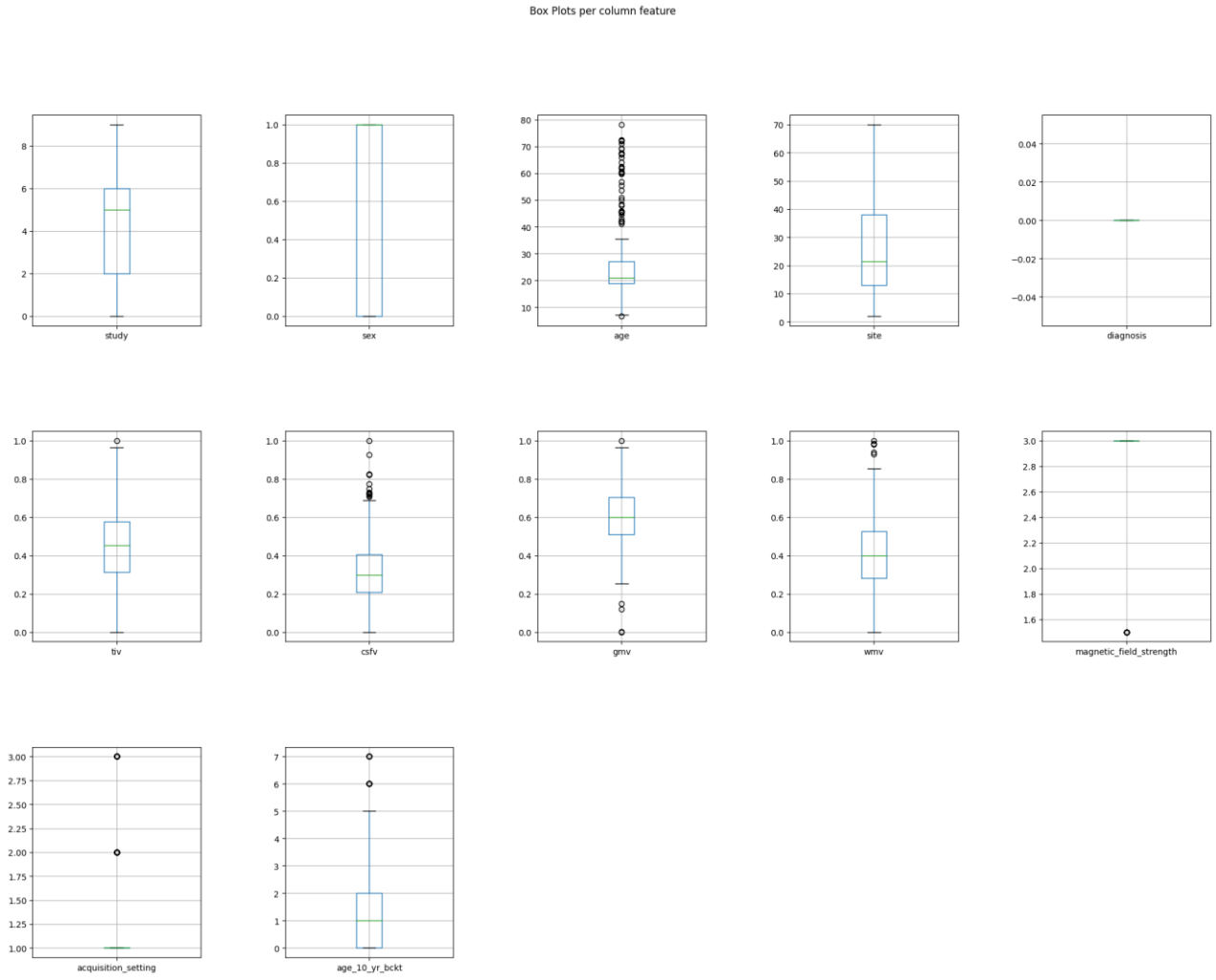
Coursework 2: Report on CNN + Age Regressor
FGZN0

Part 1: Dataset analysis and define a suitable setup

Data Analysis:

Prior to any sort of data analysis, I always split the dataset into training, validation, and test splits, where there is an approximate 75/25 ratio between training and testing, and within the training split an 85/15 ratio between training and validation. The following data analysis only applies to the training split.
First, we focus on the tabular meta-data. We perform some exploratory analysis to check whether I have a balanced dataset. If we group the patients by age intervals, we find that the training meta data is unbalanced with a left skew, as shown by the boxplots afterwards. Most of my patients are between the ages of 0 – 30, which means that my model's age predictions from brain scans may not generalize well to older patients.



Box plots per feature. Can zoom in if font is too small.

```
(466, 13)
age_10_yr_bckt_bg_70
(20, 30]     220
(10, 20]     152
(30, 40]      24
(0, 10]       21
(60, 70]      18
(40, 50]      14
(50, 60]       9
(70, 110]      8
Name: count, dtype: int64
age_10_yr_bckt
(20, 30]     220
(10, 20]     152
(30, 40]      24
(0, 10]       21
(60, 70]      18
(40, 50]      14
(50, 60]       9
(70, 80]       8
(80, 90]       0
(90, 100]      0
Name: count, dtype: int64
```

Count of patients per age group in the training set

I also must take care when making the train-validation split to ensure that all age intervals are present in both splits, which means that I need to ***stratify*** based on age intervals to ensure there is a representative sample per age group per split.

```
study
number of unique values in training split:  10
number of unique values in validation split:  9
sex
number of unique values in training split:  2
number of unique values in validation split:  2
diagnosis
number of unique values in training split:  1
number of unique values in validation split:  1
age_10_yr_bckt_bg_70
number of unique values in training split:  8
number of unique values in validation split:  7
age_10_yr_bckt
number of unique values in training split:  8
number of unique values in validation split:  7
```

Notice that in age_10_yr_bckt, there is an age group absent in the validation split but present in the training split. Stratifying could help avoid this problem.

Our target variable age is a continuous variable, which guides us to use the MSE as a training loss function. In practice we both use the mean-square error for training and mean-absolute error for reporting performance in the validation set. The use of both loss functions is well-justified: MSE has nice mathematical properties for stochastic gradient descent, though MAE is robust to outliers and is preferrable in this case where there is data skewness owed to age intervals because it penalizes less for

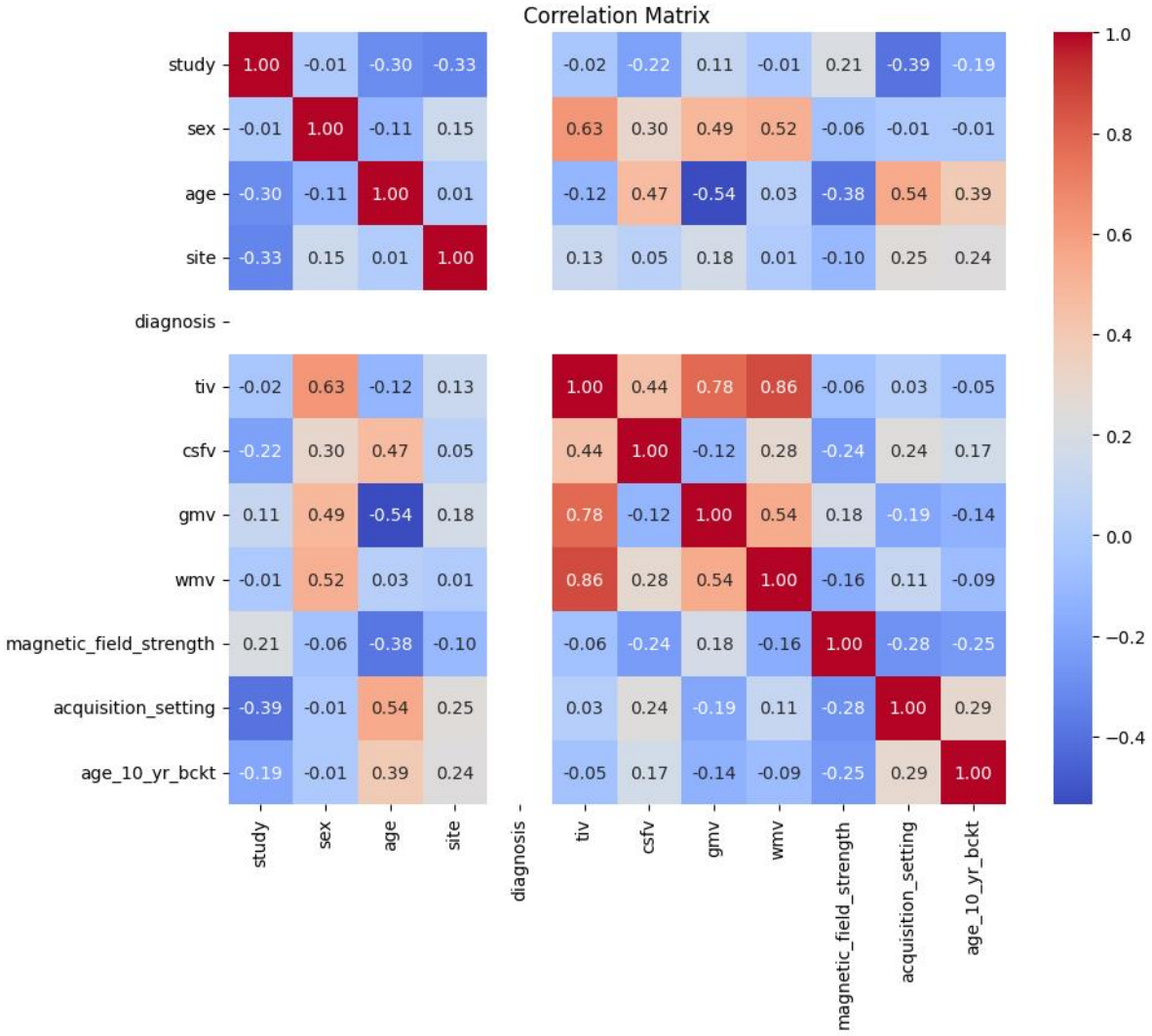
errors compared to the MSE. MAE has also been used in prior [work](https://www.nature.com/articles/s41467-019-13163-9) regarding age prediction from brain scans.

In addition to age, other relevant variables include sex, total intracranial, white matter, gray matter, and cerebrospinalfluid volumes, although only the last 3 would be used to predict age later in the report. These 3 variables need to be rescaled through min-max scaling since they are on a different scale compared to other variables, as shown by the summary stats. This is to stabilize the training of the MLP regressor afterwards.

	study	sex	age	site	diagnosis	tiv	csfv	gmv	wmv	magnetic_field_strength	acquisition_setting	age_10_yr_bckt
min	0.000000	0.000000	6.685832	2.000000	0.0	0.000000	0.000000	0.000000	0.000000	1.500000	1.000000	0.000000
max	9.000000	1.000000	78.203970	70.000000	0.0	1.000000	1.000000	1.000000	1.000000	3.000000	3.000000	7.000000
mean	4.270202	0.530303	24.619896	26.757576	0.0	0.449065	0.324212	0.607331	0.412818	2.924242	1.242424	1.527778
std	2.173540	0.499712	12.679297	17.929590	0.0	0.194452	0.163293	0.157528	0.182870	0.328893	0.543610	1.853286

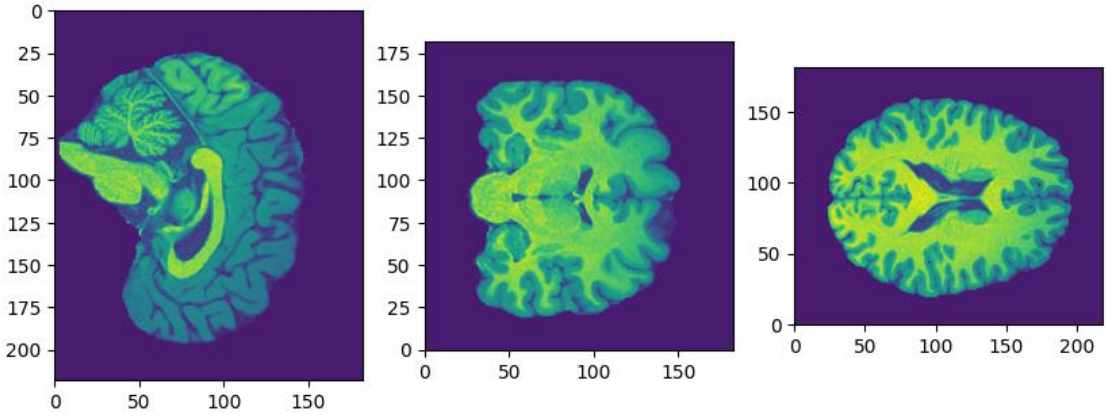
Summary stats of rescaled variables

Their rescaled version follow a Gaussian-like distribution (see boxplot), so it is reasonable to model them using the Gaussian likelihood, i.e., MSE. Arguably, irrelevant variables include patient ID, diagnosis since the metadata only contains control patients, and age_10_yr_bckt_bg_70 which is just a copy of age_10_yr_bckt (they showed a perfect positive correlation in the correlation matrix, before I removed them). The remaining variables like site and study are not used in our later analysis, though future work can explore their relevance.



Correlation matrix between relevant variables. Irrelevant ones have been dropped.

I also checked whether there are missing values, and luckily there aren't any.
The brain scans are 3D and only have 1 channel, and this influences how I design my CNN later. They are all resized to 96*96*96 pixels.



3D Brain scans are of 1 channel.

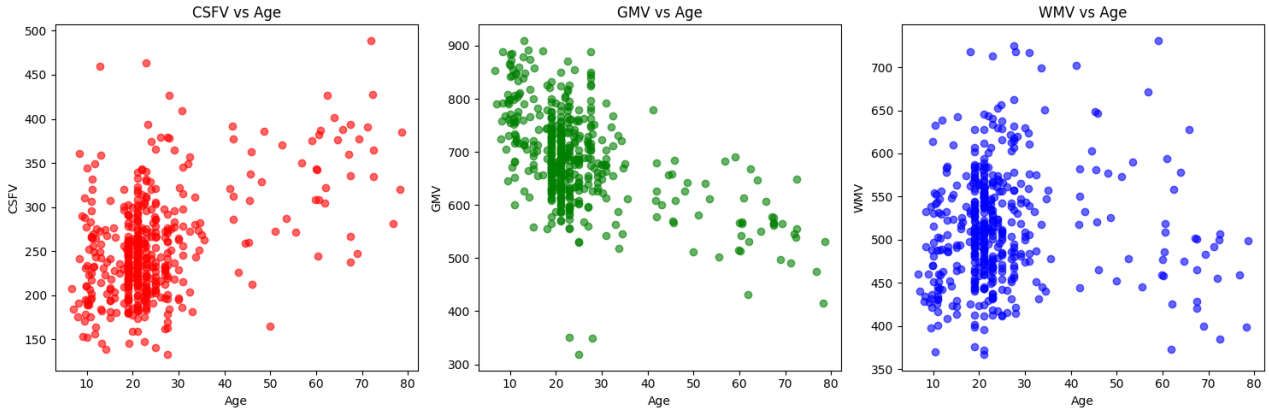
Defining a suitable setup:

I set the training set's size to be 85% of the overall training set, while the rest is given to validation split. This splitting ratio is standard practice; alternatives include 90/10 or 75/25.
The stratification variable I chose is age_10_yr_bckt because my target variable is age, and I want to make sure both the training and validation splits have representative groups per age interval. Furthermore, as mentioned and illustrated above, age groups follow a left-skewed Gaussian like distribution, so stratifying it could help balance this skew.
The test metric will be the MAE loss for reasons mentioned above, including that MAE has been used in prior work on predicting age from brain scans.

The train-test split is already provided. The train-validation split is done randomly, albeit seeded to ensure replicability following an 85/15 ratio. The training set is and will be used for exploratory data analysis as well as model training. The validation set is used for evaluating model performance because training performance metrics are not the only metrics I should report, since they're less meaningful than validation metrics. This is because training metrics are meant to be 'good' because of SGD; the validation performance is the one that sheds some insight into the generalizability of the model.

Part 2: Baseline model definition

In this report, we design a [concept-bottleneck modelling](https://arxiv.org/pdf/2007.04612.pdf) method for predicting age from 3D brain scans. Specifically, we choose to train 2 models independently, a 3D CNN and MLP Regressor, and then assemble them together. The choice of such method helps improve interpretability, because instead of mapping from images to scalar ages directly, the intermediate brain volume predictions from the brain scan help explain, to some extent, why certain age is predicted. As a side note, brain volume measurements are not needed during testing or inference. Furthermore, such architecture is encouraged as the brain volume measurements have been visualized to be to some extent correlated with age.

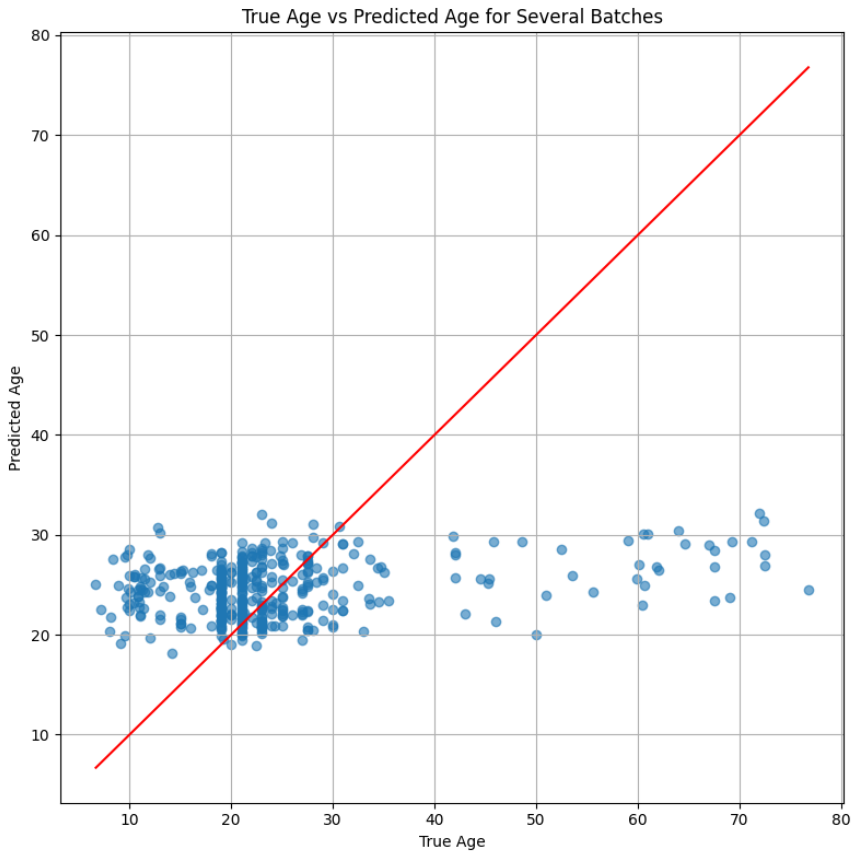


Scatterplot of each of the brain volume measurements with age

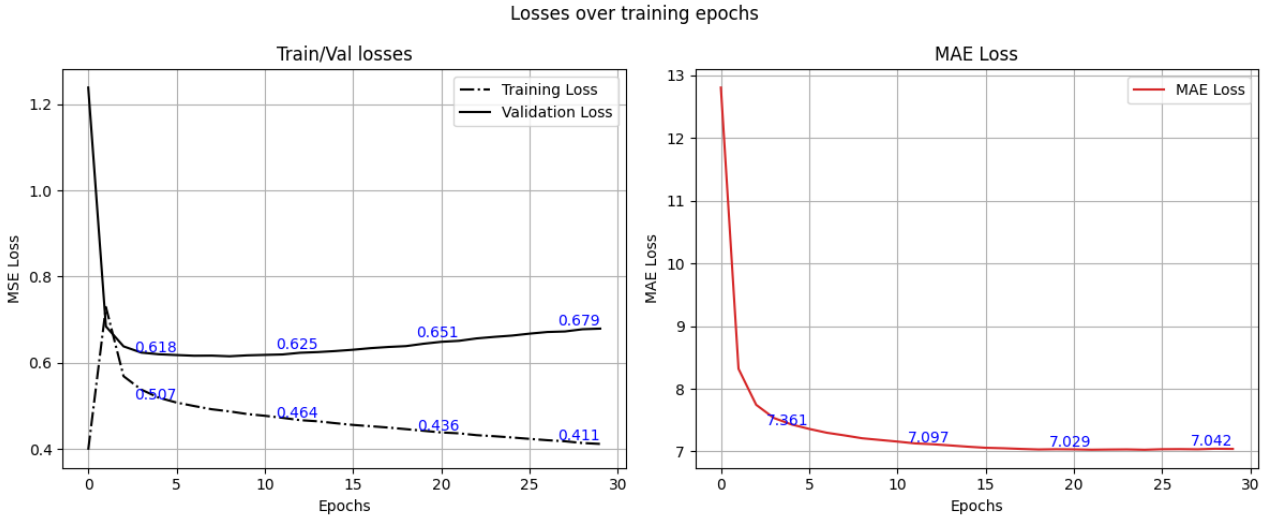
As a baseline, we separately train baseline models: a simple MLP consisting of 2 fully connected layers along with a simple 3D CNN. The MLP achieves a validation MAE of 7 after training for 30 epochs and my plots show that losses decrease smoothly during training. I train with a lr of 1e-3.

```
class MLPRegression(nn.Module):
    def __init__(self, input_dim, hidden_dim=64):
        super(MLPRegression, self).__init__()
        self.linear1 = nn.Linear(input_dim, hidden_dim)
        self.linear2 = nn.Linear(hidden_dim, 1)
        self.relu = nn.ReLU()

    def forward(self, x):
        x = self.relu(self.linear1(x))
        x = self.linear2(x)
        return x
```

Definition of the MLP



MLP's performance on predicting age.



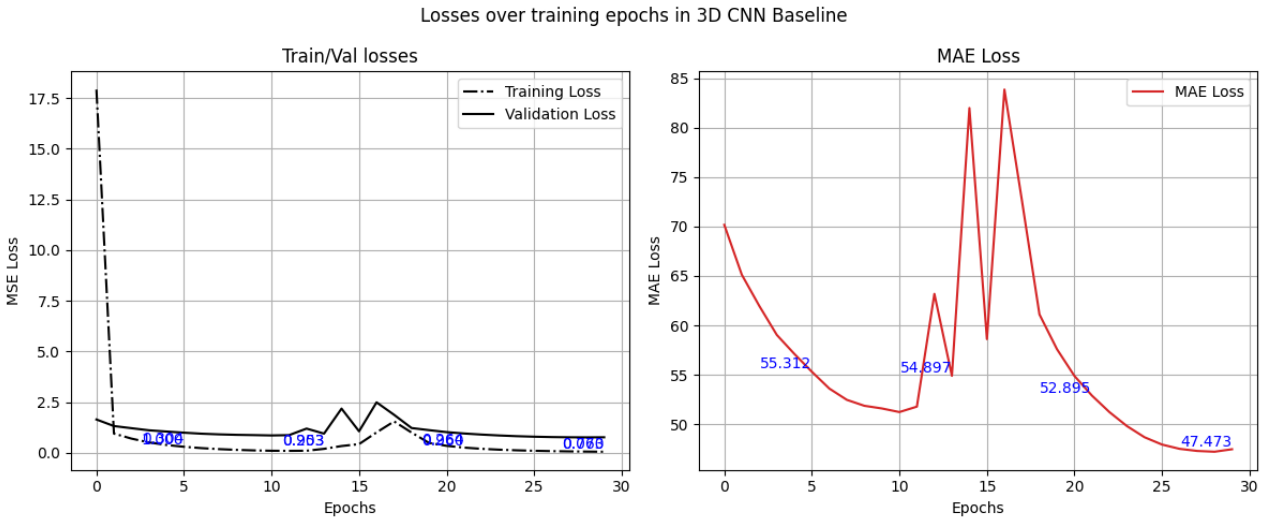
Train/val and validation MAE losses over training epochs of baseline MLP

Since we're working with 3D images, there is spatial information that the model must consider. Thus, the go-to architecture is a convolutional neural network, which in this case would be a 3D variant. Since we're designing a baseline, I chose to implement a simple 1-layer 3D CNN which has a fully connected layer as a tail that predicts 3 volume labels as per the given specifications: csfv, gmv and wmv. I also add a pooling layer to regularize the model and prevent possible overfitting to the training set, where I define overfitting as memorizing patterns in the training distribution, unable to generalize if compared to a model of lesser complexity (e.g. less number of parameters). I also use the ReLU activation unit due to standard practice.

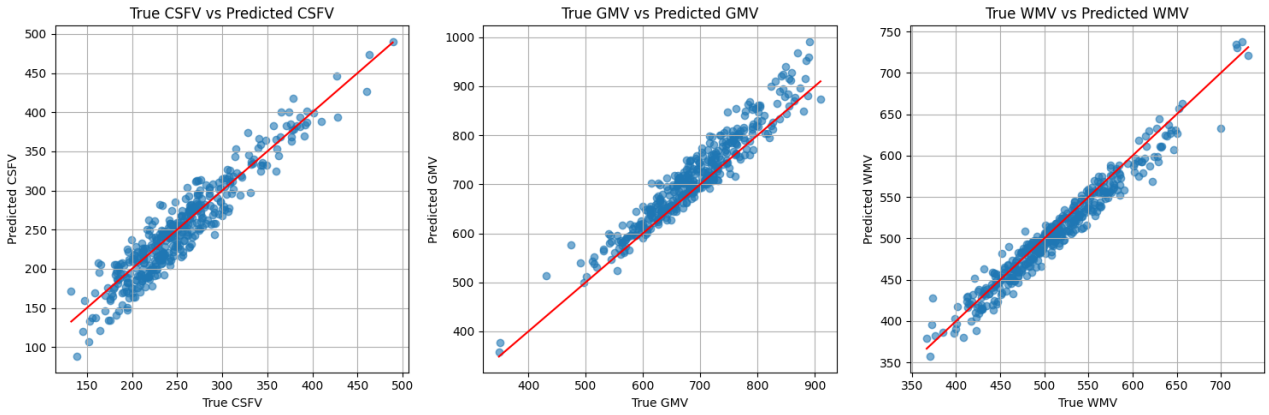
```
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
================================================================
            Conv3d-1       [-1, 2, 94, 94, 94]              56
              ReLU-2       [-1, 2, 94, 94, 94]               0
         MaxPool3d-3       [-1, 2, 47, 47, 47]               0
            Linear-4                   [-1, 3]         622,941
================================================================
Total params: 622,997
Trainable params: 622,997
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 3.38
Forward/backward pass size (MB): 26.93
Params size (MB): 2.38
Estimated Total Size (MB): 32.68
----------------------------------------------------------------
```

Architectural summary of baseline 3D CNN

I don't have an objective definition of 'reasonable' baseline. It is suggested that a 'reasonable' baseline could refer to one that performs better than random guessing or better than a linear classifier trained on images. This is a sensible approach; I *could* train a linear regressor from XGBoost on these MRI scans and see whether the 1-layer 3D CNN can outperform it and determine it is a good baseline. However, this kind of approach is not standard practice when working with images. A baseline can be defined as the first, simple model that is able to complete the task of predicting brain volume measurements given brain scan. Moreover, I argue it is a reasonable baseline given its simplicity in terms of small size (~600 thousand parameters), quick training (about 1 minute for 30 epochs with a lr of 1e-3) and steadily decreasing training and validation losses. This 1-layer 3D CNN achieves a final validation MAE of almost 50, which is very good for a baseline. I state this based on preliminary experiments that I don't report where I explored several variants such as adding few more convolutional layers, and usually being stuck at validation MAEs of around 64. Given all these, I argue it is a good baseline from which to explore improvements. I also plot the training, validation, and MAE losses, and they show steady decrease over the training epochs.

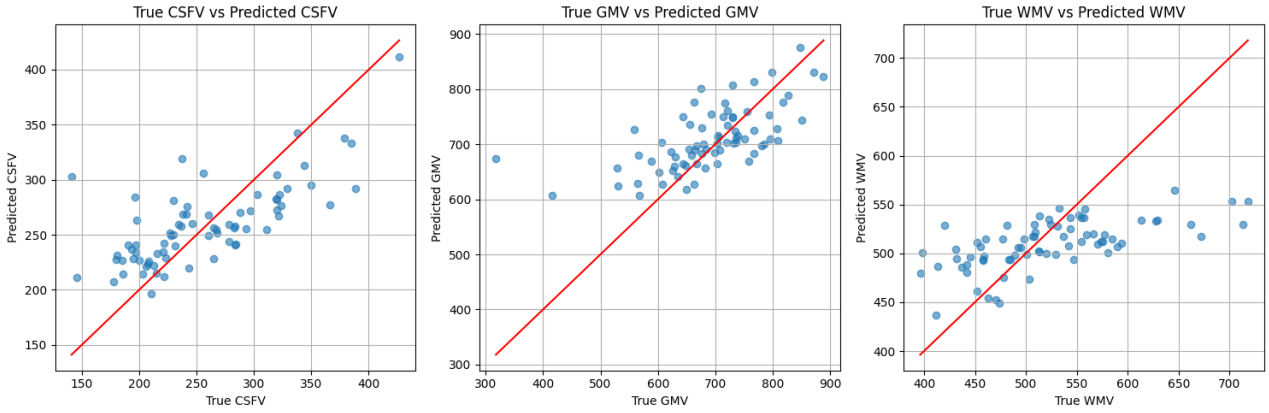


Train/val and validation MAE losses over training epochs of baseline 3D CNN



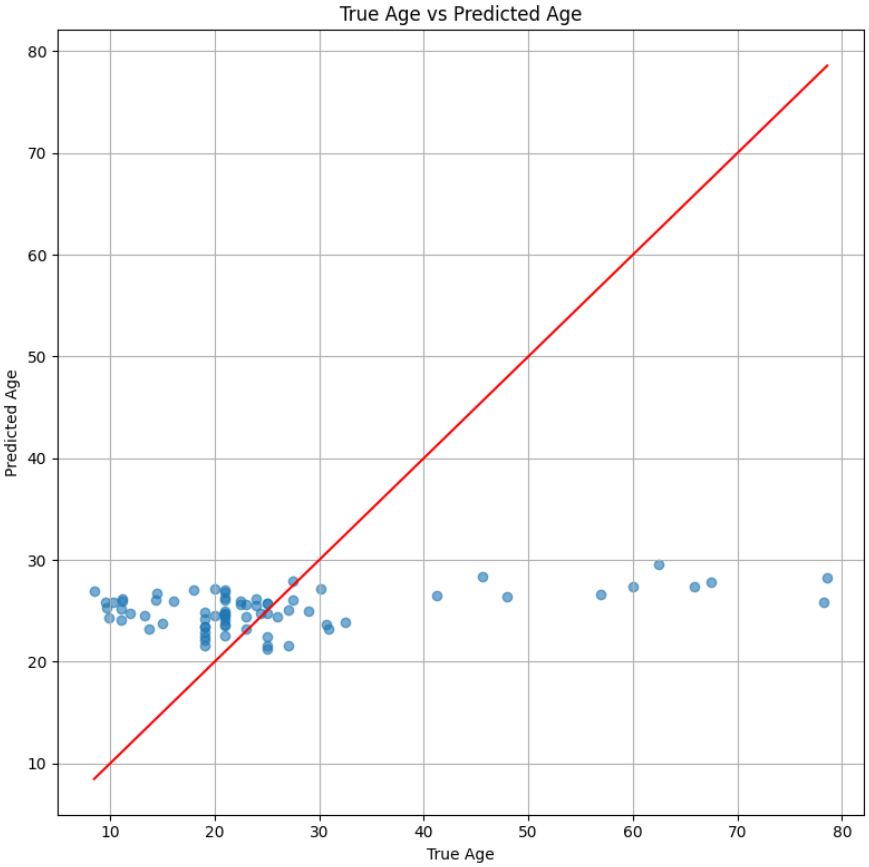
Predictive performance of the baseline 3D CNN over the training set.

There is a question when plotting the training performance. As said previously, plotting training performance can be done for illustrative purposes of the stability and progress in training the model. However, performance on the training set is often not very meaningful as it is meant to be good due to SGD. As such, it is more reasonable to report validation metrics, as I did above by reporting the MAE computed over the validation set.



Predictive performance of the baseline 3D CNN over the validation set.

The combination of both baselines 3D CNN with MLP is achieved by coupling the MLP as the “tail” of the 3D CNN, where it receives an input brain scan, outputs brain volume measurements that are fed into the MLP, to finally output an age value. This combined model shows a validation MAE of around 9.8. I can’t say whether this is a good or bad value, other than architectural improvements in Part 3 must at least perform better (lower) than this baseline performance. I plot the how well does the combined architecture predicts



Visualization of predictive performance of combined model over the validation set

A limitation of the choice of training the models separately is that I have no theoretical guarantee that independent, good performance by either component implies that together they will also perform good during inference (on the test set). Furthermore, the authors of the concept-bottleneck paper also provide alternative ways to assemble and train both models: training them sequentially (the outputs of the 3D CNN is used to train the MLP regressor), or jointly (both 3D CNN and MLP are trained end-end), although it is out-of-the scope of this report to explore the other 2 architectural variants on whether they serve as good baselines or not. Another limitation is that what we call 'baseline' defined here is constrained to analyzing the independent training of the concept-bottleneck modelling technique. In an academic paper illustrating the strengths of concept-bottleneck modelling, or maybe integration of datasets (images + tabular data), what is commonly called as 'baseline' would refer to the training of a 3D CNN to predict age directly from brain-scans, i.e., neither concept-bottleneck modelling nor integrating metadata associated to each image. I didn't try implementing this baseline due to time constraints as that would involve redefining a dataloader that puts images and ages together. Despite this, I still think I have a good baseline to improve upon.

Part 3: Improving upon the Baseline
Hypothesis 1

My first hypothesis is that a larger 3D CNN will perform better than the baseline. It is well known in the machine learning community that larger models perform better than shallower alternatives. See this [paper](https://arxiv.org/abs/2001.08361) on increased performance associated to increase language model size, or about the so-called “double-descent” phenomenon that describes a decrease in loss as model size grows. I explore this hypothesis by defining 2 additional convolutional layers with 1 additional fully connected layer to the baseline, yielding about 1 million parameters. Like the baseline, I take care in regularizing it by adding pooling layers.

```
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
================================================================
            Conv3d-1        [-1, 2, 94, 94, 94]              56
              ReLU-2        [-1, 2, 94, 94, 94]               0
         MaxPool3d-3        [-1, 2, 47, 47, 47]               0
            Conv3d-4       [-1, 16, 45, 45, 45]             880
              ReLU-5       [-1, 16, 45, 45, 45]               0
         MaxPool3d-6       [-1, 16, 22, 22, 22]               0
            Conv3d-7       [-1, 64, 20, 20, 20]          27,712
              ReLU-8       [-1, 64, 20, 20, 20]               0
         MaxPool3d-9       [-1, 64, 10, 10, 10]               0
           Linear-10                  [-1, 16]       1,024,016
             ReLU-11                  [-1, 16]               0
           Linear-12                   [-1, 3]              51
================================================================
Total params: 1,052,715
Trainable params: 1,052,715
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 3.38
Forward/backward pass size (MB): 58.78
Params size (MB): 4.02
Estimated Total Size (MB): 66.17
----------------------------------------------------------------
```

Architectural summary of larger 3D CNN

I test this hypothesis by training whilst controlling for several hyperparameters like learning rate and epochs and checking the validation MAE performance while it’s training and its validation performance when placed in the combined architecture with the MLP. Surprisingly, I observe **no** improvement over the baseline, neither during training when reporting the validation MAE (it doesn’t decrease beneath 64 > 50), nor when reporting the validation MAE when placed in the joint architecture (9.78 > 9.55, exact values may vary due to stochasticity). Despite seeing **no** improvement in all metrics, I do note this is not a definite judgement since there is still the test set where I must check whether I improved over the baseline. This is because it could be that lower error by the baseline may be due to overfitting.

Hypothesis 2

Because in the first hypothesis the simpler 1-layer 3D CNN outperformed a larger alternative, I thought about exploring a model of lower complexity compared to the MLP in terms of size of parameters. In hypothesis 2, I explore using a kernel ridge regressor of 3 parameters to check whether I can improve upon the MLP. The kernel ridge regressor trains faster as I can stack the entire dataset and estimate the optimal parameters in one iteration. Furthermore, it is more transparent than the MLP given I can analyze coefficients as a proxy in understanding how it correlates to age without non-linearities in between as in the MLP. I arbitrarily set relevant hyperparameters concerning the kernel, which I chose to be the radial basis function with gamma=0.1, and alpha which controls the regularization term to be 0.01. Similar as before, I validate this second hypothesis by monitoring validation MAE during training and validation MAE when placed together with the baseline 3D CNN. I don't explore looking at performance of combining the kernel ridge regressor with the larger 3D CNN due to time constraints.

I get a validation MAE loss of 0.47, compared to the validation MAE of ~7.5 of the MLP, though I suspect that this big disparity is because of aggregated MAEs over batches for the MLP, while for the kernel ridge regressor there is just a single, full batch. When the kernel ridge regressor is combined with the baseline 3D CNN, I get a validation MAE of 7.18, which is less than 9.56 corresponding to the baseline 3D CNN + MLP. This serves as evidence that supports hypothesis 2, although as mentioned before this is not conclusive until I check the MAE in the unseen test set.

Hypothesis 3

For hypothesis 3, I realized that models of lesser complexity, e.g., a 1 layer 3D CNN and 3 parameter kernel ridge regressor, were enough for this task of age prediction from 3D brain MRI scans. I suppose this is because the dataset we're working with is relatively small, so smaller models are enough to achieve a good performance. As such, in this last hypothesis I decided to perform hyperparameter optimization through the sophisticated way of Bayesian optimization using pre-defined libraries. The way to check whether hyperparameter tuning worked is by monitoring validation MAE as before.

I chose to optimize the alpha and gamma hyperparameters of the kernel ridge regressor as they control the regularization and expressivity of the model respectively. Alpha controls regularization as it is part of the loss function that penalizes weights to prevent overfitting, and gamma controls the width of the RBF and determines how wiggly is the function line. Bayesian optimization returns an alpha of 0.001 and gamma of 0.02, which are justifiable given there is not much need to penalize weights for such a small model trained on a relatively small dataset, though expressiveness is needed to model the relationship between brain volume measurements with age. Independently, I see the kernel ridge regressor didn't improve and got a slightly worse validation MAE loss (0.49 > 0.47) compared to hypothesis 2. When placed together with the baseline 3D CNN, I get a validation MAE of 7.70, which is unexpectedly worse than before since I believed that a sophisticated method of hyperparameter tuning would give a more expressive model.

If given enough time and computational resources, I would have also loved to explore using Bayesian optimization to find the optimal learning rate (or other hyperparameters) for the baseline 3D CNN. I wrote the code but opted to not run it given a single GPU and limited time. I expected to run for around ~300 iterations: 30 epochs by default times 10 steps in searching for next candidate lr in given search space.

Concluding discussion

There is a plethora of experiments I wasn't able to run due to computational and time constraints: I could have compared pretrained 3D CNN and/or pretrained MLPs to see how it impacts performance. I could have also used data augmentation approaches to mitigate the class skewness owed to age intervals.

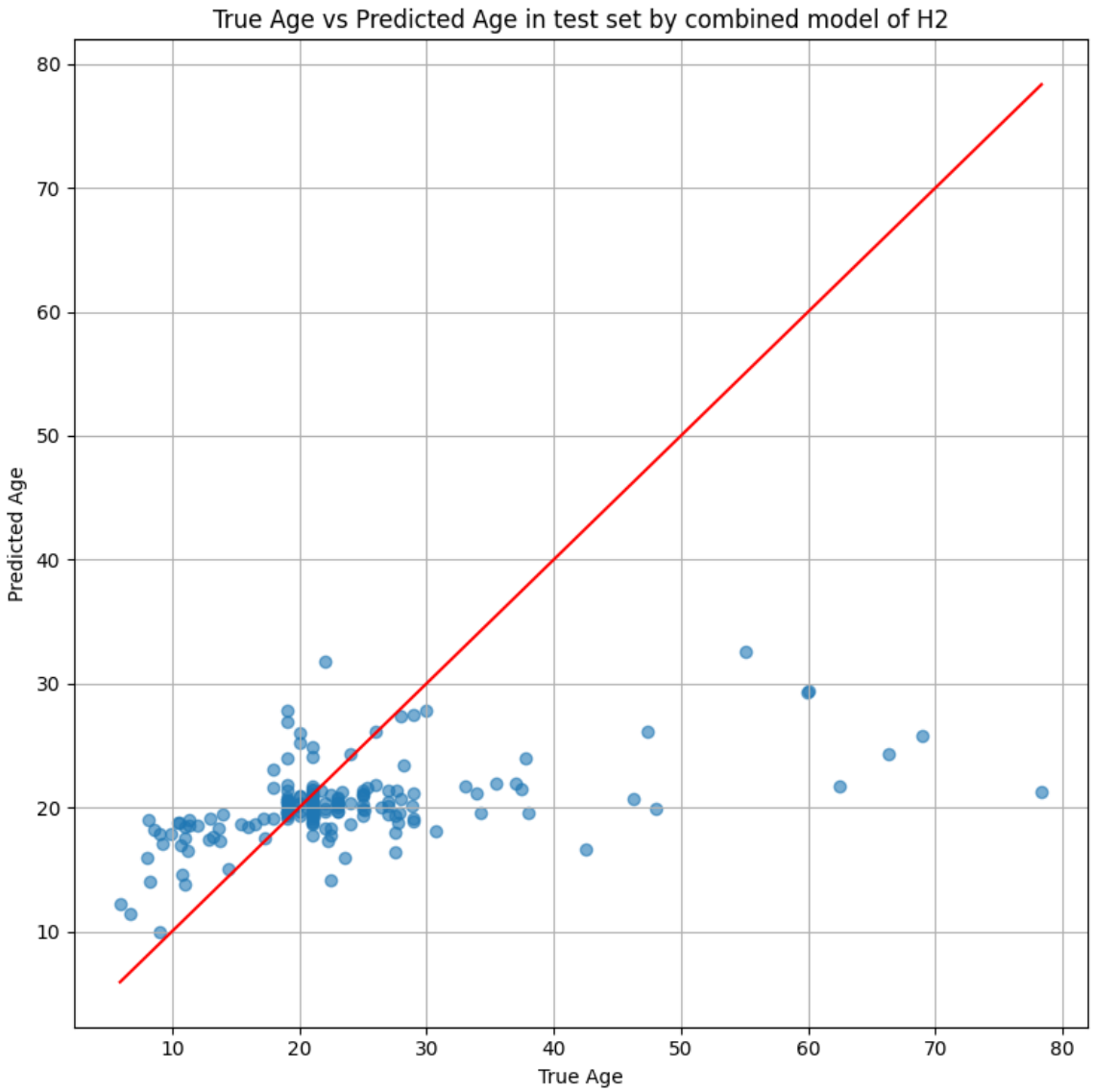
Despite this, I proceeded in making a final evaluation of my candidate models I first defined a test dataloader, appropriately normalized the age given test-set statistics and used the previously defined test metric (MAE loss) to evaluate the 4 candidate models. The second hypothesis, baseline 3D CNN + kernel ridge regressor without hyperparameter tuning yielded the best performing model, with the lowest MAE of 6.8. I argue this is because, as previously said, the MRI to age End2End dataset is relatively small, so models of lower complexity (lower number of parameters) may perform better because they converge faster and are less prone to overfit w.r.t larger models.

```
Test set metrics:
Baseline: 3D CNN + MLP
Validation loss:  0.630185, MAE:  7.198770

H1: Larger 3D CNN + MLP
Validation loss:  0.624337, MAE:  7.131959

H2: 3D CNN + kernel ridge regressor
Validation loss:  0.598969, MAE:  6.842181

H3: 3D CNN + hparam optimization of kernel ridge regressor
Validation loss:  0.632278, MAE:  7.222672
```

Performance on the test set by the 4 candidate models

Surprisingly, the second performing model was the larger 3D CNN coupled with the MLP. I say it is surprising because according to validation metrics, it had the worst MAE of ~9.8. This highlights the interesting phenomenon that bad performance during training and validation doesn't necessarily mean bad generalization as often some error can be tolerated in training/validation to avoid memorizing the training distribution. This result also opens new experiments: I could experiment coupling the larger 3D CNN with the kernel ridge regressor with and without hyperparameter tuning.

Finally, I also plotted the true vs. predicted ages of the best performing model.



Predictive performance of the best performing model: baseline 3D CNN + kernel ridge regressor with no hyperparameter tuning

In conclusion, in this report we ran a series of experiments to design a joint architecture for predicting age from 3D MRI scans, probably inspired by concept-bottleneck modelling.

CW2 - Coding Part 2 (30 points)

Variational Autoencoders

Build a Convolutional Variational AutoEncoder and achieve best possible reconstruction and latent space disentanglement. Then answer the questions.

In [ ]:
```
import os
import numpy as np
import torch
import torch.nn as nn
from torchvision import datasets, transforms
from torchvision.transforms import ToTensor
from torchvision.utils import make_grid
from torchsummary import summary

import matplotlib.pyplot as plt
import pandas as pd
import altair as alt
```

In [ ]:
```
# Use GPU if available
device = "cuda" if torch.cuda.is_available() else "cpu"
print(f"Using {device} device")
```

```
Using cuda device
```

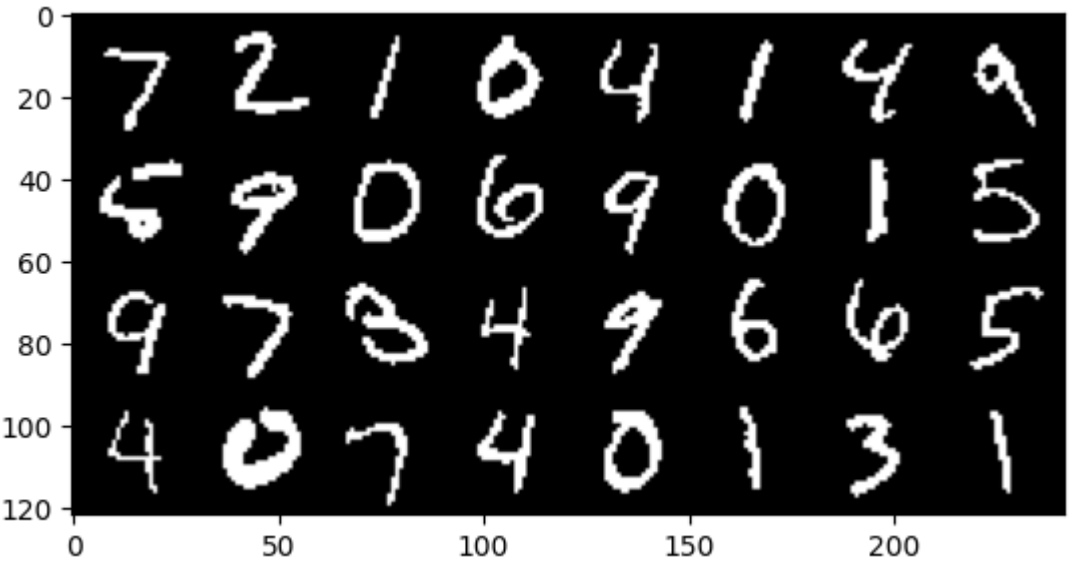
In [ ]:
```
def show(img):
    npimg = img.cpu().numpy()
    plt.imshow(np.transpose(npimg, (1,2,0)))
```

In [ ]:
```
# Load the data

########################################################################
#                       ** START OF YOUR CODE **
########################################################################

#                  ** MODIFY CODE HERE IF NECESSARY **
# import torchvision.transforms as transforms
class Binarize(object):
    def __call__(self, image):
        threshold = 0.5
        return (image > threshold).float()

batch_size = 64

data_transforms = transforms.Compose(
    [
        transforms.ToTensor(),
        Binarize()
    ]
)

def denormalize(x):
    return x

########################################################################
#                       ** END OF YOUR CODE **
########################################################################
```

```
training_data = datasets.MNIST(
    root="data",
    train=True,
    download=True,
    transform=data_transforms,
)

train_dataloader = torch.utils.data.DataLoader(
    training_data,
    batch_size=batch_size,
    shuffle=True,
)

# Download test data
test_data = datasets.MNIST(
    root="data",
    train=False,
    download=True,
    transform=data_transforms,
)

test_dataloader = torch.utils.data.DataLoader(
    test_data,
    batch_size=batch_size,
)
```

In [ ]:

```
sample_inputs, _ = next(iter(test_dataloader))
fixed_input = sample_inputs[0:32, :, :, :]
# visualize the original images of the last batch of the test set
img = make_grid(denormalize(fixed_input), nrow=8, padding=2, normalize=False,
                scale_each=False, pad_value=0)
plt.figure()
show(img)
```



Variational Auto Encoders (VAEs)

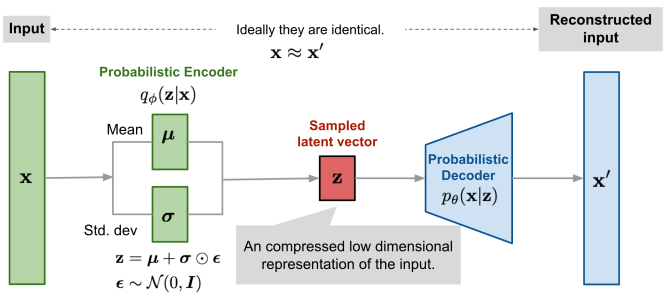


Fig.1 - VAE Diagram (with a Guassian prior), taken from 2.

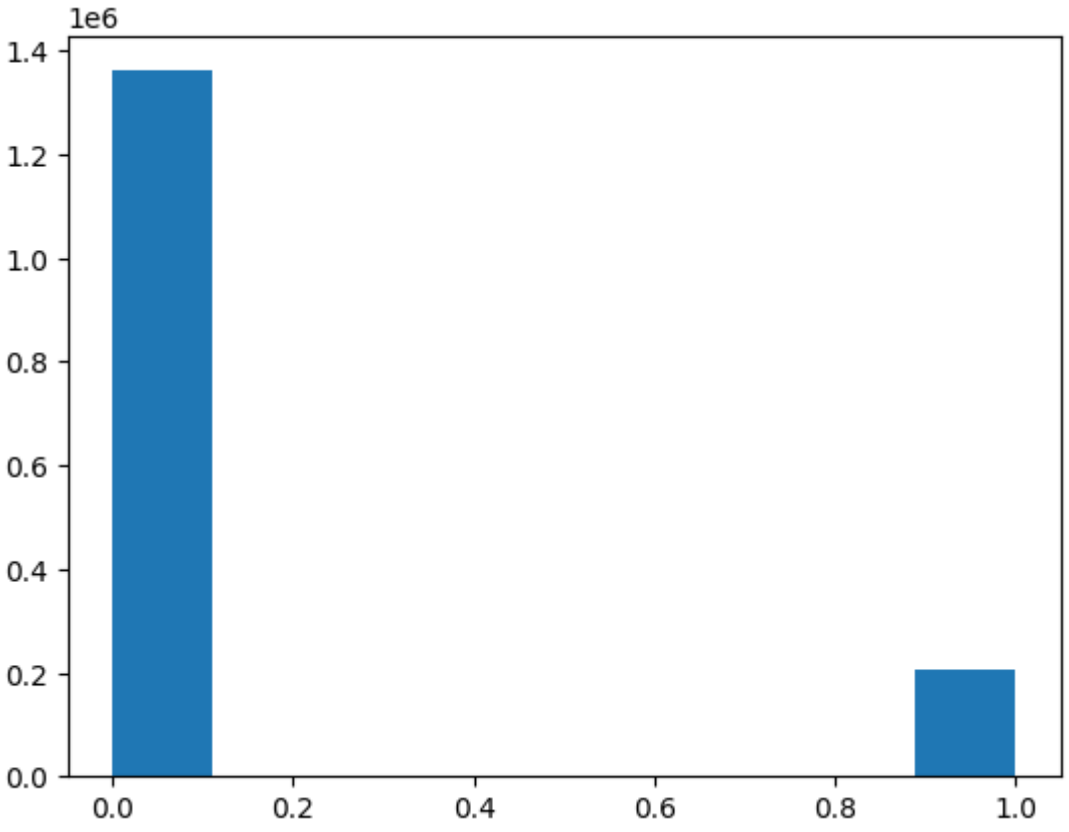
Build a convolutional VAE (5 points)

The only requirement is that it contains convolutions both in the encoder and decoder. You can still use some linear layers if needed.

In [ ]:
```
training_data[0][0].shape
28*28
all_data = torch.vstack([x for x, _ in training_data])
print('Min value:', all_data.min().item())
print('Max value:', all_data.max().item())

# Plot histogram for a random subset
subsample_size = 2000
indices = np.random.choice(all_data.shape[0], size=subsample_size, replace=False)
plt.hist(all_data[indices].flatten().numpy(), bins=np.linspace(0, 1, num=10))
```

```
Min value: 0.0
Max value: 1.0
```

Out[ ]:
```
(array([1361454.,       0.,       0.,       0.,       0.,       0.,
              0.,       0.,  206546.]),
 array([0.        , 0.11111111, 0.22222222, 0.33333333, 0.44444444,
        0.55555556, 0.66666667, 0.77777778, 0.88888889, 1.        ]),
 <BarContainer object of 9 artists>)
```



In [ ]:
```
import pdb
import torch.nn.functional as F
# Convolutional VAE implementation here

### VAE CODE IS RECYCLED FROM https://github.com/rasbt/stat453-deep-learning-ss21/blob/main/L1
class Reshape(nn.Module):
    def __init__(self, *args):
        super().__init__()
        self.shape = args

    def forward(self, x):
        return x.view(self.shape)
```

```python
class Trim(nn.Module):
    def __init__(self, *args):
        super().__init__()

    def forward(self, x):
        return x[:, :, :28, :28]


class VAE(nn.Module):
    def __init__(self, latent_dim = 2):
        super(VAE, self).__init__()
        ############################################################################
        #                          ** START OF YOUR CODE **
        ############################################################################

        self.latent_dim = latent_dim

        ### ENCODER
        self.enc_model = nn.Sequential(
                nn.Conv2d(1, 16, stride=(1, 1), kernel_size=(3, 3), padding=1),
                nn.LeakyReLU(0.01),
                nn.Conv2d(16, 32, stride=(2, 2), kernel_size=(3, 3), padding=1),
                nn.LeakyReLU(0.01),
                nn.Conv2d(32, 32, stride=(2, 2), kernel_size=(3, 3), padding=1),
                nn.LeakyReLU(0.01),
                nn.Conv2d(32, 32, stride=(1, 1), kernel_size=(3, 3), padding=1),
                nn.Flatten(),
        )
        # Create separate final layers for each parameter (mean and log-variance)
        # I use log-variance to unconstrain the optimisation of the positive-only variance par
        self.enc_mean = nn.Linear(32 * 7 * 7, self.latent_dim)
        self.enc_logvar = nn.Linear(32 * 7 * 7, self.latent_dim)

        ### DECODER
        self.dec_model = nn.Sequential(
                torch.nn.Linear(self.latent_dim, 32 * 7 * 7),
                Reshape(-1, 32, 7, 7),
                nn.ConvTranspose2d(32, 32, stride=(1, 1), kernel_size=(3, 3), padding=1),
                nn.LeakyReLU(0.01),
                nn.ConvTranspose2d(32, 32, stride=(2, 2), kernel_size=(3, 3), padding=1),
                nn.LeakyReLU(0.01),
                nn.ConvTranspose2d(32, 16, stride=(2, 2), kernel_size=(3, 3), padding=0),
                nn.LeakyReLU(0.01),
                nn.ConvTranspose2d(16, 1, stride=(1, 1), kernel_size=(3, 3), padding=0),
                Trim(),  # 1x29x29 -> 1x28x28
                nn.Sigmoid()
                )


        ############################################################################
        #                          ** END OF YOUR CODE **
        ############################################################################

    def encode(self, x):
        ############################################################################
        #                          ** START OF YOUR CODE **
        ############################################################################
        '''
        x (B, C, H, W): Batch of input MNIST digits
        '''
        features = self.enc_model(x)
        mean = self.enc_mean(features)
        logvar = self.enc_logvar(features)
```

```
        return mean, logvar

        ##############################################################################
        #                          ** END OF YOUR CODE **
        ##############################################################################

    def reparametrize(self, mu, logvar):
        ##############################################################################
        #                          ** START OF YOUR CODE **
        ##############################################################################
        '''
        mu, logvar are the outputs of the encoder
        '''
        std = torch.exp(0.5*logvar)
        eps = torch.randn(mu.size(0), mu.size(1)).to(mu.device)
        Z = mu + eps*std
        return Z.to(device=std.device)

        ##############################################################################
        #                          ** END OF YOUR CODE **
        ##############################################################################

    def decode(self, z):
        ##############################################################################
        #                          ** START OF YOUR CODE **
        ##############################################################################
        # pdb.set_trace()
        '''
        z is the latent from which to reconstruct the input
        '''
        features = self.dec_model(z)
        # pdb.set_trace()
        return features

        ##############################################################################
        #                          ** END OF YOUR CODE **
        ##############################################################################

    def forward(self, x):
        ##############################################################################
        #                          ** START OF YOUR CODE **
        ##############################################################################
        '''
        x (B, C, H, W): Batch of input MNIST digits
        '''
        mu, logvar = self.encode(x)         # (B, H) , (B, H)
        z = self.reparametrize(mu, logvar) # (M, B, H); z is of size (B, H=2)
        recon_x = self.decode(z)            # recon_x (B, C, H, W)
        # pdb.set_trace()

        ###

        return recon_x, mu, logvar
        ##############################################################################
        #                          ** END OF YOUR CODE **
        ##############################################################################


##############################################################################
#                          ** START OF YOUR CODE **
##############################################################################

latent_dim = 2

##############################################################################
#                          ** END OF YOUR CODE **
```

```
#####################################################################
print(device)
model = VAE(latent_dim).to(device)
summary(model, (1, 28, 28))
```

```
cuda
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
================================================================
            Conv2d-1          [-1, 16, 28, 28]             160
         LeakyReLU-2          [-1, 16, 28, 28]               0
            Conv2d-3          [-1, 32, 14, 14]           4,640
         LeakyReLU-4          [-1, 32, 14, 14]               0
            Conv2d-5            [-1, 32, 7, 7]           9,248
         LeakyReLU-6            [-1, 32, 7, 7]               0
            Conv2d-7            [-1, 32, 7, 7]           9,248
           Flatten-8                 [-1, 1568]               0
            Linear-9                    [-1, 2]           3,138
           Linear-10                    [-1, 2]           3,138
           Linear-11                 [-1, 1568]           4,704
          Reshape-12            [-1, 32, 7, 7]               0
  ConvTranspose2d-13            [-1, 32, 7, 7]           9,248
         LeakyReLU-14            [-1, 32, 7, 7]               0
  ConvTranspose2d-15          [-1, 32, 13, 13]           9,248
         LeakyReLU-16          [-1, 32, 13, 13]               0
  ConvTranspose2d-17          [-1, 16, 27, 27]           4,624
         LeakyReLU-18          [-1, 16, 27, 27]               0
  ConvTranspose2d-19           [-1, 1, 29, 29]             145
             Trim-20           [-1, 1, 28, 28]               0
          Sigmoid-21           [-1, 1, 28, 28]               0
================================================================
Total params: 57,541
Trainable params: 57,541
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 0.00
Forward/backward pass size (MB): 0.66
Params size (MB): 0.22
Estimated Total Size (MB): 0.88
----------------------------------------------------------------
```

In [ ]:
```
### debugging
fst_batch = next(iter(train_dataloader))
fst_batch = fst_batch[0].to('cuda')
recon_x , mu, logvar= model(fst_batch)
torch.sum(recon_x < 0.5)
```

Out[ ]:
```
tensor(37941, device='cuda:0')
```

Briefly Explain your architectural choices

YOUR ANSWER

First, because there exists a plethora of tutorials of VAEs trained on the MNIST dataset, I simply recycled existing code on the internet. Namely, I used code from this tutorial and here. I can try explaining their architectural choices: for a convolution based VAE, there has to be convolutional layers, whereby layers in the decoder are essentially the transpose to those of the encoder. Dimensions such as number of channels are arbitrarily set. There are some slight fixes to be made such as Trim() to ensure that the output of the VAE is the same size as the input, in this case (1, 28, 28). Another important addition is the sigmoid activation function on the decoder's last layer. This is because I'm modelling binarized MNIST pixel values, where each pixel has been preprocessed to be either 0 or 1 as per a 0.5 threshold, as shown in the histogram above.

Defining a Loss (6 points)

The Beta VAE loss, with encoder q and decoder p:

$$L = \mathbb{E}_{q_\phi(z|X)}[\log p_\theta(X \mid z)] - \beta D_{KL}[q_\phi(z \mid X) \| p_\theta(z)]$$

The loss you implement depends on your choice of latent prior and model outputs.

There exist different solutions that are equally correct. Depending on your assumptions you might want to do a data preprocessing step.

In [ ]:
```
def loss_function_VAE(recon_x, x, mu, logvar, beta):
        ##########################################################################
        #                        ** START OF YOUR CODE **
        ##########################################################################
    '''
    B = 64, C = 1, H = W = 28
    recon_x: (B, C, H, W) output of my conv. VAE
    x: (B, C, H, W) ground truth binarized MNIST digit
    mu, logvar: parameters of my variational distribution p(z|x)
    beta: hyperparamter controlling the trade-off between the
          reconstruction and the regularization loss.
    '''
    # KL divergence between learned latent distribution
    # and the prior distribution p(z)
    kld = -0.5 * torch.sum(1 + logvar - mu.pow(2) - logvar.exp())           # scalar

    # reconstruction loss or negative cross entropy. use bce
    # for binarized mnist digits
    neg_cross_entropy = F.binary_cross_entropy(recon_x, x, reduction='sum') # scalar; loss for

    # Beta VAE loss or Langragian
    langragian = neg_cross_entropy - beta * kld                             # scalar
    avg_langragian = langragian.mean()

    # pdb.set_trace()
    # use the opposite sign because standard optimizers minimize, but I want to maximize the L
    loss =  neg_cross_entropy + beta * kld
    return avg_langragian, loss, neg_cross_entropy, kld

        ##########################################################################
        #                        ** END OF YOUR CODE **
        ##########################################################################
```

In [ ]:
```
fst_batch.shape
elbo, loss, neg_cross_entropy, kld = loss_function_VAE(recon_x, fst_batch, mu, logvar, 0.5)
print(loss, elbo, neg_cross_entropy, kld)
```

```
tensor(35150.9609, device='cuda:0', grad_fn=<AddBackward0>) tensor(35150.7812, device='cuda:0
', grad_fn=<MeanBackward0>) tensor(35150.8711, device='cuda:0', grad_fn=<BinaryCrossEntropyBac
kward>) tensor(0.1835, device='cuda:0', grad_fn=<MulBackward0>)
```

Briefly answer the following:

a. Explain what are the possible choices of reconstruction loss, and which one you choose. Explain how it relates to

1. Your choice of VAE prior
2. The output data domain
3. The latent space disentanglement

Feel free to try and train with different reconstruction losses to see which one works best

YOUR ANSWER

a. There are different reconstruction losses depending on the assumptions made on the support of each pixel value of the MNIST image. I **binarized** the MNIST digits, and thus each pixel value is {0, 1}, i.e. a Bernoulli variable. Thus, for reconstruction loss it'd be most appropriate to model each pixel using the Bernoulli distribution, which is equivalent to using the binary cross entropy as the reconstruction loss. If I didn't binarize them, I should have used the continuous Bernoulli distribution. If the theoretical domain of each pixel was $(-\infty, +\infty)$, then we could use the mean squared error as a reconstruction loss, as it's derived from the Gaussian likelihood. Additionally, I can also choose what reduction method to use, in which I opted for the 'sum' method instead of the 'mean' because I argue that each pixel in the image represents a separate binary classification problem, so I treat them as separate datapoints.

1. The choice of VAE prior, or the prior of the latent $p(z)$, is by common practice a standard Normal (zero mean and unit variance) and thus it is used regardless of which reconstruction loss I choose. A standard Gaussian prior encourages disentanglement of latent factors by pushing them to be independent and not correlated with each other through the Kullback–Leibler divergence. From another perspective, the KL divergence can also be thought of as a regularization term to prevent the latents from memorizing an input to be reconstructed.
2. The choice of reconstruction loss is deeply related to the output/input domain. As said before, I binarized the MNIST digits as a preprocessing step. Therefore, it is mathematically recommended using the Bernoulli distribution to model the pixel values. The binary cross entropy measures the difference between the predicted probabilities given by the sigmoid and the actual binary labels of the image.
3. First, disentanglement of the latent space is defined as being able to learn a latent distribution $q(z|x)$ that closely resembles the VAE prior $p(z)$ by minimizing $KL(q(z|x)||p(z))$. This provides interpretability as it leads to finding independent latent factors correlated to variations in the original data. This KL divergence term is aggregated with the reconstruction loss into the joint loss function defined above, called the Lagrangian. It has a hyperparameter β to actively balance a trade-off between building a disentangled latent space whilst minimizing reconstruction loss, i.e, if I want greater disentanglement of latent space I use a larger β value that may sacrifice reconstruction quality.

I choose not to train with different reconstruction losses as I prefer to match the probability distribution with the pixel values' domain.

Train and plot

Train the VAE and plot:

1. The total loss curves for train and test (on the same plot)
2. The reconstruction losses for train and test (on the same plot)
3. The KL losses for train and test (on the same plot)

(x-axis: epochs, y-axis: loss)

You may want to have different plots with differente values of β.

Hint: You can modify the training scripts provided in previous tutorials to record the required information, and use matplotlib to plot them Hint: If you plan on doing hyperparameter tuning, it might be a good idea to split the training set and create a validation set

In [ ]:
```
from torch.utils.data import random_split, DataLoader

# Define the sizes of the training and validation sets
train_size = int(0.8 * len(training_data))
val_size = len(training_data) - train_size

# Split the training_data into training and validation sets
train_data, val_data = random_split(training_data, [train_size, val_size])

# Create data loaders for training and validation sets
train_loader = DataLoader(train_data, batch_size=batch_size, shuffle=True)
val_loader = DataLoader(val_data, batch_size=batch_size, shuffle=False)
```

In [ ]:
```
from tqdm import tqdm
from copy import deepcopy
from IPython import display
import matplotlib as mpl
from torch import nn, optim
```

In [ ]:
```
# # Training code

# ################################################################################
# #                        ** START OF YOUR CODE **
# ################################################################################

### The training and plotting code below is taken from https://github.com/vsimkus/pmr2023-vae.
### please ignore the naming of some variables as I made minimal additions without replacing
### previous variable names. For example, the elbo refer to the lagrangian defined above, and
### test set refer to validation set.
def train_vae(beta):
    fig, ax = plt.subplots(1, 3, figsize=(15, 8))
    model = VAE().to(device)  # Assuming VAE class is defined
    optimizer = optim.Adam(model.parameters(), lr=1e-3)
    # hparams
    num_epochs = 5
    beta = beta
    train_epochs = []
    train_elbos = []
    train_avg_epochs = []
    train_avg_elbos = []
    test_avg_epochs = []
    test_avg_elbos = []

    ### my additional metrics
    train_recon_losses = []
    train_klds = []

    val_epochs = []
    test_recon_losses = []
    test_klds = []
```

```
    # We will use these to track the best performing model on test data
    best_avg_test_elbo = float('-inf')
    best_epoch = None
    best_model_state = None
    best_optim_state = None

    pbar = tqdm(range(1, num_epochs + 1))
    for epoch in pbar:
        # Train
        model.train()
        epoch_train_elbos = []
        epoch_train_recon_loss = []
        epoch_train_klds = []
        # We don't use labels hence discard them with a _
        for batch_idx, (mbatch, _) in enumerate(train_loader):
            mbatch = mbatch.to(device)
            # Reset gradient computations in the computation graph
            optimizer.zero_grad()

            # Compute the loss for the mini-batch
            recon_x, mu, logvar = model(mbatch)
            # pdb.set_trace()
            elbo, loss, recon_loss, kld  = loss_function_VAE(recon_x, mbatch, mu, logvar, beta

            # Compute the gradients using backpropagation
            loss.backward()
            # Perform an SGD update
            optimizer.step()

            epoch_train_elbos += [elbo.detach().item()]
            epoch_train_recon_loss += [recon_loss.detach().item()]
            epoch_train_klds += [kld.detach().item()]

            pbar.set_description((f'Train Epoch: {epoch} [{batch_idx * len(mbatch)}/{len(train
                                  f'({100. * batch_idx / len(train_loader):.0f}%)] Lagrangia

        # Test
        if val_data is not None:
            with torch.no_grad():
                model.eval()
                epoch_test_elbos = []
                epoch_test_recon_loss = []
                epoch_test_klds = []
                for batch_idx, (mbatch, _) in enumerate(val_loader):
                    mbatch = mbatch.to(device)
                    # Compute the loss for the test mini-batch
                    recon_x, mu, logvar = model(mbatch)
                    # pdb.set_trace()
                    elbo, loss, recon_loss, kld = loss_function_VAE(recon_x, mbatch, mu, logva

                    epoch_test_elbos += [elbo.detach().item()]
                    epoch_test_recon_loss += [recon_loss.detach().item()]
                    epoch_test_klds += [kld.detach().item()]
                    pbar.set_description((f'Validation Epoch: {epoch} [{batch_idx * len(mbatch
                                          f'({100. * batch_idx / len(val_loader):.0f}%)] Lag

        # Store epoch summary in list
        train_avg_epochs += [epoch]
        train_avg_elbos += [np.mean(epoch_train_elbos)]
        train_epochs += np.linspace(epoch-1, epoch, len(epoch_train_elbos)).tolist()
        train_elbos += epoch_train_elbos
        ### additional metrics: recon_loss and kld
        train_recon_losses += epoch_train_recon_loss
        train_klds += epoch_train_klds
```

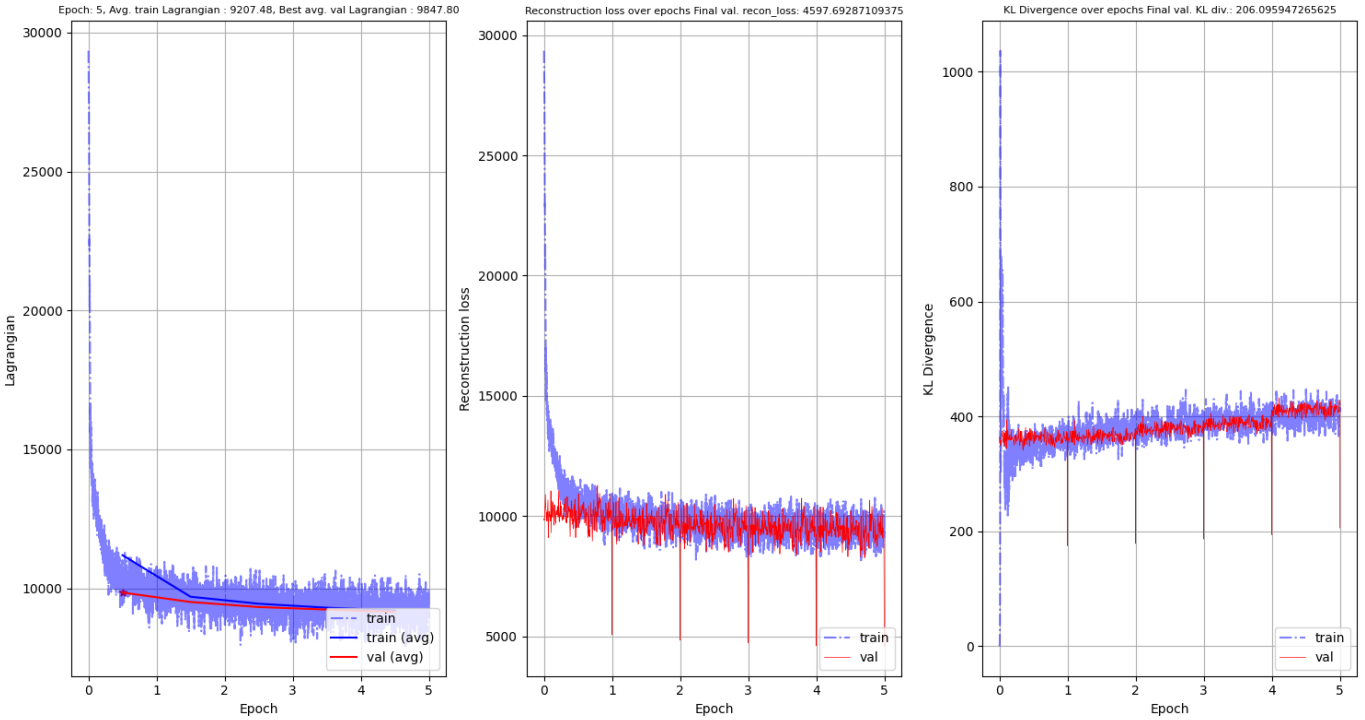
```
        val_epochs += np.linspace(epoch-1, epoch, len(epoch_test_elbos)).tolist()
        test_recon_losses += epoch_test_recon_loss
        test_klds += epoch_test_klds
        if val_data is not None:
            test_avg_epochs += [epoch]
            epoch_avg_test_elbo = np.mean(epoch_test_elbos)
            test_avg_elbos += [epoch_avg_test_elbo]

            # Snapshot best model
            if epoch_avg_test_elbo > best_avg_test_elbo:
                best_avg_test_elbo = epoch_avg_test_elbo
                best_epoch = epoch

                best_model_state = deepcopy(model.state_dict())
                best_optim_state = deepcopy(optimizer.state_dict())

        # Update learning curve figure
        ax[0].clear()
        ax[0].plot(train_epochs, train_elbos, 'b-.', alpha=0.5, label='train')
        ax[0].plot(np.array(train_avg_epochs)-0.5, train_avg_elbos, color='b', label='train (a
        if len(test_avg_elbos) > 0:
            ax[0].plot(np.array(test_avg_epochs)-0.5, test_avg_elbos, color='r', label='val (a
        ax[0].grid(True)
        ax[0].xaxis.set_major_locator(mpl.ticker.MaxNLocator(integer=True))
        ax[0].legend(loc='lower right')
        ax[0].set_ylabel('Lagrangian')
        ax[0].set_xlabel('Epoch')


        ### plotting additional metrics: recon_losses and klds
        ### reconstruction loss
        ax[1].clear()
        ax[1].plot(train_epochs, train_recon_losses, 'b-.', alpha=0.5, label='train')
        ax[1].plot(val_epochs, test_recon_losses, 'r-', label='val', linewidth=0.5)
        # ax[0].plot(np.array(train_avg_epochs)-0.5, train_avg_elbos, color='b', label='train
        # if len(test_avg_elbos) > 0:
        #     ax[0].plot(np.array(test_avg_epochs)-0.5, test_avg_elbos, color='r', label='val
        ax[1].grid(True)
        ax[1].xaxis.set_major_locator(mpl.ticker.MaxNLocator(integer=True))
        ax[1].legend(loc='lower right')
        ax[1].set_ylabel('Reconstruction loss')
        ax[1].set_xlabel('Epoch')
        ### KL divergence
        ax[2].clear()
        ax[2].plot(train_epochs, train_klds, 'b-.', alpha=0.5, label='train')
        ax[2].plot(val_epochs, test_klds, 'r-', label='val', linewidth=0.5)

        ax[2].grid(True)
        ax[2].xaxis.set_major_locator(mpl.ticker.MaxNLocator(integer=True))
        ax[2].legend(loc='lower right')
        ax[2].set_ylabel('KL Divergence')
        ax[2].set_xlabel('Epoch')


        fig_title = f'Epoch: {epoch}, Avg. train Lagrangian : {np.mean(epoch_train_elbos):.2f}
        # If we are tracking best model, then also highlight it on the plot and figure title
        if best_avg_test_elbo != float('-inf'):
            fig_title += f', Best avg. val Lagrangian : {best_avg_test_elbo:.2f}'
            ax[0].scatter(best_epoch-0.5, best_avg_test_elbo, marker='*', color='r')


        # fig.suptitle(fig_title, size=13)
        ax[0].set_title(fig_title, fontdict={'fontsize': 8})
        fig.tight_layout()
        display.clear_output(wait=True)
        if epoch != num_epochs:
```

```
            # Force display of the figure (except last epoch, where
            # jupyter automatically shows the contained figure)
            display.display(fig)

    # Reset gradient computations in the computation graph
    optimizer.zero_grad()
    overall_title = f'Losses over epochs for beta = {beta}'

    fig.suptitle(overall_title, size=13, va='top', y=1.05)
    ax[1].set_title("Reconstruction loss over epochs " + f'Final val. recon_loss: {test_recon_
    ax[2].set_title("KL Divergence over epochs " + f'Final val. KL div.: {test_klds[-1]}', for
    if best_model_state is not None and best_epoch != num_epochs:
        print(f'Loading best model state from epoch {best_epoch}.')
        model.load_state_dict(best_model_state)
    if best_optim_state is not None and best_epoch != num_epochs:
        print(f'Loading best optimizer state from epoch {best_epoch}.')
        optimizer.load_state_dict(best_optim_state)

    out = {
        'train_avg_epochs': train_avg_epochs,
        'train_avg_elbos': train_avg_elbos,
        'train_epochs': train_epochs,
        'train_elbos': train_elbos,
        'train_recon_losses': train_recon_losses,
        'train_klds': train_klds,
        'val_avg_epochs': test_avg_epochs,
        'val_avg_elbos': test_avg_elbos,
        'val_recon_losses': test_recon_losses,
        'val_klds': test_klds
    }


    return model, optimizer, out, fig

# ##########################################################################
# #                       ** END OF YOUR CODE **
# ##########################################################################
```

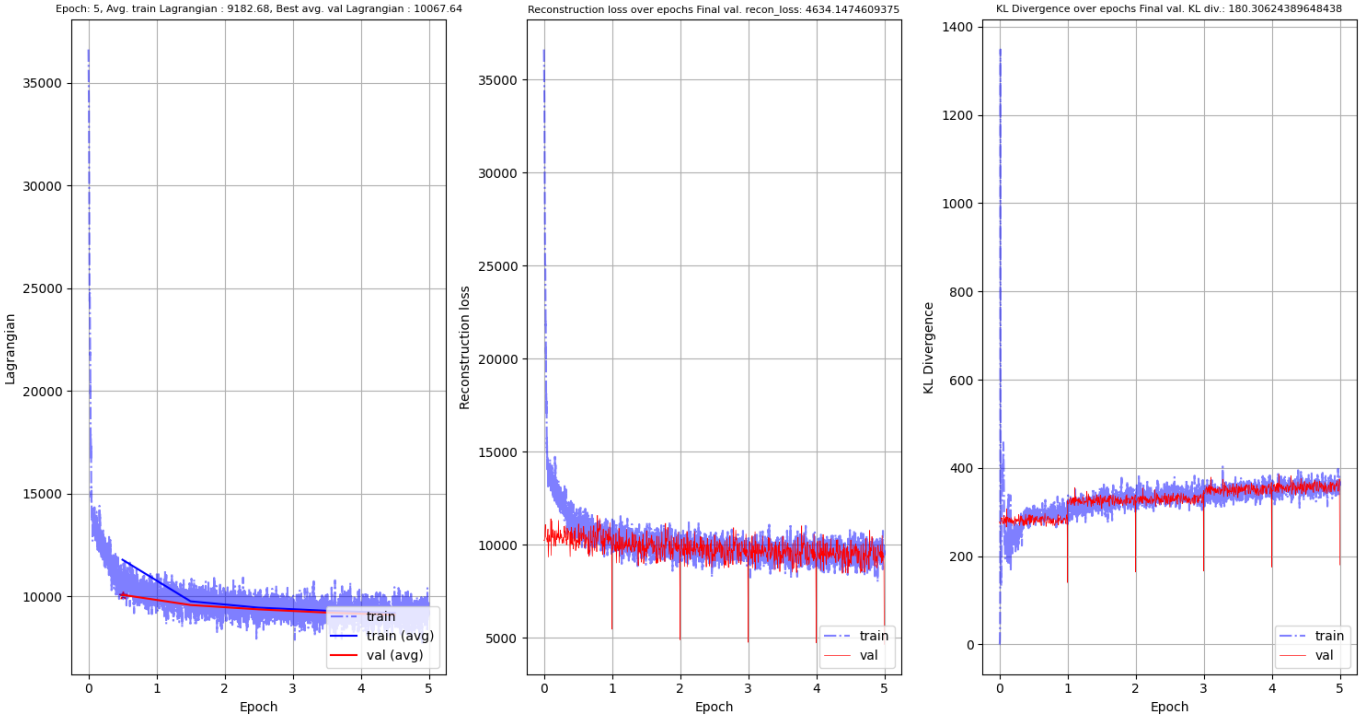
In [ ]:
```
betas = np.linspace(0.6 , 1.8, 4)
# betas = [1]
vae_models = []
vae_outs = []
for beta in betas:

    best_vae, _, out, _ = train_vae(beta)
    vae_models.append(best_vae)
    vae_outs.append(out)
```

```
Validation Epoch: 5 [5984/12000 (99%)] Lagrangian: 4339.916992: 100%|██████████| 5/5 [03:43<0
0:00, 44.77s/it]
Loading best model state from epoch 1.
Loading best optimizer state from epoch 1.
```

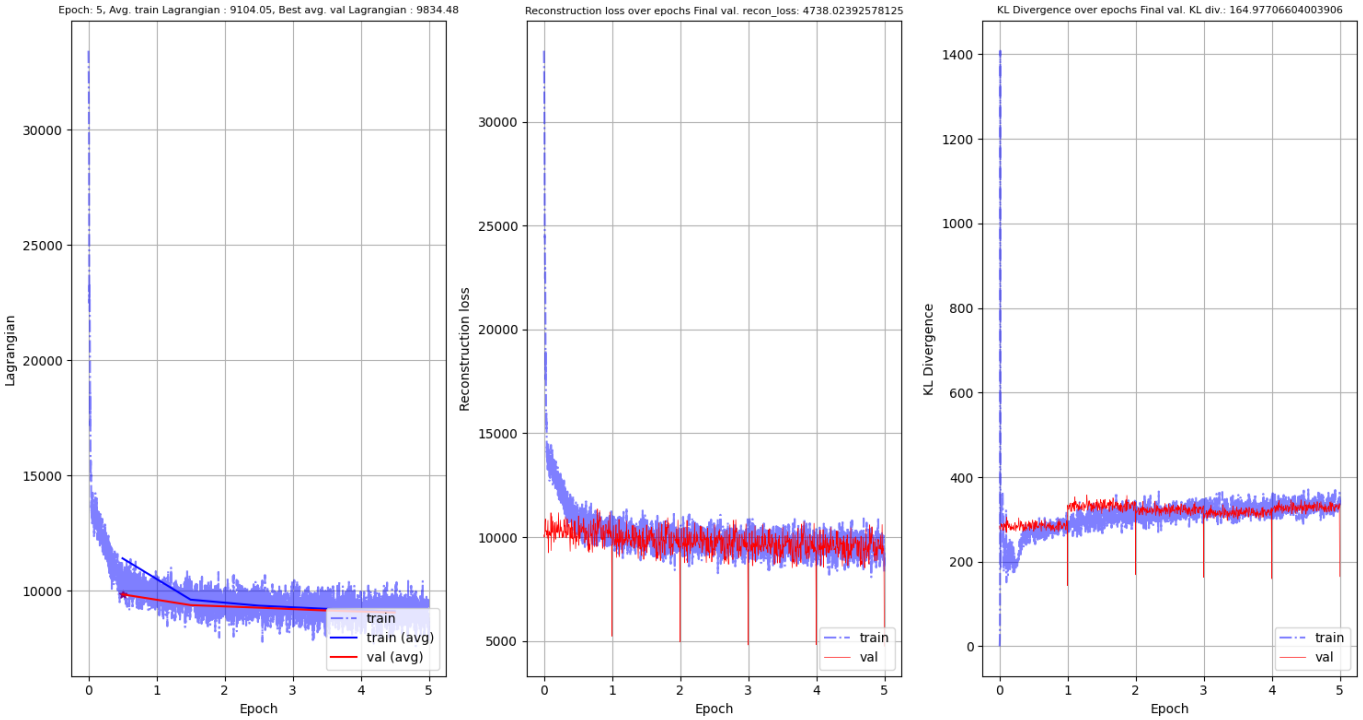
Losses over epochs for beta = 0.6



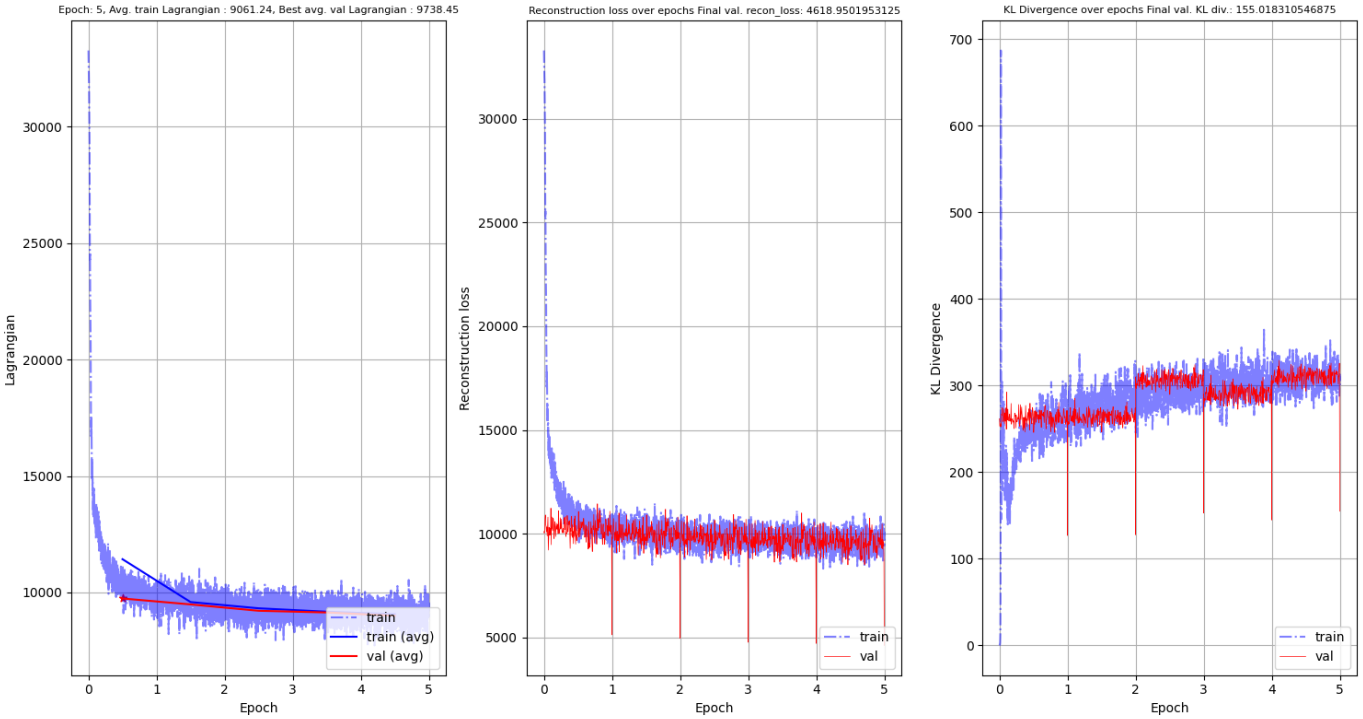
Losses over epochs for beta = 1.0



Losses over epochs for beta = 1.4000000000000001



Losses over epochs for beta = 1.8



In [ ]:
```
# # Plotting code

# ########################################################################
# #                       ** START OF YOUR CODE **
# ########################################################################

### I TRAIN AND PLOT JOINTLY. PLEASE SEE ABOVE FOR THE PLOTS

# ########################################################################
# #                       ** END OF YOUR CODE **
# ########################################################################
```

Plot loss (3 points)

Analyze and discuss:

1. Loss curves (reconstruction and KL divergence)

2. Explain how different values of β affect your training.

YOUR ANSWER

I train the conv. VAE over 5 epochs with fixed learning rate of 0.001 and latent dimension of 2, over 4 values of beta in [0.6, 1, 1.4, 1.8] and notice $\beta = 1.8$ to be the best value that balances the trade of reconstruction loss and KL divergence, i.e. it achieves the second-lowest reconstruction loss, lowest KL divergence and overall lowest Lagrangian. The first panel plots 3 curves: the pointwise train Lagrangian, the average train and validation Lagrangian over the training batch. In the second I plot 2 curves, the pointwise training and validation reconstruction losses over epochs and in the third panel I plot the KL divergence.

1. For all β values, both loss curves (2nd and 3rd panel in each figure corresponding to reconstruction loss and KL divergence, respectively) decrease, indicating the VAE is learning to both reconstruct the MNIST digits, and encouraging disentanglement of latent space. A common pattern is this great leap from a very high loss to a very low value within 1 epoch, albeit afterwards there is a lot of variance during updates. Such variance is partly due to the VAE trying to balance the reconstruction loss and KL divergence, as minimizing one often involves compromising the other, yet they have to be jointly minimized in the Lagrangian term.
2. β controls the trade-off between reconstruction loss and disentanglement of latent space. A large β value encourages disentanglement, such as in $\beta = 1.8$ achieving a KL divergence of 164, however, this can be at the expense of reconstruction quality and thus slow-down the convergence of the reconstruction loss. Similar reasoning applies for small β whereby a model ignores the KL divergence and prioritize reconstruction quality (recon_loss of 4621 for $\beta = 0.6$), which hinders interpretability and may lead to memorizing certain digits that are reconstructed very well (i.e. lead to overfitting). A $\beta = 1$ leads to the Lagrangian objective function become the ELBO or Evidence of Lower Bound, a lower bound approximation to the log-likelihood of the data $p(x)$.

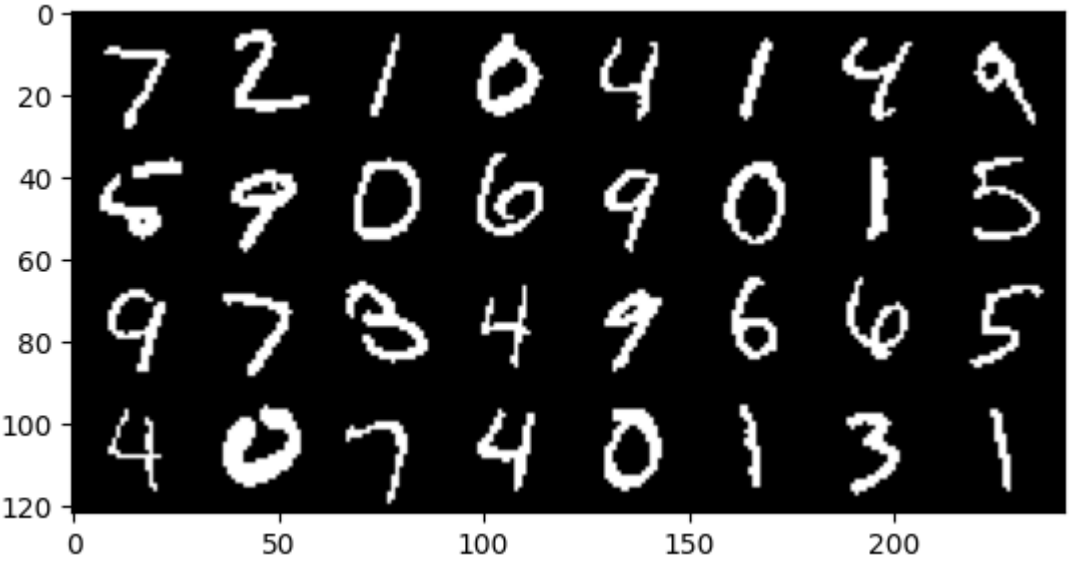
There are also some low spikes which are only present in the validation (red) curves at the end of an epoch, which I'm not sure what is the cause. Achieving a low validation loss at the end of the training epoch could be a sign of memorizing the training distribution, though I wouldn't worry too much since the validation curve behaves normally after the epoch starts again.

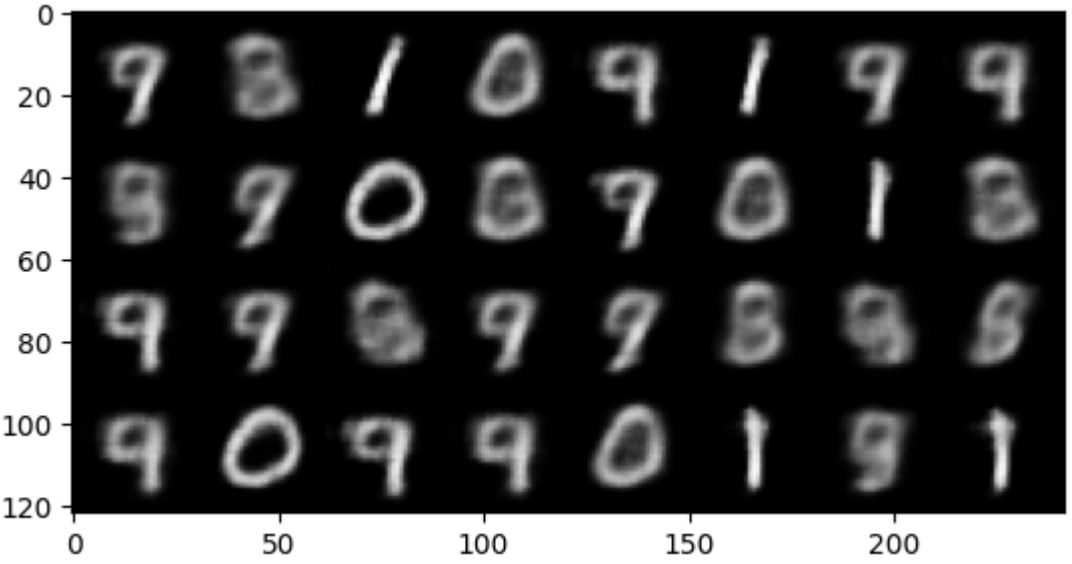
Sample and reconstruction quality (6 points)

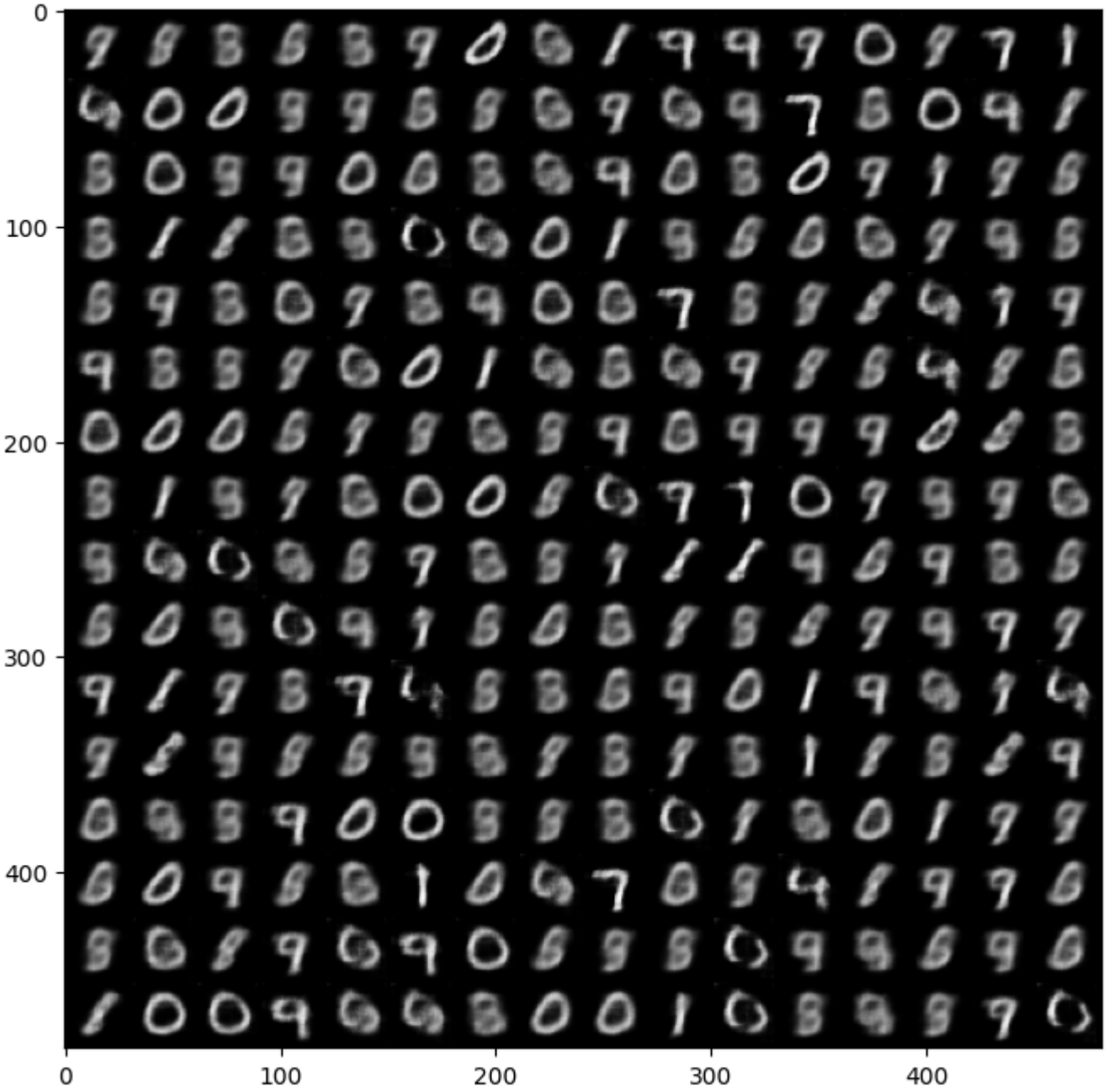
Simply run the below cell to show the output

In [ ]:
```
# Input images
model = vae_models[-1] # best model seemed to be that of beta = 1.8, i.e., the last model
model.eval()
sample_inputs, _ = next(iter(test_dataloader))
fixed_input = sample_inputs[0:32, :, :, :]

# visualize the original images of the last batch of the test set
img = make_grid(denormalize(fixed_input), nrow=8, padding=2, normalize=False,
                scale_each=False, pad_value=0)
plt.figure()
show(img)

# Reconstructed images
with torch.no_grad():

    recon_batch, mu, logvar  = model(sample_inputs.to(device))
```

```
    recon_batch = recon_batch.unsqueeze(1).reshape(-1,1,28,28)
    recon_batch = recon_batch[0:32, :, :, :]
    recon_batch = recon_batch.cpu()
    recon_batch = make_grid(denormalize(recon_batch), nrow=8, padding=2, normalize=False,
                            scale_each=False, pad_value=0)
    # pdb.set_trace()
    plt.figure()
    show(recon_batch)

# Generated Images
n_samples = 256
z = torch.randn(n_samples,latent_dim).to(device)
with torch.no_grad():

    samples = model.decode(z)
    samples = samples.unsqueeze(1).reshape(-1,1,28,28)
    samples = samples.cpu()
    samples = make_grid(denormalize(samples), nrow=16, padding=2, normalize=False,
                            scale_each=False, pad_value=0)
    plt.figure(figsize = (8,8))
    show(samples)
```







Reconstruction and generated samples discussion (5 points)

Analyze and briefly discuss:

1. Reconstruction quality
2. Generated samples quality

Explain in your answers how they relate to different values of β, latent dimension and VAE architecture

YOUR ANSWER

1. The reconstruction quality (second row of images) of $\beta = 1.8$ seems a bit blurrier compared to $\beta = 0.6$. For this value of β, the digits are easier to be distinguished between one another, 0 from 1 from 9. This is expected given that larger β values prioritize latent disentanglement even if it's at the expense of reconstruction quality. A larger size of the latent dimension of z can also improve reconstruction quality by allowing more intricate reconstructions.
2. For $\beta = 0.6$, I observe several generated samples are zeros. Each zero is reconstructed with

high quality. This shows that by compromising latent disentanglement, the VAE memorized certain digits in order to increase their reconstruction quality, thus lacking diversity in its output. The size of the latent dimension of z can also impact the generated sample quality, as a larger latent space can provide more flexibility in generating diverse samples, albeit it might be slower to train than using a smaller latent dimension. Furthermore, for larger z, sampling becomes harder and can not guarantee good coverage in the latent space.

I think for both reconstruction and generated sample quality would see a big improvement if I use a more expressive VAE encoder and decoder, along with a larger latent dimension instead of 2. As it is now, there are only ~50000 parameters in the VAE, which is very low. I could improve by adding more convolutional layers, training for longer epochs, and performing data augmentation techniques on the training data, such as rotation (taking care of 6 and 9), translation, blur, adding noise, among others so that the VAE learns to reconstruct data with greater diversity. Although this comes at the expense of consuming more computational resources, as well as more intricate considerations such as how to prevent overfitting, gradient vanishing, sampling efficiency, etc.

T-SNE on Embeddings (5 points)

Extract the latent representations of the test set and visualize them using T-SNE

Run the below cells (no coding required).

Qualitatively assess the learned representations of your model using the T-SNE plots.

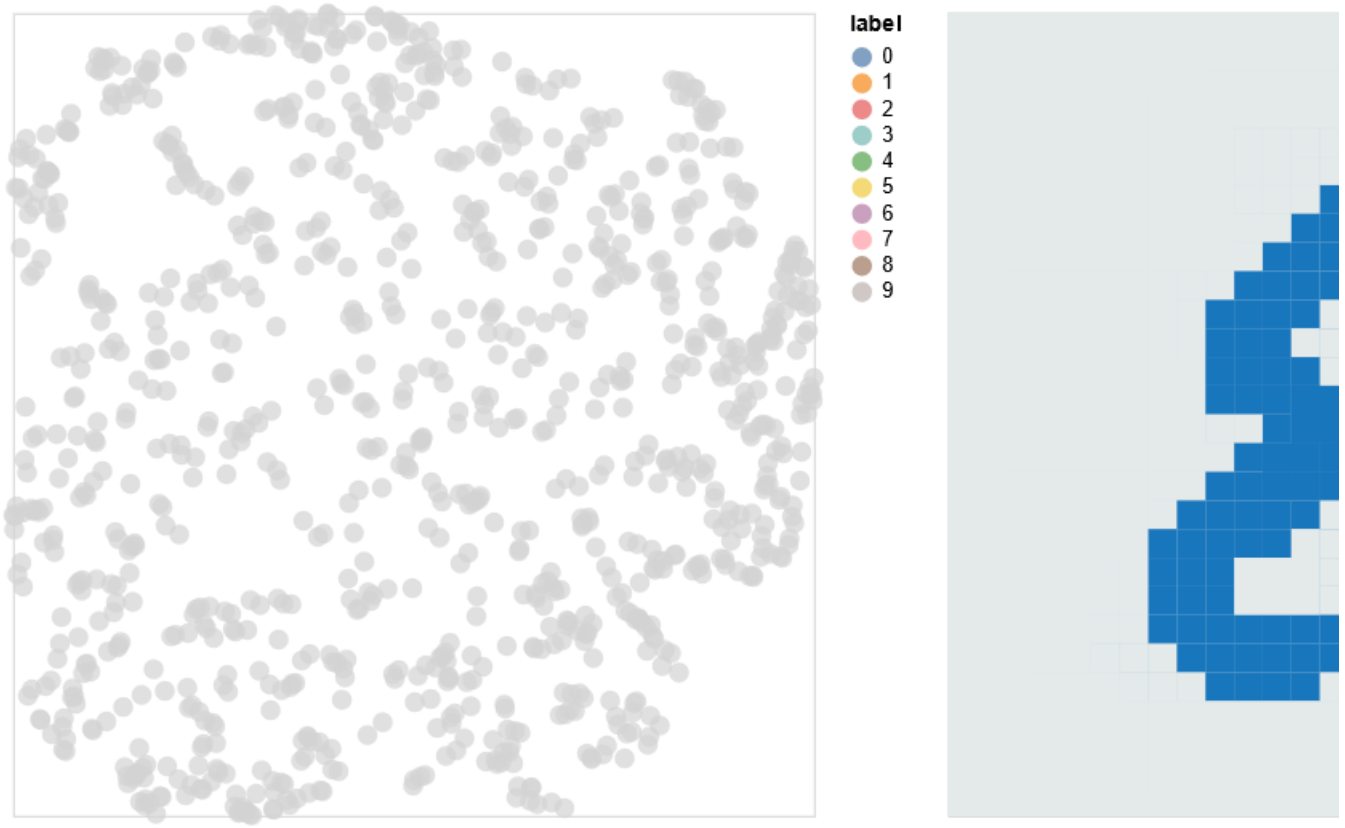
In [ ]:
```
alt.data_transformers.disable_max_rows()

def plot_tsne(tsne_xy, dataloader, num_points=1000):

    images, labels = zip(*[(x[0].numpy()[0,:,:,None], x[1]) for x in dataloader.dataset])

    num_points = min(num_points, len(labels))
    data = pd.DataFrame({'x':tsne_xy[:, 0], 'y':tsne_xy[:, 1], 'label':labels,
                         'image': images})
    data = data.sample(n=num_points, replace=False)

    alt.renderers.set_embed_options('light')
    selection = alt.selection_point(on='mouseover', clear='false', nearest=True)
                                    # init={'x':data['x'][data.index[0]], 'y':data['y'][data.i
    scatter = alt.Chart(data).mark_circle().encode(
        alt.X('x:N',axis=None),
        alt.Y('y:N',axis=None),
        color=alt.condition(selection,
                            alt.value('lightgray'),
                            alt.Color('label:N')),
        size=alt.value(100),
        tooltip='label:N'
    ).add_params(
        selection
    ).properties(
        width=400,
        height=400
    )

    digit  = alt.Chart(data).transform_filter(
        selection
    ).transform_window(
        index='count()'           # number each of the images
    ).transform_flatten(
```

```
        ['image']                 # extract rows from each image
    ).transform_window(
        row='count()',            # number the rows...
        groupby=['index']         # ...within each image
    ).transform_flatten(
        ['image']                 # extract the values from each row
    ).transform_window(
        column='count()',         # number the columns...
        groupby=['index', 'row']  # ...within each row & image
    ).mark_rect(stroke='black',strokeWidth=0).encode(
        alt.X('column:O', axis=None),
        alt.Y('row:O', axis=None),
        alt.Color('image:Q',sort='descending',
            scale=alt.Scale(scheme=alt.SchemeParams('lightgreyteal',
                            extent=[1, 0]),

            ),
            legend=None
        ),
    ).properties(
        width=400,
        height=400,
    )

    return scatter | digit
```

In [ ]:
```
# TSNE
from sklearn.manifold import TSNE

for t, (x, y) in enumerate(test_dataloader):
    if t == 0:
        data = x
        labels = y
    else:
        data = torch.cat((data, x))
        labels = torch.cat((labels, y))

# Then let's apply dimensionality reduction with the trained encoder

with torch.no_grad():
    data = data.to(device)
    mu, logvar = model.encode(data)
    z = (model.reparametrize(mu, logvar)).cpu().detach().numpy()

z_embedded = TSNE(n_components=2).fit_transform(z)
```

In [ ]:
```
plot_tsne(z_embedded, test_dataloader, num_points=1000)
```

Out[ ]:



Discussion

Analyze and discuss the visualized T-SNE representations

1. What role do the KL loss term and β have?
2. Can you find any outliers?

YOUR ANSWER

1. Because β moderates the importance of the KL divergence, and the KL divergence determines the disentanglement of the latent space, both these terms affect whether in regions of dots of certain color, say orange dots, I'm able to find only a particular digit. In my plot, for instance, I mostly find 1 in the orange region in the upper left. As we go closer to the center, we observe disentanglement to be more difficult, as the latent space tend to conflate number 6 with 8 and 3 or 1 with 7, which is understandable given they look alike. A larger beta, coupled with a larger dimension for z in the KL loss term could help disentangle furthermore the points above.
2. It depends on what you mean by outlier. By only looking at the T-SNE representations, we can define an outlier as a digit which is placed far away from its well-defined cluster, into a region of digits that are clearly different to it. For example, a 1 appearing very far from the orange region would be an outlier. Following this definition, I can identify some orange dots corresponding to 1 in the middle left region that are clearly far away from the main cluster of 1 in the upper left region. These digits 1s are placed close to 9, 4 and 7, probably because image-wise they look alike. However, this definition of outlier is disputable given that conventionally, an outlier could refer to one of the extremely unlikely instances where a digit is mislabeled, such as a digit 1 mislabeled as a 3. However, whether we are able to identify this from the embedding space is disputable since the influence of outliers may have been smoothed given a larger batch of correctly labeled training data.