Variational Autoencoders: From Theory to Practice

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Overview

1. Variational Autoencoder - The Idea
   - Autoencoder
   - VAE framework
   - Some use cases
   - Mathematical foundations
2. Enhancing the model
   - Tweaking the variational distribution
   - Building better estimators
   - Questioning our priors
3. VAE in Practice with Pythae

Autoencoder

- The objective $\Longrightarrow$ Dimensionnality Reduction

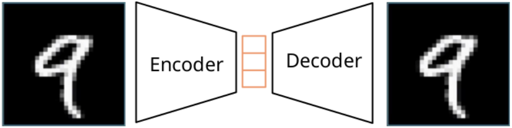

Figure: Simple Autoencoder

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

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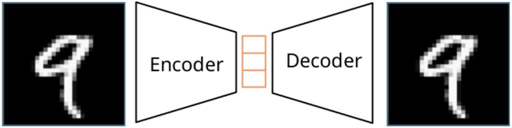

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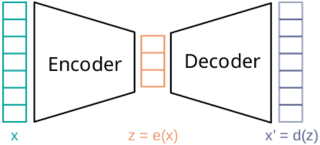

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Autoencoder

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:

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

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

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

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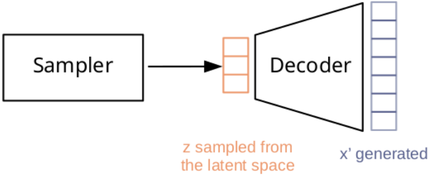

Figure: Generation procedure ?

- How to sample form the latent space?
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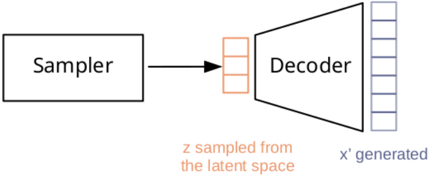

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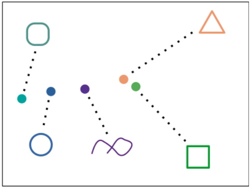

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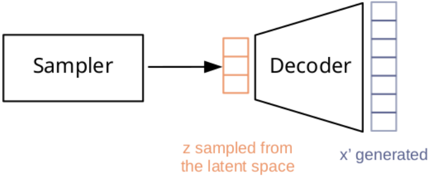

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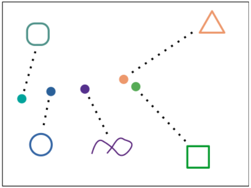

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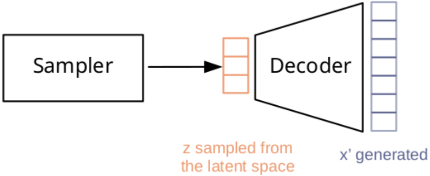

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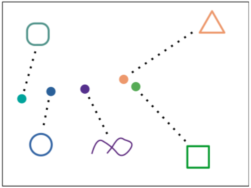

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- An autoencoder based model...

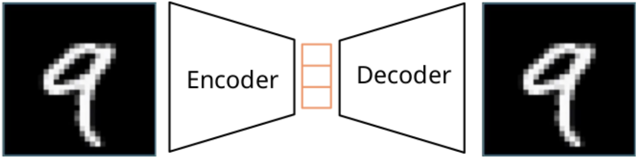

Figure: Simple autoencoder

- ... but where an input data point is encoded as a **distribution** defined over the latent space [17, 27]

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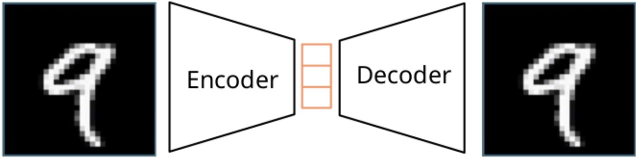

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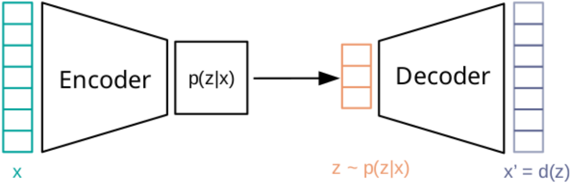

Figure: VAE framework

VAE - Use Cases

- The VAE is a very versatile model that can be used to model complex distributions [18] such as *images* [34, 33], time series [5, 13], natural language [2], chemical structures [30], shapes [4] ...
- It can be used for various tasks as well!

Image Synthesis

- VAE as a generative model for image data

Figure: Samples from NVAE [33] on FFHQ [16]

Data Augmentation

- VAE for Data Augmentation of 3D MRIs to enhance Alzheimer's disease automatic diagnosis [7]

training set	data set	ADNI sensitivity	ADNI specificity	ADNI balanced accuracy	AIBL sensitivity	AIBL specificity	AIBL balanced accuracy
train-50	real	70.3 ± 12.2	62.4 ± 11.5	66.3 ± 2.4	60.7 ± 13.7	73.8 ± 7.2	67.2 ± 4.1
	real (high-resolution)	78.5 ± 9.4	57.4 ± 8.8	67.9 ± 2.3	57.2 ± 11.2	75.8 ± 7.0	66.5 ± 3.0
	500 synthetic + real	71.9 ± 5.3	67.0 ± 4.5	69.4 ± 1.6	55.9 ± 6.8	81.1 ± 3.1	68.5 ± 2.5
	2000 synthetic + real	72.2 ± 4.4	70.3 ± 4.3	71.2 ± 1.6	66.6 ± 7.1	79.0 ± 4.1	72.8 ± 2.2
	5000 synthetic + real	$\mathbf{74.7 \pm 5.3}$	$\mathbf{73.5 \pm 4.8}$	$\mathbf{74.1 \pm 2.2}$	$\mathbf{71.7 \pm 10.0}$	80.5 ± 4.4	$\mathbf{76.1 \pm 3.6}$
	10000 synthetic + real	74.7 ± 7.0	73.4 ± 6.1	74.0 ± 2.7	69.1 ± 9.9	$\mathbf{80.7 \pm 5.1}$	74.9 ± 3.2

Figure: Classification results with state-of-the-art CNN for Alzheimer disease from [7]

Clustering

- VAE for clustering

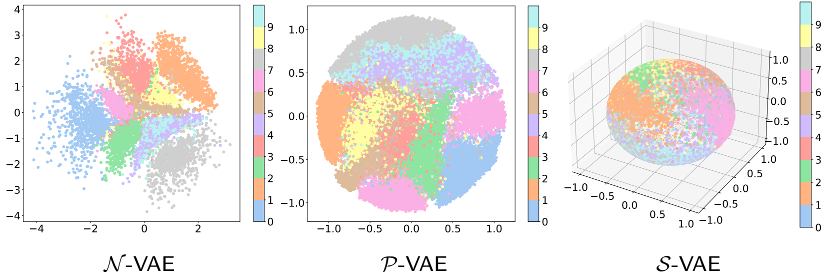

Figure: 2-dimensional latent spaces learned by a vanilla VAE ($\mathcal{N}$-VAE), Poincaré VAE ($\mathcal{P}$-VAE) and Hyperspherical VAE ($\mathcal{S}$-VAE) on MNIST. The colors represent the digits. Plots are made using [8]

Feature Extraction

- VAE used as feature extractor (*e.g.* Stable diffusion) [28]

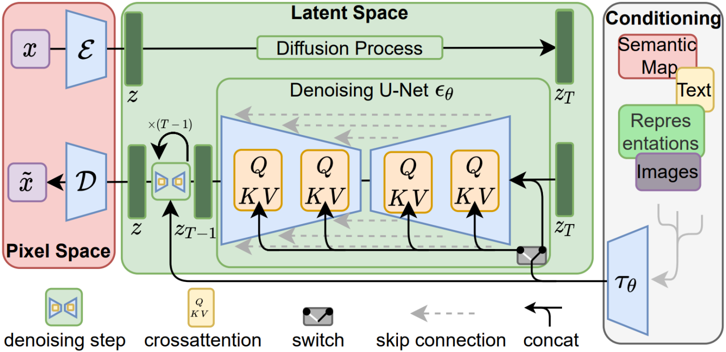

Figure: Latent Diffusion Model architecture [28]

VAE - Mathematical Considerations

- Let $x \in \mathcal{X}$ be a set of data and $\{P_\theta, \theta \in \Theta\}$ be a parametric model
- We assume there exists latent variables $z \in \mathcal{Z}$ living in a smaller space such that the marginal likelihood writes

$$p_\theta(x) = \int p_\theta(x|z) q_{\text{prior}}(z) dz \,,$$

  where q_{prior} is a prior distribution over the latent variables and $p_\theta(x|z)$ is referred to as the decoder
- Example:

$$q_{\text{prior}} = \mathcal{N}(0, I), \qquad p_\theta(x|z) = \prod_{i=1}^{D} \mathcal{B}(\pi_{\theta_i(z)})$$

Objective:

- Maximizing the likelihood of the model

Problem: The integral is often intractable.

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&\geq \int\left(\log\frac{p_\theta(x,z)}{q(z)}\right)q(z)dz\text{ , using Jensen's inequality} \\
&\geq \int\left(\log p_\theta(x,z)\right)q(z)dz - H(q(z))
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with H the entropy of $q(z)$.

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

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The ELBO

- Well-know issue: the posterior $q(z) = p_\theta(z|x)$ is intractable.
  $\longrightarrow$ use Expectation-Maximisation algorithms (up to the MCMC-SAEM version)
- **OR** approximate this posterior with amortised variational inference $\rightarrow$ ELBO
- Introduce a parametric approximation:

$$q_\phi(z|x) \simeq p_\theta(z|x)\,,$$

  where $q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \Sigma_\phi(x))$
- This leads to an unbiased estimate of the log-likelihood

$$\widehat{p_\theta}(x) = \frac{p_\theta(x,z)}{q_\phi(z|x)}, \qquad \mathbb{E}_{z\sim q_\phi(z|x)}[\widehat{p_\theta}(x)] = p_\theta(x)\,,$$

- and the definition of the **Evidence Lower Bound** (ELBO):

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

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Variational inference: The ELBO

Objective:

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

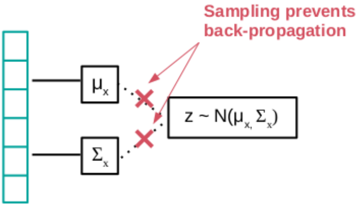
   Use stochastic gradient descent in both θ and ϕ

The Reparametrisation Trick for stochastic gradient descent

- Recall the ELBO

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

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



(a) Back-propagation impossible

$\Longrightarrow$

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

Objective $\Longrightarrow$ OK

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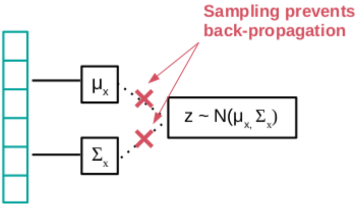
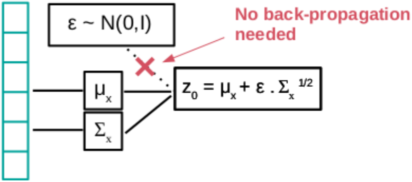


(a) Back-propagation impossible

$\Longrightarrow$



(b) Back-propagation possible

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

Objective $\Longrightarrow$ OK

The Reparametrisation Trick for stochastic gradient descent

- Recall the ELBO

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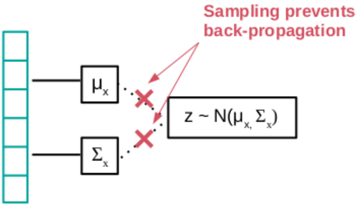

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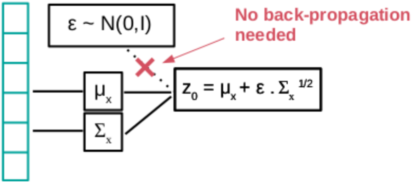

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Generating new samples

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

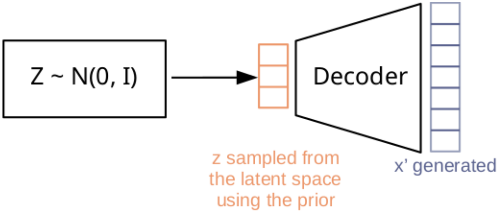

Figure: Generation procedure using prior

Pros:

- Very simple to use in practice

Cons:

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

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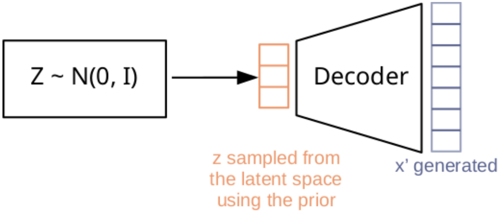

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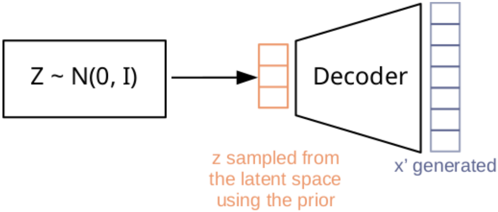

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Improving the model

Can we do better?

Tweaking the Approximate Posterior Distribution

- The ELBO can written as

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

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Normalizing Flows

- The idea is to use smooth invertible parameterised mappings f_ψ to "sample" z [26]
- K transformations are then applied to a latent variable z_0 drawn from an initial distribution q (here $q = q_\phi$) leading to a final random variable $z_K = f_x^K \circ \cdots \circ f_x^1(z_0)$ whose density writes

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

- *E.g.* Planar flows [26], NICE [10], radial flows [26], RealNVP [11], Masked Autoregressive Flows (MAF) [23] or Inverse Autoregressive Flows (IAF) [19]

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- Idea: Work with an extended space by adding an *auxiliary* continuous random variable $u \in \mathcal{U}$ and consider an augmented inference model [29, 20, 24]

$$q_\phi(u, z|x) = q_\phi(u|x) q_\phi(z|u, x) \,.$$

- u allows to access to a potentially richer class of $q_\phi(z|x)$ since

$$q_\phi(z|x) = \int_{\mathcal{U}} q_\phi(u, z|x) du \,.$$

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Building Better Estimators

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- Several approached proposed to build more complex estimators of the marginal likelihood $p_\theta(x)$ [3, 21, 12, 31]
- *E.g* Importance Weighted AutoEncoder (IWAE) that uses an ELBO derived from the K-sample importance weighted estimator.

$$\widehat{p}_\theta(x) = \frac{1}{K}\sum_{i=1}^{K}\frac{p_\theta(x,z_i)}{q_\phi(z_i|x)} \text{ and } \mathbb{E}_{z_1,\dots,z_K\sim q_\phi(z|x)}\left[\widehat{p}_\theta\right] = p_\theta(x)\,.$$

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- Recall the vanilla VAE ELBO

$$\mathcal{L}(\theta, \phi, x) = \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}(q_\phi(z|x)||p(z)) \, .$$

- One may show that the prior maximising the ELBO is given by the *aggregated* posterior [15, 32]

$$q^{\mathrm{avg}}(z) = \frac{1}{N}\sum_{i=1}^{N} q_\phi(z|x_i)$$

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Several axis of development were proposed in the literature to improve the generative capability of the model and reduce the regularisation coming from the prior.

- Approximate the *aggregated posterior* [32]:

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  where λ corresponds to the prior's parameters $\lambda = \{\phi, u_1, \ldots, u_K\}$.
- Learn the prior during training [9, 25, 22, 1]
- *post*-training density estimation with Gaussian mixture or flows [34, 14]
  $\Longrightarrow$ Estimate density of the latent code

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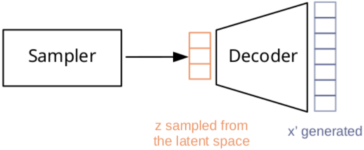

Training VAEs wit Pythae

Let's Train VAEs

What is Pythae?

- Pythae is a Python library that implements some of the most common VAEs models

pypi package 0.1.0 | python 3.7|3.8|3.9+ | docs passing | license Apache-2.0
code style black | codecov 97% | Open in Colab

Documentation

pythae

This library implements some of the most common (Variational) Autoencoder models under a unified implementation. In particular, it provides the possibility to perform benchmark experiments and comparisons by training the models with the same autoencoding neural network architecture. The feature *make your own autoencoder* allows you to train any of these models with your own data and own Encoder and Decoder neural networks. It integrates experiment monitoring tools such wandb, mlflow or comet-ml 🧪 and allows model sharing and loading from the HuggingFace Hub 🤗 in a few lines of code.

News 📢

As of v0.1.0, `Pythae` now supports distributed training using PyTorch's DDP. You can now train your favorite VAE faster and on larger datasets, still with a few lines of code. See our speed-up benchmark.

Why Pythae ?

- **Unifying implementations**
  - × Existing implementations may be *difficult to adapt* to other use-cases, be in *different frameworks* or *no longer maintained*.
  - ✓ **Pythae**'s **brick-like structure** allows for seamless but efficient interchange between models, sampling techniques, network architectures, model hyper-parameters and training schemes.
- **A reproducible research environment**
  - × Reproducibility is hard: implementations may *no longer maintained* or *unavailable*.
  - ✓ **Pythae** reproduced most of the most popular GAE methods (when code was available or enough information provided in the paper).
- **Usable by all**
  - × Existing codes may only allow reproduction of specific results available in the paper.
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Pythae - Code structure

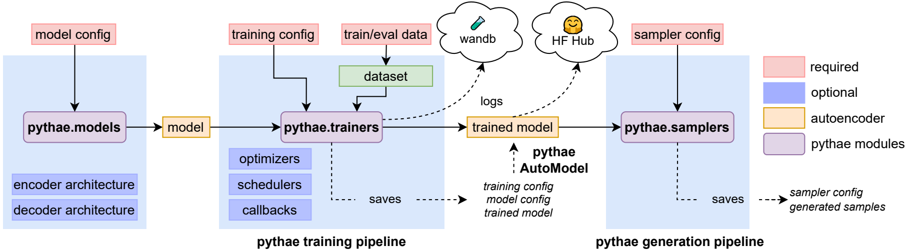

Figure: Code structure

Pythae - API

Architecture Definition

```python
from pythae.models.nn import BaseEncoder, BaseDecoder
from pythae.models.base.base_utils import ModelOutput

# Define encoder architecture
class My_Encoder(BaseEncoder):
    def __init__(self):
        BaseEncoder.__init__(self)
        self.layers = my_nn_layers()

    def forward(self, x: torch.Tensor) -> ModelOutput:
        out = self.layers(x)
        output = ModelOutput(embedding=out)
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class My_Decoder(BaseDecoder):
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Training

```python
from pythae.pipelines import TrainingPipeline
from pythae.models import VAE, VAEConfig
from pythae.trainers import BaseTrainerConfig

# Set up the training configuration
my_training_config = BaseTrainerConfig(...)

# Set up the model configuration
model_config = VAEConfig(...)

# Build the model
my_vae_model = VAE(
    model_config=my_vae_config,
    encoder=my_encoder,
    decoder=my_decoder
)

# Build the pipeline
pipeline = TrainingPipeline(
    training_config=my_training_config,
    model=my_vae_model
)

# Launch the pipeline
pipeline(
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Data Generation

```python
from pythae.models import AutoModel
from pythae.samplers import GaussianMixtureSamplerConfig
from pythae.pipelines import GenerationPipeline

# Retrieve the trained model
my_trained_vae = AutoModel.load_from_folder(
  'path/to/your/trained/model'
)

# Set up the sampler configuration
my_sampler_config = GaussianMixtureSamplerConfig(
    n_components=10
)

# Build the pipeline
pipeline = GenerationPipeline(
    model=my_trained_vae,
    sampler_config=my_sampler_config
)

# Launch data generation
generated_samples = pipeline(
    num_samples=100,
    return_gen=True
    train_data=train_data,
    eval_data=None,

)
```

Zoom on Configurations

- How to define my training configuration?

```python
from pythae.trainers import BaseTrainerConfig

# Set up the training configuration
my_training_config = BaseTrainerConfig(
    output_dir='my_model',
    num_epochs=50,
    learning_rate=1e-3,
    per_device_train_batch_size=200,
    per_device_eval_batch_size=200,
    train_dataloader_num_workers=2,
    eval_dataloader_num_workers=2,
    steps_saving=20,
    optimizer_cls="AdamW",
    optimizer_params={"weight_decay": 0.05, "betas": (0.91, 0.995)},
    scheduler_cls="ReduceLROnPlateau",
    scheduler_params={"patience": 5, "factor": 0.5}
)
```

Figure: Example of a training configuration

Zoom on Configurations

- How to define my model configuration?

```
from pythae.models import WAE_MMD, WAE_MMD_Config

# Set up the model configuration
my_wae_config = WAE_MMD_Config(
    input_dim=(1, 28, 28),
    latent_dim=10,
    kernel_choice="imq",
    reg_weight=0.01
)

# Build the model
my_wae_model = WAE_MMD(
    model_config=my_wae_config,
    encoder=my_encoder, # pass your encoder as argument when building the model
    decoder=my_decoder # pass your decoder as argument when building the model
 )
```

Figure: Example of a model configuration

Distributed Training with Pythae

- Pythae also support distributed training using PyTorch DDP

```
training_config = BaseTrainerConfig(
     num_epochs=10,
     learning_rate=1e-3,
     per_device_train_batch_size=64,
     per_device_eval_batch_size=64,
     train_dataloader_num_workers=8,
     eval_dataloader_num_workers=8,
     dist_backend="nccl", # distributed backend
     world_size=8 # number of gpus to use (n_nodes x n_gpus_per_node),
     rank=5 # process/gpu id,
     local_rank=1 # node id,
     master_addr="localhost" # master address,
     master_port="12345" # master port,
)
```

Figure: Training configuration in a distributed setting

Distributed Training with Pythae

- Pythae also support distributed training using PyTorch DDP

Table 1: Training time of a Vector Quantized VAE (VQ-VAE) with Pythae on V100 GPU(s) on MNIST (100 epochs), FFHQ (50 epochs) and ImageNet-1k (20 epochs).

Dataset	Data Type (train size)	1 GPU	4 GPUs	2x4 GPUs
MNIST	28x28 images (50k)	221.01s	60.32s	34.50s
FFHQ	1024x1024 RGB images (60k)	19h 1min	5h 6min	2h 37min
ImageNet-1k	128x128 RGB images (≈ 1.2M)	6h 25min	1h 41min	51min 26s

Figure 1: Reconstructions on FFHQ-1024.

Pythae - Implemented Models

GAE Model	Pythae model
Autoencoder	AE
Variational Autoencoder	VAE
Beta Variational Autoencoder	BetaVAE
VAE with Linear Normalizing Flows	VAE_LinNF
VAE with Inverse Autoregressive Flows	VAE_IAF
Disentangled β-VAE	DisentangledBetaVAE
Disentangling by Factorising	FactorVAE
Beta-TC-VAE	BetaTCVAE
Importance Weighted Autoencoder	IWAE
Multiply Importance Weighted Autoencoder	MIWAE
Partially Importance Weighted Autoencoder	PIWAE
Combination Importance Weighted Autoencoder	CIWAE
VAE with perceptual metric similarity	MSSSIM_VAE
Wasserstein Autoencoder	WAE
Info Variational Autoencoder	INFOVAE_MMD
VAMP Autoencoder	VAMP
Hyperspherical VAE	SVAE
Poincaré Disk VAE	PoicaréVAE
Adversarial Autoencoder	Adversarial_AE
Variational Autoencoder GAN	VAEGAN
Vector Quantized VAE	VQVAE
Hamiltonian VAE	HVAE
Regularized AE with L2 decoder param	RAE_L2
Regularized AE with gradient penalty	RAE_GP
Riemannian Hamiltonian VAE	RHVAE

Figure: 25 implemented models

Pythae - Experiments monitoring

Pythae integrates experiment monitoring tools

W&B

```python
from pythae.trainers.training_callbacks import WandbCallback

callbacks = []

# Build the callback
wandb_cb = WandbCallback()

# Set up the callback
wandb_cb.setup(
    training_config=your_training_config,
    model_config=your_model_config,
    project_name="your_wandb_project",
    entity_name="your_wandb_entity",
)

# Add it to the callbacks list
callbacks.append(wandb_cb)
```

mlflow

```python
from pythae.trainers.training_callbacks import MLFlowCallback

callbacks = []

# Build the callback
mlflow_cb = MLFlowCallback() # Build the callback

# Set up the callback
mlflow_cb.setup(
    training_config=your_training_config,
    model_config=your_model_config,
    run_name="mlflow_cb_example",
)

# Add it to the callbacks list
callbacks.append(wandb_cb)
```

comet

```python
from pythae.trainers.training_callbacks import CometCallback

callbacks = []

# Build the callback
comet_cb = CometCallback() # Build the callback

# Set up the callback
comet_cb.setup(
    training_config=training_config,
    model_config=model_config,
    api_key="your_comet_api_key",
    project_name="your_comet_project",
)

# Add it to the callbacks list
callbacks.append(wandb_cb)
```

Callback set-up

Pythae - Experiments monitoring

Pythae integrates experiment monitoring tools

W&B

```python
from pythae.trainers.training_callbacks import WandbCallback

callbacks = []

# Build the callback
wandb_cb = WandbCallback()

# Set up the callback
wandb_cb.setup(
    training_config=your_training_config,
    model_config=your_model_config,
    project_name="your_wandb_project",
    entity_name="your_wandb_entity",
)

# Add it to the callbacks list
callbacks.append(wandb_cb)
```

mlflow

```python
from pythae.trainers.training_callbacks import MLFlowCallback

callbacks = []

# Build the callback
mlflow_cb = MLFlowCallback() # Build the callback

# Set up the callback
mlflow_cb.setup(
    training_config=your_training_config,
    model_config=your_model_config,
    run_name="mlflow_cb_example",
)

# Add it to the callbacks list
callbacks.append(wandb_cb)
```

comet

```python
from pythae.trainers.training_callbacks import CometCallback

callbacks = []

# Build the callback
comet_cb = CometCallback() # Build the callback

# Set up the callback
comet_cb.setup(
    training_config=training_config,
    model_config=model_config,
    api_key="your_comet_api_key",
    project_name="your_comet_project",
)

# Add it to the callbacks list
callbacks.append(wandb_cb)
```

Callback set-up

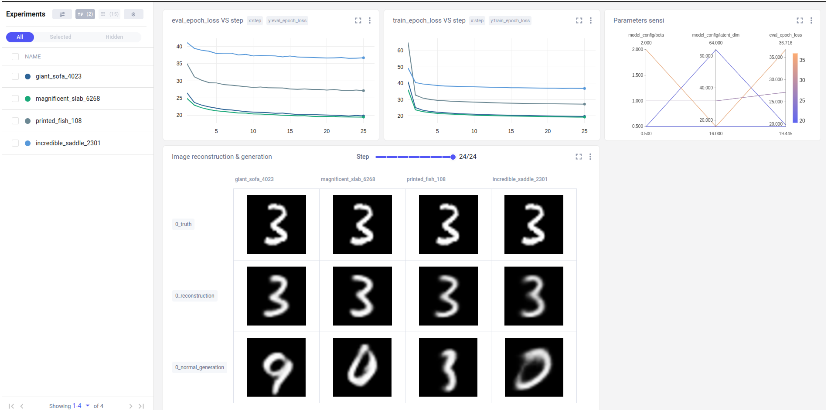
```python
pipeline = TrainingPipeline(
    training_config=config,
    model=model
)

pipeline(
    train_data=train_dataset,
    eval_data=eval_dataset,
    callbacks=callbacks
)
```

```python
pipeline = TrainingPipeline(
    training_config=config,
    model=model
)

pipeline(
    train_data=train_dataset,
    eval_data=eval_dataset,
    callbacks=callbacks
)
```

```python
pipeline = TrainingPipeline(
    training_config=config,
    model=model
)

pipeline(
    train_data=train_dataset,
    eval_data=eval_dataset,
    callbacks=callbacks
)
```

Callback usage

Pythae - Experiments monitoring



Pythae - Model sharing

Pythae allows model sharing through the HuggingFace Hub

```
my_vae_model.push_to_hf_hub(hf_hub_path="your_hf_username/your_hf_hub_repo")
```

Model saving

Pythae - Model sharing

Pythae allows model sharing through the HuggingFace Hub

```
my_vae_model.push_to_hf_hub(hf_hub_path="your_hf_username/your_hf_hub_repo")
```

Model saving

```
from pythae.models import AutoModel
my_downloaded_vae = AutoModel.load_from_hf_hub(hf_hub_path="path_to_hf_repo")
```

Model loading

Pythae - Resources

Thank you!

- ✓ Github: `https://github.com/clementchadebec/benchmark_VAE`
- ✓ Online documentation: `https://pythae.readthedocs.io/en/latest/`
- ✓ Pypi project page: `https://pypi.org/project/pythae/`
- ✓ Open to contributors!

```
pip install pythae
```

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