PART V: A VERY BRIEF INTRODUCTION TO DEEP UNSUPERVISED LEARNING

*elements taken from D. Kirkby lectures at KSPA

WHAT DOES MACHINE LEARNING DO?

the machine is told what to look for

SUPERVISED

the machine is NOT told what to look for

UN-SUPERVISED

TWO VERY BROAD TYPES OF MACHINE LEARNING ALGORITHMS

WHAT DOES MACHINE LEARNING DO?

the machine is told what to look for

SUPERVISED

LEARNS A MAP FROM X [FEATURES] TO Y [LABELS]

$$P(X|Y)$$

the machine is NOT told what to look for

UN-SUPERVISED

NO LABELS - DISCOVER PATTERNS

$$P(X)$$

IT IS AN ACTIVE FIELD OF RESEARCH BECAUSE LABELLING IS ONE OF THE MAIN BOTTLENECKS OF MACHINE LEARNING

- **"Pure" Reinforcement Learning (cherry)**
  - The machine predicts a scalar reward given once in a while.
  - **A few bits for some samples**
- **Supervised Learning (icing)**
  - The machine predicts a category or a few numbers for each input
  - Predicting human-supplied data
  - **10→10,000 bits per sample**
- **Self-Supervised Learning (cake génoise)**
  - The machine predicts any part of its input for any observed part.
  - Predicts future frames in videos
  - **Millions of bits per sample**

@ Y. LECUN

IN THIS LAST PART WE ARE GOING TO BRIEFLY INTRODUCE CURRENT TECHNIQUES OF UNSUPERVISED LEARNING WITH NEURAL NETWORKS

THERE ARE 3 MAJOR APPLICATIONS TO ASTRONOMY (THAT I CAN THINK OF):

- **DIMENSIONALITY REDUCTION:** HOW CAN I REPRESENT MY COMPLEX DATA MORE EFFICIENTLY TO GET NEW INSIGHTS INTO ITS STRUCTURE?

- **GENERATIVE MODELING:** HOW CAN I INTERPOLATE / EXTRAPOLATE A (SMALL, SPARSE) DATASET TO GENERATE NEW DATA SAMPLED FROM THE SAME (UNKNOWN) DISTRIBUTION?

- **PROBABILISTIC MODELING:**WHAT IS THE PROBABILITY THAT A NEW OBSERVATION IS DRAWN FROM THE SAME (UNKNOWN) DISTRIBUTION AS SOME REFERENCE (SMALL, SPARSE) DATASET?

DIMENSIONALITY REDUCTION

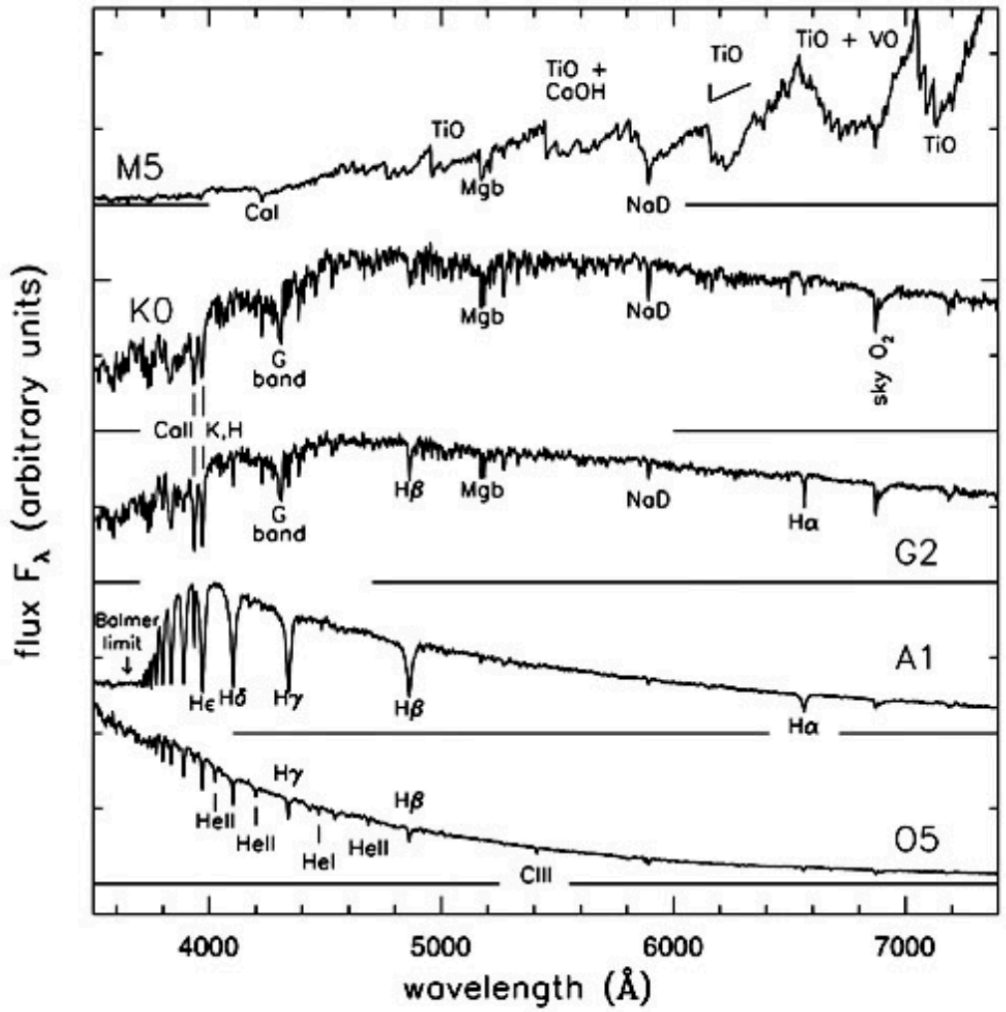
NEED OF REPRESENTING THE DATA IN A SMALLER DIMENSIONALITY SPACE

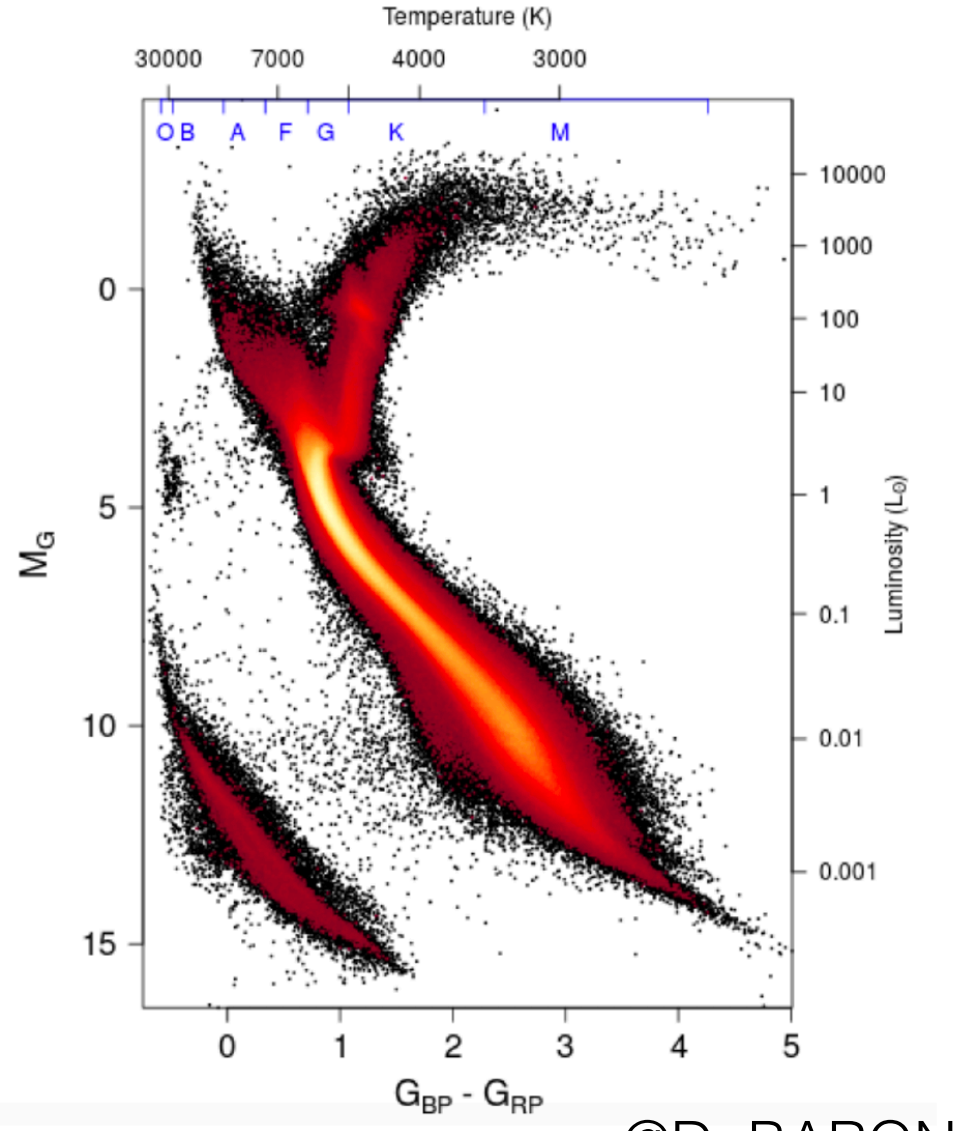
$$G_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}$$

@D. BARON

MOST OF THE SCIENTIFIC WORK IS ABOUT COMPRESSION OF NATURE IN SOME EXPLANATORY EQUATIONS

From: Gaia Collaboration et al. 2018





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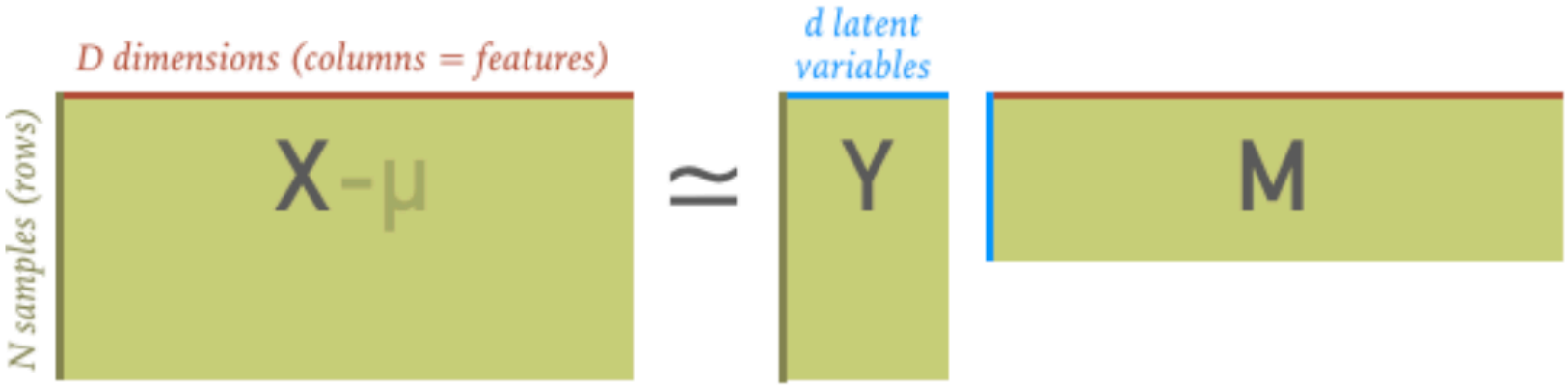
THE STELLAR MAIN SEQUENCE IS A DIMENSIONALITY REDUCTION



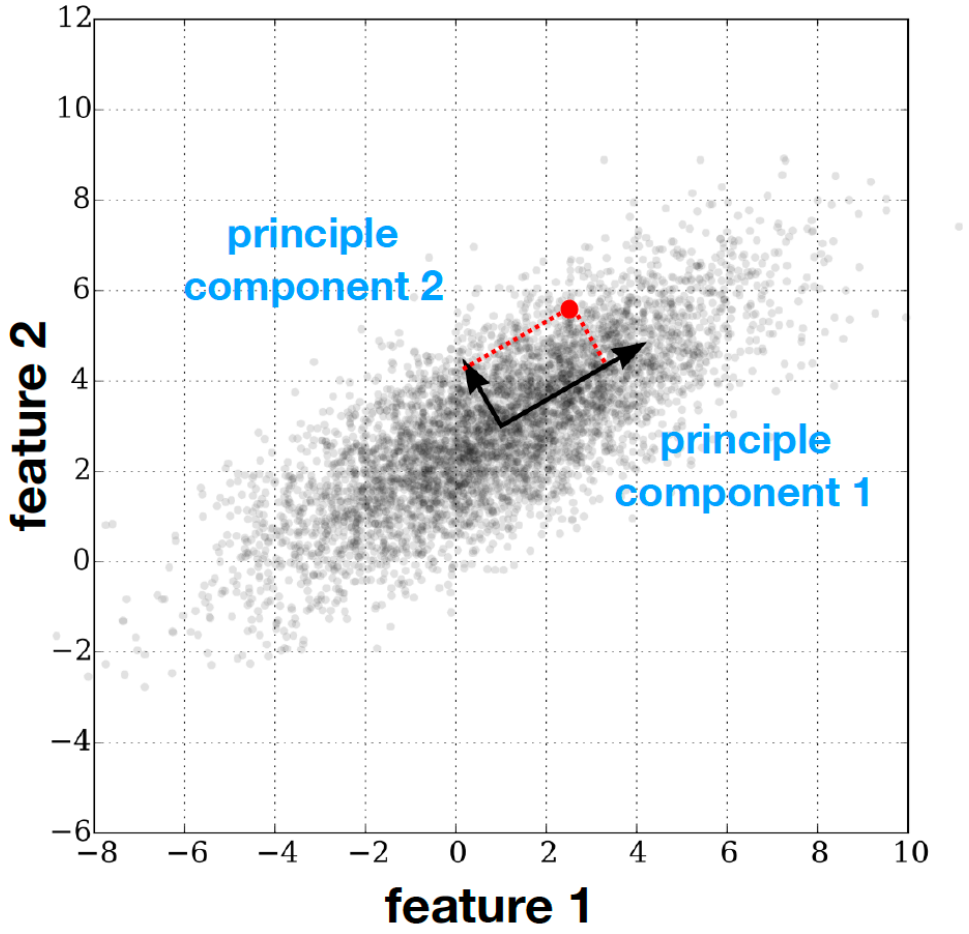
CLASSICAL METHODS FOR DIMENSIONALITY REDUCTION SEEK A LINEAR DECOMPOSITION THAT BEST EXPLAINS THE OBSERVATIONS X IN TERMS OF **LATENT VARIABLES Y**

PRINCIPAL COMPONENT ANALYSIS

PCA CONVERT A SET OF (CORRELATED) VARIABLES INTO A SET OF VALUES LINEARLY UNCORRELATED

1. THE FIRST PRINCIPLE COMPONENT ("PROTOTYPE"), HAS THE LARGEST POSSIBLE VARIANCE

2. THE FOLLOWING COMPONENTS HAVE THE LARGEST VARIABLES WITH THE ADDITIONAL CONSTRAIN THAT THEY ARE ORTHOGONAL TO THE PRECEDING COMPONENTS



PRINCIPAL COMPONENT ANALYSIS

1. COMPUTE THE **COVARIANCE MATRIX** OF YOUR DATA

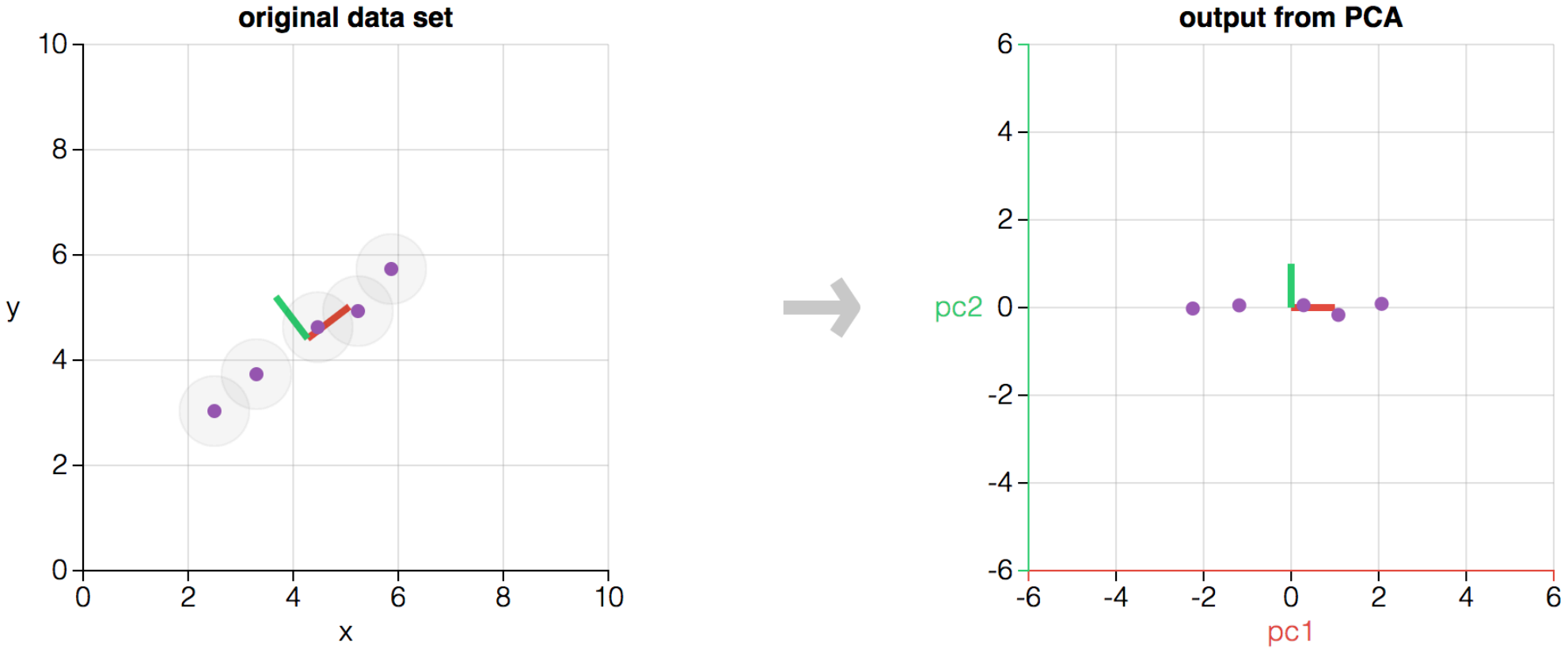
2. COMPUTE THE **EIGENVALUES AND EIGENVECTORS** OF THE **COVARAINCE MATRIX**

3.THE **EIGENVECTORS** PROVIDE THE DIRECTION OF MAXIMUM VARIANCE AND THE **EIGENVALUES** THE ‘IMPORTANCE’ OF THAT PARTICULAR FEATURE

REMEMBER, THE COVARIANCE MATRIX IS NOTHING ELSE THAN THAT:

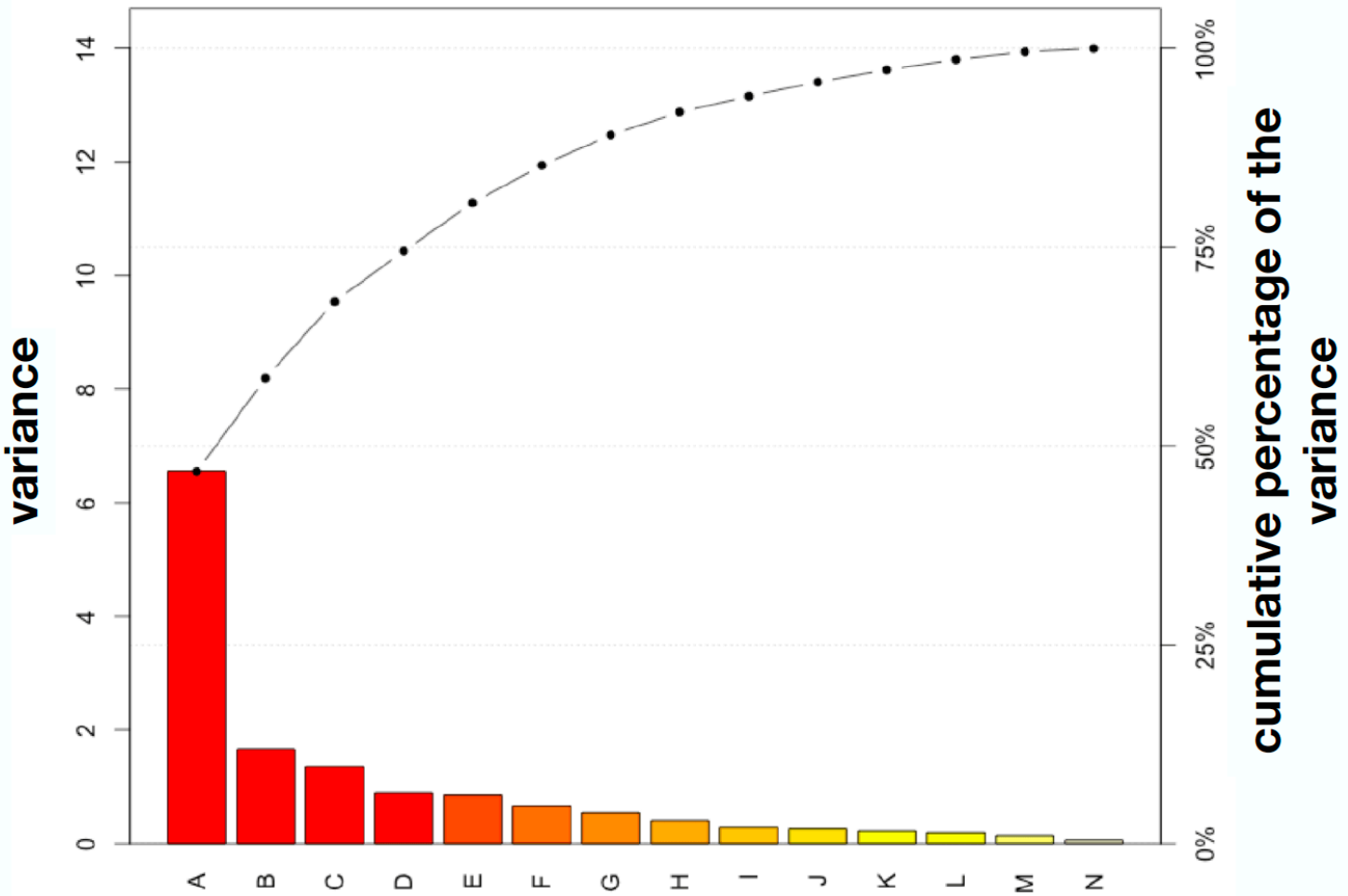
$$\mathrm{K}_{\mathbf{XX}} = \begin{bmatrix} \mathrm{E}[(X_1 - \mathrm{E}[X_1])(X_1 - \mathrm{E}[X_1])] & \mathrm{E}[(X_1 - \mathrm{E}[X_1])(X_2 - \mathrm{E}[X_2])] & \cdots & \mathrm{E}[(X_1 - \mathrm{E}[X_1])(X_n - \mathrm{E}[X_n])] \\ \mathrm{E}[(X_2 - \mathrm{E}[X_2])(X_1 - \mathrm{E}[X_1])] & \mathrm{E}[(X_2 - \mathrm{E}[X_2])(X_2 - \mathrm{E}[X_2])] & \cdots & \mathrm{E}[(X_2 - \mathrm{E}[X_2])(X_n - \mathrm{E}[X_n])] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n - \mathrm{E}[X_n])(X_1 - \mathrm{E}[X_1])] & \mathrm{E}[(X_n - \mathrm{E}[X_n])(X_2 - \mathrm{E}[X_2])] & \cdots & \mathrm{E}[(X_n - \mathrm{E}[X_n])(X_n - \mathrm{E}[X_n])] \end{bmatrix}$$

https://en.wikipedia.org/wiki/Covariance_matrix



https://setosa.io/ev/principal-component-analysis/

PRINCIPAL COMPONENT ANALYSIS



IT RESULTS IN DATA COMPRESSION, BY REPRESENTING EACH OBJECT AS A PROJECTION OF THE FIRST PRINCIPLE COMPONENTS

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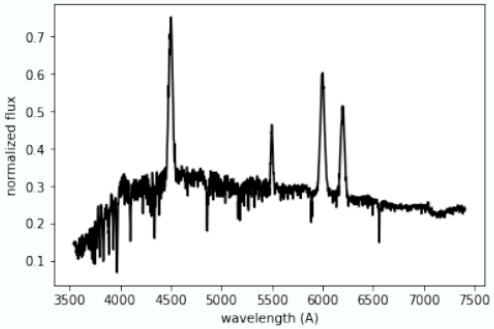
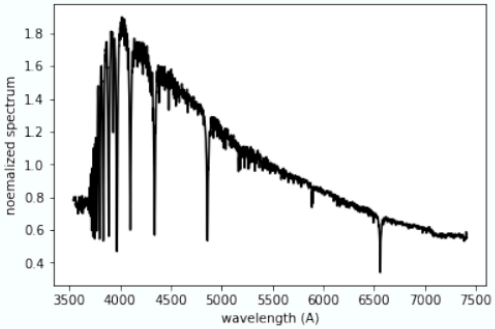
PRINCIPAL COMPONENT ANALYSIS

observed object



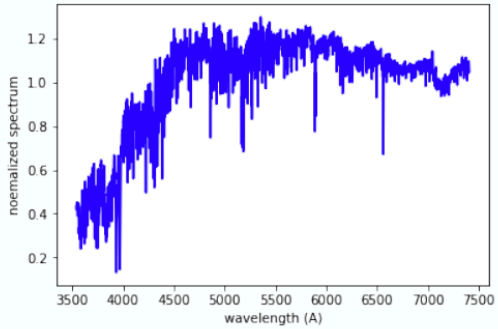
= A *

principle comp. 1



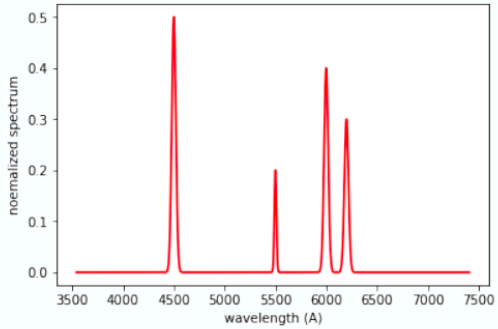
+ B *

principle comp. 2



+ C *

principle comp. 3



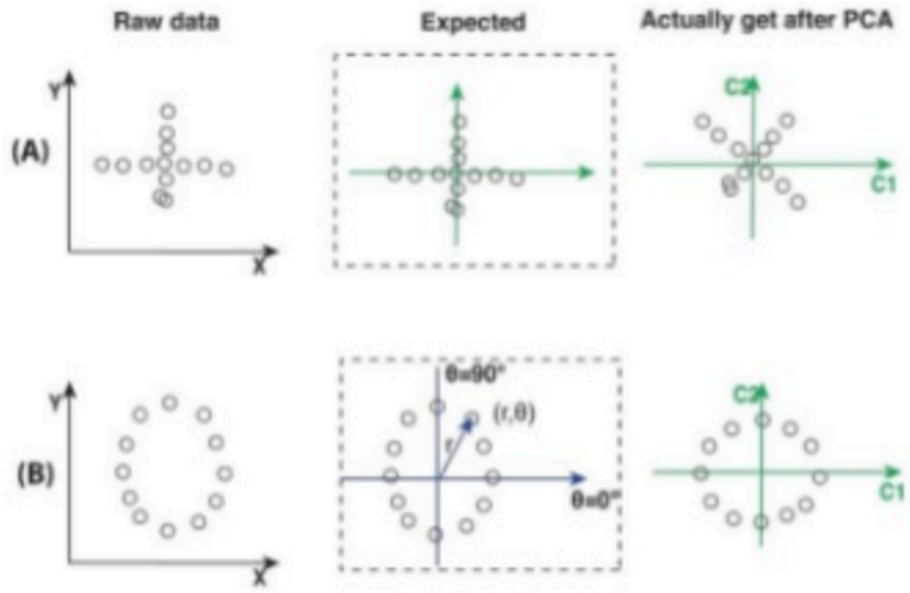
OBJECTS ARE DIVIDED INTO MAJOR PROTOTYPES AND ALL OBJECTS CAN BE OBTAINED AS LINEAR COMBINATIONS

@D. BARON

LIMITATIONS OF PCA

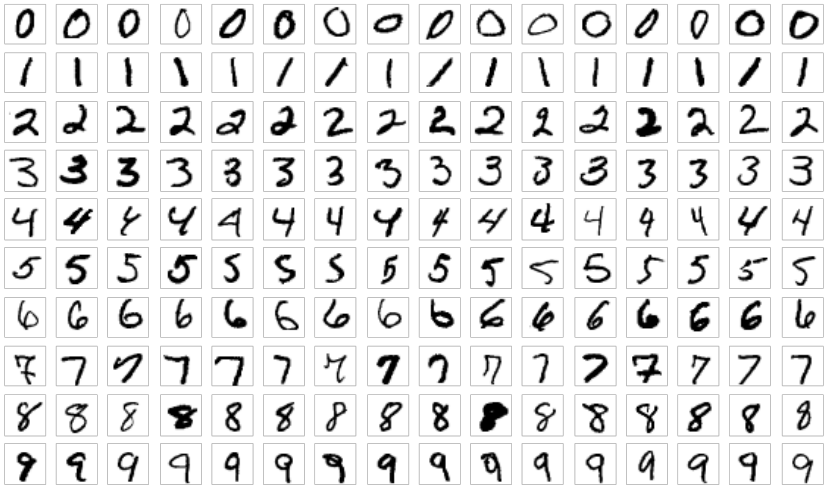
PCA APPLY LINEAR TRANSFORMATIONS

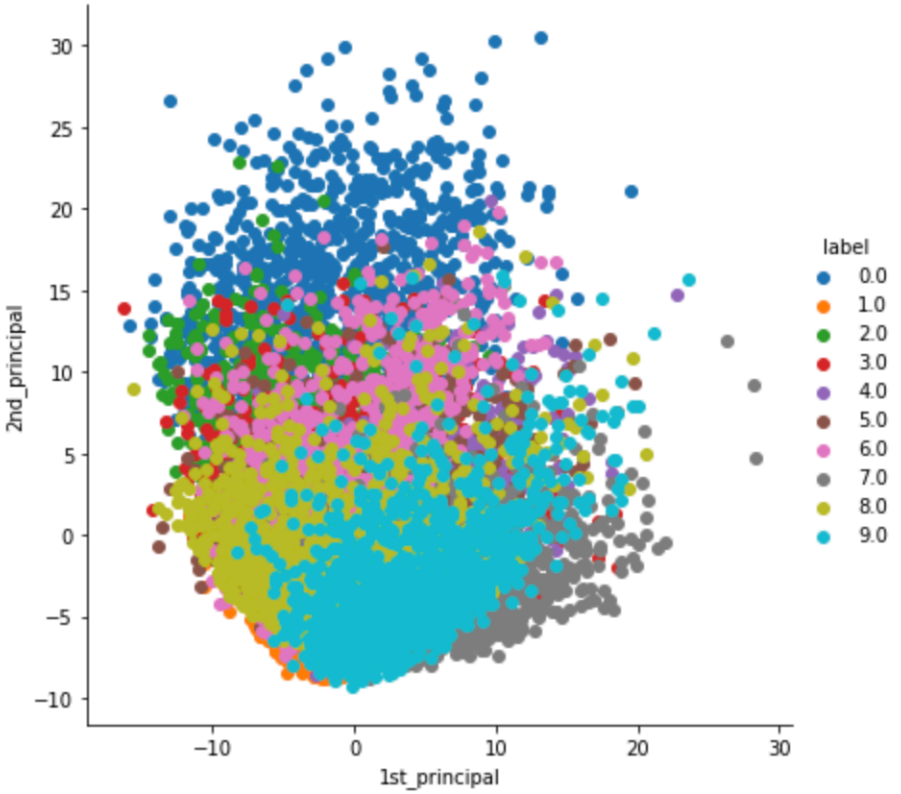
SINCE WE USE THE COVARIANCE MATRIX, IT ASSUMES THAT THE DATA FOLLOWS A **MULTIDIMENSIONAL NORMAL DISTRIBUTION**



LIMITATIONS OF PCA

AND DATA IS NOT ALWAYS GAUSSIAN….

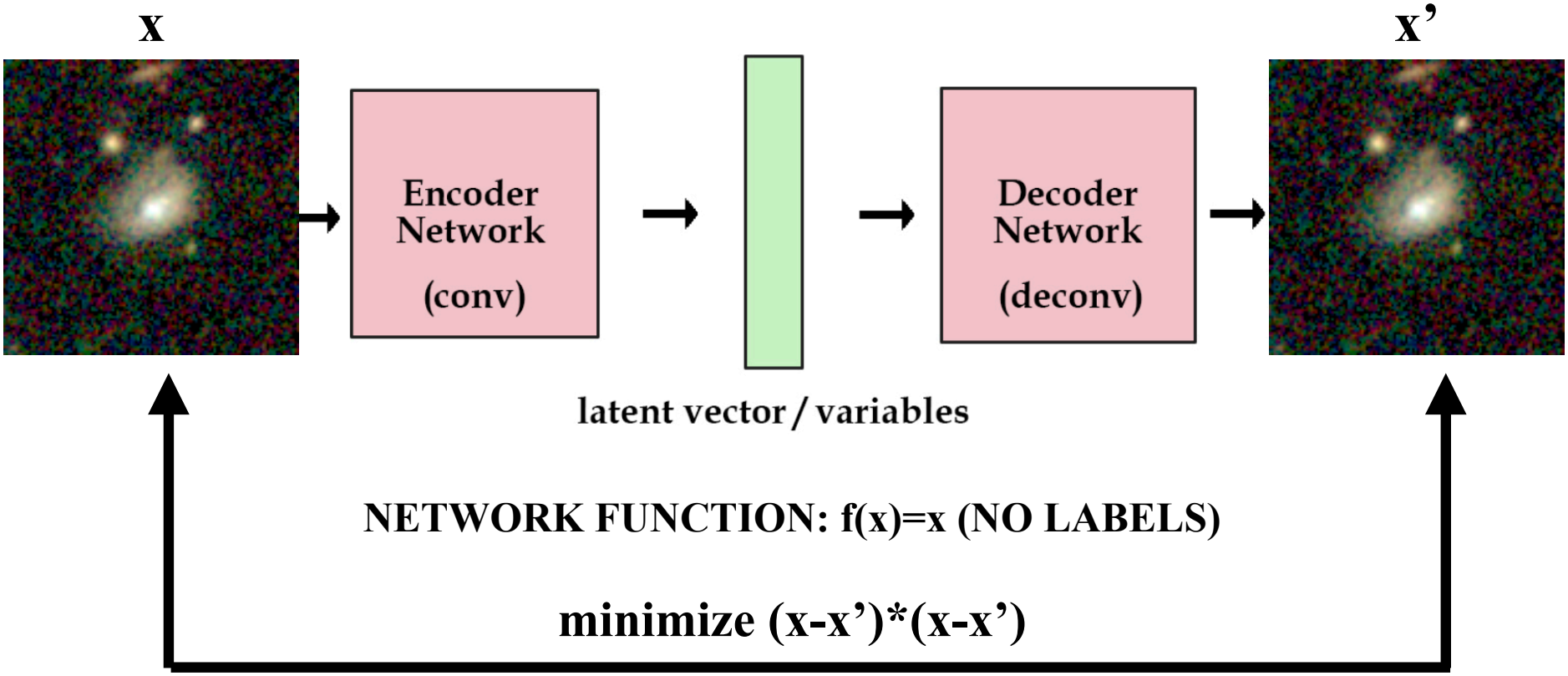




https://medium.com/analytics-vidhya/principal-component-analysis-pca-with-code-on-mnist-dataset-da7de0d07c22

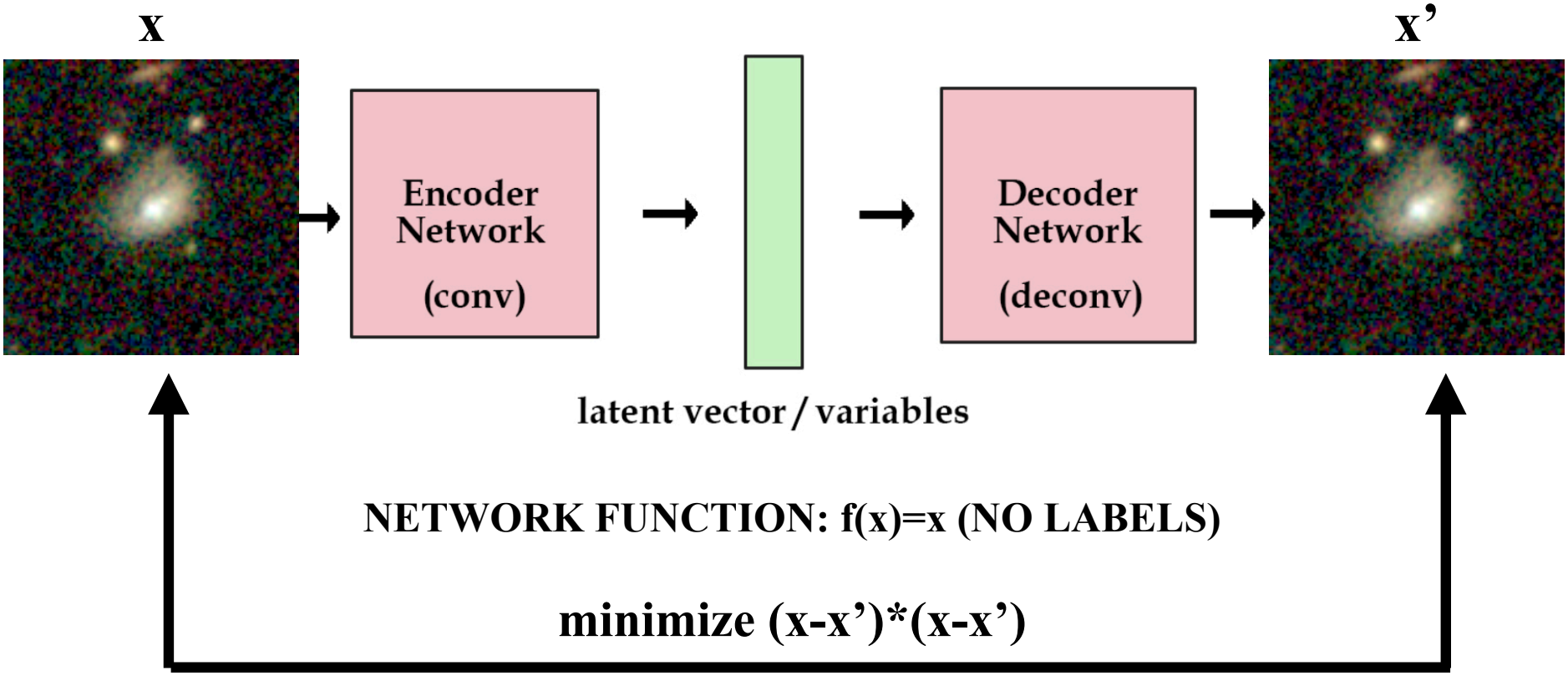
CAN WE GENERALIZE THAT?

CONVOLUTIONAL AUTO-ENCODER



AN AUTO-ENCODER IS ANY NETWORK WITH IDENTICAL INPUT AND OUTPUT

CONVOLUTIONAL AUTO-ENCODER



BY REDUCING THE DIMENSIONALITY IN THE LATENT SPACE WE FORCE THE NETWORK TO LEARN A REPRESENTATION OF THE INPUT DATA IN A LOWER DIMENSIONALITY SPACE

* NO NEED TO BE CONVOLUTIONAL - ANY NEURAL NETWORK WITH A BOTTLENECK WILL DO THE JOB

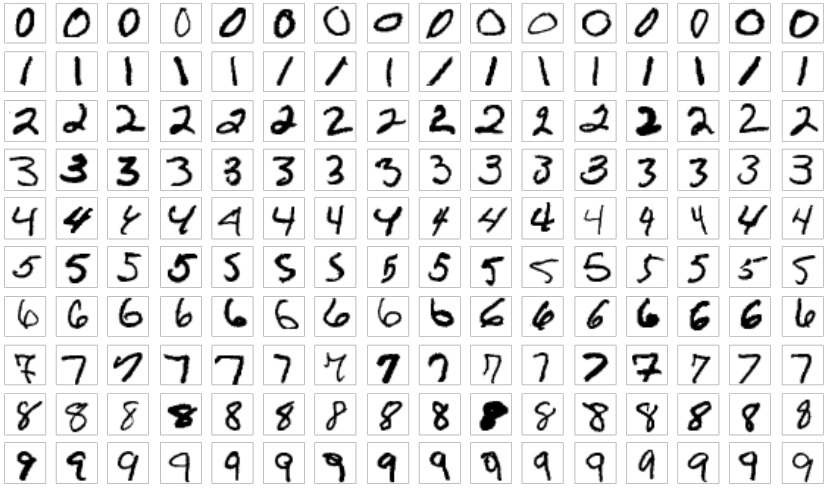
* **QUESTION**: WHAT WOULD HAPPEN IF WE SET AN AUTOENCODER WITH NO ACTIVATION FUNCTIONS?

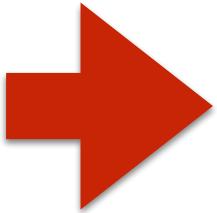
SEE EXAMPLE FROM TUTORIALS FOR STAR-GALAXY SEPARATION

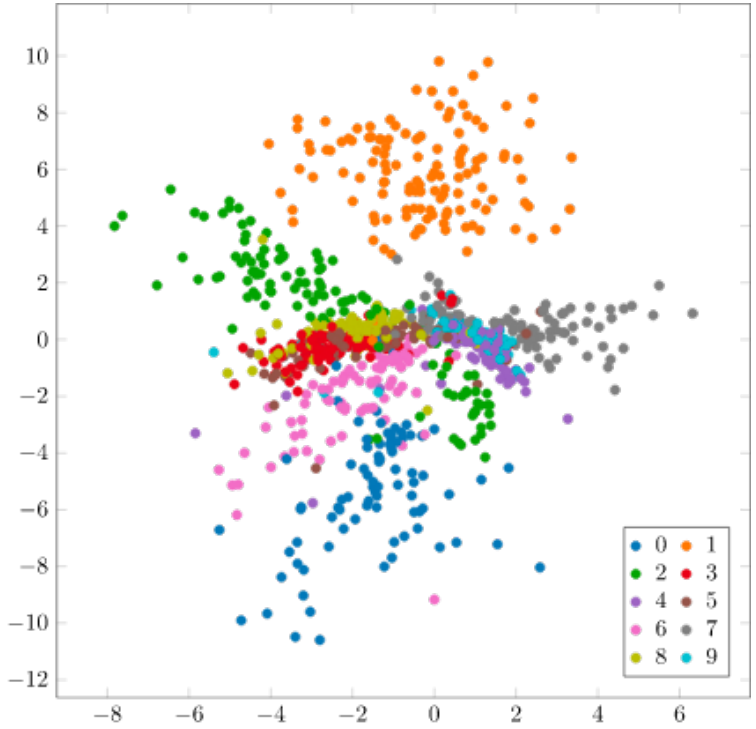
What would happen if we set an auto-encoder with no activation functions?

- nothing special - it would be a linear model
- PCA
- Depends on the input data
- Don't know

AUTOENCODER REPRESENTATION OF MNIST

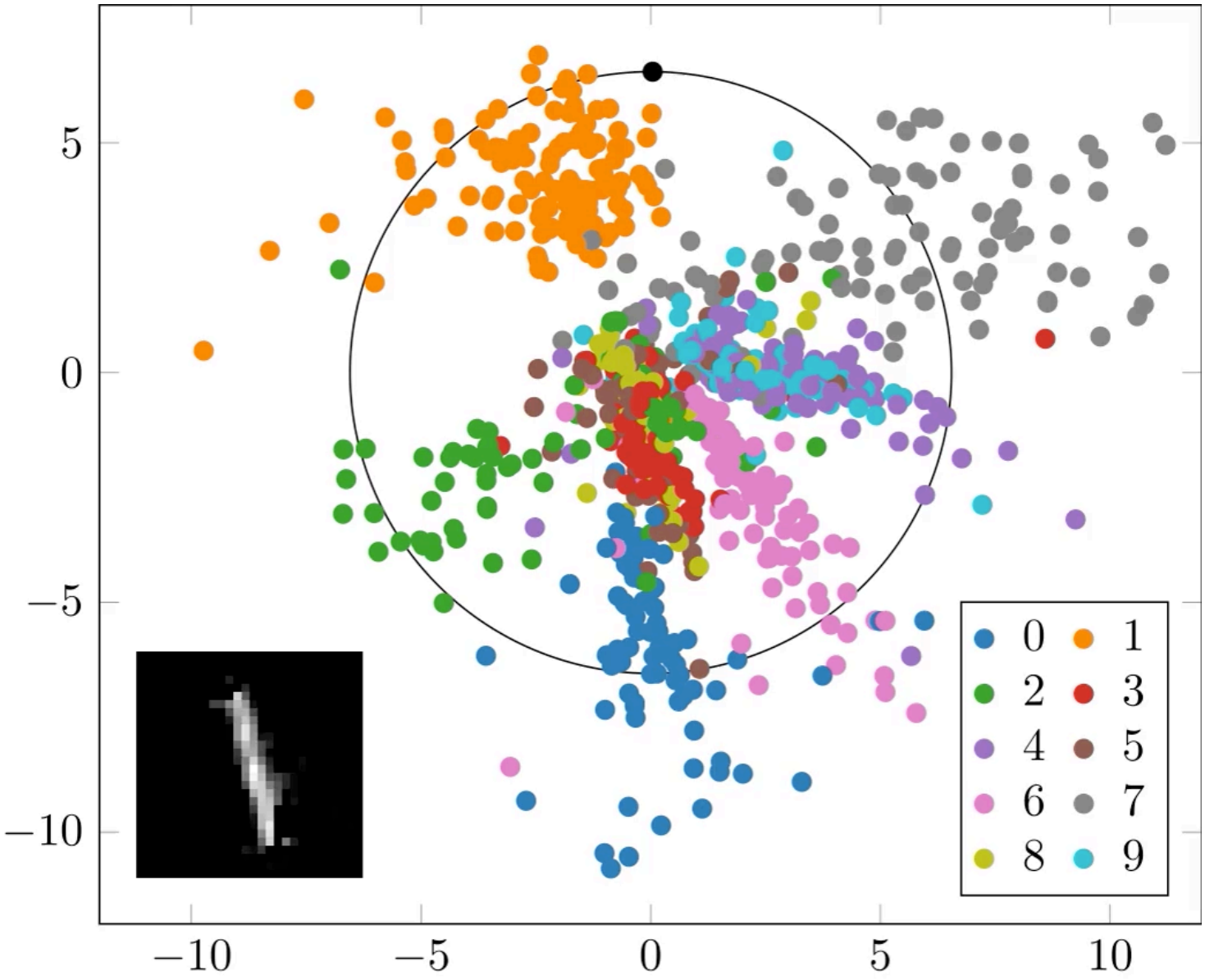




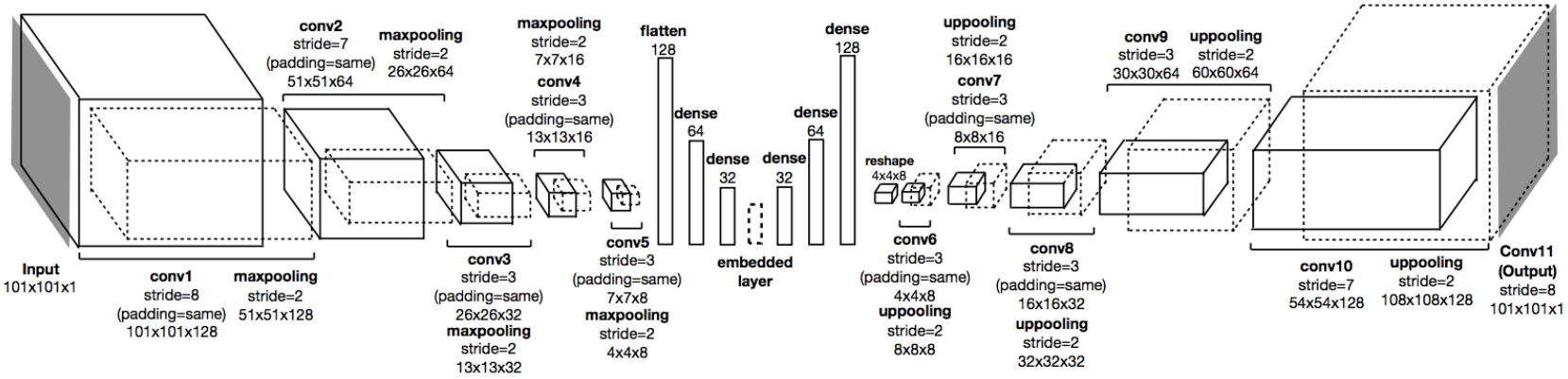


https://gertjanvandenburg.com/blog/autoencoder/

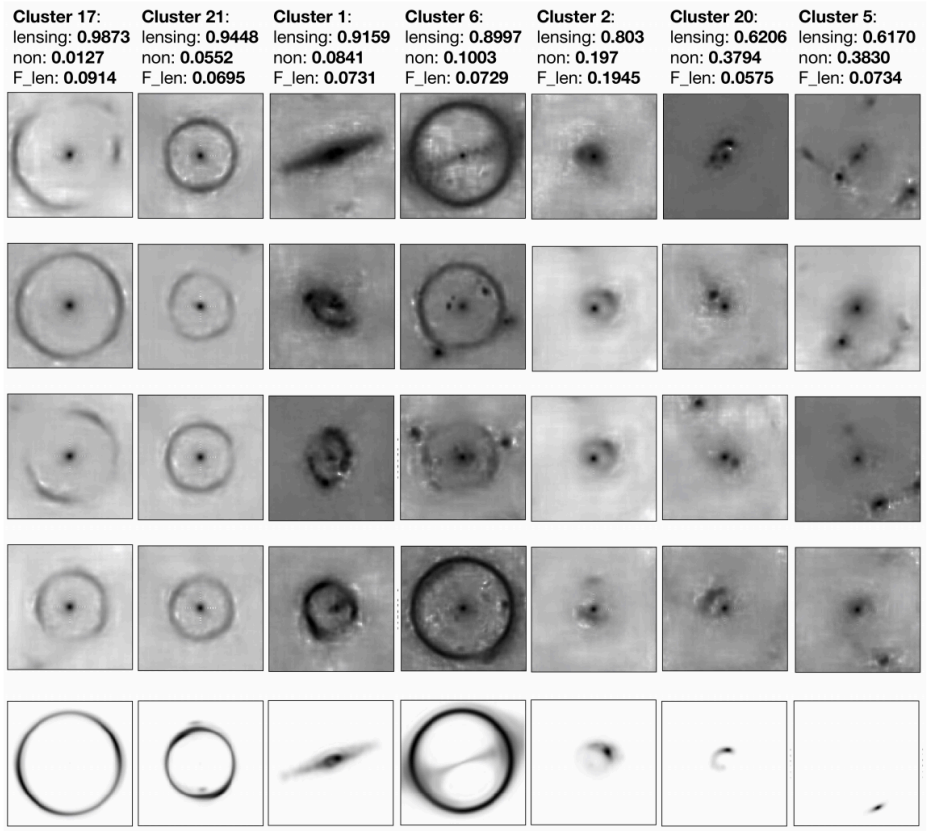
AUTOENCODER REPRESENTATION OF MNIST



https://gertjanvandenburg.com/blog/autoencoder/


Input
101x101x1
conv1
stride=8
(padding=same)
101x101x128
maxpooling
stride=2
51x51x128
conv2
stride=7
(padding=same)
51x51x64
maxpooling
stride=2
26x26x64
conv3
stride=3
(padding=same)
26x26x32
maxpooling
stride=2
13x13x32
maxpooling
stride=2
7x7x16
conv4
stride=3
(padding=same)
13x13x16
conv5
stride=3
(padding=same)
7x7x8
maxpooling
stride=2
4x4x8
flatten
128
dense
64
dense
32
embedded
layer
dense
32
dense
64
dense
128
reshape
4x4x8
conv6
stride=3
(padding=same)
4x4x8
uppooling
stride=2
8x8x8
uppooling
stride=2
16x16x16
conv7
stride=3
(padding=same)
8x8x16
conv8
stride=3
(padding=same)
16x16x32
uppooling
stride=2
32x32x32
conv9
stride=3
30x30x64
uppooling
stride=2
60x60x64
conv10
stride=7
54x54x128
uppooling
stride=2
108x108x128
Conv11
(Output)
stride=8
101x101x1

Cheng+20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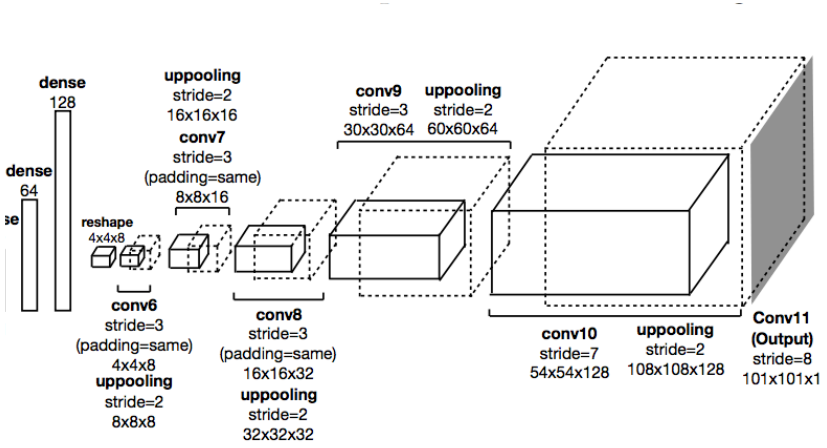
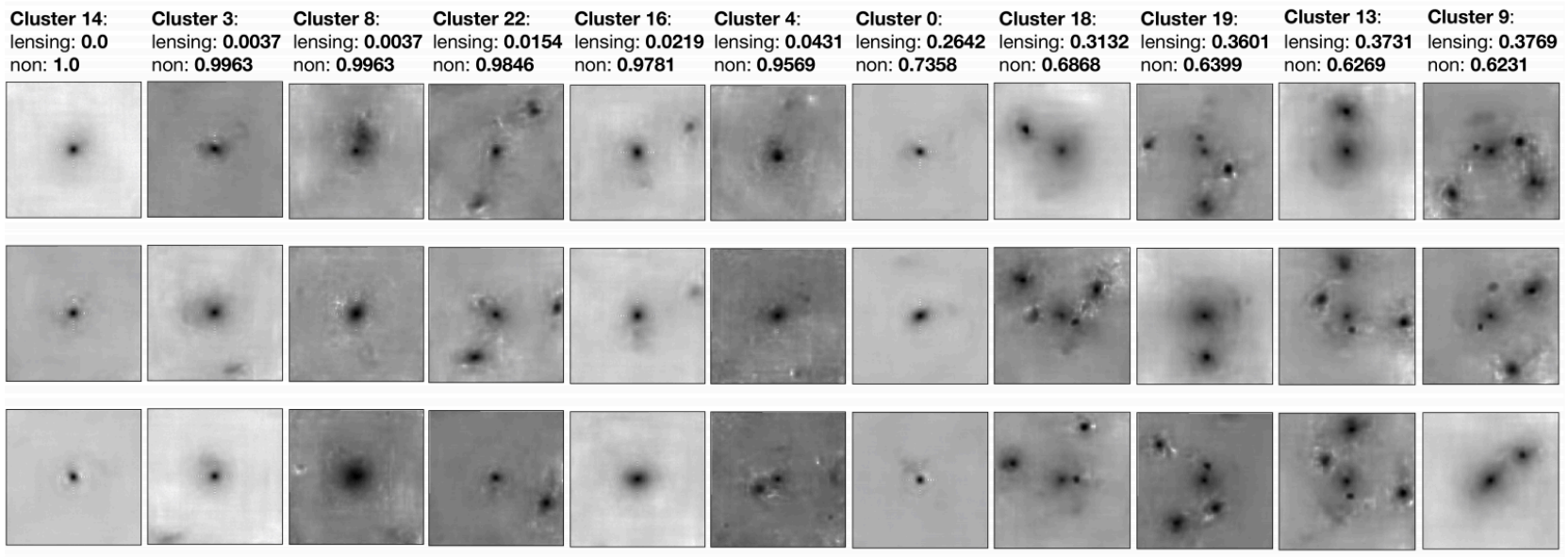
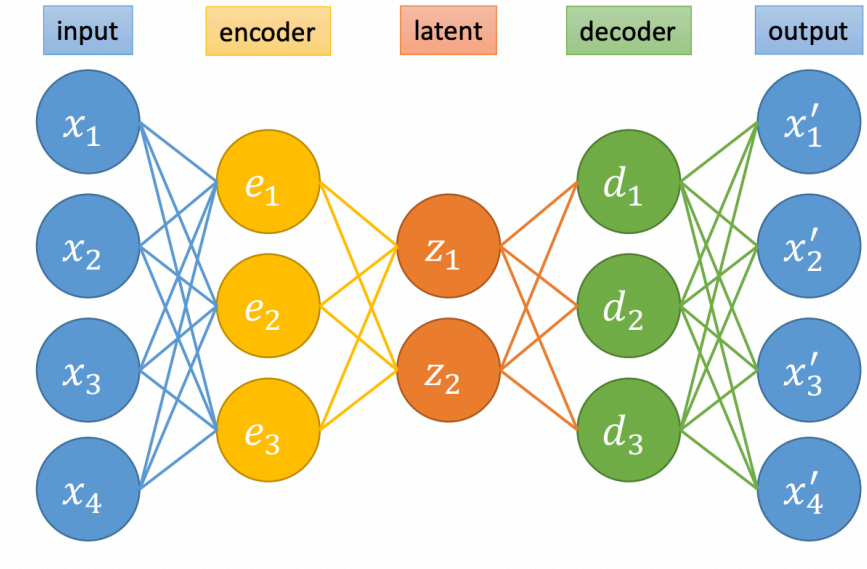
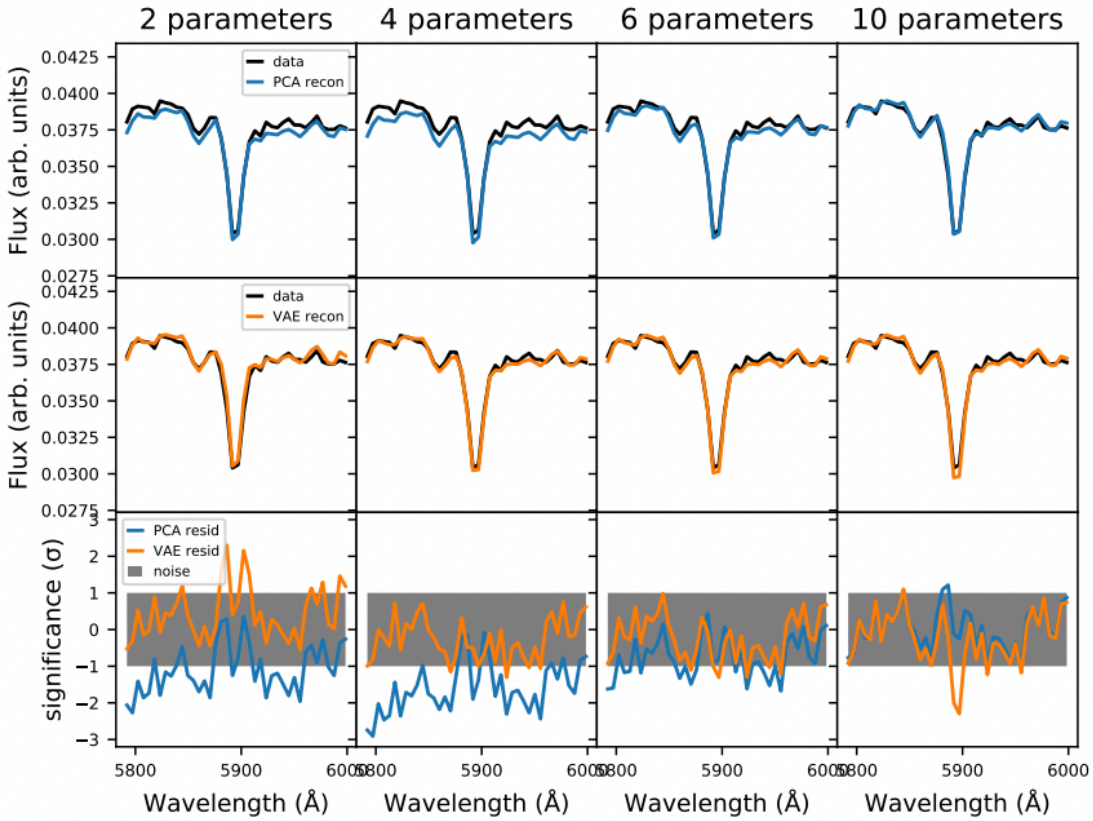
Cluster 21: lensing: 0.9448 non: 0.0552 F_len: 0.0695
Cluster 1: lensing: 0.9159 non: 0.0841 F_len: 0.0731
Cluster 6: lensing: 0.8997 non: 0.1003 F_len: 0.0729
Cluster 2: lensing: 0.803 non: 0.197 F_len: 0.1945
Cluster 20: lensing: 0.6206 non: 0.3794 F_len: 0.0575
Cluster 5: lensing: 0.6170 non: 0.3830 F_len: 0.0734


dense
128
dense
64
reshape
4x4x8
conv6
stride=3
(padding=same)
4x4x8
uppooling
stride=2
8x8x8
uppooling
stride=2
16x16x16
conv7
stride=3
(padding=same)
8x8x16
conv8
stride=3
(padding=same)
16x16x32
uppooling
stride=2
32x32x32
conv9
stride=3
30x30x64
uppooling
stride=2
60x60x64
conv10
stride=7
54x54x128
uppooling
stride=2
108x108x128
Conv11
(Output)
stride=8
101x101x1


Cluster 14: lensing: 0.0 non: 1.0
Cluster 3: lensing: 0.0037 non: 0.9963
Cluster 8: lensing: 0.0037 non: 0.9963
Cluster 22: lensing: 0.0154 non: 0.9846
Cluster 16: lensing: 0.0219 non: 0.9781
Cluster 4: lensing: 0.0431 non: 0.9569
Cluster 0: lensing: 0.2642 non: 0.7358
Cluster 18: lensing: 0.3132 non: 0.6868
Cluster 19: lensing: 0.3601 non: 0.6399
Cluster 13: lensing: 0.3731 non: 0.6269
Cluster 9: lensing: 0.3769 non: 0.6231

Cheng+20


input
encoder
latent
decoder
output
x_1
x_2
x_3
x_4
e_1
e_2
e_3
z_1
z_2
d_1
d_2
d_3
x'_1
x'_2
x'_3
x'_4


2 parameters
4 parameters
6 parameters
10 parameters
Flux (arb. units)
data
PCA recon
data
VAE recon
PCA resid
VAE resid
noise
significance (σ)
Wavelength (Å)

Portillo+21

UMAP AND T-SNE ARE ALSO TWO USEFUL TECHNIQUES TO VISUALIZE LARGE DIMENSIONAL SPACES

INSTEAD OF MATRIX FACTORIZATION SUCH AS PCA, THEY ARE BASED ON GRAPH LAYOUT

1. WE BUILD A GRAPH OF OUR HIGH-DIMENSIONALITY DATA

2. WE OPTIMIZE TO GET THE MOST SIMILAR GRAPH IN TWO DIMENSIONS

https://lvdmaaten.github.io/tsne/

https://umap-learn.readthedocs.io/en/latest/how_umap_works.html

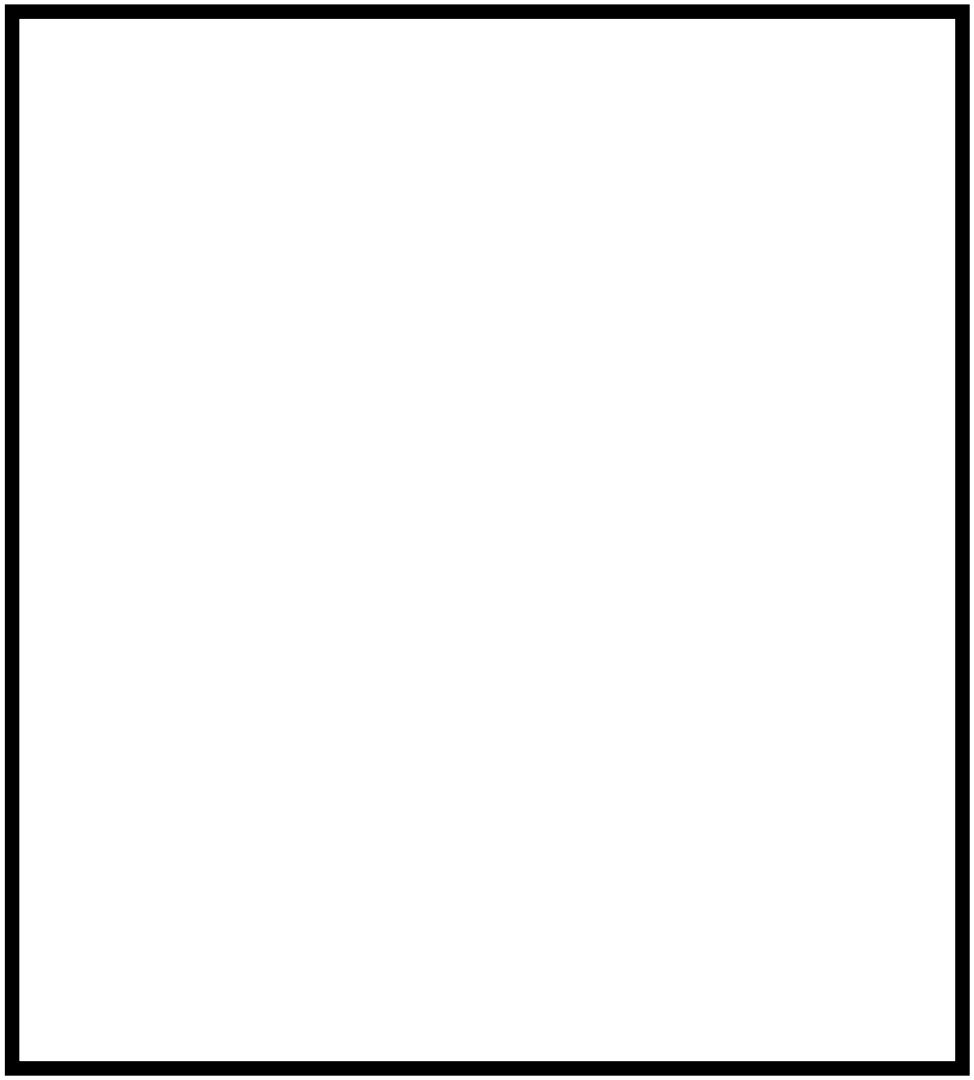
UMAP EXAMPLES AND EXPLANATIONS;

https://pair-code.github.io/understanding-umap/#:~:text=In%20the%20simplest%20sense%2C%20UMAP,behind%20them%20is%20remarkably%20simple.

LEARNING REPRESENTATIONS THROUGH CONTRASTIVE LEARNING

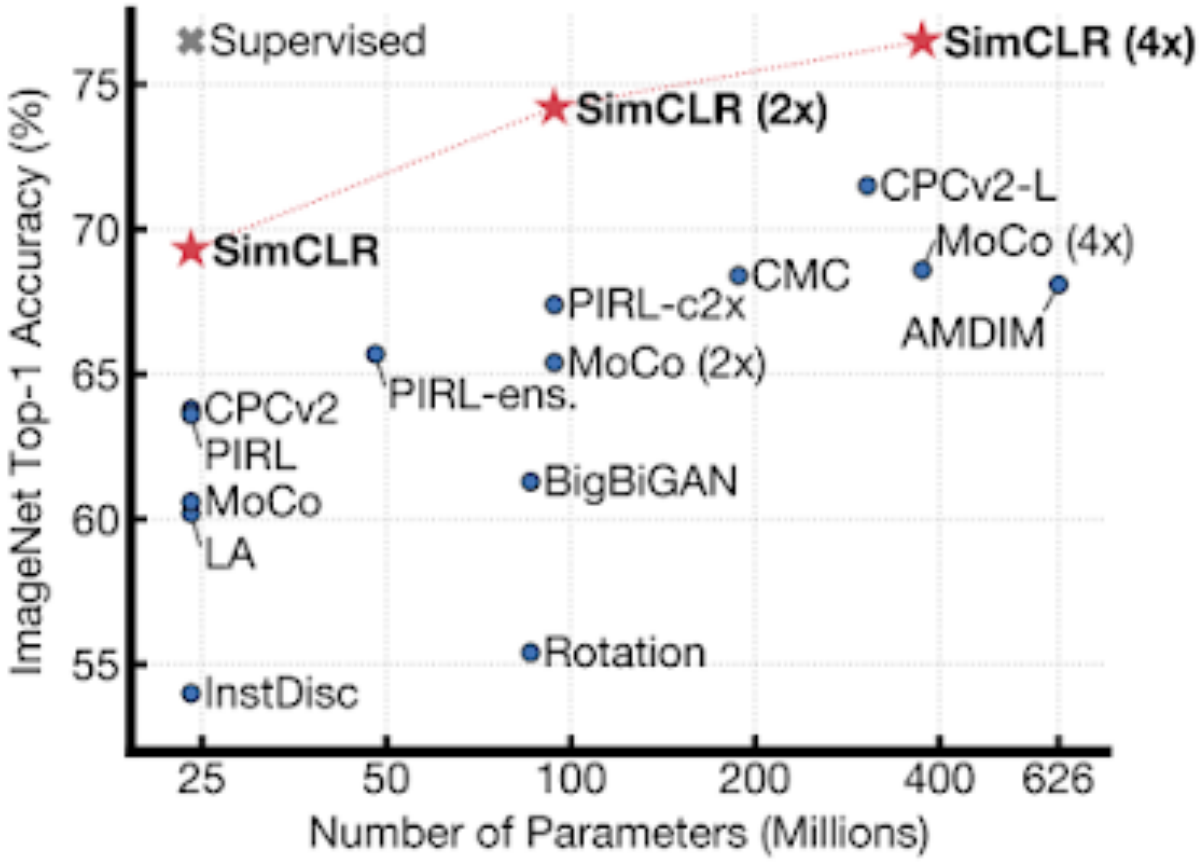
CONTRASTIVE LOSS:

$$l_{i,j} = -\log \frac{\exp(\langle z_i, z_j \rangle / h)}{\Sigma_{k=1,k\neq i}^{2N} \exp(\langle z_i, z_k \rangle / h)},$$

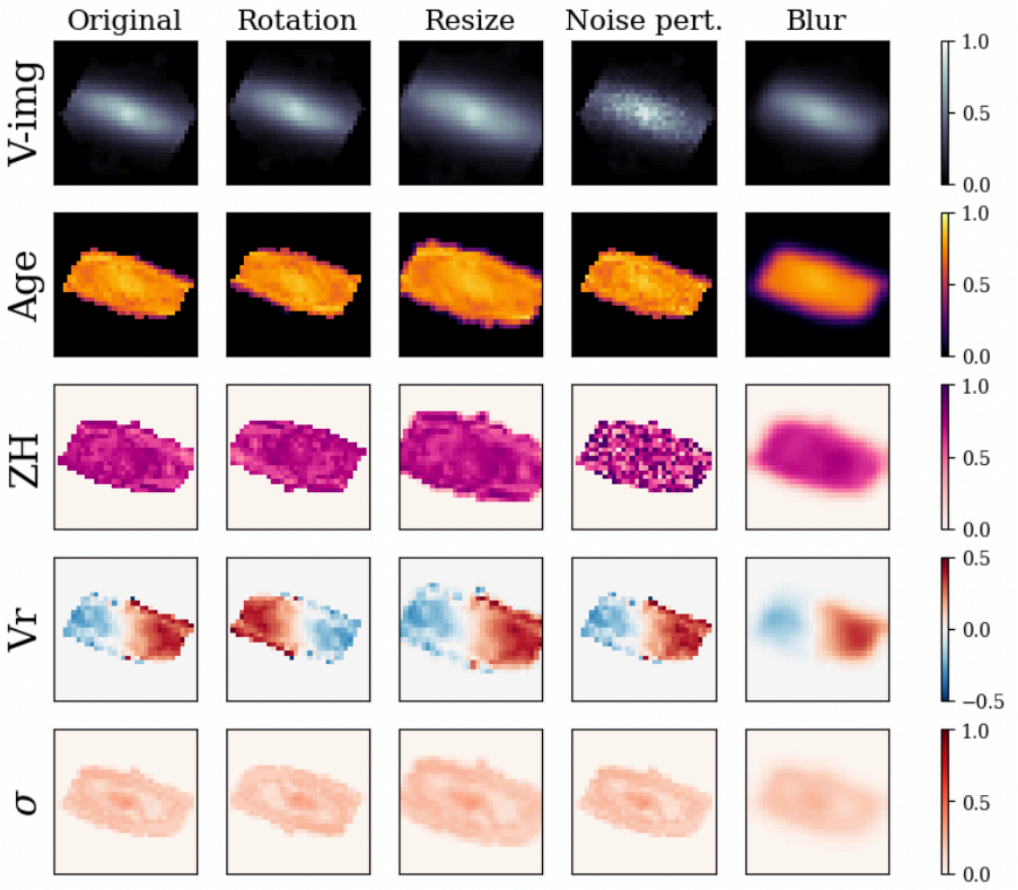


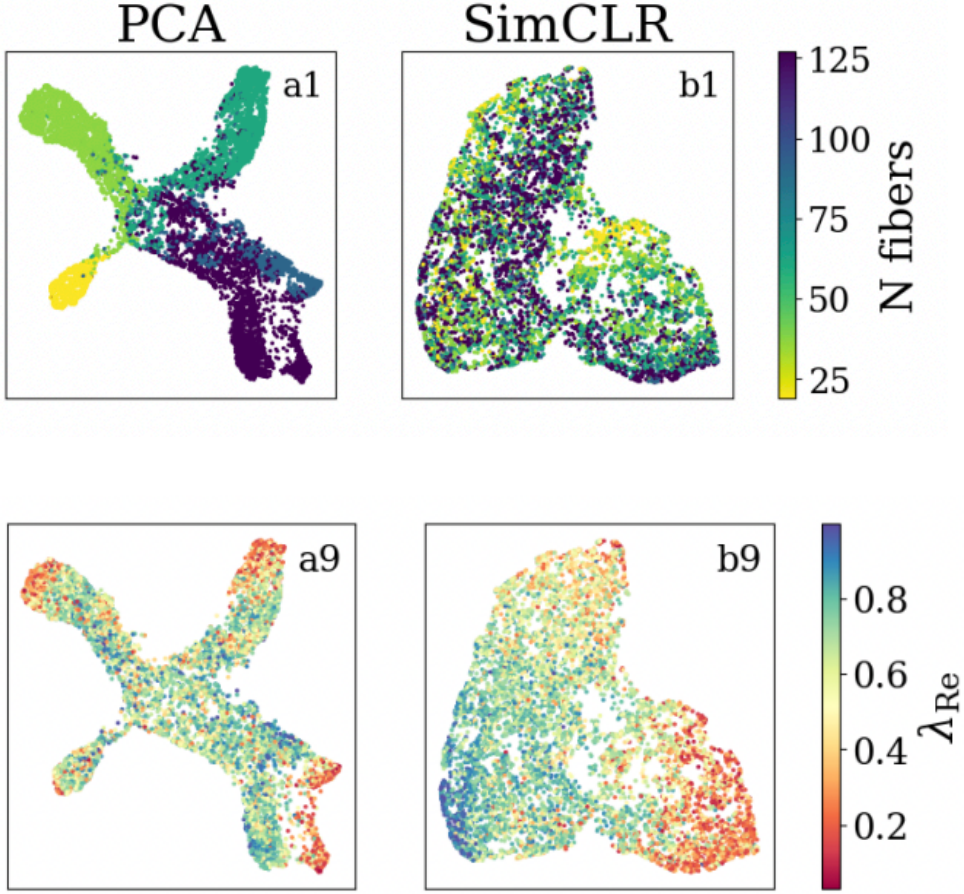
Chen+20

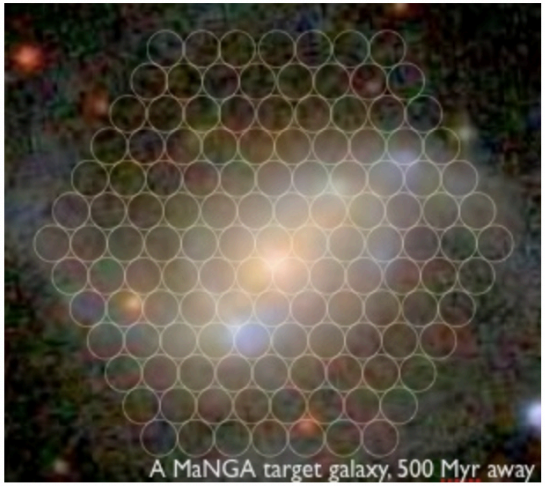
SELF-SUPERVISED LEARNING REACHES COMPARABLE ACCURACY TO FULLY SUPERVISED APPROACHES…



Chen+20







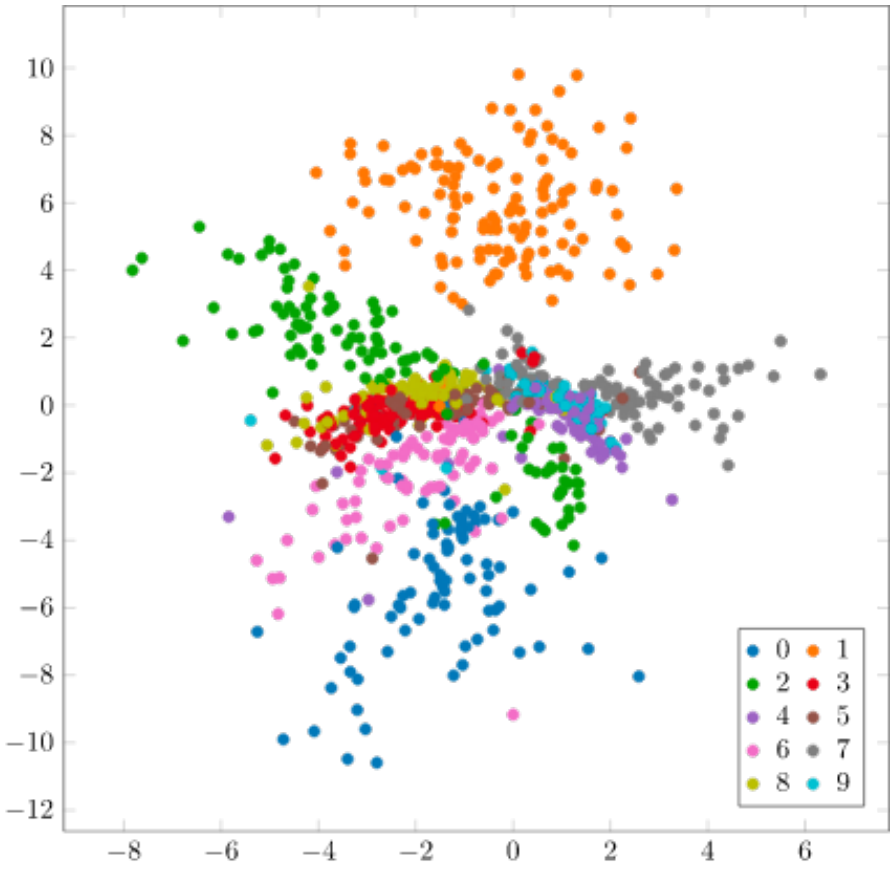
Contrastive learning representation of Manga galaxies

Sarmiento+21

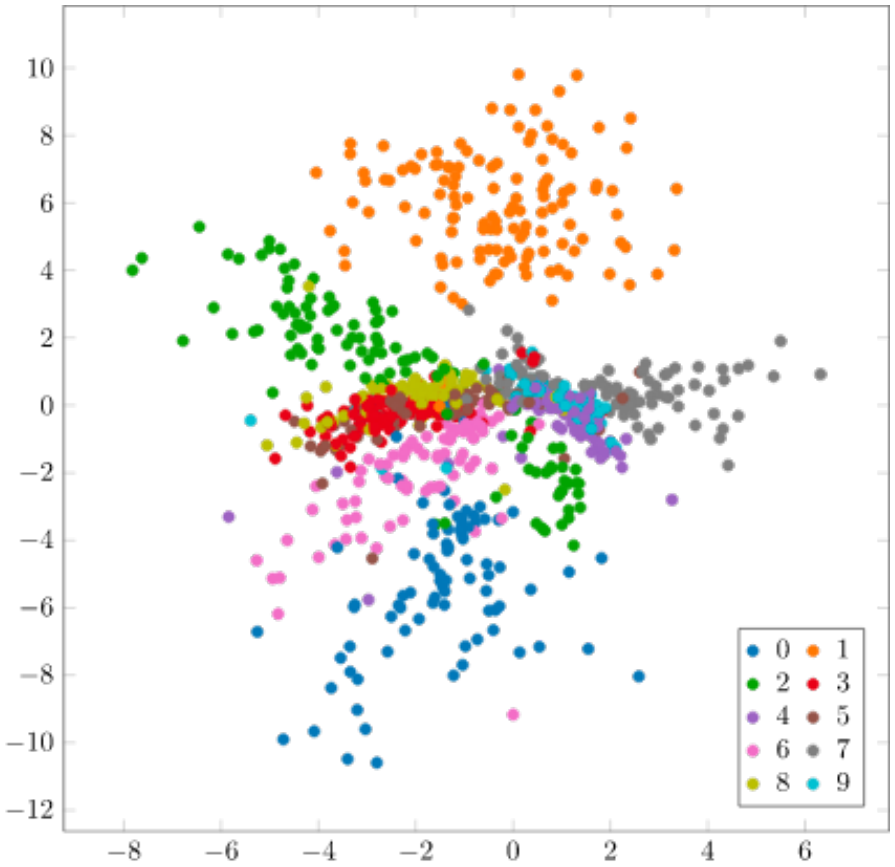
HOW MIGHT YOU SOLVE THESE RELATED PROBLEMS ONCE YOU HAVE THE LATENT SPACE COORDINATES FOR YOUR TRAINING SAMPLE?

GENERATE A RANDOM SAMPLE DRAWN FROM THE INPUT DISTRIBUTION ("**GENERATIVE MODEL**")

ESTIMATE THE PROBABILITY DENSITY OF AN ARBITRARY INPUT, RELATIVE TO THE INPUT DISTRIBUTION ("**PROBABILISTIC MODEL**")



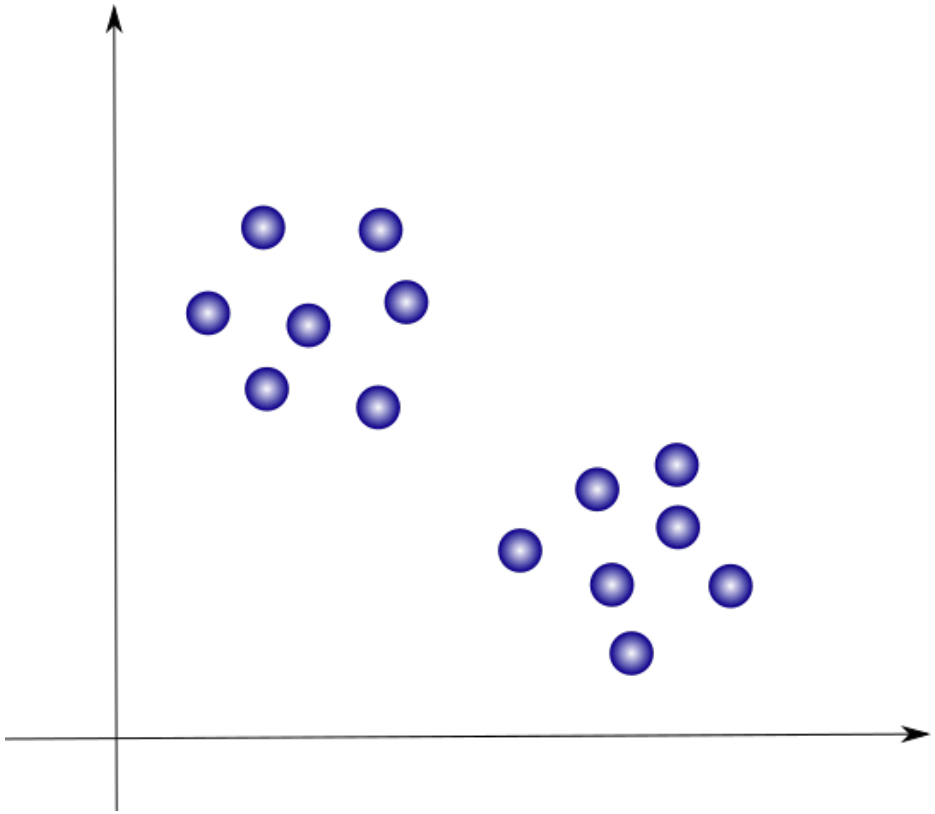
HOW CAN I ESTIMATE P(X)?

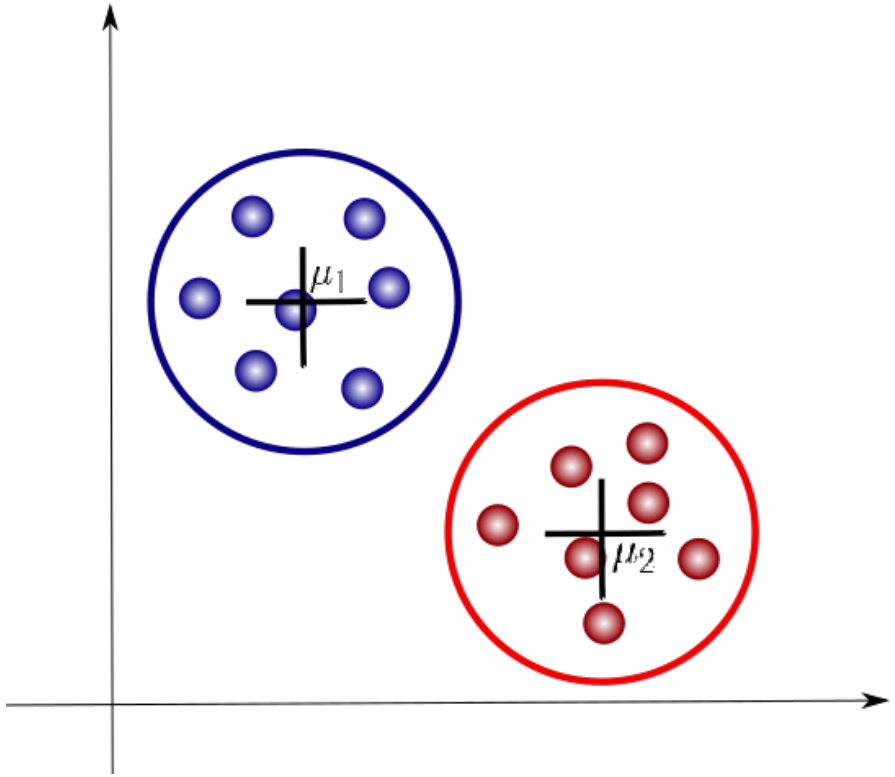


HOW CAN I ESTIMATE P(X)?

WHEN YOU DON'T KNOW, ASSUME IT IS GAUSSIAN….

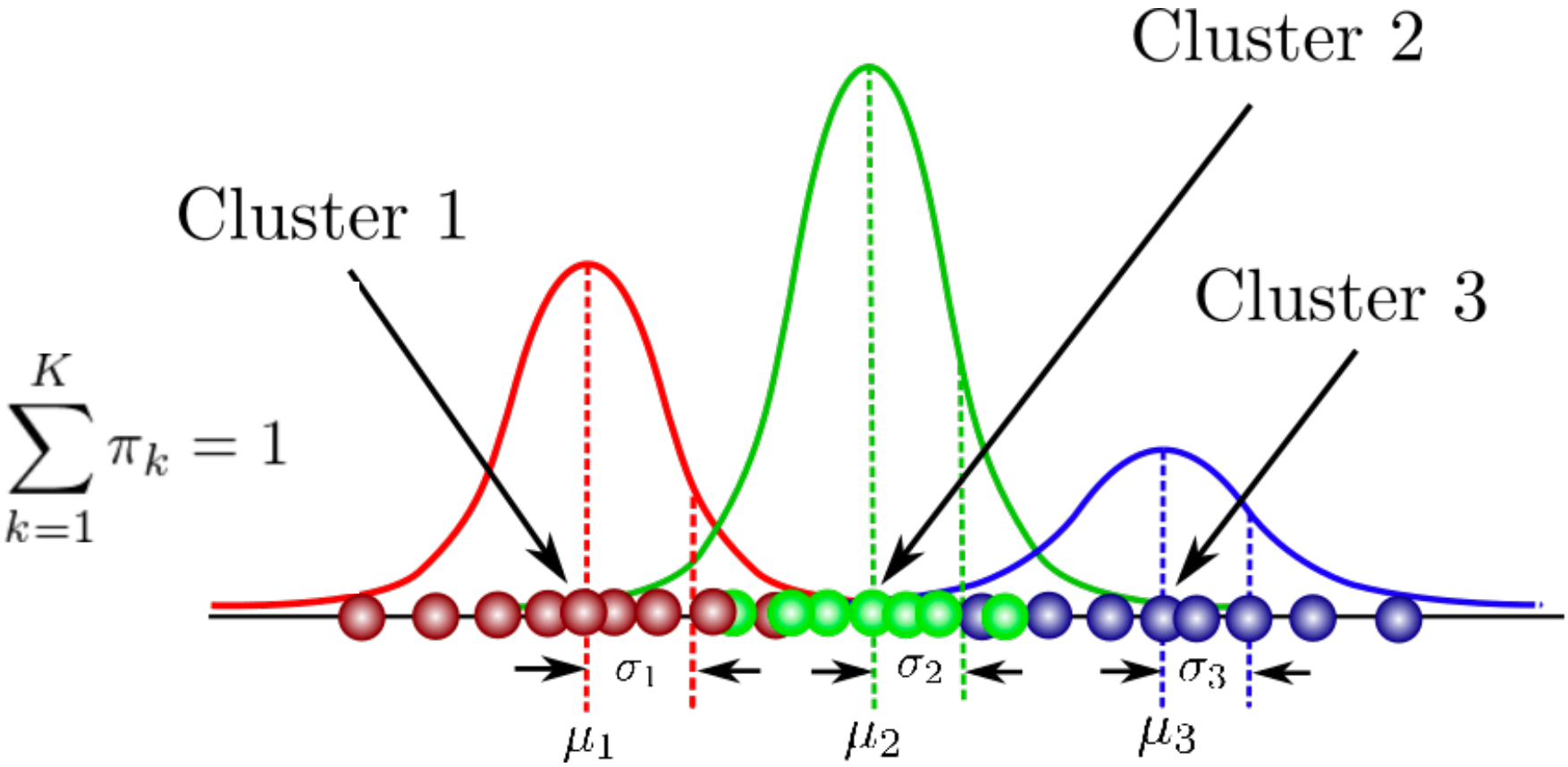
GAUSSIAN MIXTURE MODELS (GMMs) ARE DENSITY ESTIMATOR METHODS THAT FIT MULTIPLE GAUSSIANS TO THE REPRESENTATION





https://towardsdatascience.com/gaussian-mixture-models-explained-6986aaf5a95

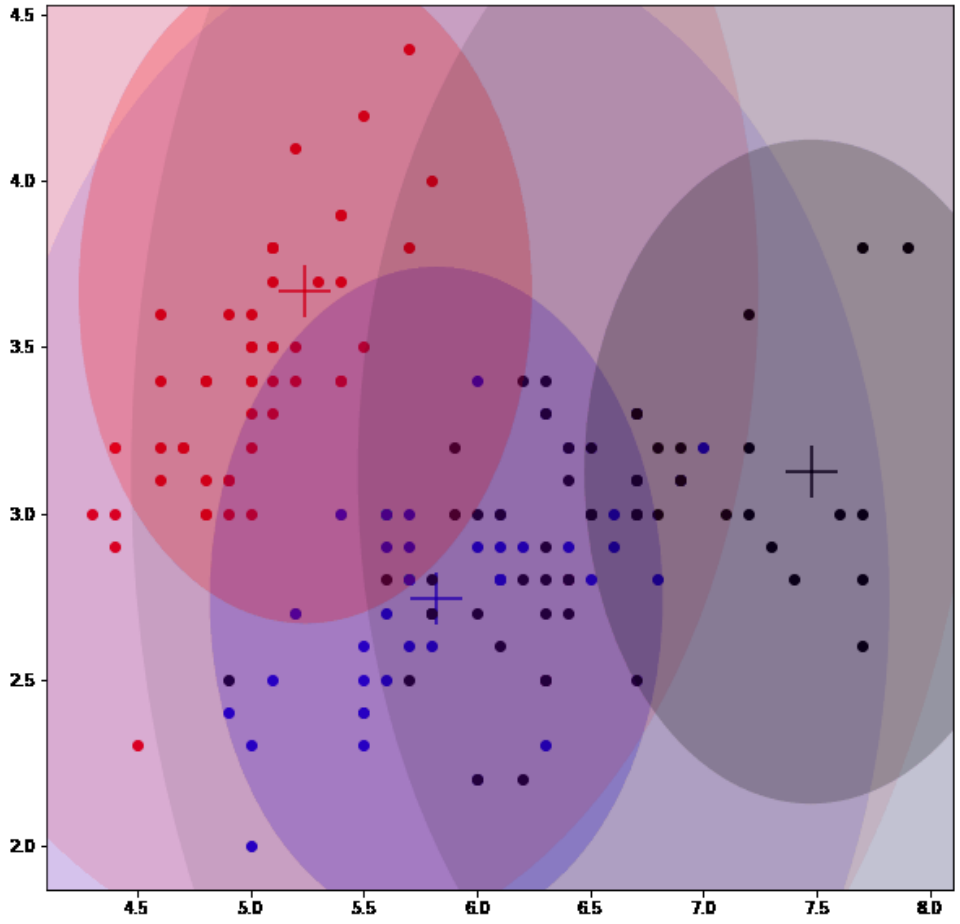
GAUSSIAN MIXTURE MODELS (GMMs) ARE DENSITY ESTIMATOR METHODS THAT FIT MULTIPLE GAUSSIANS TO THE REPRESENTATION



means, sigmas and scale factors of each gaussian are free parameters

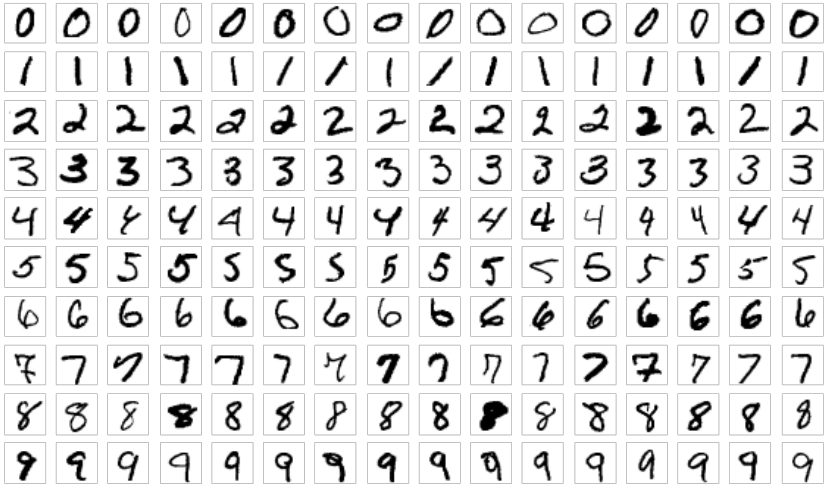
https://towardsdatascience.com/gaussian-mixture-models-explained-6986aaf5a95

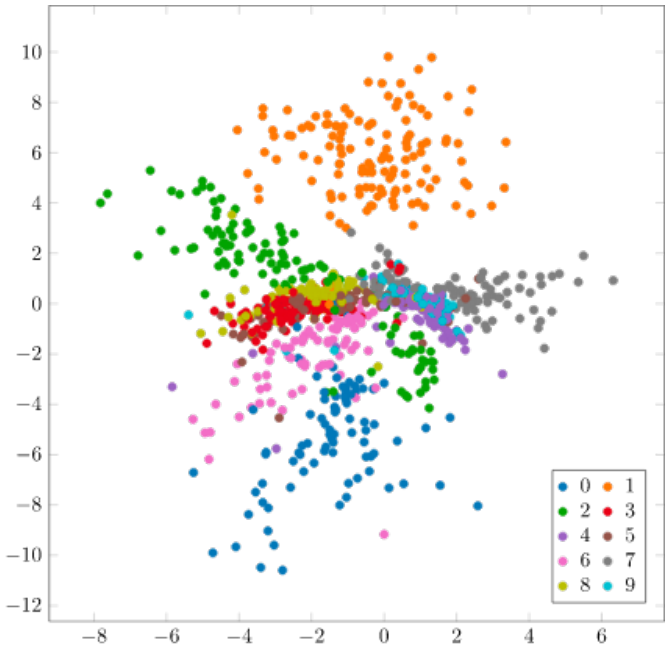
GAUSSIAN MIXTURE MODELS (GMMs) ARE DENSITY ESTIMATOR METHODS THAT FIT MULTIPLE GAUSSIANS TO THE REPRESENTATION



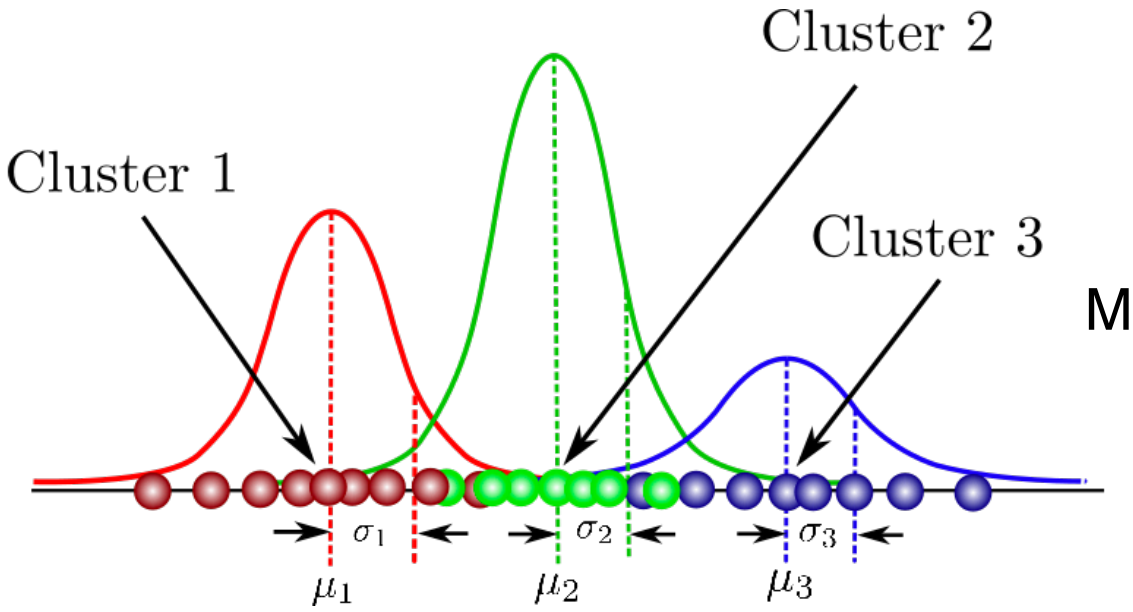
https://towardsdatascience.com/gaussian-mixture-models-explained-6986aaf5a95

DATA



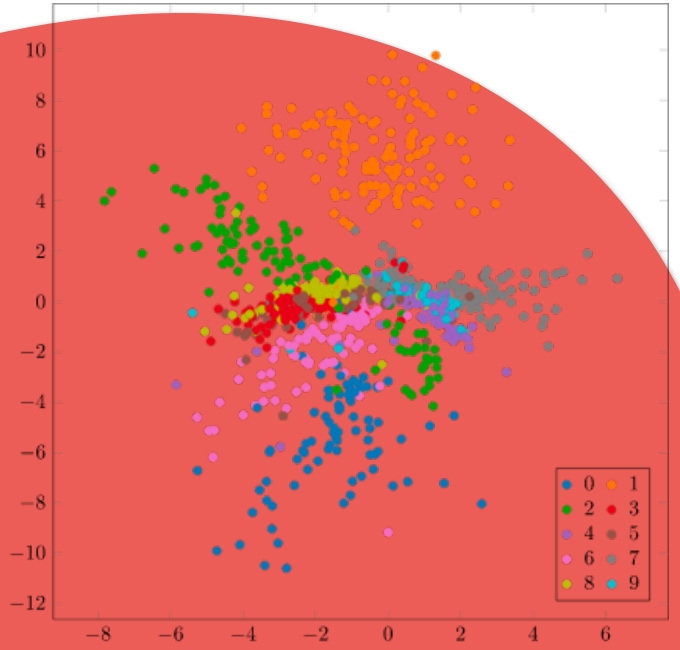


REPRESENTATION
(AUTOENCODER)



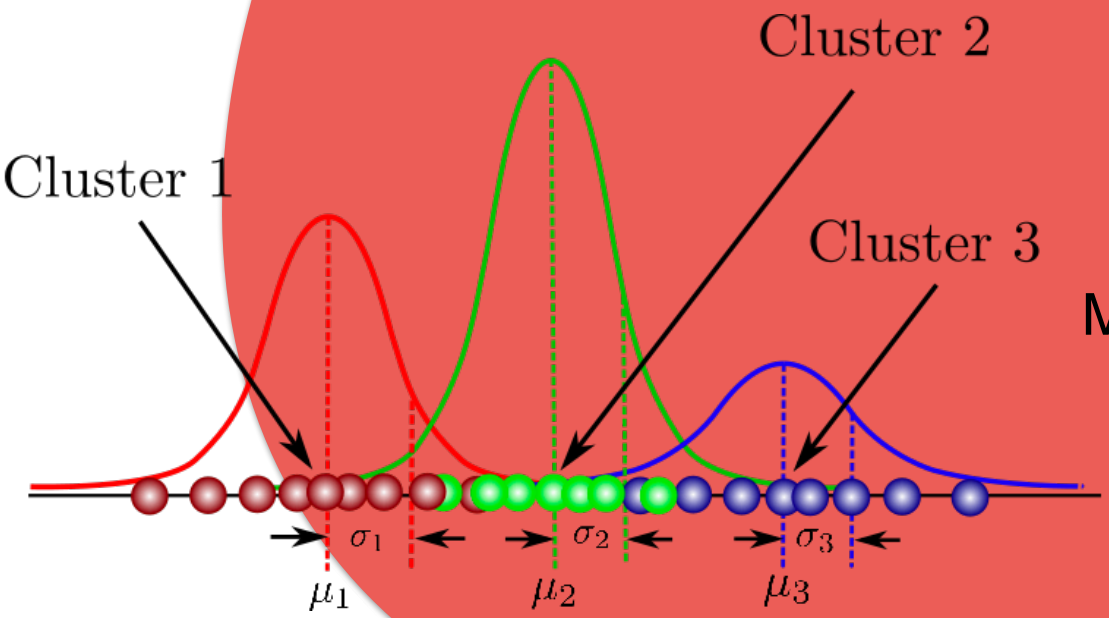
MODELING OF P(X) WITH GMMs

DATA



REPRESENTATION
(AUTOENCODER)

WE COMBINE THESE 2 STEPS?



MODELING OF P(X) WITH GMMs

Much of the recent progress in unsupervised deep learning has been to invent network architectures that are capable of solving either or both of these related problems directly, without resorting to any auxiliary methods

VAE

(VARIATIONAL AUTOENCODER)

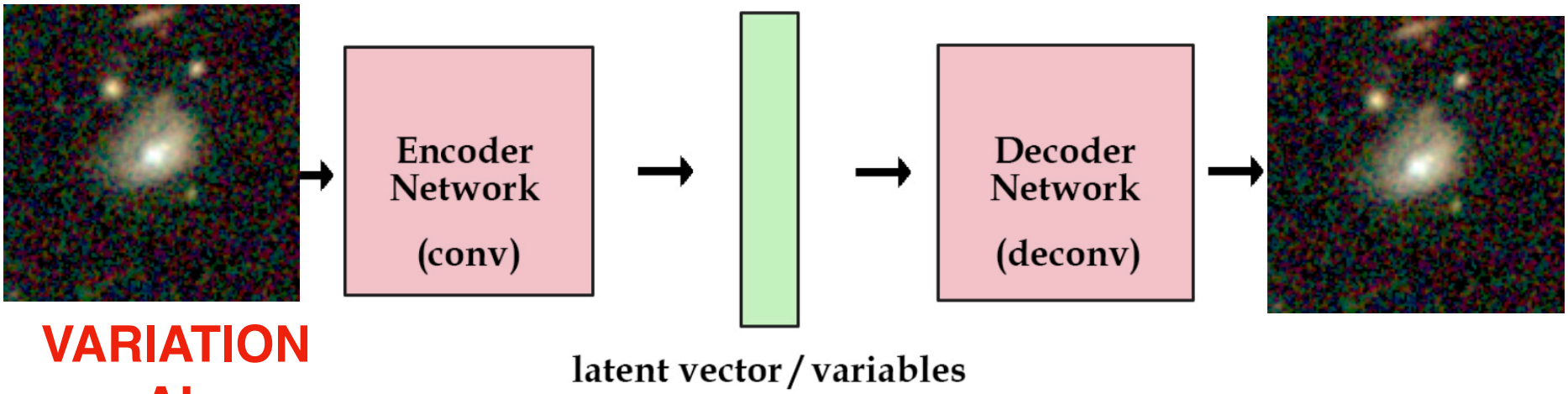
GAN

(GENERATIVE ADVERSARIAL NETOWRK)

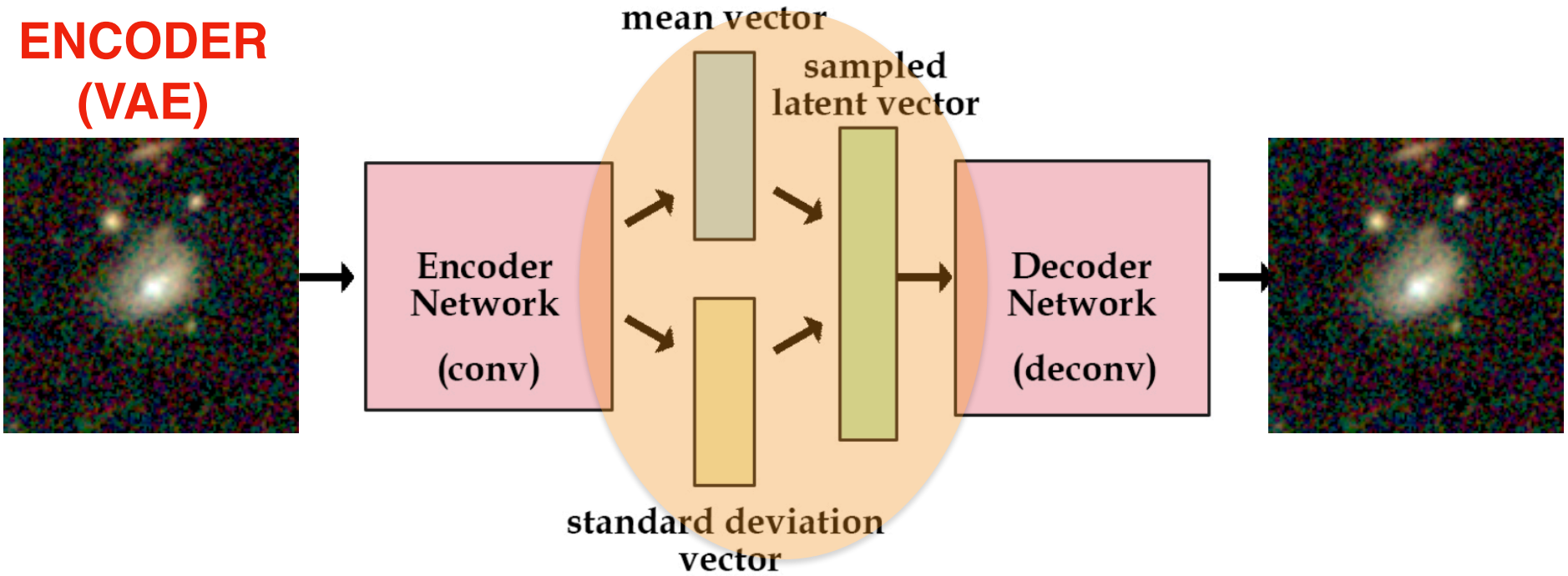
ARF

(AUTOREGRESSIVE FLOWS)

AUTO-ENCODER

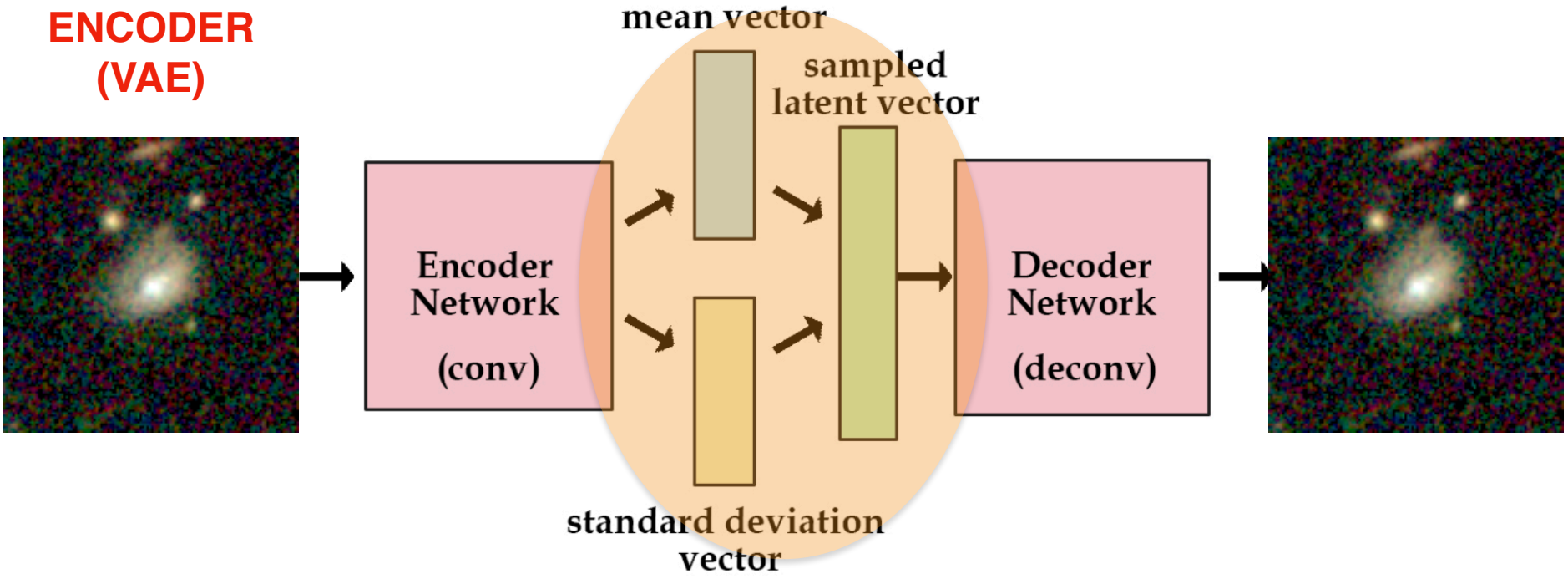


VARIATIONAL AUTO-ENCODER (VAE)



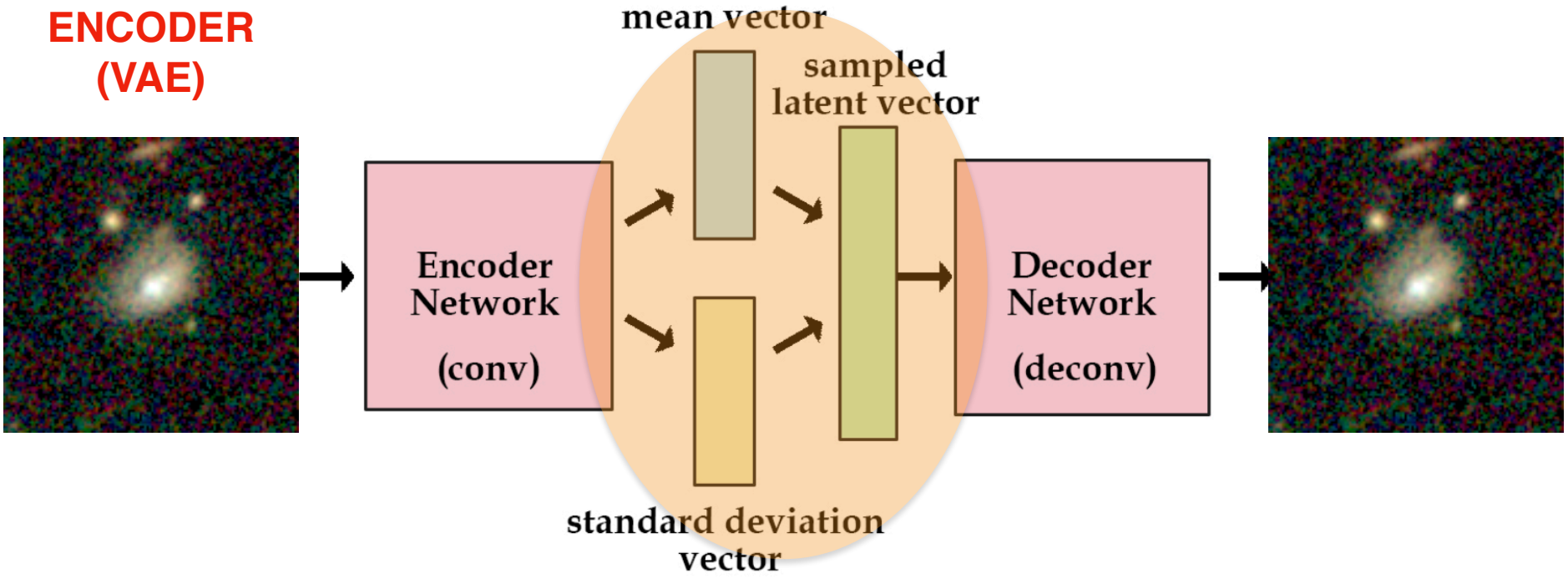
LET'S MODEL THE LATENT SPACE WITH A MIXUTRE OF GAUSSIANS

VARIATIONAL AUTO-ENCODER (VAE)



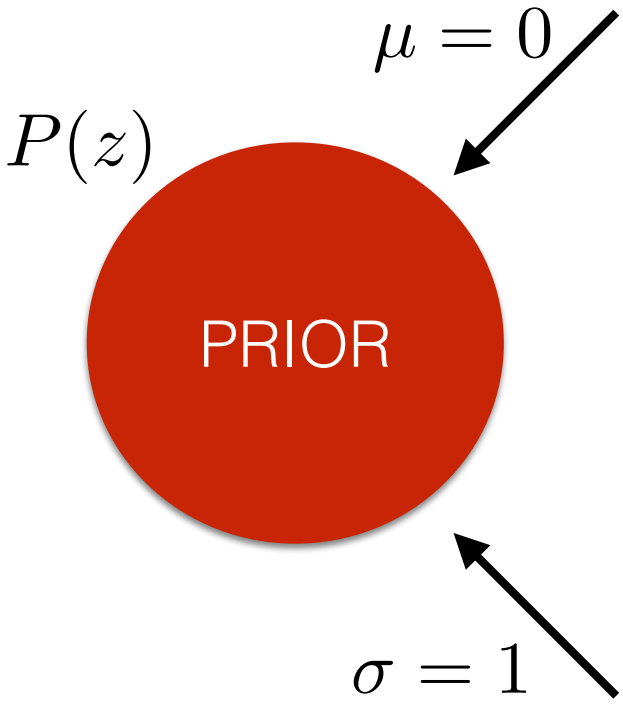
HOWEVER, NOTHING GUARANTEES US THAT THE LATENT SPACE CAN BE MODELLED BY A MIXTURE OF GAUSSIANS….

VARIATIONAL AUTO-ENCODER (VAE)

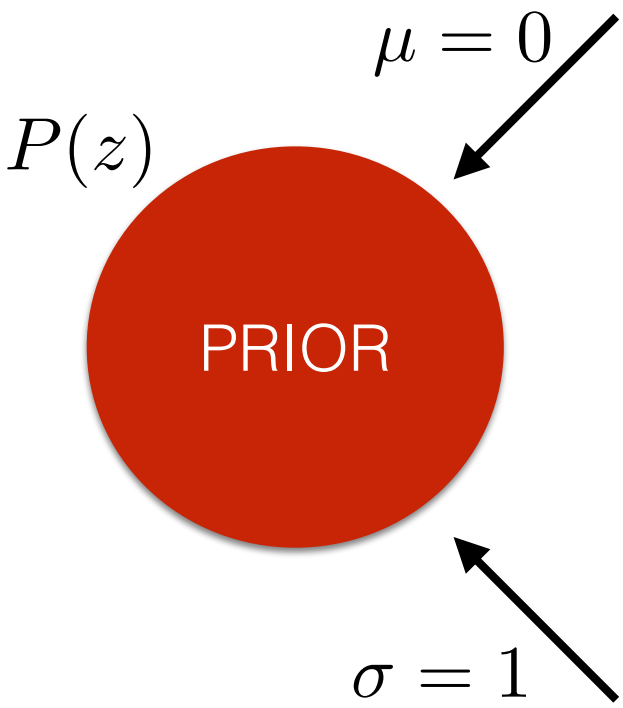


HOWEVER, NOTHING GUARANTEES US THAT THE LATENT SPACE CAN BE MODELLED BY A MIXTURE OF GAUSSIANS….

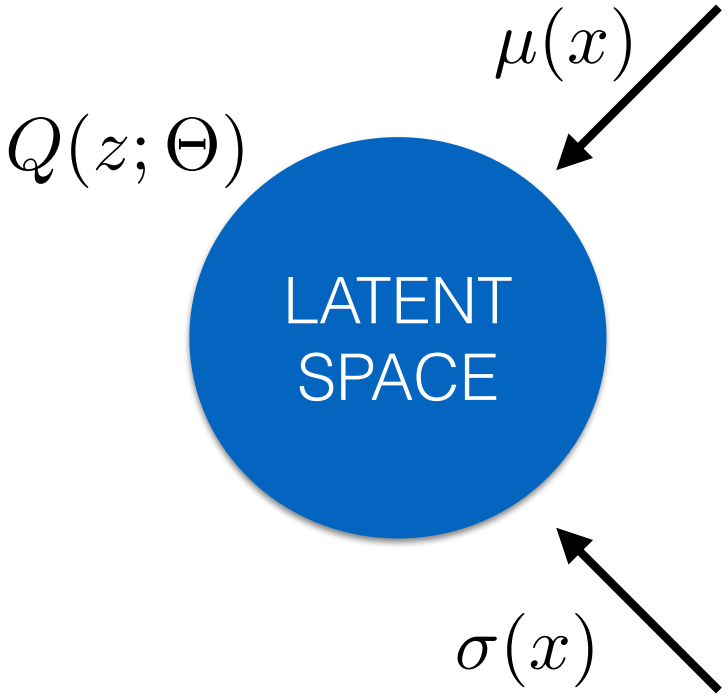
… LET'S FORCE IT TO BE GAUSSIAN LIKE!



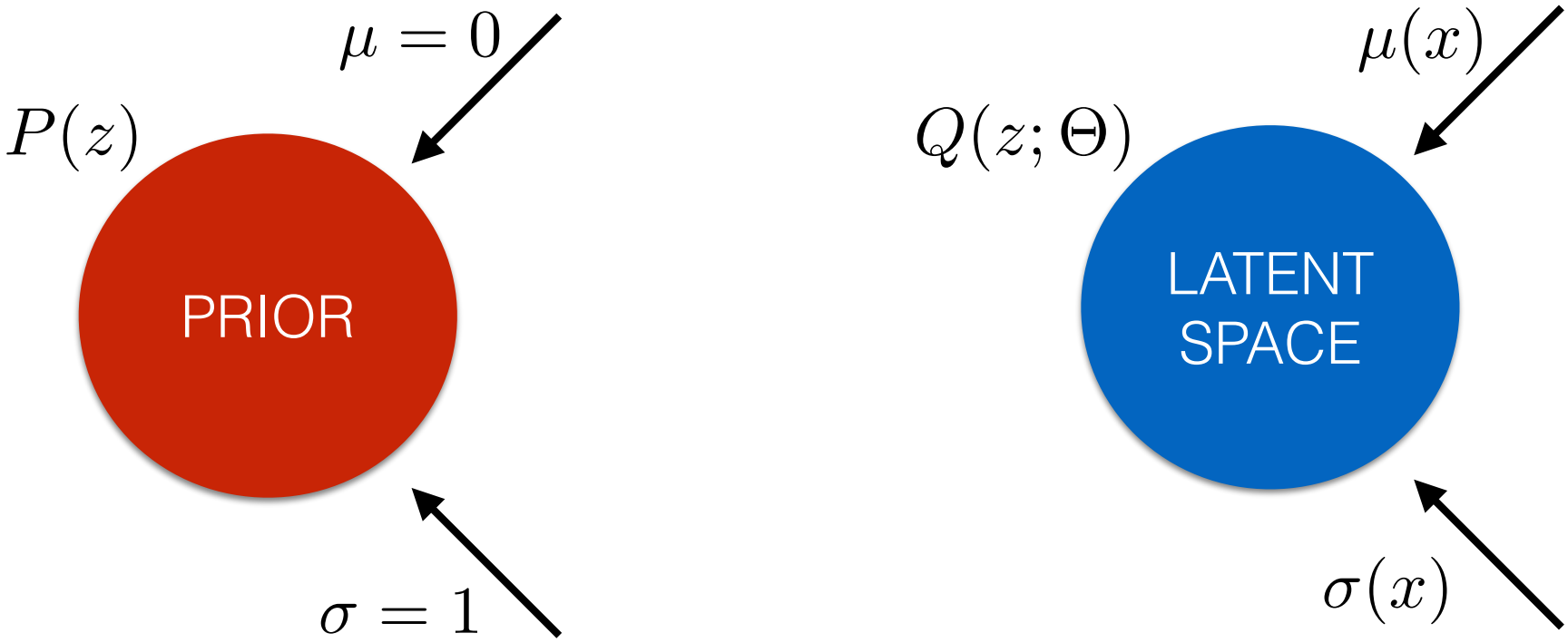
WE ASSUME A SIMPLE PRIOR



WE ASSUME A SIMPLE PRIOR

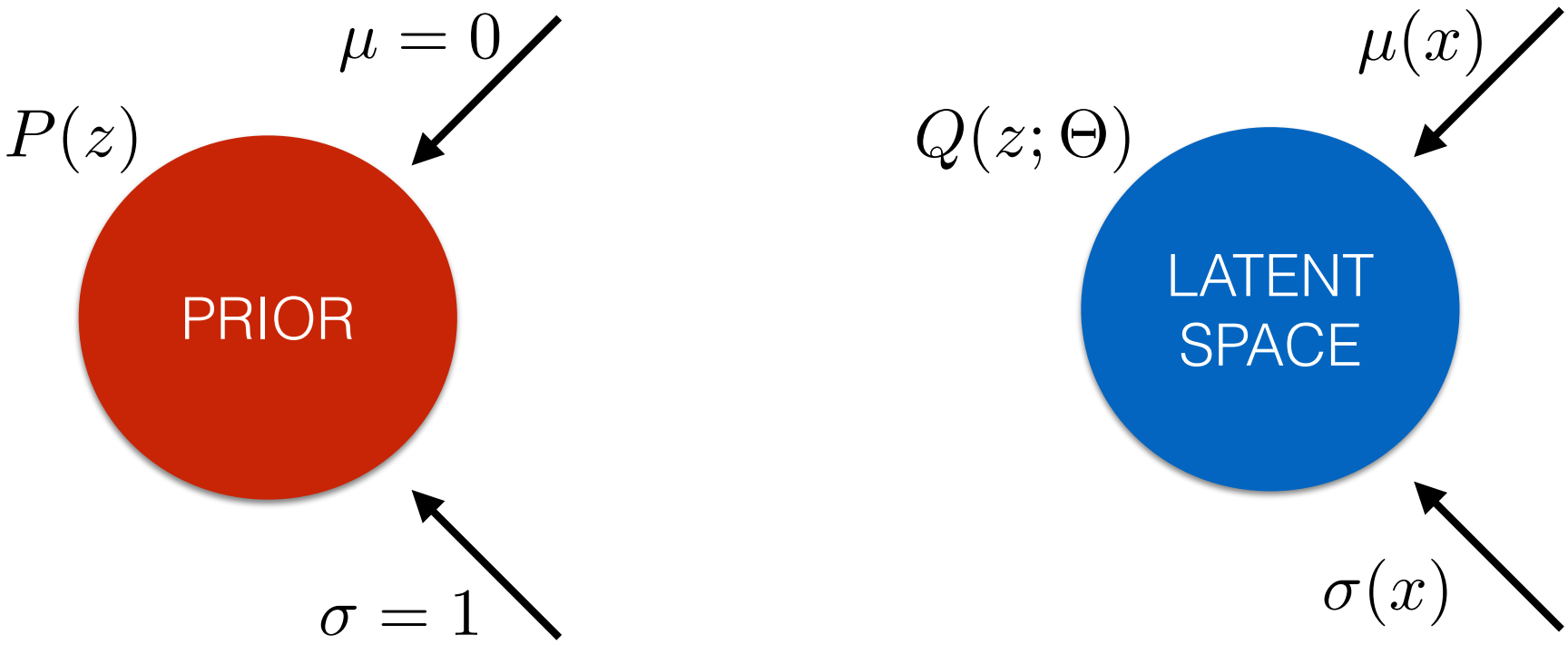


LATENT SPACE MODELING



WE ASSUME A SIMPLE PRIOR ⟺ LATENT SPACE MODELLING

WE WANT Q TO BE CLOSE TO THE PRIOR…



WE ASSUME A SIMPLE PRIOR ⟺ LATENT SPACE MODELLING

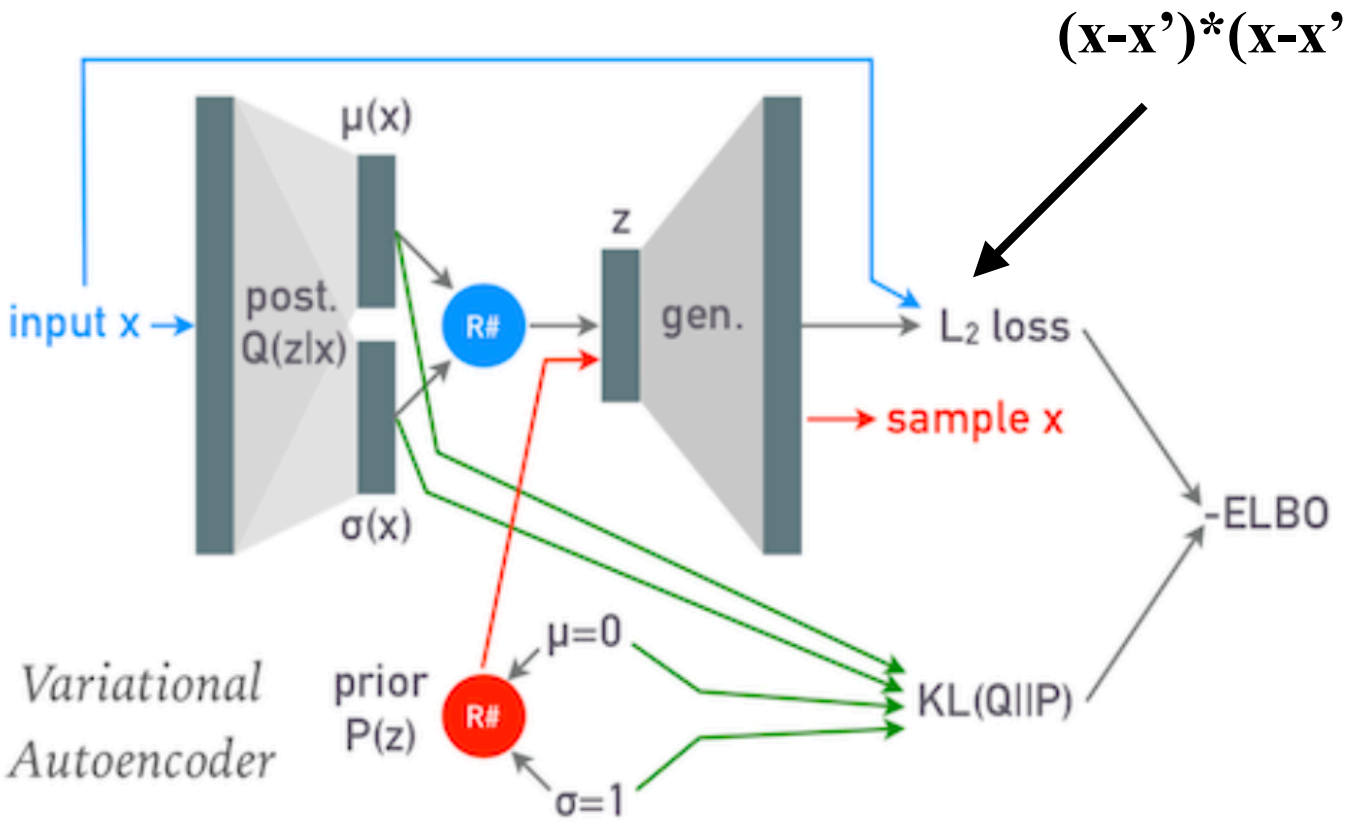
WE WANT Q TO BE CLOSE TO THE PRIOR…

$$D_{\mathrm{KL}}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \log\left(\frac{P(x)}{Q(x)}\right).$$

$$D_{\mathrm{KL}}(P \parallel Q) = \int_{\mathcal{X}} \log\left(\frac{dP}{dQ}\right) \frac{dP}{dQ}\, dQ,$$

WE MINIMIZE THE K-L DIVERGENCE BETWEEN P AND Q

WHAT WOULD BE THEN THE LOSS FUNCTION OF A VAE?

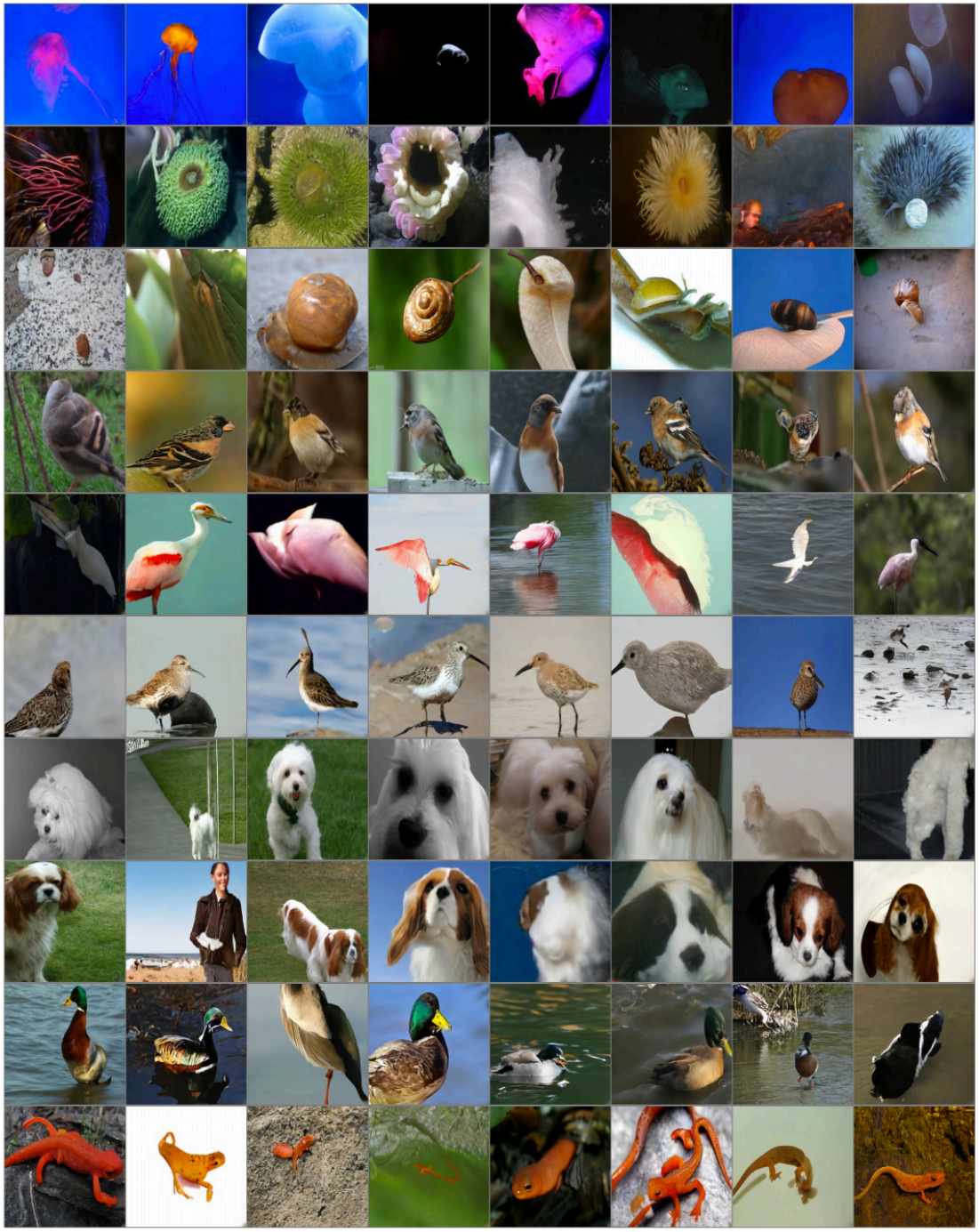


The key insight of VAE is that we are actually performing **variational inference** here, which then tells us what the loss function should be...

$$-\text{ELBO} = \langle \log P(\mathbf{x} \mid \mathbf{z}) \rangle_{z \sim Q} + \text{KL}\left(Q(\mathbf{z}; \Theta) \parallel P(\mathbf{z})\right) \ ,$$

L2 LOSS

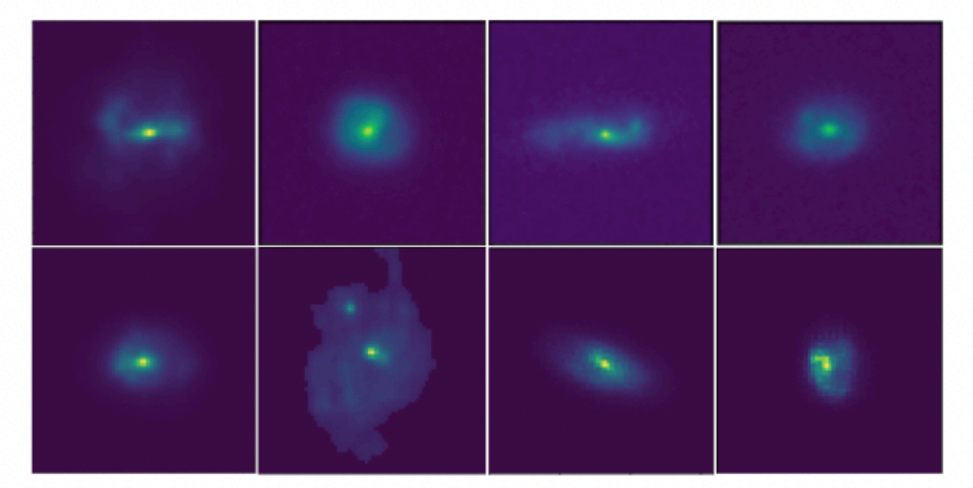
REGULARIZATION TERM



(VQ-VAE)

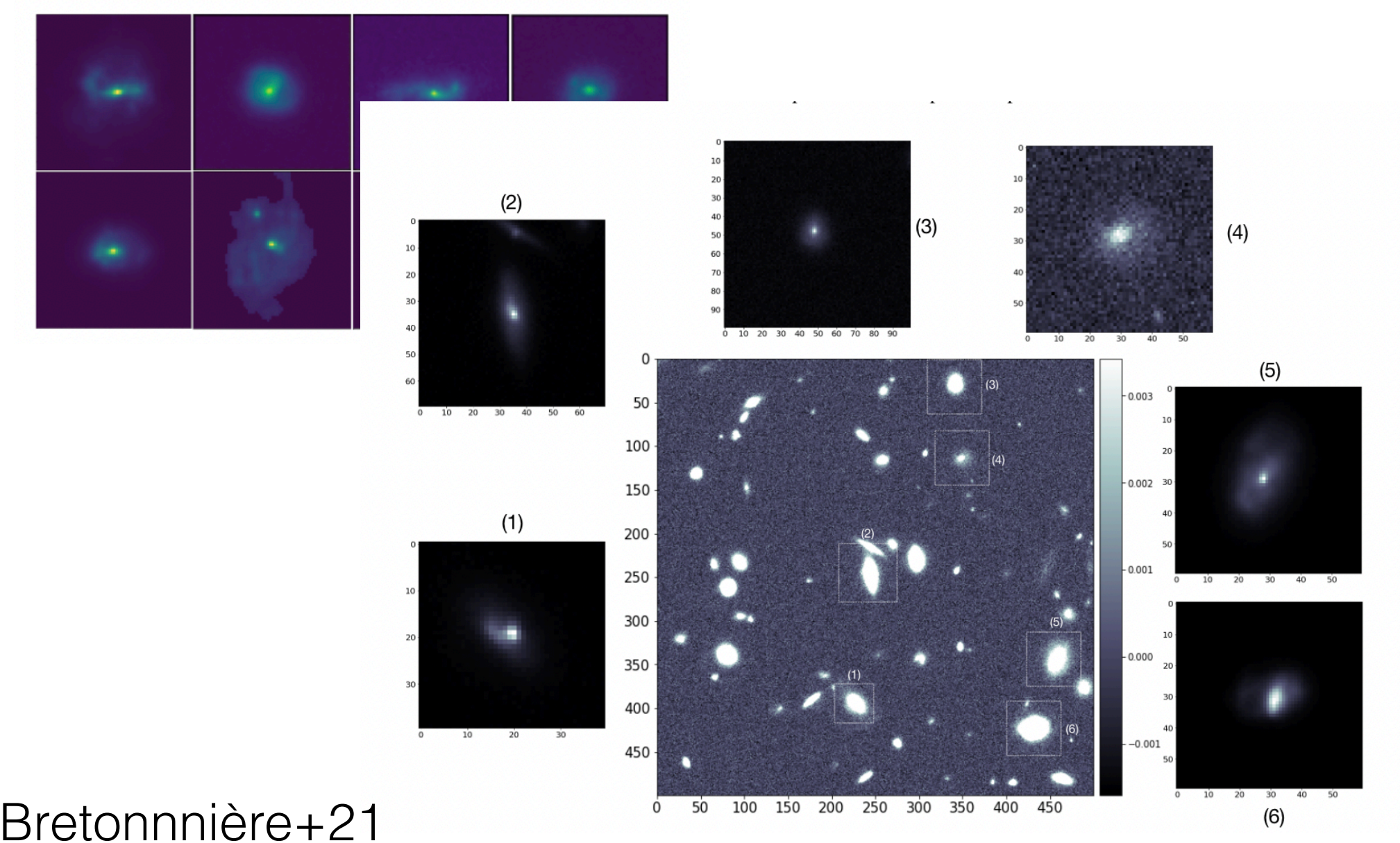
Razavi+19
(deepmind)

VAE GENERATED EUCLID REALSITIC GALAXIES

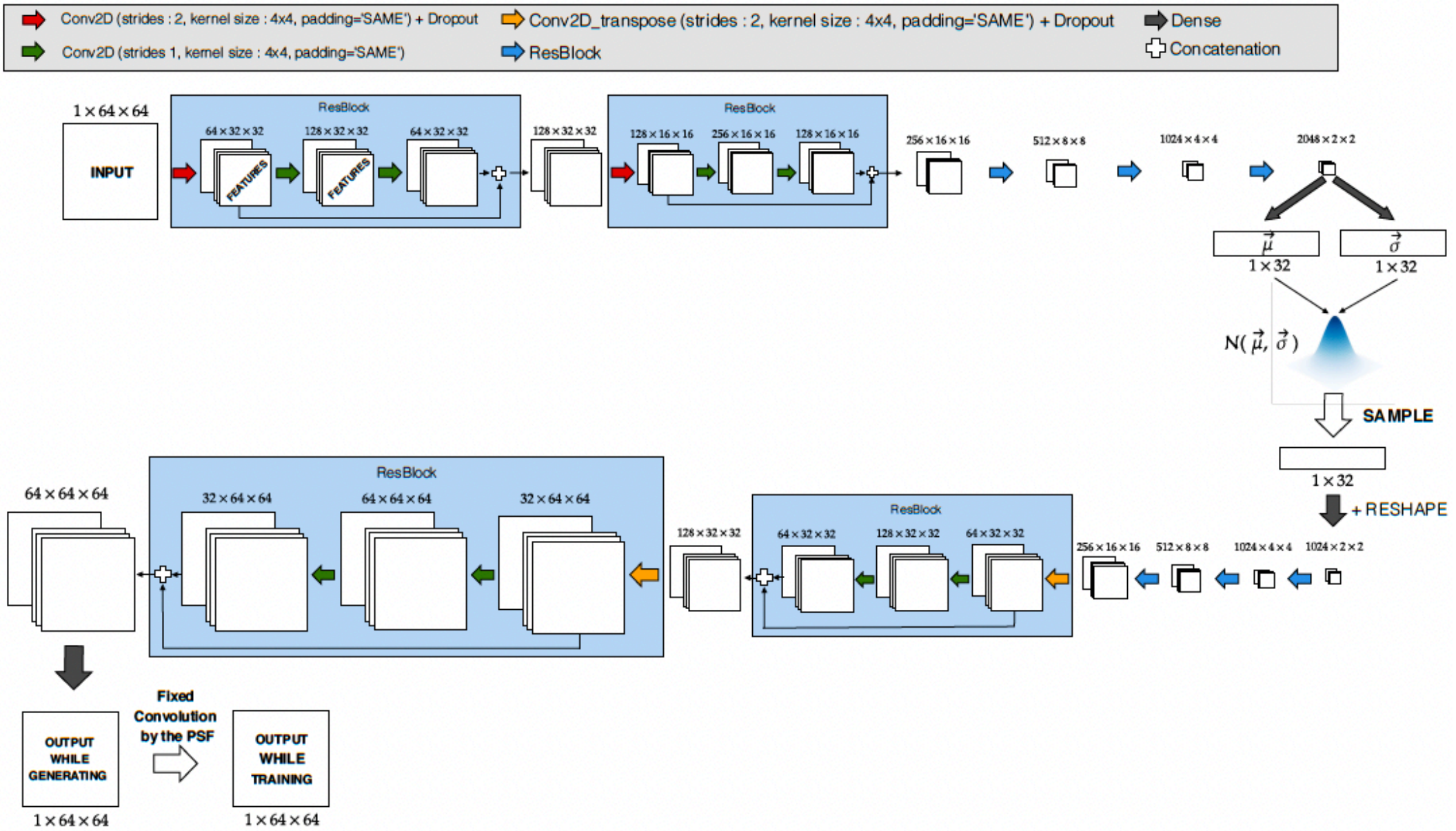


Bretonnnière+21

VAE GENERATED EUCLID REALSITIC GALAXIES



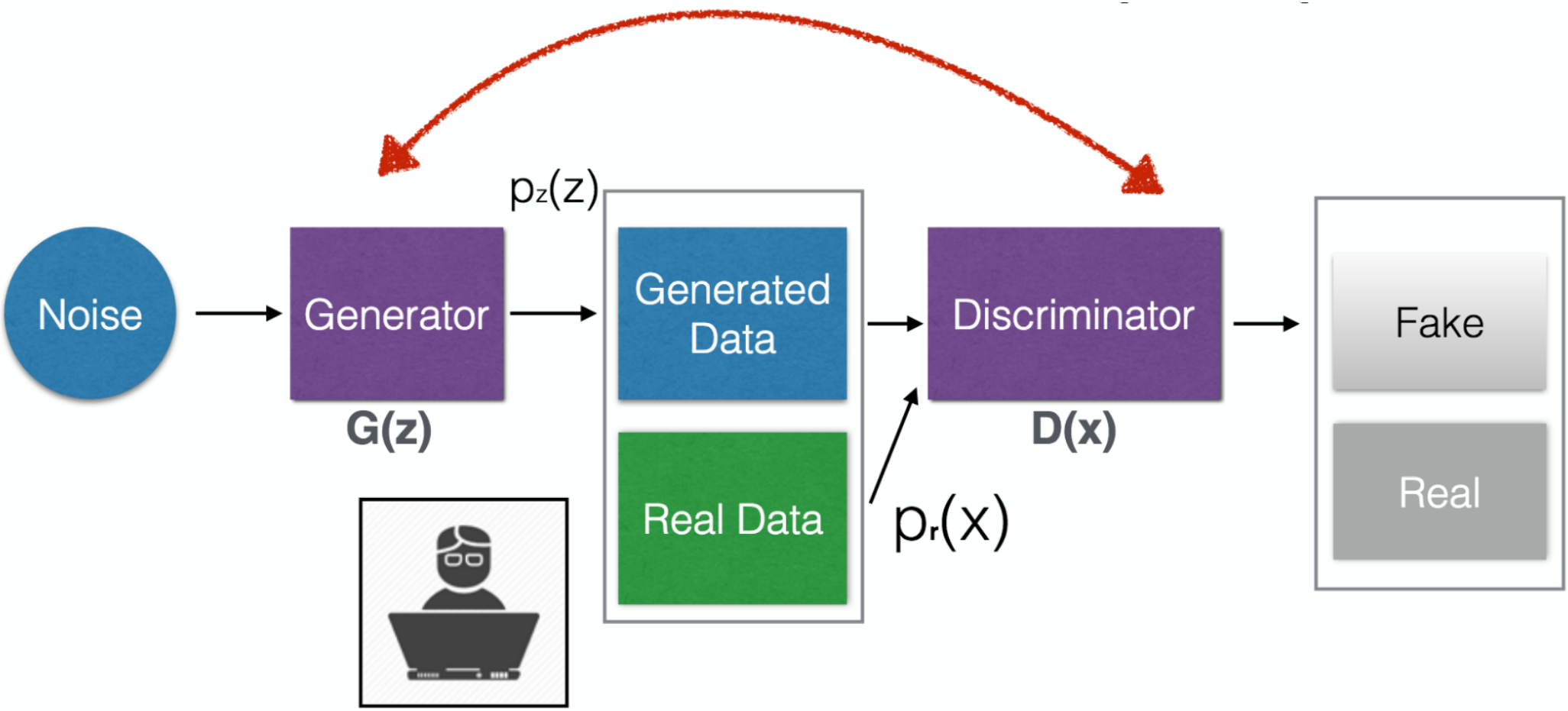
Bretonnnière+21



Bretonnnière+21

GENERATIVE ADVERSARIAL NETWORKS

(Goodfellow+14)

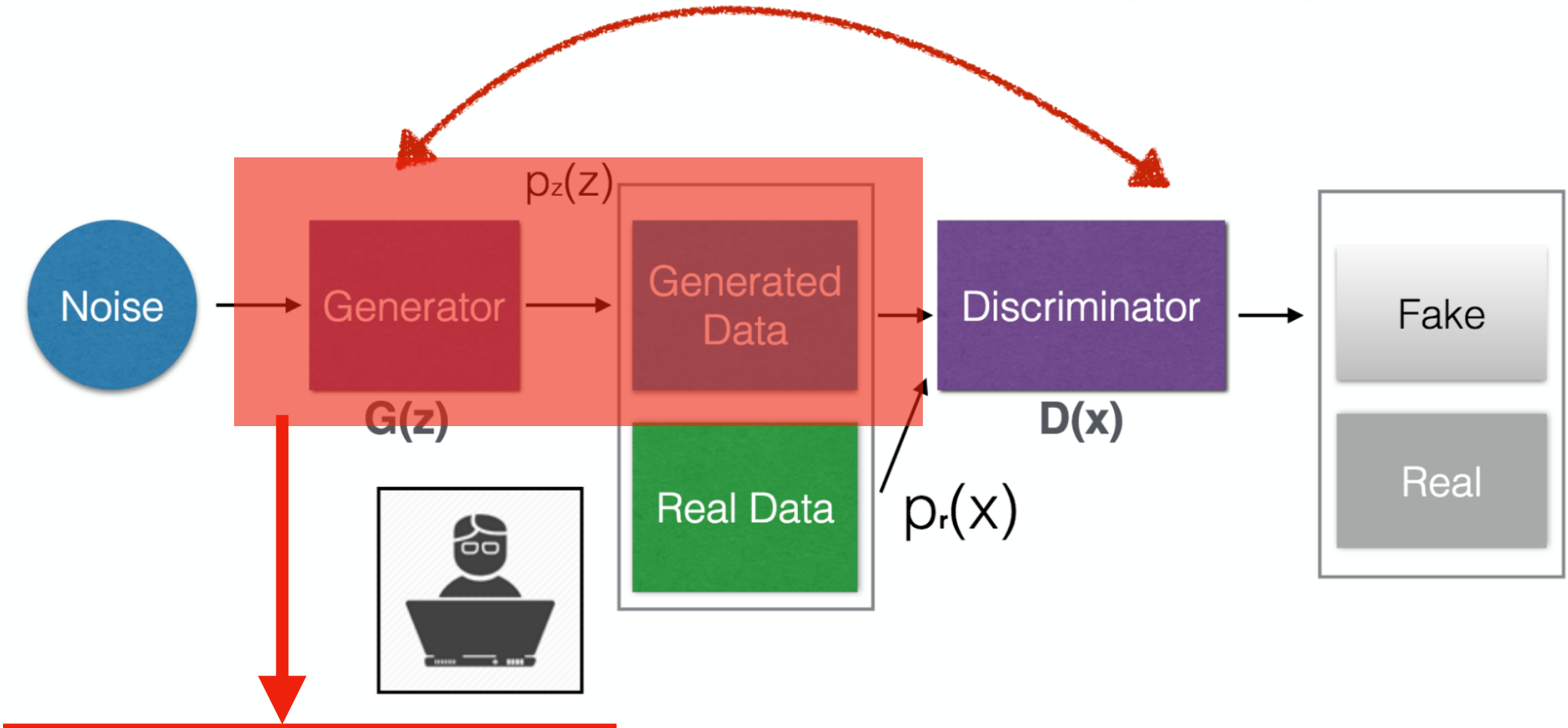


TWO COMPETING NETWORKS

GENERATIVE ADVERSARIAL NETWORKS

(Goodfellow+)

TWO COMPETING NETWORKS

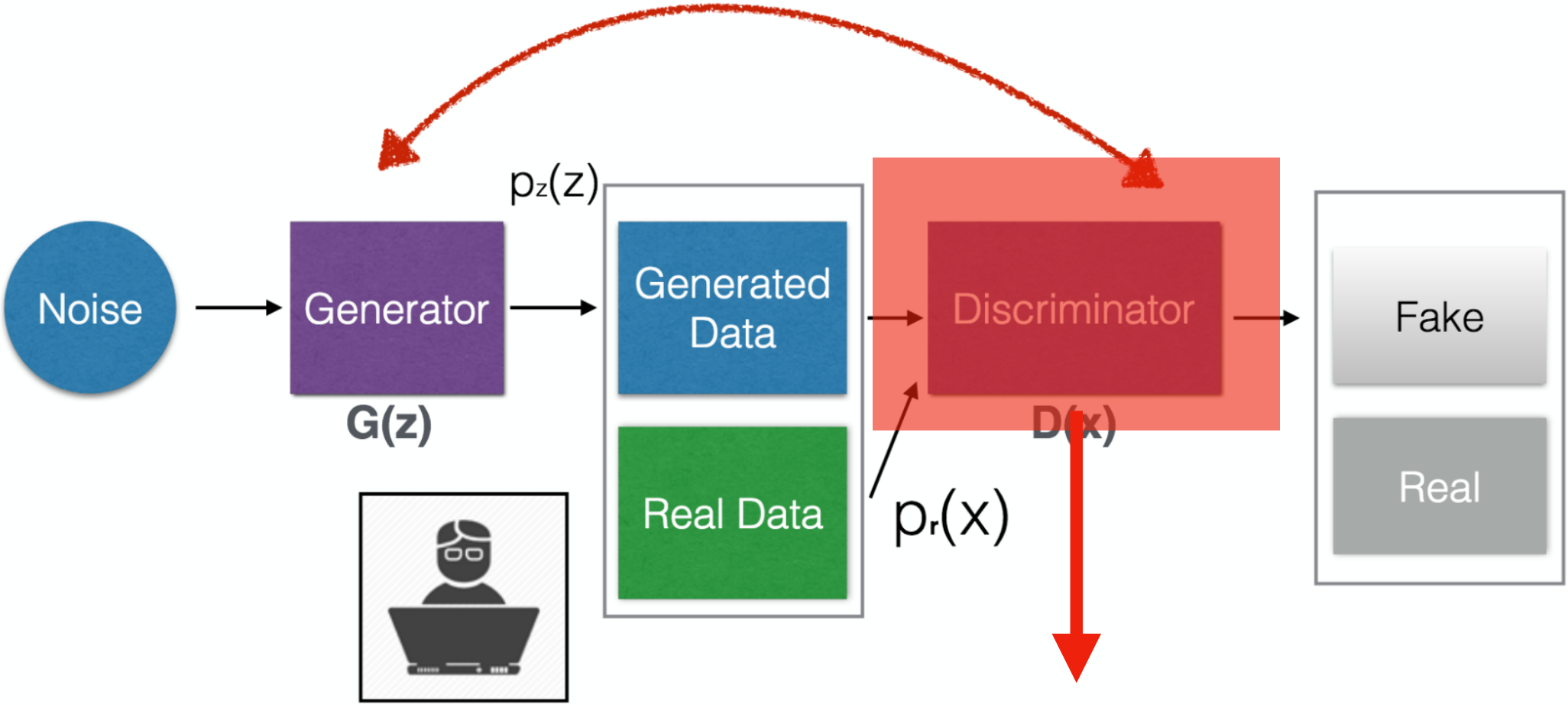


Every N iterations the generator is trained to force the discriminator to classify as real

GENERATIVE ADVERSARIAL NETWORKS

(Goodfellow+)

TWO COMPETING NETWORKS

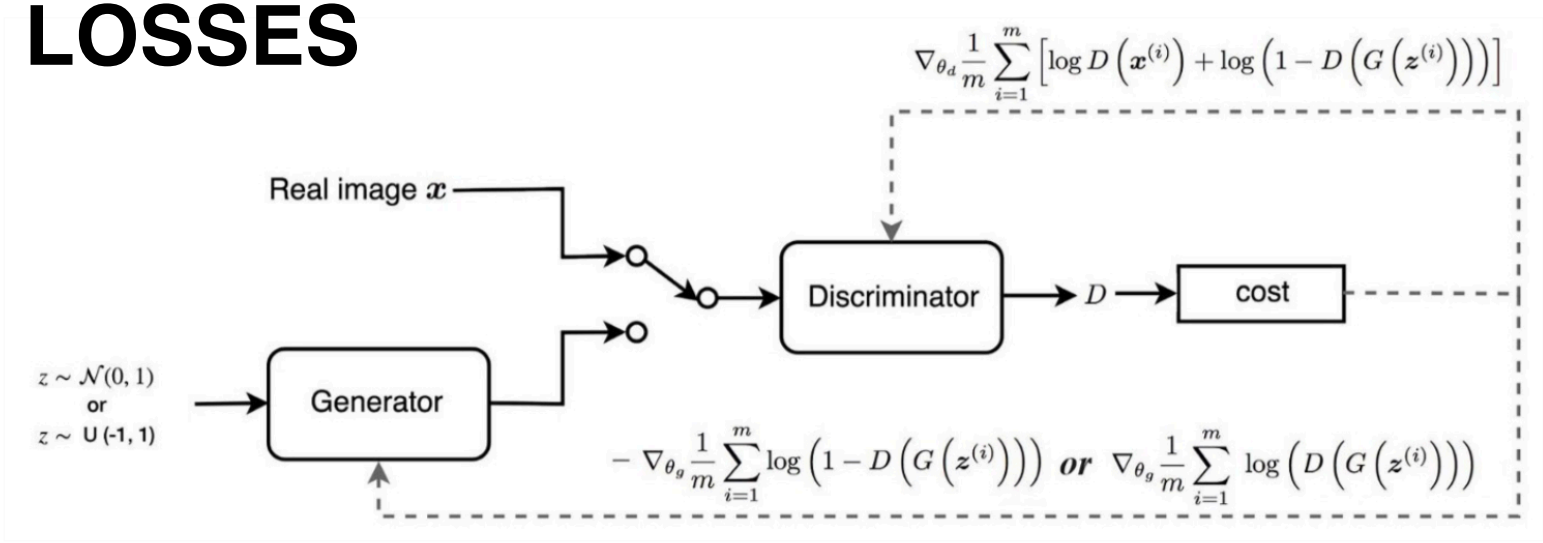


Every N iterations the discriminator is trained to force to distinguish between real and fake

IN PRACTICE

DISCRIMINATOR LOSS (CROSS-ENTROPY)

GAN LOSSES



GENERATOR LOSS

GANs CAN ACHIEVE IMPRESSIVE RESULTS…

Karras+19

THEY ARE ALSO VERY HARD TO TRAIN

1. IT IS HARD TO REACH EQUILIBRIUM AND IT IS ACTUALLY NOT GUARANTEED…

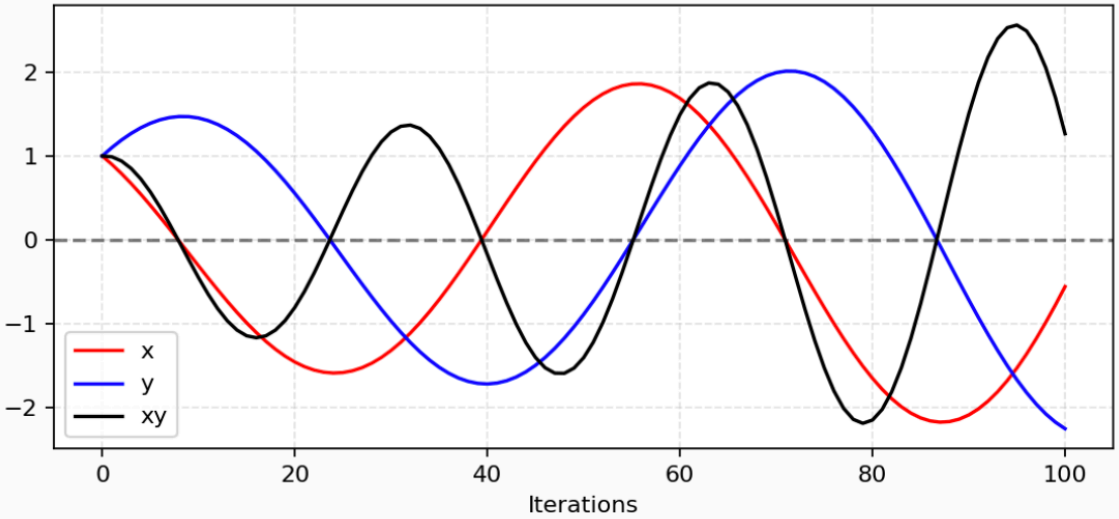


Fig. 3. A simulation of our example for updating x to minimize xy and updating y to minimize $-xy$. The learning rate $\eta = 0.1$. With more iterations, the oscillation grows more and more unstable.

https://lilianweng.github.io/lil-log/2017/08/20/from-GAN-to-WGAN.html

SALIMANS+16

THEY ARE ALSO VERY HARD TO TRAIN

2. LOW DIMENSIONAL SUPPORTS

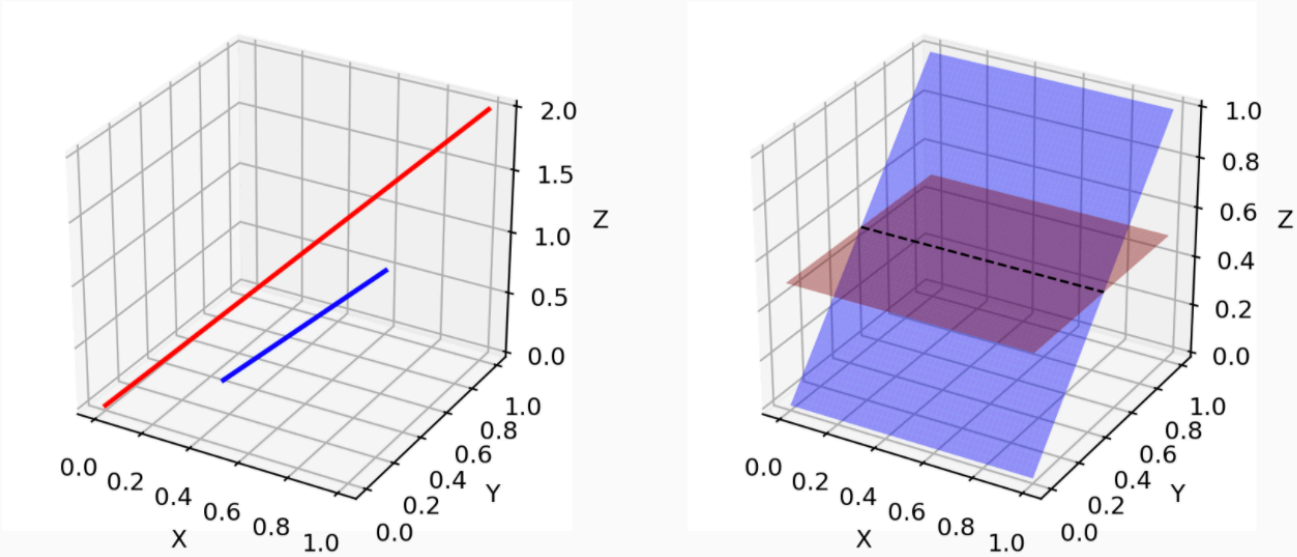


Fig. 4. Low dimensional manifolds in high dimension space can hardly have overlaps. (Left) Two lines in a three-dimension space. (Right) Two surfaces in a three-dimension space.

https://lilianweng.github.io/lil-log/2017/08/20/from-GAN-to-WGAN.html

ARJOVSKI+17

THEY ARE ALSO VERY HARD TO TRAIN

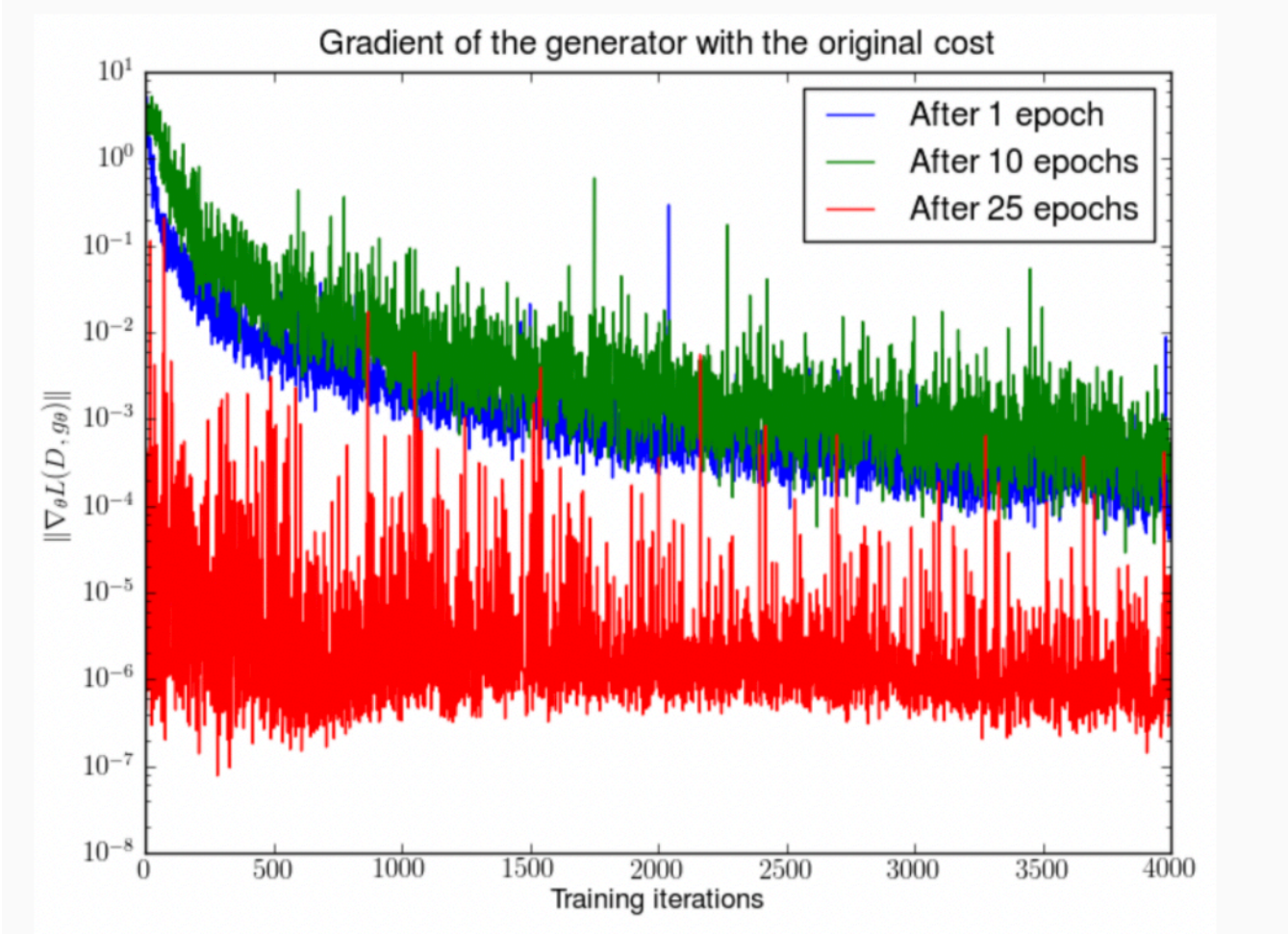
3. MODE COLLAPSE

https://lilianweng.github.io/lil-log/2017/08/20/from-GAN-to-WGAN.html

razavi+19

THEY ARE ALSO VERY HARD TO TRAIN

4. VANISHING GRADIENT

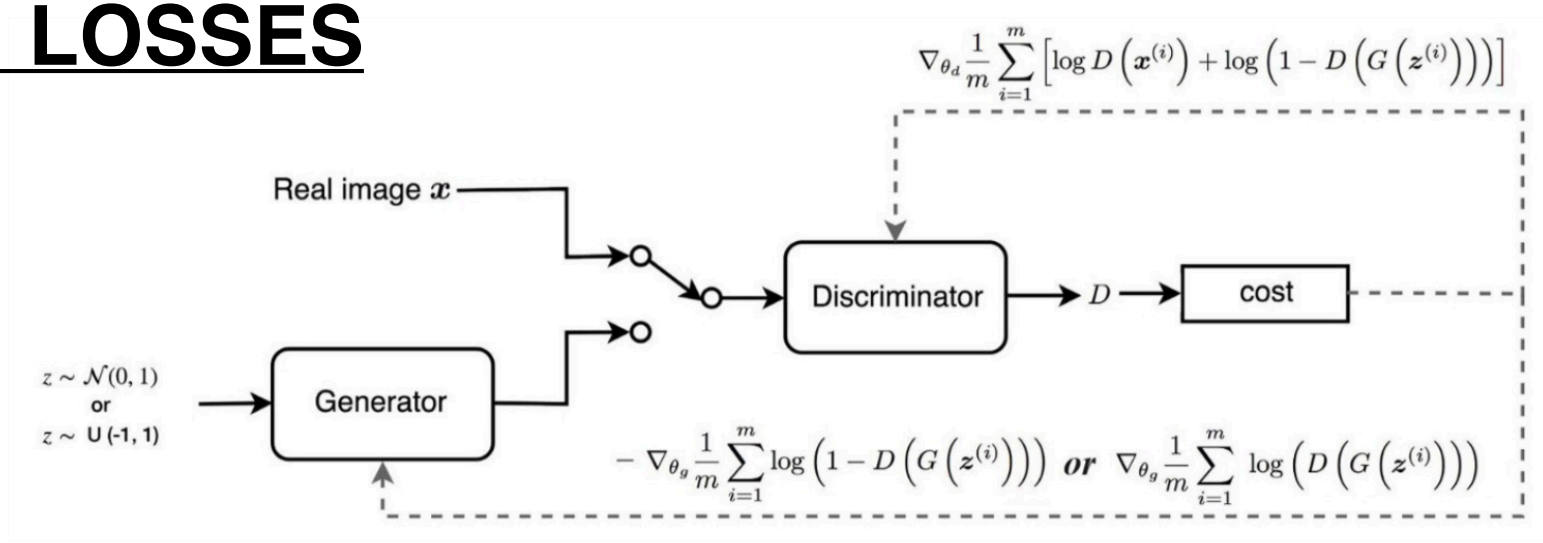


When the discriminator becomes perfect, there are no more gradients to update

IN PRACTICE

GAN LOSSES

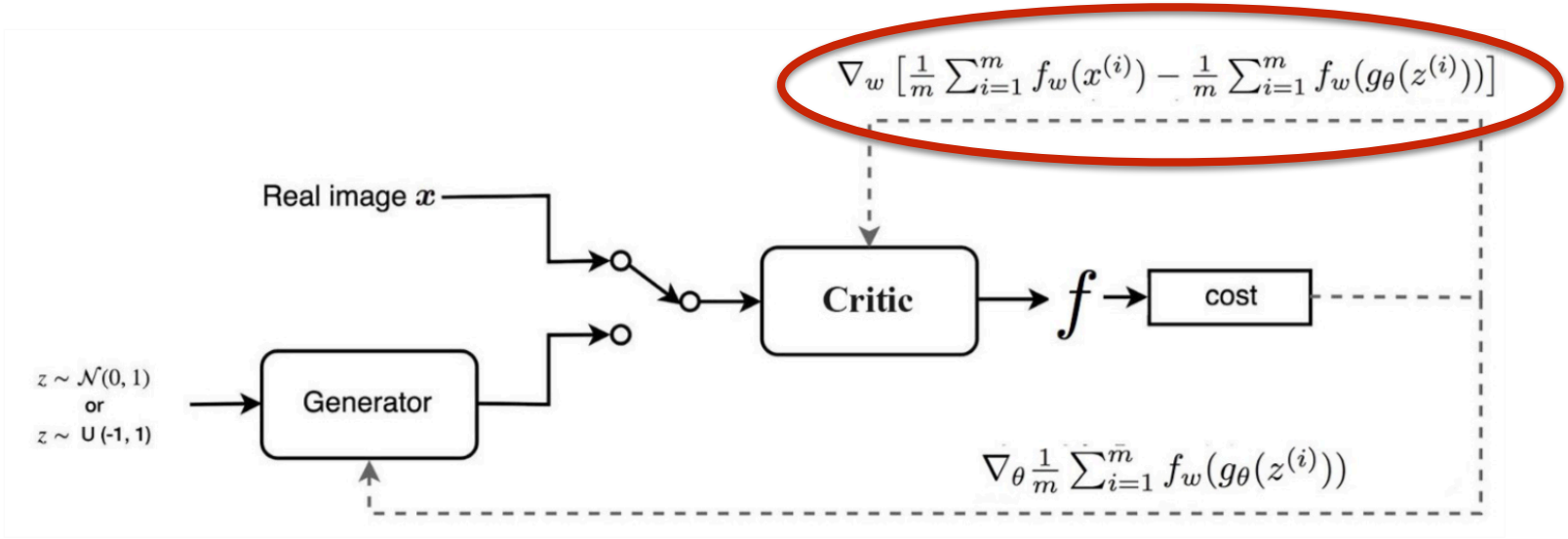
DISCRIMINATOR LOSS (CROSS-ENTROPY)



GENERATOR LOSS

WASSERSTEIN GAN LOSSES

K-L DIvergence is replaced by Wasserstein distance



A USEFUL APPLICATION (BESIDES GENERATING NICE IMAGES) IS ESTIMATING THE PROBABILITY DENSITY OF AN ARBITRARY INPUT, RELATIVE TO THE INPUT DISTRIBUTION

ANOMALY DETECTION IN ASTRONOMY

- FUTURE BIG-DATASETS WILL BE PROCESSED THROUGH AUTOMATED (ML) METHODS - MOST OF THE DATA WILL NEVER BE LOOKED BY HUMANS
- UNKNOWN UNKNOWNS IS WHERE INTERESTING (NEW) SCIENCE WILL BE FOUND
- EFFICIENT ANOMALY DETECTION IS CRUCIAL TO UNLOCK THE DISCOVERY POTENTIAL OF FUTURE SURVEYS