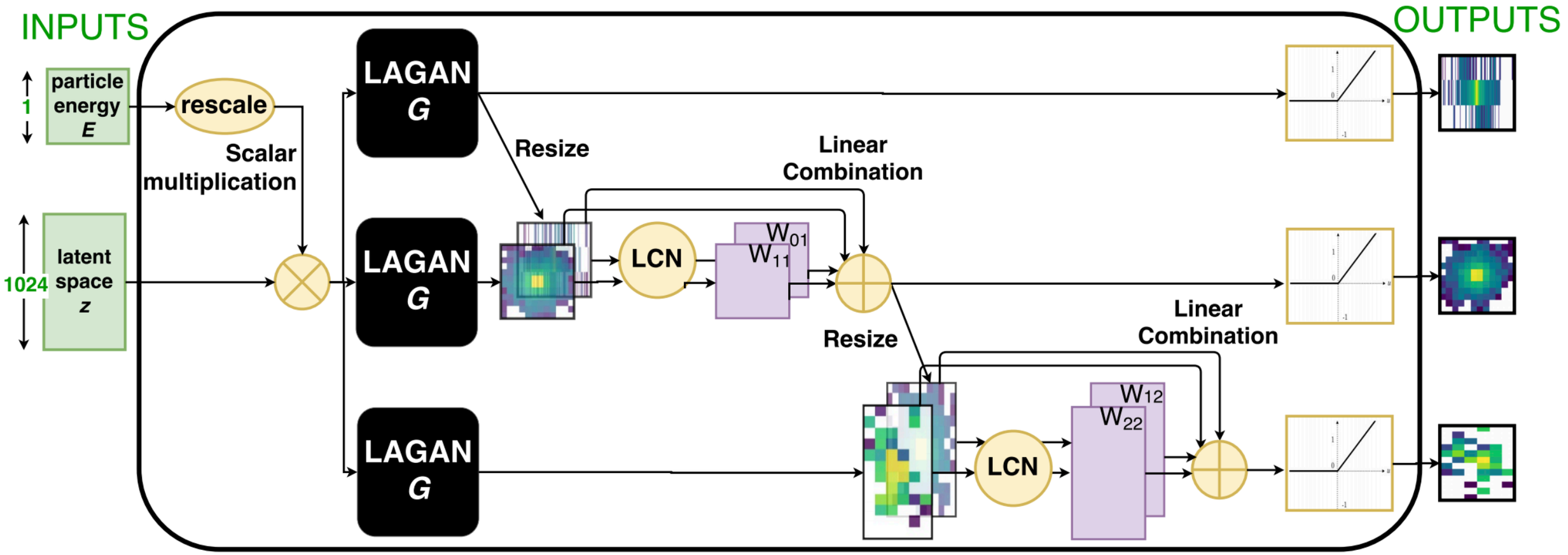
*Task: to efficiently model the **propagation of high energy particles** (and their interaction) within the layers of electromagnetic and hadronic calorimeters*

GANs for detector simulation in HEP

- Use GANs as a tool to **speed up full simulation of particle showers** in a HEP calorimeter
- The generator G learns a map from **a latent space** to space of **generated samples** for training
- Carefully understanding the **underlying physics of particle propagation** in a detector is crucial to optimise the training strategy, *e.g.* relationships between neighbouring detector layers

Generator Network

Output: ***generated samples*** *to be used for training D*



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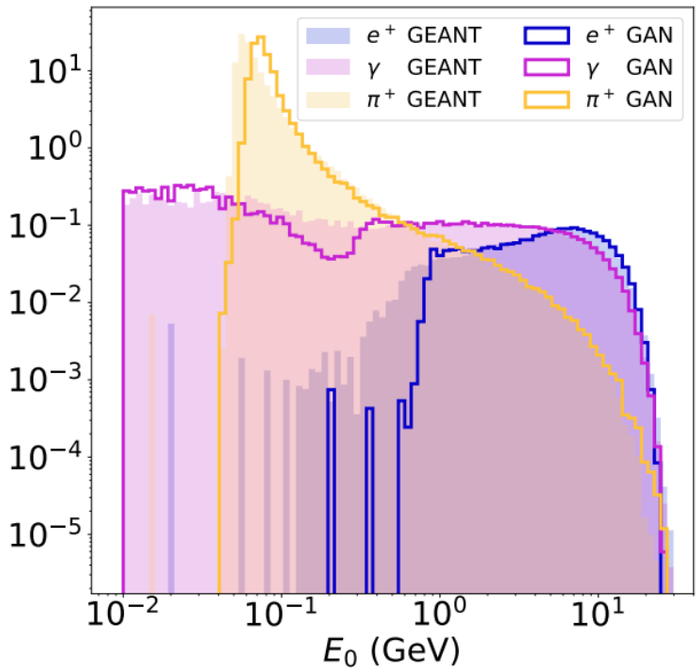
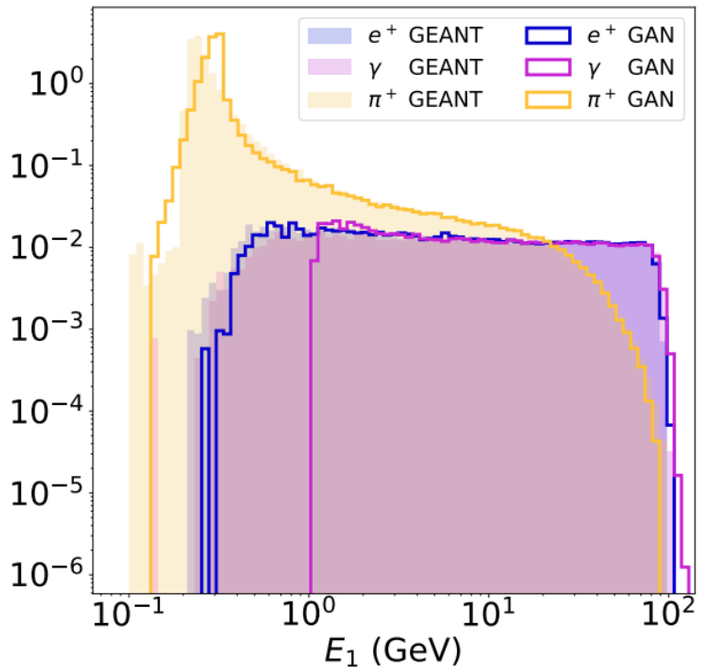
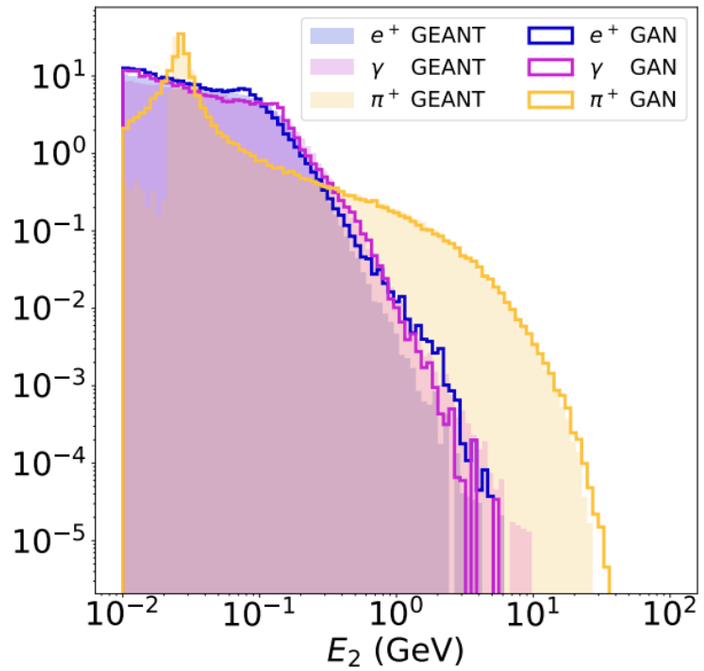
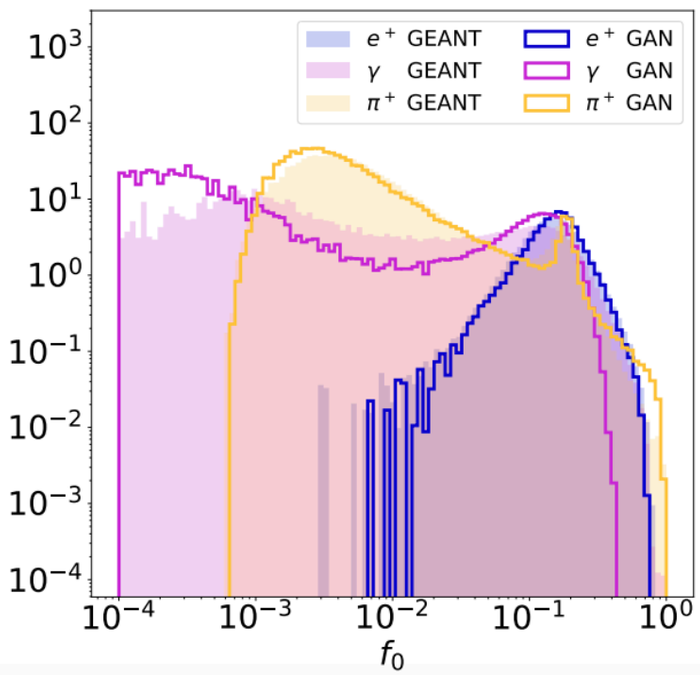
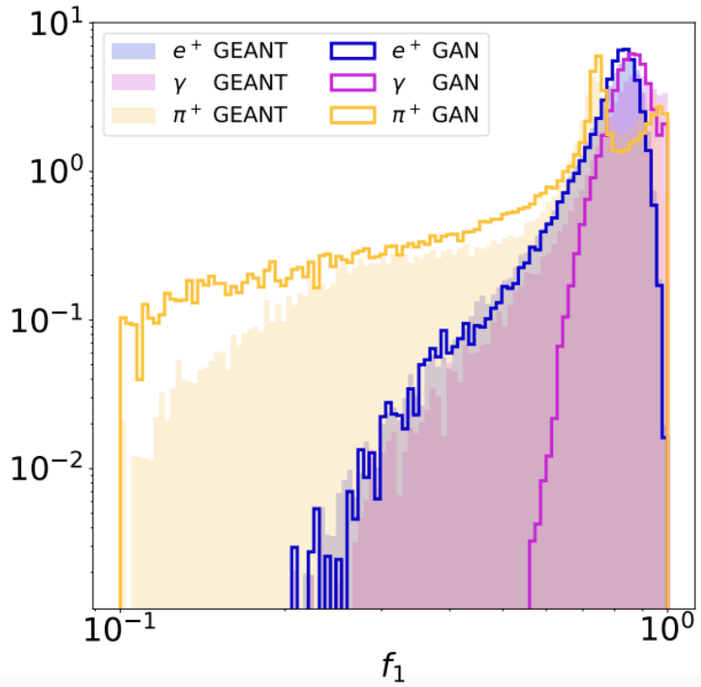
GANs for detector simulation in HEP

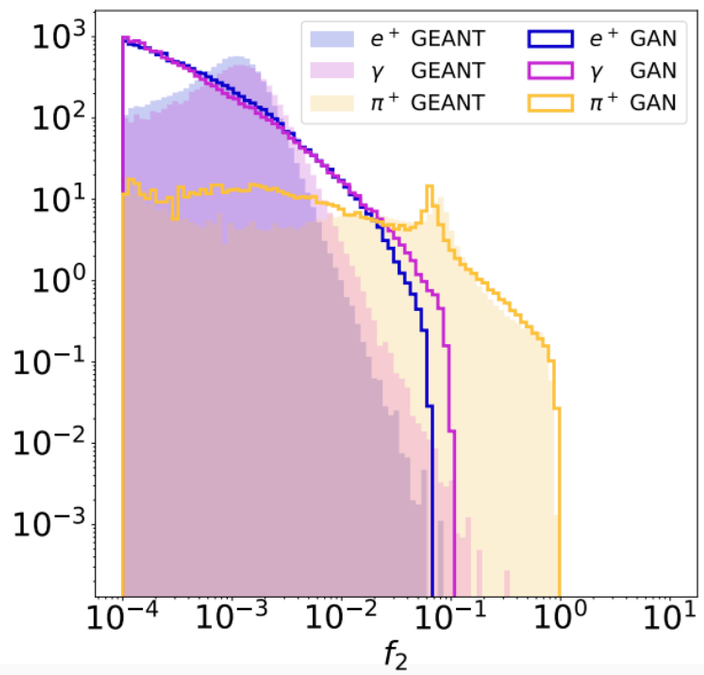












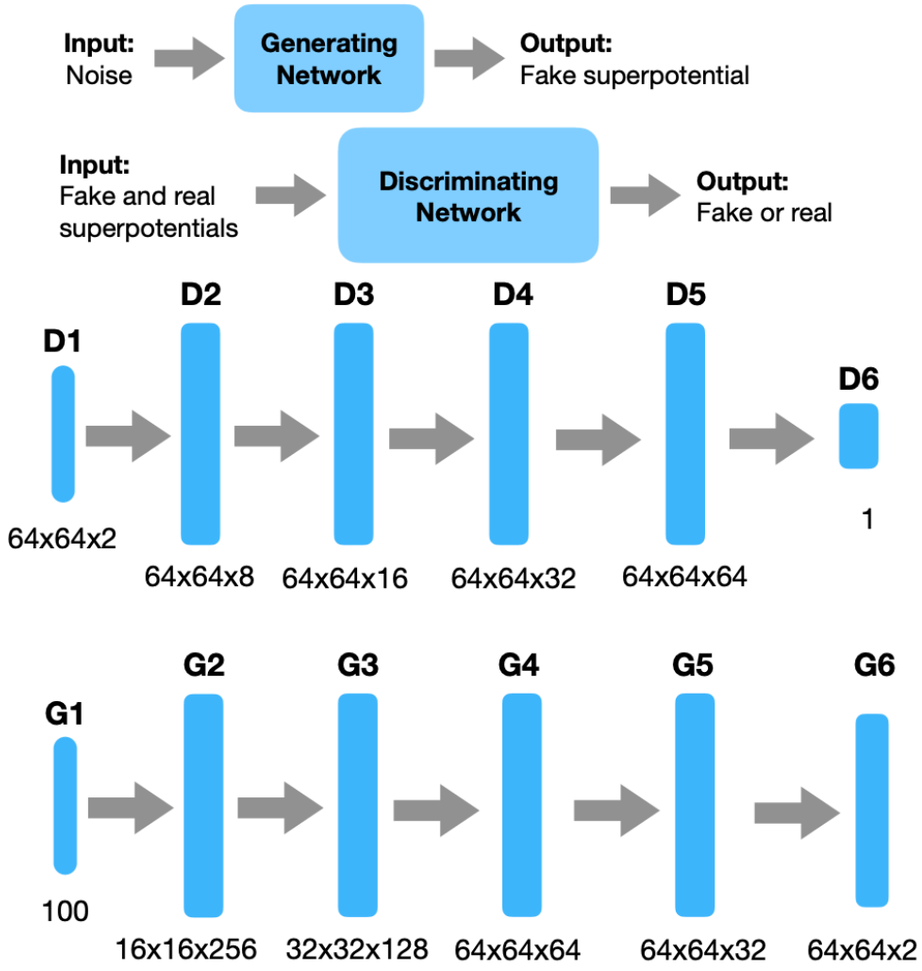
GANs for detector simulation in HEP

Simulator	Hardware	Batch Size	ms/shower
GEANT4	CPU	N/A	1772
CALOGAN	CPU	1	13.1
		10	5.11
		128	2.19
		1024	2.03
	GPU	1	14.5
		4	3.68
		128	0.021
		512	0.014
		1024	0.012

Speed-up by several orders of magnitude, specially when running in GPUs

(More) Applications of ML to Theoretical Physics

GANs for generating EFT models



- Starting from examples of **known SUSY QFTs** (with generating superpotentials) train GANs to generate other, equally consistent, theories

- After training the generator outputs new superpotentials that correspond to **new SUSY theories** not present in the training sample

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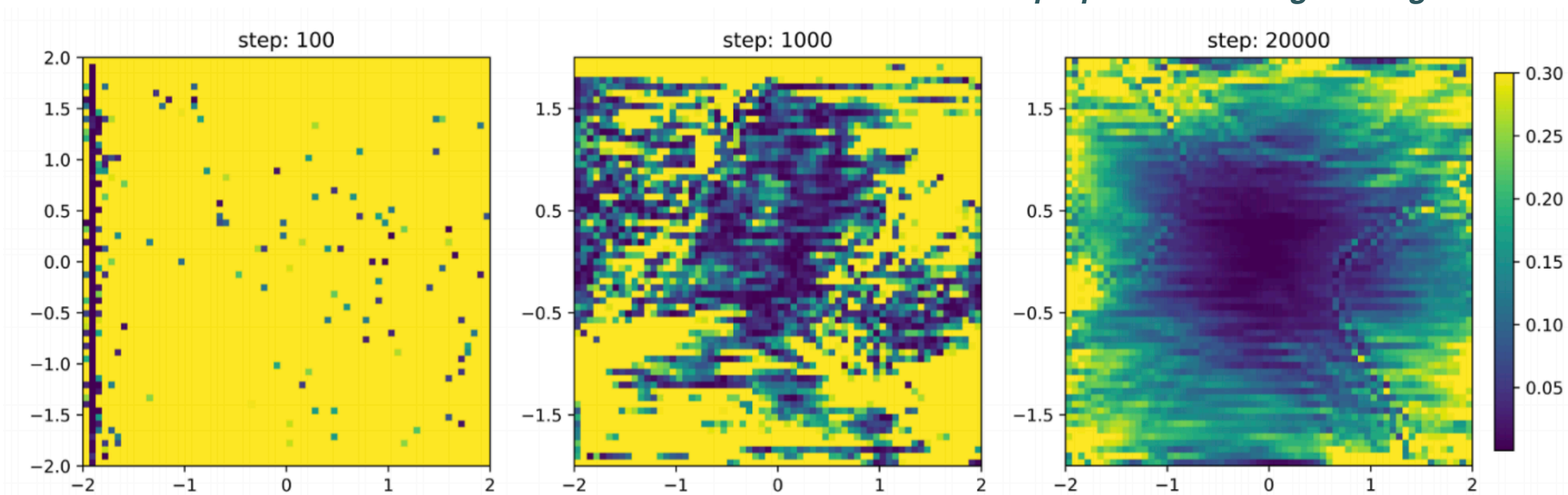
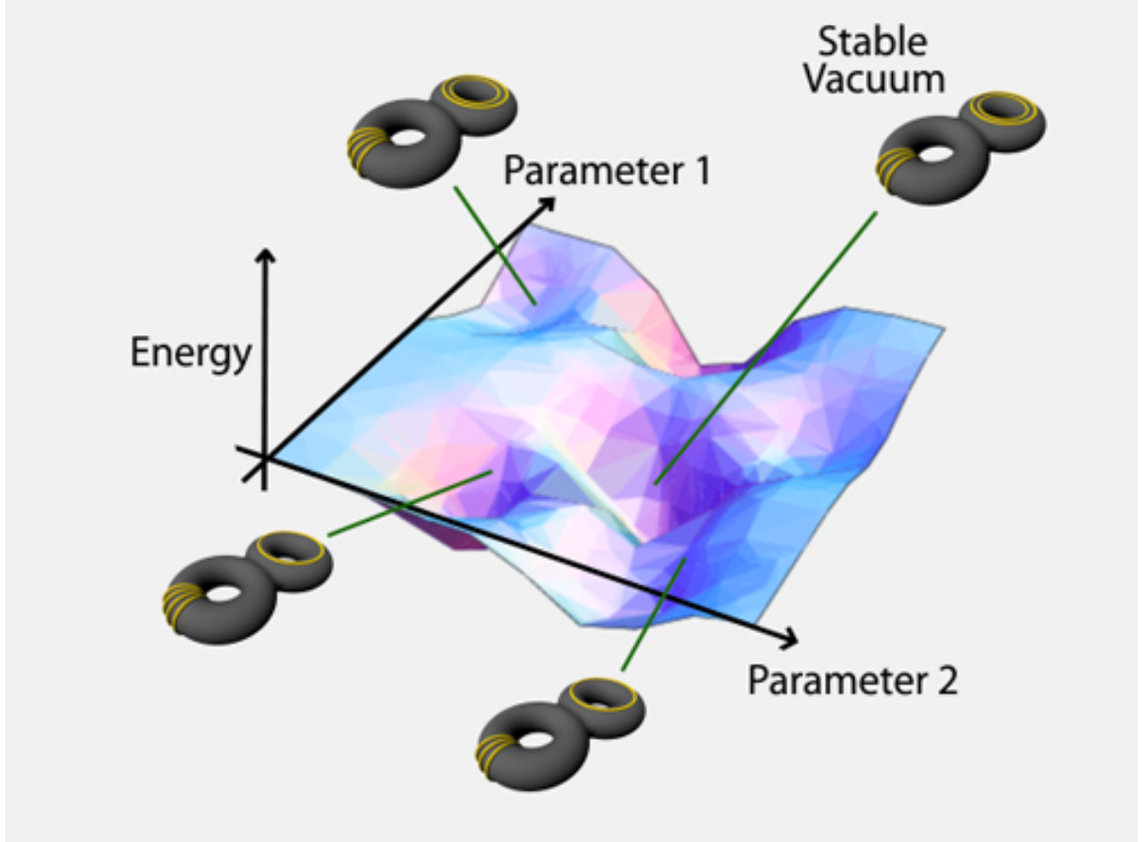
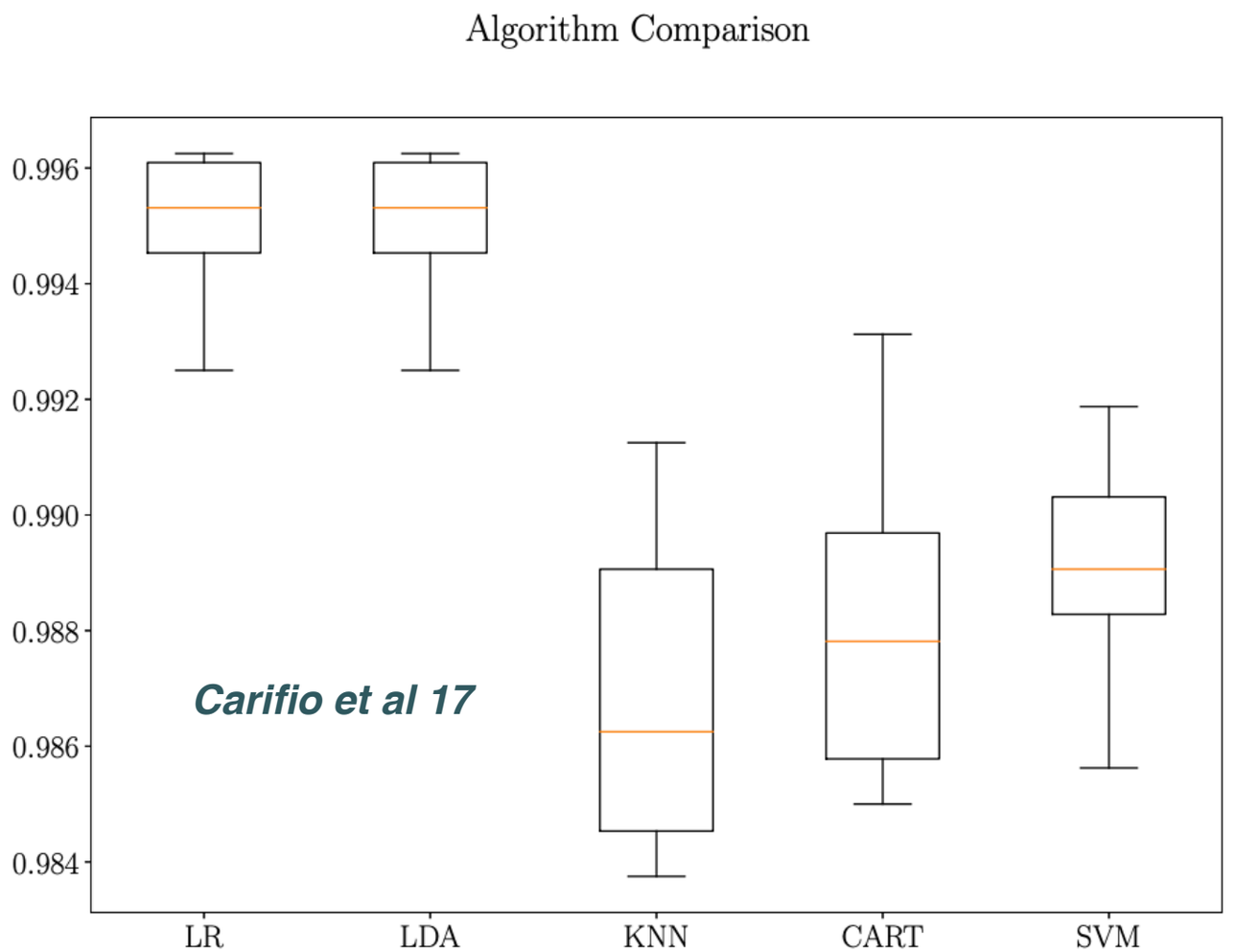
evolution of superpotential during training



Machine Learning the String Landscape

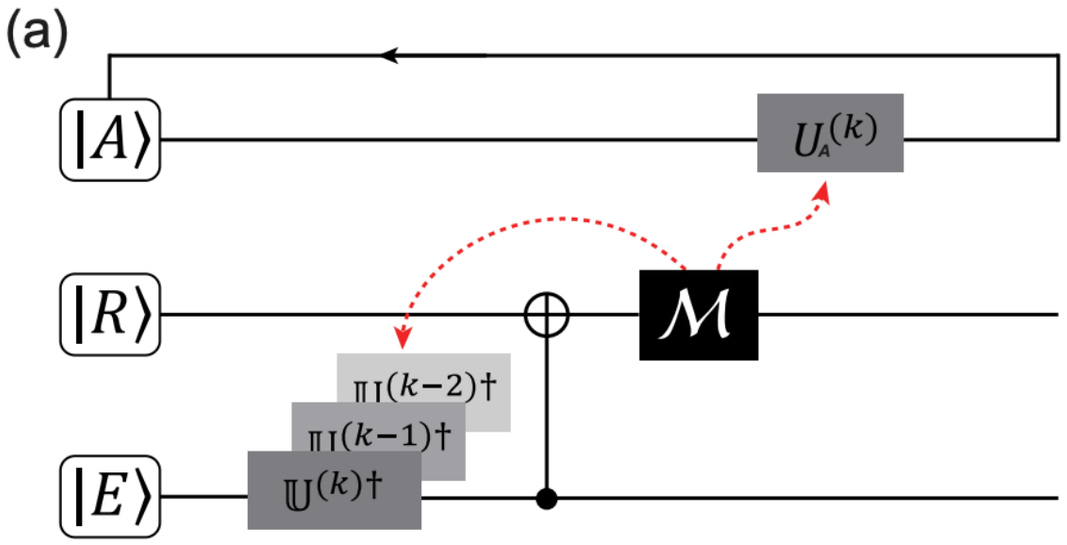
- Numerical exploration of the string theory landscape
- **Formulation and verification of conjectures** about the properties of the landscape
- Using regression, K-means clustering, decision trees, Linear Discriminant Analysis …..

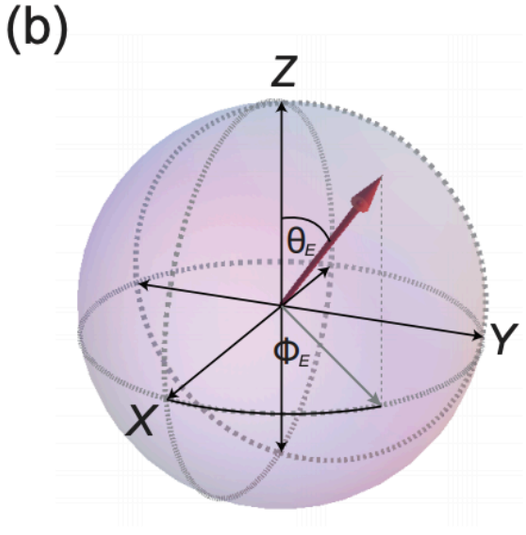


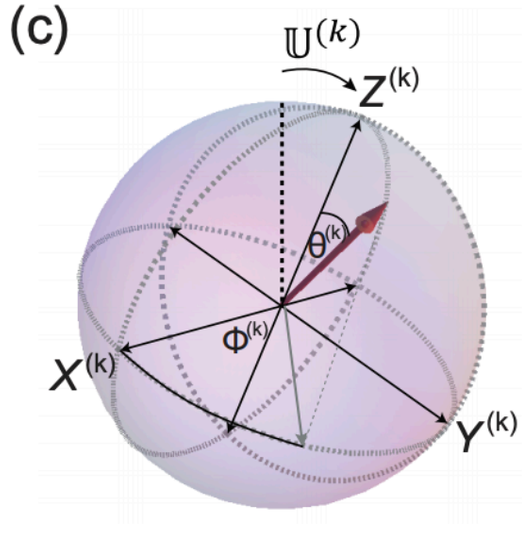


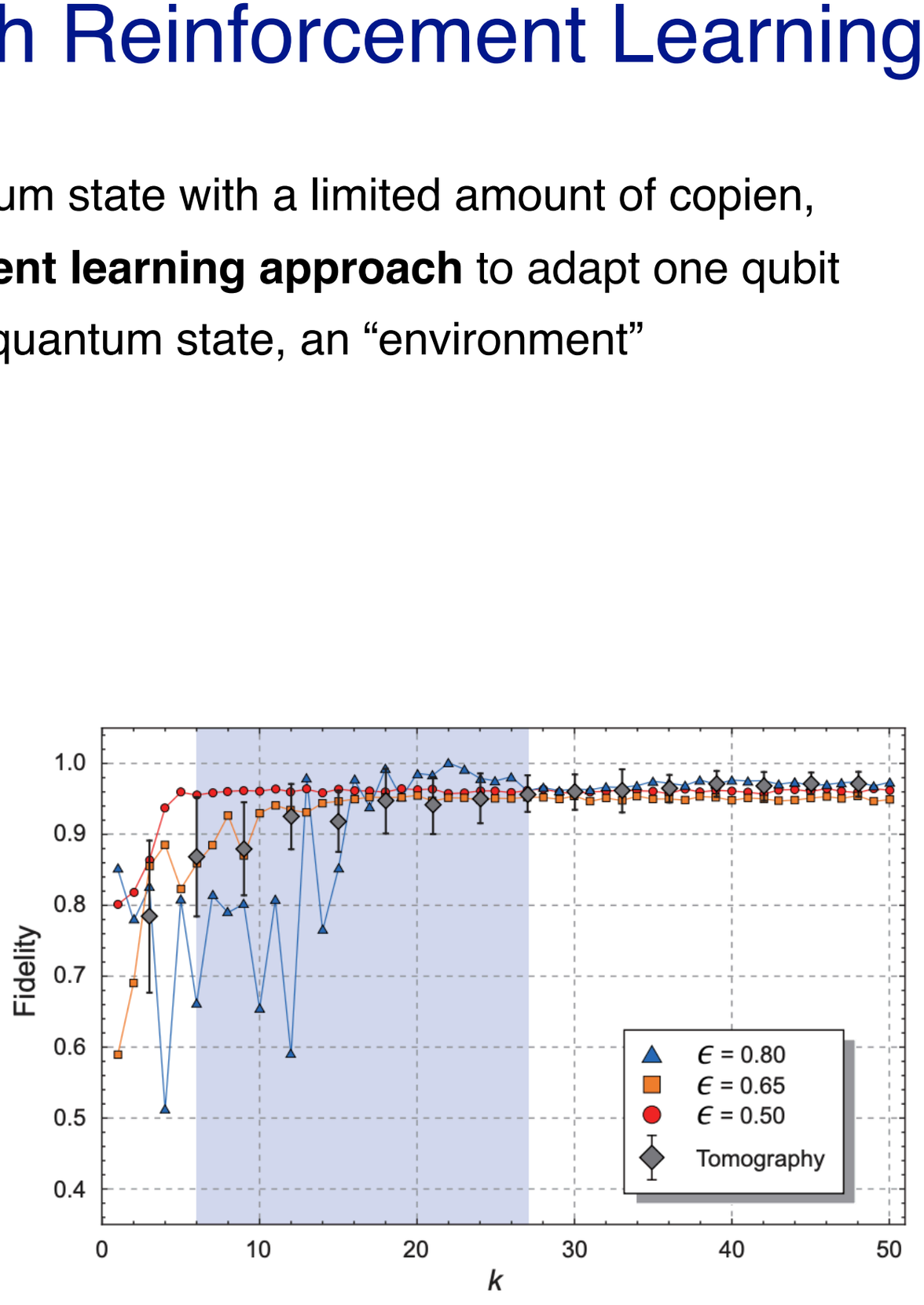
Qubit Reconstruction with Reinforcement Learning

to reconstruct an unknown photonic quantum state with a limited amount of copien, one employs a **semi-quantum reinforcement learning approach** to adapt one qubit state, an “agent”, to an unknown quantum state, an “environment”









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More Examples

Machine learning and the physical sciences

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