Geometry-Aware Variational Autoencoders for Medical Data Augmentation.

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Overview

Main Challenges

Main challenges with medical data

- Small number of subjects:
  - potential poor population representativity
  - no statistically significant results
  - overfitting

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Issue

- Most of the time, unable to generate faithfully with small data sets

Classic Data Augmentation

- Adding some geometric transformations (shift, rotations ...)
- Adding noise, blur ...

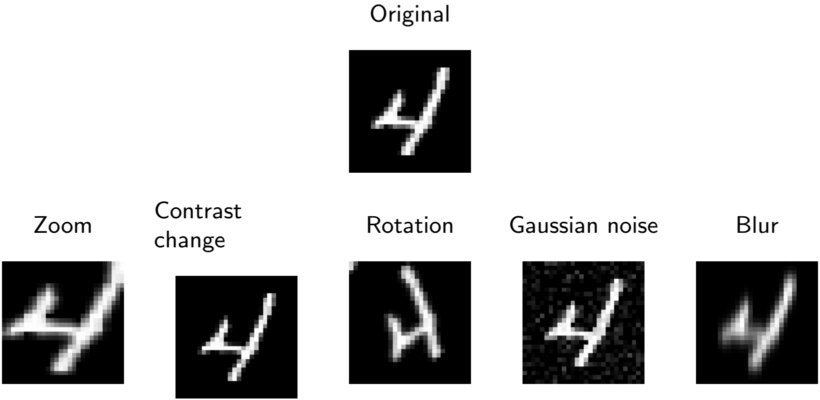

Figure: Examples of transformations

Classic Data Augmentation - Shortcomings

Classic DA

- Is data set dependent
- May require the intervention of an expert “knowledge”

Figure: Nine figure rotated.

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An attractive solution?

- Generative models (Generative Adversarial Networks, Variational Auto-Encoders ...)

Use of Generative Models for DA

GANs: wide use in many fields of application including medicine [YWB19]:

- Magnetic Resonance Images (MRI) [STR$^+$18, CMST17]
- Computed Tomography (CT) [FADK$^+$18, SYPS19]
- X-ray [MMKSM18, SVD$^+$18, WGG$^+$20],
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$\Longrightarrow$ Use VAEs!

Auto-Encoder

- The objective $\Longrightarrow$ Dimensionnality Reduction

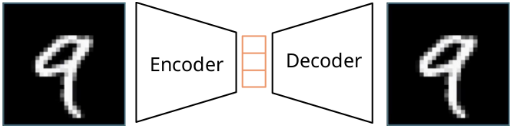
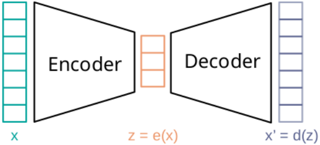


Figure: Simple Auto-Encoder

- Need for a representation of the image $\Longrightarrow$ vectors



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AutoEncoder

Assumptions:

- Let $x \in \mathcal{X}$ be a set a data. We assume that there exists $z \in \mathcal{Z}$ such that z is a low dimensional representation of x
- The encoder e_θ and decoder d_ϕ are functions modelled by neural networks (NNs) such that θ and ϕ are the weights of the NNs
- Let x' be the reconstructed samples, the objective is to have $x \simeq x'$

The Objective function writes:

$$\mathcal{L} = \|x - x'\|^2 = \|x - d_\phi(z)\|^2 = \|x - d_\phi(e_\theta(x))\|^2$$

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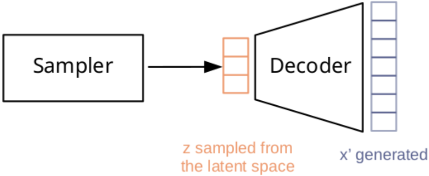
$\Longrightarrow$ The networks are optimised using stochastic gradient descent

$$\phi \leftarrow \phi - \varepsilon \cdot \nabla_\phi \mathcal{L}$$
$$\theta \leftarrow \theta - \varepsilon \cdot \nabla_\theta \mathcal{L}$$

AutoEncoder - Shortcomings

- How to generate new data ?



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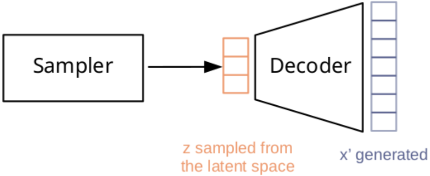

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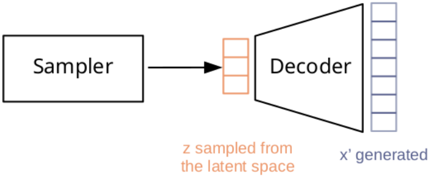

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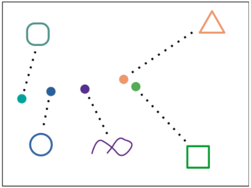

Figure: Potential latent space

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- The AutoEncoder was just trained to encode and decode the **input data** without information on its structure or distribution.

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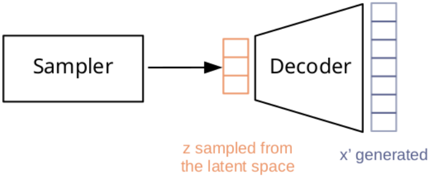

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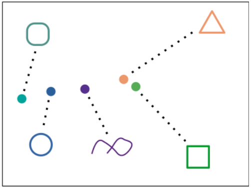

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$\Longrightarrow$ Need for a new framework

VAE - The Idea

- An auto-encoder based model...

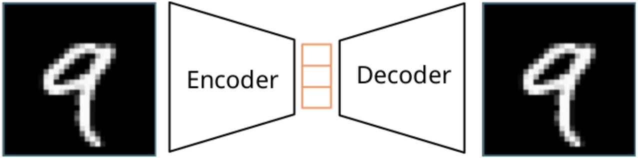

Figure: Simple Auto-Encoder

- ... but where an input data point is encoded as a **distribution** defined over the latent space [KW14, RMW14]

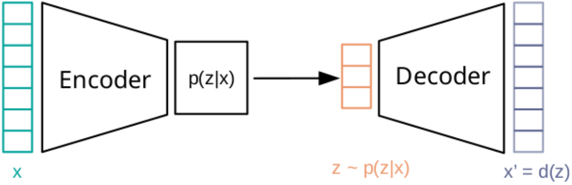

Figure: VAE framework

VAE - Mathematical Considerations

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Problem: The integral is often intractable.

Variational inference

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The equality holds for $q(z) = q_\theta(z|x)$.

Variational inference: The ELBO

- Well-know issue: the posterior $q(z) = q_\theta(z|x)$ is intractable.
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- and the definition of the **Evidence Lower Bound** (ELBO):

$$\begin{aligned}\log p_\theta(x) &\geq \mathbb{E}_{z\sim q_\phi(z|x)}[\log(p_\theta(x,z)) - \log(q_\phi(z|x))]\\ &\geq ELBO\end{aligned}$$

Variational inference: The ELBO

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Use stochastic gradient descent in both θ and ϕ

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1. Optimize the ELBO **as a function** instead of the target distribution

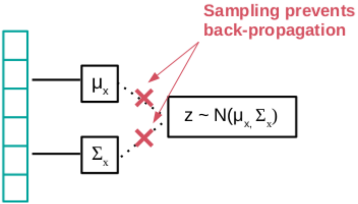
   Use stochastic gradient descent in both θ and ϕ

2. Optimize the ELBO **as a bound** to get closer to the target

   Use sampling methods to produce samples $z \sim q_\theta(z|x)$

The Reparametrization Trick for stochastic gradient descent

- Since $z \sim \mathcal{N}(\mu_\phi(x), \Sigma_\phi(x))$, the model is not amenable to gradient descent



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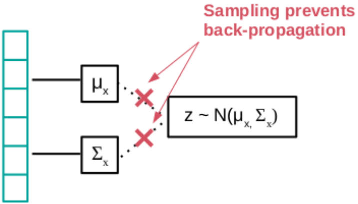

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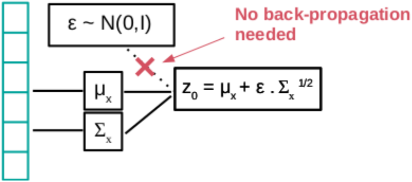

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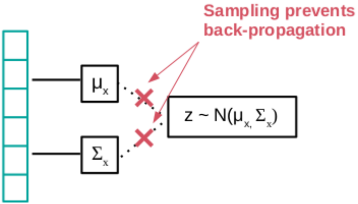

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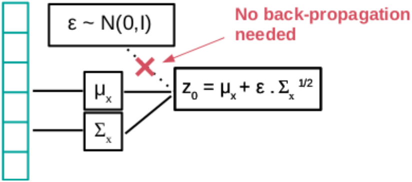


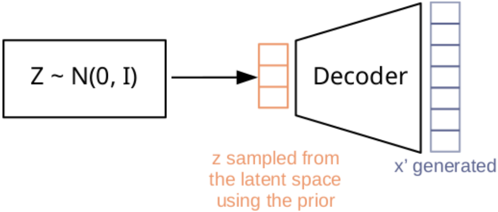
(b) Back-propagation possible

$\Longrightarrow$ Optimization with respect to encoder and decoder parameters made possible !

Objective 1.

Generating new samples

- We only need to sample $z \sim \mathcal{N}(0, I)$ and feed it to the decoder.



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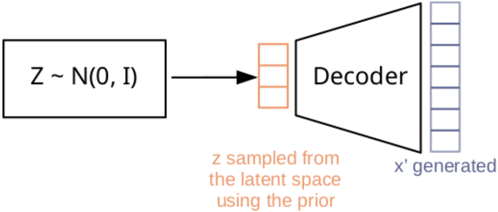

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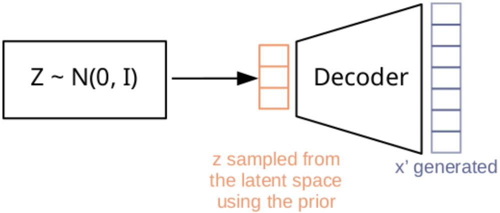

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Pros:

- Very simple to use in practice

Cons:

- The prior and posterior are not expressive enough to capture complex distributions
- Poor latent space prospecting

Tweaking the Approximate Posterior Distribution

Concerning Objective 2.

- The ELBO can written as

$$ELBO = \log p_\theta(x) - \underbrace{\mathrm{KL}(q_\phi(z|x)||p_\theta(z|x))}_{\approx 0 \text{ if } q_\phi(z|x) \approx p_\theta(z|x)} .$$

- Kullback-Leiber divergence $\geq 0 \Rightarrow$ make it vanish by tweaking the approximate posterior $q_\phi(z|x)$

- Produce variables z which targets the true posterior $p_\theta(z|x)$ using a sample $z_0 \sim q_{init}$

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- How? and how to ensure that the model would still be amenable to the back-propagation ?

Solution 1: Normalizing Flows

- Use smooth invertible parametrized mappings f_ψ to "sample" z [RM15]

- Apply K transformations to $z_0 \sim q_{init}$ (here $q_{init} = q_\phi$)
- Final random variable $z_K = f_x^K \circ \cdots \circ f_x^1(z_0) \sim q_\phi(z_K|x)$ with

$$q_\phi(z_K|x) = q_\phi(z_0|x) \prod_{k=1}^{K} |\det \mathbf{J}_{f_x^k}|^{-1}, \tag{1}$$

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Objective 2.

although difficult to compute the Jacobian of these maps f_1^K

Solution 2: Hamiltonian VAE

- Idea = Hybrid Monte Carlo Sampler [No11, DMS17, LBB$^+$19],
- Target density

$$p_\theta(z|x) = \frac{p_\theta(x,z)}{p_\theta(x)} \propto p_\theta(x,z) = \pi_x(z)\,.$$

- Introduce an auxiliary random variable $\rho \sim \mathcal{N}(0, \mathbf{M})$ called "momentum"
- Write the Hamiltonian:

$$\begin{aligned} H_x(z,\rho) &= -\log \pi_x(z,\rho) \\ &= -\log \pi_x(z) + \frac{1}{2}\log((2\pi)^d|\mathbf{M}|) + \rho^\top \mathbf{M}^{-1}\rho \\ &= U_x(z) + \kappa(\rho)\,. \end{aligned}$$

- Sample (z, ρ) with this dynamic.

Solution 2: Hamiltonian VAE

- Use a discretization scheme

$$
\begin{aligned}
\rho(t+\varepsilon/2) &= \rho(t) - \frac{\varepsilon}{2} \cdot \nabla_z H(z(t), \rho(t))\,, \\
z(t+\varepsilon) &= z(t) + \varepsilon \cdot \nabla_\rho (H(z(t), \rho(t+\varepsilon/2)))\,, \\
\rho(t+\varepsilon) &= \rho(t+\varepsilon/2) - \frac{\varepsilon}{2} \cdot \nabla_z H(z(t+\varepsilon), \rho(t+\varepsilon/2))\,,
\end{aligned}
\tag{2}
$$

- A proposal $(\widetilde{z}, \widetilde{\rho})$ is accepted with probability:

$$
\alpha = \min\Big(1, \exp\left(-H(\widetilde{z}, \widetilde{\rho}) + H(z, \rho)\right)\Big)
$$

$\Longrightarrow$ Creates an ergodic, time-reversible Markov Chain having π_x as stationary distribution.

Hamiltonian VAE

- The graphical scheme [CDS18]

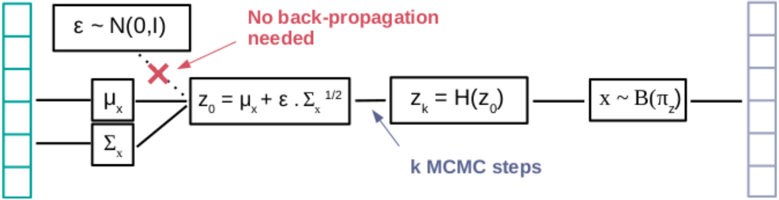

Figure: Hamiltonian VAE

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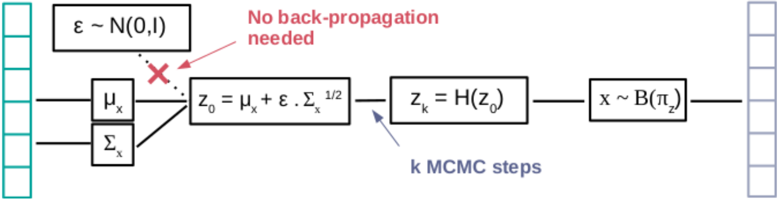

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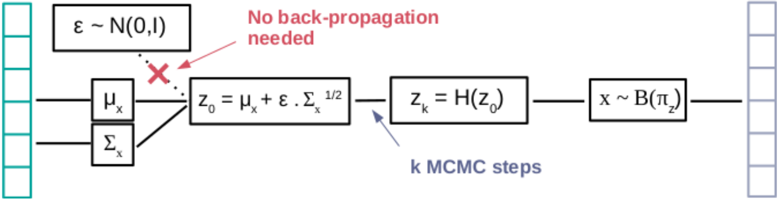

Figure: Hamiltonian VAE

Issue: Perform poorly when trained on small data set and so we need to define a new framework

What about geometry?

Defining a New Framework

Assumptions:

- As of now the latent space structure was supposed to be Euclidean (i.e. $\mathcal{Z} = \mathbb{R}^d$)

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2. Learn the metric defined in the latent space [CMA20]
3. Use the learned geometry to generate instead of the prior [CTSBA21]

Riemanian geometry principles

- Riemanian manifold: (reduced to our model) $\mathbb{R}^d$ endowed with a metric $\mathbf{G}$: $\mathcal{M} = (\mathbb{R}^d, \mathbf{G})$.
  $\Longrightarrow \mathbb{R}^d$ not flat anymore, curved space (as montains)

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- Geodesic curves:
  - Length of a curve $\gamma : [0, 1] \to \mathcal{M}$ from z_1 to z_2 living in a Riemannian manifold $\mathcal{M}$

$$L(\gamma) = \int_0^1 \sqrt{\langle \gamma'(t), \gamma'(t) \rangle_{\gamma(t)}} dt \qquad \gamma(0) = z_1, \gamma(1) = z_2 \,. \tag{3}$$

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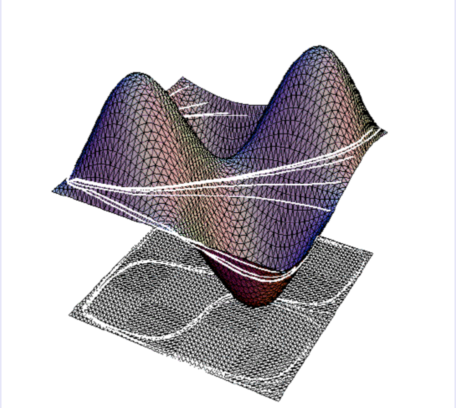
  - or equivalently minimizing the curve energy

$$E(\gamma) = \int_0^1 \langle \gamma'(t), \gamma'(t) \rangle_{\gamma(t)} dt \qquad \gamma(0) = z_1, \gamma(1) = z_2 \,.$$

Riemanian geometry principles



Shortest path geodesic on sinusoidal surface. See Ref. 1 below.

Figure: Image taken from: Fast Marching Methods on Triangulated Domains : Kimmel, R., and Sethian, J.A., Proceedings of the National Academy of Sciences, 95, pp. 8341-8435, 1998

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$$U(z) = -\log p_{\mathrm{target}}(z), \qquad K(v, z) = \frac{1}{2} v^\top \mathbf{G}^{-1}(z) v\,.$$

- Position-specific random momentum $\rho \sim \mathcal{N}(0, \mathbf{G}(z))$ introduced
- The Hamiltonian writes

$$H_x^{Riem}(z, \rho) = U_x(z) + \frac{1}{2} \log((2\pi)^D \det \mathbf{G}(z)) + \frac{1}{2} \rho^\top \mathbf{G}(z)^{-1} \rho\,.$$

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Pros:

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Cons:

- The metric is unknown

2) Learn the Metric - The Choice of the Metric

- Parametric metric: [Lou19]:

$$\mathbf{G}^{-1}(z) = \sum_{i=1}^{N} L_{\psi_i} L_{\psi_i}^{\top} \exp\Big(- \frac{\|z - c_i\|_2^2}{T^2} \Big) + \lambda I_d \ ,$$

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Pros:

- Closed-form expression of the inverse metric $\Longrightarrow$ useful for geodesic computation
- Geodesics travel through most populated areas.

The Model - Riemannian Hamiltonian VAE

- The graphical scheme

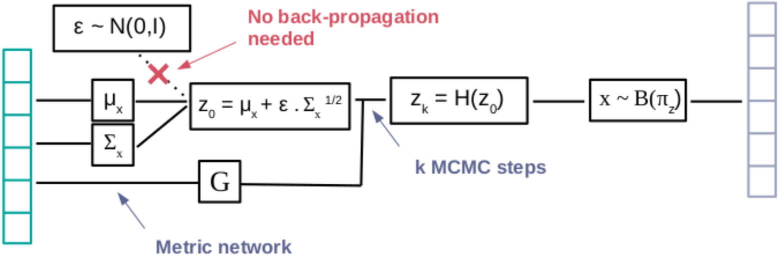
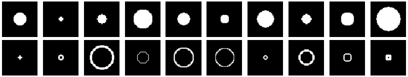


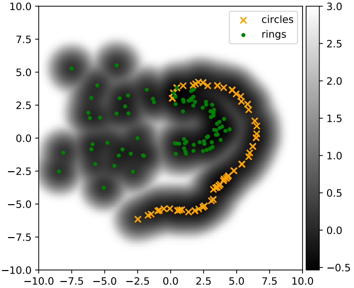
Figure: Riemannian Hamiltonian VAE.

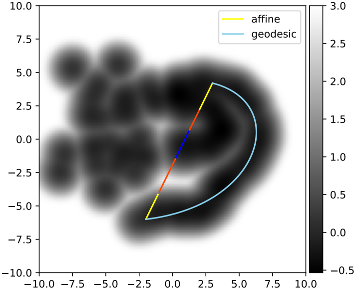
The Learned Latent Space examples

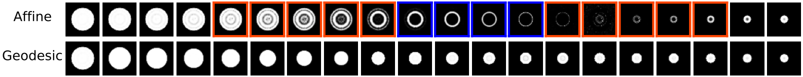
Training samples:



Latent space and interpolations:







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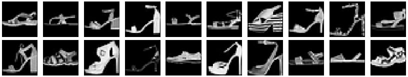

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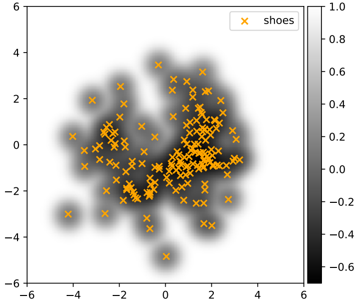
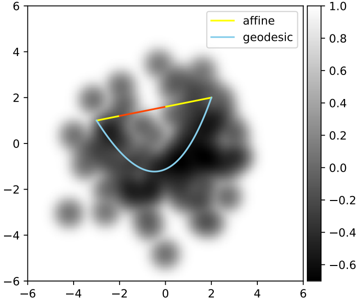
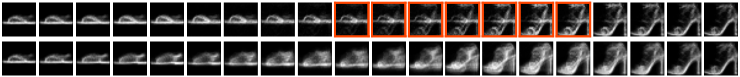




Affine

Geodesic



3) Improve Data Generation - Sample With the Metric

Idea:

- Use a geometry-based sampling procedure: pdf driven by the metric

$$p(z) = \frac{\mathbb{1}_S(z)\sqrt{\det \mathbf{G}^{-1}(z)}}{\int\limits_{\mathbb{R}^d} \mathbb{1}_S(z)\sqrt{\det \mathbf{G}^{-1}(z)dz}} ,$$

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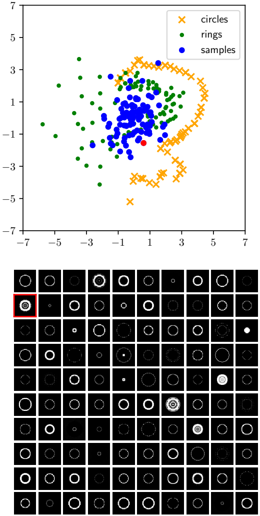
  where S is a compact set and $\mathbb{1}_S(z) = 1$ if $z \in S$, 0 otherwise.
- Use of classic MCMC sampler (e.g. Hamiltonian Monte Carlo)

Pros:

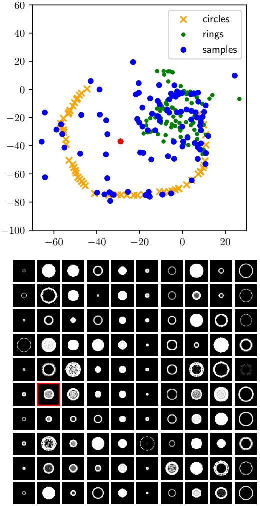
- $\mathbf{G}^{-1}$ easily computable
- Samples "close" to the data

Sampling Comparison

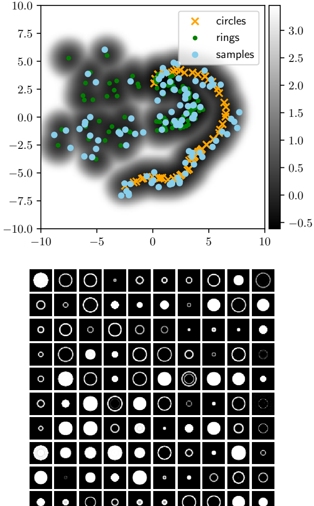
(a) VAE - $\mathcal{N}(0, I)$



(b) VAE - VAMP (multimodal conditional prior)

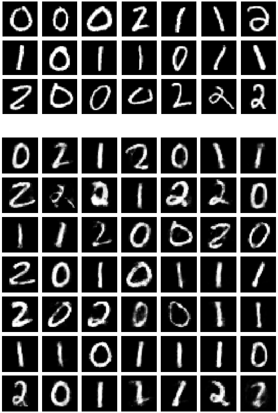


(c) Ours

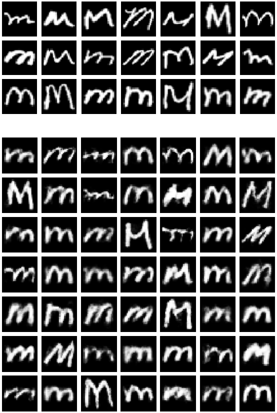


Sampling Comparison - Higher Dimension

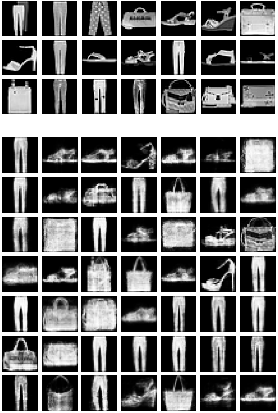
(a) *reduced* MNIST (120)



(b) *reduced* EMNIST (120)



(c) *reduced* Fashion (120)



Data Augmentation

Data Augmentation

1. Framework
2. Toy Data
3. Medical Imaging

Data Augmentation - Framework

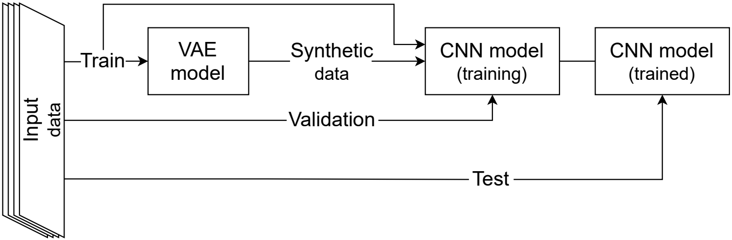


Figure: Data Augmentation pipeline

Performances are estimated using cross-validation.

Data Augmentation

1. Framework
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3. Medical Imaging

Robustness Across Data Sets

Table: Classification results on *reduced* data sets ($\sim$ 50 samples per class)

	MNIST	MNIST (unbal.)	EMNIST (unbal.)	FASHION
Baseline	89.9 ± 0.6	81.5 ± 0.7	82.6 ± 1.4	76.0 ± 1.5
Baseline + Synthetic				
Basic Augmentation (X5)	92.8 ± 0.4	86.5 ± 0.9	85.6 ± 1.3	77.5 ± 2.0
Basic Augmentation (X10)	88.2 ± 2.2	82.0 ± 2.4	85.7 ± 0.3	79.2 ± 0.6
Basic Augmentation (X15)	92.8 ± 0.7	85.8 ± 3.4	86.6 ± 0.8	80.0 ± 0.5
VAE - 200*	88.5 ± 0.9	84.0 ± 2.0	81.7 ± 3.0	78.6 ± 0.4
VAE - 2k*	92.2 ± 1.6	88.0 ± 2.2	86.0 ± 0.2	79.3 ± 1.1
Ours-200	91.0 ± 1.0	84.1 ± 2.0	85.1 ± 1.1	77.0 ± 0.8
Ours-500	92.3 ± 1.1	87.7 ± 0.9	85.1 ± 1.1	78.5 ± 0.9
Ours-1k	93.2 ± 0.8	**89.7 ± 0.8**	87.0 ± 1.0	**80.2 ± 0.8**
Ours-2k	**94.3 ± 0.8**	89.1 ± 1.9	**87.6 ± 0.8**	78.1 ± 1.8

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* Using a standard normal prior to generate

- Classic DA is data set dependent
- Vanilla VAE performs as well as classic DA

Robustness Across Data Sets

Table: Classification results on *reduced* data sets ($\sim$ 50 samples per class) **on synthetic samples only**

	MNIST	MNIST (unbal.)	EMNIST (unbal.)	FASHION
Baseline	89.9 ± 0.6	81.5 ± 0.7	82.6 ± 1.4	76.0 ± 1.5
Synthetic Only				
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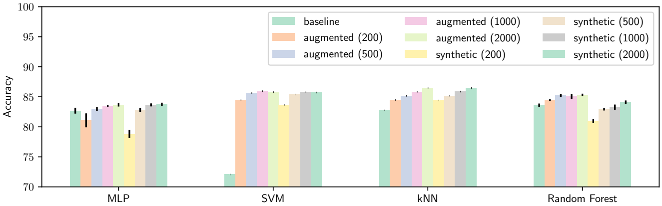
* Using a standard normal prior to generate

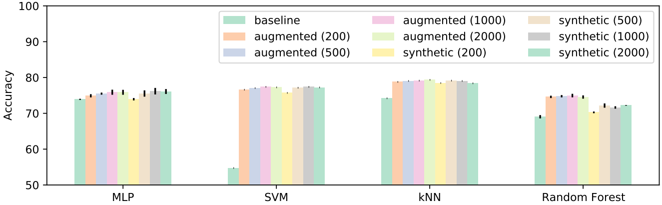
- The proposed model seems to create diverse samples relevant to the classifier

Robustness Across Classifiers

(a) *reduced* MNIST balanced



(b) *reduced* MNIST unbalanced



A Note on the Method Scalability

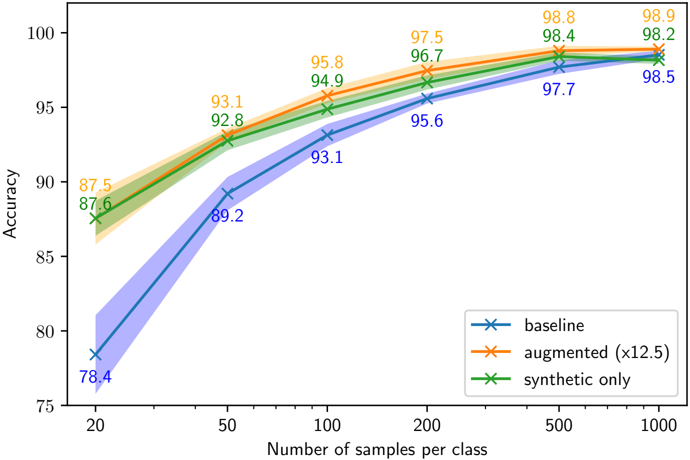


Figure: Benchmark classifier accuracy according to the number of samples in the training set on MNIST.

Data Augmentation

1. Framework
2. Toy Data
3. Medical Imaging

Datasets and classification task

Classification task: Alzheimer's disease patients (**AD**) vs Cognitively Normal participants (**CN**) using T1-weighted MR images.

Table: Summary of participant demographics, mini-mental state examination (MMSE) and global clinical dementia rating (CDR) scores at baseline.

Data set	Label	Obs.	Age	Sex M/F	MMSE	CDR
ADNI	CN	403	73.3 ± 6.0	185/218	29.1 ± 1.1	0: 403
	AD	362	74.9 ± 7.9	202/160	23.1 ± 2.1	0.5: 169, 1: 192, 2: 1
AIBL	CN	429	73.0 ± 6.2	183/246	28.8 ± 1.2	0: 406, 0.5: 22, 1: 1
	AD	76	74.4 ± 8.0	33/43	20.6 ± 5.5	0.5: 31, 1: 36, 2: 7, 3: 2

MRI preprocessing

Bias field correction (N4ITK) + linear registration (ANTS) + cropping

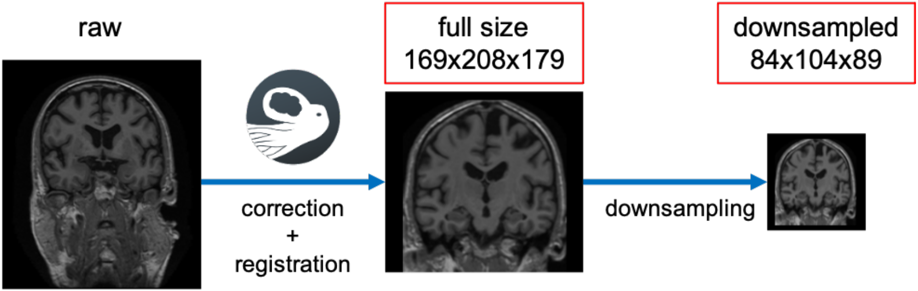
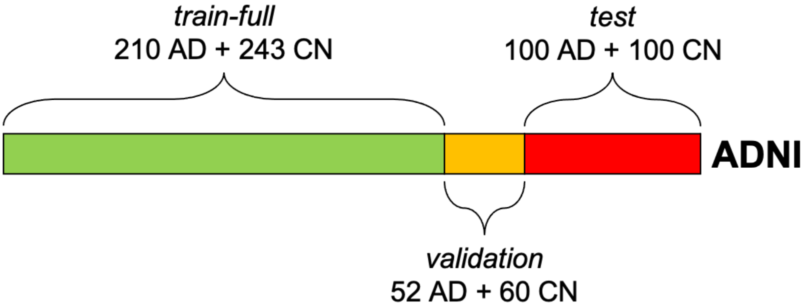


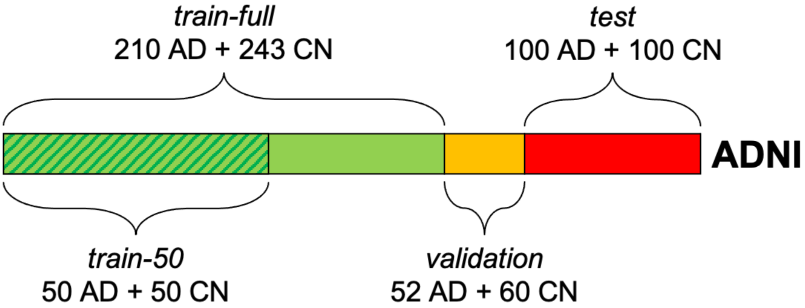
Figure: Preprocessed MRI used in the study

Find wonderful data at:
`/network/lustre/dtlake01/aramis/datasets/adni/caps/caps_v2021`

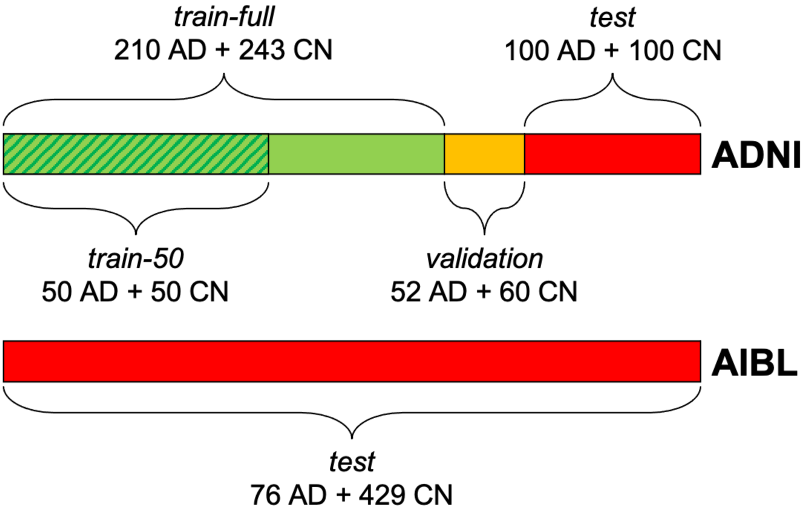
Evaluation procedure



Evaluation procedure

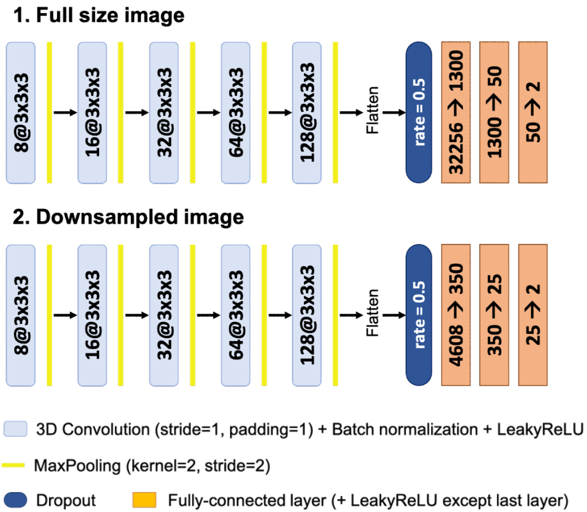


Evaluation procedure



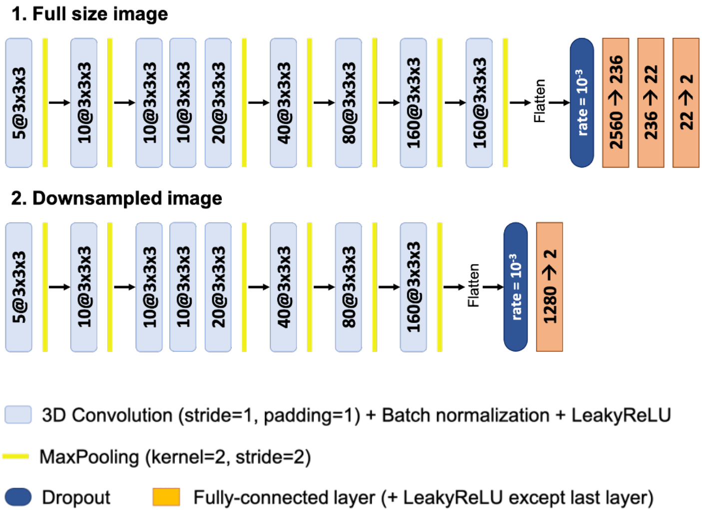
CNN architectures

Baseline architectures provided by a previous study [WTSDM+20]



CNN architectures

Optimized architectures opitmize with random search procedure for this training set (ClinicaDL)



Experiments

Four series of experiments:

- **baseline** architecture on *train-50*
- **baseline** architecture on *train-full*
- **optimized** architecture on *train-50*
- **optimized** architecture on *train-full*

For each experiment 20 CNNs are run and the performance is the mean value of the 20 performance values.

Synthesized images

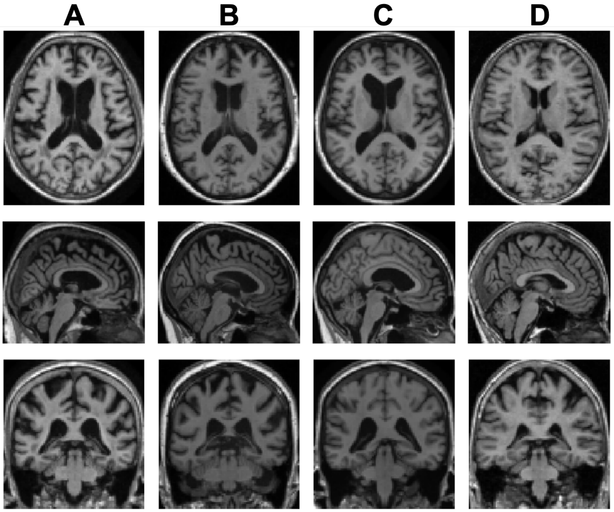


Figure: Example of two *true* patients compared to two generated by our method. Can you find the intruders ?

Synthesized images

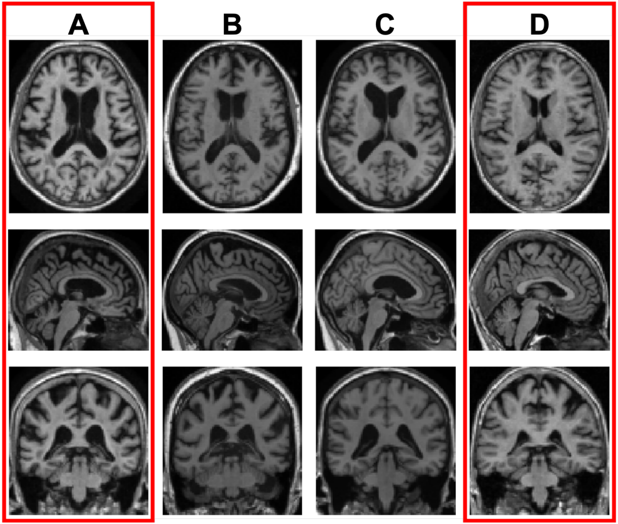


Figure: Example of two *true* patients compared to two generated by our method. Can you find the intruders ?

Results on train-50 with baseline CNN

Table: Mean test performance of each series of 20 runs trained with the **baseline** hyperparameters on *train-50* set.

data set	ADNI balanced accuracy	AIBL balanced accuracy
real	66.3 ± 2.4	67.2 ± 4.1
real (high-resolution)	67.9 ± 2.3	66.5 ± 3.0
500 synthetic + real	69.4 ± 1.6	68.5 ± 2.5
1000 synthetic + real	70.5 ± 2.1	70.6 ± 3.1
2000 synthetic + real	71.2 ± 1.6	72.8 ± 2.2
3000 synthetic + real	72.6 ± 1.6	73.6 ± 3.0
5000 synthetic + real	$\mathbf{74.1 \pm 2.2}$	$\mathbf{76.1 \pm 3.6}$
10000 synthetic + real	74.0 ± 2.7	74.9 ± 3.2

Increase of balanced accuracy of 6.2 points on ADNI and 8.9 points on AIBL

Results on train-full with baseline CNN

Table: Mean test performance of each series of 20 runs trained with the **baseline** hyperparameters on *train-full* set.

data set	ADNI balanced accuracy	AIBL balanced accuracy
real	77.7 ± 2.5	78.4 ± 2.4
real (high-resolution)	80.6 ± 1.1	80.4 ± 2.6
500 synthetic + real	82.2 ± 2.4	82.9 ± 2.5
1000 synthetic + real	84.4 ± 1.8	83.7 ± 2.3
2000 synthetic + real	85.9 ± 1.6	83.8 ± 2.2
3000 synthetic + real	85.8 ± 1.7	84.4 ± 1.8
5000 synthetic + real	85.7 ± 2.1	84.2 ± 2.2
10000 synthetic + real	**86.3 ± 1.8**	**85.1 ± 1.9**

Increase of balanced accuracy of 5.7 points on ADNI and 4.7 on AIBL

Results on train-50 with optimized CNN

Table: Mean test performance of each series of 20 runs trained with the **baseline** hyperparameters on *train-50* set.

data set	ADNI balanced accuracy	AIBL balanced accuracy
real	75.5 ± 2.7	75.6 ± 4.1
real (high-resolution)	72.1 ± 3.1	71.2 ± 5.1
500 synthetic + real	75.6 ± 2.5	76.0 ± 4.2
1000 synthetic + real	77.8 ± 2.3	80.9 ± 3.2
2000 synthetic + real	76.9 ± 2.4	80.0 ± 3.6
3000 synthetic + real	77.8 ± 1.9	81.2 ± 3.7
5000 synthetic + real	76.9 ± 2.5	80.9 ± 2.7
10000 synthetic + real	**78.0±2.1**	**81.9±2.2**

Increase of balanced accuracy of 2.5 points on ADNI and 6.3 points on AIBL

Results on train-full with optimized CNN

Table: Mean test performance of each series of 20 runs trained with the **baseline** hyperparameters on *train-full* set.

data set	ADNI balanced accuracy	AIBL balanced accuracy
real	85.5 ± 2.4	81.9 ± 3.2
real (high-resolution)	85.7 ± 2.5	84.4 ± 1.7
500 synthetic + real	86.0 ± 1.8	83.2 ± 2.4
1000 synthetic + real	86.5 ± 1.9	83.7 ± 2.0
2000 synthetic + real	**87.2 ± 1.7**	84.0 ± 2.0
3000 synthetic + real	85.8 ± 2.6	83.6 ± 3.2
5000 synthetic + real	86.4 ± 1.3	83.5 ± 2.2
10000 synthetic + real	86.7 ± 1.8	**84.3 ± 1.8**

Increase of balanced accuracy of 1.5 point on ADNI and -0.1 point on AIBL

Conclusion

We have proposed

- a new geometry aware VAE-based data augmentation framework relevant for representing and classifying data in the HDLSS setting.
- Validated on classification tasks on *toy* and *real-life* data sets.

Conclusion

We have proposed

- a new geometry aware VAE-based data augmentation framework relevant for representing and classifying data in the HDLSS setting.
- Validated on classification tasks on *toy* and *real-life* data sets.

Strengths:

- Independent on the nature of the data set: from 2D images (MNIST, EMNIST, FASHION) to 3D medical images (ADNI and AIBL),
- Relevant synthetic data: classifiers achieved a similar or better classification performance when trained only on synthetic data than on the *real* train set.
- Classifier independence: MLP, random forest, k-NN and SVM (on toy data sets) ; baseline and optimized parameters (on medical images).

Conclusion

We have proposed

- a new geometry aware VAE-based data augmentation framework relevant for representing and classifying data in the HDLSS setting.
- Validated on classification tasks on *toy* and *real-life* data sets.

Limitations - what could be improved:

- No extensive search on VAE architecture.
- Would it benefit from the use of longitudinal data?
- *train-50* is still large compared to some medical data sets...

Implementation

All this is available as a Python library named Pyraug:

Training Pipeline:

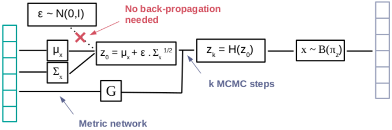
```
>>> from pyraug.pipelines import TrainingPipeline
>>> pipeline = TrainingPipeline()
>>> pipeline(train_data=dataset_to_augment)
```

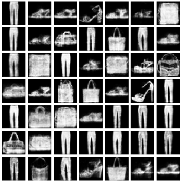
Data sampler:

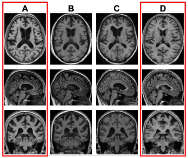
```
>>> from pyraug.pipelines import GenerationPipeline
>>> from pyraug.models import RHVAE
>>> model = RHVAE.load_from_folder('path/to/your/trained/model') # reload the model
>>> pipe = GenerationPipeline(model=model) # define pipeline
>>> pipe(samples_number=10) # This will generate 10 data points
```

Available (upon request by email) and soon for download under licence on Pypi and github with documentation and tutorials.

Thank you!







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References I

Christoph Baur, Shadi Albarqouni, and Nassir Navab, *Generating highly realistic images of skin lesions with GANs*, OR 2.0 Context-Aware Operating Theaters, Computer Assisted Robotic Endoscopy, Clinical Image-Based Procedures, and Skin Image Analysis, Springer, 2018, pp. 260–267.

Lei Bi, Jinman Kim, Ashnil Kumar, Dagan Feng, and Michael Fulham, *Synthesis of Positron Emission Tomography (PET) Images via Multi-channel Generative Adversarial Networks (GANs)*, Molecular Imaging, Reconstruction and Analysis of Moving Body Organs, and Stroke Imaging and Treatment, LNCS, Springer, 2017, pp. 43–51.

Anthony L Caterini, Arnaud Doucet, and Dino Sejdinovic, *Hamiltonian variational auto-encoder*, Advances in Neural Information Processing Systems, 2018, pp. 8167–8177.

Clment Chadebec, Clment Mantoux, and Stphanie Allassonnire, *Geometry-aware hamiltonian variational auto-encoder*, arXiv:2010.11518 [cs, math, stat] (2020).

References II

- Francesco Calimeri, Aldo Marzullo, Claudio Stamile, and Giorgio Terracina, *Biomedical data augmentation using generative adversarial neural networks*, International conference on artificial neural networks, Springer, 2017, pp. 626–634.
- Clément Chadebec, Elina Thibeau-Sutre, Ninon Burgos, and Stéphanie Allassonnière, *Data augmentation in high dimensional low sample size setting using a geometry-based variational autoencoder*, arXiv preprint arXiv:2105.00026 (2021).
- Alain Durmus, Eric Moulines, and Eero Saksman, *On the convergence of hamiltonian monte carlo*, arXiv preprint arXiv:1705.00166 (2017).
- Maayan Frid-Adar, Idit Diamant, Eyal Klang, Michal Amitai, Jacob Goldberger, and Hayit Greenspan, *GAN-based synthetic medical image augmentation for increased CNN performance in liver lesion classification*, Neurocomputing **321** (2018), 321–331.

References III

- Mark Girolami and Ben Calderhead, *Riemann manifold langevin and hamiltonian monte carlo methods*, Journal of the Royal Statistical Society: Series B (Statistical Methodology) **73** (2011), no. 2, 123–214.
- Mark Girolami, Ben Calderhead, and Siu A Chin, *Riemannian manifold hamiltonian monte carlo*, arXiv preprint arXiv:0907.1100 (2009).
- Dimitrios Korkinof, Tobias Rijken, Michael O'Neill, Joseph Yearsley, Hugh Harvey, and Ben Glocker, *High-resolution mammogram synthesis using progressive generative adversarial networks*, arXiv preprint arXiv:1807.03401 (2018).
- Diederik P. Kingma and Max Welling, *Auto-encoding variational bayes*, arXiv:1312.6114 [cs, stat] (2014).
- Samuel Livingstone, Michael Betancourt, Simon Byrne, Mark Girolami, and others, *On the geometric ergodicity of hamiltonian monte carlo*, Bernoulli **25** (2019), no. 4, 3109–3138.

References IV

Maxime Louis, *Computational and statistical methods for trajectory analysis in a Riemannian geometry setting*, PhD Thesis, Sorbonnes universits, 2019.

Yufei Liu, Yuan Zhou, Xin Liu, Fang Dong, Chang Wang, and Zihong Wang, *Wasserstein gan-based small-sample augmentation for new-generation artificial intelligence: a case study of cancer-staging data in biology*, Engineering **5** (2019), no. 1, 156–163.

Ali Madani, Mehdi Moradi, Alexandros Karargyris, and Tanveer Syeda-Mahmood, *Chest x-ray generation and data augmentation for cardiovascular abnormality classification*, Medical Imaging 2018: Image Processing, vol. 10574, International Society for Optics and Photonics, 2018, p. 105741M.

Radford M Neal and others, *MCMC using hamiltonian dynamics*, Handbook of Markov Chain Monte Carlo **2** (2011), no. 11, 2.

References V

Danilo Rezende and Shakir Mohamed, *Variational inference with normalizing flows*, International Conference on Machine Learning, PMLR, 2015, pp. 1530–1538.

Danilo Jimenez Rezende, Shakir Mohamed, and Daan Wierstra, *Stochastic backpropagation and approximate inference in deep generative models*, International conference on machine learning, PMLR, 2014, pp. 1278–1286.

Hoo-Chang Shin, Neil A Tenenholtz, Jameson K Rogers, Christopher G Schwarz, Matthew L Senjem, Jeffrey L Gunter, Katherine P Andriole, and Mark Michalski, *Medical image synthesis for data augmentation and anonymization using generative adversarial networks*, International Workshop on Simulation and Synthesis in Medical Imaging, LNCS, Springer, 2018, pp. 1–11.

References VI

Hojjat Salehinejad, Shahrokh Valaee, Tim Dowdell, Errol Colak, and Joseph Barfett, *Generalization of deep neural networks for chest pathology classification in x-rays using generative adversarial networks*, 2018 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, 2018, pp. 990–994.

Veit Sandfort, Ke Yan, Perry J. Pickhardt, and Ronald M. Summers, *Data augmentation using generative adversarial networks (CycleGAN) to improve generalizability in CT segmentation tasks*, Scientific reports **9** (2019), no. 1, 16884.

Abdul Waheed, Muskan Goyal, Deepak Gupta, Ashish Khanna, Fadi Al-Turjman, and Plcido Rogerio Pinheiro, *Covidgan: data augmentation using auxiliary classifier gan for improved covid-19 detection*, Ieee Access **8** (2020), 91916–91923.

References VII

- Junhao Wen, Elina Thibeau-Sutre, Mauricio Diaz-Melo, Jorge Samper-Gonzlez, Alexandre Routier, Simona Bottani, Didier Dormont, Stanley Durrleman, Ninon Burgos, and Olivier Colliot, *Convolutional neural networks for classification of Alzheimer's disease: Overview and reproducible evaluation*, Medical Image Analysis **63** (2020), 101694.
- Eric Wu, Kevin Wu, David Cox, and William Lotter, *Conditional infilling gans for data augmentation in mammogram classification*, Image analysis for moving organ, breast, and thoracic images, Springer, 2018, pp. 98–106.
- Xin Yi, Ekta Walia, and Paul Babyn, *Generative adversarial network in medical imaging: A review*, Medical image analysis **58** (2019), 101552.

Clustering

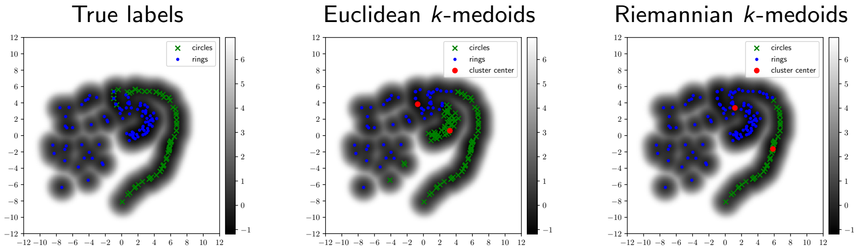

Figure: Euclidean and Riemannian k-medoids custering.

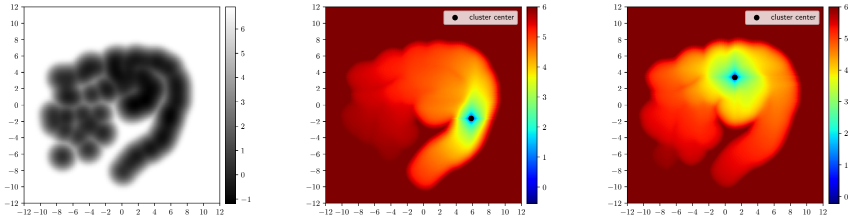

Figure: Distance maps.

Results - Clustering

Data set	Model	Subset 1	Subset 2	Subset 3	Mean
Synthetic data	linear	53.88	62.52	71.63	62.68
	geodesic	**71.41**	**81.39**	**79.49**	**77.43**
MNIST 1	linear	89.73	93.11	91.80	91.55
	geodesic	**91.68**	**94.51**	**95.63**	**93.94**
MNIST 2	linear	68.24	69.22	79.05	71.17
	geodesic	**70.35**	**71.34**	**79.64**	**73.78**
MNIST 3	linear	75.55	75.76	81.70	77.67
	geodesic	**76.08**	**77.94**	**81.96**	**78.66**
FashionMNIST 1	linear	90.47	91.63	86.78	89.63
	geodesic	**91.44**	**92.55**	**87.46**	**90.48**
FashionMNIST 2	linear	92.20	91.26	93.30	92.25
	geodesic	**93.56**	**91.80**	**94.12**	**93.16**
FashionMNIST 3	linear	72.46	79.58	83.16	78.40
	geodesic	**74.89**	**81.88**	**84.83**	**80.53**

Table: F1-Scores.