

## Searching for new physics without knowing the signal model

- Machine Learning
- Automatization
- Data Derived Signal Regions

**Sascha Caron**  
**(Radboud University**  
**and Nikhef)**

# Outline

- 1. Introduction:
- 2. Particle Physics (Particle DM)  
situation in 2019
- 3. DM searches with Deep Networks
- 4. Learning DM/HEP models
- 5. Unsupervised searches
- 6. Simulation without MC simulators

Very personal selection of topics/papers/etc.  
No real overview talk...



# The situation in 2011

## What do we expect to find at the LHC?



One physicist's schematic view of particle physics in the 21st century  
(Courtesy of Hitoshi Murayama)

# 2019: What has changed ?

- **We have not seen any signs of new physics (no SUSY and no convincing signal of anything else !)**
- **We got a “toolbox” from the future**



# 2019: What has changed ?

- **We have not seen any signs of new physics (no SUSY and no convincing signal of anything else !)**

**→ Was that expected ?**

**→ Maybe yes ...**

Higgs: You got a new toy, it's a playmobil castle with a size between 1-100 cm. Can you find it ?





Today: I have a new toy for you, I put it somewhere in your room. The size is 0.1-100 cm. Can you find it ?



**Could work to implement more of automatization for particle physics to „scan“ the full room for something interesting...**

**→ This can help LHC, but might also work for astrophysics**

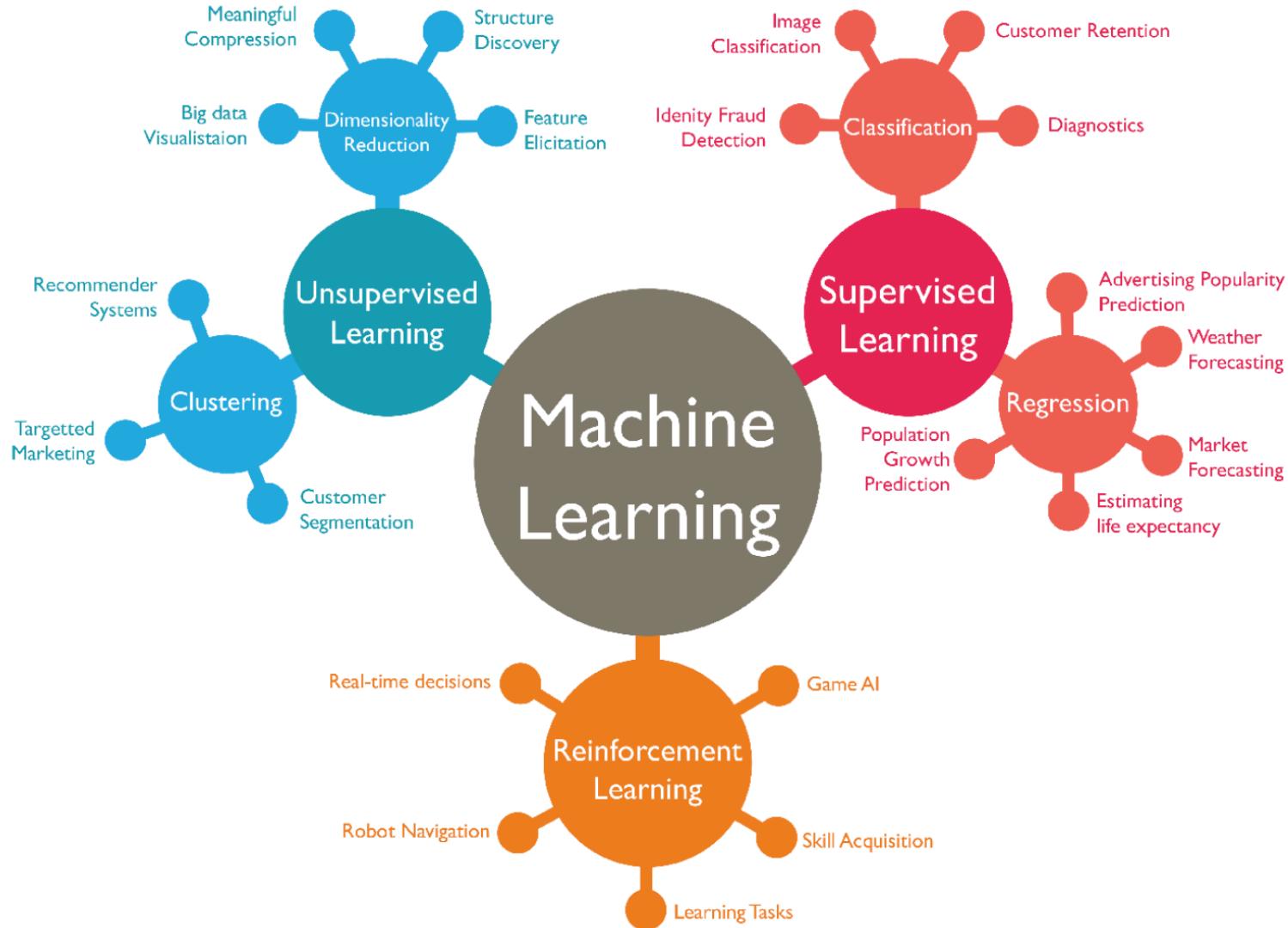
**→ We can embed into this “scan” our prejudice how new physics looks like, e.g. in this case it would be „toy“ detection software trained on all known toys...**



# 1. Machine Learning or toys from the future



# What is Machine Learning ?





# Most important example: Supervised Learning

## Computer systems “learn” with data

Actually the computer “learn/derives and fits”  
a continuous estimator  $\hat{\mathbf{f}}(\vec{x})$  for an unknown function  $\mathbf{f}(\vec{x})$   
from  $i$  discrete data points  $\vec{x}_i$  with known function values  $\mathbf{f}(\vec{x}_i)$ .

$i$  discrete data points  $\vec{x}_i$  with known function values  $\mathbf{f}(\vec{x}_i)$ .

is called the “**training set**”.

Determining  $\hat{\mathbf{f}}(\vec{x})$  is called “**training**”.

The axis values of the  $\vec{x}_i$  values are called “**features**”.

# Neural Networks

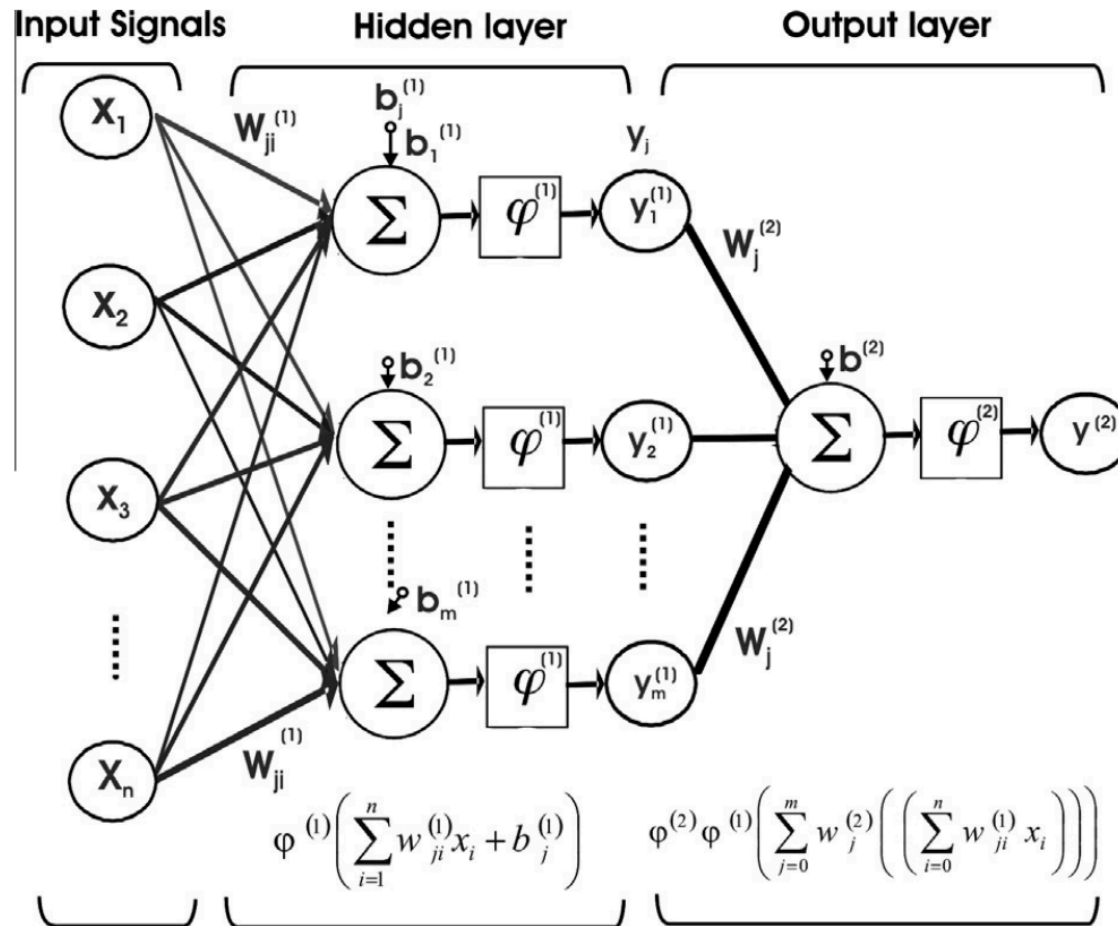
- Let us now make the basis function itself nonlinear combinations of its inputs

$$\begin{aligned} y^{(2)} &= \varphi^{(2)} \left( \sum_{j=1}^m \left( w_j^{(2)} y_j^{(1)} + b^{(2)} \right) \right) \\ &= \varphi^{(2)} \left( \sum_{j=1}^m w_j^{(2)} \varphi^{(1)} \left( \sum_{i=1}^n w_{ji}^{(1)} x_i + b_j^{(1)} \right) + b^{(2)} \right) \end{aligned}$$

And phi is a non-linear activation function, b is called bias

*(bias allows to “shift” the activation function)*

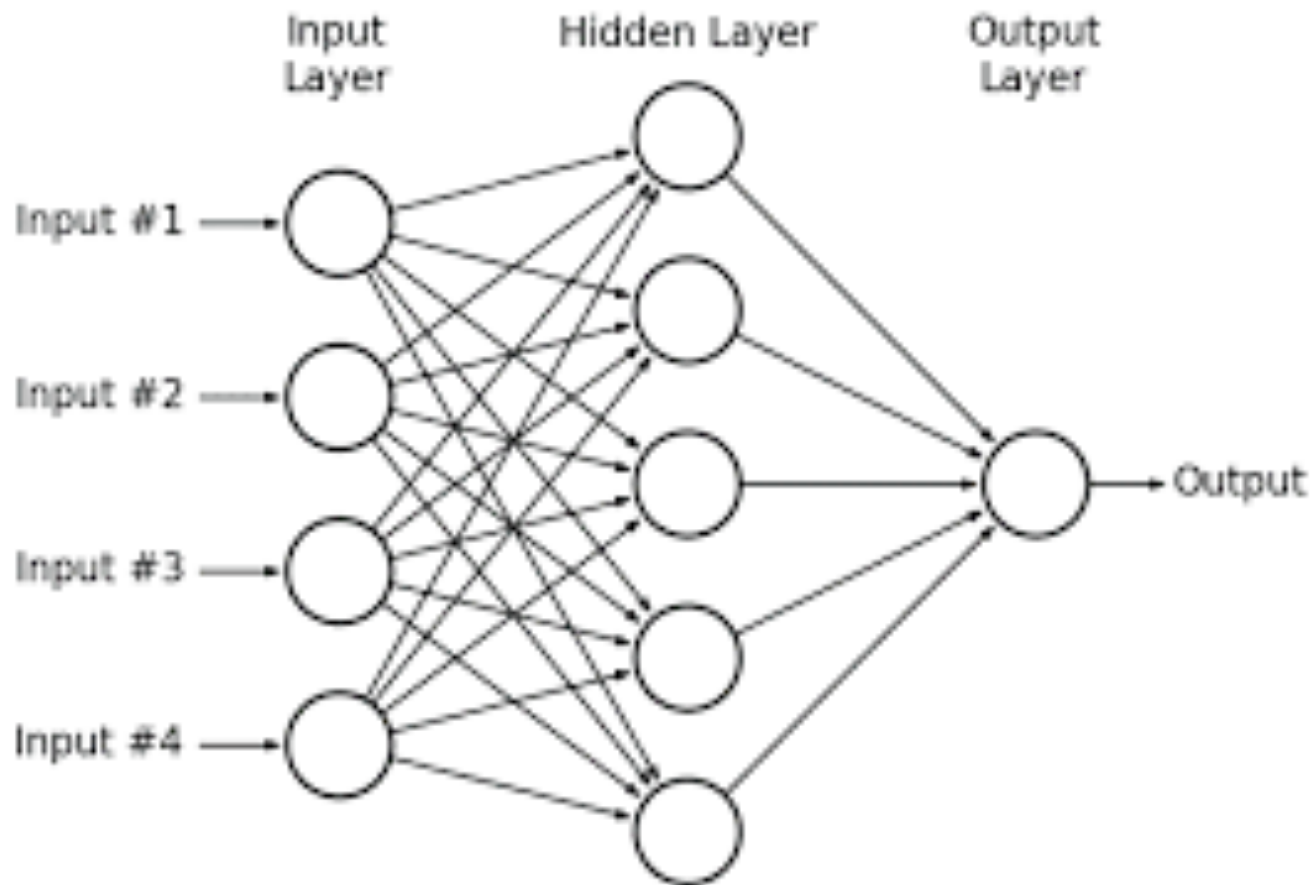
$$\begin{aligned}
 y^{(2)} &= \varphi^{(2)} \left( \sum_{j=1}^m \left( w_j^{(2)} y_j^{(1)} + b^{(2)} \right) \right) \\
 &= \varphi^{(2)} \left( \sum_{j=1}^m w_j^{(2)} \varphi^{(1)} \left( \sum_{i=1}^n w_{ji}^{(1)} x_i + b_j^{(1)} \right) + b^{(2)} \right)
 \end{aligned}$$



y



$$\begin{aligned}
 y^{(2)} &= \varphi^{(2)} \left( \sum_{j=1}^m \left( w_j^{(2)} y_j^{(1)} + b^{(2)} \right) \right) \\
 &= \varphi^{(2)} \left( \sum_{j=1}^m w_j^{(2)} \varphi^{(1)} \left( \sum_{i=1}^n w_{ji}^{(1)} x_i + b_j^{(1)} \right) + b^{(2)} \right)
 \end{aligned}$$



This is a 3 layer (1 hidden layer) feedforward (multilayer) perceptron

→ This is the “simplest network”

**“Training”:**

Finding the set of weights which minimize the error function

# Example: NNpdfs

Fitting pdfs without assuming the underlying function

## 10. Parton distributions for the LHC Run II

NNPDF Collaboration ([Richard D. Ball](#) (U. Edinburgh, Higgs Ctr. Theor. Phys. & CERN) *et al.*). Oct 31, 2014. 138 pp.

Published in **JHEP 1504 (2015) 040**

EDINBURGH-2014-15, IFUM-1034-FT, CERN-PH-TH-2013-253, OUTP-14-11P, CAVENDISH-HEP-14-11

DOI: [10.1007/JHEP04\(2015\)040](https://doi.org/10.1007/JHEP04(2015)040)

e-Print: [arXiv:1410.8849](https://arxiv.org/abs/1410.8849) [hep-ph] | [PDF](#)

[References](#) | [BibTeX](#) | [LaTeX\(US\)](#) | [LaTeX\(EU\)](#) | [Harvmac](#) | [EndNote](#)

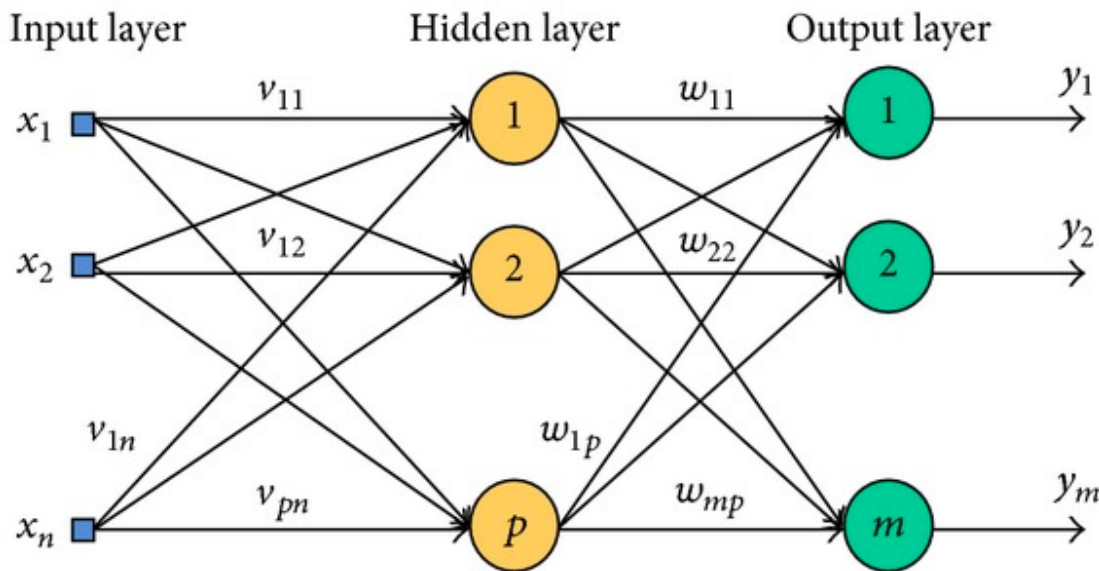
[CERN Document Server](#); [ADS Abstract Service](#); [Link to Article from SCOAP3](#)

[Detailed record](#) - [Cited by 1054 records](#) 1000+



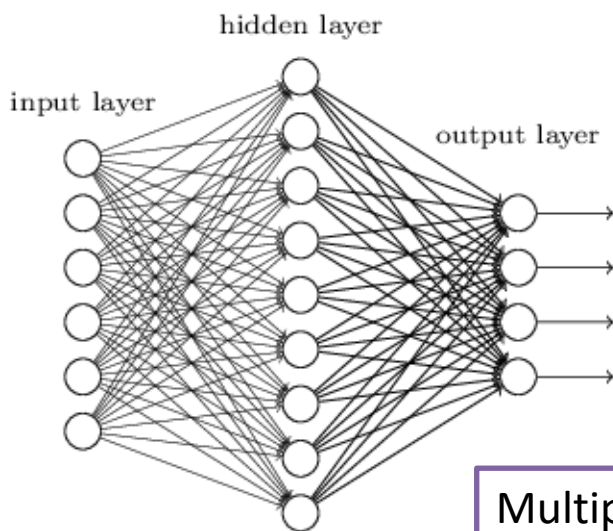
# Neural Networks

- Of course we can have multiple output nodes



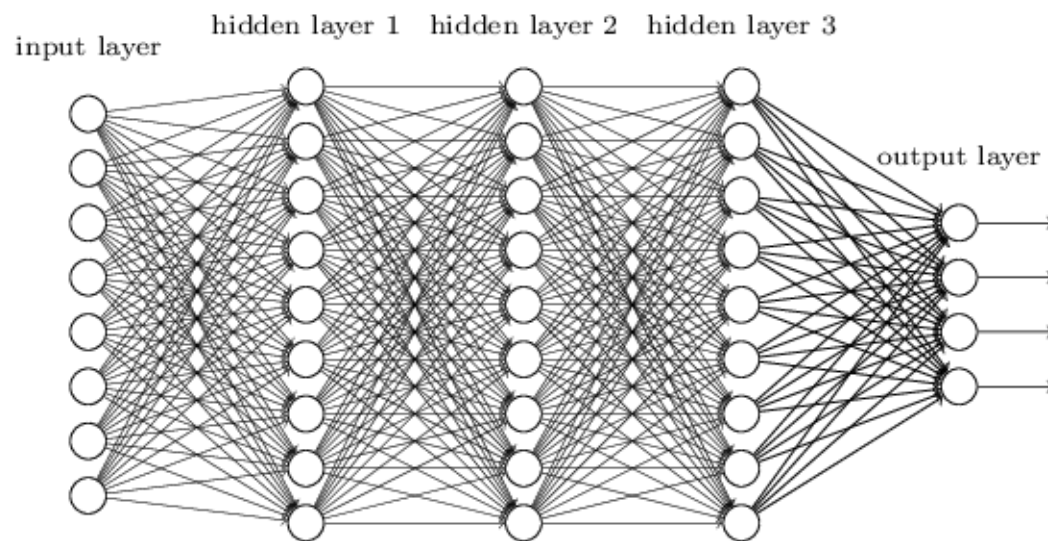
... or multiple hidden layers...

"Non-deep" feedforward  
neural network



Multiple  
Output  
Nodes !

Deep neural network



We often use 5-10 layers

# 2014 First deep network in HEP (begin 2018 we had 50 on arxiv)

## Searching for Exotic Particles in High-Energy Physics with Deep Learning

P. Baldi,<sup>1</sup> P. Sadowski,<sup>1</sup> and D. Whiteson<sup>2</sup>

<sup>1</sup>*Dept. of Computer Science, UC Irvine, Irvine, CA 92617\**

<sup>2</sup>*Dept. of Physics and Astronomy, UC Irvine, Irvine, CA 92617†*

Collisions at high-energy particle colliders are a traditionally fruitful source of exotic particle discoveries. Finding these rare particles requires solving difficult signal-versus-background classification problems, hence machine learning approaches are often used. Standard approaches have relied on ‘shallow’ machine learning models that have a limited capacity to learn complex non-linear functions of the inputs, and rely on a pain-staking search through manually constructed non-linear features. Progress on this problem has slowed, as a variety of techniques have shown equivalent performance. Recent advances in the field of deep learning make it possible to learn more complex functions and better discriminate between signal and background classes. Using benchmark datasets, we show that deep learning methods need no manually constructed inputs and yet improve the classification metric by as much as 8% over the best current approaches. This demonstrates that deep learning approaches can improve the power of collider searches for exotic particles.

AUC			
Technique	Low-level	High-level	Complete
BDT	0.73 (0.01)	0.78 (0.01)	0.81 (0.01)
NN	0.733 (0.007)	0.777 (0.001)	0.816 (0.004)
DN	0.880 (0.001)	0.800 (< 0.001)	0.885 (0.002)

Discovery significance			
Technique	Low-level	High-level	Complete
NN	2.5 $\sigma$	3.1 $\sigma$	3.7 $\sigma$
DN	4.9 $\sigma$	3.6 $\sigma$	5.0 $\sigma$

Important:  
Input only 4 vectors !!!!  
No knowledge about physics !!!!



# Then ..hyped in QCD ... jet algorithms.. ... top taggers.. Showering and calorimeters

**Machine Learning for Jet Physics**

11 Dec 2017, 01:15 → 13 Dec 2017, 18:00 US/Pacific

2-100 (Lawrence Berkeley National Laboratory)

Benjamin Nachman, Kyle Cranmer, Matt Dolan, Timothy Cohen (Princeton/IAS)

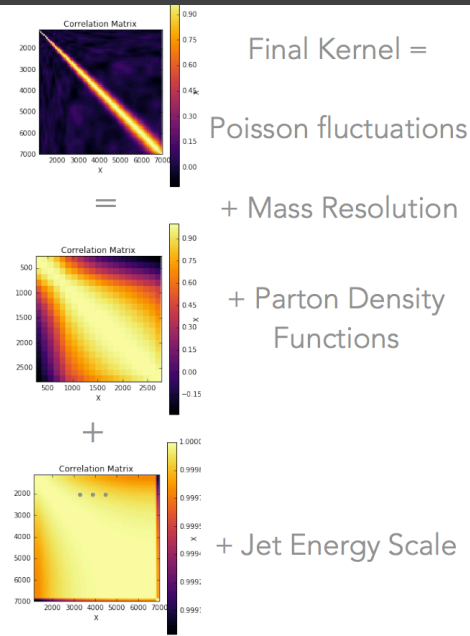
**Description** There has been a recent surge of interest in developing and applying advanced machine learning techniques in HEP, and jet physics is a domain at the forefront of the excitement. The goal of this workshop is to gather experts and new-comers to discuss progress, new ideas, and common challenges. The workshop is open to the community; we invite contributions and will try to accommodate everyone within reason.

Slides

**Participants**

Anders Andreassen, Andrew Larkoski, Aviv Cukierman, Benjamin Nachman, Bryan Ostdiek, Charilou Labitan, Christine McLean, Christopher Frye, Eric Metodiev, Felix Ringer, Francesco Rubbo, Frederic Dreyer, Gabriela Lima Lichtenstein, Gregor Kasieczka, Hulin Ou, Ian Mould, Isaac Henlon, Jack Collins

Discussed in  
talk by Michael Kagan



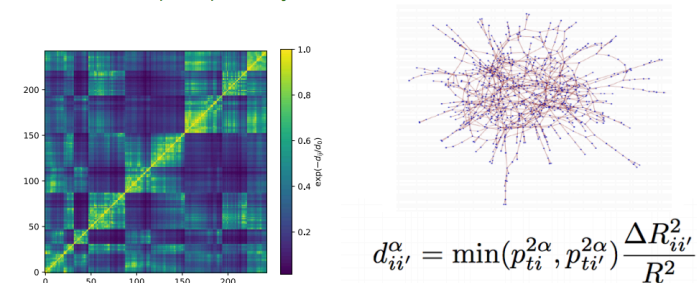
## MACHINE LEARNING

ways of injecting physics knowledge into  
well...

QCD-Aware recursive neural networks  
arXiv:1702.00748

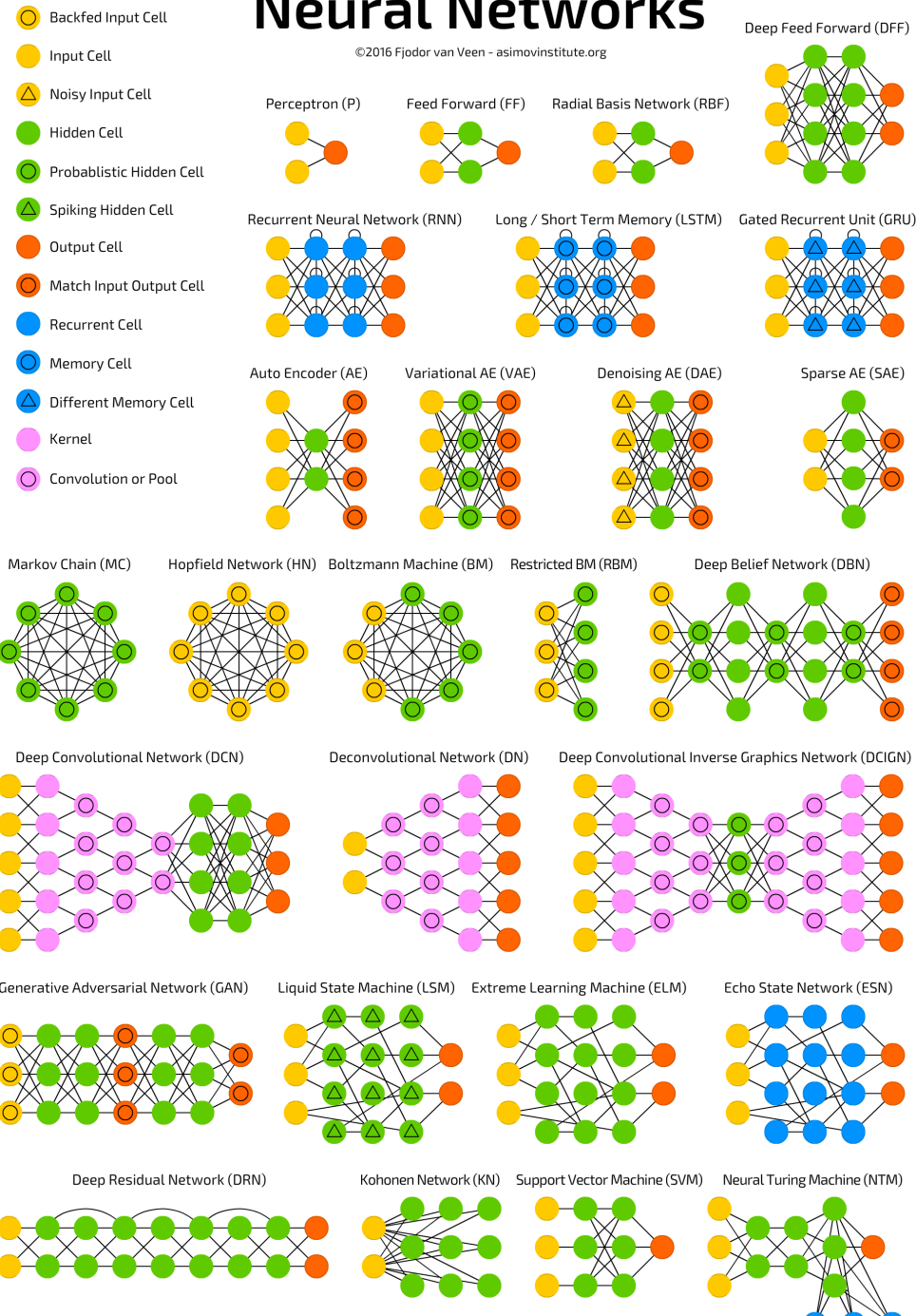


QCD-Aware graph convolutional neural networks  
NIPS2017 workshop [<http://bit.ly/2AkwYRG>]



# Neural Networks

©2016 Fjodor van Veen - asimovinstitute.org





## 2. Astroparticle DM searches with Machines



## About Dark Machines

Dark Machines is a research collective of physicists and data scientists. We are curious about the universe and want to answer cutting edge questions about Dark Matter with the most advanced techniques that data science provides us with.

[Visit our indico page](#)



**Dark Machines**  
@dark\_machines



The strong lensing subgroup of the DarkMachines project ([darkmachines.org](https://darkmachines.org)) will be holding a kick-off video-meeting for the strong lens challenge on Tuesday, August 7th, 7am PDT (California time).



Aug 3, 2018



Dark Machines Retweeted



**Gianfranco Bertone**  
@gfbertone

Nice summary on [@nature](#) of the challenges and opportunities that come with the use of machine learning at the frontiers of particle physics  
[nature.com/articles/s4158...](https://nature.com/articles/s4158...)



Machine learning at the energy and intensity frontiers of...

# Deep Convolutional Networks

Actually Alpha-go used a deep convolutional network...  
What is this ?

2015-2017: First deep learning attempts

We used deep convolutional networks to analyse gamma  
ray images for  
Dark Matter

<https://arxiv.org/abs/1708.06706>

# Convolutional Networks

- Convolutional networks have convolution layers based on “filters”, a filter (a **matrix**) maps “a group of numbers” to “a number” reducing the data → CONV layers
- There are also layers which only do a downsampling (lower the dimensionality) POOL or “fully connected layers” to process the final numbers...

important paper: LeCun, Yann. "LeNet-5, convolutional neural networks". Retrieved 16 November 2013.



# Filters (Matrix)

- Unity

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



“Edge detector”:

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$



“Convolutional” Network use “invariances” (rotation, translation) in data (e.g. images)

## CONV layer

Input Volume (+pad 1) (7x7x3)

$x[:, :, 0]$

0	0	0	0	0	0	0
0	1	2	2	2	2	0
0	2	1	0	0	1	0
0	0	1	2	2	1	0
0	1	1	2	2	0	0
0	0	1	2	0	0	0
0	0	0	0	0	0	0

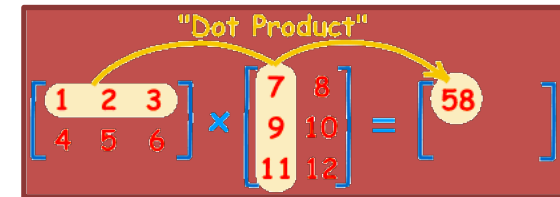
Filter  $W_0$  (3x3x3)

$w_0[:, :, 0]$

1	0	-1
1	0	-1
0	0	0

$w_0[:, :, 1]$

1	0	1
-1	0	-1
-1	0	1



+ adding bias vector + applying  
e.g. RELU as non-linearity

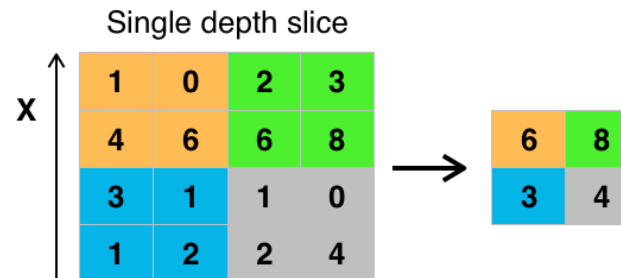
Filter coefficients  
learned by  
backpropagation

Followed by

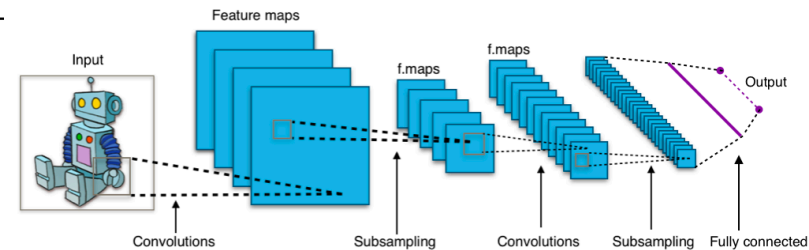
a POOLING layer

(partition the input matrix into  
Submatrices, here max POOL, i.e.

Storing the maximum)



Y



(you can have Red, Green and Blue matrices)

# Use case: gamma rays from galactic center

A method to investigate the origin of an excess emission of GeV  $\gamma$  rays in the direction of the Galactic Center  
( reported by several groups by analyzing Fermi-LAT data)

Interpretations of this excess include  $\gamma$  rays created **by the annihilation of dark matter particles** and  $\gamma$  rays originating from a **collection of unresolved point sources, such as millisecond pulsars.**

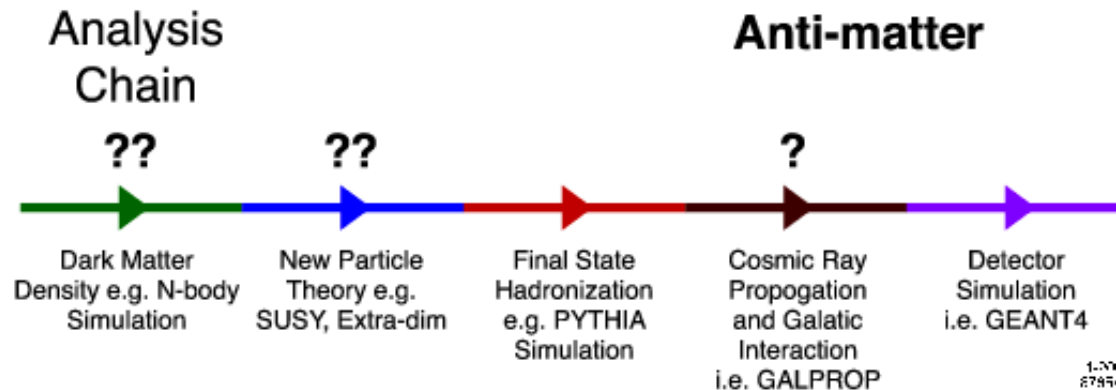
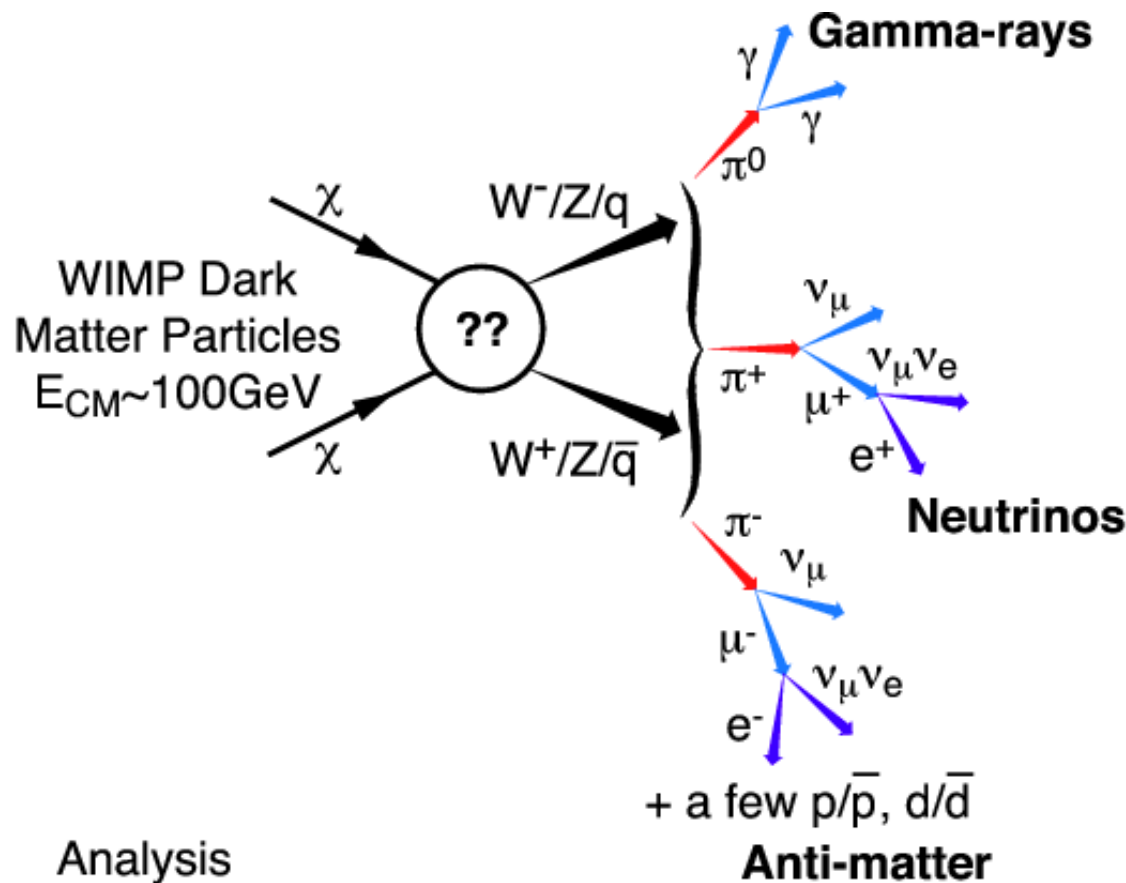
## What have we done ?

Simulated Fermi-LAT images based on point and diffuse emission models of the Galactic Center tuned to measured  $\gamma$  ray data

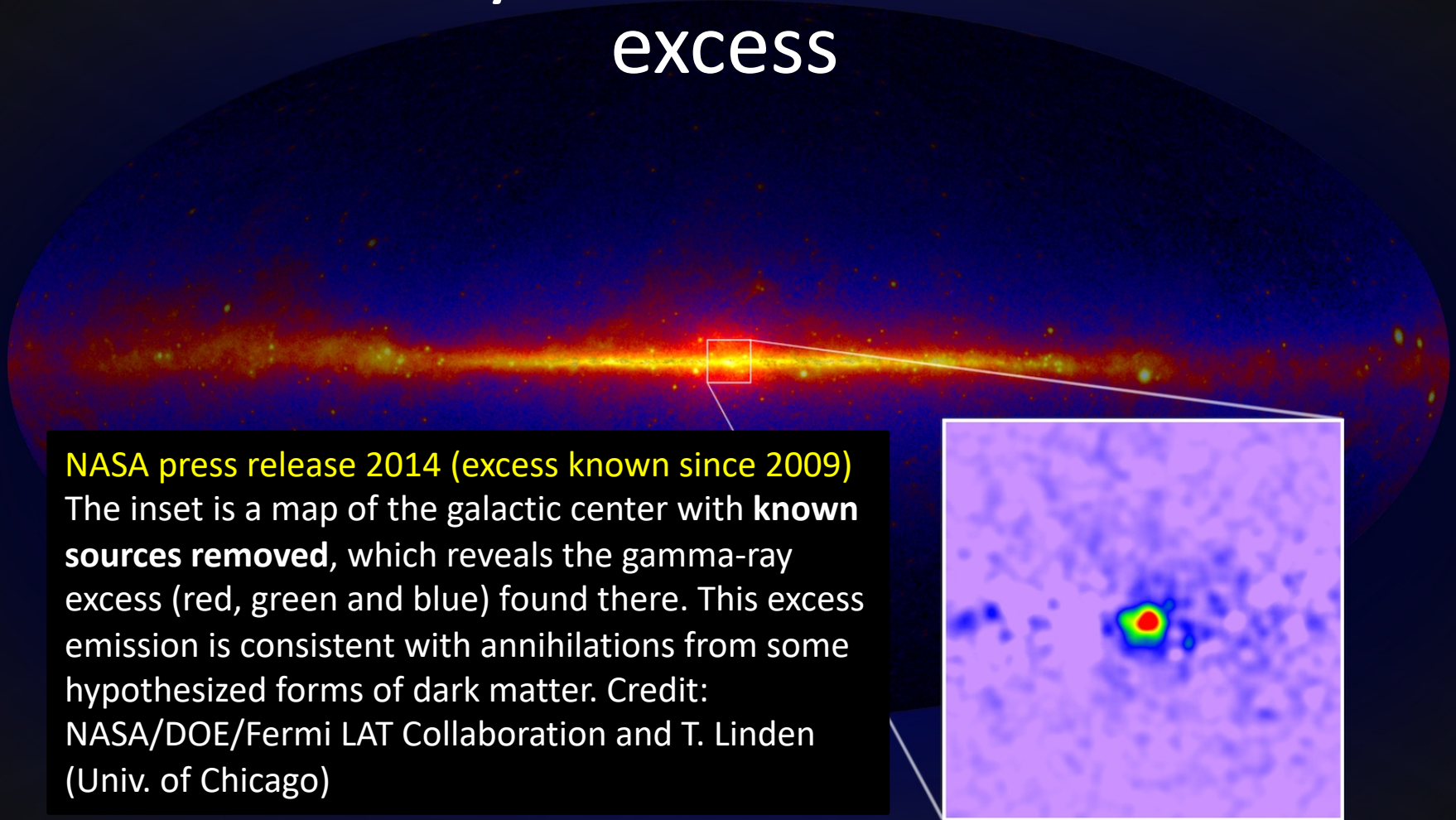
➔ Train and test convolutional Network on this



# WIMP Astrophysics



# Gamma rays & the Galactic Center excess



**NASA press release 2014 (excess known since 2009)**

The inset is a map of the galactic center with **known sources removed**, which reveals the gamma-ray excess (red, green and blue) found there. This excess emission is consistent with annihilations from some hypothesized forms of dark matter. Credit: NASA/DOE/Fermi LAT Collaboration and T. Linden (Univ. of Chicago)

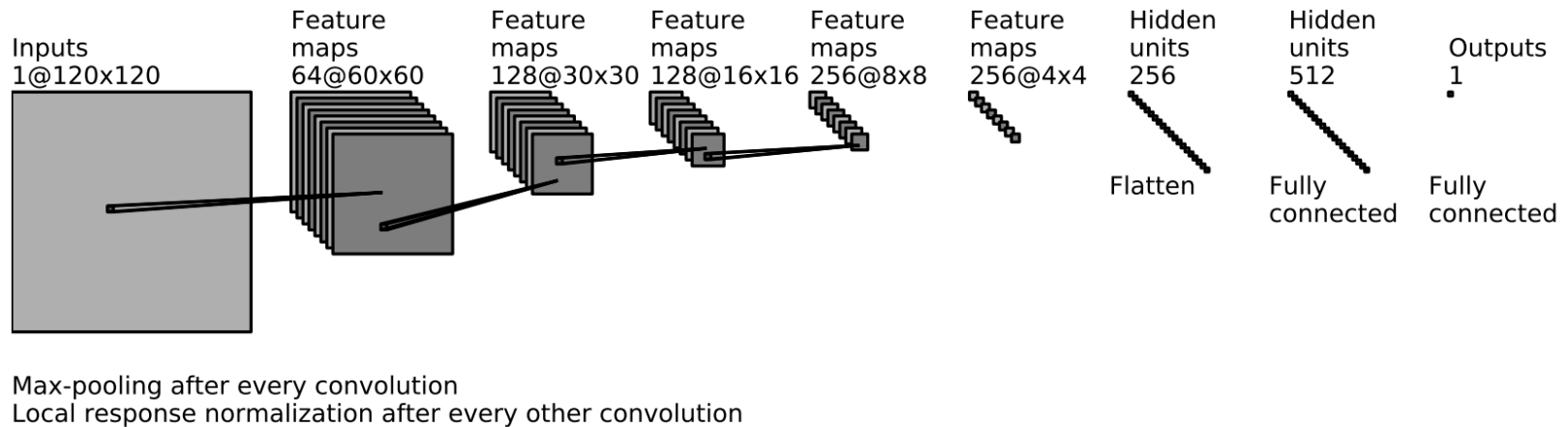
Official paper in 2015

**Fermi-LAT Observations of High-Energy Gamma-Ray Emission Toward the Galactic Center**

Fermi-LAT Collaboration (M. Ajello (Clemson U.) *et al.*). Nov 9, 2015. 29 pp.

e-Print: [arXiv:1511.02938](https://arxiv.org/abs/1511.02938) [astro-ph.HE] | [PDF](#)

# Our convolutional network (convnet)



**Figure 6:** Visualization of the convolutional neural network. The network consists of an input layer, 5 convolutional + pooling layers, 2 fully connected layers and finally an output layer.

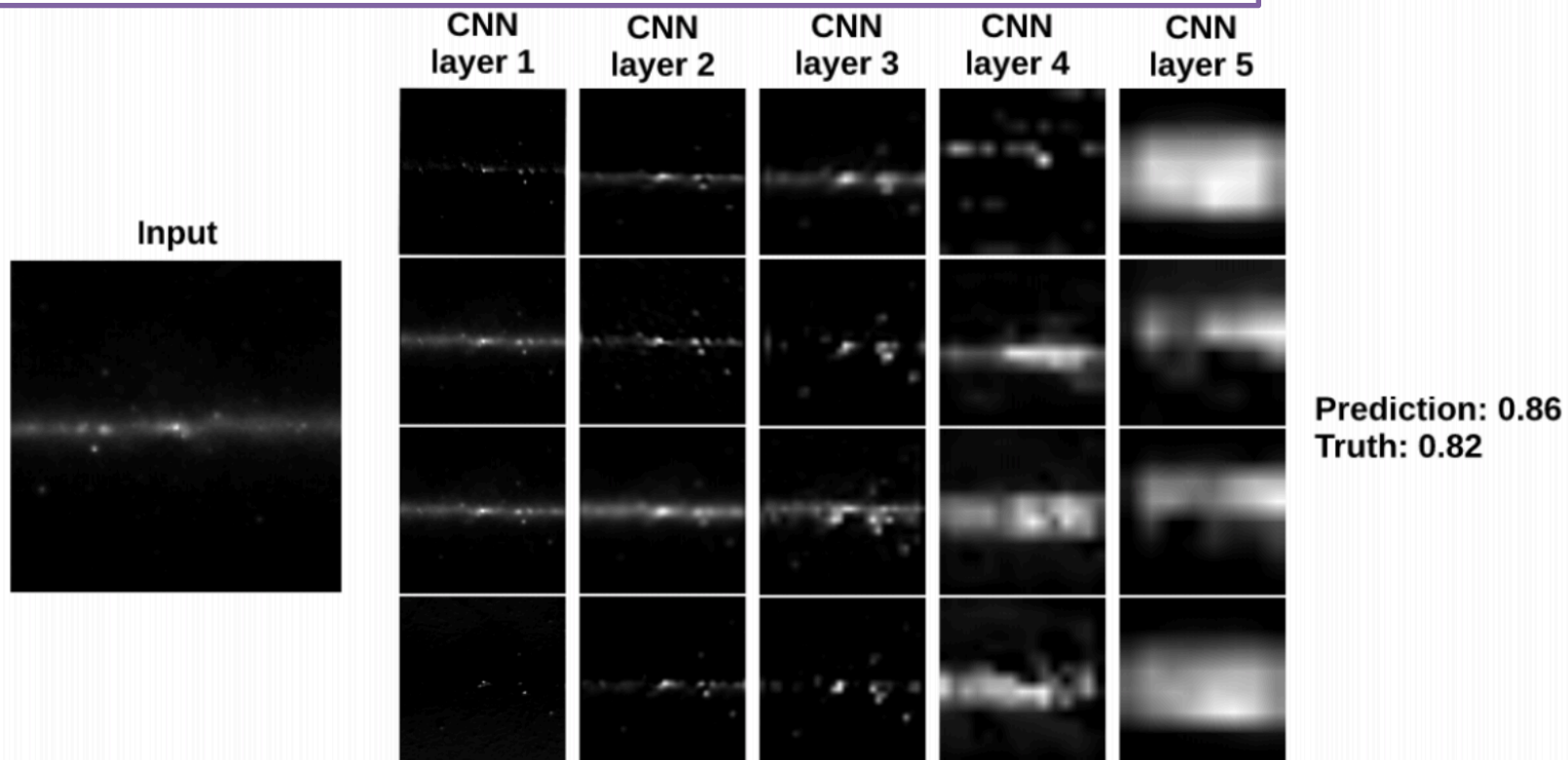
Hierarchical/compositional structure → smaller to larger structures  
(reason: visible system is hierarchical as well...)

*In comparison: GoogleLeNet has like 30 layers...*



# Isotropic or point sources: A Deep Convolutional Network approach

Output of the 5 convolutional layers can be “visualized” per event.

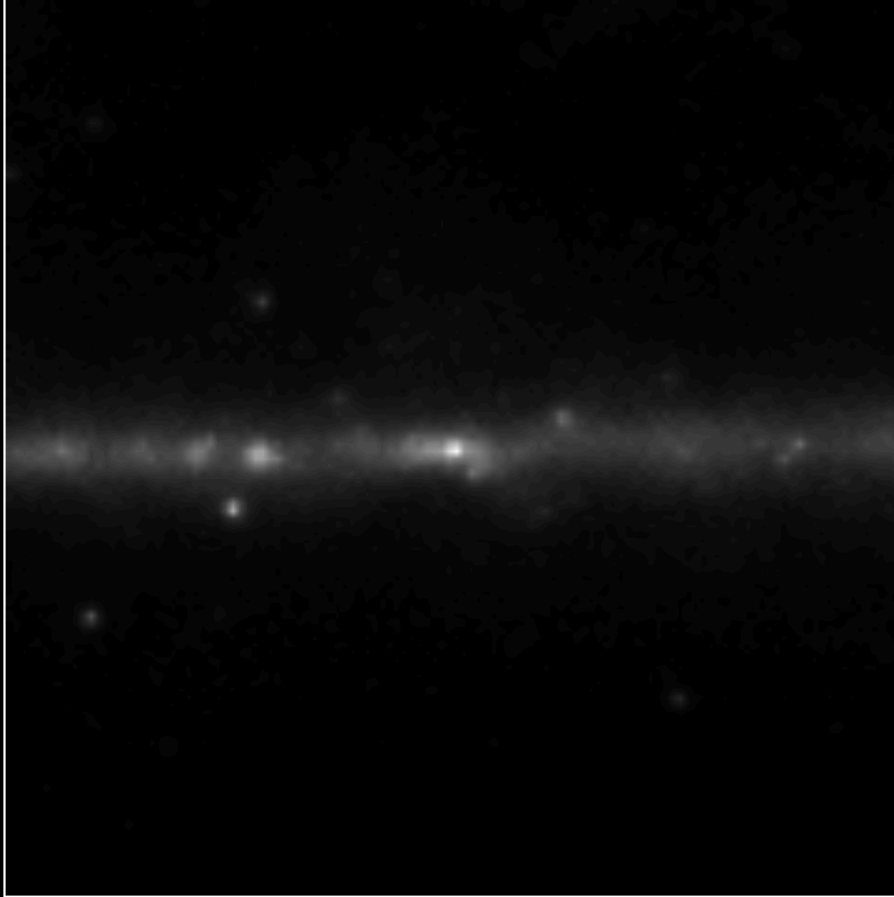


Activations of the network. Only four filters per layers are shown for clarity, between 256 and 65 filters are used for the different layers

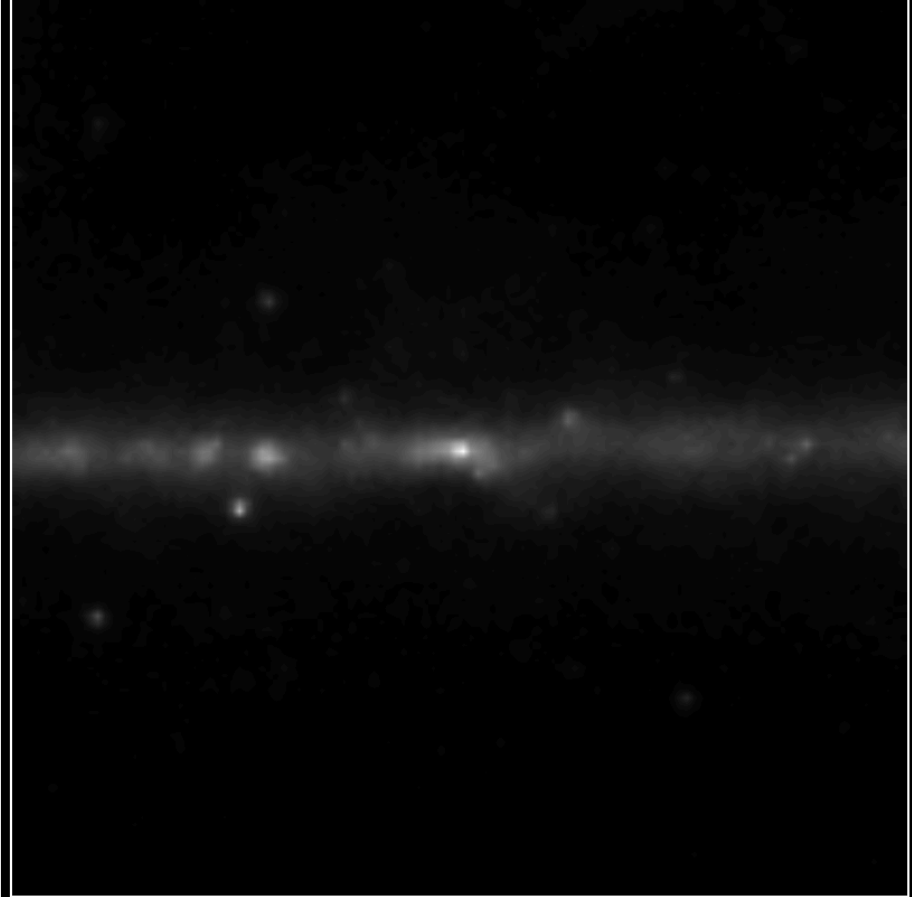
# Guess the fraction of point sources

[www.mydarkmachine.org](http://www.mydarkmachine.org)

What is this fraction?



This is 0.5



Your prediction:

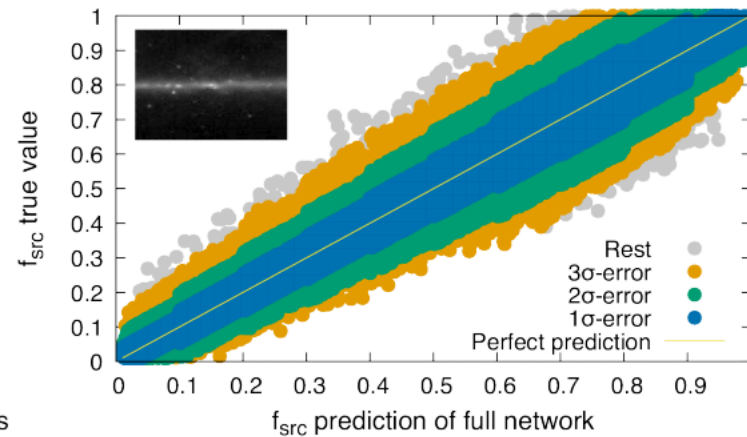
Invert image: ☐

Guess

What is this fraction?

This is 0.5

Network can generalize over randomness



(b) Prediction of the full network versus true values.

Your prediction:

Invert image: ☐

Truth: 0.052

Network: 0.1230

Your guess: 0.5

Who is better? The network

Interpretation here is frequentists and relies on the model to be correct (uncertainties from toy experiments, no p-value yet)



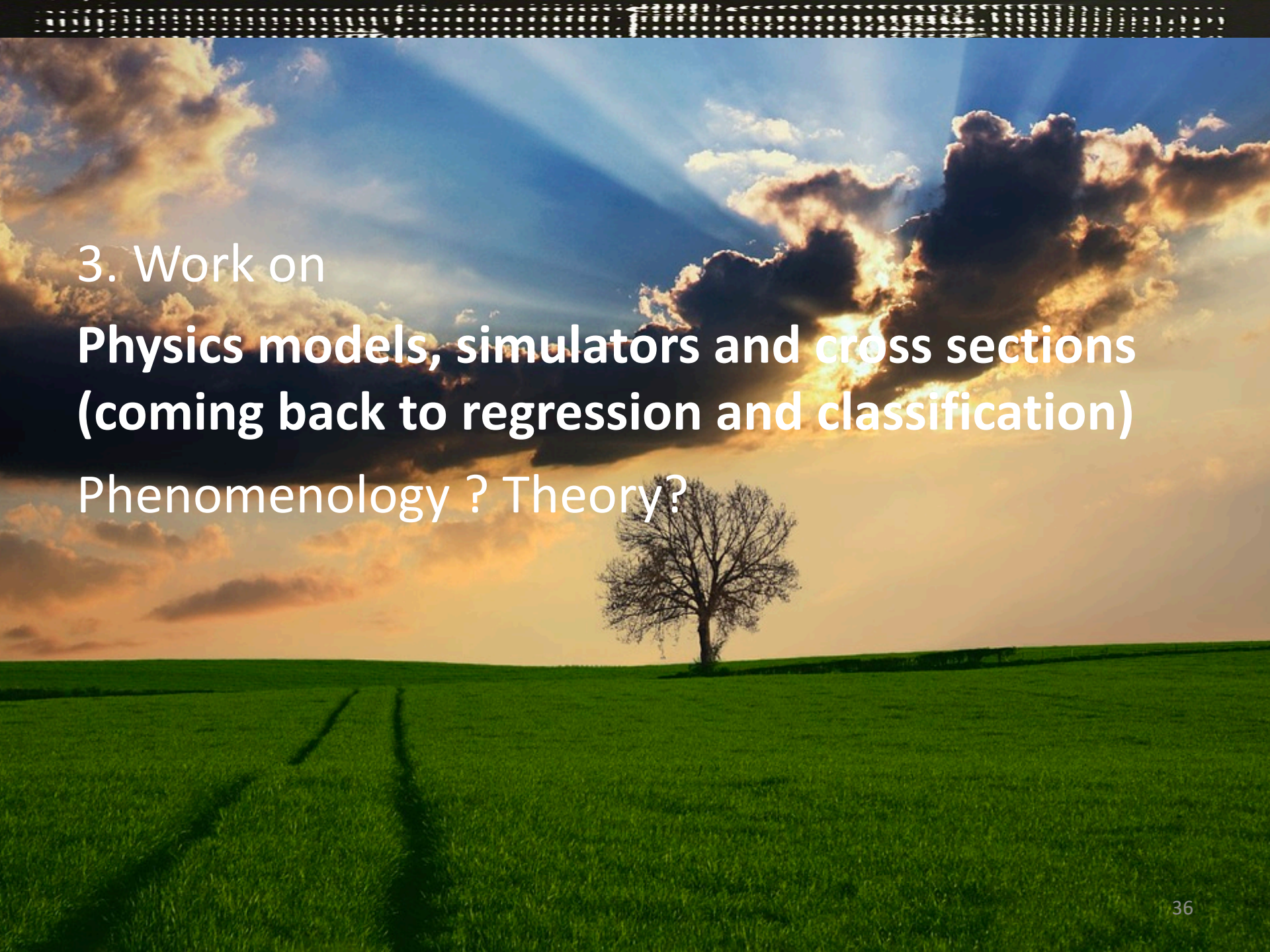
# Next steps

- Categorize objects on the gamma-ray sky



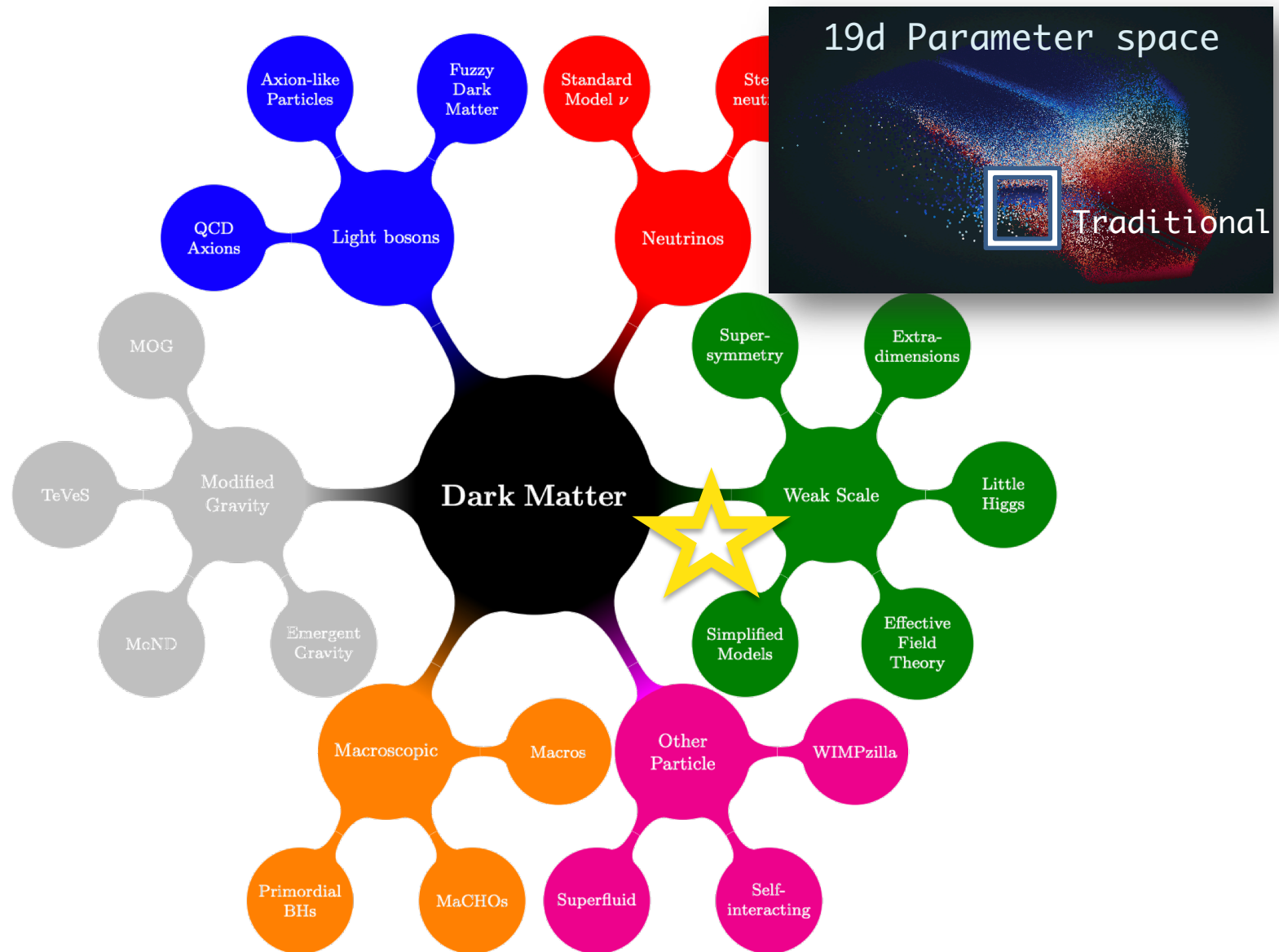
Also point source detection now → see e.g. recent paper called “deepsources”  
<https://arxiv.org/abs/1807.02701>





3. Work on  
**Physics models, simulators and cross sections**  
**(coming back to regression and classification)**  
Phenomenology ? Theory?

# What could it be? Dark Matter models

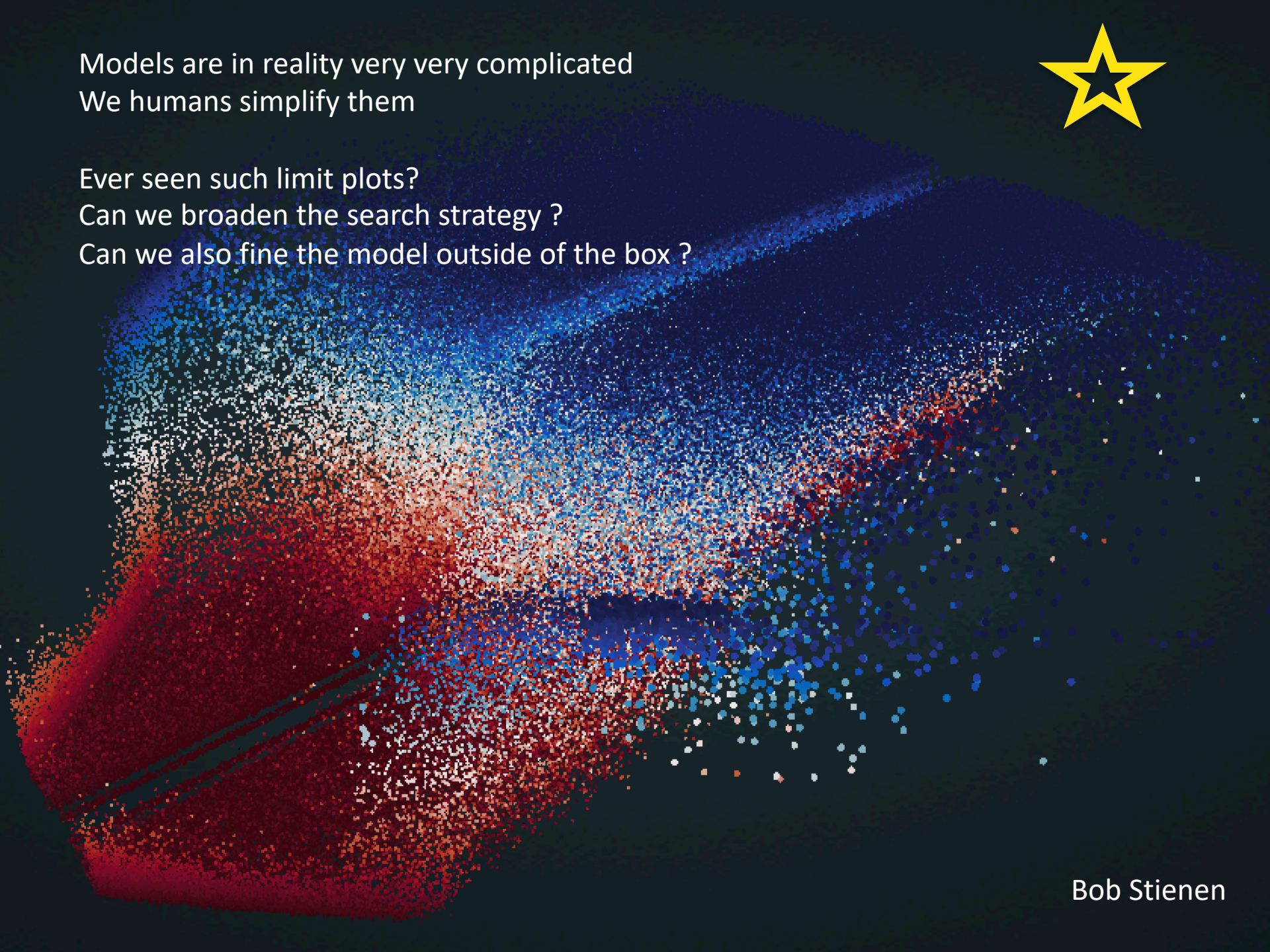




Models are in reality very very complicated  
We humans simplify them



Ever seen such limit plots?  
Can we broaden the search strategy ?  
Can we also fine the model outside of the box ?



# Accelerating searches

Inputs → *Long simulations + many programs* → Output

Train classification / regression tool to replace *this* by ML

Advantages:

- **Speed !**
- **Generality !**

# Coupling Theory and Machine Learning part 1

“Learning a function” from datasets with known labels sounds boring and old-fashioned.

However we can couple it to simulators+ experiments + phenomenology ....





# Coupling Theory and Machine Learning part 1

“Learning a function” from datasets with known labels sounds boring and old-fashioned.

However we can couple it to simulators+ experiments + phenomenology ....



# Coupling Theory and Machine Learning part 1

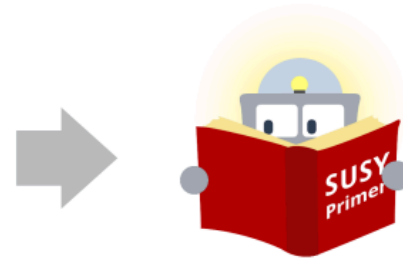
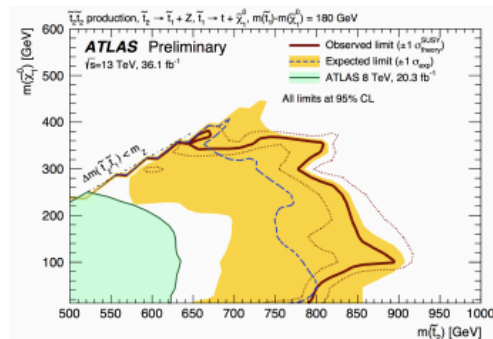
“Learning a function” from datasets with known labels sounds boring and old-fashioned.

However we can couple it to simulators+ experiments + phenomenology ....



# SUSY-AI

- Exclusion determination in 19d pMSSM
- 310,324 model points with known exclusion as data input
- Algorithm: a collection of decision trees (Random Forest)
- **Idea: going from 2d slices to N-dim representations**



**Prevent overfitting:** Boosting: many trees + not subset of all features for each tree  
Bagging: random picking training data -> each tree of the forest sees only 0.68\*data (see extra slides)

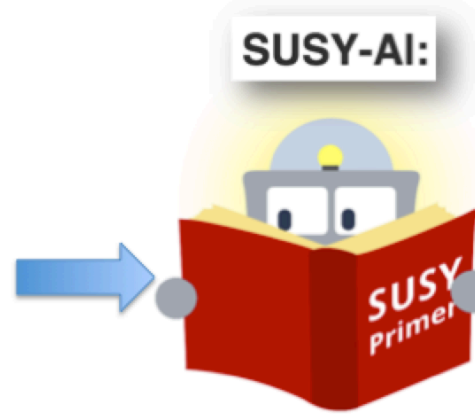


# SUSY-AI

Encoding of model constraints with Machine Learning

Aim: Generic framework (**all** models)

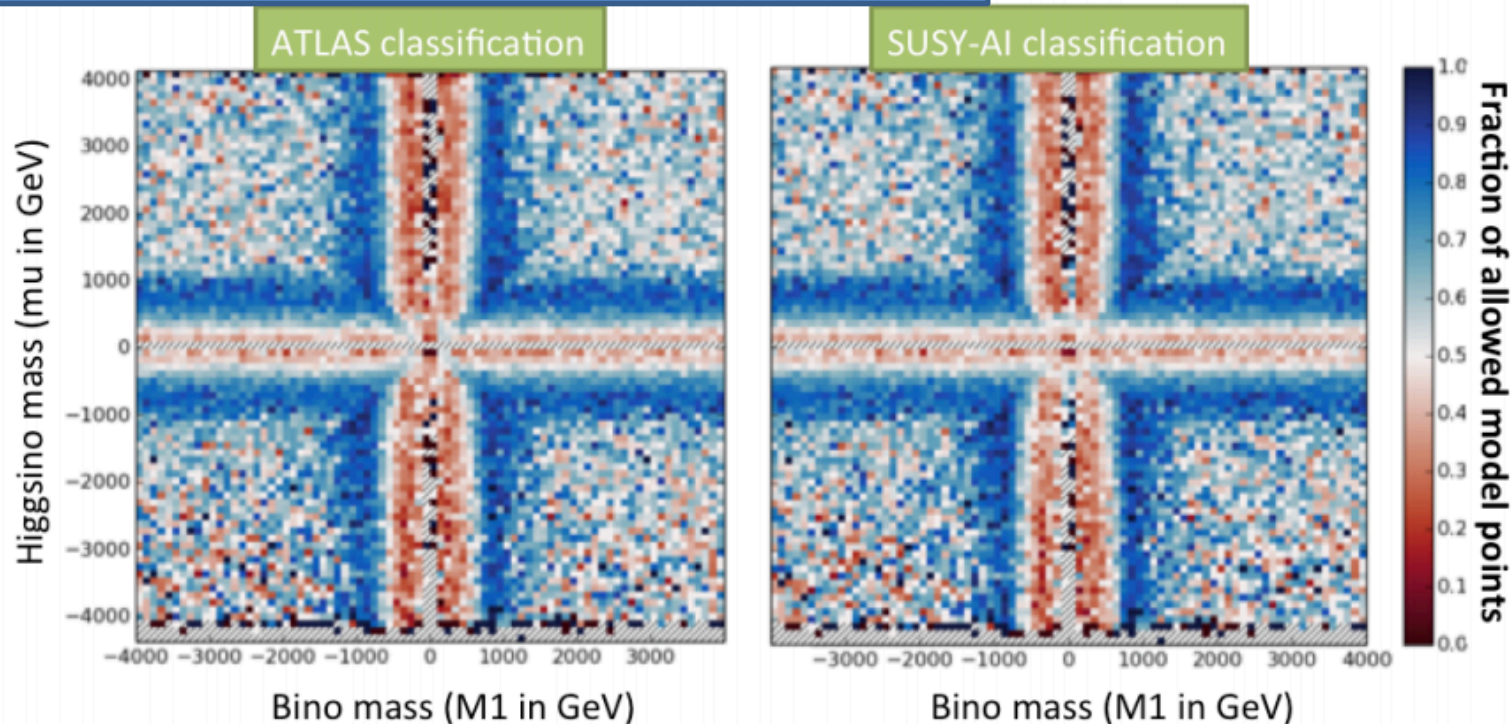
Les Houches  
Accord File

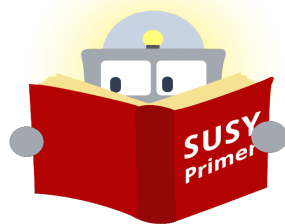


Bob Stienen, >10 collaborators

Determine  
Confidence Level

*Testing with out-of-bag estimation (remember 0.68!)*



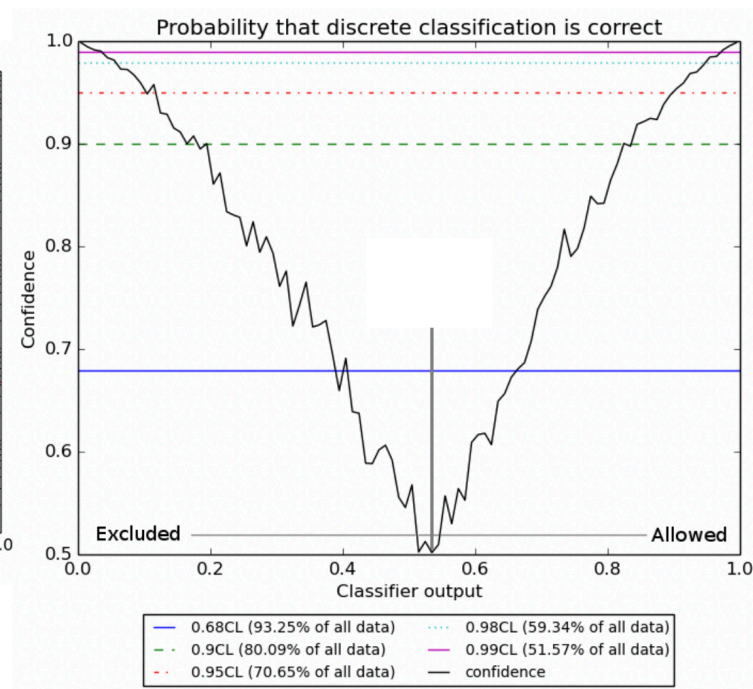
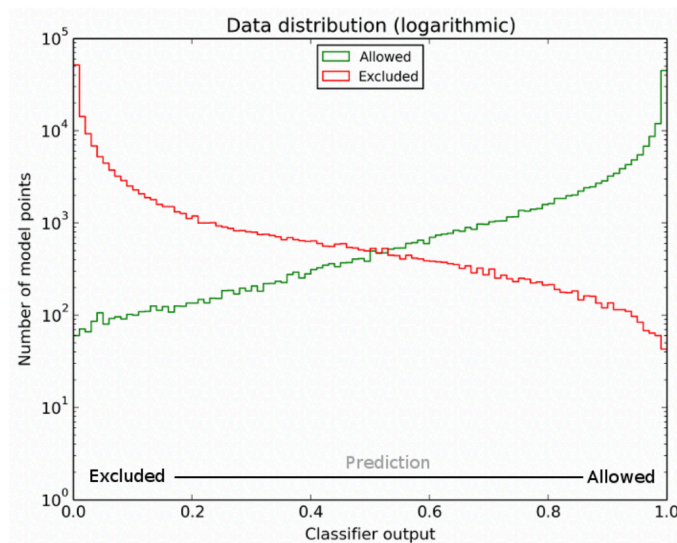


Used training data to learn classification

It determines a **confidence** level of its **classification** using the training data.

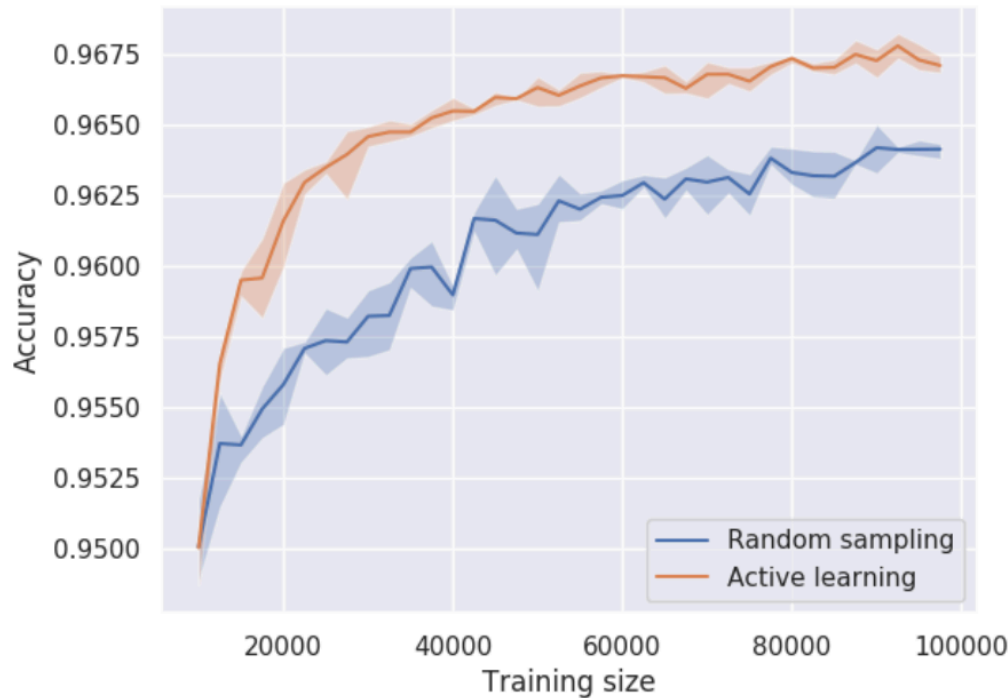
→ Need **more points** in regions of low certainty

Ratio of majority class per bin



## Active learning

[arXiv:1905.08628](https://arxiv.org/abs/1905.08628) , mainly  
Bob Stienen



Query-by-Dropout-Committee

FIG. 5. Accuracy development on model exclusion of the 19-dimensional model for new physics (pMSSM) for random sampling and active learning using a dropout Neural Network with infinite pool. True labeling was provided by a machine learning algorithm trained on model points and labels provided by ATLAS [1]. The gain of active learning with respect to random sampling (as described by Equation 2) is 3 to 4. The bands show the range in which all curves of that colour lay when the experiment was repeated 7 times.

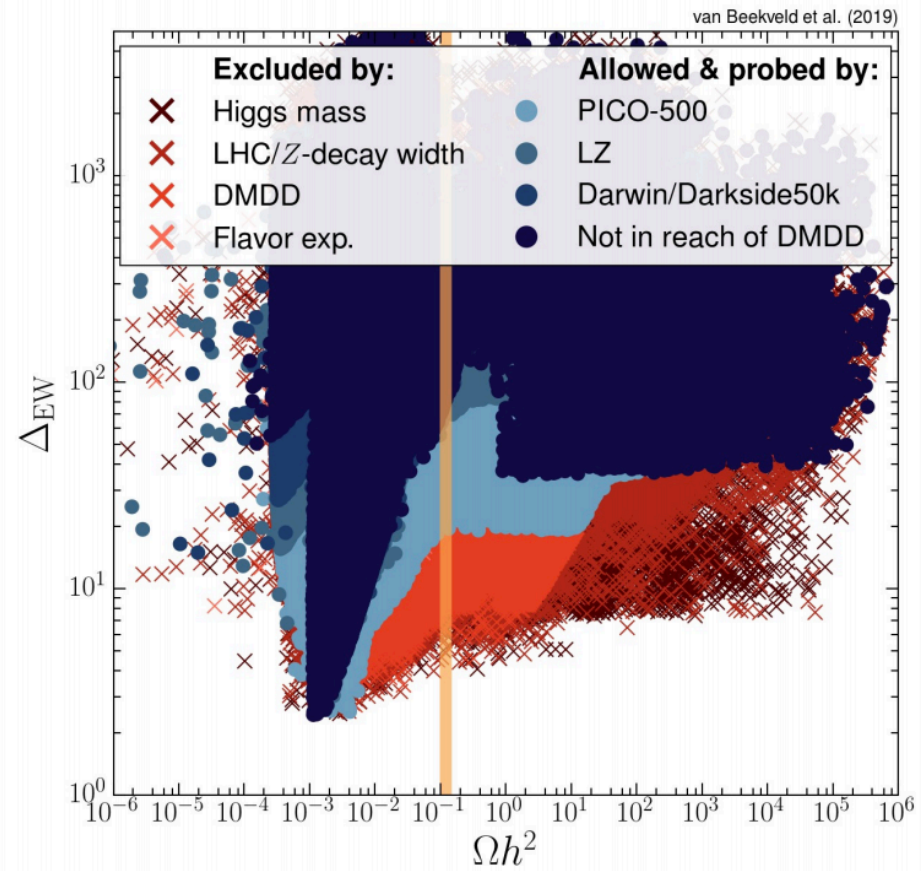
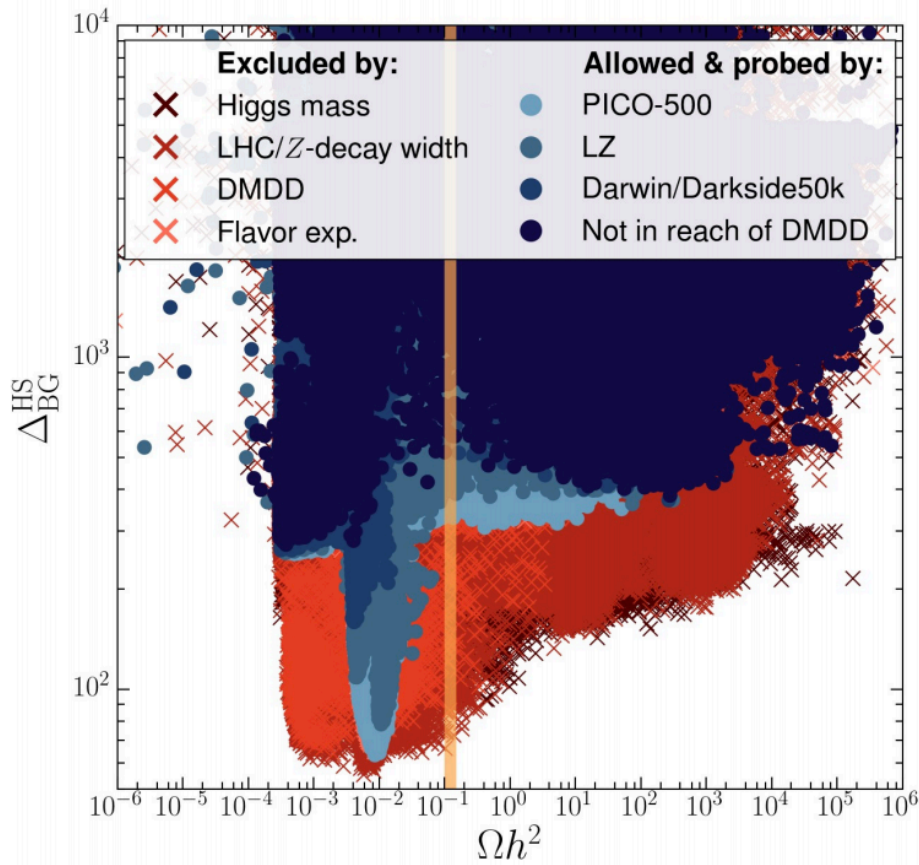


Why are you still interested in SUSY ?

Because ...

Use cases → How fine-tuned is Supersymmetry in the 19d MSSM ?

<https://arxiv.org/pdf/1906.10706.pdf>



# Les Houches project: SUSY-AI --> PhenoAI

- Encoding model constraints for everybody in the full model parameter space (e.g. LHC constraints on various high-dimensional models)
- No simplifications of models needed !
- "model-space" can provide training data



# Need to store pheno data

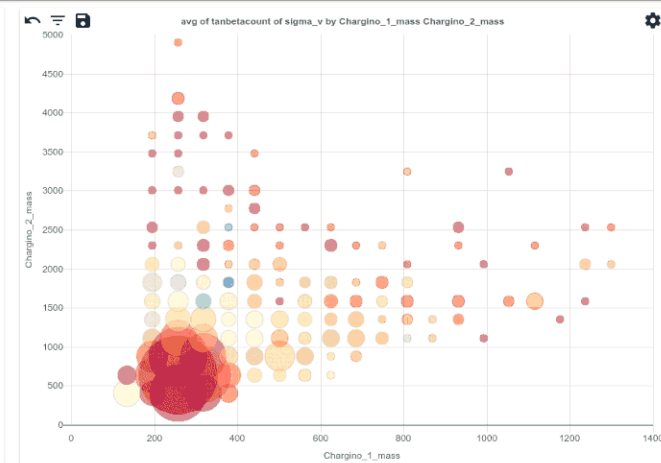
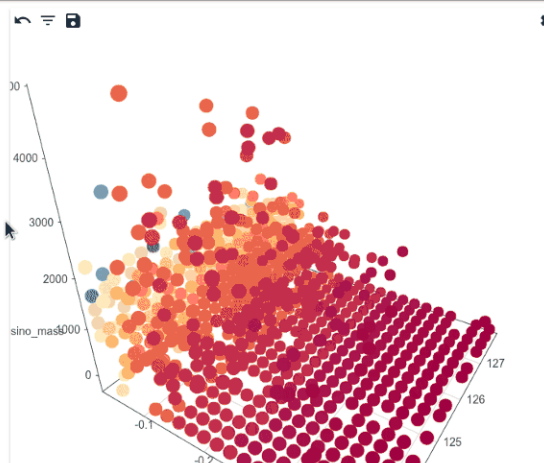
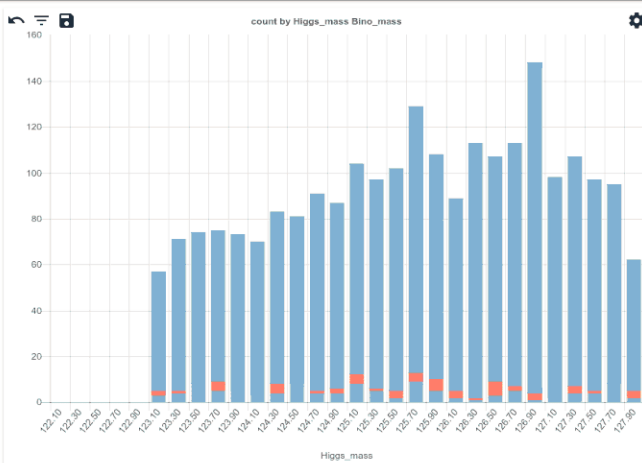
- Remember the animated newspapers from Harry Potter ?



# Pheno model database ?

Analyze

2331 total, 2331 selected (100%)



Within  
idark project  
Dutch escience  
Center

Faruk Diblen  
Jisk Attema

Collect model solutions in a database

Use them as target !

Use Machine Learning to interpolate between them → Generalization of DM searches

[www.idarksurvey.com](http://www.idarksurvey.com)

# DeepXs: DM Cross sections

- Running NLO code to derive SUSY cross sections can take up to 10 minutes
- Can we “learn the cross sections” and derive in a microsecond for *any* model parameter set? ➔ <https://arxiv.org/abs/1810.08312>



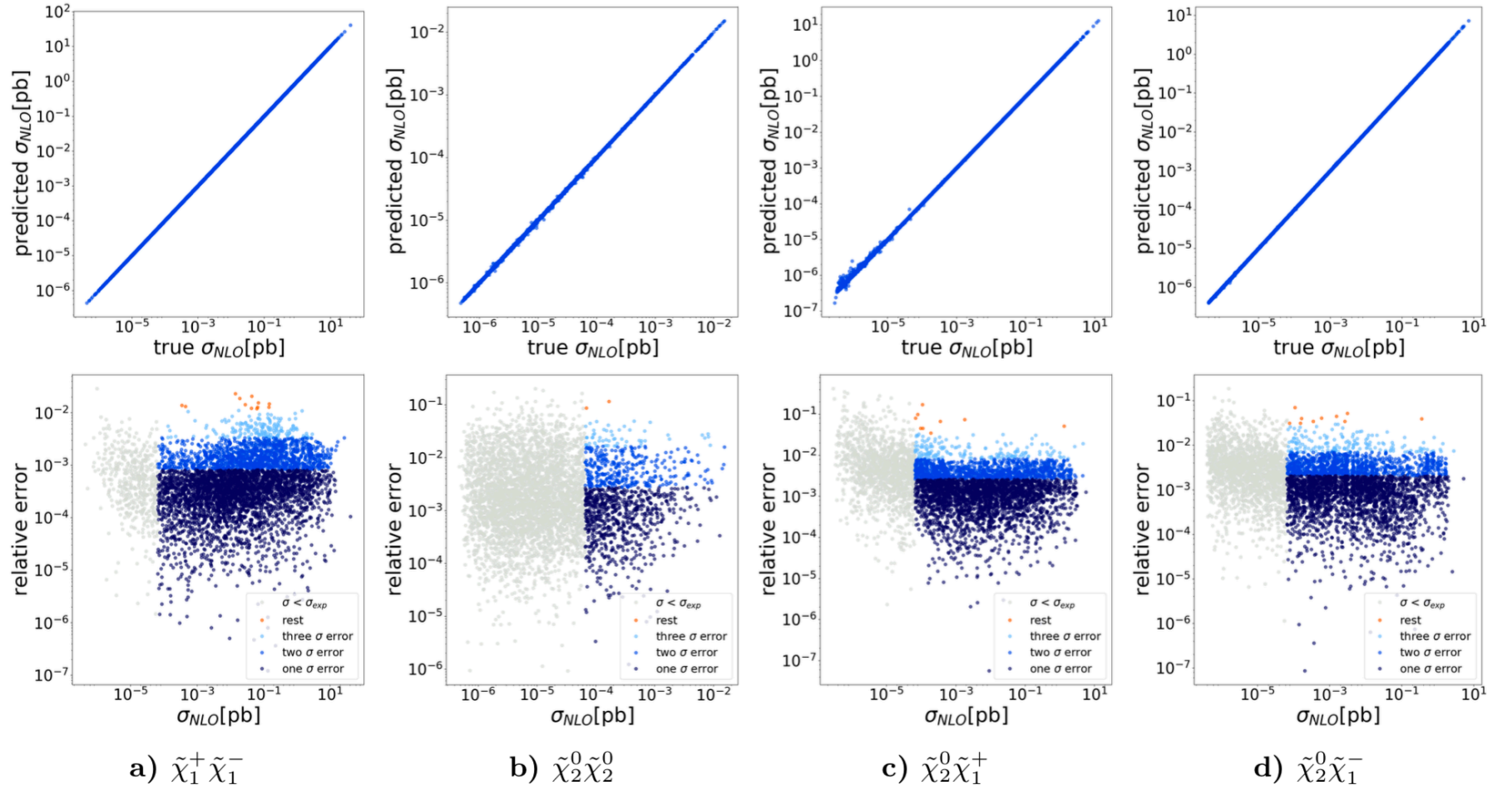


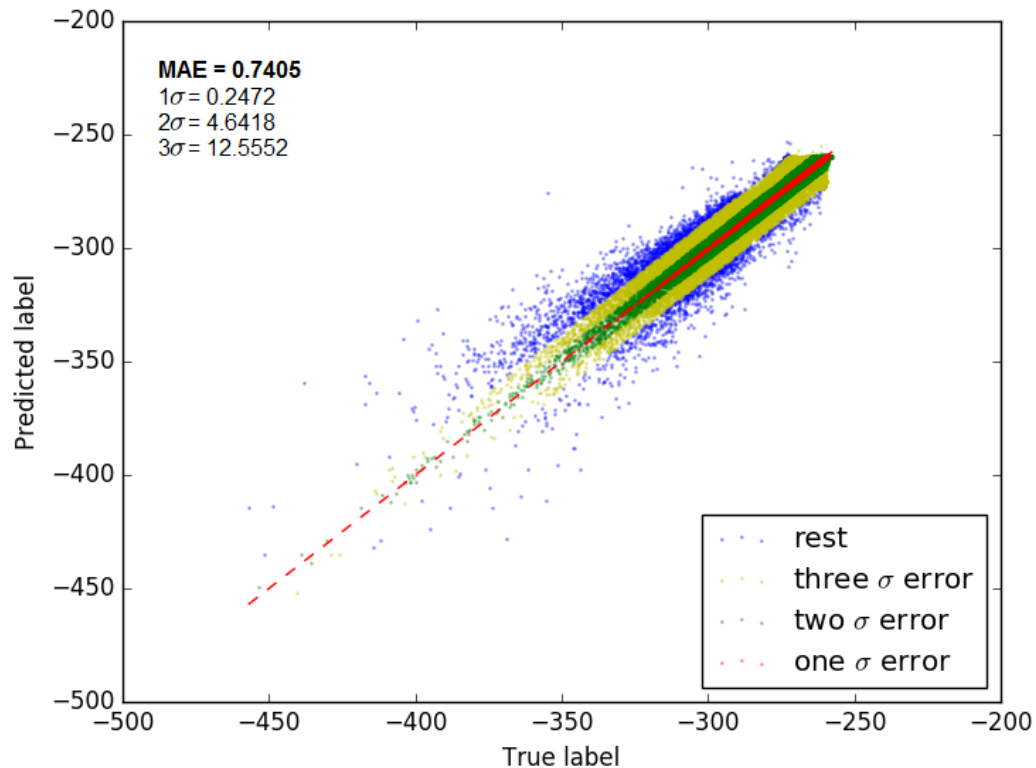
FIG. 1: The true vs. predicted NLO cross-sections (top) and the relative error vs. true NLO cross-section with confidence intervals (bottom) for the same  $10^4$  samples in both plots

inference at NLO with inference times that improve the Monte Carlo integration procedures that have been available so far by a factor of  $\approx 6.9$  million from  $\approx 3$  minutes to  $\approx 26\mu s$  per evaluation.

# Regression: Likelihoods

- Fitting groups derive likelihood plots for given models
- Can we “learn the likelihoods” in return in a microsecond for *any* model parameter set ?

## BSM-AI regression example... Learning GAMBIT likelihoods



MSSM - 7

<https://arxiv.org/abs/1705.07917>

Plot by Sydney Otten



## 5. (Unknown) data anomalies



# Model parameter space (pre- LHC)



# Unknown signals/ unknown labels

Typical task at the LHC is **supervised discrimination of signal and background** (particle ID, Higgs search)

→ Discriminator

(typically BDT/TMVA, now Deep Network)

## Interesting:

What can we do if the signal is unknown ?

*Related to a simpler question:*

What can we do if the signal is vaguely known (i.e. a simulation is possible) ?



Today: I have a new toy for you, I put it somewhere in your room. The size is 0.1-100 cm. Can you find it ?



We propose to construct an **automatized**  
**„scan“ of the full room/data for something interesting...**

→ This may help LHC to find new physics

→ We can embed into this “scan” our prejudice how new physics could look like, e.g. in the example on the previous slide this could be done via a „toy“ detection software trained on all known toys with the ability to do some extrapolation and interpolation ...

# Many hypotheses ...

Searching for new physics with ,minimal/less‘ assumptions on the signal

Consequences:

Less signal assumptions → more hypothesis tests (multiple testing)  
→ more/all channels and data selections

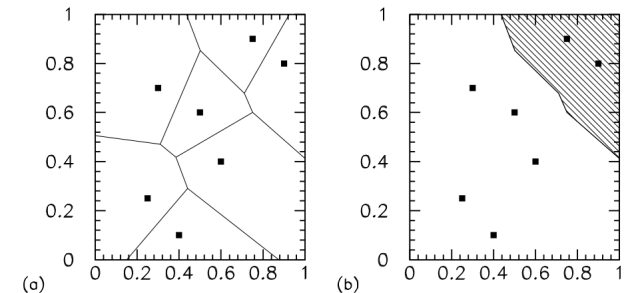
Implementations:

- Search with an “algorithm|: **automatizing data selections and testing**
- **Automatize/Generalize** the construction of **the background model**

# Automatized generic searches in HEP: history

- Before **2000**: Some (unpublished) ideas and work (e.g. by Thomas Hebbeker and M.W. Krasny) to construct generic (non-model dependent searches) by comparing data with background expectation in a broad class of high pt events
- **2000**: First „automatized search without fixed model assumptions“ in HEP  
→ **Sherlock/Sleuth at D0** experiment/ Tevatron (B. Knuteson and others)

Partition of events into (many !) Voronoi regions defined by data (N=1 region, N=2 regions, etc.)



Criteria which regions are interested (e.g. corners, high pt...) and should be considered for hypothesis tests (p-value to test if data is consistent with SM expectation)

→ Select region with smallest p-value

→ **Problem: (Too) many trials + Needs multivariate understanding of backgrounds**



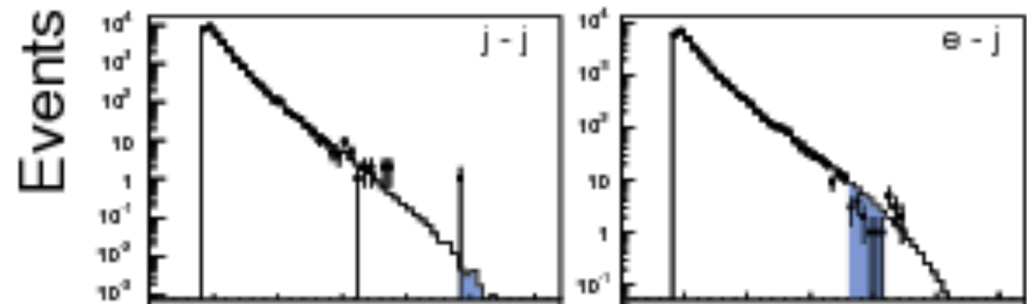
# Automatized generic searches in HEP: history

- 2004: **General Search at H1** experiment at HERA. (*2nd paper 2009*)

All “HERA channels” 1-d search algorithm with smaller trial factor

-> similar/better sensitivity

- simpler to understand the background



- 2007: **Global Searches at CDF** with 1-d algorithms (one algorithm became “bumphunter” in 2011)
- 2010-2016: Start of work for LHC (several internal notes in ATLAS, one in CMS)
- 2011: First public **ATLAS** CONF note ( $4.7 \text{ fb}^{-1}$  with 7 TeV)
- 2011: **CMS** PAS note (“Music”) (MC note in 2008)
- 2011: Second ATLAS CONF note ( $20 \text{ fb}^{-1}$  with 8 TeV)
- 2016-2018: **ATLAS released paper to arxiv (submitted to EPJ-C)** , 13 TeV data, 2015 data)

# **A strategy for a general search for new phenomena using data-derived signal regions and its application within the ATLAS experiment**

## **Goal:**

Strategy paper. Generalize previous attempts.

Define a “meta-algorithm” for

automated / generic / unsupervised LHC searches

Show with 2015 data that this is - in principle – possible

<https://arxiv.org/pdf/1807.07447.pdf>

# A strategy for a general search for new phenomena using data-derived signal regions and its application within the ATLAS experiment

Define a 2-step approach:

First put available resources on generality

Then use available resources to test most interesting deviations...

**1. General Search:** Automatically testing a large set of signal regions

Observation of one or more significant deviations in some phase-space region(s)

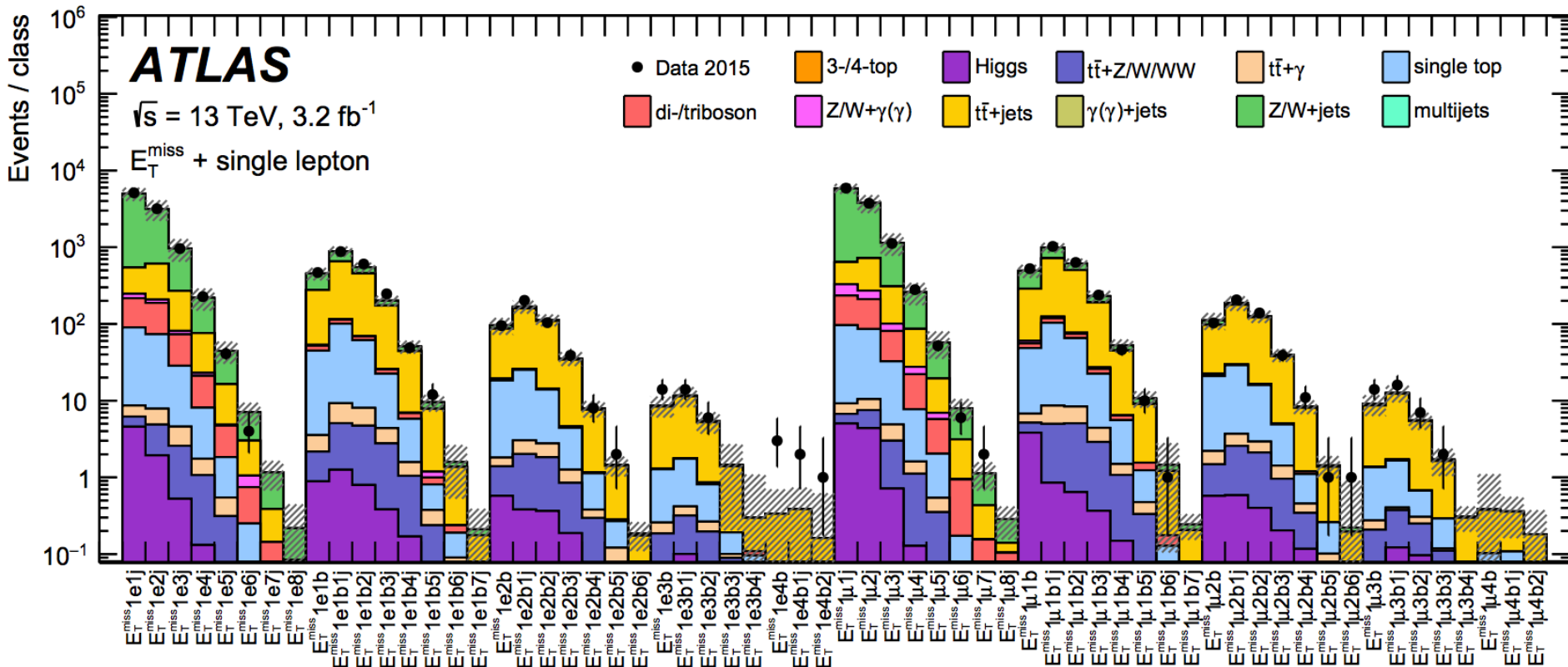
➔ Trigger to perform dedicated and model-dependent analyses

where these **'data-derived' phase-space region(s) can be used as signal regions**

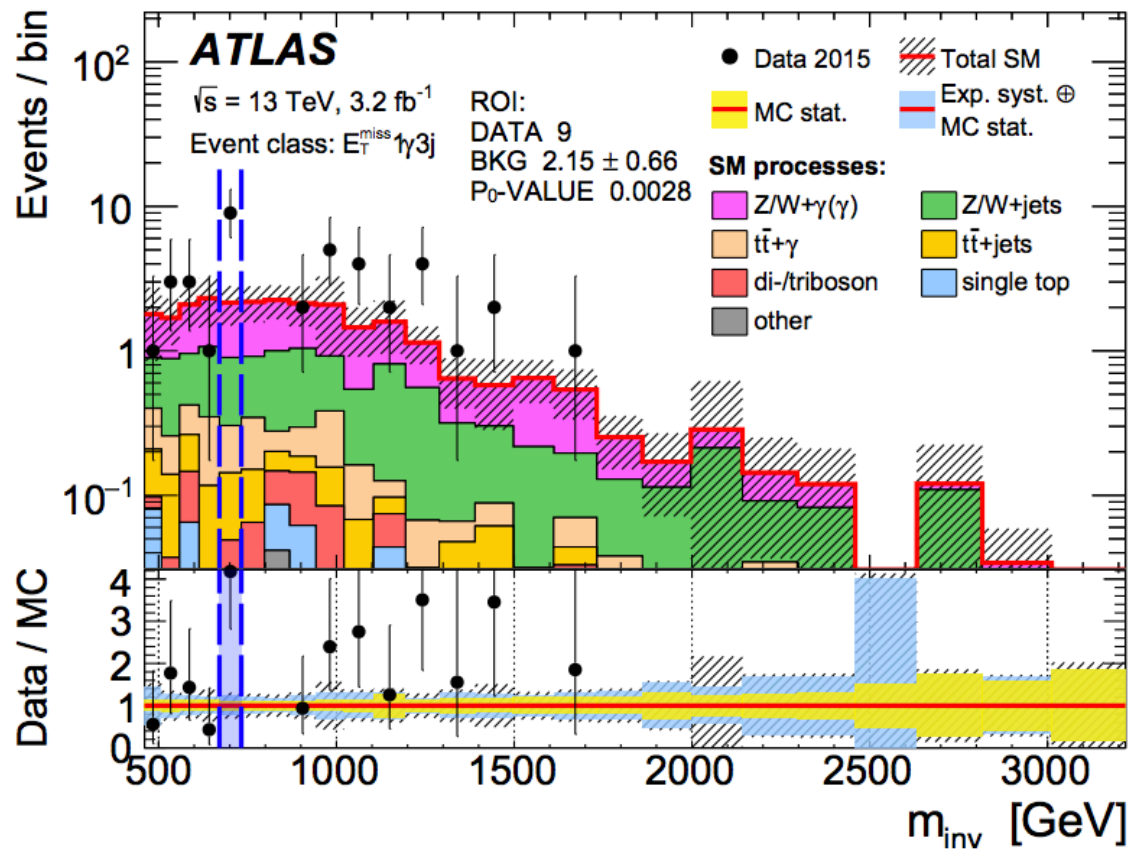
In ATLAS > 800 channels !

>  $10^5$  regions !



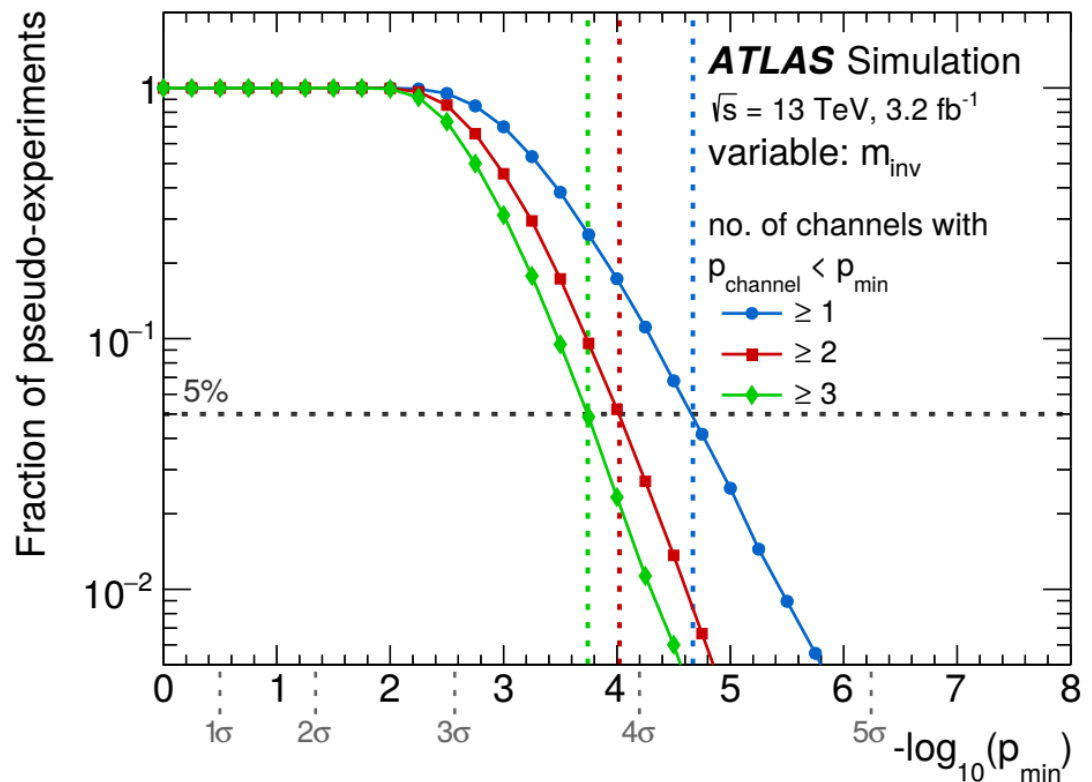


> 800 channels .... (plot shows a small selection)



> 30000 regions (hypothesis tests)

Determine  $p$ -value thresholds by asking how many toy datasets would give such a deviation  
 → A regions is interesting if you find channels with  $p$ -values more significant than in 95% of the toys



# A strategy for a general search for new phenomena using data-derived signal regions and its application within the ATLAS experiment

Define a 2-step approach:

First put available resources on generality

Then use available resources to test most interesting deviations...

**1. General Search:** Automatically testing a large set of signal regions

Observation of one or more significant deviations in some phase-space region(s)

➔ Trigger to perform dedicated and model-dependent analyses

where these **'data-derived' phase-space region(s) can be used as signal regions**

**2. Dedicated Search**

- "Wave function collapsed" to test most interesting deviations with available resources

- On 2<sup>nd</sup> dataset (➔ Statistically independent, unbiased p-value !!)



## Dataset 1 signal regions





Dataset 1 signal regions

Dataset 1 signal regions  
Colour code – p-value



## Dataset 1 step 2 -> dedicated search

Dedicated  
Searches -->

(e.g. defining  
control regions or  
signal hypothesis)



*(in the toy example the kids are counting the Lego figures and  
are trying to estimate how many they had ...)*

## Dataset 1 step 2 -> dedicated search

Assume two regions have  
Background issues  
→ Dedicated search does  
not confirm deviation





## step 2 -> test in independent dataset 2

P-value =  $10^{-7}$

In independent dataset

→ Publish

→ Follow up with CMS



*(in the toy example the kids are asking their father for confirmation)*

# ATLAS scan 2015 data results

Table 4: List of the three channels with the smallest  $p_{\text{channel}}$ -values in the scan of the  $m_{\text{inv}}$  distributions.

Largest deviations in $m_{\text{inv}}$ scan				
Channel	$p_{\text{channel}} (\cdot 10^{-3})$	$N_{\text{obs}}$	$N_{\text{SM}} \pm \delta N_{\text{SM}}$	Region [GeV]
$E_{\text{T}}^{\text{miss}} 1\gamma 3j$	2.81	9	$2.15 \pm 0.66$	670–732
$1\mu 1e 4b 2j$	2.91	2	$0.042 \pm 0.037$	1227–1569
$1e 1b 4j$	3.44	160	$105 \pm 14$	726–809

Table 5: List of the three channels with the smallest  $p_{\text{channel}}$ -values in the scan of the  $m_{\text{eff}}$  distributions.

Largest deviations in $m_{\text{eff}}$ scan				
Channel	$p_{\text{channel}} (\cdot 10^{-3})$	$N_{\text{obs}}$	$N_{\text{SM}} \pm \delta N_{\text{SM}}$	Region [GeV]
$1\mu 1e 4b 2j$	2.66	2	$0.040 \pm 0.036$	992–1227
$1\mu 1\gamma 5j$	3.98	4	$0.45 \pm 0.18$	750–895
$3b 1j$	4.87	4	$0.42 \pm 0.24$	3401–3923

No deviation above threshold ...  
 → No data-derived signal region yet

Need better variables, “smarter” regions.. Better background model  
Supervised ? Unsupervised ? Reinforcement learning task ?

→ Need community effort to help

→ Need > 1 algorithm !(and comparison)



# New ideas for searches with unknown signal -> Selection of recent developments in 2017/2018 !

- Fit a ML based background model to be less sensitive on MC prediction (gaussian processes in [arXiv:1709.05681](#) )
- Autoencoders as “filters” for SM events [1808.08992](#)
- Unsupervised techniques (clustering as hypothesis test...)

*K- Nearest Neighbour to estimate the point density of two samples, KL-test statistics to compare the samples*

- Classification without Labels (CWOLA) [arXiv:1805.02664](#):

*Here the idea is to train a NN to separate signal region + sideband region (as two samples) --> this can be possible due to a signal in the signal region ...*

- “Novelty detection algorithm” [arXiv:1807.10261](#) ,
- unsupervised KL divergence [arXiv:1807.06038](#)
- Self-organizing maps...outlier detection with autoencoders ...
- ... various more !!! (can't catch up anymore, can you ?)
- **Which one is good ? Which one to use ? Need comparison !!!**



# Next steps: Compare / Optimize different approaches

e.g. in „unsupervised searches“ group of darkmachines

(Amir Farbin, Erzebet Merenyi, Andrea di Simone, Maurizio Pierini)

e.g. in ATLAS with General Search as prototype data ?

The image shows a screenshot of the Dark Machines website and a tweet. The website has a dark blue background with a starry sky pattern. The header includes the name 'Dark Machines' and navigation links: 'About', 'News', 'Events', 'Projects', 'Researchers', 'White paper', 'Mailinglist', and 'Contribute'. A Twitter icon is also present. The main content area is titled 'About Dark Machines' and contains the text: 'Dark Machines is a research collective of physicists and data scientists. We are curious about the universe and want to answer cutting edge questions about Dark Matter with the most advanced techniques that data science provides us with.' Below this text is a button that says 'Visit our indico page'. To the right of the website content is a tweet from 'Dark Machines' (@dark\_machines) dated August 3, 2018. The tweet text is: 'The strong lensing subgroup of the DarkMachines project ([darkmachines.org](https://darkmachines.org)) will be holding a kick-off video-meeting for the strong lens challenge on Tuesday, August 7th, 7am PDT (California time).' Below the tweet is a retweet from 'Gianfranco Bertone' (@gfbertone) with the text: 'Nice summary on @nature of the challenges and opportunities that come with the use of machine learning at the frontiers of particle physics [nature.com/articles/s4158...](https://nature.com/articles/s4158...)'. At the bottom of the tweet is a small image of a book cover titled 'Machine learning at the energy and intensity frontiers of...'. The page number '78' is visible in the bottom right corner.

Dark Machines

About News Events Projects Researchers White paper Mailinglist Contribute

## About Dark Machines

Dark Machines is a research collective of physicists and data scientists.  
We are curious about the universe and want to answer cutting edge questions about Dark Matter with the most advanced techniques that data science provides us with.

Visit our indico page

**Dark Machines**  
@dark\_machines

The strong lensing subgroup of the DarkMachines project ([darkmachines.org](https://darkmachines.org)) will be holding a kick-off video-meeting for the strong lens challenge on Tuesday, August 7th, 7am PDT (California time).

Aug 3, 2018

Dark Machines Retweeted

**Gianfranco Bertone**  
@gfbertone

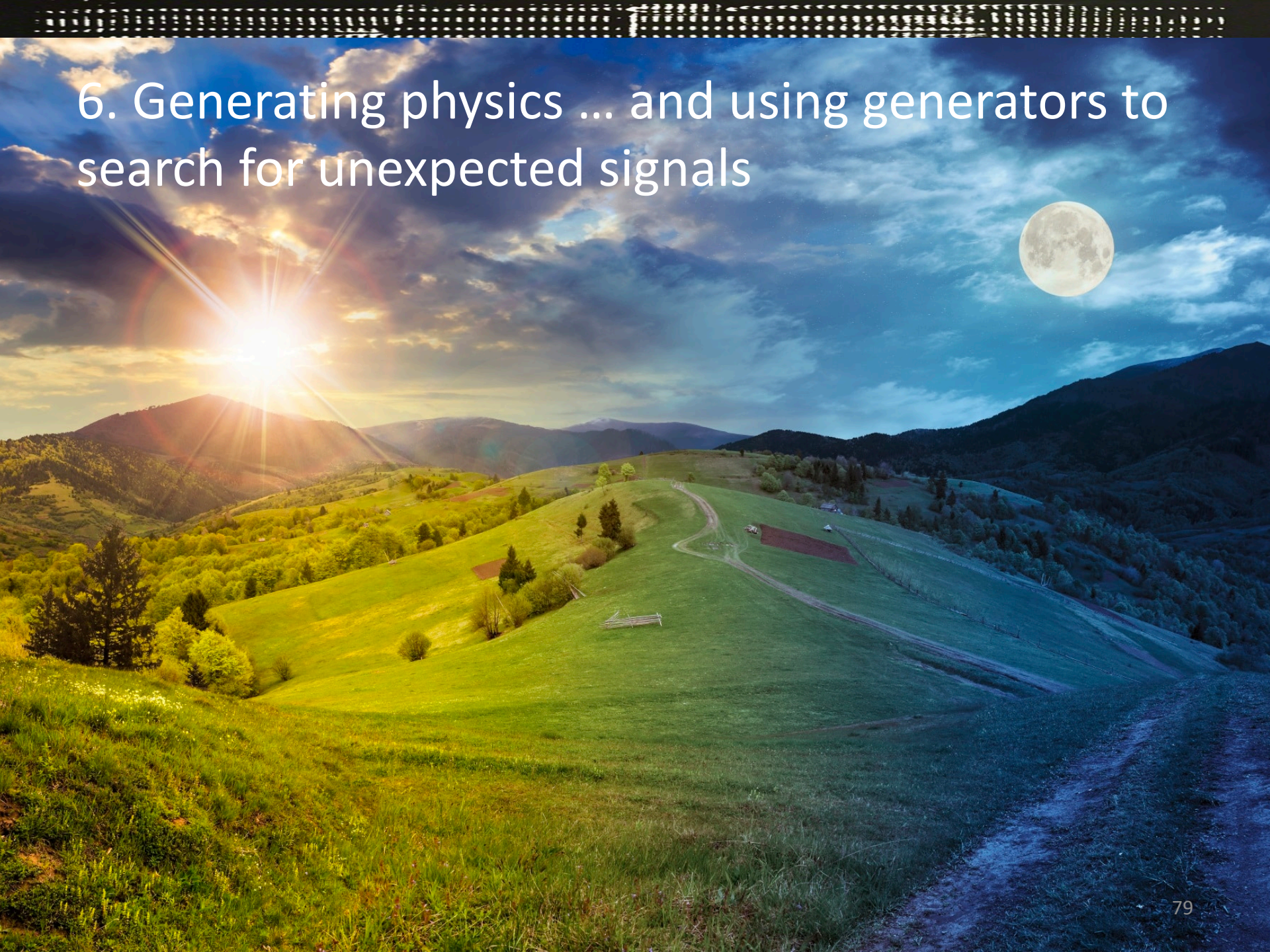
Nice summary on @nature of the challenges and opportunities that come with the use of machine learning at the frontiers of particle physics  
[nature.com/articles/s4158...](https://nature.com/articles/s4158...)

Machine learning at the energy and intensity frontiers of...

78



## 6. Generating physics ... and using generators to search for unexpected signals





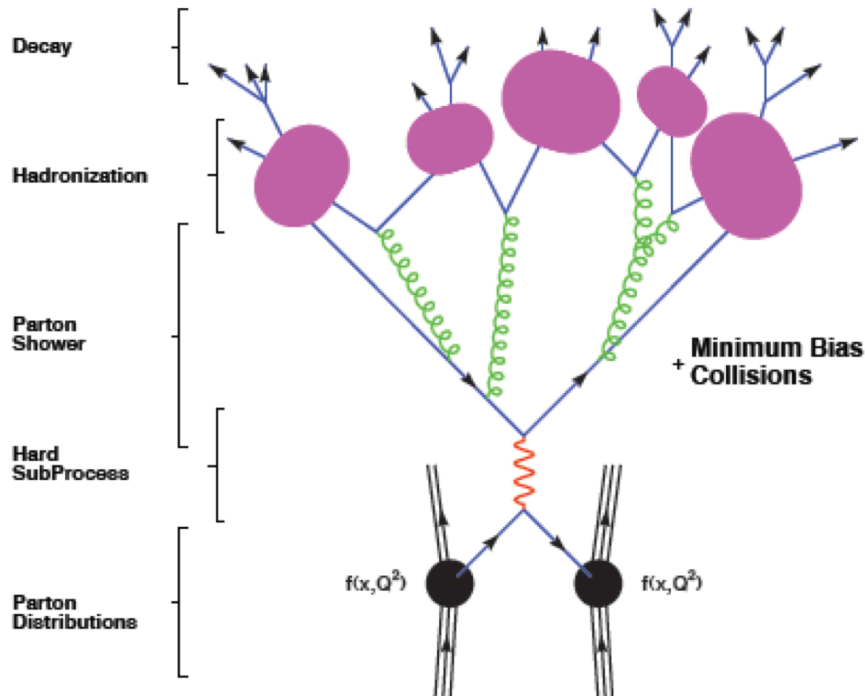
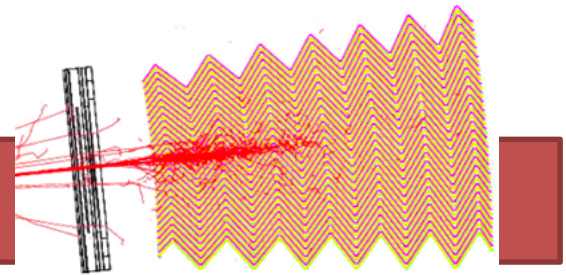
Question: Can we make physical  
(collider, astroparticle, etc) events  
with a generative model ?

# Simulation: Traditional

Energy and angles of reconstructed particles



Detector Simulator

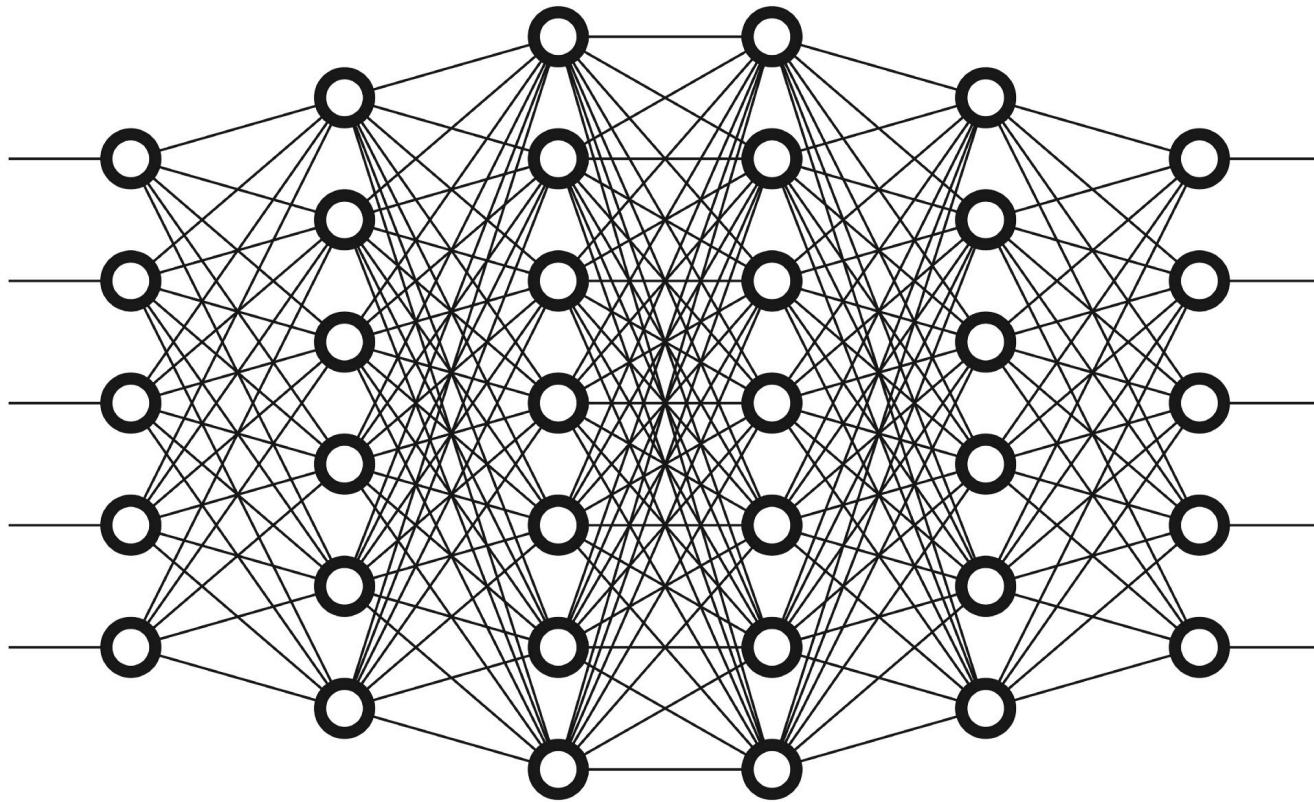


Input:  
Random numbers



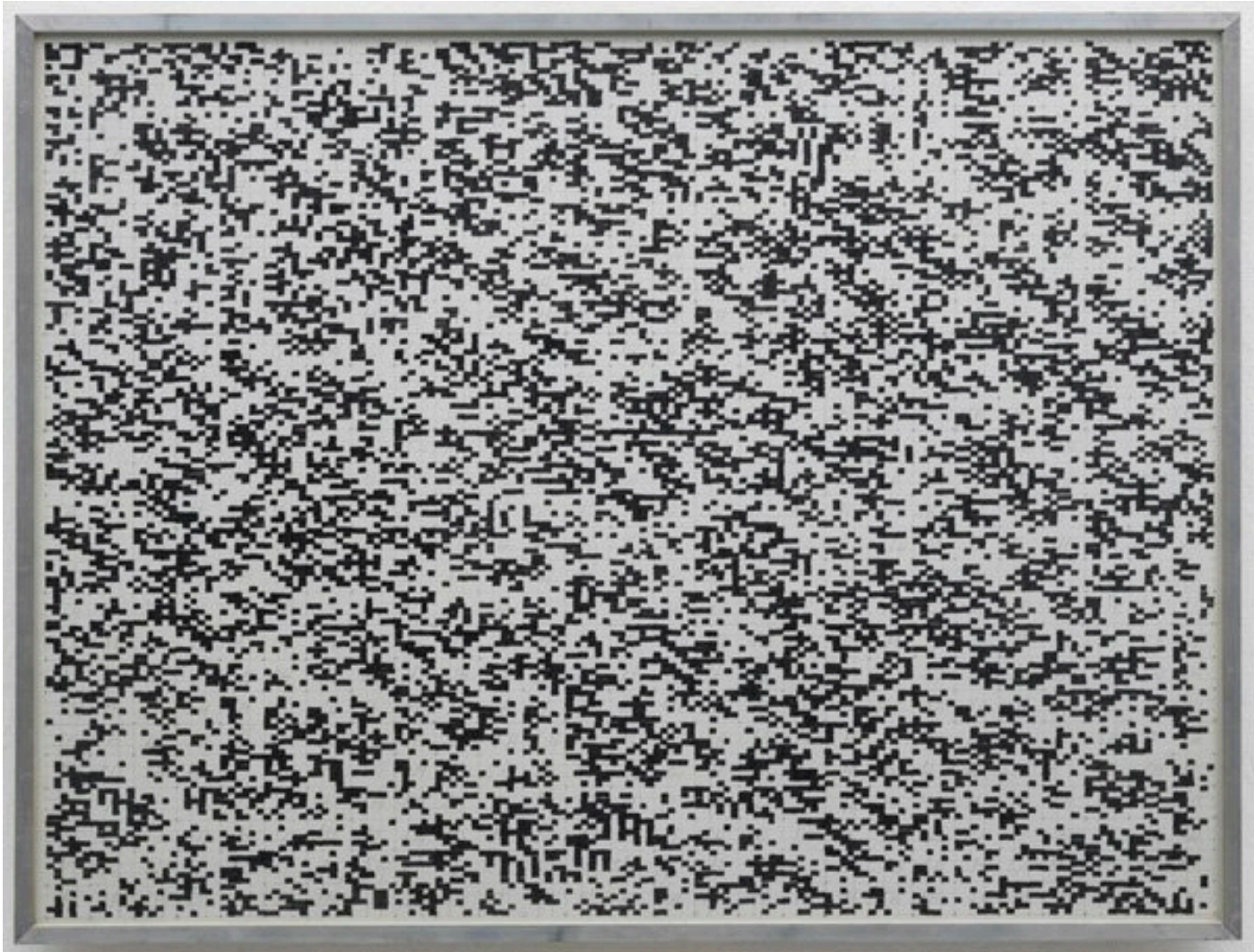
# Simulation: Us

Energy and angles of reconstructed particles



Input:  
Random numbers

# Random numbers...



Götz, Karl Otto: Statistisch-metrischer  
Versuch 4:2:2:1, Entwurf Sommer 1959



# Random input → Art

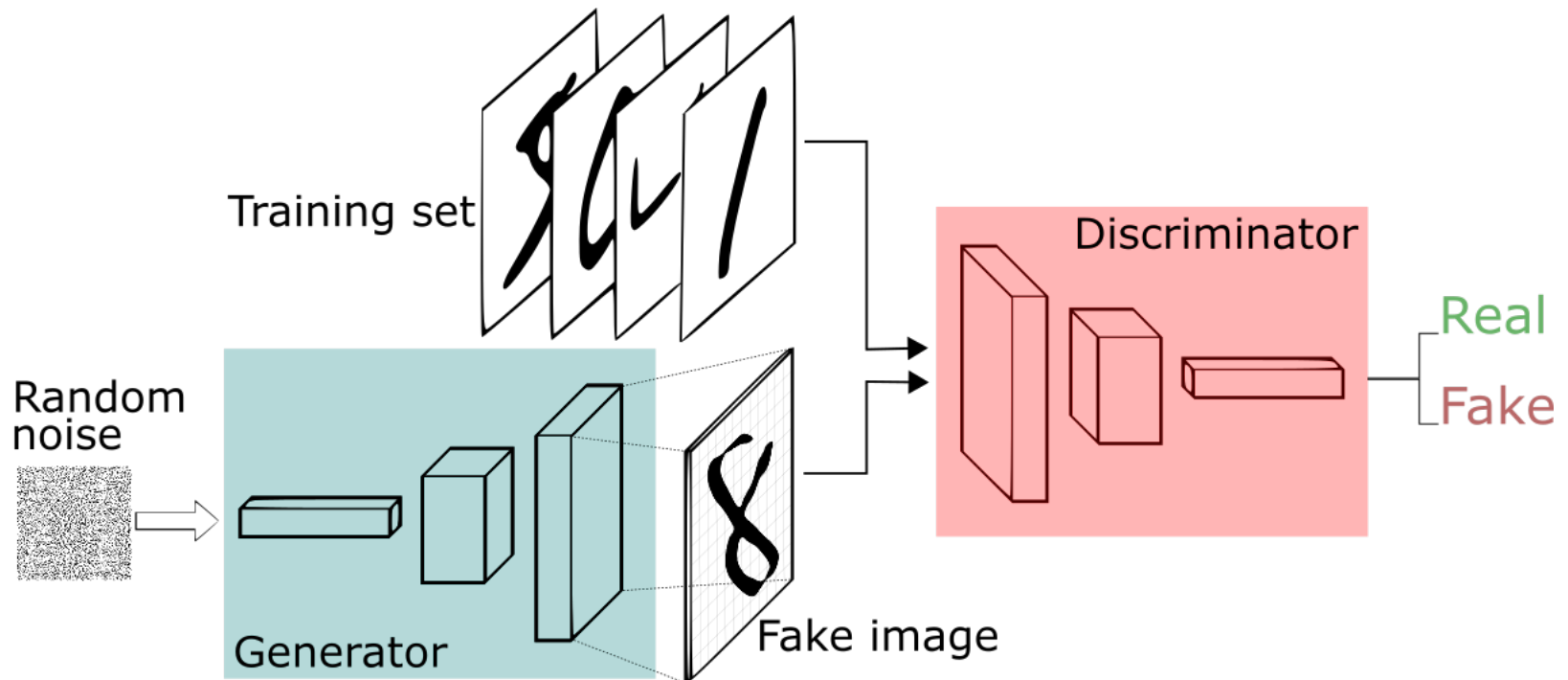


Tinguely, Meta Matics



# Network simulations ?

Generative Adversarial Networks state of the art:



1812.04948

source

destination



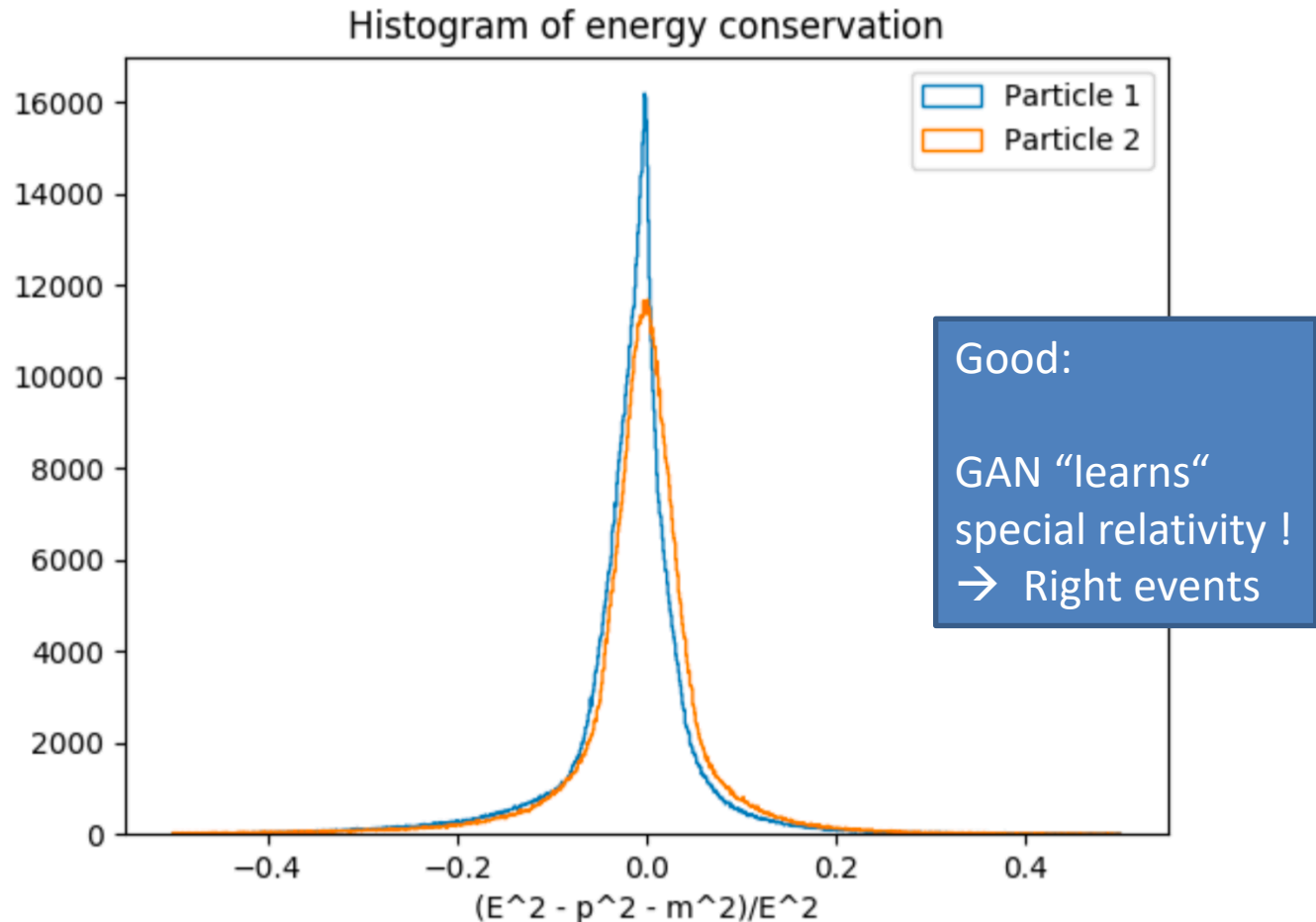
Coarse styles copied



Middle styles copied

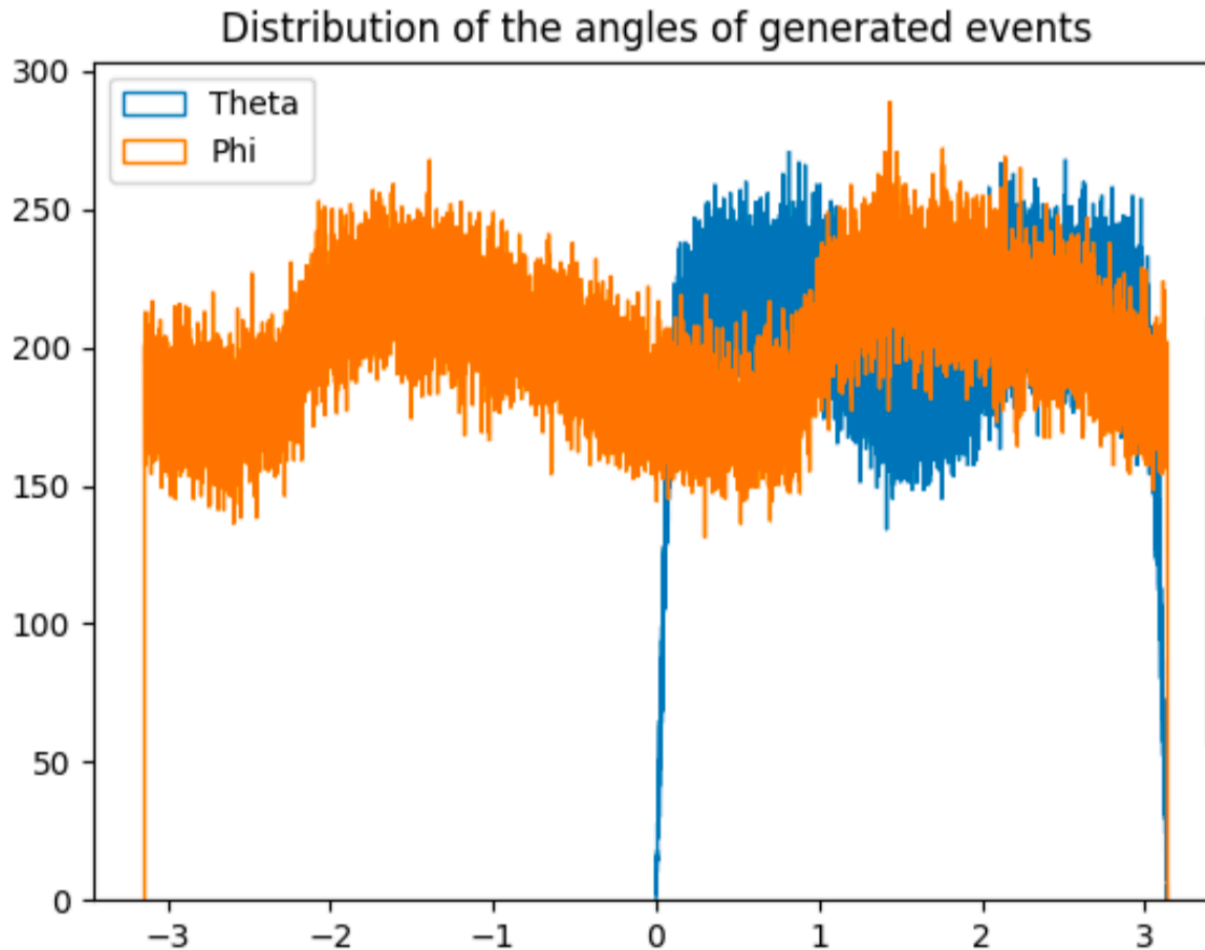


# Distributions of Particle Collision “Events” with GANs





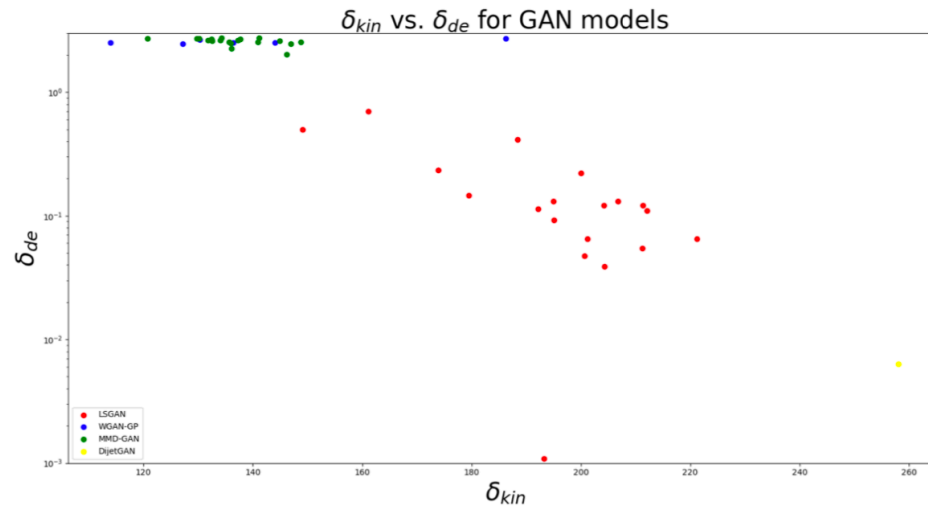
# Distributions of Particle Collision “Events” with GANs



BAD:

GAN does not  
make  
events of different  
types with right  
frequencies !

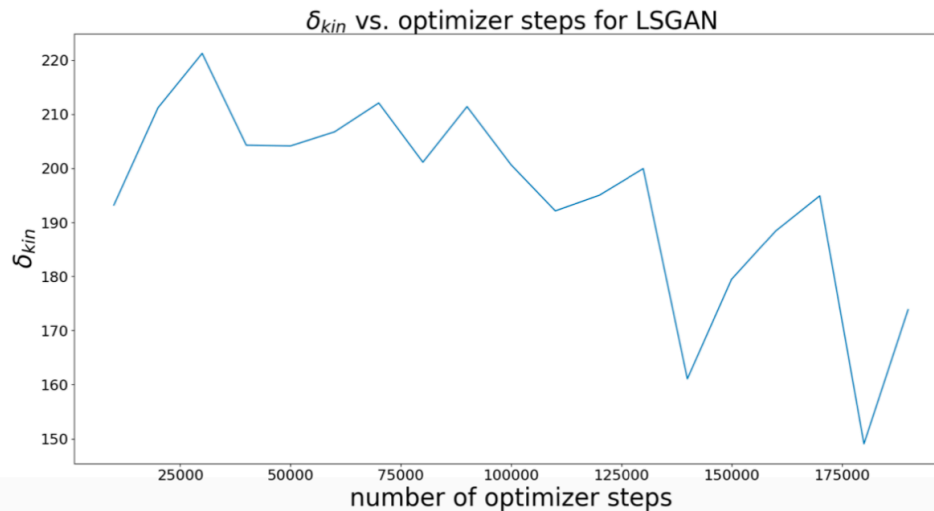
# Our GAN attempt



Tried 5 different  
GAN architectures

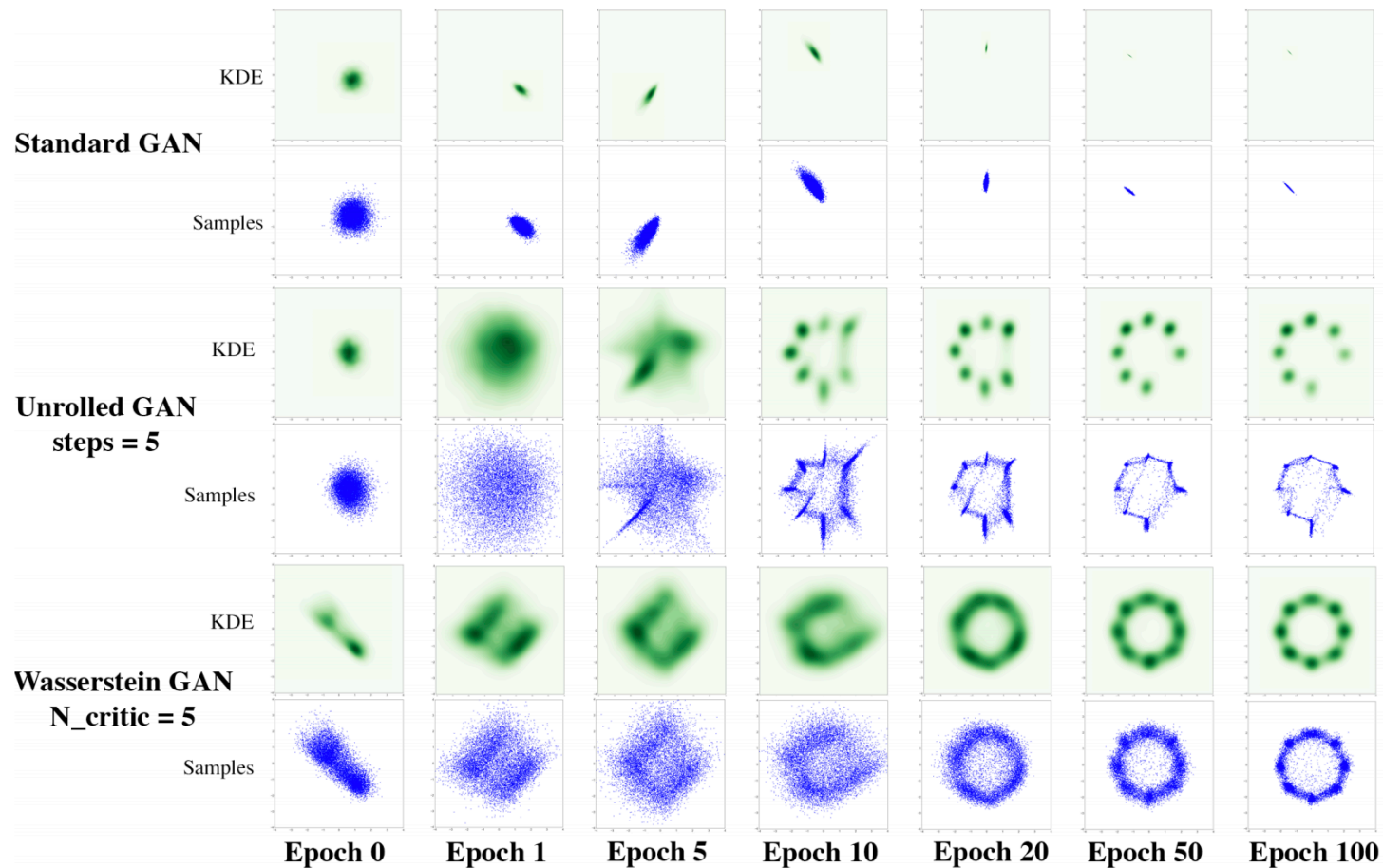
Training highly unstable

Not able to sample 25d  
density



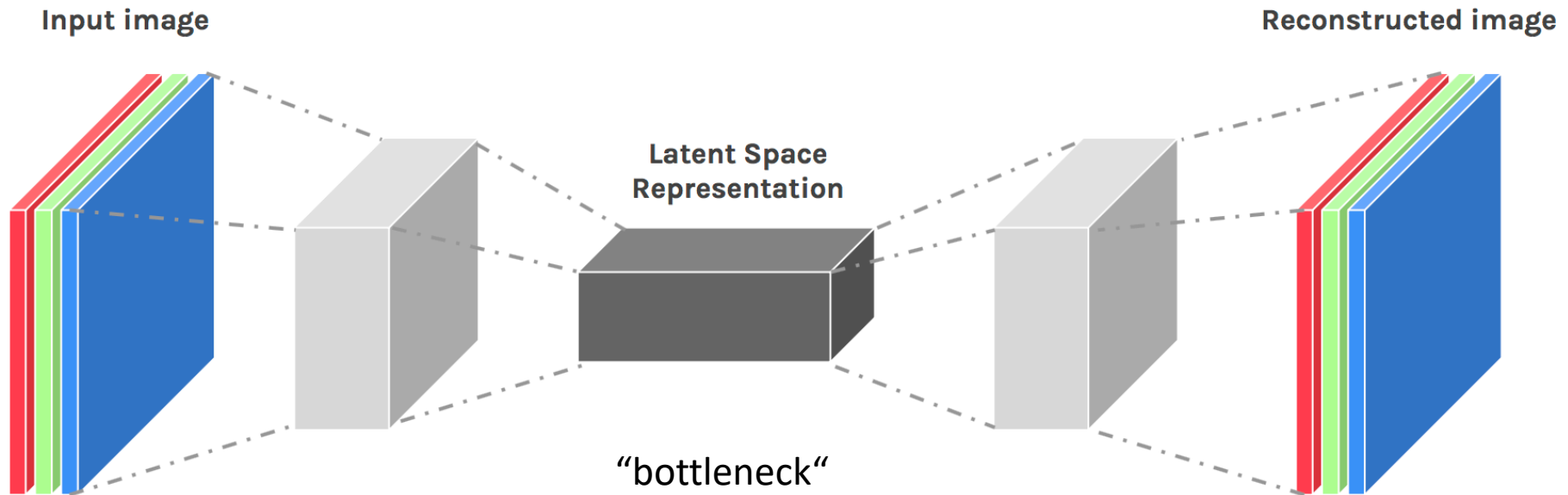
# Densities with GANs

<http://proceedings.mlr.press/v70/arjovsky17a/arjovsky17a.pdf>





# Autoencoders



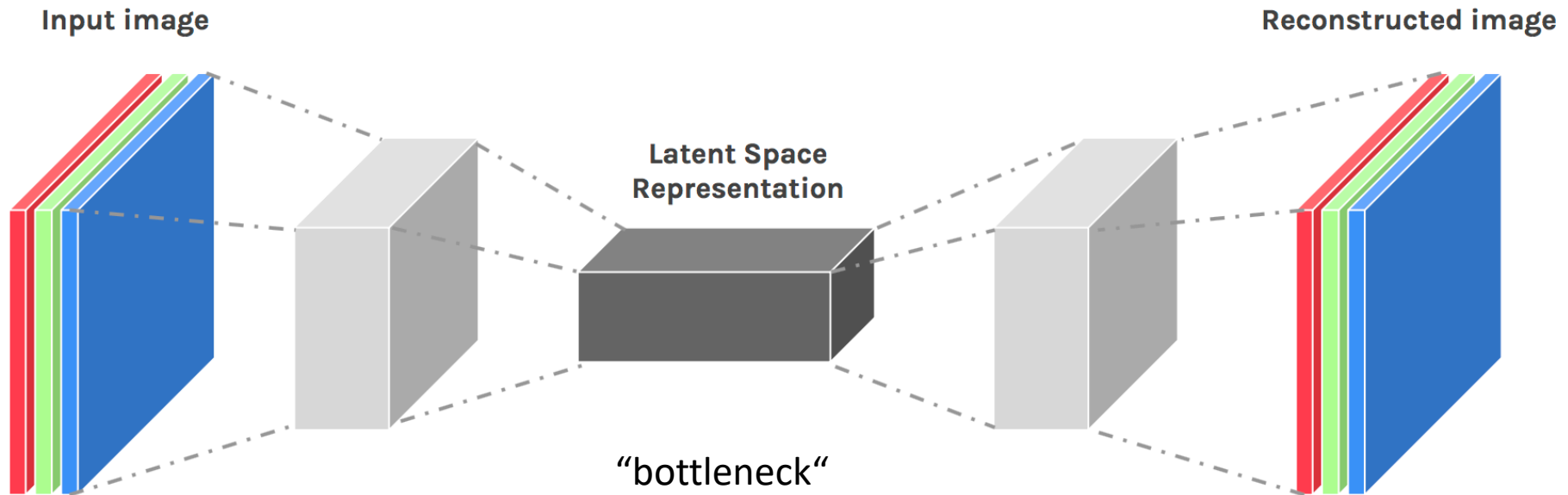
Can find new physics  
with reconstruction Loss

We actually use a better version:

**„Dutch“ Autoencoder**

(Variational Autoencoder by Diederik Kingma and Max Welling)

# Variational Autoencoders



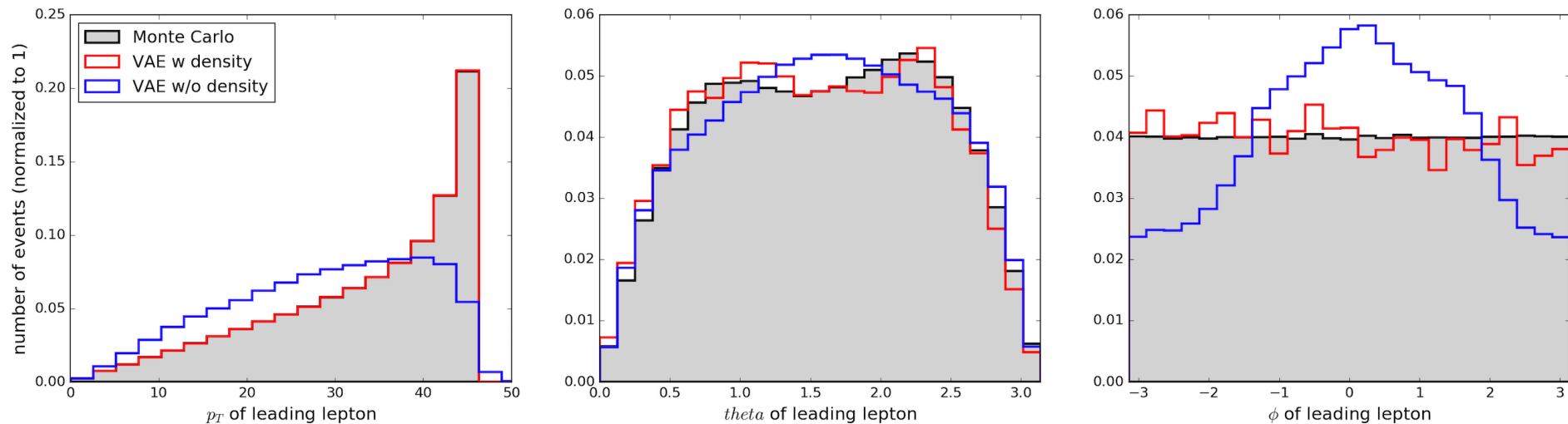
Encoder output is the mean and the variance of  $d$  Gaussians

Decoder input is  $z$  : a sample drawn from these  $d$  Gaussians

We proposed to use  
B-VAE ( $B \ll 1$ )

$$L = \frac{1}{M} \sum_{i=1}^M (1 - B) \cdot MSE + B \cdot D_{KL}.$$

# Distributions of Particle Collision “Events” with variational autoencoders

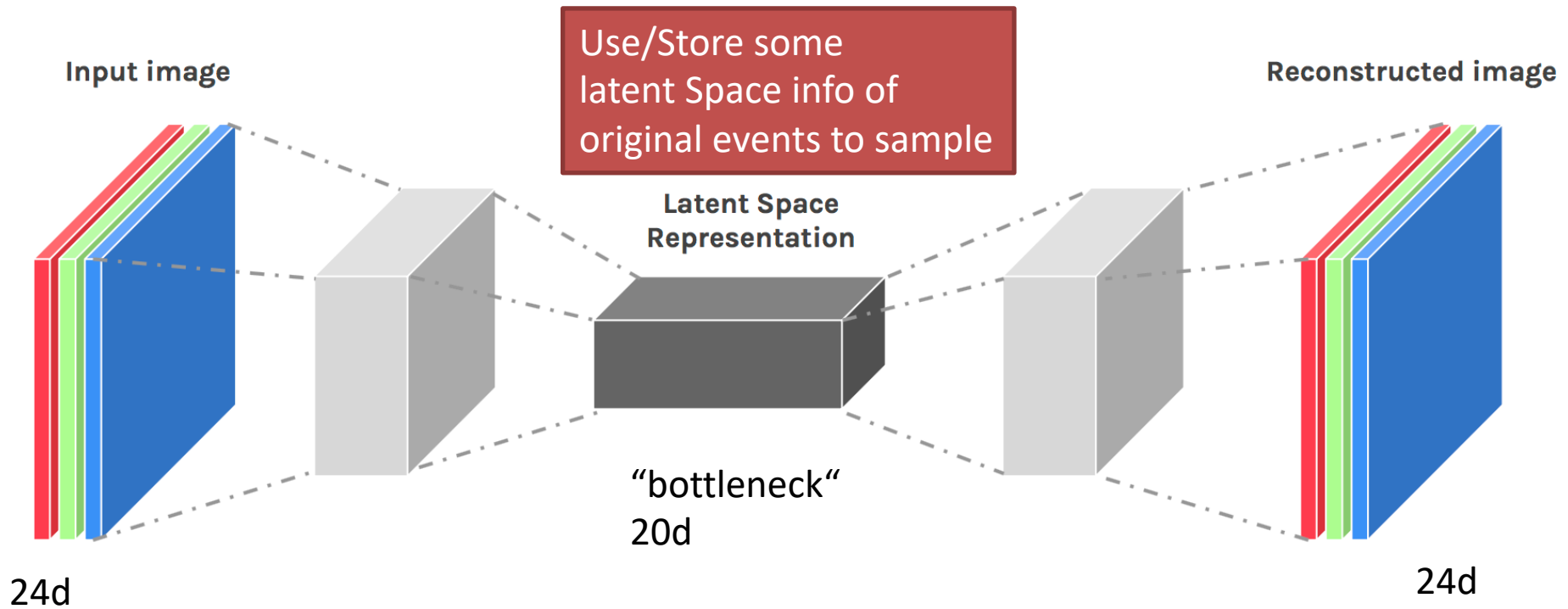


BAD:

Autoencoder typically does not  
make events of different types with right  
frequencies !



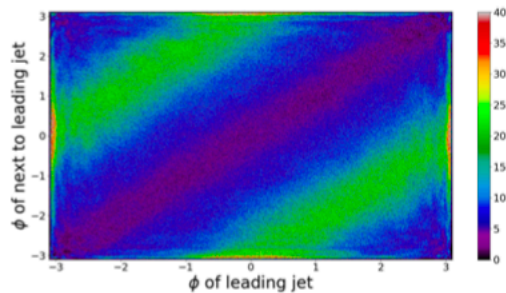
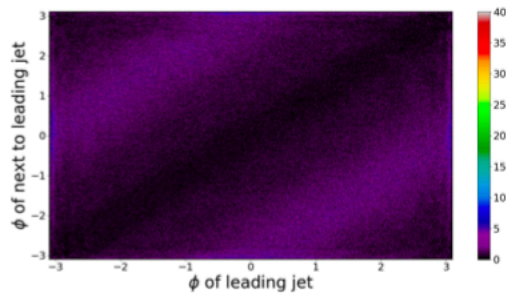
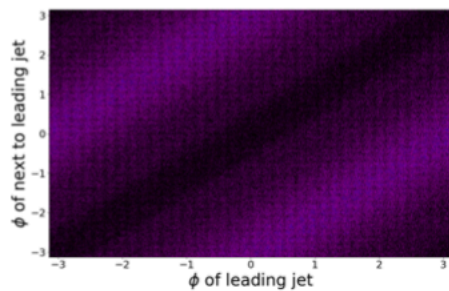
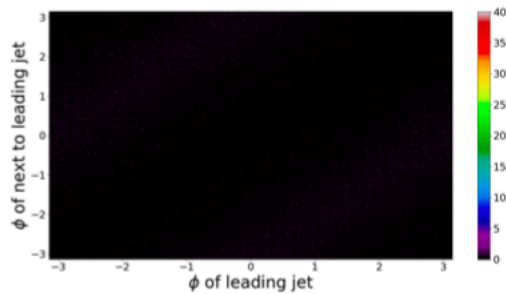
# Autoencoder (+ event info in latent space )



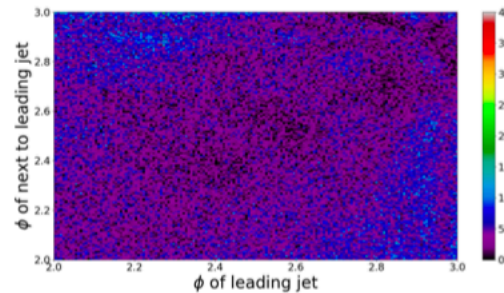
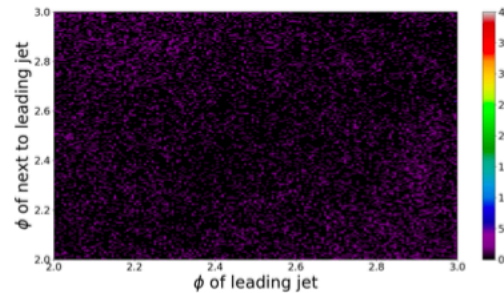
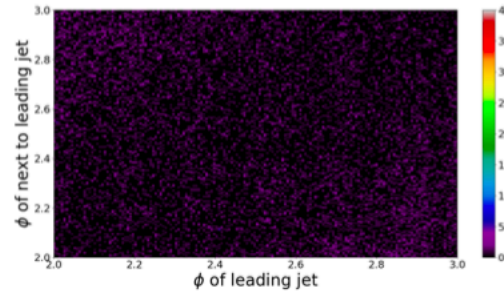
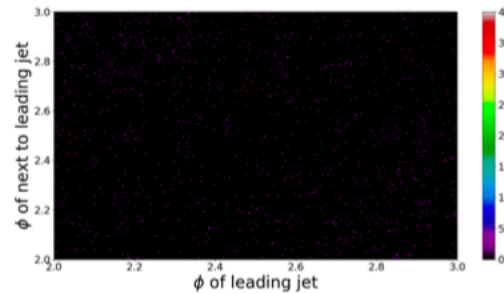
VAE:  $p(z)$  is typically from  $d$  dimensional gauss,

VAE with buffer:

$$p_{\phi, X_L}(z) = \sum_{i=1}^m q_{\phi}(z|x^i)p(x^i) \text{ with } p(x^i) = \frac{1}{m}.$$



a) full range



b) zoom in on  $[2, 3] \times [2, 3]$

Training data  
100k

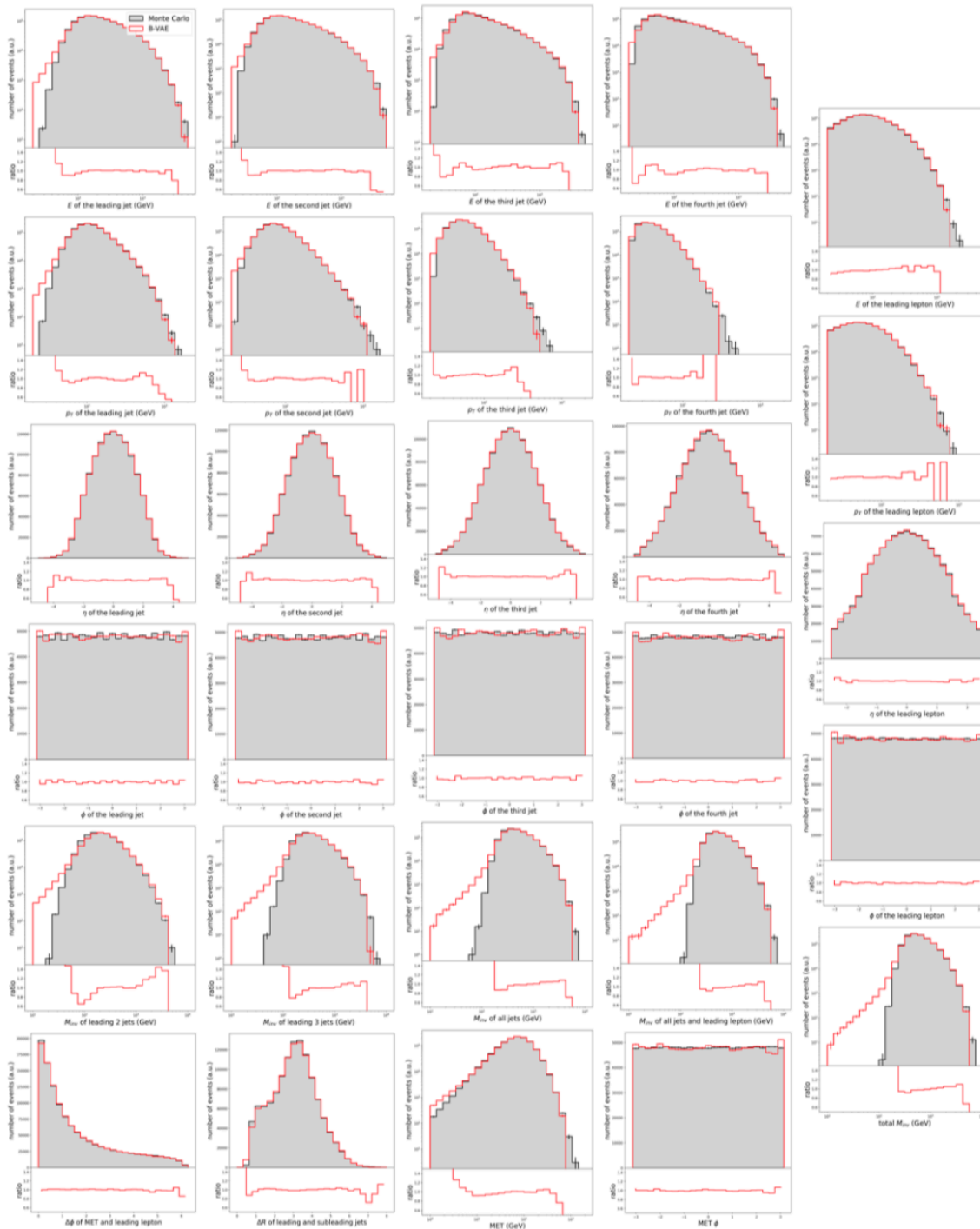
2d projection  
of density

Monte Carlo  
1M events

B-VAE  
1M events

B-VAE  
12M events

# Sampling top top -> 6 particles



<https://arxiv.org/abs/1901.00875>

1d distributions :

Red: B-VAE

Grey: MC (Madgraph+Delphes)

Rank	$(\dim(z), B, \alpha = 1, \gamma)$	$\delta_{kin}$	$\delta_{de}$
1	$(20, 10^{-6}, 1, 0.01)$	483.5	0.0067
2	$(20, 10^{-7}, 1, 0.01)$	481.2	0.0068
3	$(16, 10^{-7}, 1, 0.01)$	471.8	0.0081

Model	$\delta_{kin}$	$\delta_{de}$
KDE	249.0	0.4934
GMM, 50	279.9	1.4457
GMM, 100	291.2	1.5141
GMM, 1000	307.1	1.5232
5 % Smearing	505.3	0.1316
10 % Smearing	442.6	0.3186

TABLE I: KDE and GMM model performance evaluated on figures of merit  $\delta_{kin}$  and  $\delta_{de}$ .



# Noise input vs True events input $\rightarrow$ B-VAE as anomaly detector

15

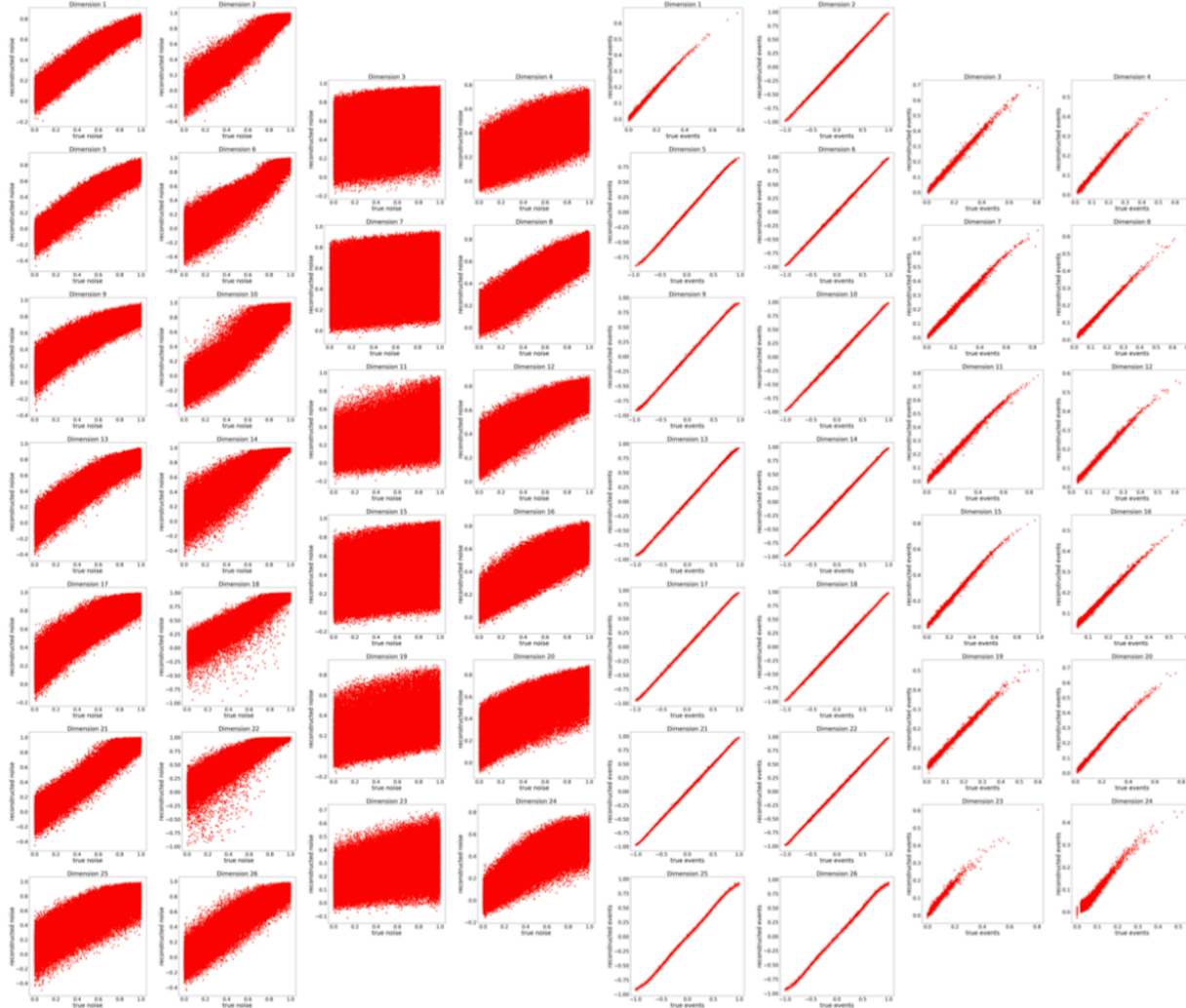


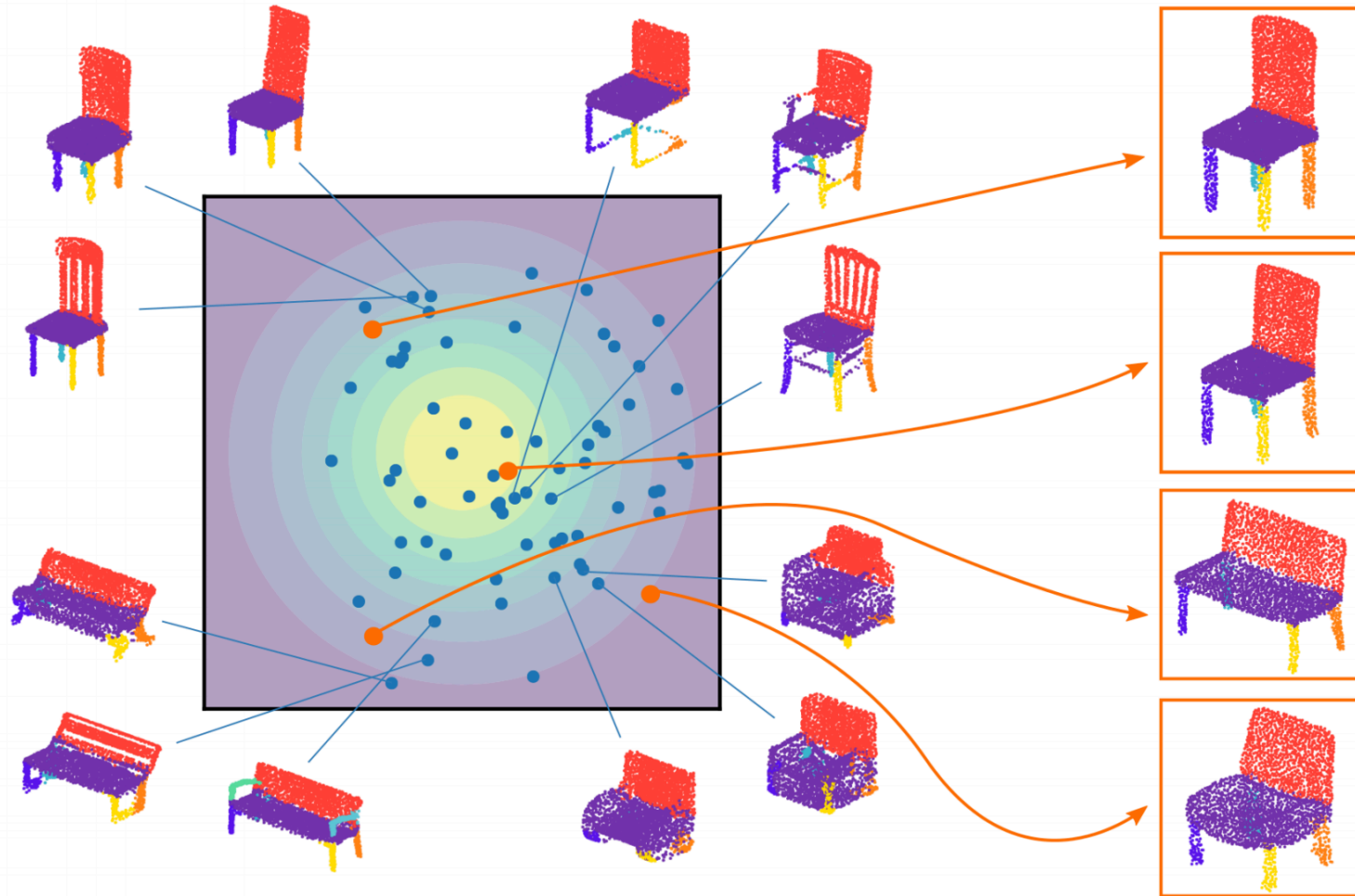
FIG. 1: Input vs. Reconstruction of uniform noise  $x \sim U(0, 1)$  (first four columns) and real events (last four columns) for a VAE with  $\dim(z) = 20$  and  $B = 10^{-6}$ .

# Why is this useful ?

Can „store“ events in *lower dimensional* latent space and interpolate between them

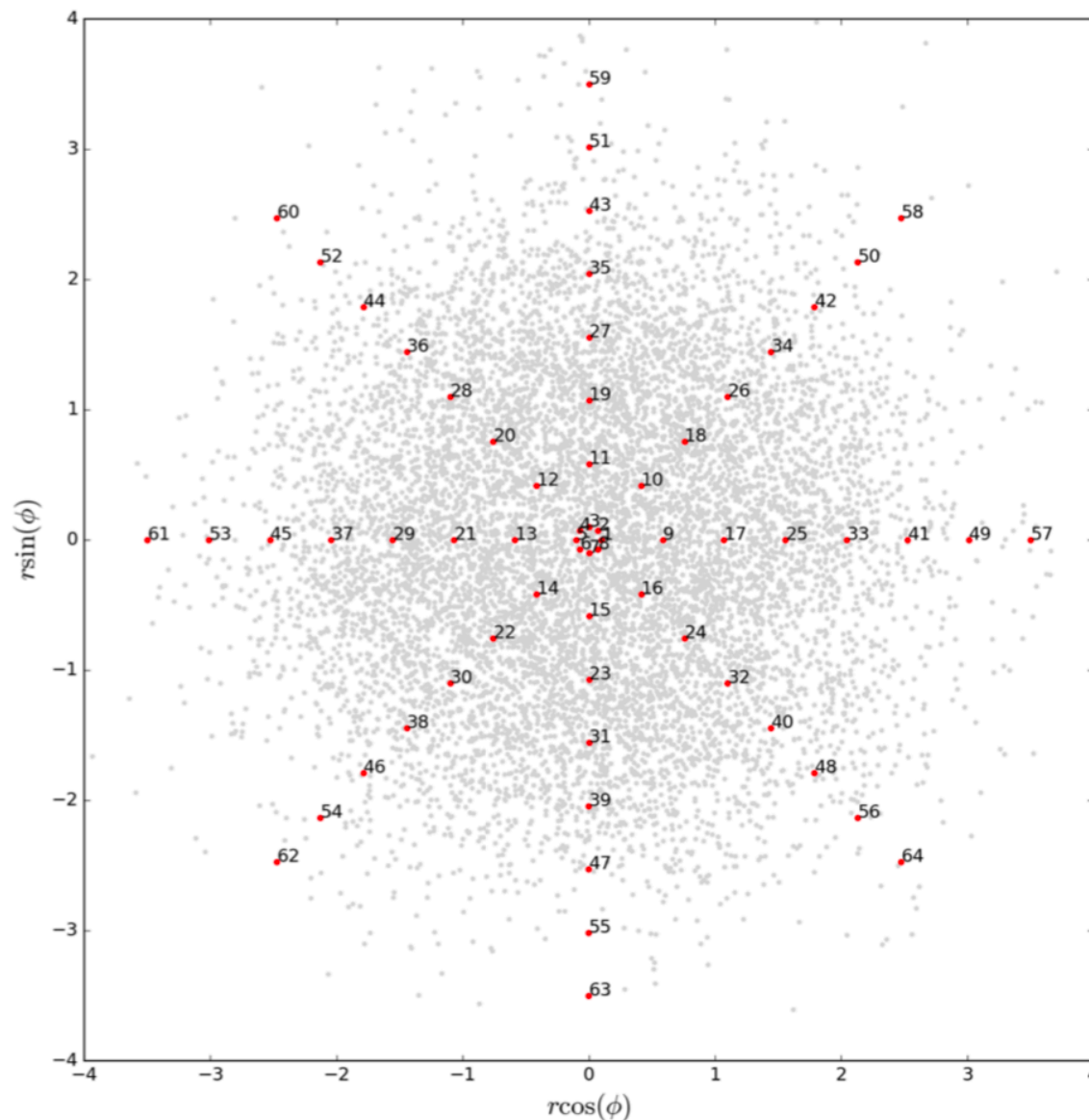
- New events (by interpolation and compression/decompression)
- New concepts (by interpolation)
- New models (by interpolation)
- Better random number sampling
- Ultrafast (Million events per second compared to 1 event per minute ...)

# Concept of a latent space of sofas and chairs





# Top top Latent space PCA1 vs PCA2



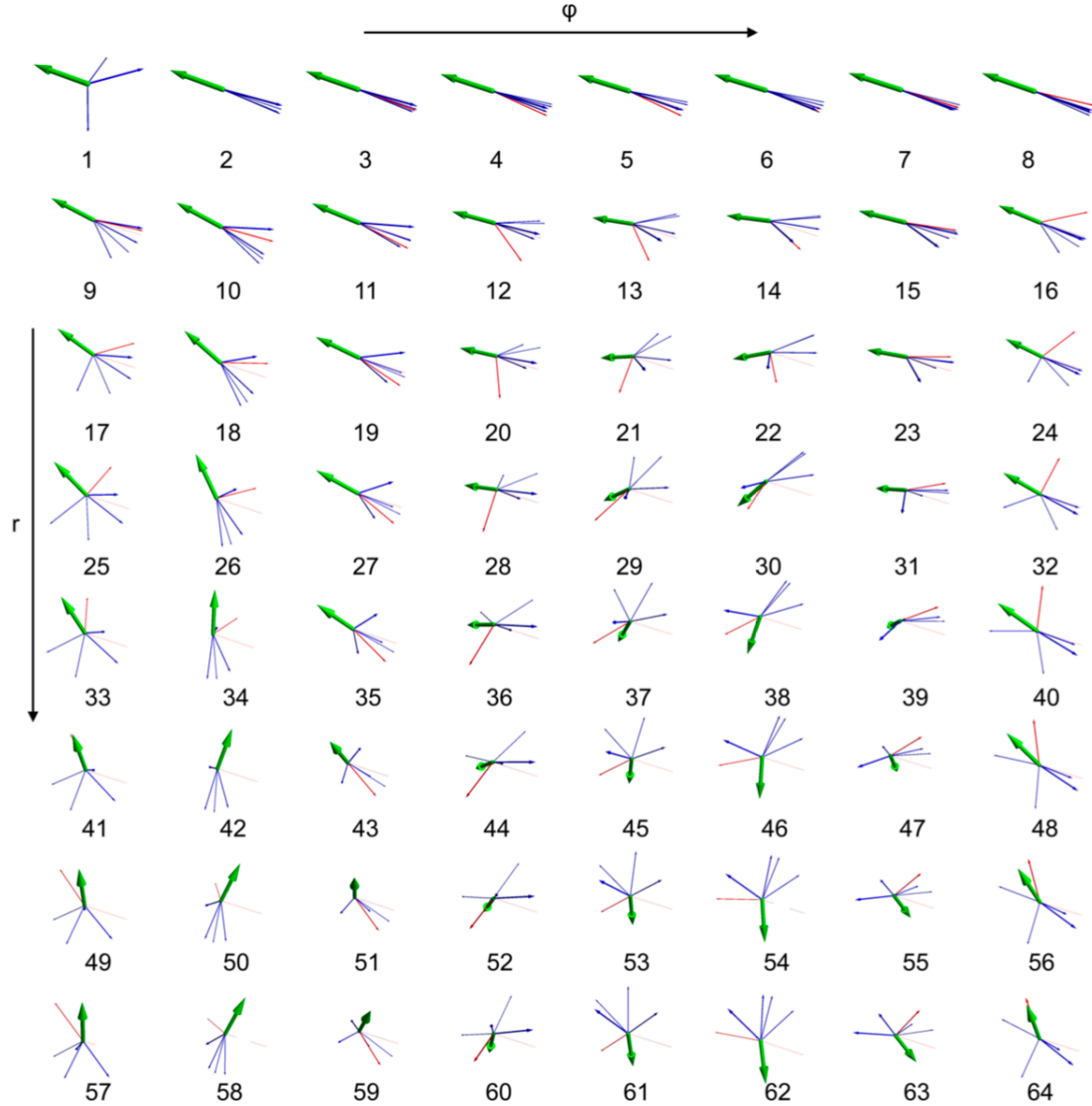


FIG. 7: Visualization of the first two components of a principal component analysis of encoded Monte Carlo events in latent space. This shows an  $8 \times 8$  grid of event displays following the red dots in Figure 6. These 64 points chosen

# Summary

1. Automatization
  2. Data derived signal regions
  3. Learn the model space
  4. Learn the simulator
- Use this for your search



# Extra Slides

# Main message: Parameter determination of the physical model with a Neural Network

- Finally our goal is to **determine the model parameters** from 1 image (“real data”)
- We do this by **training the network on “simulation”** (“simulated data”)
- We need to **ensure that simulation agrees with data**: *Is the true image in the simulation parameter space of images ? If not DM parameters maybe wrong !*

In simple words we do a “fit” to the image including all kinds of “unknown correlations” using a deep convolutional network trained on simulations