# **DD-GAN-AE**

Release 1.0.0

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**CHAPTER** 

ONE

# **MODELS**

This package contains three models that can readily be used with user defined or imported network architectures. These consist of: adversarial autoencoder, convolutional autoencoder, and SVD autoencoder.

# 1.1 Adversarial Autoencoder

Implementation of two classes with a slightly different version of the adversarial autoencoder model. The former corresponds to the original paper on adversarial autoencoders:

https://arxiv.org/abs/1511.05644

and the second is an adaptation with weighted losses inspired by:

https://arxiv.org/abs/2104.06297

class models.aae.AAE (encoder, decoder, discriminator, optimizer, seed=None)

Adversarial autoencoder class

compile (input\_shape)

Compilation of models according to original paper on adversarial autoencoders

Parameters input\_shape (tuple) - Shape of input data

train (train\_data, epochs, val\_data=None, batch\_size=128, val\_batch\_size=128, wandb\_log=False)
Training model according to original paper on adversarial autoencoders

#### **Parameters**

- train\_data (np.ndarray) Train dataset
- **epochs** (*int*) Number of training epochs to execute
- val\_data (np.ndarray, optional) Validation dataset. Defaults to None.
- batch\_size (int, optional) Training batch size. Defaults to 128.
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.
- wandb\_log (bool, optional) Whether to log results to wandb. Note function needs to be called in wandb.init() scope for this to work. Defaults to False.

validate (val\_dataset, val\_batch\_size=128)

Validate model on previously unseen dataset.

- val\_dataset (np.ndarray) Validation dataset
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.

**Returns** Validation losses and accuracies

Return type tuple

**class** models.aae.**AAE\_combined\_loss** (encoder, decoder, discriminator, optimizer, seed=None) Adversarial autoencoder with combined loss class

compile(input shape)

Compilation of models where we use a training method that weights the losses of the discriminator and autoencoder and as such combines them into one loss and trains on them simultaneously.

Parameters input\_shape (tuple) - Shape of input data

Training model with combined loss strategy

#### **Parameters**

- train\_data (np.ndarray) Train dataset
- epochs (int) Number of training epochs to execute
- val\_data (np.ndarray, optional) Validation dataset. Defaults to None.
- batch\_size (int, optional) Training batch size. Defaults to 128.
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.
- wandb\_log (bool, optional) Whether to log results to wandb. Note function needs to be called in wandb.init() scope for this to work. Defaults to False.

**validate** (val dataset, val batch size=128)

Validate model on previously unseen dataset.

#### **Parameters**

- val\_dataset (np.array) Validation dataset
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.

**Returns** Validation losses and accuracies

Return type tuple

models.aae.plot\_losses (*d\_loss*, *g\_loss*, *liveloss*, *d\_loss\_val=None*, *g\_loss\_val=None*) Convenience function to plot a set of losses. Can be used by adversarial type of networks

#### **Parameters**

- d loss (float) Discriminator loss value
- **g\_loss** (float) Generator loss value
- livaloss (object) livelossplot class instance
- d\_loss\_val (float, optional) Validation discriminator loss value. Defaults to None.
- g\_loss\_val(float, optional) Validation generator loss value. Defaults to None.

models.aae.print\_losses(d\_loss, g\_loss, epoch, d\_loss\_val=None, g\_loss\_val=None)

Convenience function to print a set of losses. Can be used by adversarial type of networks

# **Parameters**

- **d\_loss** (float) Discriminator loss value
- **g\_loss** (float) Generator loss value

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- **epoch** (*int*) Current epoch
- d\_loss\_val (float, optional) Validation discriminator loss value. Defaults to None.
- g\_loss\_val(float, optional) Validation generator loss value. Defaults to None.

# 1.2 Convolutional Autoencoder

Convolutional autoencoder model.

class models.cae.CAE (encoder, decoder, optimizer, seed=None)

Convolutional autoencoder class

compile (input\_shape, pi\_loss=False)

Compile model

#### **Parameters**

- input\_shape (tuple) Shape of input data
- **pi\_loss** (bool, optional) Whether to use physics informed loss, note this is currently in experimental stage. Defaults to False.

## predict (data)

Convenience function that gives class predict method that just does forward pass through model.

Parameters data (np. ndarray) - Input grids that are to be reconstructed by this model

Returns Reconstructed grids

Return type np.ndarray

train (train\_data, epochs, val\_data=None, batch\_size=128, val\_batch\_size=128, wandb\_log=False)
Training convolutional autoencoder model

## **Parameters**

- train\_data (np.ndarray) Train dataset
- epochs (int) Number of training epochs to execute
- val\_data (np.ndarray, optional) Validation dataset. Defaults to None.
- batch\_size (int, optional) Training batch size. Defaults to 128.
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.
- wandb\_log (bool, optional) Whether to log results to wandb. Note function needs to be called in wandb.init() scope for this to work. Defaults to False.

 $\verb|train_generate| (data\_file\_base, val\_data, epochs, regen\_epochs)|$ 

Train and every regen\_epochs epochs generate a new training set from available vtu files.

Currently in development.

- data\_file\_base (string) Path to vtu files
- val data (np.array) Array to use as validation dataset
- **epochs** (*int*) Number of total epochs to do
- regen\_epochs (int) Interval at which to regenerate a new dataset

```
validate(val dataset)
```

Validate model on validation dataset.

#### **Parameters**

- val\_dataset (np.ndarray) Validation dataset
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.

**Returns** Validation losses and accuracies

Return type tuple

# 1.3 SVD Autoencoder

SVD autoencoder model. Can be used with any of the dense (or 1D convolutional) encoder and decoder architectures in architectures directory.

class models.svdae.SVDAE (encoder, decoder, optimizer, seed=None)

SVD Autoencoder class

calc\_pod (snapshots, nPOD=-2, cumulative\_tol=0.99)

Calculate POD coefficients and basis functions

#### **Parameters**

- **snapshots** (*list of ndarrays*) List of arrays with subgrid snapshots. shape: (n\_grids, n\_nodes, n\_timelevels)
- **nPOD** (*int*) number of pod coefficients to use. Set to -2 for dynamic setting where a tolerance determines the number of POD coefficients. Defaults to -2.
- **cumulative\_tol** (*float*) Tolerance value to use if this option is selected in *nPOD* parameter.

**Returns** POD coefficients per subgrid

**Return type** list of ndarrays

compile (nPOD, weight\_loss=False)

Compile SVD autoencoder

#### **Parameters**

- nPOD (int) Number of POD coefficients to use
- weight\_loss (bool, optional) Whether to weight losses by singular value magnitudes, note this feature is currently in experimental phase. Defaults to False.

predict (data)

Pass a collection of grids through the model

Parameters data (np.ndarray) - Dataset that is to be passed through the model

Returns Reconstructed dataset

Return type np.ndarray

```
predict_single (snapshot)
```

Pass single array through full model including POD and the autoencoder

Parameters snapshot (np.ndarray) - Grid to be predicted

Returns Grid reconstructed by SVD autoencoder

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# **Return type** np.ndarray

#### reconstruct from pod(R)

Convenience function to reconstruct a grid from bases and coefficients

#### **Parameters**

- coeffs (np.ndarray) POD coefficients
- R (np.ndarray) POD basis matrix

Returns Grid reconstructed through POD

Return type np.ndarray

train (train\_data, epochs, val\_data=None, batch\_size=128, val\_batch\_size=128, wandb\_log=False)
Training SVD autoencoder model

#### **Parameters**

- train\_data (np.ndarray) Train dataset
- epochs (int) Number of training epochs to execute
- val\_data (np.ndarray, optional) Validation dataset. Defaults to None.
- batch\_size (int, optional) Training batch size. Defaults to 128.
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.
- wandb\_log (bool, optional) Whether to log results to wandb. Note function needs to be called in wandb.init() scope for this to work. Defaults to False.

## validate(val\_dataset)

Validate model on validation dataset.

Parameters val\_dataset (np.ndarray) - Validation dataset

**Returns** Validation losses and accuracies

Return type tuple

models.svdae.plot\_losses(loss, liveloss, loss\_val=None)

Convenience function to plot a set of losses. Can be used by SVD autoencoder.

#### **Parameters**

- loss (float) loss value
- livaloss (object) livelossplot class instance
- loss val(float, optional) Validation loss value. Defaults to None.

models.svdae.print\_losses(loss, epoch, loss\_val=None)

Convenience function to print a set of losses. can be used by SVD autoencoder.

#### **Parameters**

- loss (float) Loss value
- epoch (int) Current epoch

# 1.4 Predictive models

Predictive Models. Note that these models contain multiple vestigial elements from having been autoencoders before. For example the naming of the attributes on the classes, e.g. "encoder" and "decoder". Note that in a production

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release these would likely be named differently. However, since other students rely on this code in their codebases and use the present version such a change would require a coordination with other students as well, for which there was no time in this project.

class models.predictive.Predictive(encoder, decoder, optimizer, seed=None)

Predictive Neural Network class

compile (nPOD, increment=False)

Compile the model

# **Parameters**

- nPOD (np.ndarray) Number of input coefficients, can be POD coefficients but also latent variables
- increment (bool, optional) Whether to predict and train on increments or whole values. Defaults to False.

Predict in time using boundaries and initial values for a certain number of timesteps. The timestep shifts will be done in this function

#### **Parameters**

- **boundaries** (np.ndarray) Boundaries in shape (nboundaries (2), nvars, ntimesteps)
- init\_values (np.ndarray) Initial values in shape (ngrids, nvars)
- timesteps (int) Number of timesteps to predict
- **iters** (*int*) Number of iterations to do before a prediction. Defaults to 5.
- **sor** (*float*) Successive overrelaxation factor. Defaults to 1.
- **timestep\_print\_interval** (*int*) Interval at which to print the current timestep to see progress, defaults to None.

# preprocess (input\_data)

Preprocessing function to transform dataset.

**Parameters input\_data** (np.ndarray) - Input data in shape (<number of domains>, <number of pod

coeffcients or latent variables per domain>, <number of timesteps>)

**Returns** Tuple containing x (samples) and y (targets) datasets

# Return type tuple

train (input\_data, epochs, interval=5, val\_size=0, val\_data=None, batch\_size=128, val\_batch\_size=128, wandb\_log=False, n\_discriminator=5, n\_gradient\_ascent=inf, noise\_std=0)

Train the model and do preprocessing within this function.

#### **Parameters**

- input\_data (np.ndarray) Input data in shape
- epochs (int) Number of epochs to train for
- interval (int, optional) Interval at which to train data. Defaults to 5.
- **val\_size** (*float*, *optional*) Relative size of validation set, if not supplied as the next argument. Number between 0 and 1. Defaults to 0.

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- val\_data (np.ndarray, optional) User-supplied validation dataset, mutually exclusive with val size > 0. Defaults to None.
- batch\_size (int, optional) [description]. Defaults to 128.
- val\_batch\_size (int, optional) Batch size on the validation set. Defaults to 128.
- wandb\_log(bool, optional) Whether to log results to wandb, needs to be called within wandb context if set to true. Defaults to False.
- n\_discriminator (int, optional) Interval at which discriminator is trained, i.e. it is trained on every n\_discriminator batches. Defaults to 5.
- n\_gradient\_ascent (int, optional) Interval at which discriminator is made to do a step of gradient ascent, i.e. it does a step of gradient ascent every n\_gradient\_ascent batches. Defaults to np.inf.
- noise\_std (float, optional) Standard deviation of Gaussian noise applied to training dataset, is reapplied uniquely every epoch. Defaults to 0.

validate(val dataset, val batch size)

Validate model on validation dataset.

#### **Parameters**

- val\_dataset (np.ndarray) Validation dataset
- val batch size (int, optional) Validation batch size. Defaults to 128.

**Returns** Validation losses and accuracies

Return type tuple

Predictive Adversarial Neural Network class

compile (nPOD, increment=False)

Compile the model with a weighted loss between the autoencoder and generator

#### **Parameters**

- nPOD (np.ndarray) Number of input coefficients, can be POD coefficients but also latent variables
- increment (bool, optional) Whether to predict and train on increments or whole values. Defaults to False.

classmethod from\_save(dirname, optimizer)

Load model from savefile and override default constructor

#### Parameters

- dirname (str) Name of directory where model is saved
- **optimizer** (Object) Tensorflow optimizer

# **Parameters**

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- **boundaries** (np.ndarray) Boundaries in shape (nboundaries (2), nvars, ntimesteps)
- init\_values (np. ndarray) Initial values in shape (ngrids, nvars)
- timesteps (int) Number of timesteps to predict
- iters (int) Number of iterations to do before a prediction. Defaults to 5.
- **sor** (*float*) Successive overrelaxation factor. Defaults to 1.
- **pre\_interval** (bool) Whether intervals have already been applied outside of this function. If False, this function will do it. Defaults to False.
- **timestep\_print\_interval** Interval at which to print the current timestep to see progress, defaults to None.

#### preprocess (input\_data)

Preprocessing function to transform dataset. Will be called on input data when function *train* is called. Will not be used when *train\_preprocessed* is used instead, as the latter assumes the user has done the preprocessing in advance.

**Parameters input\_data** (np.ndarray) - Input data in shape (<number of domains>, <number of pod

coeffcients or latent variables per domain>, <number of timesteps>)

**Returns** Tuple containing x (samples) and y (targets) datasets

#### Return type tuple

**save** (dirname='model')
Saves the model

#### **Parameters**

- dirname (str, optional) Directory to save model in. Defaults to
- "model" -

train(input\_data, epochs, interval=5, val\_size=0, val\_data=None, batch\_size=128,
 val\_batch\_size=128, wandb\_log=False, n\_discriminator=5, n\_gradient\_ascent=inf,
 noise\_std=0)

Train the model and do preprocessing within this function.

#### **Parameters**

- input\_data (np.ndarray) Input data in shape
- epochs (int) Number of epochs to train for
- interval (int, optional) Interval at which to train data. Defaults to 5.
- **val\_size** (*float*, *optional*) Relative size of validation set, if not supplied as the next argument. Number between 0 and 1. Defaults to 0.
- val\_data (np.ndarray, optional) User-supplied validation dataset, mutually exclusive with val size > 0. Defaults to None.
- batch\_size (int, optional) [description]. Defaults to 128.
- val\_batch\_size (int, optional) Batch size on the validation set. Defaults to 128.
- wandb\_log (bool, optional) Whether to log results to wandb, needs to be called within wandb context if set to true. Defaults to False.

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- n\_discriminator (int, optional) Interval at which discriminator is trained, i.e. it is trained on every *n* discriminator batches. Defaults to 5.
- n\_gradient\_ascent ([type], optional) Interval at which discriminator is made to do a step of gradient ascent, i.e. it does a step of gradient ascent every n\_gradient\_ascent batches. Defaults to np.inf.
- noise\_std (float, optional) Standard deviation of Gaussian noise applied to training dataset, is reapplied uniquely every epoch. Defaults to 0.

train\_preprocessed ( $x_full$ ,  $y_full$ , epochs, interval=5,  $val\_size=0$ ,  $val\_data=None$ , batch\_size=128,  $val\_batch\_size=128$ ,  $wandb\_log=False$ ,  $n\_discriminator=5$ ,  $n\_gradient\_ascent=inf$ ,  $noise\_std=0$ )
Train the model and do no preprocessing.

#### **Parameters**

- input\_data (np.ndarray) Input data
- epochs (int) Number of epochs to train for
- interval (int, optional) Interval at which to train data. Defaults to 5.
- **val\_size** (*float*, *optional*) Relative size of validation set, if not supplied as the next argument. Number between 0 and 1. Defaults to 0.
- val\_data (np.ndarray, optional) User-supplied validation dataset, mutually exclusive with val size > 0. Defaults to None.
- batch\_size (int, optional) [description]. Defaults to 128.
- val\_batch\_size (int, optional) Batch size on the validation set. Defaults to 128.
- wandb\_log (bool, optional) Whether to log results to wandb, needs to be called within wandb context if set to true. Defaults to False.
- n\_discriminator (int, optional) Interval at which discriminator is trained, i.e. it is trained on every n\_discriminator batches. Defaults to 5.
- n\_gradient\_ascent ([type], optional) Interval at which discriminator is made to do a step of gradient ascent, i.e. it does a step of gradient ascent every n\_gradient\_ascent batches. Defaults to np.inf.
- noise\_std (float, optional) Standard deviation of Gaussian noise applied to training dataset, is reapplied uniquely every epoch. Defaults to 0.

validate(val dataset, val batch size)

Validate model on validation dataset.

#### **Parameters**

- val\_dataset (np.ndarray) Validation dataset
- val\_batch\_size (int, optional) Validation batch size. Defaults to 128.

**Returns** Validation losses and accuracies

Return type tuple

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# HYPERPARAMETER OPTIMIZATION

This package contains some functionality for doing hyperparameter optimization with the Weights and Biases platform. Below is the documentation for the functions that handle this for the flow past cylinder and slug flow problems.

# 2.1 Flow Past Cylinder

Functions used for weights and biases hyperparameter optimization of autoencoders on FPC dataset.

```
wandb.train_wandb_fpc.train_wandb_aae(config=None)
```

Construct and subsequently train the model while reporting losses to weights and biases platform. Weights and biases also controls hyperparameters.

**Parameters config** (dict, optional) – Dictionary with hyperparameters, set by weights and biases. Defaults to None.

```
wandb.train wandb fpc.train wandb cae(config=None)
```

Construct and subsequently train the model while reporting losses to weights and biases platform. Weights and biases also controls hyperparameters.

**Parameters config** (dict, optional) – Dictionary with hyperparameters, set by weights and biases. Defaults to None.

```
wandb.train wandb fpc.train wandb svdae(config=None)
```

Construct and subsequently train the model while reporting losses to weights and biases platform. Weights and biases also controls hyperparameters.

**Parameters config**(dict, optional) – Dictionary with hyperparameters, set by weights and biases. Defaults to None.

# 2.2 Slug Flow

Functions used for weights and biases hyperparameter optimization of autoencoders on slug flow dataset

```
wandb.train_wandb_sf.train_wandb_aae(config=None)
```

Construct and subsequently train the model while reporting losses to weights and biases platform. Weights and biases also controls hyperparameters.

**Parameters config**(dict, optional) – Dictionary with hyperparameters, set by weights and biases. Defaults to None.

```
wandb.train_wandb_sf.train_wandb_cae(config=None)
```

Construct and subsequently train the model while reporting losses to weights and biases platform. Weights and biases also controls hyperparameters.

**Parameters config** (dict, optional) – Dictionary with hyperparameters, set by weights and biases. Defaults to None.

wandb.train\_wandb\_sf.train\_wandb\_svdae(config=None)

Construct and subsequently train the model while reporting losses to weights and biases platform. Weights and biases also controls hyperparameters.

**Parameters config** (dict, optional) – Dictionary with hyperparameters, set by weights and biases. Defaults to None.

**CHAPTER** 

# **THREE**

# **UTILITIES**

This package also contains some utilities for printing, loss functions, etc...

General utilities for package

utils.calc\_pod(snapshots, nPOD=-2, cumulative\_tol=0.99, R=None)

Calculate POD coefficients and basis functions

**Parameters** snapshots (list of ndarrays) – List of arrays with subgrid snapshots. shape: (n\_grids, n\_nodes\*n\_scalar, n\_timelevels)

Returns POD coefficients per subgrid

Return type list of ndarrays

class utils.mse\_PI(dx=None, dy=None)

Mean squared error loss class.

class utils.mse\_weighted

Custom weighted mean squared error loss

utils.reconstruct\_pod(coeffs, R)

Reconstruct grid from POD coefficients and transormation matrix R.

## **Parameters**

- coeffs (np.array) POD coefficients
- R (np.array) Transformation matrix R

Returns Reconstructed grid

Return type np.array

Collection of preprocessing utilities. Further preprocessing utilities can be found in DD-GAN submodule.

preprocessing.utils.convert\_2d(subgrid\_snapshots, shape, timesteps)

Utility to convert list of grids to list of 2d grids

#### **Parameters**

- subgrid\_snapshots (List) List of subgrids
- **shape** (*Tuple*) Shape of 2d grid, e.g. (nFields, nx, ny)
- timesteps (Int) Number of timesteps

**Returns** List of converted subgrids

Return type List

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**CHAPTER** 

**FOUR** 

# LIBRARY OF ARCHITECTURES

While the package is built in such a way that the user can easily use the architectures they designed. This package also includes a set of premade architectures. These are listed below.

# 4.1 Convolutional Architectures

Note that we have different architectures for the flow past cylinder and slug flow problems.

# 4.1.1 Two Dimensional (Flow Past Cylinder)

Collection of encoders and decoders that can readily be imported and used by the 2D adversarial and convolutional autoencoder and predictive models.

Note that these models are currently adjusted to a 55 by 42 input shape.

```
architectures.cae.D2.cae.build_agostini_encoder_decoder(input_shape, latent_dim, initializer, info=False)
```

This encoder-decoder pair currently works for 221 by 42 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.

Returns encoder, decoder pair

# Return type tuple

```
architectures.cae.D2.cae.build_custom_conv_decoder(latent_dim, initializer, info=False)
```

Builds a 2D convolutional decoder

#### **Parameters**

- latent dim(int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.

Returns encoder

Return type tf.keras.Model

architectures.cae.D2.cae.build\_custom\_conv\_encoder(input\_shape, latent\_dim, initial-izer.info=False)

Builds a 2D convolutional encoder

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.

#### Returns encoder

# Return type tf.keras.Model

```
architectures.cae.D2.cae.build_deeper_omata_encoder_decoder(input_shape, latent_dim, initializer, info=False, act='elu', dense_act=None)
```

This encoder-decoder pair currently works for 55 by 42 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

Returns encoder, decoder pair

#### Return type tuple

```
architectures.cae.D2.cae.build_denser_omata_encoder_decoder (input_shape, latent_dim, initializer, info=False, act='elu', dense_act=None)
```

This encoder-decoder pair currently works for 55 by 42 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

Returns encoder, decoder pair

#### Return type tuple

```
architectures.cae.D2.cae.build_densest_omata_encoder_decoder (input_shape, latent_dim, initial-izer, info=False, act='elu', dense act=None)
```

This encoder-decoder pair currently works for 55 by 42 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

Returns encoder, decoder pair

# Return type tuple

```
architectures.cae.D2.cae.build_mnist_wide_omata_encoder_decoder (input_shape, latent_dim, initializer, info=False)
```

This encoder-decoder pair currently works for 28 by 28 grids so can work on MNIST dataset as a test

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- $\bullet \ \textbf{initializer} \ (\textit{tf.keras.initializers.Initializer}) \textbf{Weights initializer} \\$
- info (bool, optional) Whether to print info. Defaults to False.

**Returns** encoder, decoder pair

# Return type tuple

```
architectures.cae.D2.cae.build_omata_encoder_decoder(input_shape, latent_dim, ini-
tializer, info=False, act='elu',
dense act=None)
```

This encoder-decoder pair currently works for 55 by 42 grids

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- $\bullet \ \ \textbf{initializer} \ (\textit{tf.keras.initializers.Initializer}) \textbf{Weights initializer} \\$
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

Returns encoder, decoder pair

# Return type tuple

```
architectures.cae.D2.cae.build_wide_omata_encoder_decoder(input_shape, latent_dim, initializer, info=False, act='elu', dense act=None)
```

This encoder-decoder pair currently works for 55 by 42 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

Returns encoder, decoder pair

# Return type tuple

```
architectures.cae.D2.cae.build_wider_omata_encoder_decoder(input_shape, latent_dim, initializer, info=False, act='elu', dense act=None)
```

This encoder-decoder pair currently works for 55 by 42 grids

# **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

Returns encoder, decoder pair

Return type tuple

# 4.1.2 Three Dimensional (Slug Flow)

Collection of encoders and decoders that can readily be imported and used by the 3D adversarial and convolutional autoencoder and predictive models.

Note that these models are currently adjusted to a 60 by 60 by 20 input shape.

```
architectures.cae.D3.cae.build_deeper_omata_encoder_decoder (input_shape, latent_dim, initializer, info=False, act='elu', dense_act=None, final act='linear')
```

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

# Return type tuple

```
architectures.cae.D3.cae.build_denser_omata_encoder_decoder (input_shape, latent_dim, initial-izer, info=False, act='elu', dense_act=None, final_act='linear')
```

This encoder-decoder pair currently works for 60 by 20 by 20 grids

# **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

**Returns** encoder, decoder pair

Return type tuple

```
architectures.cae.D3.cae.build_densest_omata_encoder_decoder (input_shape, latent_dim, initial-izer, info=False, act='elu', dense_act=None, final act='linear')
```

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

## Return type tuple

```
architectures.cae.D3.cae.build_densest_thinner_omata_encoder_decoder (input_shape, la-
la-
tent_dim,
initial-
izer,
info=False,
act='elu',
dense_act=None,
fi-
nal_act='linear')
```

This encoder-decoder pair currently works for 60 by 20 by 20 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

Return type tuple

```
architectures.cae.D3.cae.build_omata_encoder_decoder(input_shape, initializer, info=False, act='elu', dense_act=None, final_act='linear')
```

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

## Return type tuple

```
architectures.cae.D3.cae.build_wide_omata_encoder_decoder(input_shape, latent_dim, initializer, info=False, act='elu', dense_act=None, final act='linear')
```

This encoder-decoder pair currently works for 60 by 20 by 20 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

Return type tuple

# 4.2 Discriminator Architectures

Collection of discriminators that can readily be imported and used by the adversarial autoencoder and predictive models

architectures.discriminators.discriminators.build\_custom\_discriminator ( $latent\_dim$ , ini-tial-izer, info=False)

#### Build a discriminator

#### **Parameters**

- latent\_dim (int) Number of latent variables.
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print model info. Defaults to False.

#### **Returns** discriminator

# Return type tf.keras.Model

```
architectures.discriminators.discriminators.build_custom_wider_discriminator (latent\_dim, ini-
tial-
izer, info=False)
```

# Build a discriminator

#### **Parameters**

- latent\_dim (int) Number of latent variables.
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print model info. Defaults to False.

**Returns** discriminator

**Return type** tf.keras.Model

# 4.3 Mixed architectures for SVD Autoencoder and predictive networks

Collection of encoders and decoders that can readily be imported and used by the SVD autoencoder model.

```
architectures.svdae.svdae.build_conv_encoder_decoder(input_dim, latent_dim, initial-
izer, info=False, act='relu',
dense_act='relu', dropout=0.6,
final_act='linear')
```

Create a 1D convolutional encoder and decoder

- input dim(tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.

- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

#### Return type tuple

```
architectures.svdae.svdae.build_deeper_dense_decoder(input_dim, initializer, info=False, act='relu', dropout=0.6, final_act='linear')
```

Builds a dense decoder

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.
- **final\_act** (str, optional) Dense layer activation function to use. Defaults to "linear".

Returns encoder

# Return type tf.keras.Model

```
architectures.svdae.svdae.build_deeper_dense_encoder(latent\_dim, initializer, info=False, act='relu', dropout=0.6)
```

Builds a dense encoder

# **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- $\bullet \ \textbf{initializer} \ (\textit{tf.keras.initializers.Initializer}) \textbf{Weights initializer} \\$
- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.

Returns encoder

# Return type tf.keras.Model

```
architectures.svdae.svdae.build_dense_decoder(input_dim, latent_dim, initializer, info=False, act='relu', dropout=0.6, final_act='linear')
```

Builds a dense decoder

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer

- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (int, optional) Dropout factor to use. Defaults to 0.6.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

#### Returns encoder

#### Return type tf.keras.Model

```
architectures.svdae.svdae.build_dense_encoder(latent_dim, initializer, info=False, act='relu', dropout=0.6)
```

# Builds a dense encoder

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.

#### Returns encoder

#### Return type tf.keras.Model

```
architectures.svdae.svdae.build_slimmer_dense_decoder(input_dim, initializer, info=False, act='relu', dropout=0.6, final\_act='linear')
```

#### Builds a dense decoder

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (*int*, *optional*) Dropout factor to use. Defaults to 0.6.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

#### Returns encoder

## Return type tf.keras.Model

```
architectures.svdae.svdae.build_slimmer_dense_encoder(latent\_dim, initializer, info=False, act='relu', dropout=0.6)
```

# Builds a dense encoder

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer

- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.

## Returns encoder

# Return type tf.keras.Model

```
architectures.svdae.svdae.build_slimmer_vinicius_encoder_decoder (input_dim, latent_dim, initializer, info=False, act='elu', dense_act='elu', dropout=0.6, reg=0.001, batch-norm=True, fi-nal_act='linear')
```

This encoder-decoder pair currently works for 60 by 20 by 20 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **dropout** (*float*) Dropout factor to use in dense layers.
- **reg** (float) Level of weights regularization to use.
- batchnorm (bool, optional) Whether to use batch normalization layers. Defaults to True.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

# Return type tuple

```
architectures.svdae.svdae.build_smaller_vinicius_encoder_decoder (input_dim, latent_dim, initializer, info=False, act='elu', dense_act='elu', dropout=0.6, reg=0.001, batch-norm=True, fi-nal_act='linear')
```

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **dropout** (*float*) Dropout factor to use in dense layers.
- **reg** (float) Level of weights regularization to use.
- batchnorm (bool, optional) Whether to use batch normalization layers. Defaults to True.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

## Return type tuple

```
architectures.svdae.svdae.build_vinicius_encoder_decoder(input_dim, latent_dim, initializer, info=False, act='elu', dense_act='elu', dropout=0.6, reg=0.001, batchnorm=True, final_act='linear')
```

This encoder-decoder pair currently works for 60 by 20 by 20 grids

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **dropout** (float) Dropout factor to use in dense layers.
- **reg** (*float*) Level of weights regularization to use.
- batchnorm (bool, optional) Whether to use batch normalization layers. Defaults to True.
- **final\_act** (*str*, *optional*) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

Return type tuple

```
architectures.svdae.svdae.build_wider_conv_encoder_decoder (input_dim, latent_dim, initializer, info=False, act='relu', dense_act='relu', dropout=0.6, final act='linear')
```

Create a 1D convolutional encoder and decoder

#### **Parameters**

- input\_dim (tuple) Shape tuple of input grids
- latent dim(int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- act (str, optional) Activation function to use. Defaults to "elu".
- dense\_act (str, optional) Dense layer activation function to use. Defaults to None.
- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.
- **final\_act** (str, optional) Dense layer activation function to use. Defaults to "linear".

Returns encoder, decoder pair

# Return type tuple

```
architectures.svdae.svdae.build_wider_dense_decoder(input_dim, latent_dim, initializer, info=False, act='relu', dropout=0.6, final act='linear')
```

Builds a dense decoder

#### **Parameters**

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables
- initializer (tf.keras.initializers.Initializer) Weights initializer
- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (int, optional) Dropout factor to use. Defaults to 0.6.
- **final\_act** (str, optional) Dense layer activation function to use. Defaults to "linear".

Returns encoder

# Return type tf.keras.Model

```
architectures.svdae.svdae.build_wider_dense_encoder(latent\_dim, initializer, info=False, act='relu', dropout=0.6)
```

Builds a dense encoder

- input\_shape (tuple) Shape tuple of input grids
- latent\_dim (int) Number of latent variables

- $\bullet \ \textbf{initializer} \ (\texttt{tf.keras.initializers.Initializer}) \textbf{Weights initializer} \\$
- info (bool, optional) Whether to print info. Defaults to False.
- **dropout** (*int*, *optional*) **Dropout** factor to use. Defaults to 0.6.

Returns encoder

Return type tf.keras.Model

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