superres-ml

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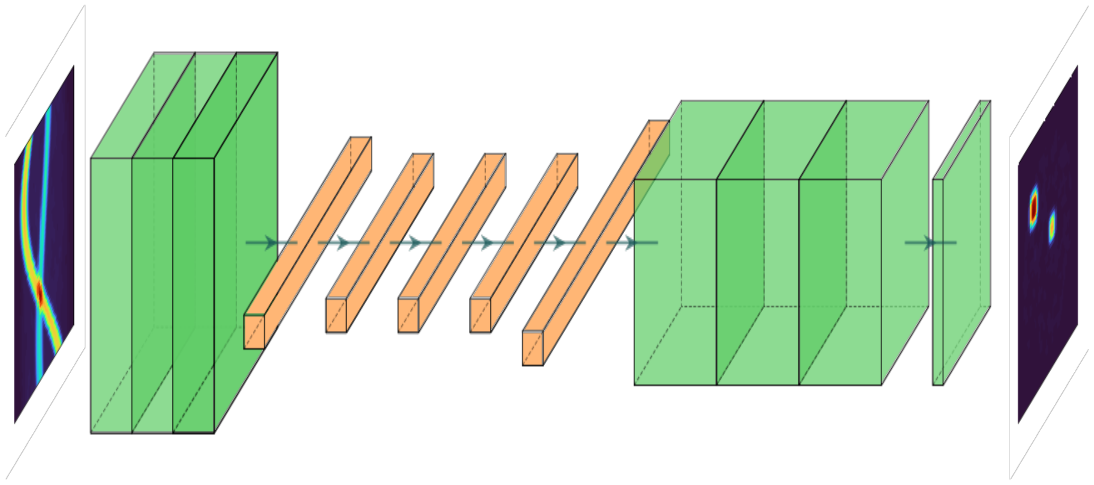
Documentation:

superres-tomo is a package of useful scripts and models for applying neural networks for tomographic reconstruction of X-ray images. The package also includes models and scripts useful for the analysis of the images generated, allowing tasks such as semantic segmentation of very large images and removing noise from low dose images.



The tasks possible with *superres-tomo* are

- Image reconstruction
- Image segmentation
- Image denoising
- Image super-resolution [coming soon]
- Image fusion for super-resolution [coming soon]

superres-tomo is a produced in collaboration between the SciML group from Rutherford Appleton Laboratory and Finden Ltd. The project has been funded by the AI3SD network

The project is also associated with a benchamrk dataset which can be used to test other super-resolution approaches on similar data.

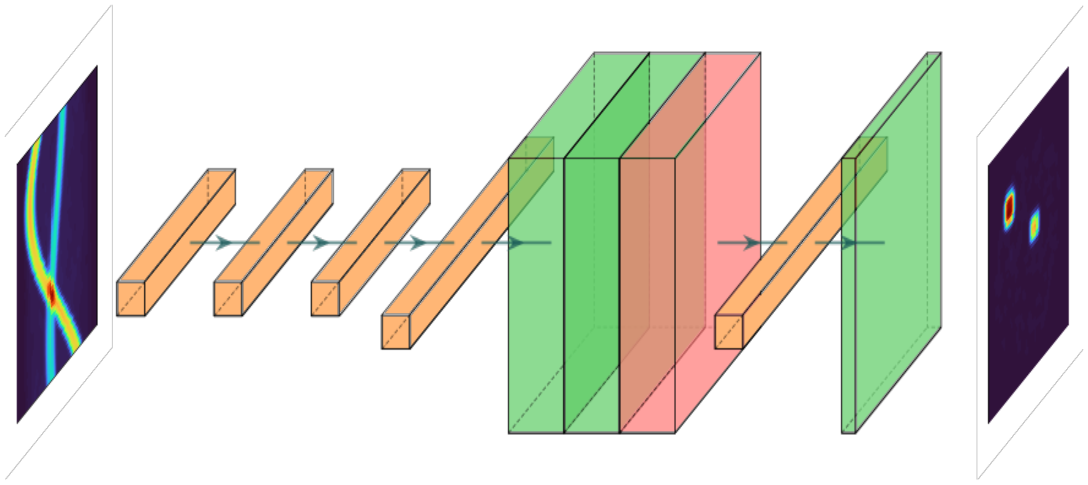
CHAPTER 1

Models available

This is a list and a brief description of the various models that are currently available in *superres-tomo*. More detailed information about each of the models can be found in their individual module documentaion. Additionally example use cases are provided in the tutorials.

1.1 Automap

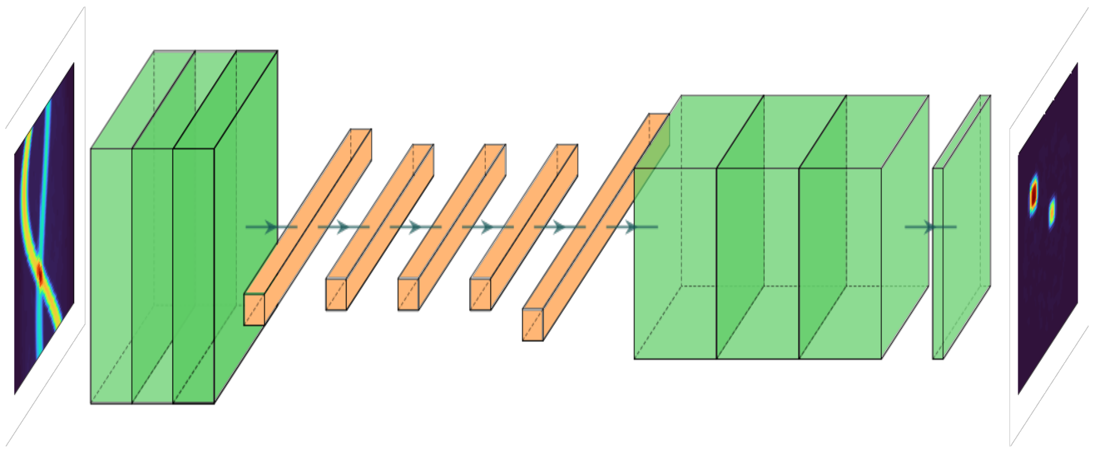
Automap is a network architecture that was specifically developed for tomogrpahic reconstruction.[1] We have implemented the architecture here. While we find that Automap does perform very well, we have alsofound that the dense connections mean that the architecture memory requirements scale very badly and it cannot deal with many typical sinograms.



[1] Bo Zhu, Jeremiah Z. Liu, Bruce R. Rosen, Matthew S. Rosen "Image reconstruction by domain transform manifold learning" https://arxiv.org/pdf/1704.08841.pdf

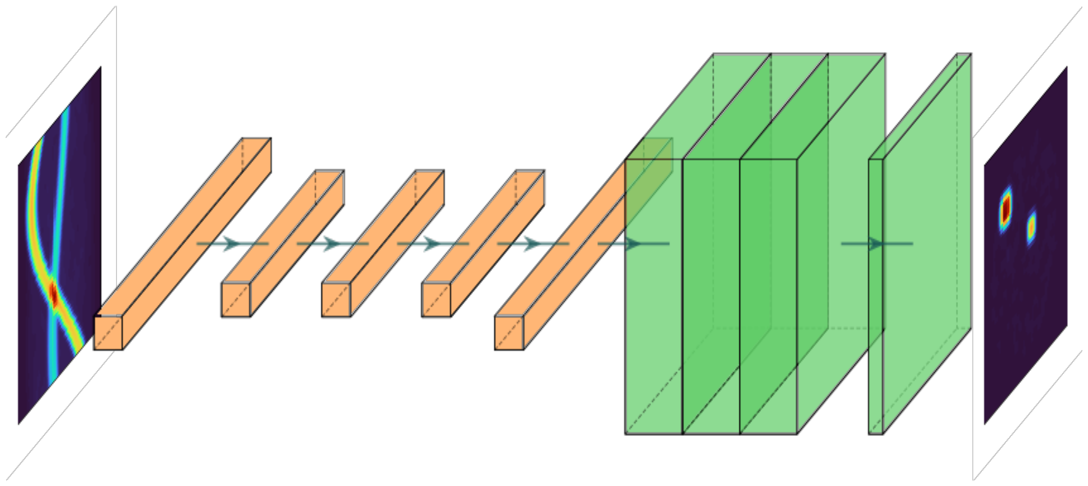
1.2 cnn_reconstruct

This module contains a CNN model for tomographic image reconstruction. For more details on how to use this follow the tutorial on reconstruction with a CNN.



1.3 dense_reconstruct

This module contains a densely connected model for tomographic image reconstruction. For more details on how to use this follow the tutorial on reconstruction with a dense network.



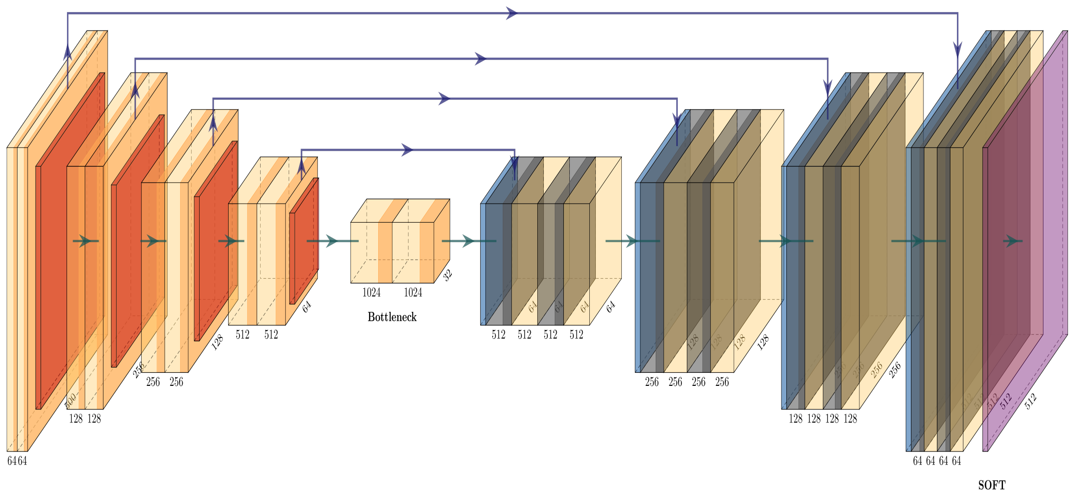
1.4 AlexNet

AlexNet is a specific instance of a CNN. It became famous in 2012, when it outperformed all of the competition in the ImageNet challenge. AlexNet contains eight layers; the first five are convolutional layers, some of them followed by max-pooling layers, and the last three are fully connected layers.[2] It uses the ReLU activation function.

[2] Krizhevsky, Alex; Sutskever, Ilya; Hinton, Geoffrey E. (2017-05-24). "ImageNet classification with deep convolutional neural networks" (PDF). Communications of the ACM. 60 (6): 84–90

1.5 U-Net

The U-net architecture is particularly popular in image segmentation tasks. The model consists of convolution layers mirrored by deconvolution layers, squeezing down and then reconstructing an image of the same size as the original. Doing this a U-Net can convert pixels in the original image into label values and segment the image. U-nets were initially developed for biomedical image segmentation.[3]



1.6 Autoencoder

An autoencoder is a type of artificial neural network used to learn efficient data codings in an unsupervised manner.[4] The aim of an autoencoder is to learn a representation (encoding) for a set of data, typically for dimensionality reduction, by training the network to ignore signal "noise". For this reason autoencoders can be used for denoising images.

1.7 References

[3] Ronneberger, Olaf; Fischer, Philipp; Brox, Thomas (2015). "U-Net: Convolutional Networks for Biomedical Image Segmentation". arXiv:1505.04597

[4] Vincent, Pascal; Larochelle, Hugo (2010). "Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion". Journal of Machine Learning Research. 11: 3371–3408

CHAPTER 2

Tutorials

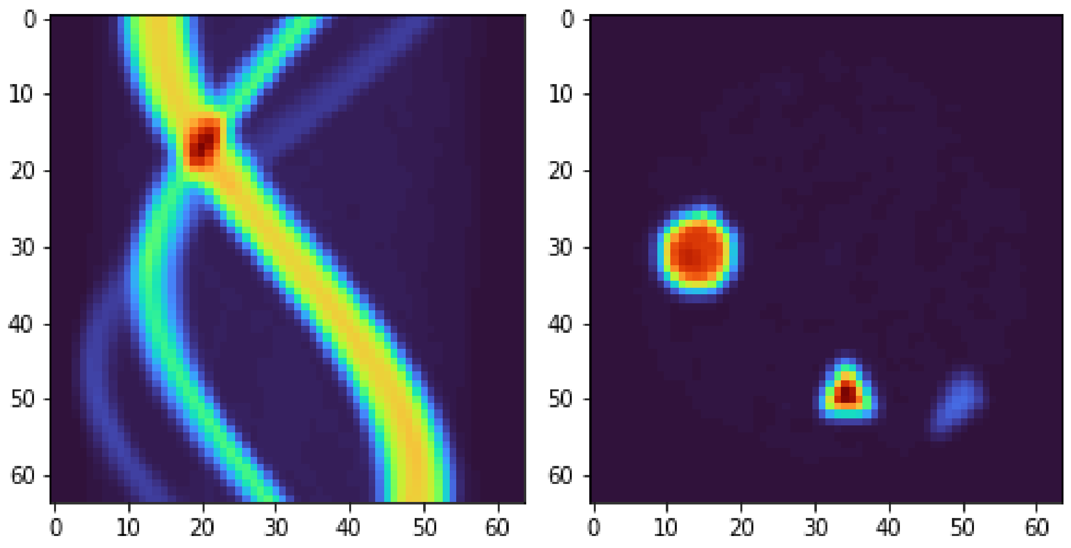
2.1 Tomographic reconstructions

2.1.1 Reconstruction with a CNN

In this tutorial we will reconstruct an image from a sinogram using a convolutional neural network. We have a network architecture for this task: *models.cnn_reconstruct.models.reconstruct_cnn*

Step 0

Generate the data. We have some scripts to generate sample data for this task. *LibShapes.py* Alternatively download sample data from here: http://tiny.cc/vdl9rz



Step 1

When the data is generated we now load it up. Use the *utils.tools.read_reconstruct_library* helper function to make this easier. We then shuffle around the image/sinogram pairs to make sure that we don't have any false ordering. We alsoe need to make sure that *superres-ml* is on our *pythonpath*. Split the data into training and test data.

```
import sys
sys.path.append('/path/to/super-resolution-ml/')
from utils.tools import read_reconstruct_library

images, sinos, nim = read_reconstruct_library('data/reconstruction/shapes_random_
↪noise_64px_norm.h5')
index = np.arange(nim)
np.random.shuffle(index)
images = images[index,:,:,:]
sinograms = sinos[index,:,:,:]
sinograms_test = sinograms[9000:]
images_test = images[9000:]
sinograms = sinograms[:9000]
images = images[:9000]
```

Step 2

Set up the network. We import the *reconstruct_cnn* netowrk from out *superres-ml* model library. We then compile the network to use the *Adam* optimiser and to monitor the *mae* and *mse* during training. We add a callback, which makes the training stop if the metrics have not improved for three steps.

```
from tensorflow.keras.optimizers import Adam
from tensorflow.keras.callbacks import EarlyStopping
from models.cnn_reconstruct.models import reconstruct_cnn

model_rec = reconstruct_cnn(sinos.shape[1], sinos.shape[2])
```

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```
model_rec.compile(optimizer = Adam(lr = 0.000025), loss = 'mean_squared_error',␣
↪metrics = ['mae', 'mse'])
my_callbacks = [EarlyStopping(patience=3)]
```

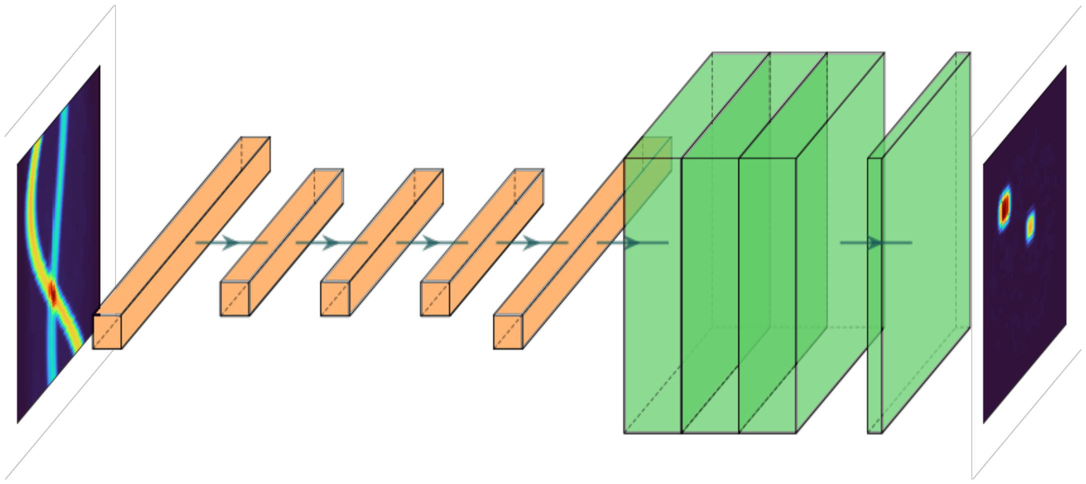
Step 3

Train the model!

```
training = model_rec.fit(sinograms, images,
                         validation_split = 0.1,
                         batch_size=32,
                         epochs = 100,
                         verbose = True,
                         callbacks=my_callbacks)
history = model_rec.history
```

2.1.2 Reconstruction with a Dense Network

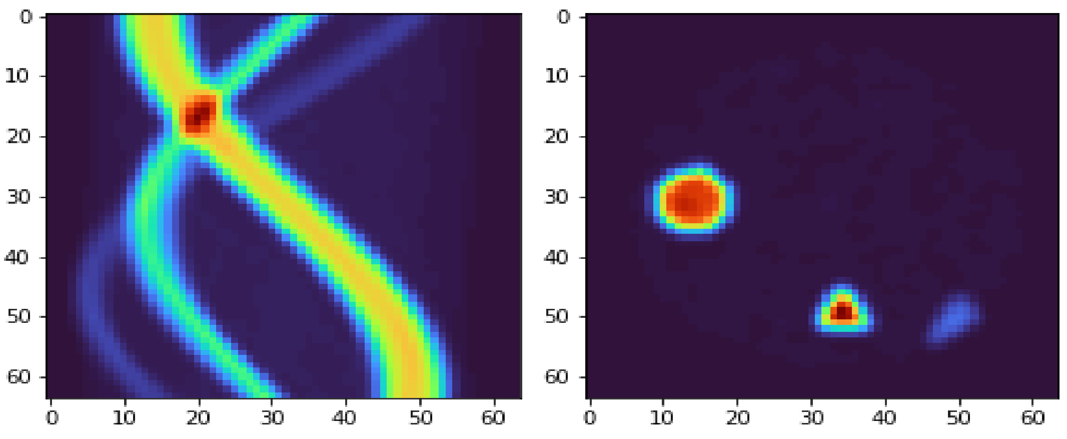
This tutorial is just like the one above, but we use a dense network at the start before convolutions. This kind of network gives very good results but requires *huge* memory for any larger images. See the architecture below.



Steps 0, 1 and 3 are the exact same as for the CNN.

Step 0

Generate the data. We have some scripts to generate sample data for this task. *LibShapes.py* Alternatively download sample data from here: http://tiny.cc/vdl9rz



Step 1

When the data is generated we now load it up. Use the *utils.tools.read_reconstruct_library* helper function to make this easier. We then shuffle around the image/sinogram pairs to make sure that we don't have any false ordering. We alsoe need to make sure that *superres-ml* is on our *pythonpath*. Split the data into training and test data.

```
from utils.tools import read_reconstruct_library
import sys
sys.path.append('/path/to/super-resolution-ml/')

images, sinos, nim = read_reconstruct_library('data/reconstruction/shapes_random_
↪noise_64px_norm.h5')
index = np.arange(nim)
np.random.shuffle(index)
images = images[index,:,:,:]
sinograms = sinos[index,:,:,:]
sinograms_test = sinograms[9000:]
images_test = images[9000:]
sinograms = sinograms[:9000]
images = images[:9000]
```

Step 2

Set up the network. We import the *reconstruct_cnn* netowrk from out *superres-ml* model library. We then compile the network to use the *Adam* optimiser and to monitor the *mae* and *mse* during training. We add a callback, which makes the training stop if the metrics have not improved for three steps.

```
from tensorflow.keras.optimizers import Adam
from tensorflow.keras.callbacks import EarlyStopping
from models.dense_reconstruct.models import dense_reconstruct

model_rec = dense_reconstruct(sinos.shape[1], sinos.shape[2])
model_rec.compile(optimizer = Adam(lr = 0.000025), loss = 'mean_squared_error',␣
↪metrics = ['mae', 'mse'])
my_callbacks = [EarlyStopping(patience=3)]
```

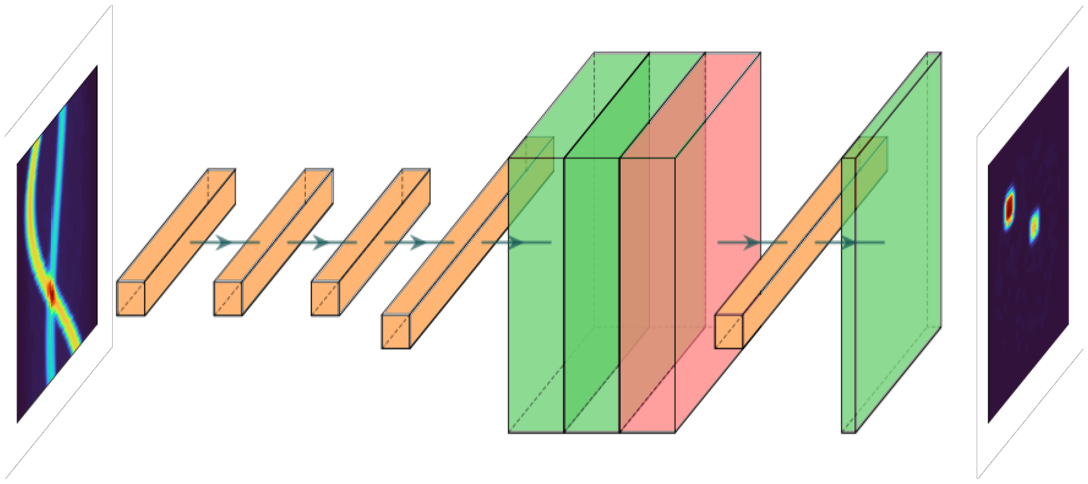
Step 3

Train the model!

```
training = model_rec.fit(sinograms, images,
                      validation_split = 0.1,
                      batch_size=32,
                      epochs = 100,
                      verbose = True,
                      callbacks=my_callbacks)
history = model_rec.history
```

2.1.3 Reconstruction with a Automap

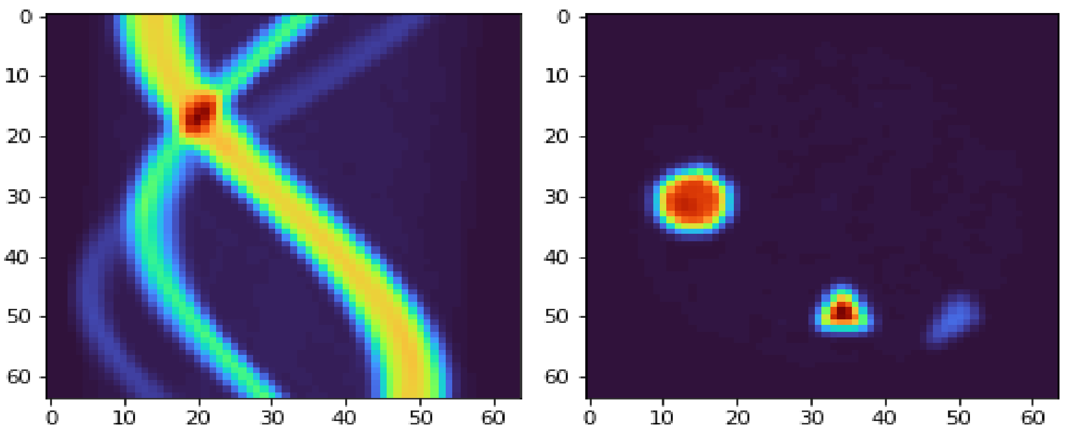
This tutorial is just like the one above, but we use a dense network at the start before convolutions. This kind of network gives very good results but requires *huge* memory for any larger images. See the architecture below.



Steps 0, 1 and 3 are the exact same as for the CNN and dense architectures.

Step 0

Generate the data. We have some scripts to generate sample data for this task. *LibShapes.py* Alternatively download sample data from here: http://tiny.cc/vdl9rz



Step 1

When the data is generated we now load it up. Use the *utils.tools.read_reconstruct_library* helper function to make this easier. We then shuffle around the image/sinogram pairs to make sure that we don't have any false ordering. We alsoe need to make sure that *superres-ml* is on our *pythonpath*. Split the data into training and test data.

```
from utils.tools import read_reconstruct_library
import sys
sys.path.append('/path/to/super-resolution-ml/')

images, sinos, nim = read_reconstruct_library('data/reconstruction/shapes_random_
↪noise_64px_norm.h5')
index = np.arange(nim)
np.random.shuffle(index)
images = images[index,:,:,:]
sinograms = sinos[index,:,:,:]
sinograms_test = sinograms[9000:]
images_test = images[9000:]
sinograms = sinograms[:9000]
images = images[:9000]
```

Step 2

Set up the network. We import the *reconstruct_cnn* netowrk from out *superres-ml* model library. We then compile the network to use the *Adam* optimiser and to monitor the *mae* and *mse* during training. We add a callback, which makes the training stop if the metrics have not improved for three steps.

```
from tensorflow.keras.optimizers import Adam
from tensorflow.keras.callbacks import EarlyStopping
from models.automap.models import automap

model_rec = automap(sinos.shape[1], sinos.shape[2])
model_rec.compile(optimizer = Adam(lr = 0.000025), loss = 'mean_squared_error',␣
↪metrics = ['mae', 'mse'])
my_callbacks = [EarlyStopping(patience=3)]
```

Step 3

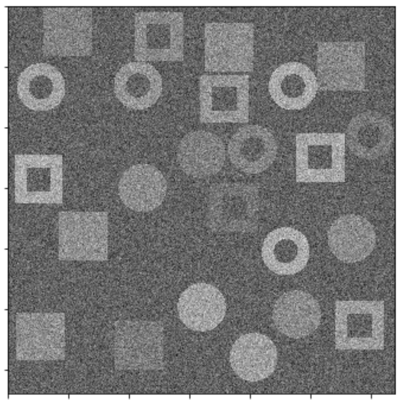
Train the model!

```
training = model_rec.fit(sinograms, images,
                      validation_split = 0.1,
                      batch_size=32,
                      epochs = 100,
                      verbose = True,
                      callbacks=my_callbacks)
history = model_rec.history
```

2.2 Segmentation of X-ray images

2.2.1 Binary segmentation

This tutorial looks at segmentation of sections of an image, for example collected from X-ray imaging. We have a set of images where we have already labelled what the different parts of the image are, now we want to train and apply a model to another set, labelling new X-ray images.



To do this we will use a U-net architecture. There is one big challenge in using most U-net architectures that you will find on the web.

> The image sizes are very large. This means that the image and the model cannot fit together in the memory.

To overcome the problem we will use a routine in *superres-tomo* to create patches from the image and learn sequentially from each patch. To do do this we have implemented the *data_handeling.generators.mask_patch_from_file* function which acts as a generator to feed the network for training.

Step 0

Generate the data. There is a helper script in the directory *data/segmentation* run this to generate the data for this tutorial. Run this script to generate the data for this tutorial.

Also make sure the *superres-ml* package is in your *pythonpath*

```
import sys
sys.path.append('/path/to/super-resolution-ml/')
```

Step 1

Once the data is in place we are ready to start setting up the U-net. Tell the code where to find the images and masks, the types of file to expect.

```
datapath= 'data/segmentation/train/' #<the root directory of images and masks for␣
↪training>
valpath= 'data/segmentation/val/' #<the root directory of images and masks for␣
↪validation>
img_dir= 'noiseless/' # <the subdirectory where images are>
mask_dir= 'label/' #<the subdirectory where masks are>
ftypes= ['./tiff'] # (<filetypes to look for>) # e.g. ('.tif')
```

Step 2

Set up the information about the size of the original image and the size of the patches to take from the image. Also here you can define a list of which patches to use. This last feature is useful when the interesting features are only in a section of the image. You can specify the particular patches to consider for the training. The numbering of patches starts from zero and proceeds left to right top to bottom. If the patch list is left empty the generator uses all patches.

```
image_shape = (1280, 1280)
patch_shape = (64, 64)
patch_range = []
```

Step 3

Set up the generator. This is the function that will flow the patches from the images to the netowrk for training.

```
from data_handeling.generators import mask_patch_from_file

myGene = mask_patch_from_file(datapath,
                           img_dir, mask_dir,
                           patch_shape, image_shape,
                           types = ftypes, patch_range=patch_range,
                           debug=False,
                           batch_size = 1,
                           normalise_images=False)

valGene = mask_patch_from_file(valpath,
                        img_dir, mask_dir,
                        patch_shape, image_shape,
                        types = ftypes, patch_range=patch_range,
                        debug=False,
                        batch_size = 1,
                        normalise_images=False)
```

Step 4

Define the netowrk architecture, the hyperparameters and the training time. Here the input size is the dimension of the patches, also we have just 1 channel as the image is greyscale. We use a standard Adam optimiser. We use *binary_crossentropy* as the loss function and also monitor the accuracy during training.

```
from models.u_net.models import unet_3layer
import models.losses.custom_loss_functions as losses
from tensorflow.keras.optimizers import Adam

model = unet_3layer(input_size = (patch_shape[0], patch_shape[1], 1))
opt = Adam()
model.compile(loss=losses.weighted_cross_entropy(2), optimizer=opt,
           metrics=["accuracy"])
```

Step 5

Train and save!

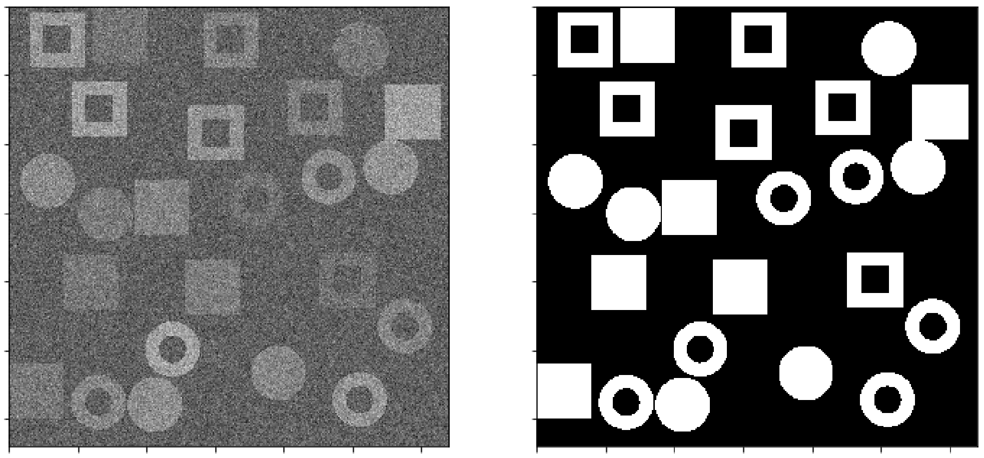
```
epochs = 6
steps_per_epoch = 2000
model.fit(myGene, steps_per_epoch=steps_per_epoch,
          epochs=epochs, validation_data=valGene, validation_steps=100)
model.save_weights('saved_weights.hdf5')
```

Step 6

Run the model for inference. Having trained the model on some images you can now try to deploy on new examples. We have the `utils.tools.inference_binary_segmentation()` helper function to do this. First we load up the saved model and weights.

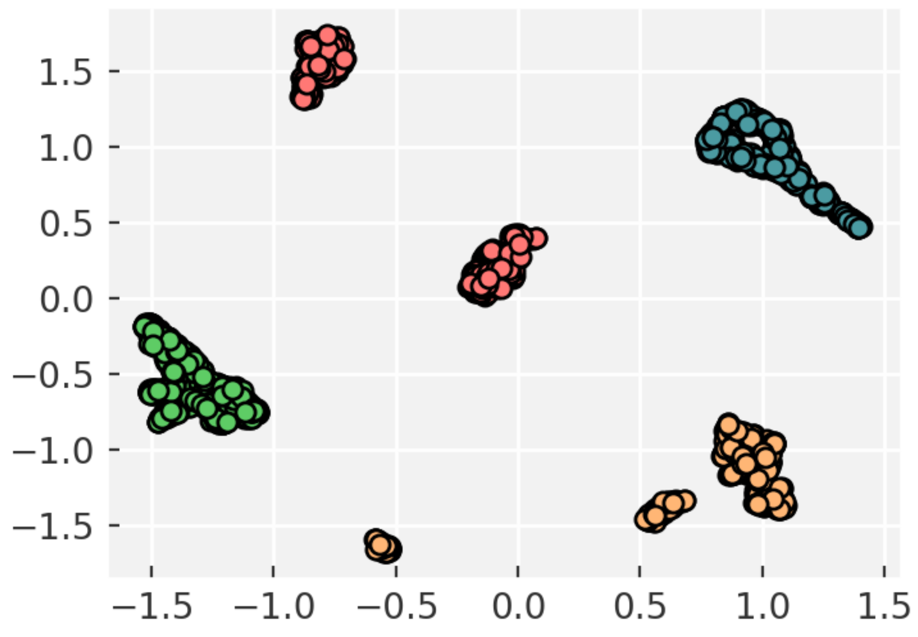
```
from  utils.tools import inference_binary_segmentation

datapath = 'data/segmentation/test/noiseless/'
patch_shape = (64, 64)
image_shape = (1280, 1280)
savepath = './inferred_masks/'

inference_binary_segmentation(datapath, patch_shape, image_shape, model,
              file_prefix='binary_mask', savepath=savepath, fig_size=(8, 8),
             normim=False)
```

In the *inferred_masks* directory there should now be a masking file something like:



2.3 Dimension reduction

This module allows one to project a dataset of images into lower dimensional space (2 or 3 D usually). It is very useful for inspeting datasets to look for outliers and anomallies. It is also useful to see if a new image is out of the training distribution, which can be a problem for CNN based reconstructions. See our paper *Identifying and avoiding training set bias in neural networks for tomographic image reconstruction* for a discussion of this.



If you do not already have the data you can download it from

- Sinograms: https://tinyurl.com/y2t56hgd
- Images: https://tinyurl.com/y2l4jvoj

Then unzip the data. It contains datasets used in our paper. In the example below we load 2000 sinograms, taken from all of the materials.

```
import sys
sys.path.append('/path/to/super-resolution-ml/')
from utils.tools import read_reconstruct_library

images, sinos, nim = read_reconstruct_library('./All_mixed_2K_sinograms_raw.h5')
```

Run the dimensionality reduction. The code below will convert each of your images to a 2D vector. You can alter the settings of the dimensionality reduction. The code uses the *scikit-learn* implementation of *tSNE* to reduce dimensions. You can change the number of desired output dimensions by passing the *n_components_tsne* to the function, by default it is 2.

```
x = dimension_reducer(sinos)
```

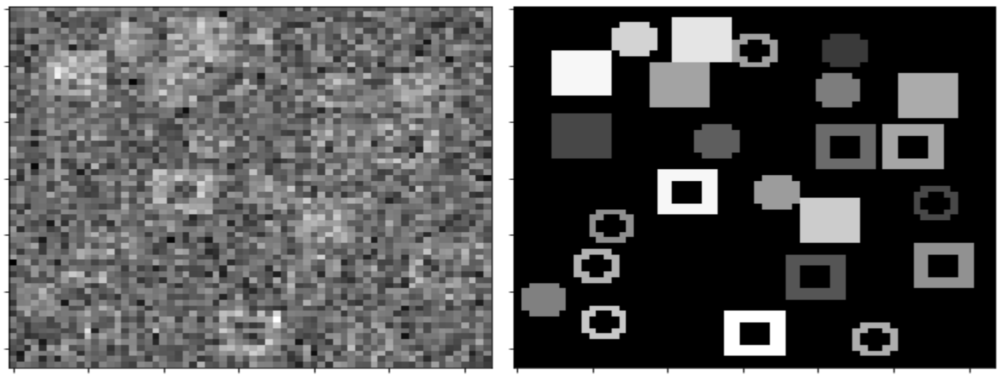
Plot and inspect your result. You can now look at the reduced dimesnion map to see if there are any outliers or anomalies.

```
plt.scatter(x[:, 0], x[:, 1])
```

2.4 Denoising of X-ray images

2.4.1 Variational Autoencoder

Often images that are reconstructed contain low signal to noise ratios, if the dose was low or the collection time short. In these cases it would often be desireable to remove the noise and accentuate the signal in an image. We can do this using a Variational Autoencoder (VAE)



Step 0

Set up the data. You can use the *data/denoising/generatedata.py* script to generate some example data. Then use the helper functions *build_list_images* and *build_autoencoder_data* to build the data set ready to train the VAE.

We need to specify the data shape with the *input_data* keyword and then specify directories to find the training and validation inputs and labels.

```
import sys
sys.path.append('/path/to/super-resolution-ml/')
from data_handeling.tools import build_list_images
from models.autoencoder.tools import build_autoencoder_data

input_data = (64, 64, 1)

datapath = '../data/denoising/train/noisy/'
Xfiles = build_list_images(datapath, types = ['.tiff'])
datapath = '../data/denoising/train/noiseless/'
yfiles = build_list_images(datapath, types = ['.tiff'])
X, labels = build_autoencoder_data(Xfiles, yfiles=yfiles, input_data=input_data)
datapath = '../data/denoising/test/noisy/'
Xfiles = build_list_images(datapath, types = ['.tiff'])
datapath = '../data/denoising/test/noiseless/'
yfiles = build_list_images(datapath, types = ['.tiff'])
xtest, ltest = build_autoencoder_data(Xfiles, yfiles, input_data=input_data)
```

Step 1

Set up the VAE. Here we import the model as well as functions to train and run the model and an optimiser. We need to set the number of units to use in the bottle-neck (latent) space.

```
from models.autoencoder.models import CVAE
from models.autoencoder.tools import vae_train, vae_inference
from tensorflow.keras.optimizers import Adam

latent_dim = 16
optimizer = Adam(lr=0.0001)
epochs = 500
model = CVAE(latent_dim, input_data)
```

Step 2

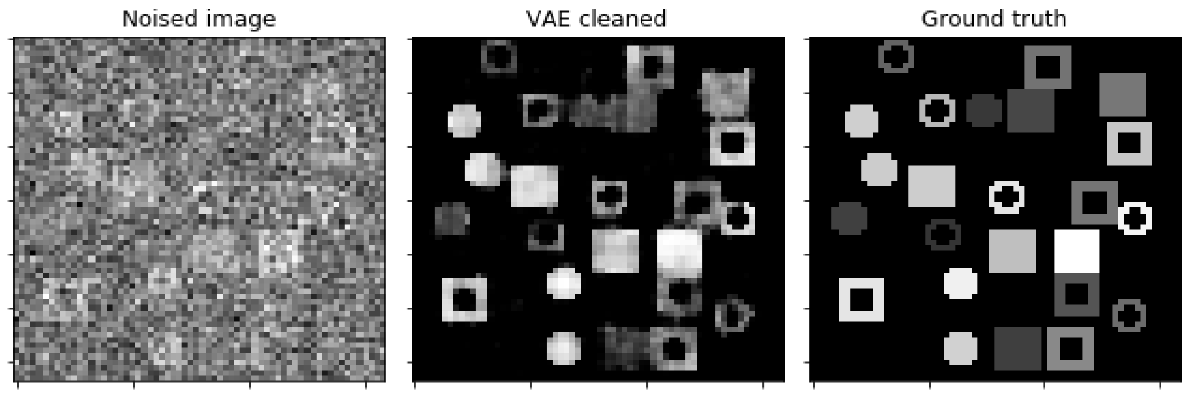
Train the model. Using the vae_train function set the model to train.

```
vae_train(model, X, labels, xtest, ltest, epochs, optimizer, sigmoid=False)
```

Step 3

Try the trained model out on some of the test data.

```
out = vae_inference(model, np.expand_dims(X[9], axis=0), sigmoid=True)
```


Noised image
VAE cleaned
Ground truth

CHAPTER 3

Loss functions

superres-tomo comes with a series of loss functions not found in the ml packages that it is built on. These are primarily useful in cases where there is class imbalance in the training/test set.

3.1 Weighted cross entropy

The weighted cross entropy (WCE) is an extension of the standard cross entropy. WCE can be used where there is a large class imbalance (excess of a particular label). In WCE all positive examples get weighted by a coefficient, which can be set in inverse proportion to the amount of a given label in the training set.

WCE is defined as

$$WCE(p, \hat{p}) = -(\beta p \log(\hat{p}) + (1 - p) \log(1 - \hat{p}))$$

To bias against false positives set $\beta < 1$ to bias against false positives set $\beta < 1$

3.2 Balanced cross entropy

Balanced cross entropy (BCE) is similar to WCE, but it also biases negatives as well as poitives.

$$BCE(p, \hat{p}) = -(\beta p \log(\hat{p}) + (1 - \beta)(1 - p) \log(1 - \hat{p}))$$

3.3 Dice Loss

The Dice loss is a loss function that is particularly useful if boundary detection is important in your image analysis. The dice loss is defined as

$$DL(p, \hat{p}) = 1 - \frac{2p\hat{p} + 1}{p + \hat{p} + 1}$$

CHAPTER 4

Benchmark Datasets

superres-tomo is assoicated with a range of benchmark datasets. These can be used to benchmark our implementations, to compare new methods, or simply as your own test.

Link	Real/Synthetic	Source	Experiment	Dimensions	Number of data	Notes
http://tiny.cc/3hydsz	Synthetic	DIV2K	n/a	64x64	180,000	Image/sinogram pairs
http://tiny.cc/m3djsz	Synthetic	Random shapes		128x128	55,000	Image/sinogram pairs
http://tiny.cc/58zdsz	Real	Micro CT	Reactor bed	185x185x1000	1000	3rd dim is the z-position
http://tiny.cc/ft0dsz	Real	Micro CT	Reactor bed	369x369x1000	1000	Same experiment as above; higher res
http://tiny.cc/0a0dsz	Real	XRD-CT	Reactor bed	75x75x2038	1	From same experiment as the data above. 3rd dim is the diffraction pattern.
http://tiny.cc/jd0dsz	Real	XRD-CT	Reactor bed	149x149x2038	1	Same experiment as above; higher-res

CHAPTER 5

super-resolution-ml

5.1 data_handeling package

5.1.1 Submodules

5.1.2 data_handeling.generators module

5.1.3 data_handeling.tools module

5.1.4 Module contents

5.2 models package

5.2.1 Subpackages

models.alex_net package

Submodules

models.alex_net.models module

Module contents

models.autoencoder package

Submodules

models.autoencoder.models module

models.autoencoder.tools module

Module contents

models.automap package

Submodules

models.automap.models module

Module contents

models.cnn_reconstruct package

Submodules

models.cnn_reconstruct.models module

Module contents

models.dense_reconstruct package

Submodules

models.dense_reconstruct.models module

Module contents

models.losses package

Submodules

models.losses.custom_loss_functions module

Module contents

models.u_net package

Submodules

models.u_net.models module

Module contents

5.2.2 Module contents

CHAPTER 6

Indices and tables

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