



Artificial Neural Networks with small Datasets. A practical Approach

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Kufstein, 31. October 2021

Paul Leitner, BA

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List of Acronyms

CNN Convolutional Neural Network

GB Gradient Boosting

nn Neural Network

ml Machine Learning

SMOTE synthetic minority oversampling technique

GAN Generative Adversarial Network

DCGAN Deep Convolutional GAN

EM Earth Mover's Distance

FH Kufstein Tirol

Data Science & Intelligent Analytics

Abstract of the thesis: **Artificial Neural Networks with small Datasets. A practical Approach**

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After giving a summary on the literature and history of neural networks, I elucidate the trade-offs between deep learning and other machine learning approaches. I show that machine learning approaches such as Gradient Boosting (GB) mostly trade increased data requirements in favor of data scientist worktime in data preparation and feature engineering. I then investigate whether more complicated Neural Networks (nns) may be used by synthetically enlarging the training data present and thereby achieving comparable accuracy while saving data preparation time, effectively trading processing time (synthetic data enlargement being resource-intensive) for manual feature-engineering time by creating a nn model and benchmarking it against a GB reference model on a standard Machine Learning (ml) dataset with small data, the diabetic retinopathy dataset.

insert result - how much better does this perform? tradeoffs!

note - synthetic data [Hittmeir et al. \(2019\)](#)

31. October 2021

1. Introduction

In 2012 Krizhevsky and his colleagues entered and won the ImageNet classification contest with a deep convolutional neural network Convolutional Neural Network (CNN), outperforming other models by a significant margin Krizhevsky et al. (2012). This marked a turning point in machine learning in general, and in perceptual tasks specifically.

Pereira et al. (2009) is often invoked as a shorthand to the core problem of Machine Learning, the fact that a larger training corpus would always be preferable.

Currently, data scientists spend a significant amount (how much? sources!) of their time, when solving 'shallow' machine learning tasks (such as???) in feature engineering / preprocessing. Source! examples! This is due to the fact that shallow approaches such as decision trees, GBM and SVM models require features that 'directly' connect the prepared data to the searched-for outcome. (source)

Deep learning (neural networks) create intermediate representations via **stacked layers** at the cost of increased training data (source). Thereby enabling a more abstract understanding of patterns within the data.

Shearer (2000)

1.1 Problem Situation

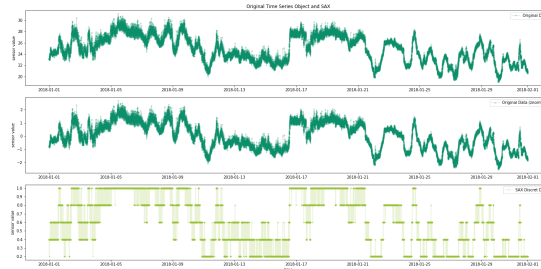


Figure 1: Sax approximation of a time series

As can be seen in Figure 1 ...

1.2 Objectives

1.3 Methods

1.4 Structure

1.5 Tables

Table 1 shows an example table.

Table 1: This is a table		
Column 1	Column 2	Column 3
A	B	C
D	E	F
G	H	I

1.6 Source Code

Listing 1: Hello World in Java

```
1 public class Hello {  
2     public static void main(String[] args) {  
3         System.out.println("Hello World");  
4     }  
5 }
```

Listing 1 shows the classic Hello World in Java.

Listing 2: Hello World in Python

```
1 # This is a comment  
2 print('Hello World')
```

Listing 2 shows the classic Hello World in Python.

2. Synthetic Data in Privacy

cite -> paper from source, different models on synthetic data!

2.1 Synthetic Data for model performance

When training [nn](#)s for image classification, (source) a common practice is **data augmentation**, a range of random transformation applied to images in order to synthetically increase the breadth of data that the model is exposed to. Such operations include

- rotation
- shearing
- zoom
- height & width shift

effectively, these operations transform an Image while preserving the underlying signals in the data. However, with other types of data this might be possible. Attributes of another dataset may not be feasibly 'shifted' in one direction or another without fundamentally changing the signal and misleading the model.

note - the infeasibility of pretraining on non-image datasets - representations of the visual world

2.2 Deep Learning

3. Comparison with other solutions to the small data problem

- synthetic minority oversampling technique ([SMOTE](#))
- crossvalidation (k-fold, single holdout)
- transfer learning (word embeddings, image filter layers)
- wholesale synthetic data approaches, [Hittmeir et al. \(2019\)](#) **more sources needed**

3.1 Data Enhancement for image data

4. Technical Application

4.1 Theoretical applicability

In their landmark paper in 2014, [Goodfellow et al. \(2014\)](#) demonstrated the viability of Generative Adversarial Networks ([GANs](#)) on creating image data on the classic MNIST dataset ([Deng \(2012\)](#)), by generating - among other things - convincing handwritten digits. As mentioned in [3.1](#), some of the architecture specifics and evaluation are quite specific to image data in that

- the data contains a notion of locality, as neighboring data points (i.e. pixels) are strongly dependent
- dimensionality of the generated data is higher than the **latent space**
- results lend themselves to visual quality inspection by humans (it is easy to see even degrees of quality between different architectures)

specifically the former points are strongly relevant to [GAN](#) architecture, as will become obvious shortly.

4.2 Technical implementation steps

Since the goal of this paper is to evaluate whether or not [GAN](#) may be used to not only generate more data of a small non-image dataset (which is fairly trivial) but whether or not this data actually serves to **boost model performance** of models trained on the resulting data, a small, well-understood standard dataset was used to develop the initial architecture; [Farag and Hassan \(2018\)](#). Specifically, the iconic titanic dataset constitutes a binary classification problem, which facilitates quick model evaluation and ameliorates some of the more typical difficulties of training [GANs](#) - see below.

The first attempts to create a basic, dense [GAN](#) actually failed to converge for a significant number of experiments with different amounts of layers, neurons and size of the latent space. Somewhat unsurprisingly, achieving the classic Nash Equilibrium between discriminator and generator was fairly difficult and the initial models all proved unstable. [GANs](#) provide several unique challenges, and/or failure modes:

- mode collapse [Che et al. \(2017\)](#)
- oscillation and general instability of the model [Liang et al. \(2018\)](#)
- catastrophic forgetting [McCloskey and Cohen \(1989\)](#)

Mode collapse is especially relevant in a task like MNIST, where there are multiple classes to be generated, and the generator becomes increasingly proficient in generating one class explicitly - thankfully, this is less of an issue in a binary classification task.

4.2.1 Network Architecture

The other failure modes, however **did** all make an appearance at one time or another, after the initial data preparation. It was fairly clear that the initial network, with one layer each for the generator and the discriminator each, and 64 neurons had insufficient representational power to converge on creating convincing samples as can be seen in 2:

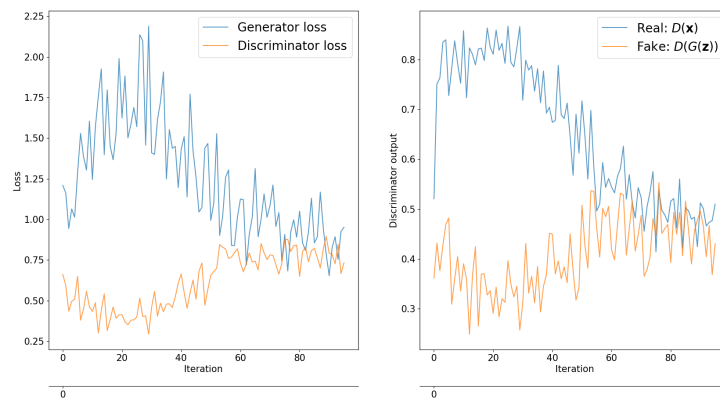


Figure 2: Initial simple dense GAN - left side shows the losses of generator and discriminator, right side shows the probabilities assigned to real and fake samples by the discriminator

Further experiments, with increased numbers of layers and neurons, produced first a very textbook oscillation pattern, shown in 3:

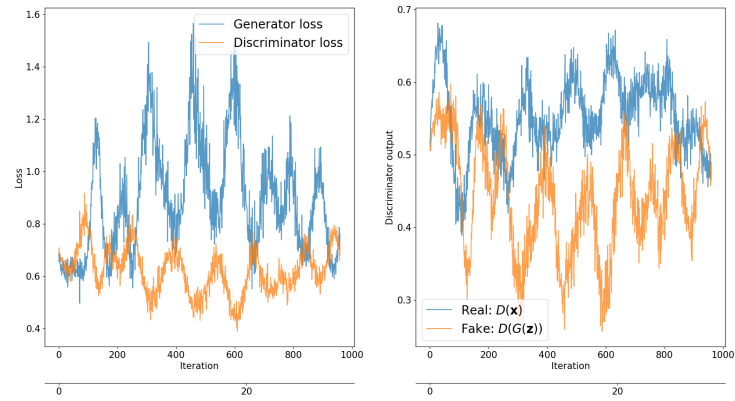


Figure 3: Dense GAN, 3 layers, 64 neurons/layer; left - losses of generator/discriminator right - the probabilities real/fake assigned by the discriminator

Finally, it has to be stressed that finding the ideal combination learning rates, dropout in the discriminator and number of training epochs, is really quite difficult, especially since there appears no good substitute to visually examining the pattern that is produced by a given architecture and then to adjust. A process that has to be iterated for quite a while, and is fairly manual and heavy on trial-and-error.

Ultimately, a promising architecture appeared to be dense networks with 3 layers each, but a higher number of neurons, and still these networks diverged rather quickly shown here 4:

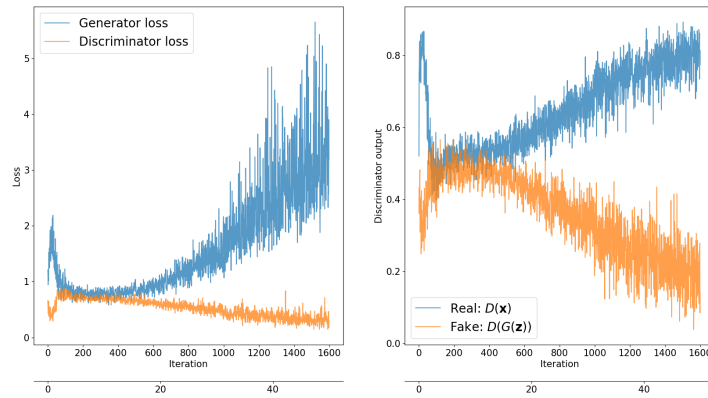


Figure 4: Dense GAN, 3 layers, 128 neurons/layer, reduced learning rate and dropout in discriminator - losses of generator/discriminator right - the probabilities real/fake assigned by the discriminator

Unfortunately, from here on out simply optimizing the number of neurons and learning rate and learning rate scheduling was not enough to mitigate this divergence. Although implementing the popular 1Cycle learning rate decay (described by [Smith \(2018\)](#)) did ameliorate the issue somewhat, it did not fix the network.

What ultimately made the difference is an adaptation of the architecture proposed by [Radford et al. \(2016\)](#). The architecture proposed here for image generation constitutes a **symmetrical** upsampling from the latent space in the generator (in case of images, a **transposed convolution**) and downsampling in the discriminator. As shown by [Suh et al. \(2019\)](#) here:

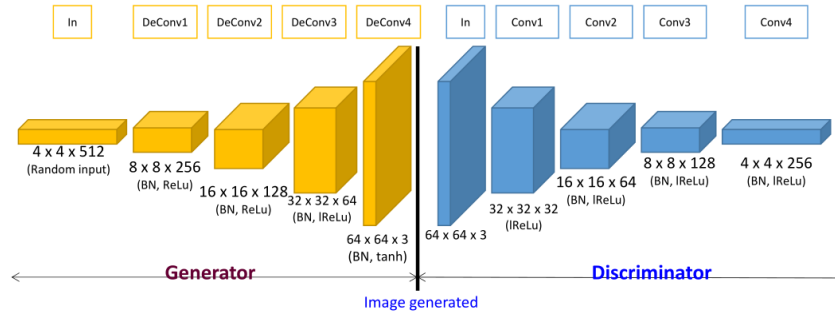


Figure 5: Architecture of Discriminator and Generator

Initially, implementing convolution actually deteriorated performance and completely prevented convergence of the network, a probable explanation would be the fact that convolution and transposed convolution not only up-sample the latent space but more fundamentally relate to locality in the data; i.e. multiple convolutional layers over a picture effectively create hierarchical feature extraction. A paper that illustrates the mechanics of this fairly well was [Dumoulin and Visin \(2018\)](#). Effectively, these convolutions would initially find small features in images, subsequent convolutions would assemble these features into feature maps and their presence would indicate the presence of objects in an image. The entire concept of strides and adjacent data points however, does not make sense in the concept of a dataset where an observation consists of a feature vector, in which the order does not convey any information. While 1D convolutions are quite widely used in sequence and time-series processing - which are quite comfortably out of scope of this paper - they fundamentally seem unsuited to a dataset which would not lose any information if the order of its' attributes was permuted.

What **did** make a difference was implementing the symmetry of upsampling and condensing in the generator and discriminator.

Furthermore, [Radford et al. \(2016\)](#) propose other guidelines for building Deep Convolutional GANs (DCGANs) which proved helpful:

- implementing BatchNormalization in the generator and discriminator [Ioffe and Szegedy \(2015\)](#)
- using ReLU activation in all layers in the generator except for the output, which would use tanh
- using LeakyReLU in all layers in the discriminator, except for the output which uses sigmoid

After implementing these guidelines, using Binary Categorical Crossentropy loss, the generator and discriminator actually converged fairly well already, as seen in [6](#)

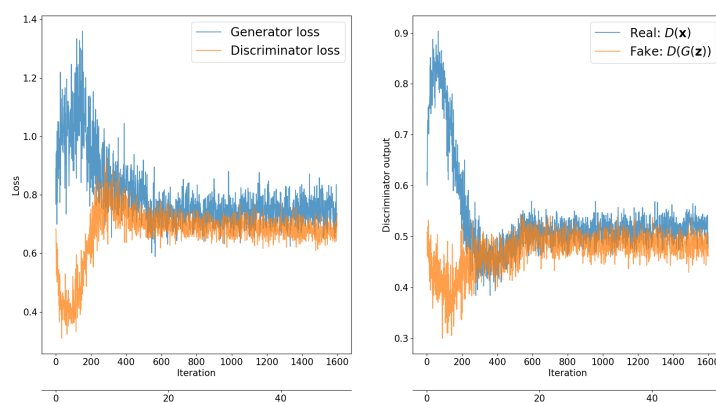


Figure 6: Dense GAN, 2 layers, 32 neurons/layer; left - losses of generator/discriminator right - the probabilities real/fake assigned by the discriminator

Importantly, in this architecture the **generator** model starts with a dense layer containing 32 neurons, which doubles in every layer (once in this case, although

this is a variable parameter). The final dense hidden layer is then downsampled again to reflect the original data - like this:

Listing 3: generator network

```

1  import tensorflow as tf
2
3
4  def create_generator_network(
5      number_hidden_layers: int = 2,
6      number_hidden_units_power: int = 5,
7      hidden_activation_function: str = 'ReLU',
8      use_dropout: bool = False,
9      upsampling: bool = True,
10     use_batchnorm: bool = True,
11     dropout_rate: float = 0.3,
12     number_output_units: int = 12,
13     output_activation_function: str = 'tanh') -> tf.keras.Model:
14
15     model = tf.keras.Sequential()
16     for i in range(number_hidden_layers):
17
18         if upsampling:
19             # implements the guideline DCGAN - upsampling layers in the generator
20             model.add(tf.keras.layers.Dense(2 ** (number_hidden_units_power + i), use_bias=False))
21
22         else:
23             model.add(tf.keras.layers.Dense(2 ** number_hidden_units_power, use_bias=False))
24
25         if use_batchnorm:
26             model.add(tf.keras.layers.BatchNormalization())
27         else:
28             pass
29
30         model.add(tf.keras.layers.Activation(hidden_activation_function))
31
32         if use_dropout:
33             model.add(tf.keras.layers.Dropout(dropout_rate))
34         else:
35             pass
36
37     model.add(tf.keras.layers.Dense(number_output_units))
38     model.add(tf.keras.layers.Activation(output_activation_function))
39
40     return model

```

Listing 3 shows the python function which creates the generator network.

The discriminator implements the exact mirror image of this pattern, beginning with the same amount of neurons after the input layer and downsampling by half each layer;

Listing 4: discriminator network

```

1  import tensorflow as tf
2
3
4  def create_discriminator_network(
5      number_hidden_layers: int = 2,
6      number_hidden_units_power: int = 5,
7      hidden_activation_function: str = 'LeakyReLU',
8      use_dropout: bool = True,
9      upsampling: bool = True,
10     use_batchnorm: bool = True,
11     dropout_rate: float = 0.3,
12     number_output_units: int = 1) -> tf.keras.Model:
13
14     model = tf.keras.Sequential()
15
16     for i in range(number_hidden_layers):
17
18         if upsampling:
19             # implements the guideline - downsample in the discriminator network
20             model.add(tf.keras.layers.Dense(2 ** (number_hidden_units_power + number_hidden_layers - i - 1)))
21
22         else:
23             model.add(tf.keras.layers.Dense(2 ** number_hidden_units_power))
24
25         if use_batchnorm:
26             model.add(tf.keras.layers.BatchNormalization())
27         else:
28             pass
29
30         model.add(tf.keras.layers.Activation(hidden_activation_function))
31
32         if use_dropout:
33             model.add(tf.keras.layers.Dropout(dropout_rate))
34         else:
35             pass
36
37     model.add(tf.keras.layers.Dense(number_output_units, activation=None))
38
39     return model

```

Listing 4 shows the python function which creates the discriminator network.

4.2.2 Network Training Implementation

With the basic architecture for the Network in place, the functions are put together into a custom training loop. While there are multiple approaches to training GANs, starting with the seminal paper by Goodfellow et al. (2014), such as training the discriminator and generator in an epoch separately, here a custom training loop with separate optimizers was chosen from the beginning, in order to accommodate more exotic loss functions.

Since a number of experiments on the efficacy of the generated data has to be done, the entire GAN system was set up to be set up with sensible defaults, dynamically adapting to 1D datasets. Specifically Buitinck et al. (2013) suggest design lessons from scikit-learn, one of which is sensible defaults.

In order to automatically create both generators and discriminators dynamically based on input shape (but with strong default settings which ideally do not have to be adjusted during experimentation at all) a small package was created which encapsulates the entire training loop.

Key part here is the training loop shown here:

Listing 5: training loop

```

1  # lists to store losses and values
2  all_losses = []
3  all_d_vals = []
4
5  for epoch in range(1, n_epochs+1):
6      epoch_losses, epoch_d_vals = [], []
7      for i, (input_z, input_real) in enumerate(training_data):
8
9          # generator loss, record gradients
10         with tf.GradientTape() as g_tape:
11             g_output = generator_model(input_z)
12             d_logits_fake = discriminator_model(g_output, training=True)
13             labels_real = tf.ones_like(d_logits_fake)
14             g_loss = loss_fn(y_true=labels_real, y_pred=d_logits_fake)
15             # get loss derivatives from tape, only for trainable vars, in case of regularization / batchnorm
16             g_grads = g_tape.gradient(g_loss, generator_model.trainable_variables)
17
18         # apply optimizer for generator
19         g_optimizer.apply_gradients(
20             grads_and_vars=zip(g_grads, generator_model.trainable_variables))
21
22         # discriminator loss, gradients
23         with tf.GradientTape() as d_tape:
24             d_logits_real = discriminator_model(input_real, training=True)
25
26             d_labels_real = tf.ones_like(d_logits_real)
27
28             # loss for the real examples - labeled as 1
29             d_loss_real = loss_fn(
30                 y_true=d_labels_real, y_pred=d_logits_real)
31
32             # loss for the fakes - labeled as 0
33
34             # apply discriminator to generator output like a function
35             d_logits_fake = discriminator_model(g_output, training=True)
36             d_labels_fake = tf.zeros_like(d_logits_fake)
37
38             # loss function
39             d_loss_fake = loss_fn(
40                 y_true=d_labels_fake, y_pred=d_logits_fake)
41
42             # compute component loss for real & fake
43             d_loss = d_loss_real + d_loss_fake
44
45         # get the loss derivatives from the tape
46         d_grads = d_tape.gradient(d_loss, discriminator_model.trainable_variables)
47
48         # apply optimizer to discriminator gradients - only trainable :todo: add regularization here
49         d_optimizer.apply_gradients(
50             grads_and_vars=zip(d_grads, discriminator_model.trainable_variables))
51
52         # add step loss to epoch list
53         epoch_losses.append(
54             (g_loss.numpy(), d_loss.numpy(),
55              d_loss_real.numpy(), d_loss_fake.numpy()))
56
57         # probabilities from logits for predictions, using tf builtin
58         d_probs_real = tf.reduce_mean(tf.sigmoid(d_logits_real))
59         d_probs_fake = tf.reduce_mean(tf.sigmoid(d_logits_fake))
60         epoch_d_vals.append((d_probs_real.numpy(), d_probs_fake.numpy()))
61

```

```

62     # record loss
63     all_losses.append(epoch_losses)
64     all_d_vals.append(epoch_d_vals)
65     print(
66         'Epoch {:03d} | ET {:.2f} min | Avg Losses >>'
67         ' G/D {:.4f}/{:.4f} [D-Real: {:.4f} D-Fake: {:.4f}]'
68         .format(
69             epoch, (time.time() - start_time)/60,
70             *list(np.mean(all_losses[-1], axis=0))))
71     result = {
72         'all_losses': all_losses,
73         'all_d_vals': all_d_vals,
74         'generator': generator_model,
75         'discriminator': discriminator_model}
76
77     if export_generator:
78
79         print()
80         print('saving generator model')
81
82         tf.keras.models.save_model(generator_model, f'./models/generator_{model_name}.h5')
83         print(f'generator model saved to: ./models/{model_name}.h5')
84
85     return result

```

Listing 5 shows the python function which trains the network. Note that this function is **quite strongly simplified**, the actual code used can be found at https://github.com/PaulBFB/master_thesis/blob/main/train_generator.py and would not likely be germane to the paper in its' entirety in any case.

The above training loop was developed together with the network architecture and also produced the training graphics shown so far. Before it was used in experimentation however, adjusting its' loss function was tested. Specifically, as proposed by [Arjovsky et al. \(2017\)](#), implementing the Earth Mover's Distance (EM) as a loss function.

$$W(\mathbb{P}_r, \mathbb{P}_g) = \inf_{\gamma \in \Pi(\mathbb{P}_r, \mathbb{P}_g)} \mathbb{E}_{(x,y) \sim \gamma} [\|x - y\|]$$

Figure 7: Wasserstein distance formula

As mentioned in the paper, this distance denotes the amount of work that is necessary to transform one distribution in to another, given an optimal transfer plan γ which actually denotes **how** the work is done. Furthermore, and probably most importantly, the EM, in contrast to other loss functions, is actually a function of the parameters θ of the distributions in question, i.e. it can express partial derivatives with respect to the single parameters!

However, finding γ is an optimization problem by itself, since it constitutes an **optimal** solution. As [Arjovsky et al. \(2017\)](#) mention therefore, it is approximated during training. A complete explication of the metric and its' approximation is out of scope of this paper.

What this achieves in practice, is that it enables the discriminator to act as a **critic**, essentially reporting the distance that the generator has yet to move back during training, which the generator then backpropagates to its' parameters. Thereby, the loss during training actually becomes more meaningfully readable.

Arjovsky et al. (2017) recommend in their paper to clip the gradients reported back to the generator to be clipped. This led to substantial instability in the network, as can be seen here:

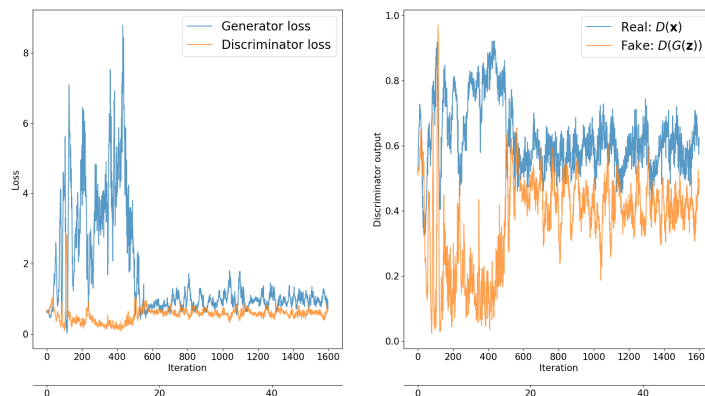


Figure 8: Wasserstein GAN, 3 layers; left - losses of generator/discriminator right - the probabilities real/fake assigned by the discriminator

As can be seen clearly here, the equilibrium between the components is fairly unstable. Gulrajani et al. (2017) pose that gradient clipping here actually leads to exploding and vanishing gradients, which seems to describe this result fairly well. In the actual implementation therefore, the **Gradient Penalty** method they recommend is implemented, namely:

- between real and fake examples in a batch, choose a random number sampled from a uniform distribution
- interpolate between real and fake examples
- calculate discriminator loss for all interpolated examples
- add the gradient penalty based on the interpolations
- remove batch normalization from the discriminator, since it shifts example gradients based on the entire batch

Therefore, the training loop was modified:

Listing 6: training loop

```

1  for epoch in range(1, n_epochs+1):
2      epoch_losses, epoch_d_vals = [], []
3      for i, (input_z, input_real) in enumerate(training_data):
4
5
6          # set up tapes for both models
7          with tf.GradientTape() as d_tape, tf.GradientTape() as g_tape:
8              g_output = generator_model(input_z, training=True)
9
10             # real and fake part of the critics output
11             d_critics_real = discriminator_model(input_real, training=True)
12             d_critics_fake = discriminator_model(g_output, training=True)
13
14             # generator loss - (reverse of discriminator, to avoid vanishing gradient)
15             g_loss = -tf.math.reduce_mean(d_critics_fake)
16
17             # discriminator losses
18             d_loss_real = -tf.math.reduce_mean(d_critics_real)
19             d_loss_fake = tf.math.reduce_mean(d_critics_fake)
20             d_loss = d_loss_real + d_loss_fake
21
22             # INNER LOOP for gradient penalty based on interpolations
23             with tf.GradientTape() as gp_tape:
24                 alpha = rng.uniform(
25                     shape=[d_critics_real.shape[0], 1, 1, 1],
26                     minval=0.0, maxval=1.0)
27
28                 # creating the interpolated examples
29                 interpolated = (
30                     alpha*tf.cast(input_real, dtype=tf.float32) + (1-alpha)*g_output)
31
32                 # force recording of gradients of all interpolations (not created by model)
33                 gp_tape.watch(interpolated)
34                 d_critics_intp = discriminator_model(interpolated)
35
36                 # gradients of the discriminator w. regard to all
37                 grads_intp = gp_tape.gradient(
38                     d_critics_intp, [interpolated,])[0]
39
40                 # regularization
41                 grads_intp_l2 = tf.sqrt(
42                     tf.reduce_sum(tf.square(grads_intp), axis=[1, 2, 3]))
43
44                 # compute penalty w. lambda hyperparam
45                 grad_penalty = tf.reduce_mean(tf.square(grads_intp_l2 - 1.0))
46
47                 # add GP to discriminator
48                 d_loss = d_loss + lambda_gp*grad_penalty

```

Note that according to [Gulrajani et al. \(2017\)](#) a λ value of 10.0 worked well in all examples, which is what was used here. Again, this is a strongly truncated version of the code, the full version can be found at https://github.com/PaulBFB/master_thesis/blob/main/train_wasserstein_generator.py - this

also contains modified functions to create a **discriminator** without BatchNormalization.

The resulting training loop with the same layers and upsampling-downsampling symmetry between generator and discriminator resulted in this:

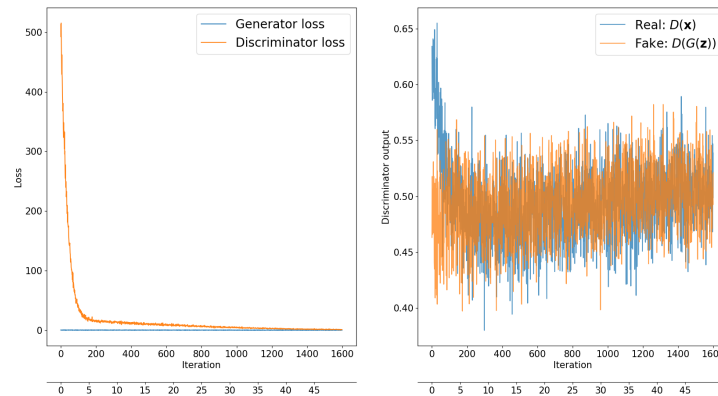


Figure 9: Wasserstein GAN with gradient penalty, 2 layers; left - losses of generator/discriminator right - the probabilities real/fake assigned by the discriminator

5. Results

6. Discussion

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A. List of Interview Partners

B. Code Table