Deep Learning Applications for collider physics Lecture 4

Maurizio Pierini

Plan for these lectures

	Day1	Day2	Day3	Day4	Day5
1st hour	Introduction	ConvNN	LHC & fast Inference	Autoencoders	Graphs
2nd hour	Dense NNNs	GANs	RNNs	Anomaly Detection	Graphs
Tutorial	Dense NNNs	ConvNN	RNNs	Autoencoders	Graphs

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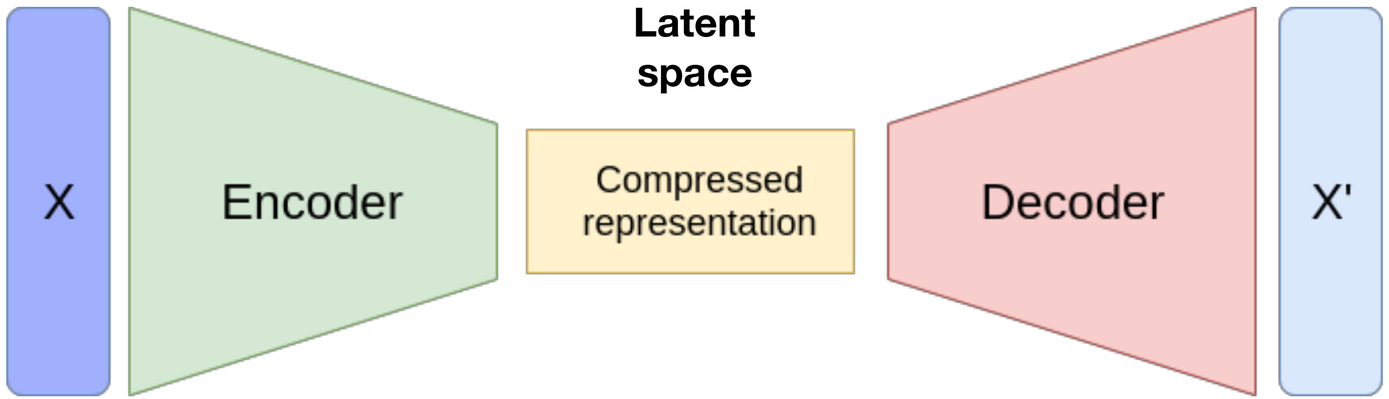
Autoencoders

- *Autoencoders are networks with a typical "bottleneck" structure, with a symmetric structure around it*
  - *They go from* $\mathbb{R}^n \rightarrow \mathbb{R}^n$
  - *They are used to learn the identity function as* $f^{-1}(f(x))$

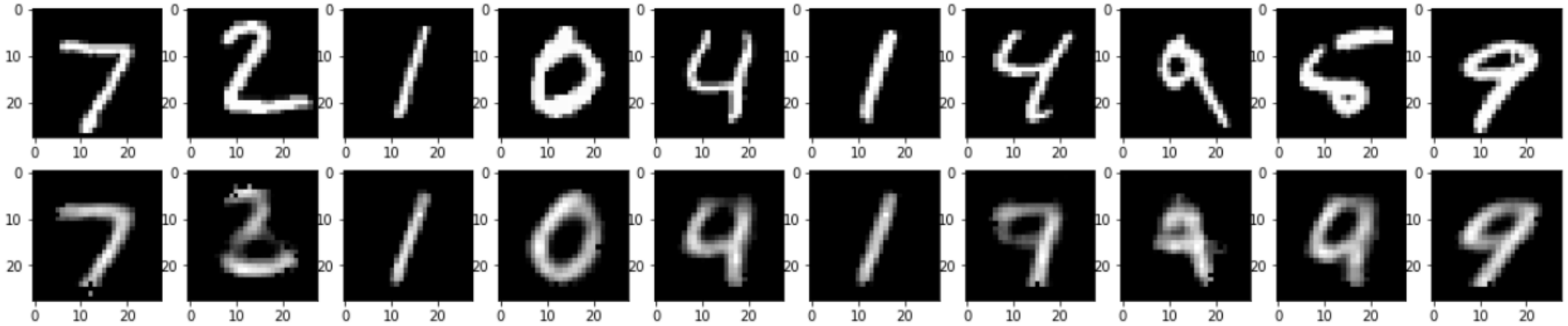
where $f: \mathbb{R}^n \rightarrow \mathbb{R}^k$ *and* $f^{-1}: \mathbb{R}^k \rightarrow \mathbb{R}^n$

- *Autoencoders are essential tools for unsupervised studies*



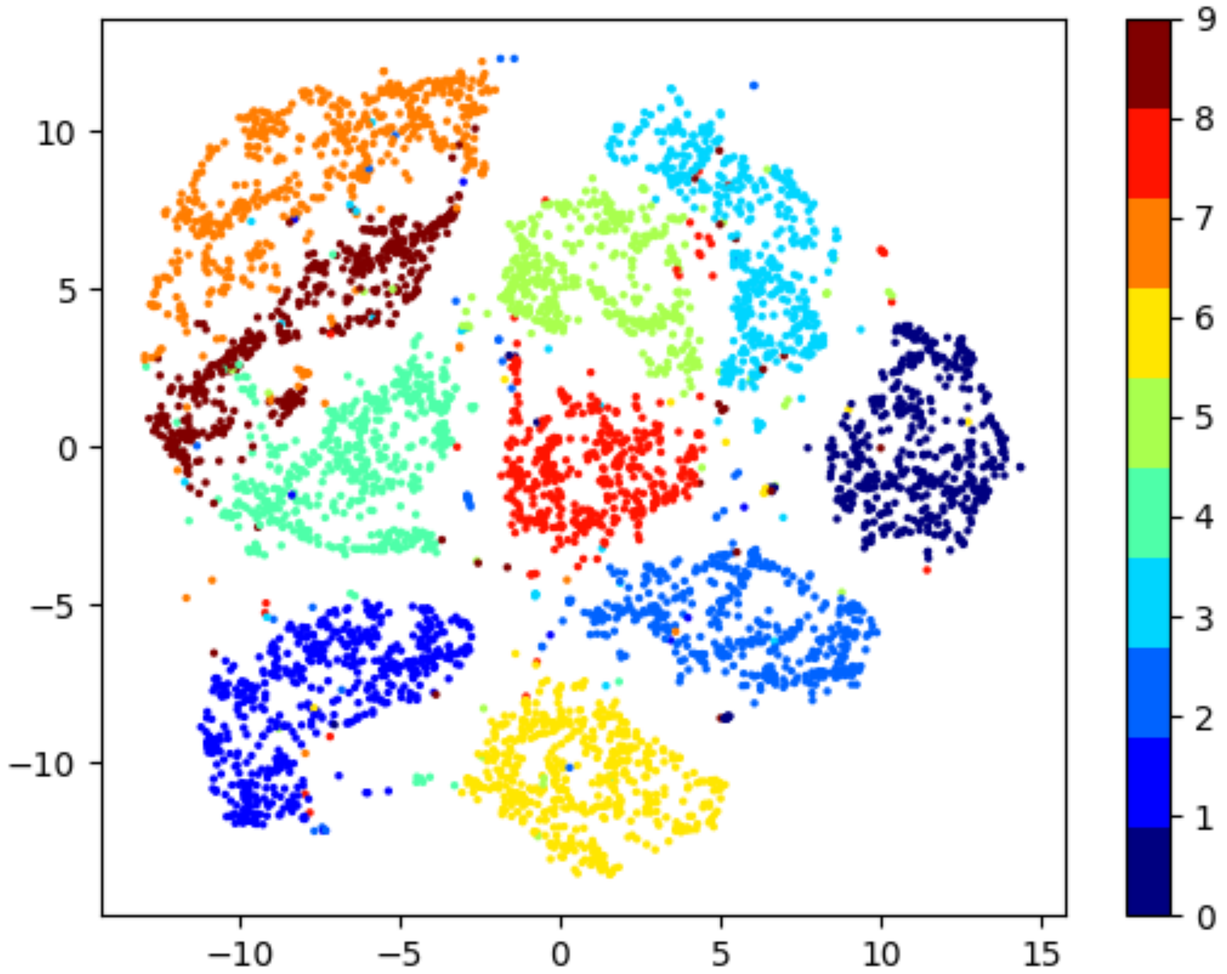
Dimensional Reduction

- *Autoencoders can be seen as compression algorithms*
  - *The n inputs are reduced to k quantities by the encoder*
  - *Through the decoder, the input can be reconstructed from the k quantities*
- *As a compression algorithm, an auto encoder allows to save (n-k)/n of the space normally occupied by the input dataset*



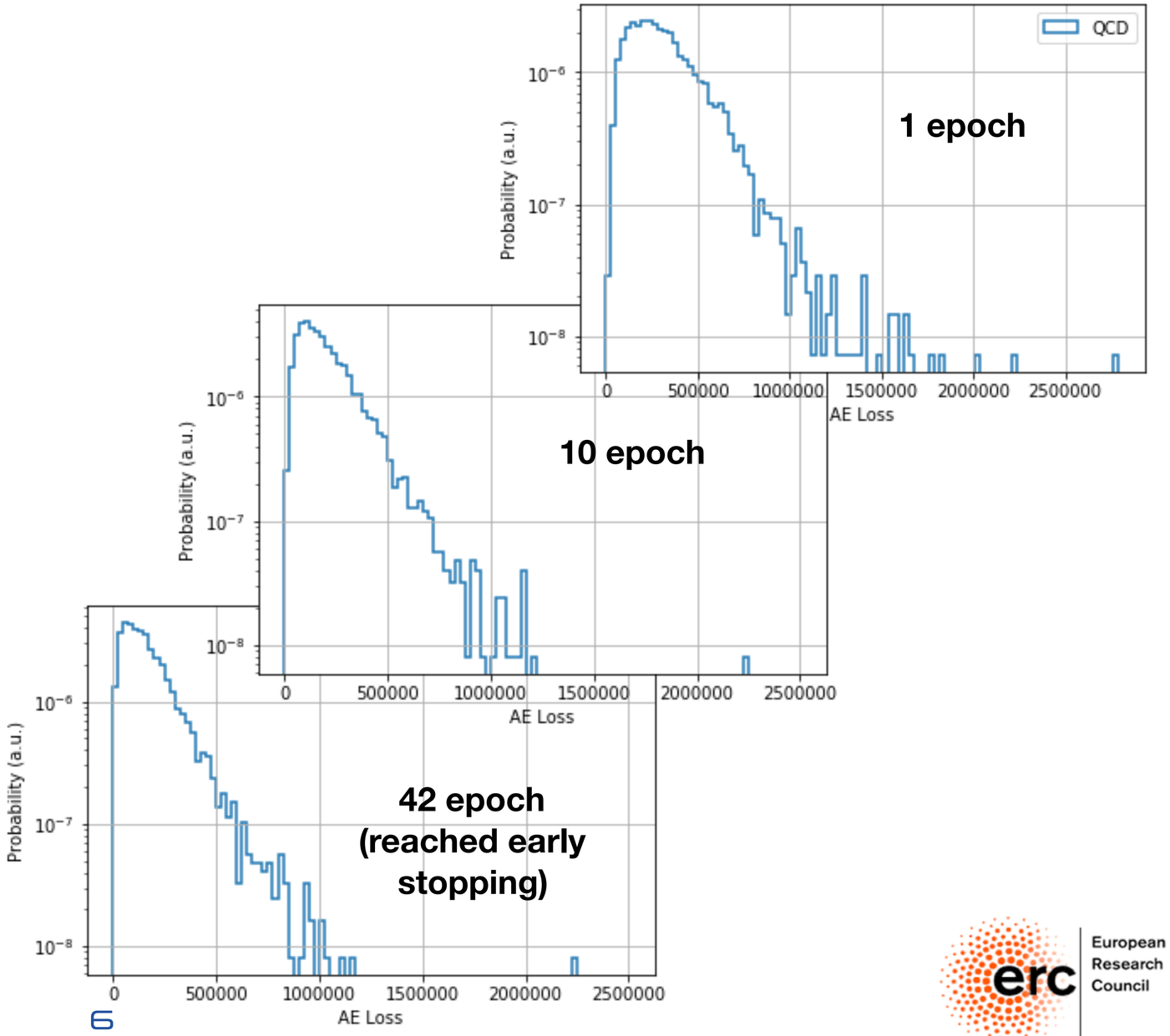
Clustering

- *The auto encoder can be used as a clustering algorithm*
  - *Alike inputs tend to populate the same region of the latent space*
  - *Different inputs tend to be far away*



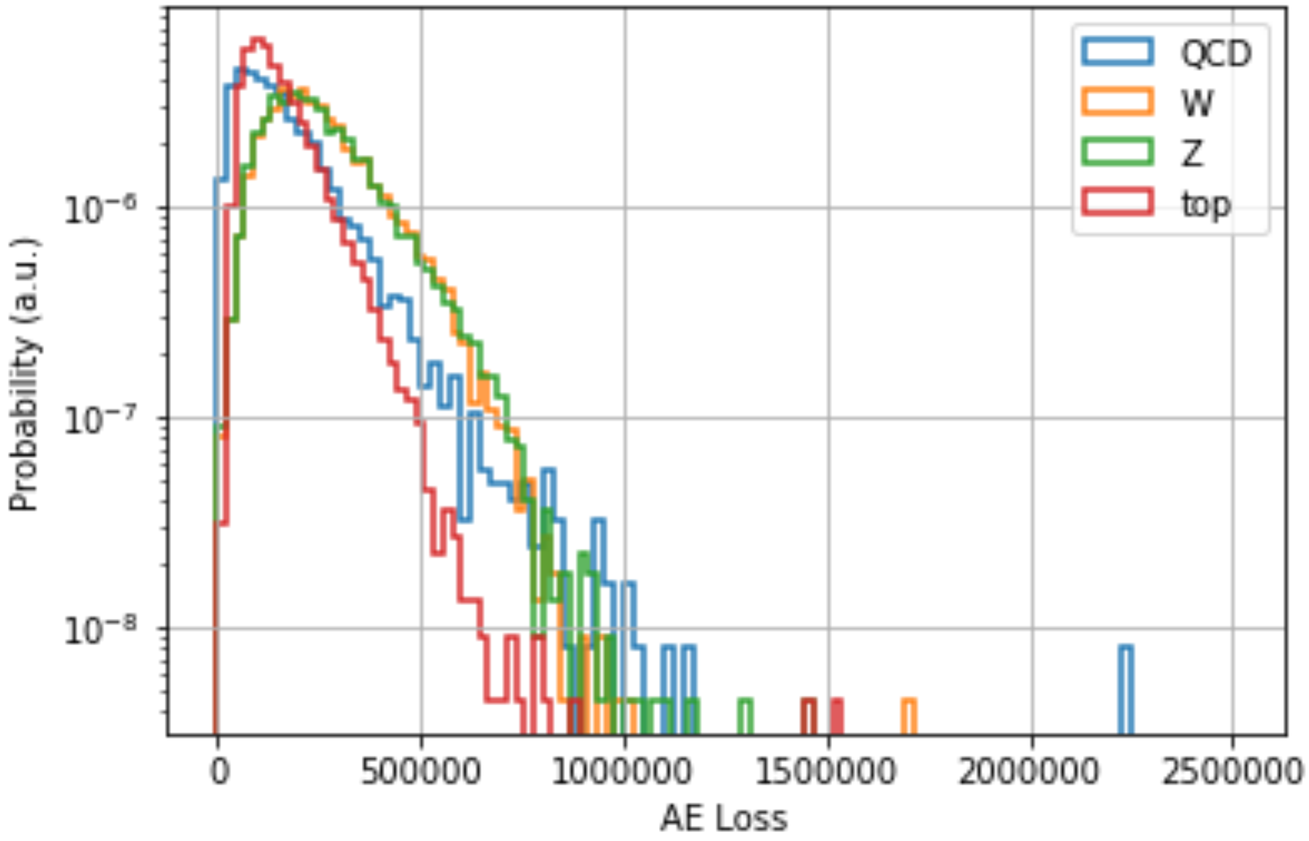
Training an Autoencoder

- *AEs are training minimizing the distance between the inputs and the corresponding outputs*
- *The loss function represents some distance metric between the two*
  - *e.g., MSE loss*
- *A minimal distance guarantees that the latent representation + decoder is enough to reconstruct the input information*



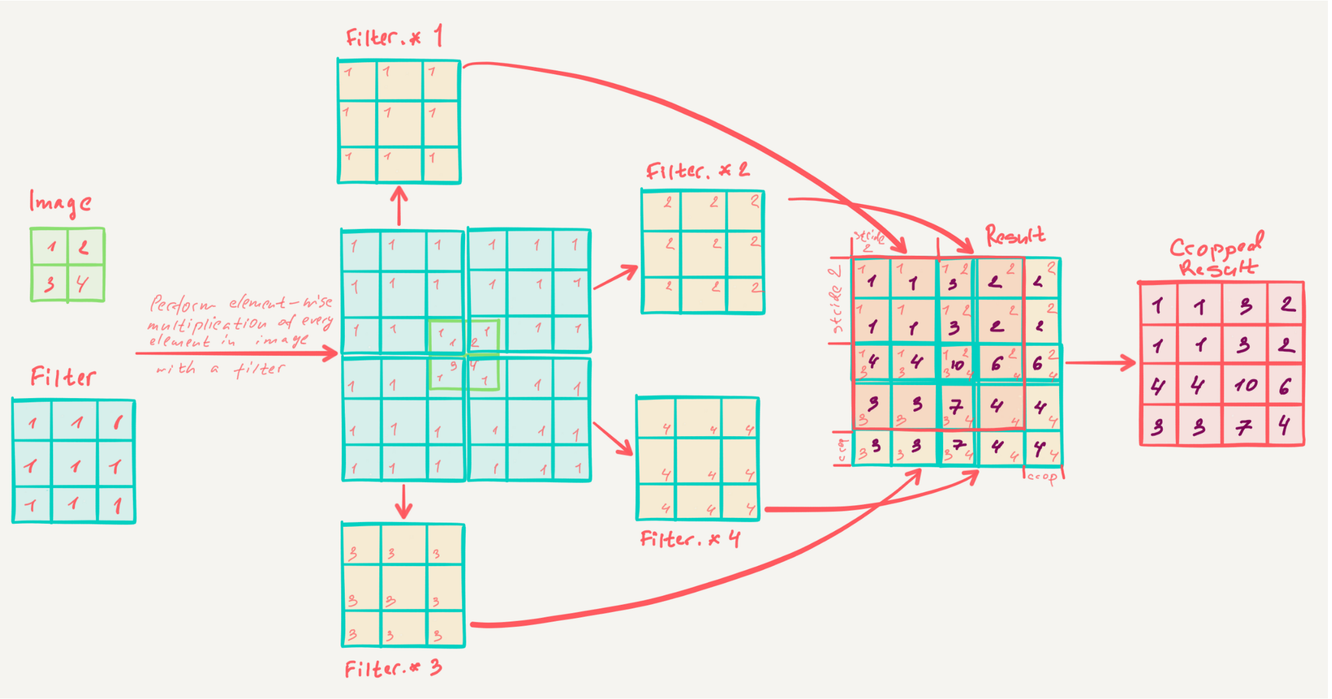
Anomaly detection

- *Once trained, an autoencoder can reproduce new inputs of the same kind of the training dataset*
  - *The distance between the input and the output will be small*
- *If presented an event of some new kind (anomaly), the encoding-decoding will tend to fail*
  - *In this circumstance, the loss (=distance between input and output) will be bigger*



Convolutional Autoencoders

- *Conv Autoencoders take images as input*
- *Through Conv and MaxPooling, they reduce it to some latent-space 1D array*
- *This 1D array is expanded using the inverse of the encoder functions*
  - *ConvTranspose (aka "Deconvolution")*
  - *Upsampling*



"Bed of Nails"

1	2
3	4

Input: 2 x 2

1	0	2	0
0	0	0	0
3	0	4	0
0	0	0	0

Output: 4 x 4

Nearest Neighbor

1	2
3	4

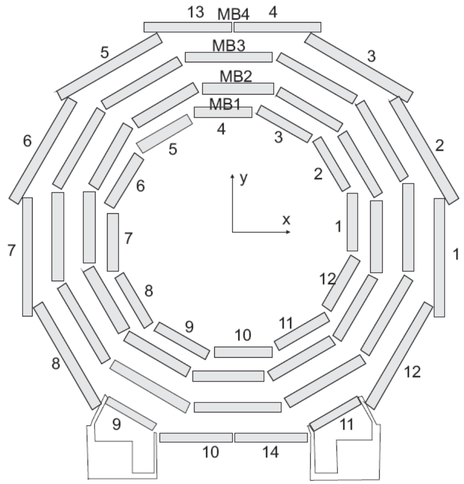
Input: 2 x 2

1	1	2	2
1	1	2	2
3	3	4	4
3	3	4	4

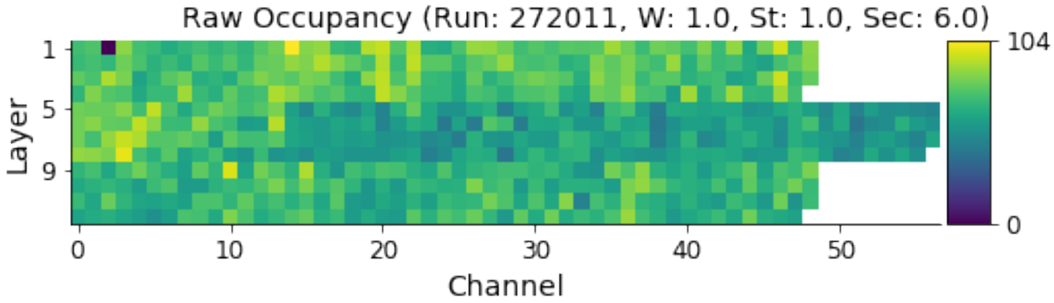
Output: 4 x 4

Example: Data Quality Monitoring

- *When taking data, >1 person watches for anomalies in the detector 24/7*
- *At this stage no global processing of the event*
- *Instead, local information from detector components available (e.g., detector occupancy in a certain time window)*



A



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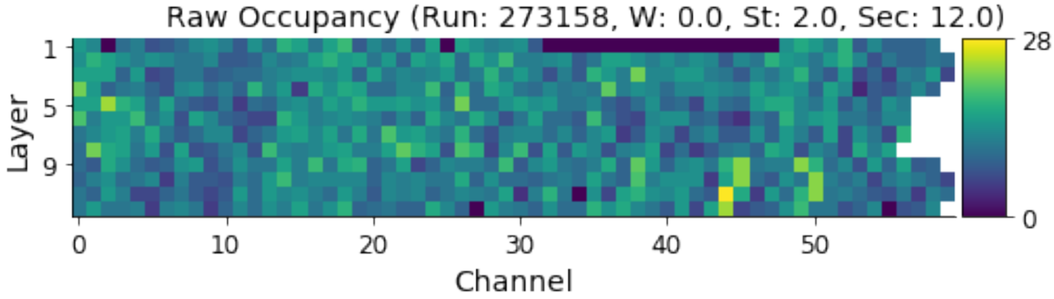

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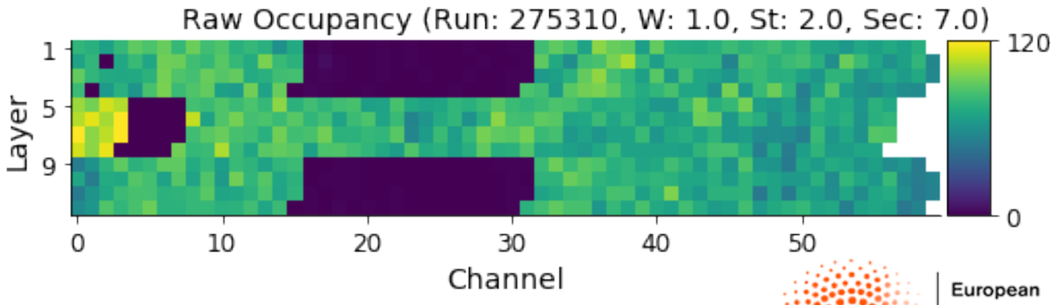
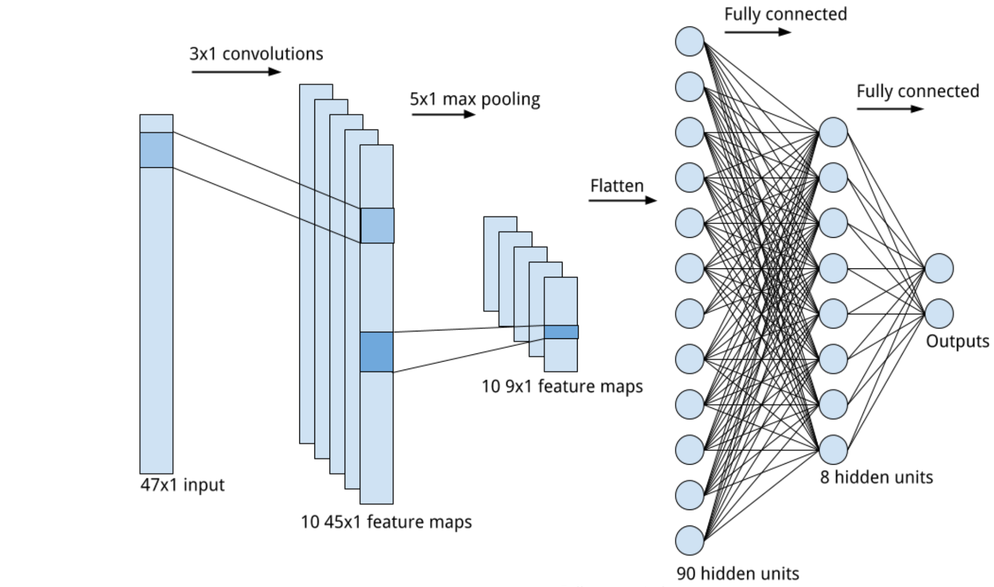


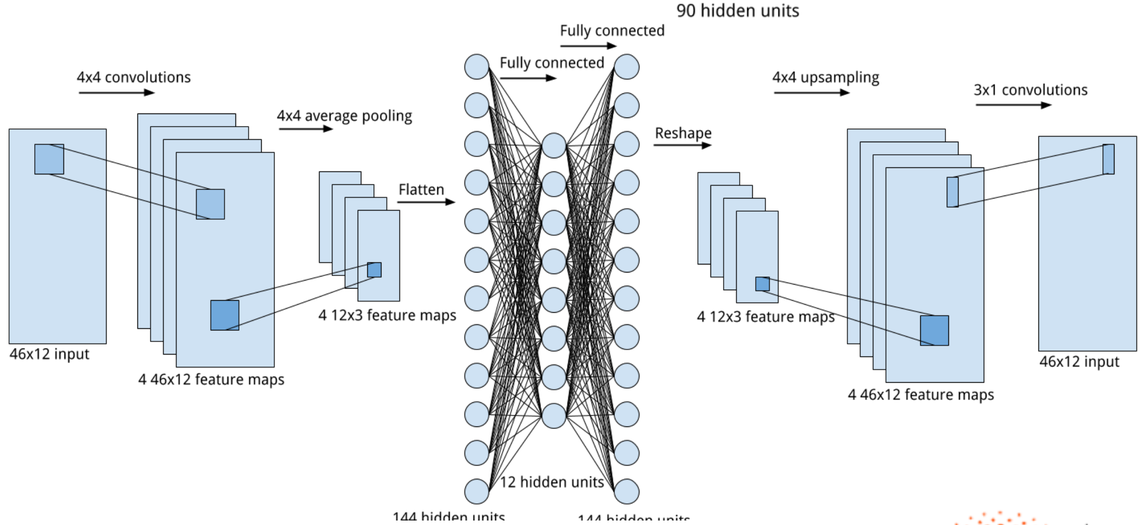
[Pol, G. Cerminara, C. Germain, MP and A. Seth arXiv:1808.00911]

Example: Data Quality Monitoring

- *Given the nature of these data, ConvNN are a natural analysis tool. Two approaches pursued*
  - *Classify good vs bad data. Works if failure mode is known*
  - *Use autoencoders to assess data "typicality". Generalises to unknown failure modes*

A. Pol et al., to appear soon





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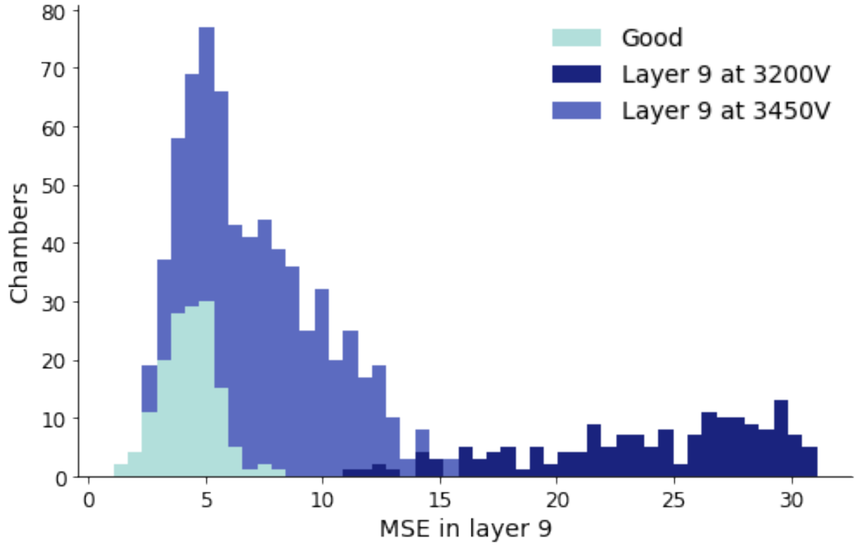

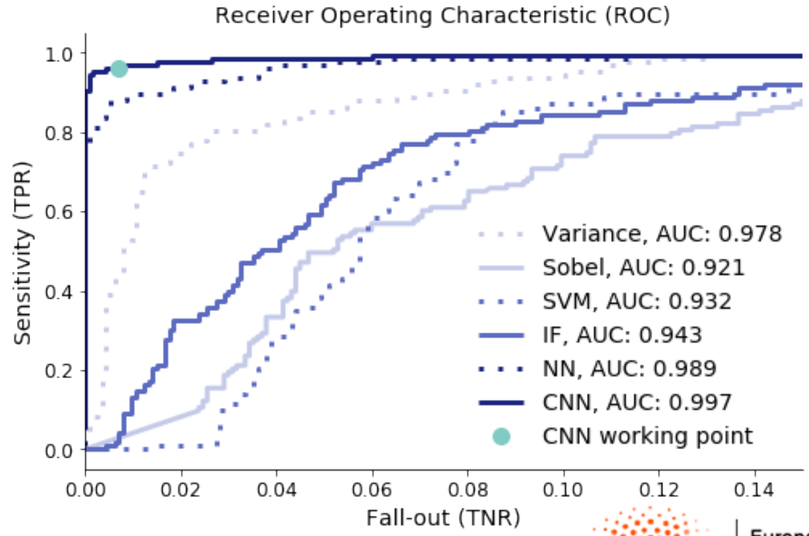

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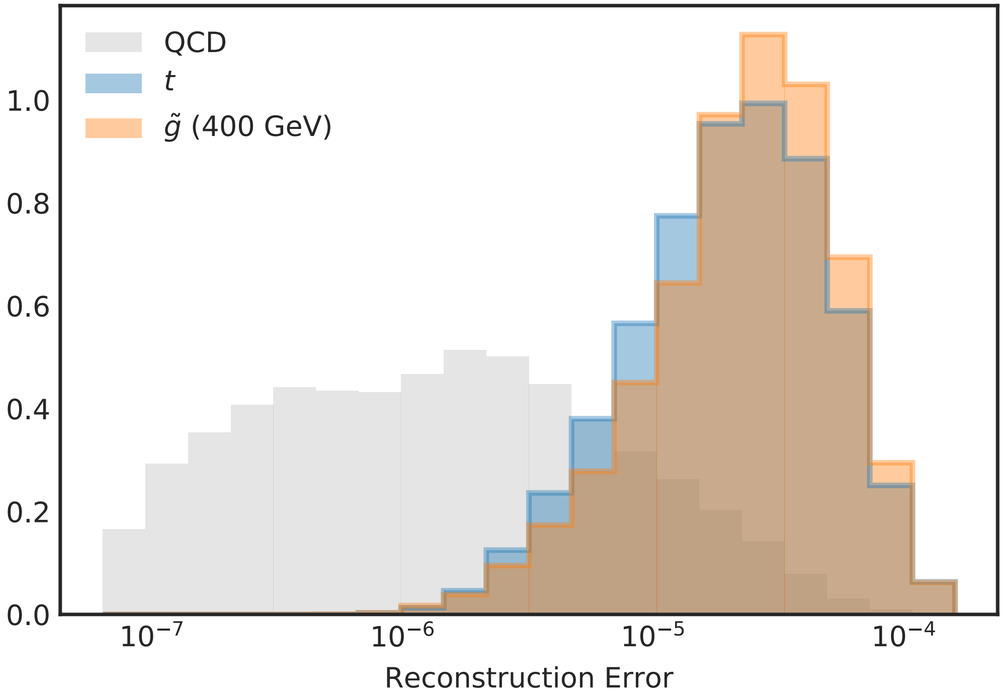
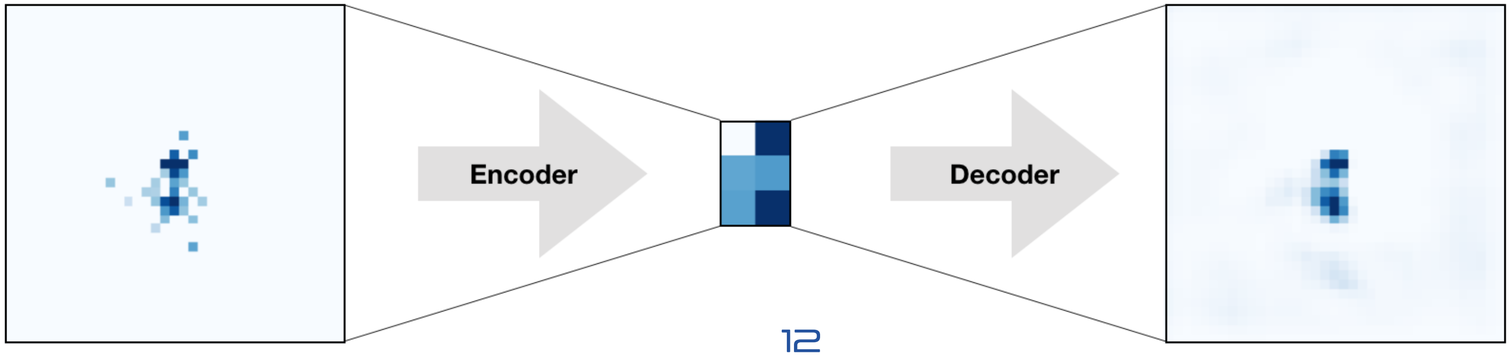
Example: Jet autoencoders

- *Idea applied to tagging jets, in order to define a QCD-jet veto*
- *Applied in a BSM search (e.g., dijet resonance) could highlight new physics signal*
- *Based on image and physics-inspired representations of jets*

Farina et al., arXiv:1808.08992

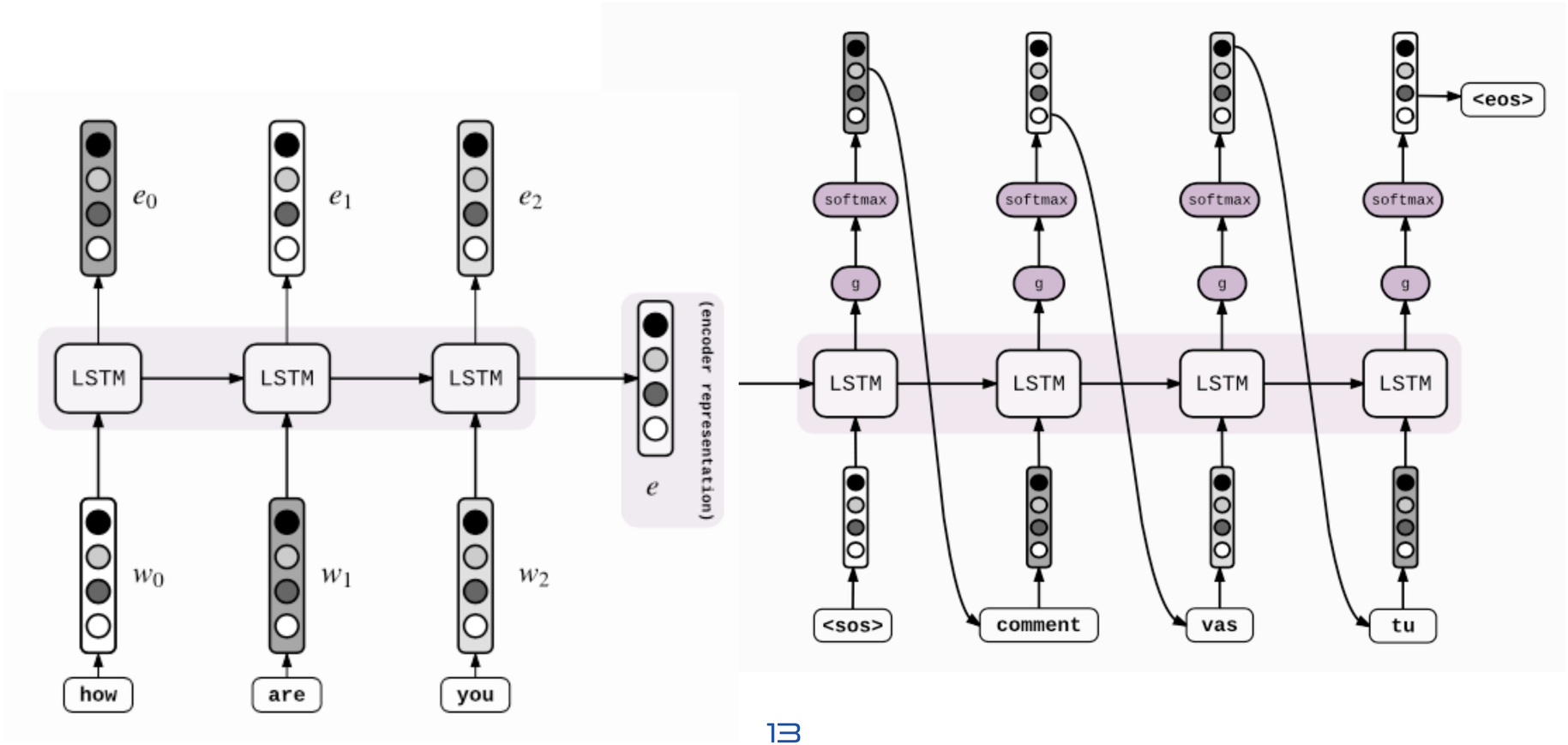
Heimel et al., arXiv:1808.08979

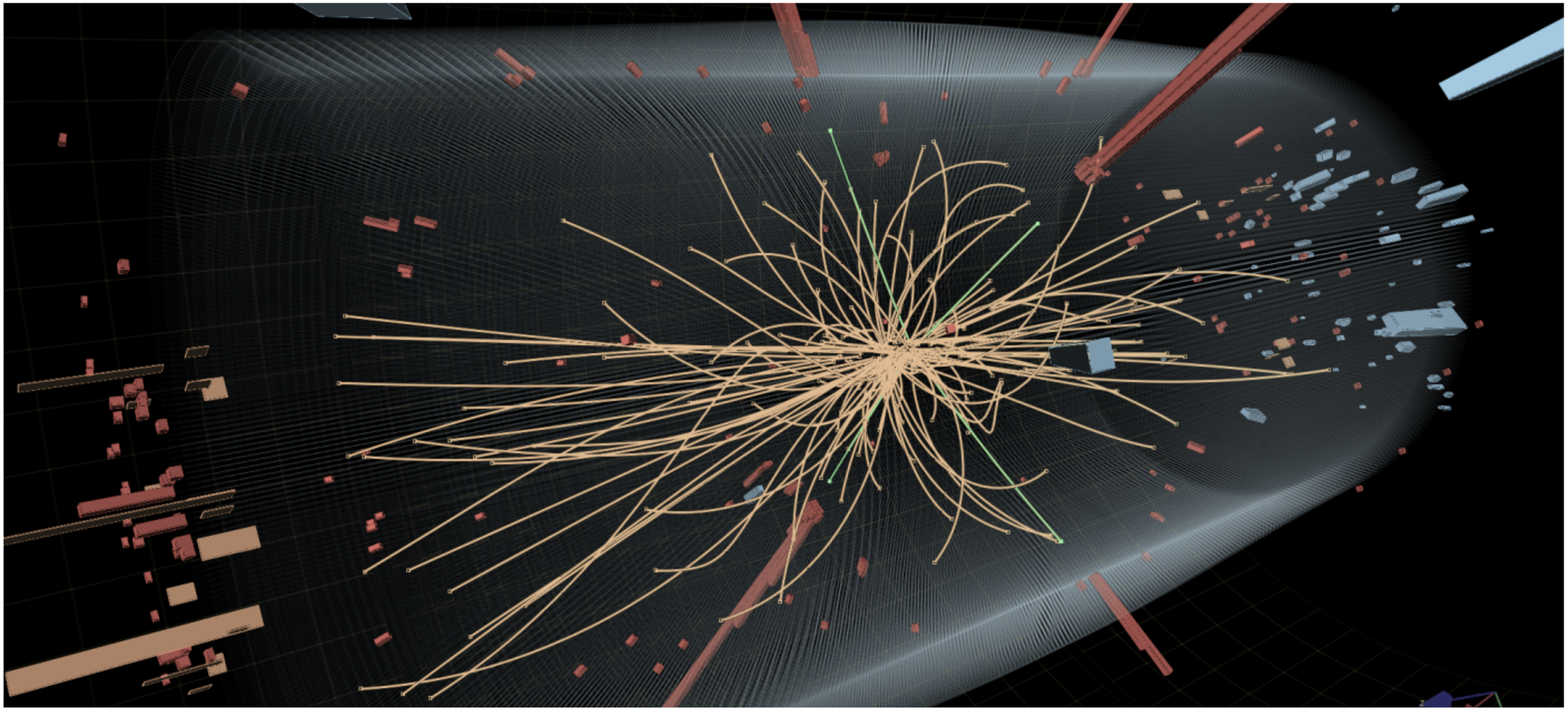




Recurrent Autoencoders

- *When given as input a sequence, the AE needs a recurrent layer to process it*
  - *The encoder is similar to the classifier we already saw*
  - *What about the decoder? This is where the serial output of the RNN comes in*





Autoencoders for New Physics searches

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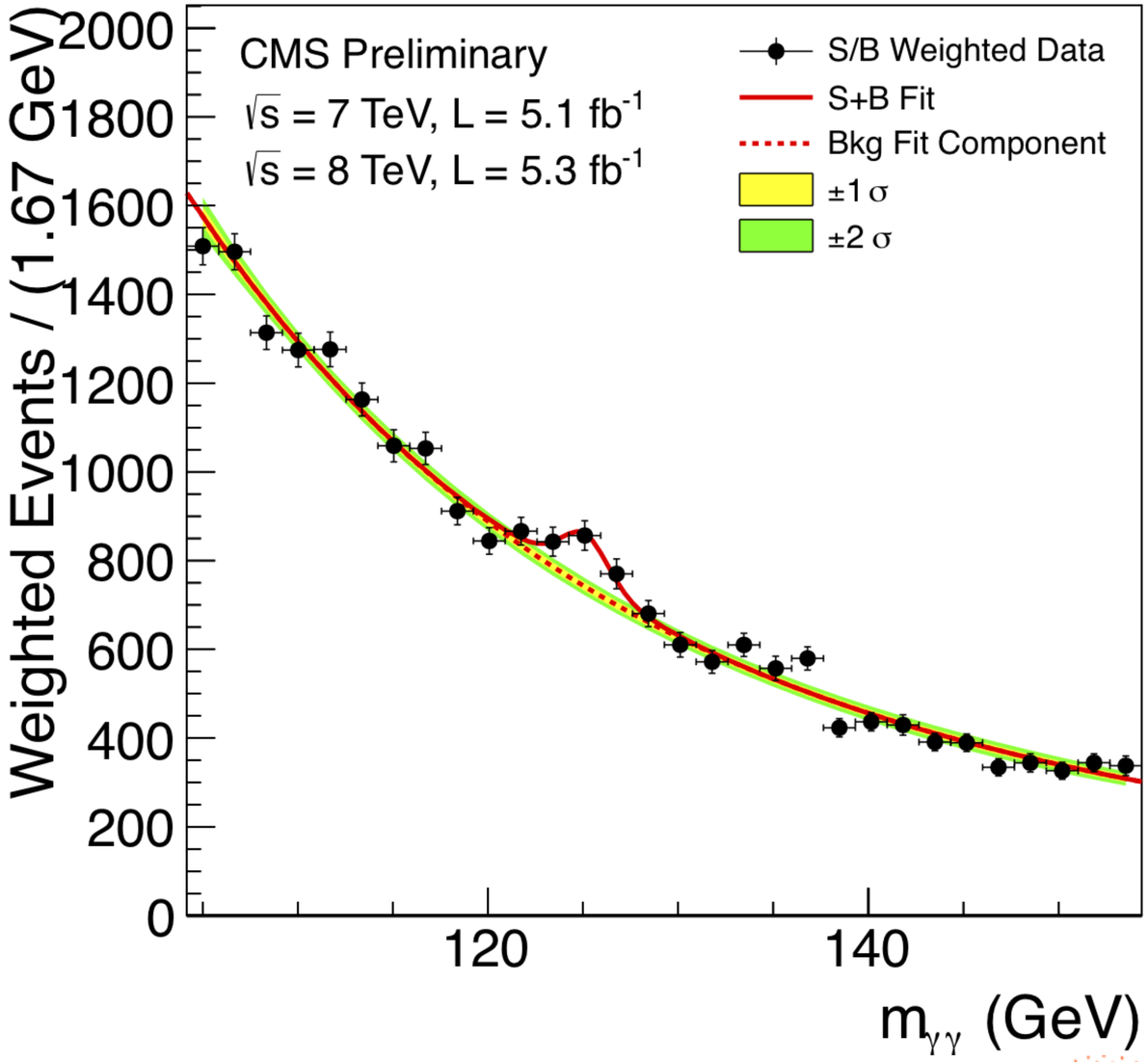
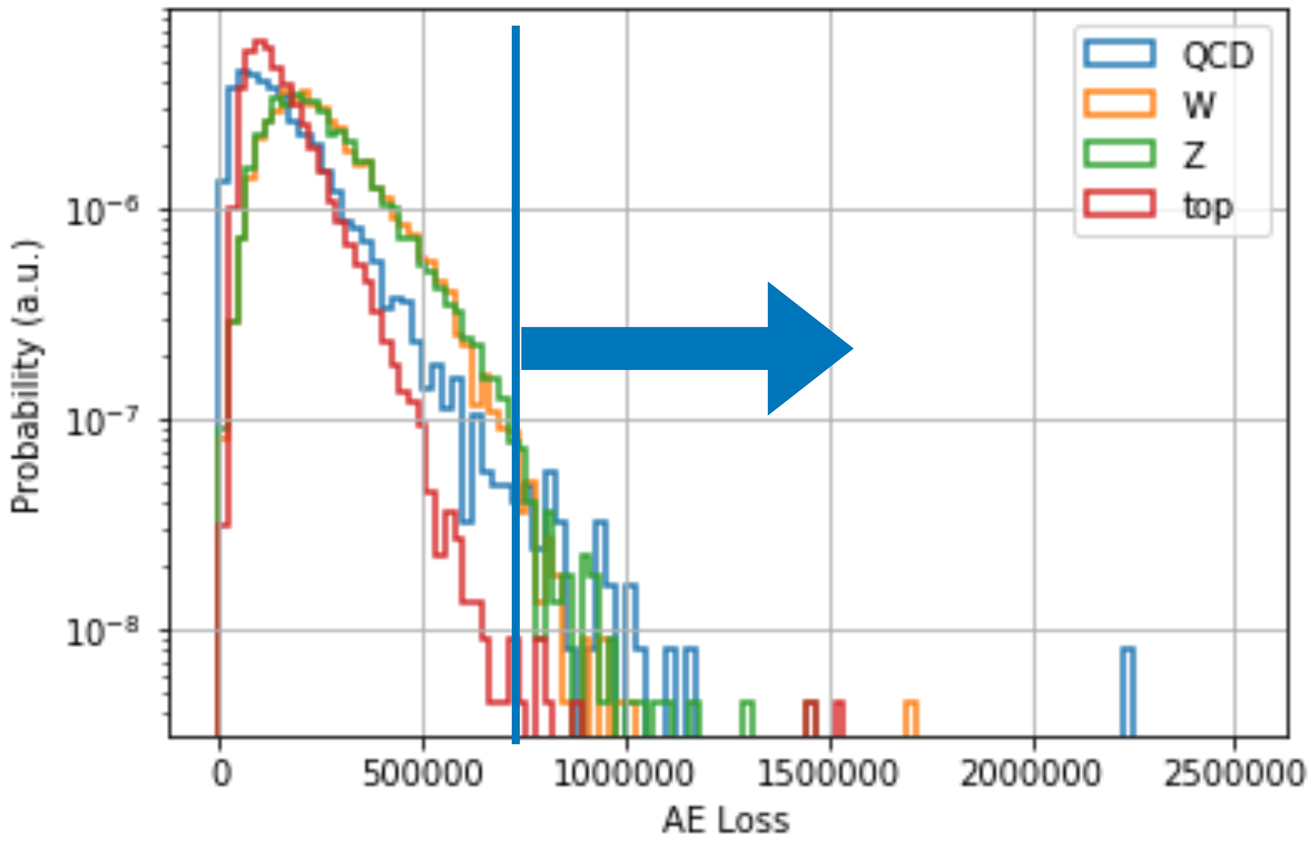
Supervised search for new physics

- *Searches for new physics are typically supervised*
  - *One knows what to look for*
  - *MC simulation provides labelled datasets to model the signal and the background*
  - *The analysis is performed as hypothesis testing*
- *The bias (what to look for) enters very early in the game (often already at trigger level). What if we are looking in the wrong place?*



Unsupervised search for new physics

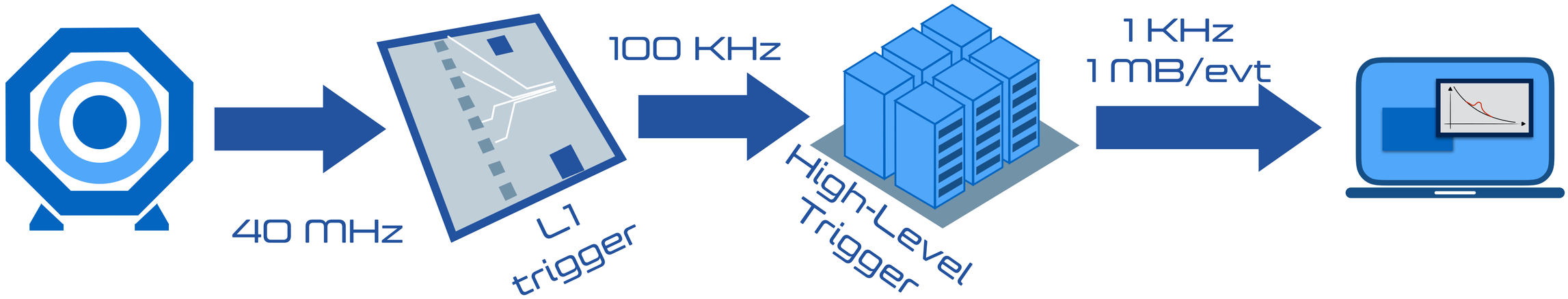
- *One can use Autoencoders to relax the assumption on the nature of new physics*
  - *Train on standard events*
  - *Run autoencoder on new events*
  - *Consider as anomalous all events with loss > threshold*



Running in the trigger

- *One needs the unsupervised algorithm to run before data are discarded*

- *This would allow to possibly notice recurrent patterns across events -> suggest explanations (new models) -> runs a classic supervised search (+ dedicated trigger) on the data to come*



Our use case: ℓ+X @HLT

- Consider a stream of data coming from L1
  - Passed L1 because of 1 lepton (e,m) with pT>23 GeV
  - At HLT, very loose isolation applied
  - Sample mainly consists of W, Z, tt & QCD (for simplicity, we ignore the rest)

Standard Model processes					
Process	Acceptance	Trigger efficiency	Cross section [nb]	Events fraction	Event /month
W	55.6%	68%	58	59.2%	110M
QCD	0.08%	9.6%	$1.6 \cdot 10^5$	33.8%	63M
Z	16%	77%	20	6.7%	12M
$t\bar{t}$	37%	49%	0.7	0.3%	0.6M

  - We consider 21 features, typically highlighting the difference between these SM processes (no specific BSM signal in mind)

- The isolated-lepton transverse momentum p_T^ℓ.
- The three isolation quantities (ChPFIso, NeuPFIso, GammaPFIso) for the isolated lepton, computed with respect to charged particles, neutral hadrons and photons, respectively.
- The lepton charge.
- A boolean flag (isEle) set to 1 when the trigger lepton is an electron, 0 otherwise.
- S_T, i.e. the scalar sum of the p_T of all the jets, leptons, and photons in the event with $p_T > 30$ GeV and $|\eta| < 2.6$. Jets are clustered from the reconstructed PF candidates, using the FASTJET [23] implementation of the anti-k_T jet algorithm [24], with jet-size parameter R=0.4.
- The number of jets entering the S_T sum (N_J).
- The invariant mass of the set of jets entering the S_T sum (M_J).
- The number of these jets being identified as originating from a b quark (N_b).
- The missing transverse momentum, decomposed into its parallel ($p_{T,\parallel}^{\text{miss}}$) and orthogonal ($p_{T,\perp}^{\text{miss}}$) components with respect to the isolated lepton direction. The missing transverse momentum is defined as the negative sum of the PF-candidate p_T vectors:

$$\vec{p}_T^{\,\text{miss}} = -\sum_q \vec{p}_T^{\,q} \,. \tag{2}$$

- The transverse mass, M_T, of the isolated lepton ℓ and the E_T^{miss} system, defined as:

$$M_T = \sqrt{2 p_T^\ell E_T^{\text{miss}} (1 - \cos\Delta\phi)} \,, \tag{3}$$

  with $\Delta\phi$ the azimuth separation between the lepton and $\vec{p}_T^{\,\text{miss}}$ vector, and E_T^{miss} the absolute value of $\vec{p}_T^{\,\text{miss}}$.
- The number of selected muons (N_μ).
- The invariant mass of this set of muons (M_μ).
- The total transverse momentum of these muons ($p_{T,TOT}^{\mu}$).
- The number of selected electrons (N_e).
- The invariant mass of this set of electrons (M_e).
- The total transverse momentum of these electrons ($p_{T,TOT}^{e}$).
- The number of reconstructed charged hadrons.
- The number of reconstructed neutral hadrons.

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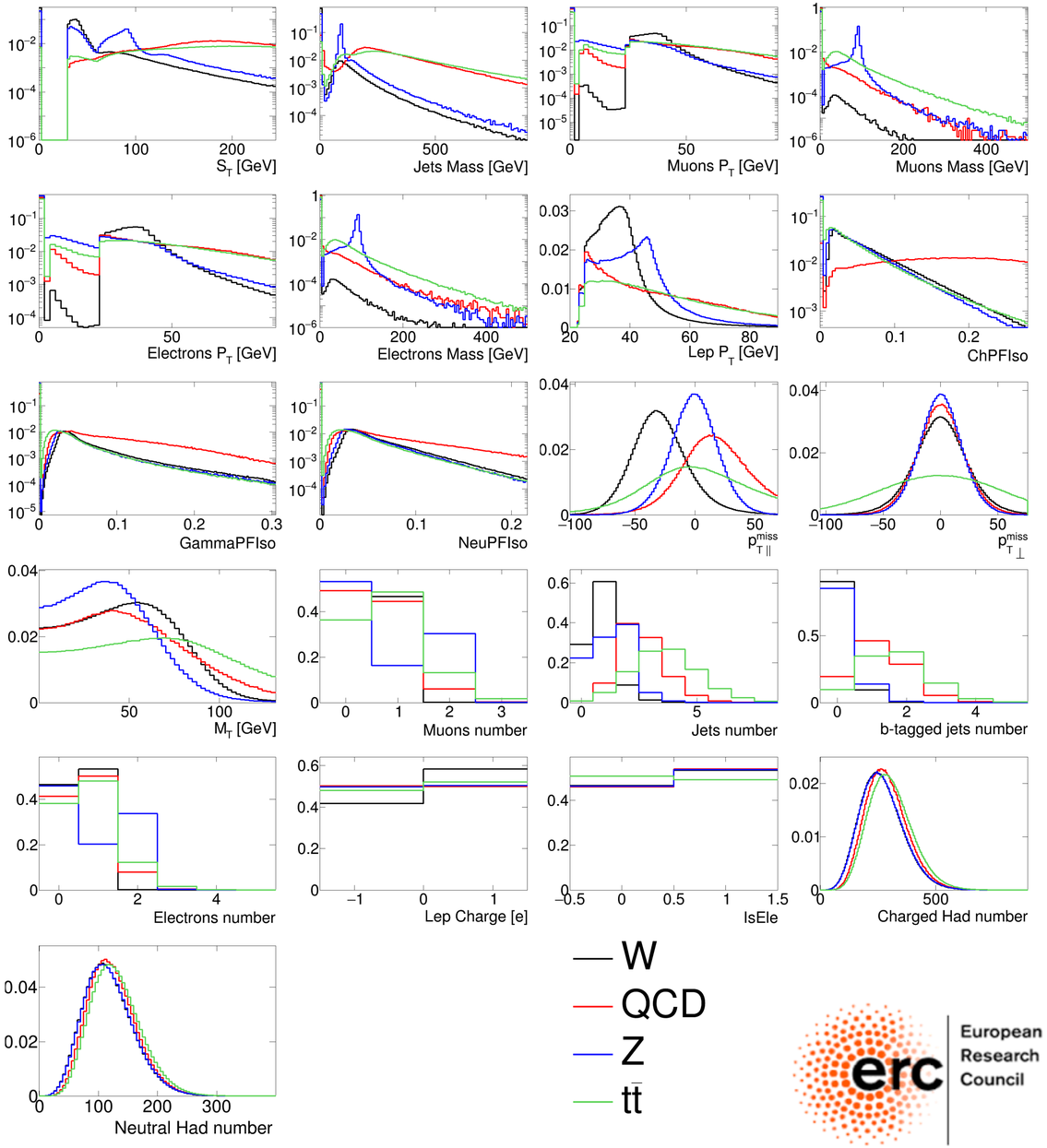
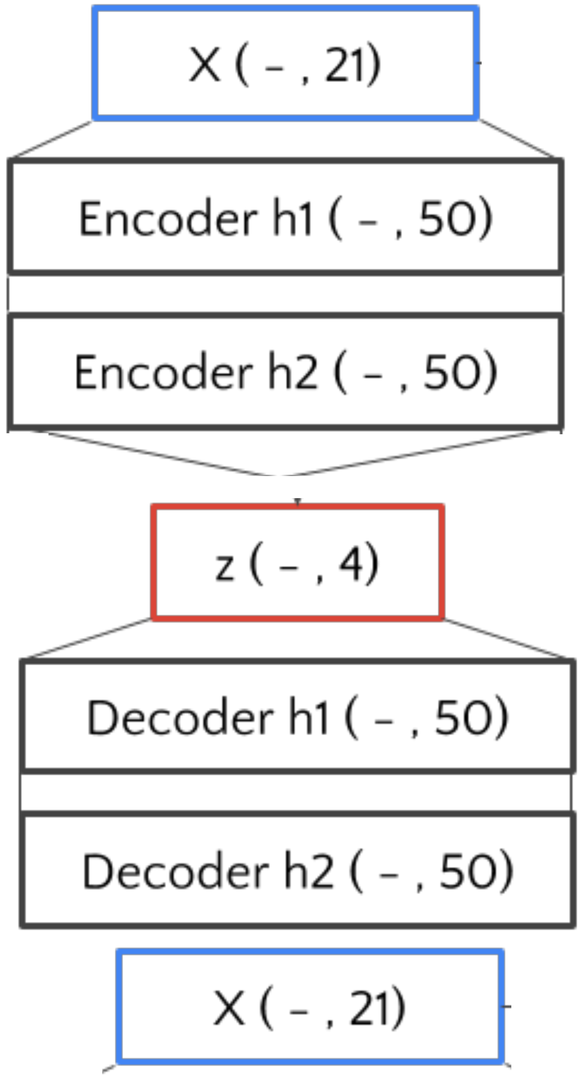


Standard Model AE

- *We train a VAE on a cocktail of SM events (weighted by xsec)*
- ***ENCODER:*** *21 inputs, 2 hidden layers → 4Dim latent space*
- ***DECODER:*** *from a random sample in the 4D space → 2 hidden layers → 21 outputs*

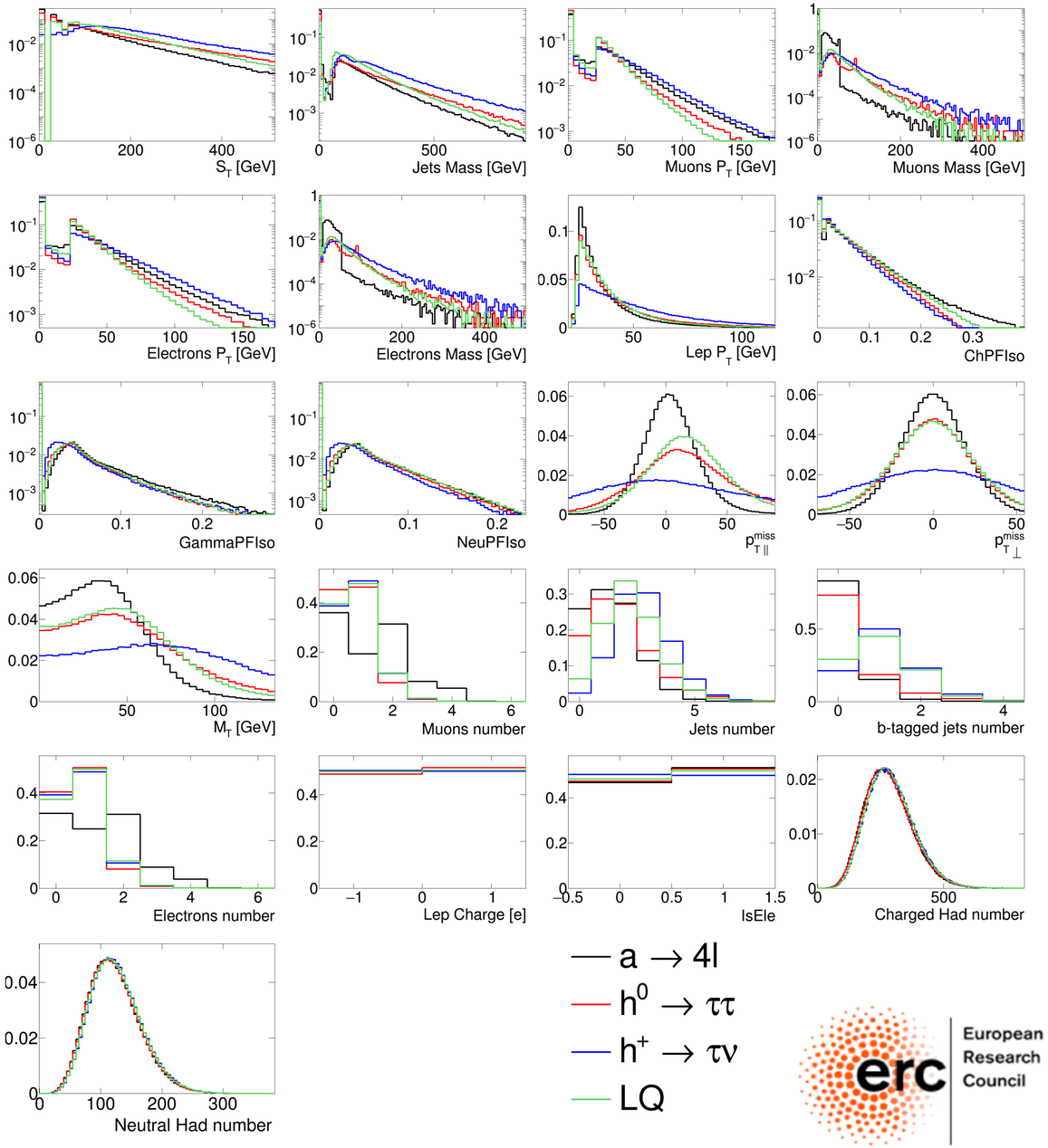


Some BSM benchmark

- *We consider four BSM benchmark models, to give some sense of VAEs potential*
  - *leptoquark with mass 80 GeV, LQ→bτ*
  - *A scalar boson with mass 50 GeV, a→Z*Z*→4ℓ*
  - *A scalar scalar boson with mass 60 GeV, h→ττ*
  - *A charged scalar boson with mass 60 GeV, h±→τν*

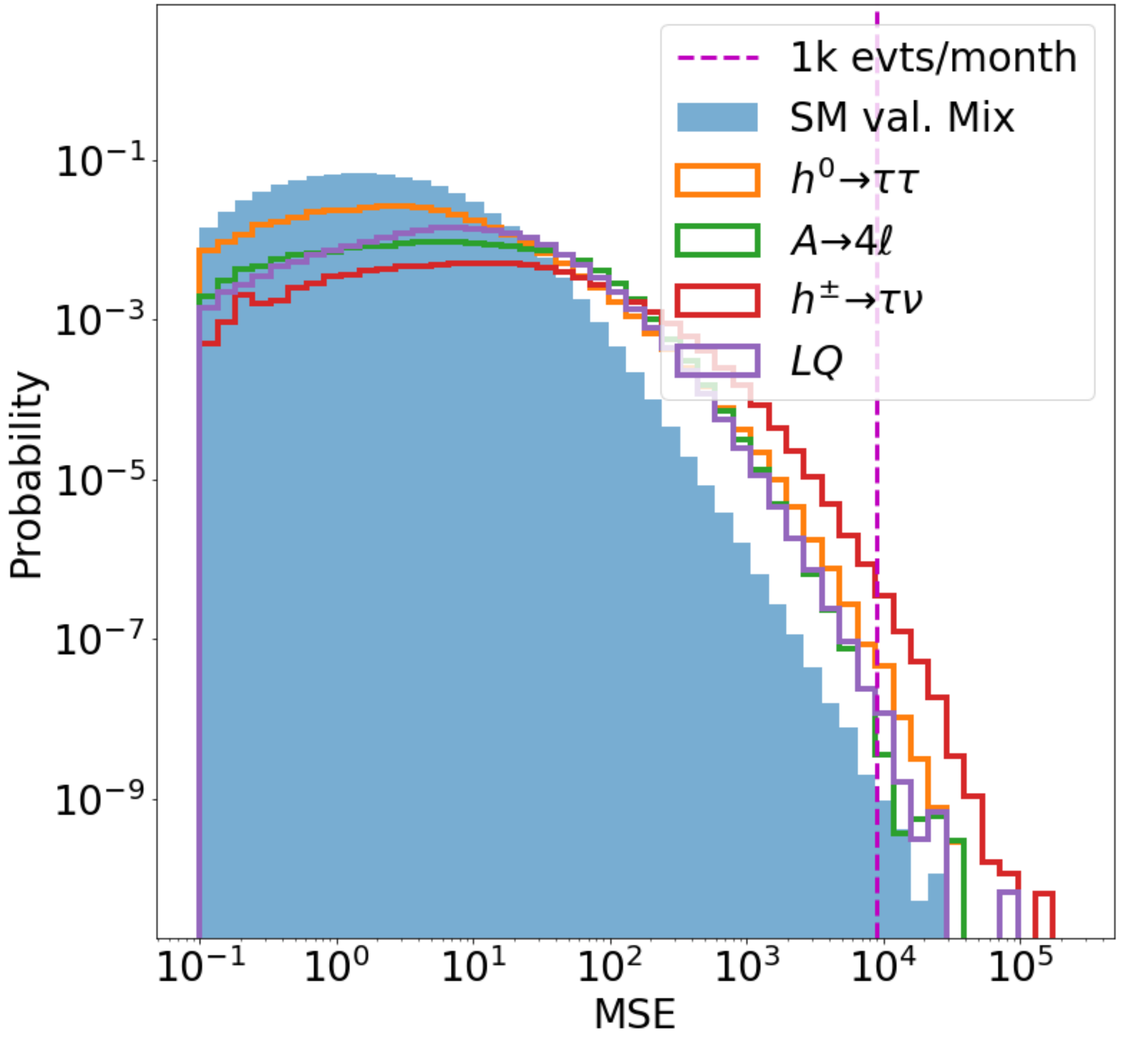
BSM benchmark processes

Process	Acceptance	Trigger efficiency	Total efficiency	Cross-section 100 events/month
$h^0 \to \tau\tau$	9%	70%	6%	335 fb
$h^0 \to \tau\nu$	18%	69%	12%	163 fb
$LQ \to b\tau$	19%	62%	12%	166 fb
$a \to 4\ell$	5%	98%	5%	436 fb



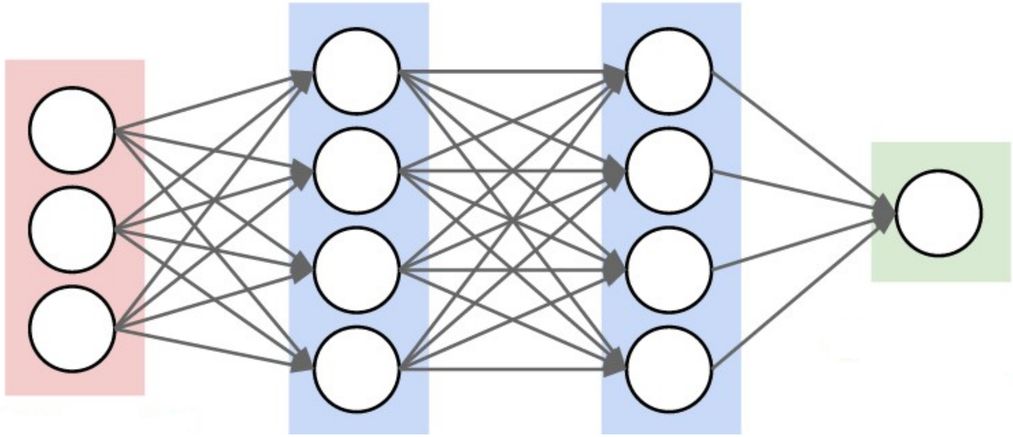
Defining anomaly

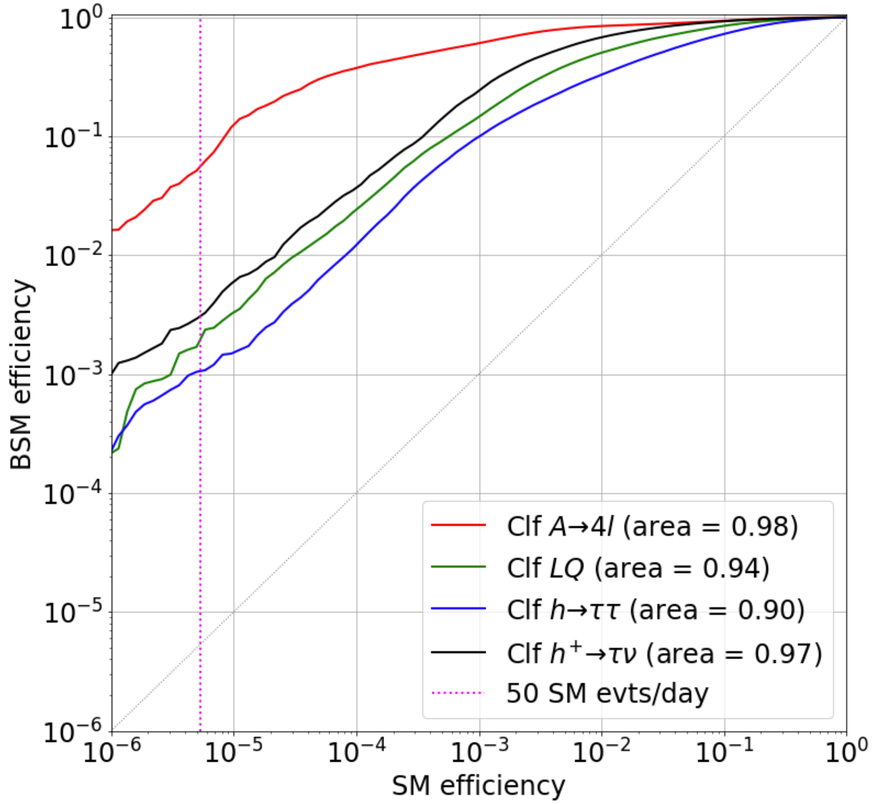
- *Anomaly defined as a p-value threshold on a given test statistics*
  - *Loss function an obvious choice*
  - *Some part of a loss could be more sensitive than others*
  - *We tested different options and found the total loss to behave better*



Benchmark comparison

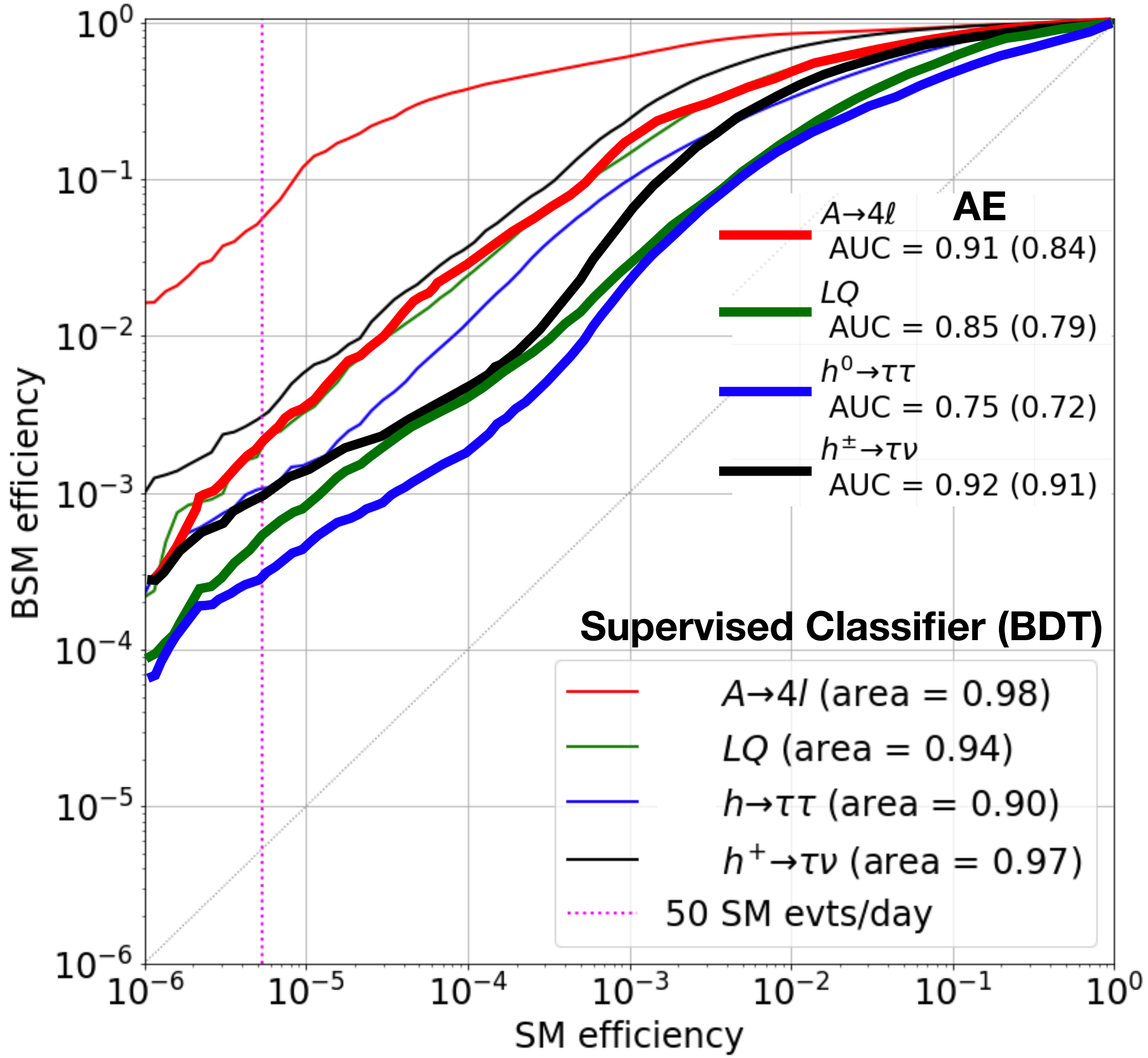
- *VAE's performances benchmarked against supervised classifiers*
- *For each BSM model*
  - *take same inputs as VAE*
  - *train a fully-supervised classifier to separate signal from background*
  - *use supervised performances as a reference to aim to with the unsupervised approach*
  - *Done for our 4 BSM models using dense neural networks*

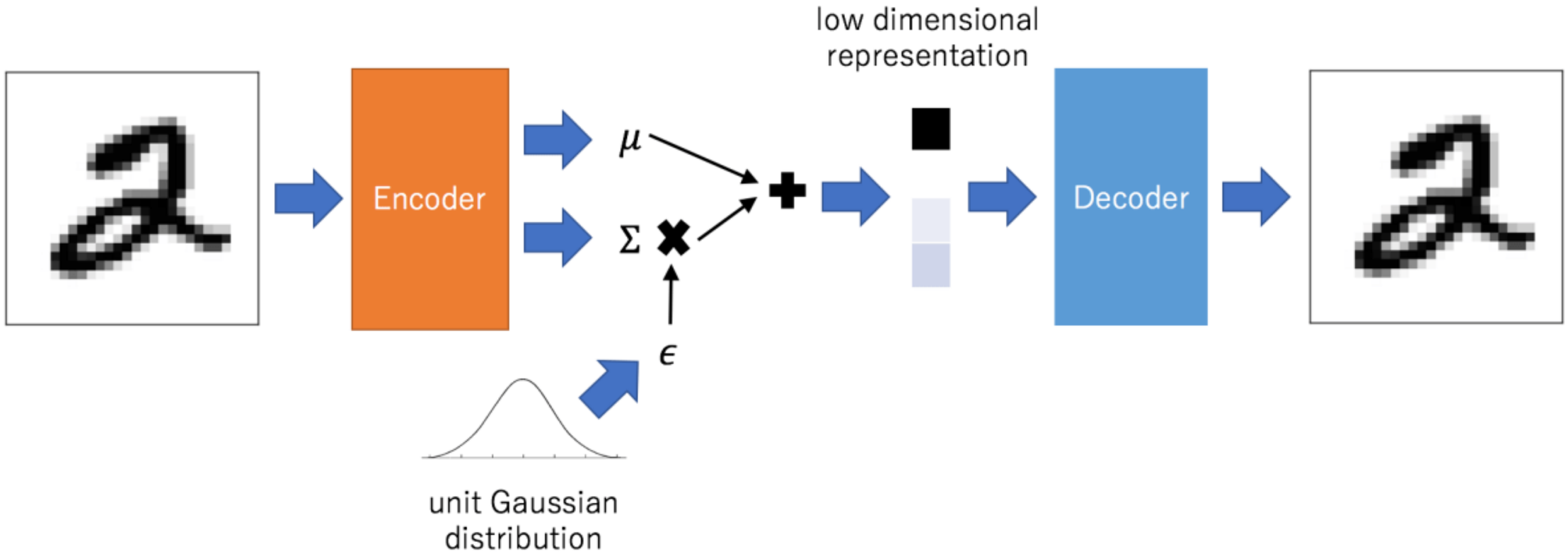




Performances

- *Evaluate general discrimination power by ROC curve and area under curve (AUC)*
  - *clearly worse than supervised*
  - *but not so far*
- *Fixing SM acceptance rate at 50 events/day*
  - *competitive results considering unsupervised nature of the algorithm*

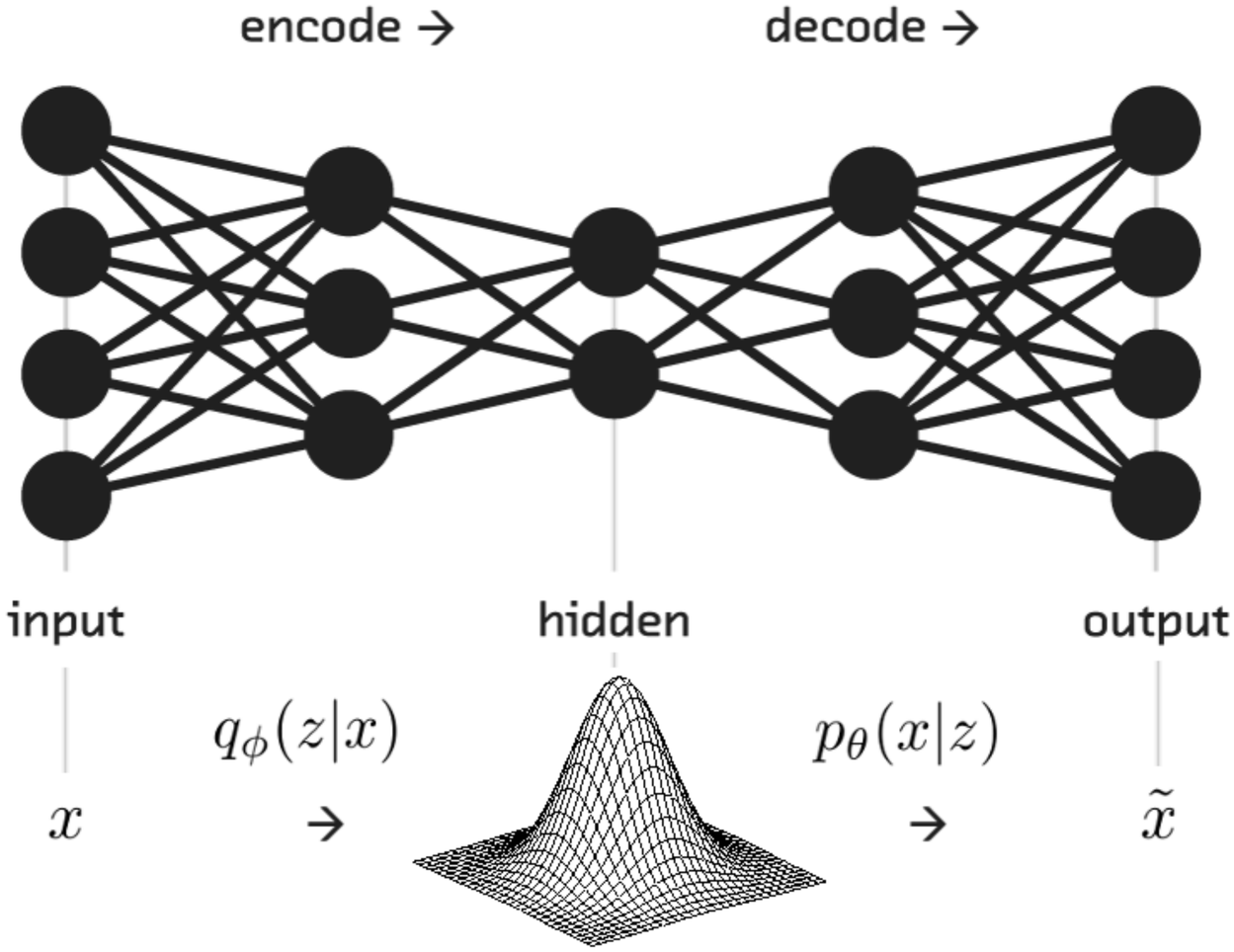




Variational Autoencoders

Variational Autoencoders

- *We investigated variational autoencoders*
- *Unlike traditional AEs, VAEs try to associate a multi-Dim pdf to a given image*
  - *can be used to generate new examples*
  - *comes with a probabilistic description of the input*
  - *tends to work better than traditional AEs*



The Loss Function

- Loss function described as the sum of two terms (scaled by a tuned λ parameter that makes the two contribution numerically similar)
  - Reconstruction loss (e.g. MSE(output-input))
  - KL loss: distance between Gaussian pdfs (assumption on prior here)
  - Why Gaussian? KL loss can be written analytically

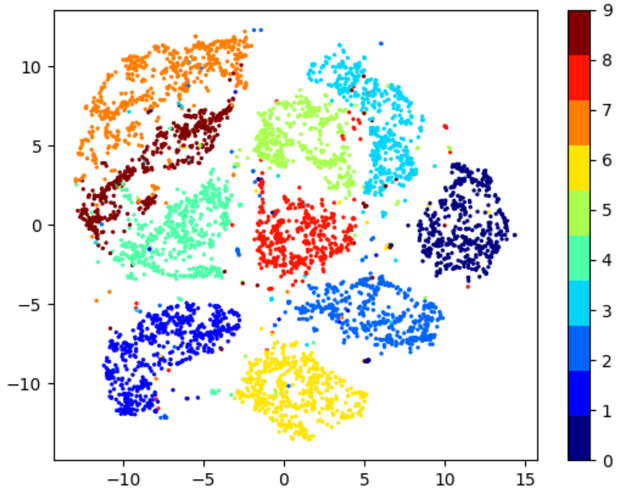
$$\mathrm{Loss}_{\mathrm{Tot}} = \mathrm{Loss}_{\mathrm{reco}} + \beta D_{\mathrm{KL}}$$

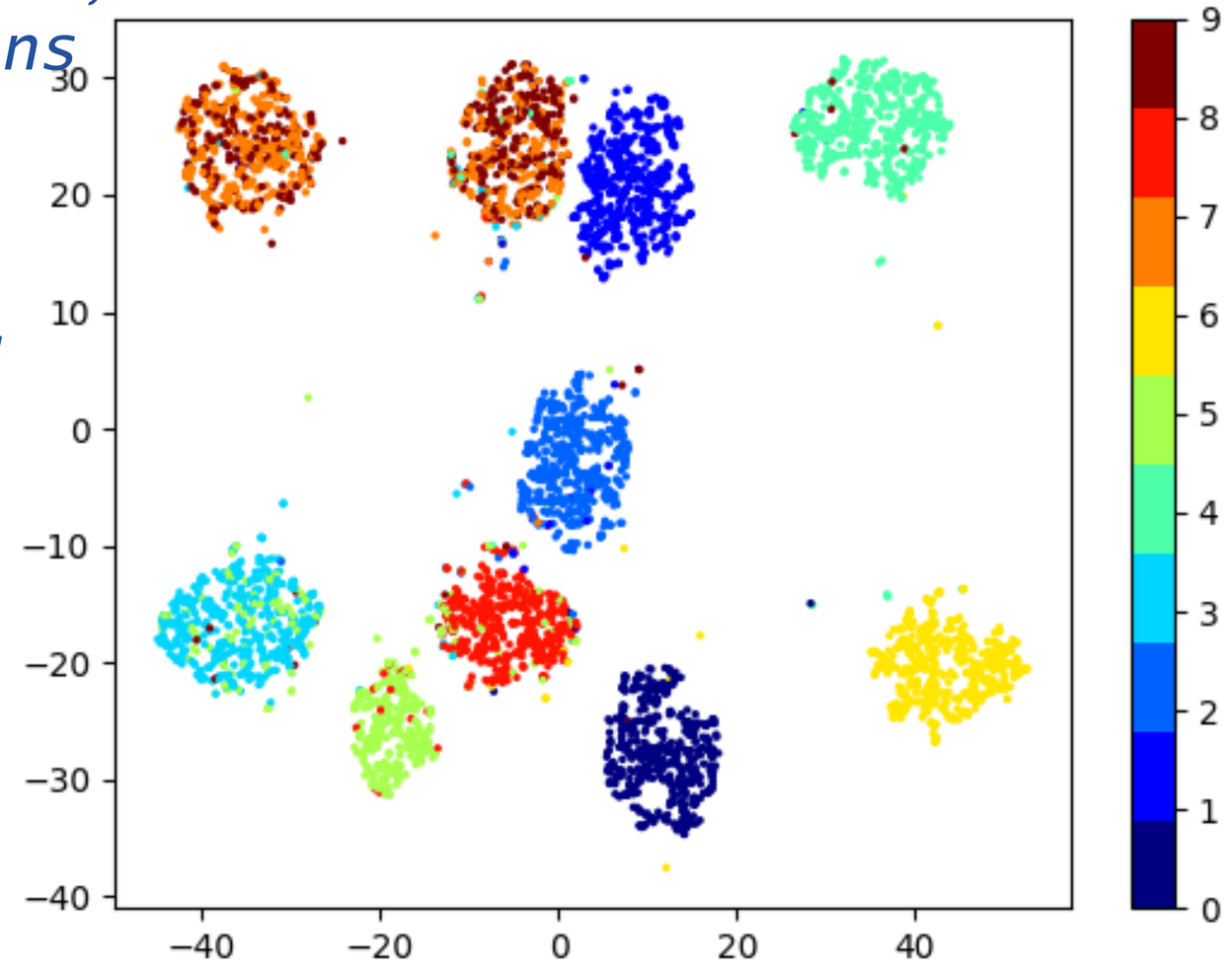
$$D_{\mathrm{KL}} = \frac{1}{k}\sum_i D_{\mathrm{KL}}\left(N(\mu_z^i, \sigma_z^i) \;||\; N(\mu_P, \sigma_P)\right)$$

$$= \frac{1}{2k}\sum_{i,j}\left(\sigma_P^j \sigma_z^{i,j}\right)^2 + \left(\frac{\mu_P^j - \mu_z^{i,j}}{\sigma_P^j}\right)^2 + \ln\frac{\sigma_P^j}{\sigma_z^{i,j}} - 1$$

Clustering with VAE

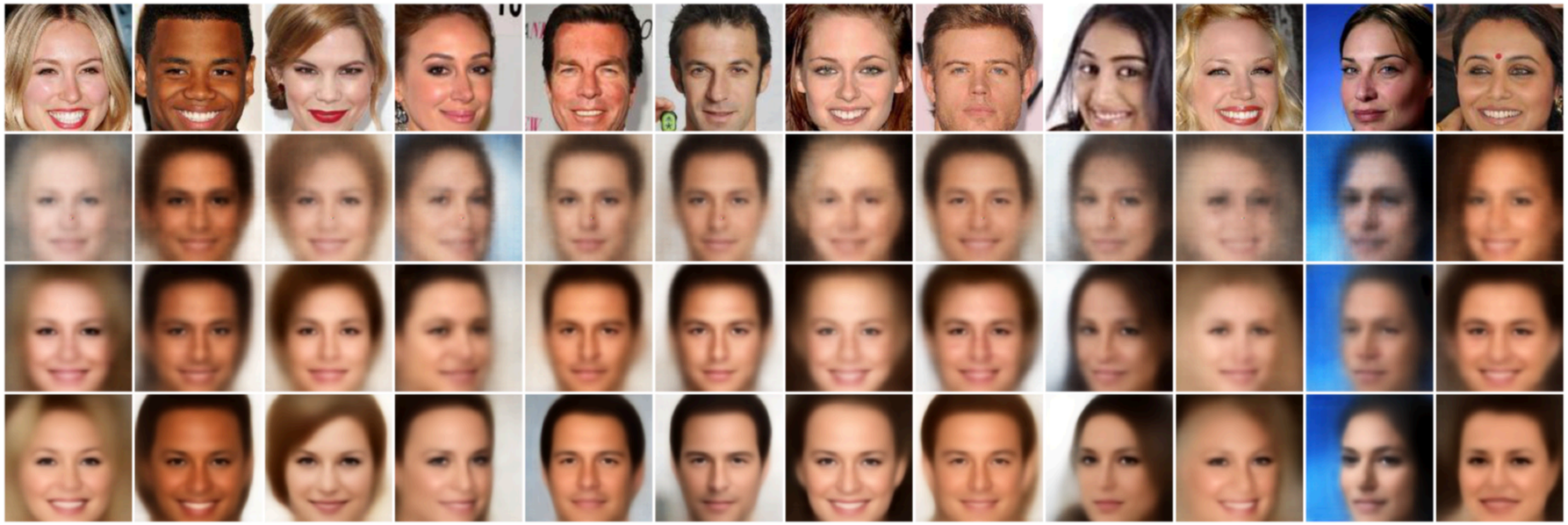
- *In the clustering example, the different populations are forced on sums of Gaussian distributions*
- *This gives more regular shape for the clusters*



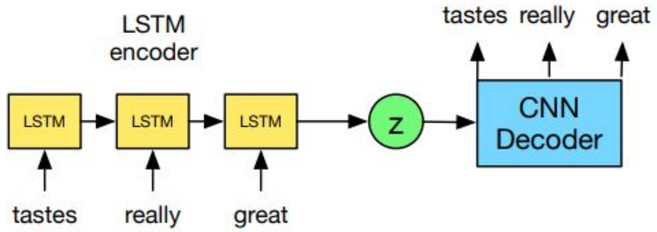


A Generative model

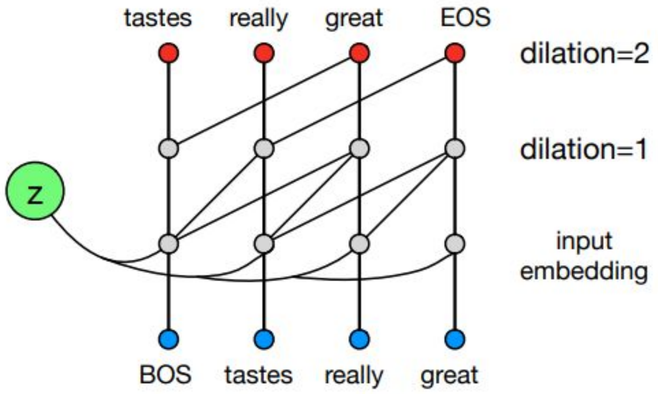
- *Now that we have a probabilistic description of the latent space, we can sample points from it*
- *These points, propagated through the decoder, will provide new examples*
- *We have defined a generative model*



More effective with sequential data

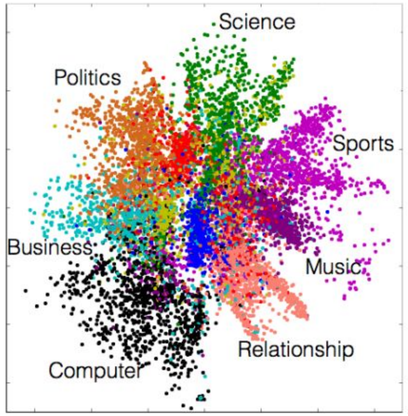


(a) VAE training graph using a dilated CNN decoder.

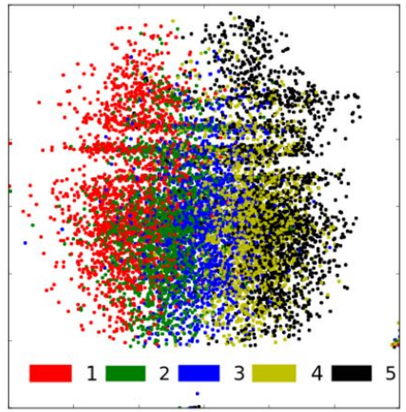


(b) Digram of dilated CNN decoder.

1 star	the food was good but the service was horrible . took forever to get our food . we had to ask twice for our check after we got our food . will not return .
2 star	the food was good , but the service was terrible . took forever to get someone to take our drink order . had to ask 3 times to get the check . food was ok , nothing to write about .
3 star	came here for the first time last night . food was good . service was a little slow . food was just ok .
4 star	food was good , service was a little slow , but the food was pretty good . i had the grilled chicken sandwich and it was really good . will definitely be back !
5 star	food was very good , service was fast and friendly . food was very good as well . will be back !



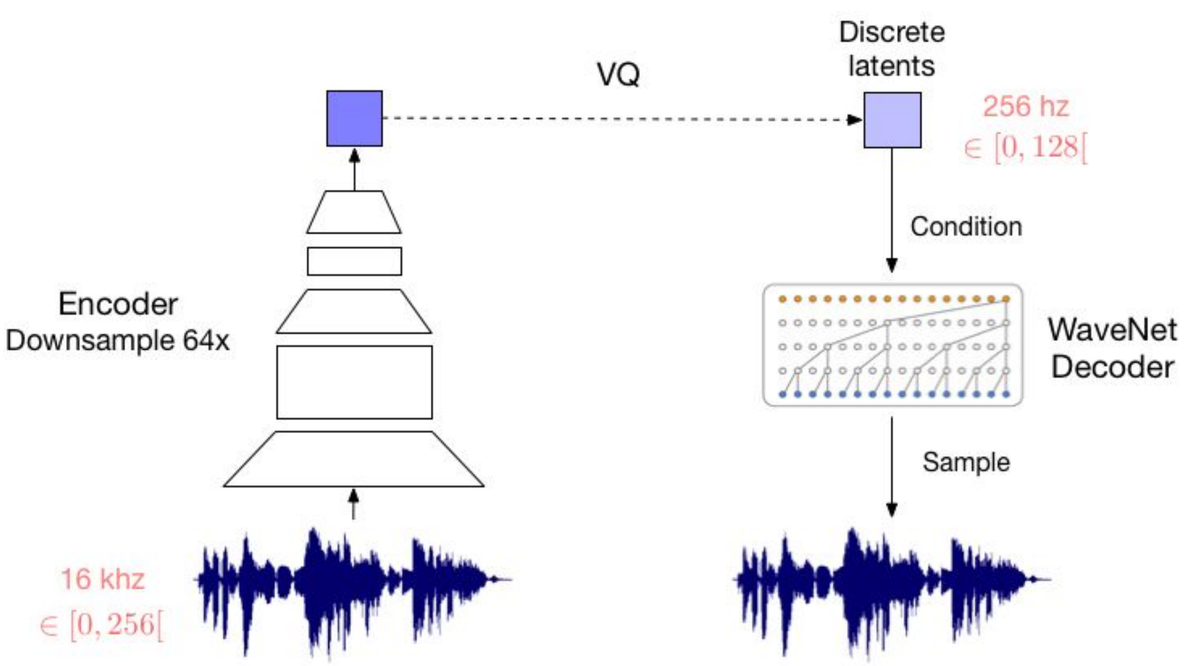
(a) Yahoo



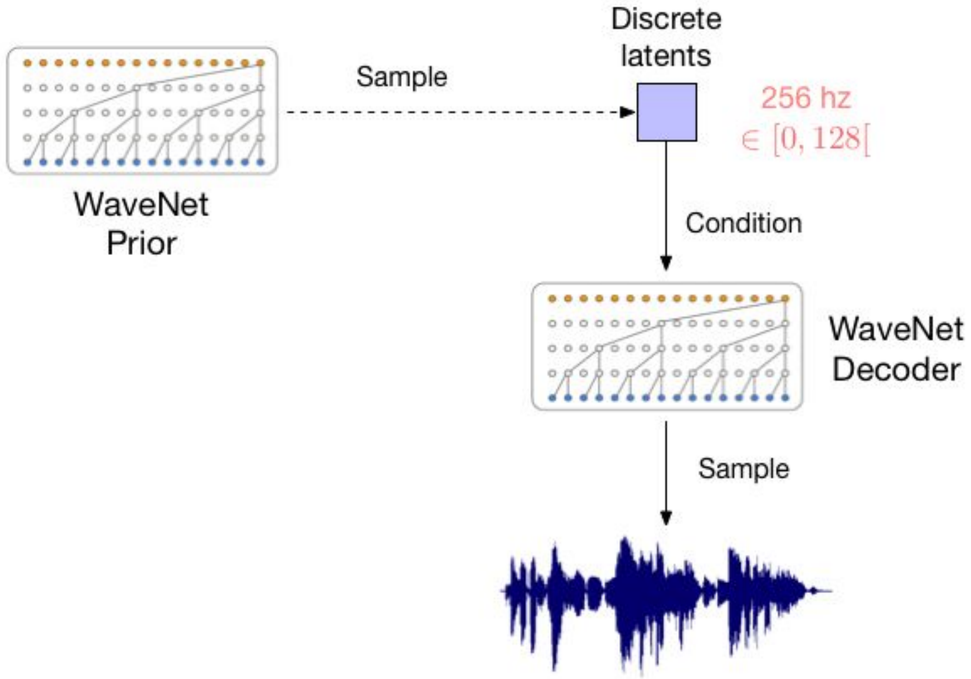
(b) Yelp

Yang, Z., Hu, Z., Salakhutdinov, R., & Berg-Kirkpatrick, T. (2017). Improved variational autoencoders for text modeling using dilated convolutions. *ICML 2017*

More effective with sequential data



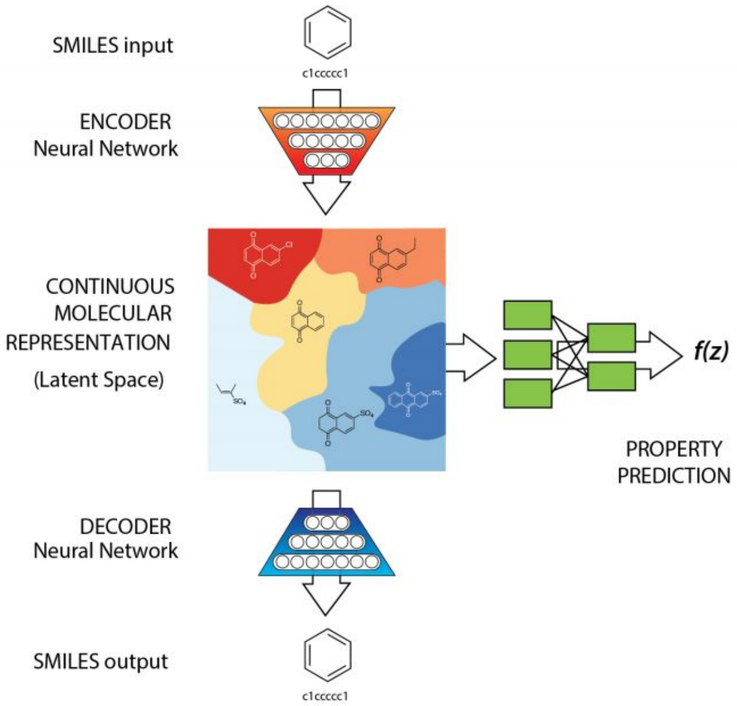
reconstruction

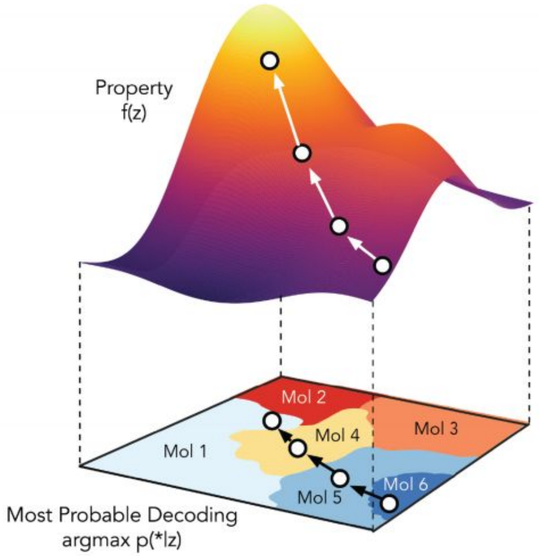


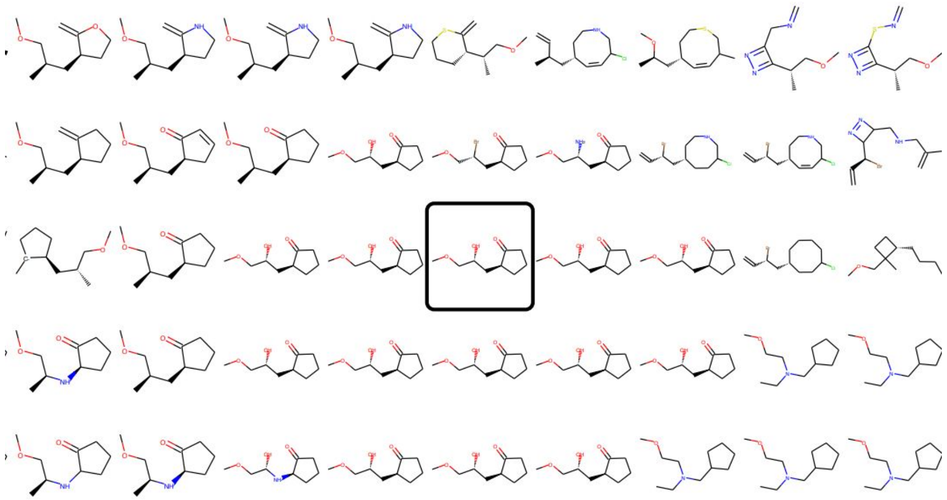
generation

van den Oord, A., & Vinyals, O. (2017). Neural discrete representation learning. *NIPS 2017*.

More effective with sequential data







Gómez-Bombarelli, R., et al. (2018). Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules ACS Cent.

Kusner, M. J., Paige, B., & Hernández-Lobato, J. M. (2017). Grammar variational autoencoder. *arXiv preprint arXiv:1703.01925*.

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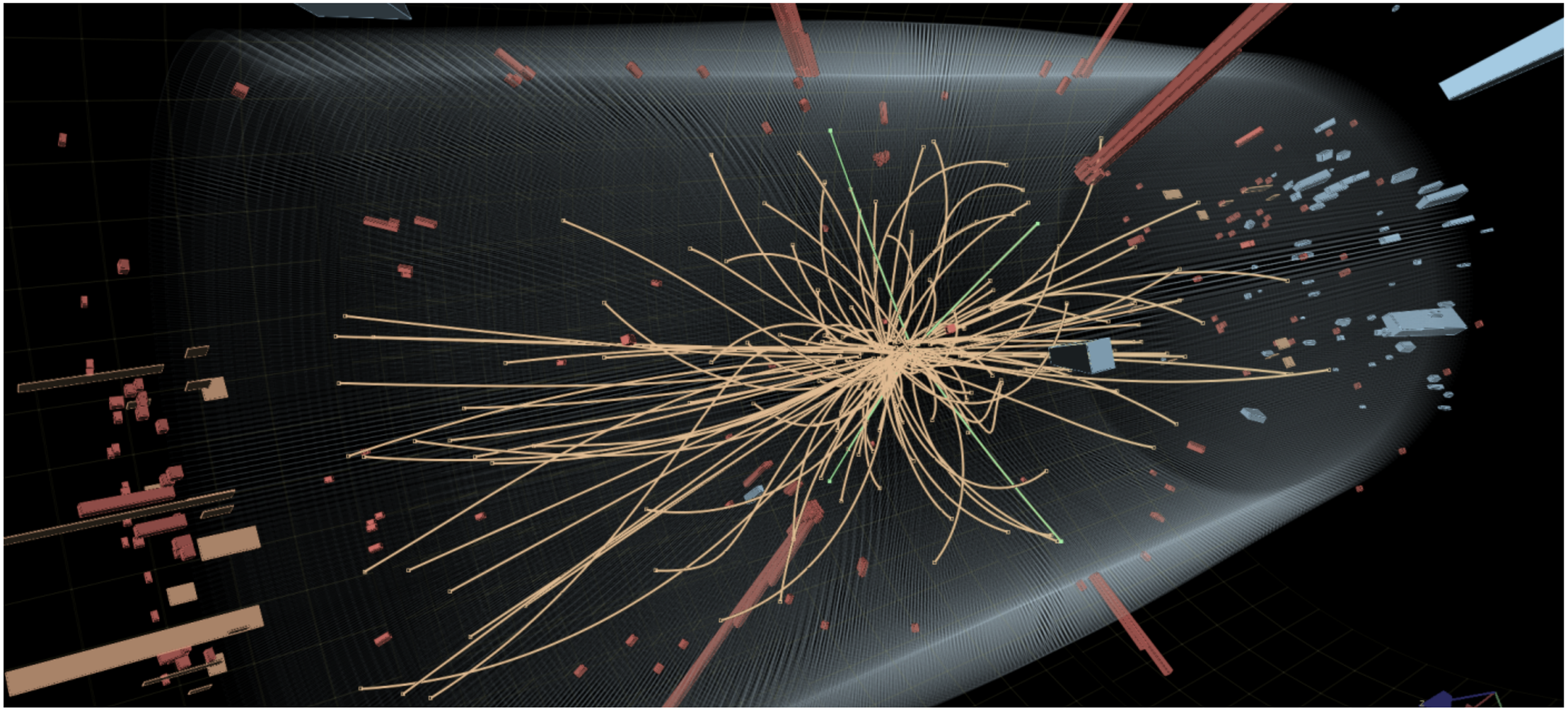
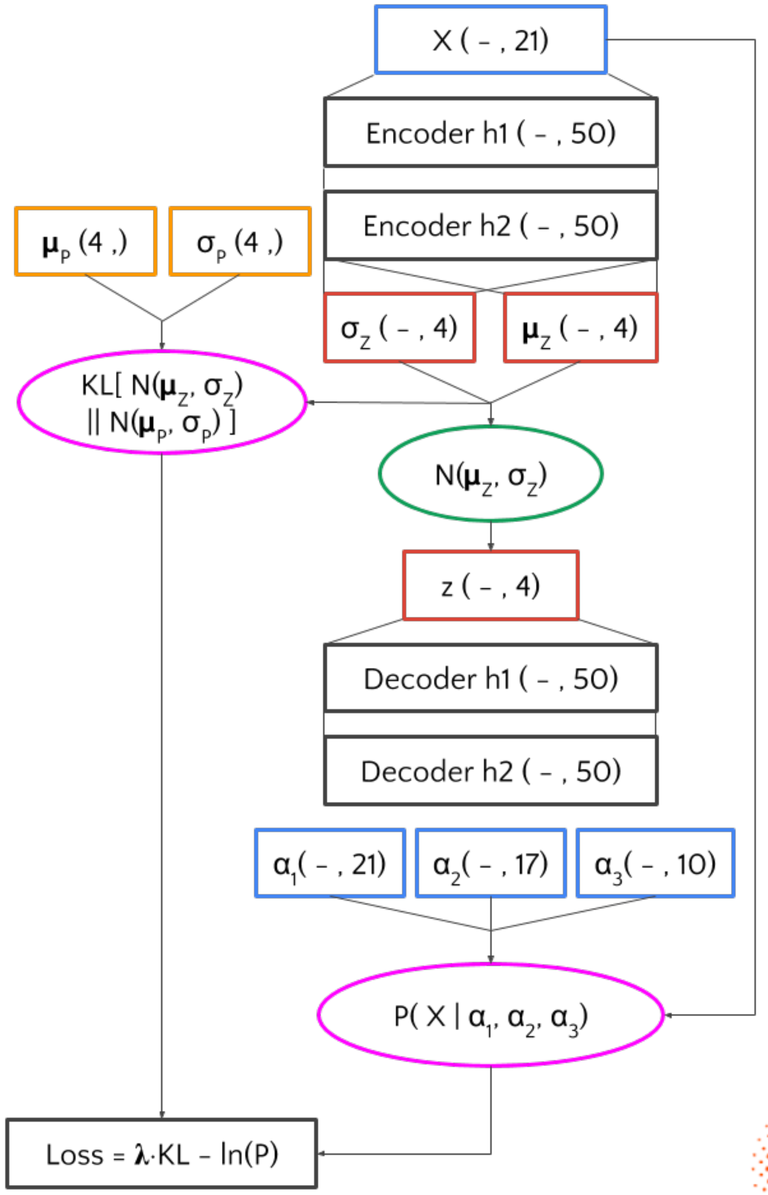


Variational Autoencoders for particle physics

European Research Council

Back to our example

- *We train a VAE on a cocktail of SM events (weighted by xsec)*
- ***ENCODER:*** *21 inputs, 2 hidden layers → 4Dim latent space*
  - *hidden nodes = μ and σ of the Gaussian pdfs describing the hidden variables*
- ***DECODER:*** *from a random sample in the 4D space → 2 hidden layers → parameters describing the shape of the 21Dim input space*



The Loss Function

- *Loss function described as the sum of two terms (scaled by a tuned λ parameter that makes the two contribution numerically similar)*
  - *Reconstruction loss: likelihood of the input 21Dim point, given the shape parameters reconstructed from it*
  - *KL loss: distance between the pdf in the latent space and an nDim Gaussian*

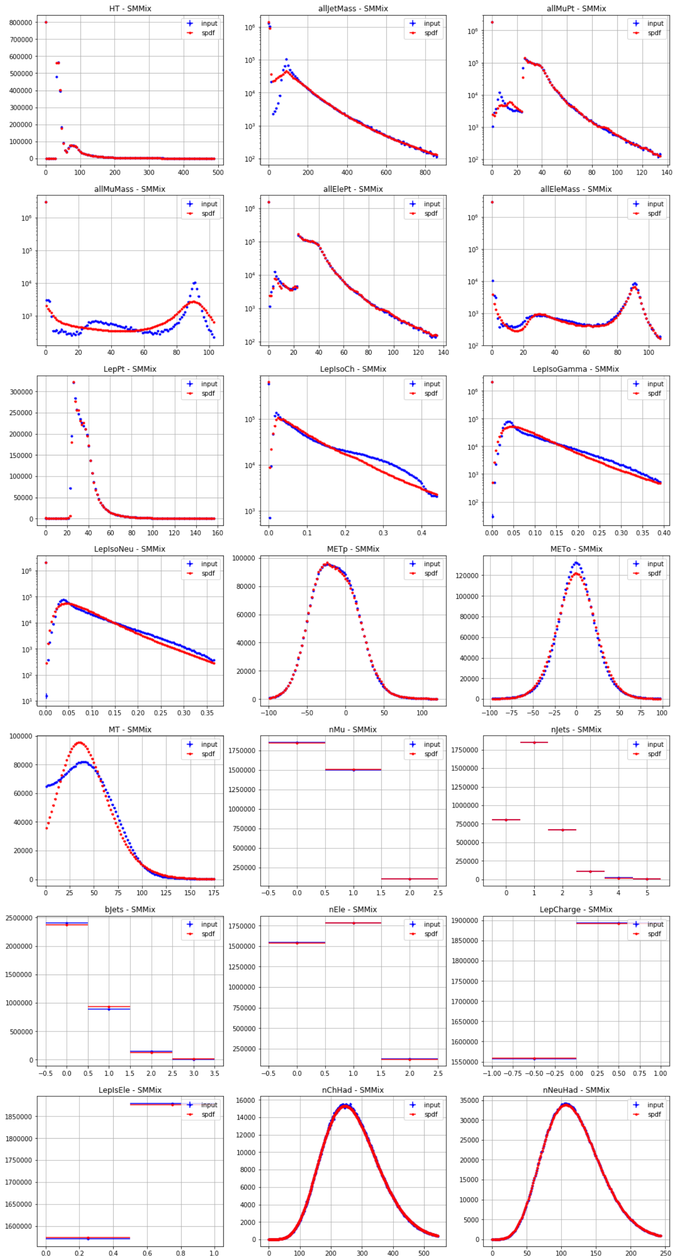
$$\text{Loss}_{\text{Tot}} = \text{Loss}_{\text{reco}} + \beta D_{\text{KL}}$$

$$\begin{aligned}\text{Loss}_{\text{reco}} &= -\frac{1}{k}\sum_{i} \ln\left(P(x \mid \alpha_1, \alpha_2, \alpha_3)\right) \\ &= -\frac{1}{k}\sum_{i,j} \ln\left(f_j(x_{i,j} \mid \alpha_1^{i,j}, \alpha_2^{i,j}, \alpha_3^{i,j})\right)\end{aligned}$$

$$\begin{aligned}D_{\text{KL}} &= \frac{1}{k}\sum_{i} D_{\text{KL}}\left(N(\mu_z^i, \sigma_z^i) \;||\; N(\mu_P, \sigma_P)\right) \\ &= \frac{1}{2k}\sum_{i,j}\left(\sigma_P^j \sigma_z^{i,j}\right)^2 + \left(\frac{\mu_P^j - \mu_z^{i,j}}{\sigma_P^j}\right)^2 + \ln\frac{\sigma_P^j}{\sigma_z^{i,j}} - 1\end{aligned}$$

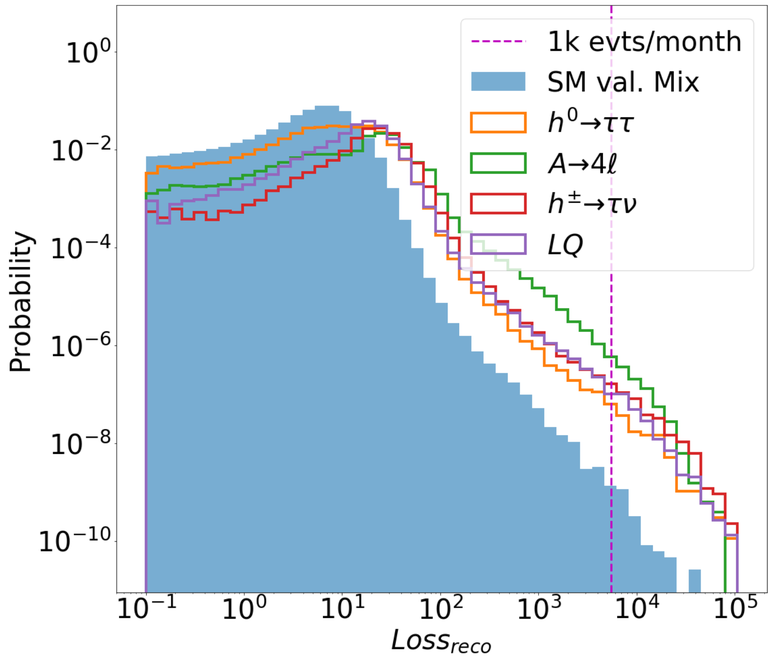
Standard Model encoding

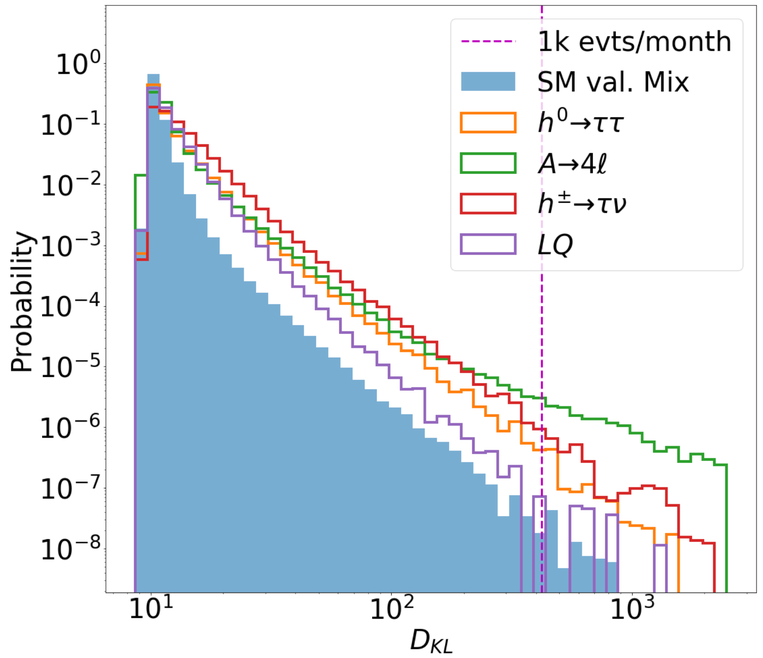
- *First post-training check consists in verifying encoding-decoding capability, comparing input data to those generated sampling from decoder*
- *Reasonable agreement observed, with small discrepancy here and there*
- *NOTICE THAT: this would be a suboptimal event generator, but we want to use it for anomaly detection*
  - *no guarantee that the best autoencoder is the best anomaly detector (no anomaly detection rate in the loss function)*
  - *pros & cons of an unsupervised/ semisupervised approach*



Defining anomaly

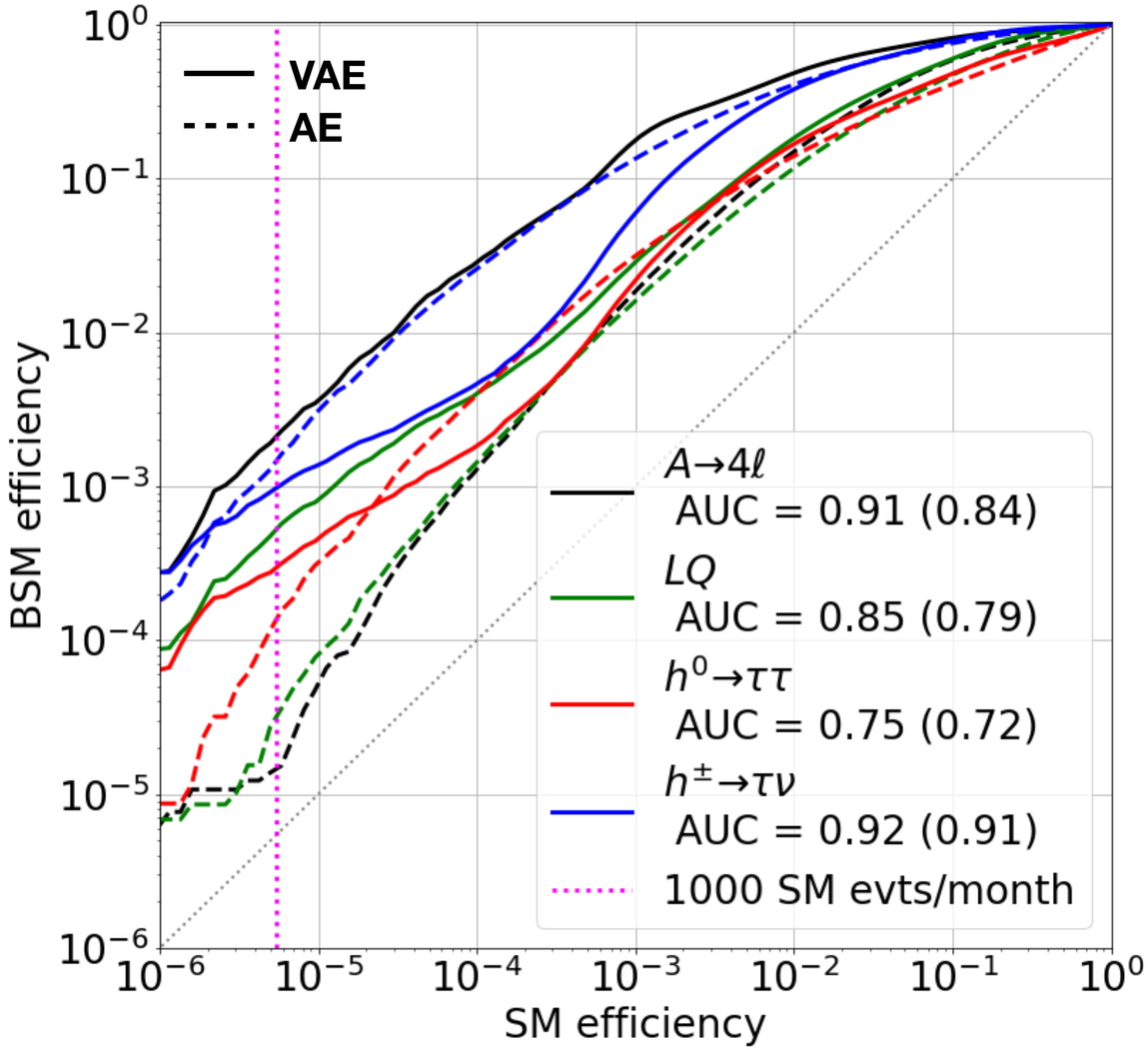
- *Anomaly defined as a p-value threshold on a given test statistics*
  - *Loss function an obvious choice*
  - *Some part of a loss could be more sensitive than others*
  - *We tested different options and found the total loss to behave better*





Performances

- *Evaluate general discrimination power by ROC curve and area under curve (AUC)*
  - *clearly worse than supervised*
  - *but not so far*
- *Fixing SM acceptance rate at 50 events/day*
  - *competitive results considering unsupervised nature of the algorithm*



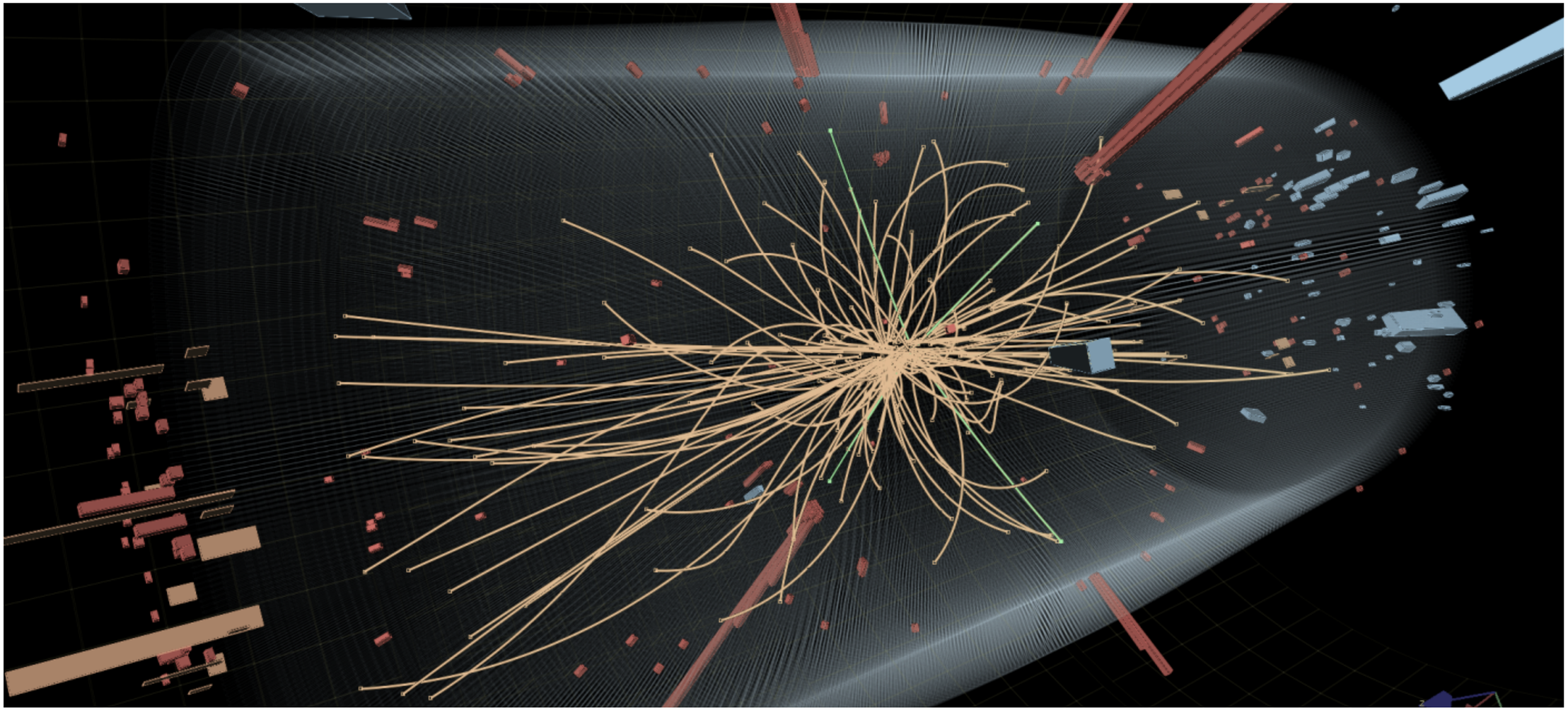
Performances

- *Small efficiency but still much larger than for SM processes*
- *Allows to probe 10-100 pb cross sections for reasonable amount of collected signal events*

Process	Efficiency for ~30 evt/day	xsec for 100 evt/ month [pb]	xsec for S/B~1/3 [pb]
$a \to 4\ell$	$2.8 \cdot 10^{-3}$	7.1	27
$LQ \to \tau b$	$6.5 \cdot 10^{-4}$	31	120
$h \to \tau\tau$	$3.6 \cdot 10^{-4}$	56	220
$h^{\pm} \to \tau\nu$	$1.2 \cdot 10^{-3}$	17	67

1/2 way to model independence

- *Procedure designed to be model independent*
  - *Training done only on SM*
  - *Algorithm that defines anomaly tuned only on number of selected SM events (false positive rate)*
- *Still, residual model dependence present*
  - *Based on physics-motivated observables*
  - *List not tailored on specific models and general enough to offer good performances in principle*
  - *But one cannot prove that performances on specific BSM models will generalise*
- *Can we go beyond this limitation and define something really BSM agnostic?*



Particle Flow, Recurrent Networks & Model Independence

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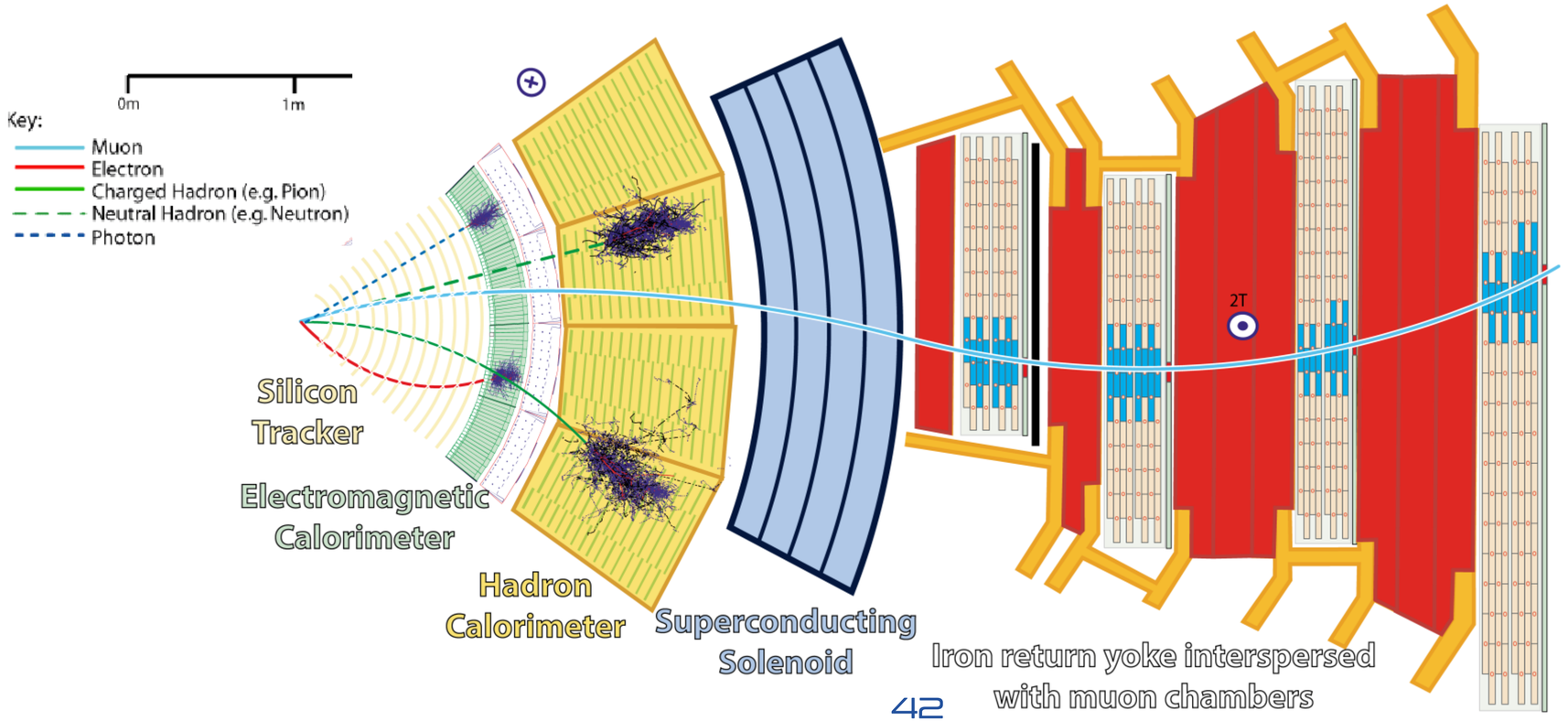
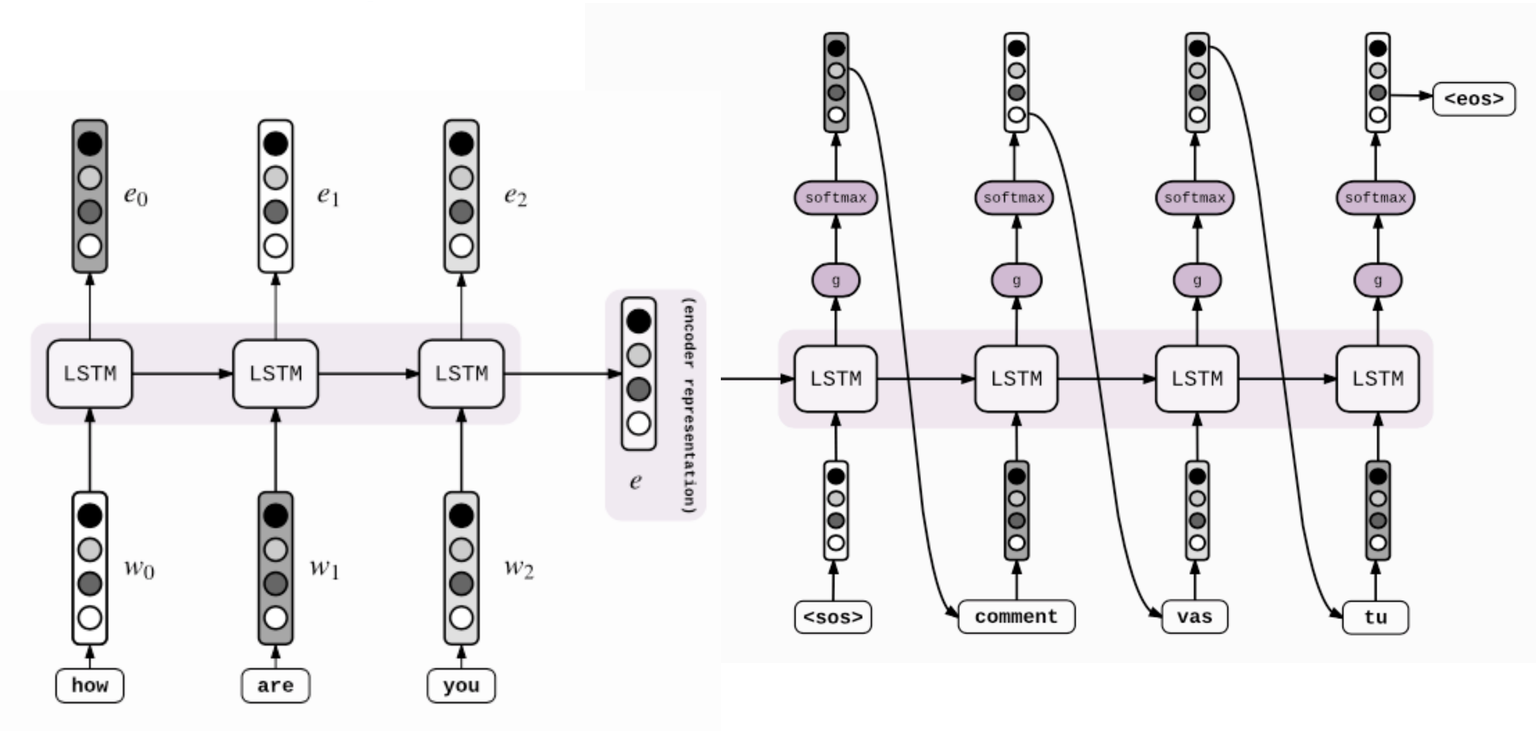
Particle Flow

- *CMS uses PF to combine sub-detector information and produce a list of reconstructed particles*
- *Anything (jets, MET, resonances, etc) is reconstructed from these particles*
- *One could generalise the VAE new-physics-detection algorithm and make it PF compliant*
  - *integrated in the reconstruction flow @HLT*
  - *can abstract from model dependence inherited by any physics-motivated HLF choice*



VAE with PF particles

- *Issues:*
  - *variable number of particles/event as input*
  - *need to return particles as output*
- *Networks used for translation*
  - *start from a sentence in language*
  - *code its meaning in some latent space z*
  - *translate to some other language, generating words from z*



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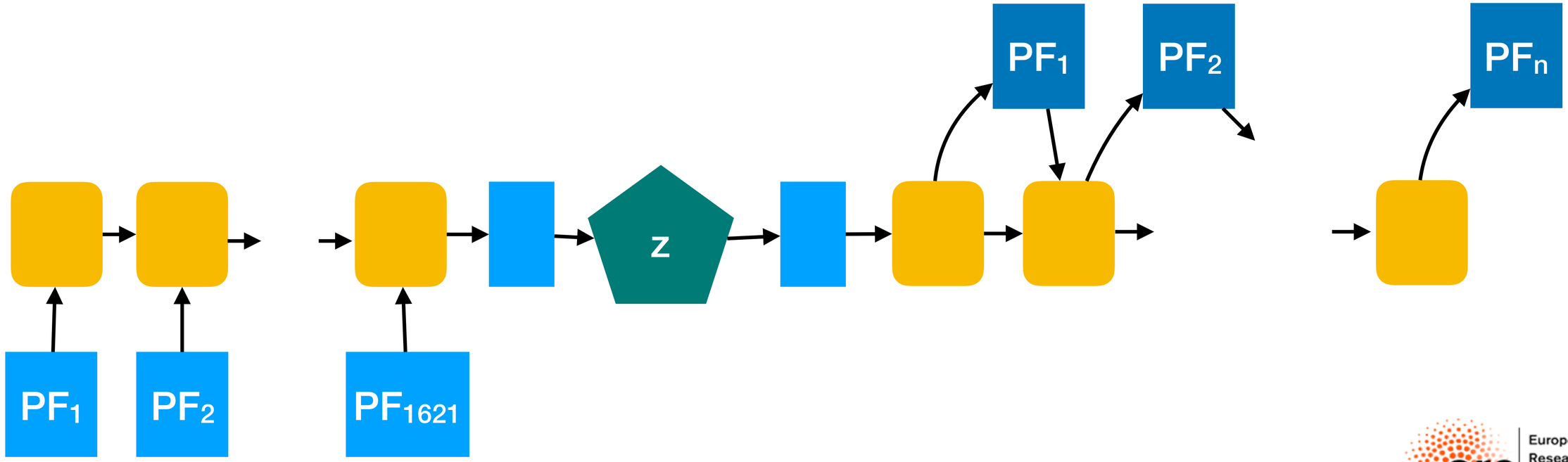
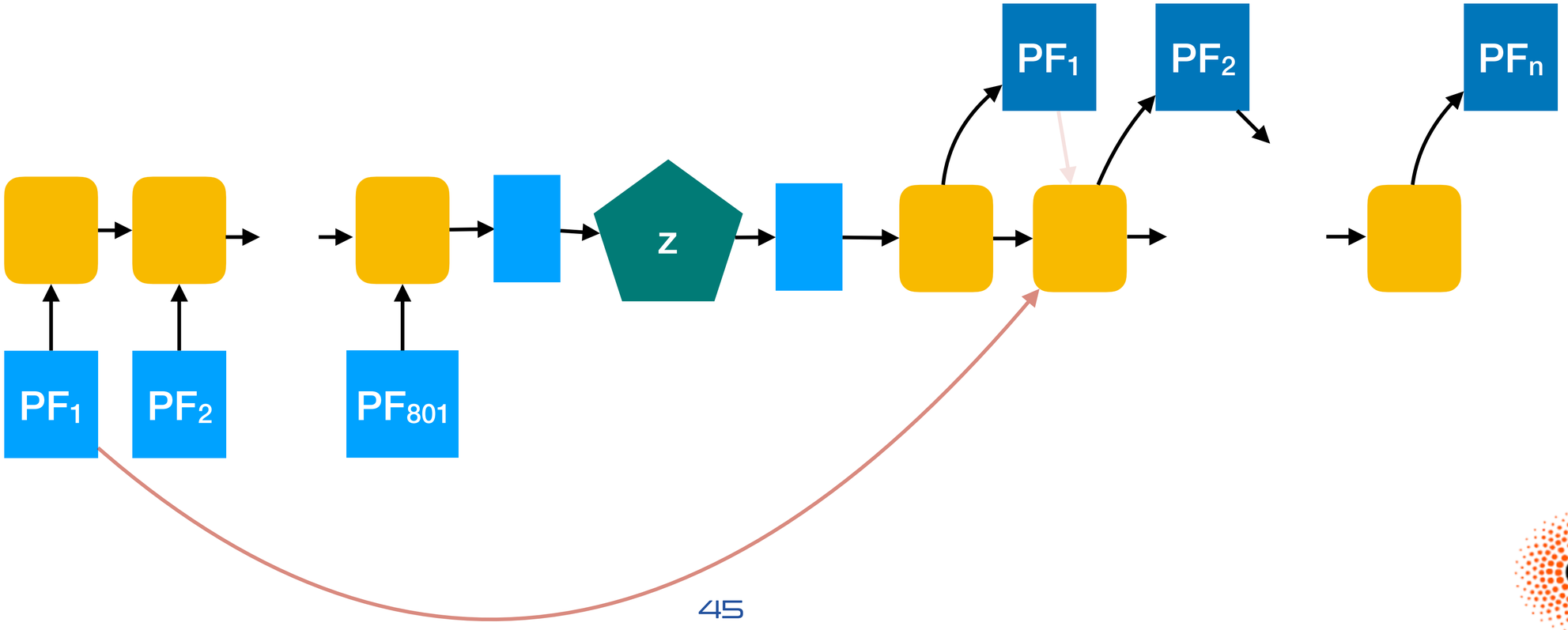


Teacher forcing

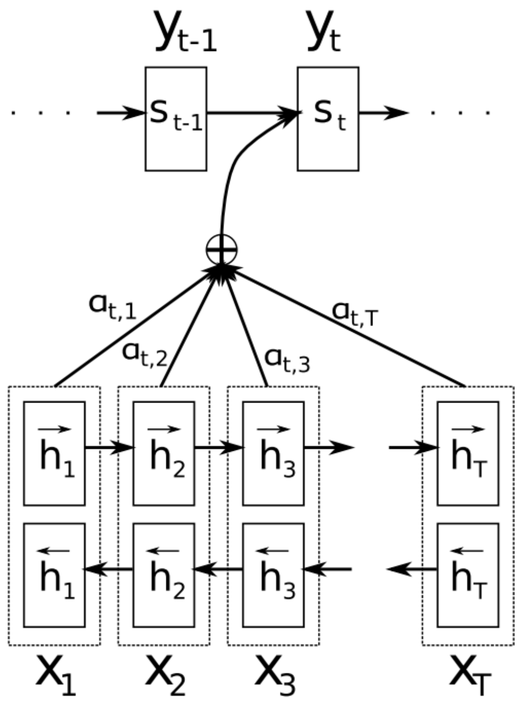
- *At early stage of training, the decoder can't reconstruct a reasonable first PF candidate; autoregressive mechanism propagates it into a wrong chain of particles.*

- ***Teacher-forcing:*** *under some probability k, feed the target as the next input instead of using the previous prediction. k decreases as the epoch number increases.*



Adding Attention

- *Attention allows the decoder to focus on which part of the inputs is relevant to the next prediction.*



the **Encoder** generates **h1,h2,h….hT** from the inputs **X1,X2,X3…XT**

a is the **Alignment model** which is a **feedforward neural network** that is trained with all the other components of the proposed system

$$e_{ij} = a(s_{i-1}, h_j)$$

The **Alignment model** scores (e) how well each encoded input (h) matches the current output of the decoder (s).

The alignment scores are normalized using a **softmax function.**

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})}$$

The context vector is a weighted sum of the **annotations** (hj) and **normalized alignment scores.**

$$c_i = \sum_{j=1}^{T_x} \alpha_{ij} h_j.$$

Bahdanau et al., arXiv:1409.0473

Adding Attention

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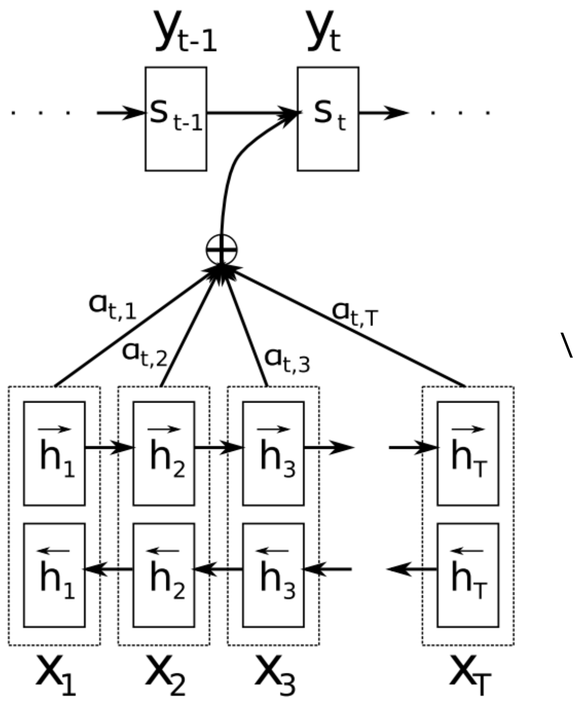

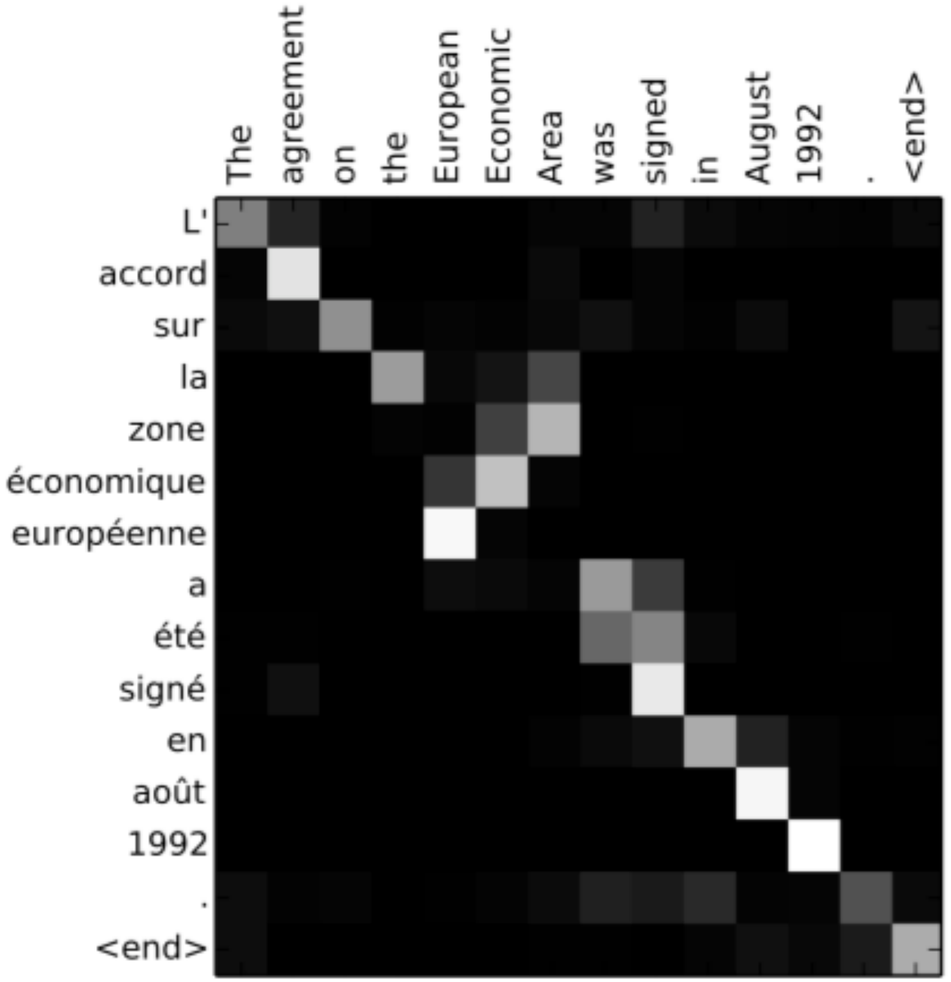

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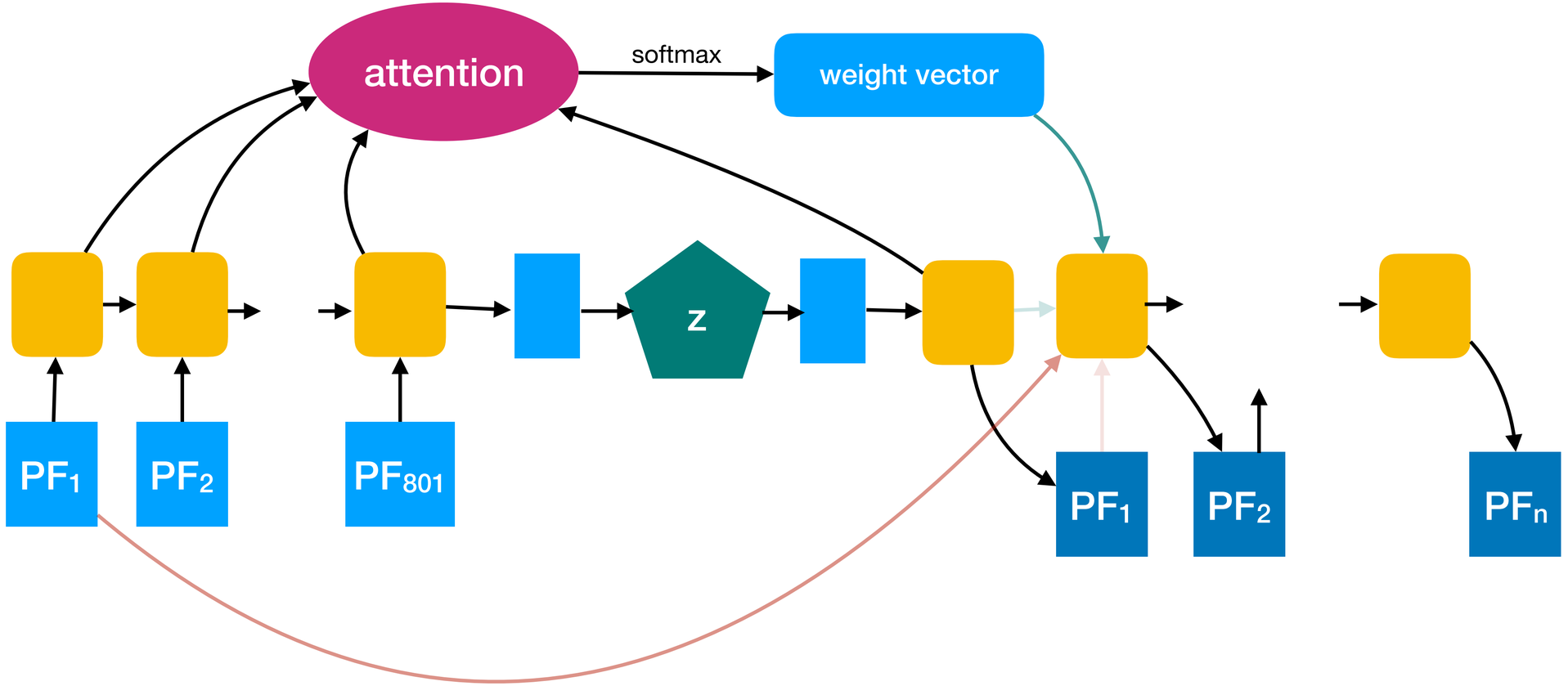
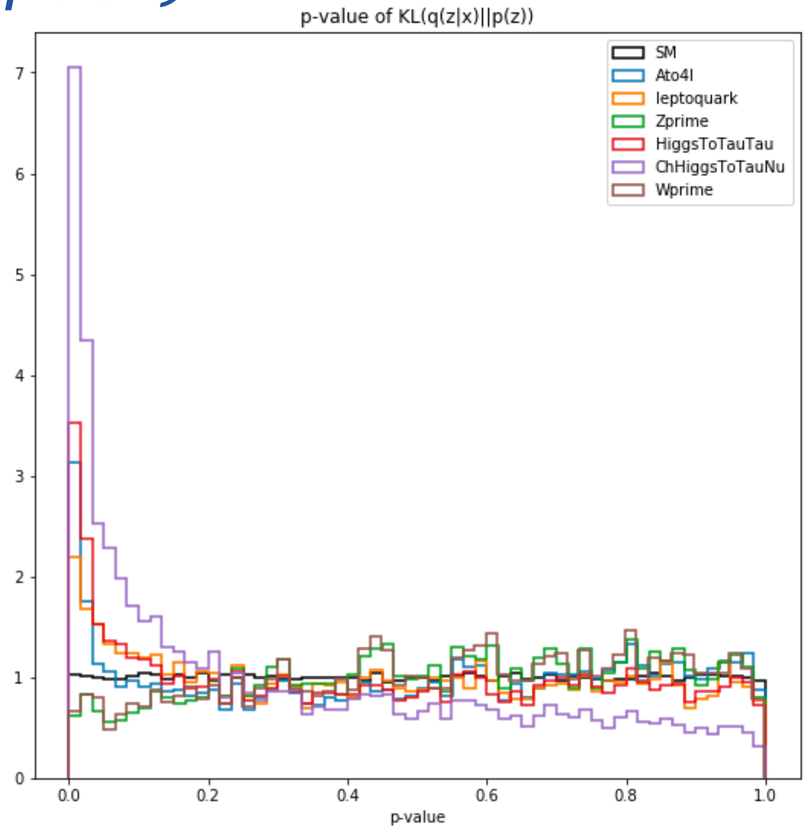
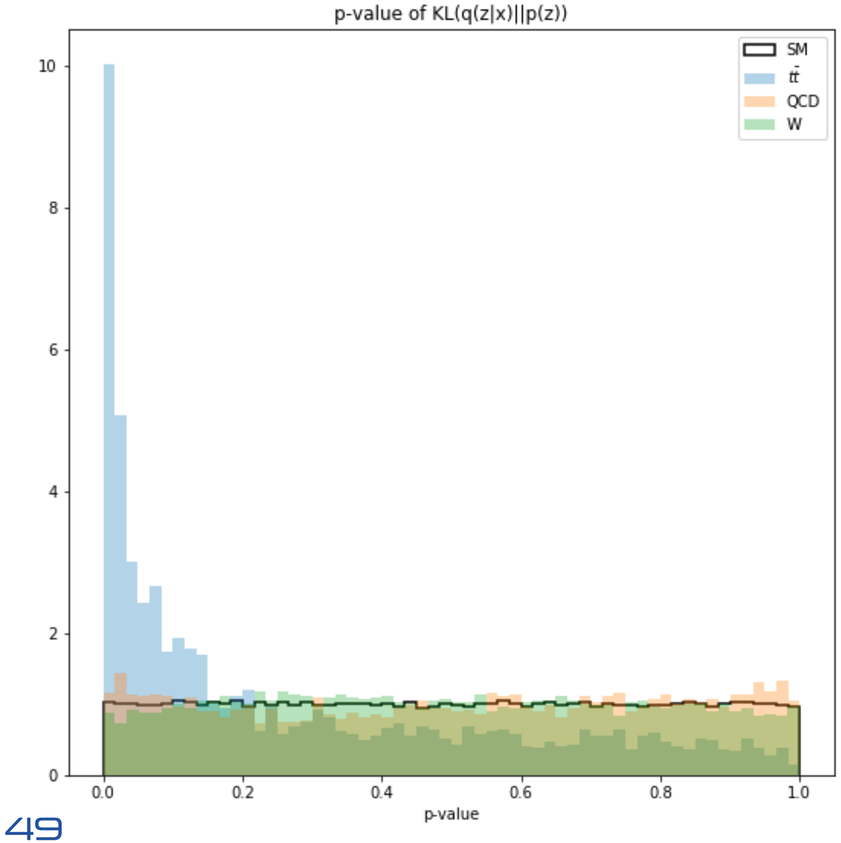


Performances

- *(Preliminary) results trained on a small subset of the initial dataset (90K events)*
- *Due to architecture complexity, training is much slower (6h/epoch)*





Performances

- *(Preliminary) results trained on a small subset of the initial dataset (90K events)*
- *Due to architecture complexity, training is much slower (6h/epoch)*

Process	Efficiency for ~300 evt/day	xsec for 10 evt/ month [pb]	xsec for S/B~1/3 [pb]
$a \to 4\ell$	$3.3 \cdot 10^{-4}$	7.2	$1.5 \cdot 10^{3}$
$LQ \to \tau b$	$5.8 \cdot 10^{-4}$	4.1	850
$h \to \tau\tau$	$1.1 \cdot 10^{-3}$	2.2	450
$h^{\pm} \to \tau\nu$	$1.4 \cdot 10^{-3}$	1.7	340

Summary

- *Autoencoders are NNs for unsupervised problems*
  - *Clustering*
  - *Dimensional reduction*
  - *Anomaly detection*
- *When adding variational functionality*
  - *Can be used as generators*
  - *Can improve robustness (e.g., anomaly detection performance)*
- *Could be relevant to reduce model dependence in searches for new physics at the LHC*

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