K. Breininger S. Vesal M. Gu Z. Pan N. Maul Z. Yang L. Reeb F. Thamm T. Würfl December 20, 2019



Regularization and the Recurrent Layer

1 Regularizers

This time we will extend our framework to include common regularization strategies. As neural networks are extremely flexible statistical models they tend to show more variance and less bias. However this also means they are very prone to overfitting. Therefore, regularization is a very important part of deep learning. Throughout this exercise you will have to use base-classes, which implement default members and methods accessible to each class derived from the respective base-class.

1.1 Refactoring

Since the behaviour of some layers changes depending on whether the network is currently training or testing, we need to refactor our layers. Moreover, we choose to introduce a "base-optimizer", which provides some basic functionality, in order to enable the use of regularizers.

Task:

All layers should be derived from a <u>base-class</u>, which defines the base-attributes they should have. For information on inheritage in python we refer to here.

- Create a <u>base-class</u> for layers "Base.py" in the "Layers" folder. All layers need to inherit from this "base-layer" so refactor them accordingly.
- Secondly, implement a class "Phase" in "Base.py", which provides two variables, namely train and test. Both variables can be defined as strings, e.g. train and test.
- The "base-layer" needs to contain a variable <u>member</u> named **phase**. Implemented as strings, possible phases are **train** or **test**. Use the training phase as default. The unittests sets the **phase** <u>member</u> according to the Phase class and its definitions for the **train** and **test** variables.
- Implement a <u>property</u> **phase** in the **NeuralNetwork** <u>class</u> setting each layer's phase. Use this method to set the phase in the **train** and **test** methods.
- Optionally you can add other members like a default weights parameter, which might come in handy.
- Create a <u>base-class</u> for optimizers in the "Optimizers.py" file. Make all optimizers inherit from this "base-optimizer".

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• The "base-optimizer" should have a method **add_regularizer(regularizer)** and a <u>member</u> storing the **regularizer**.

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1.2 Optimization Constraints

Equality and inequality constraints on the norm of the weights are well known in the field of Machine Learning. They enforce the prior assumption on the model of small weights in case of L2-regularization and sparsity in case of L1-regularization.

Task:

Implement <u>classes</u> **L2_Regularizer** and **L1_Regularizer** in the file "Constraints.py" folder "Optimization". Both have to provide the <u>methods</u> <u>calculate_gradient(weights)</u> that calculates a (sub-)gradient on the weights needed for the optimizer. Additionally they have to provide a <u>method</u> <u>norm(weights)</u>, which is used to calculate the norm enhanced loss.

- Implement the two schemes. The <u>constructor</u> of each receives an <u>argument</u> **alpha** representing the regularization weight.
- Refactor the <u>optimizers</u> to apply the new **regularizer** if it is set using the **calculate_gradient(weights)** <u>method</u>.
- Refactor the **NeuralNetwork** <u>class</u> to add the regularization loss to the data loss. Use the <u>method</u> **norm(weights)** and sum up the regularization loss created by the weights of all layers. Hint: You might want to refactor more classes to get the necessary information using base-classes.

You can verify your implementation using the provided testsuite by providing the commandline parameter **TestConstraints**.

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1.3 Dropout

Dropout is a special regularizer typical for Deep Learning. It's most often used to regularize fully connected layers. It enforces independent weights, reducing the effect of co-adaptation.

Task:

Implement a <u>class</u> **Dropout** in the file "Dropout.py" in folder "Layers". This <u>class</u> has to provide the <u>methods</u> **forward(input_tensor)** and **backward(error_tensor)**. This layer has no adjustable parameters. We choose to implement <u>inverted</u> dropout.

- Implement the <u>constructor</u> for this <u>layer</u> receiving the argument **probability** determining the fraction units to keep.
- Implement the Dropout <u>methods</u> forward(input_tensor) and backward(error_tensor) for the training phase.
- Modify the Dropout <u>method</u> forward(input_tensor) for the testing phase.

You can verify your implementation using the provided testsuite by providing the commandline parameter **TestDropout**.

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1.4 Batch Normalization

Batch Normalization is a regularization technique which is conceptually very well known in Machine Learning but specially adapted to Deep Learning.

Task:

Implement a <u>class</u> **BatchNormalization** in the file "BatchNormalization.py" in folder "Layers". This <u>class</u> has to provide the <u>methods</u> **forward(input_tensor)** and **backward(error_tensor)**.

- Implement the <u>constructor</u> for this <u>layer</u> which receives the argument **channels**. **channels** denotes the number of channels of the **input_tensor** in both, the vector and the image-case. Initialize the bias β and the weights γ according to the **channels**-size using the method **initialize**.
- Implement the method **initialize** which initializes the weights γ and the biases β . **initialize** ignores any assigned initializer and initializes always the weights γ with ones and the biases β with zeros, since you do not want the weights γ and bias β to have an impact at the beginning of the training. Make sure you optimize the weights and bias in the backward pass, but only if optimizers are defined.
- Implement the Batch Normalization <u>methods</u> forward(input_tensor) and backward(error_tensor) with independent activations for the training phase. Make sure you use an ϵ smaller than 1e-10.
- Hint: In Helpers.py we provide a <u>function</u> compute_bn_gradients(error_tensor, input_tensor, weights, mean, var) for the computation of the gradient w.r.t. inputs. Note that this function does not compute the gradient w.r.t. the weights.
- Implement the moving average estimation of training set mean and variance.
- Modify the Batch Normalization <u>method</u> **forward(input_tensor)** for the testing phase. Use an <u>online</u> estimation of the <u>mean</u> and <u>variance</u>. Initialize <u>mean</u> and <u>variance</u> with the batch mean and the batch standard deviation of the first batch used for training.
- Implement the convolutional variant. The layer should change behaviour depending on the shape of the **input_tensor**.
- Implement a method **reformat(tensor)** which receives the tensor that must be reshaped. Depending on the shape of the tensor, the method reformats the image-like tensor (with 4 dimension) into its vector-like variant (with 2 dimensions), and the same method reformats the vector-like tensor into its image-like tensor variant. Use this in the forward and the backward pass.

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You can verify your implementation using the provided test suite by providing the commandline parameter ${\bf TestBatchNorm}$.

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1.5 LeNet (optional)

By now our framework contains all the essential parts to build a convolutional neural network. However not every architecture can be trained to high performance. Therefore, successful architectures also play an important role. We implement a variant of a well known architecture called LeNet.

Task:

We implement a modification of a classic architecture called LeNet in file "LeNet.py" in folder "Models".

- Add two <u>functions</u> (This means they should not be part of the <u>class</u>.) **save(filename, net)** and **load(filename, data_layer)** to the **NeuralNetwork** <u>file</u>. Those two methods should use python's <u>pickle</u> to save and load networks. After loading the network the <u>data_layer</u> should be <u>set</u> again.
- Exclude the data_layer from saving by implementing the __getstate__() and __setstate__(state) methods. The __setstate__(state) method should initialize the dropped members with None. This needs to be done, since the data_layer is a generator-object, which cannot be processed by pickle.
- Implement the LeNet architecture as a function **build()** returning a network. Use a <u>SoftMax</u> layer and <u>ReLU</u> activation functions. Also ignore the fact, that the original architecture did not use padding for the convolution operation.
- Not typical for Deep Learning but useful, we also store the optimizer, initializer and their settings. Use the <u>ADAM</u> optimizer with a learning rate of 5^{-4} and a L₂ regularizer of weight $4 \cdot 10^{-4}$.

You can train this LeNet-variant on MNIST using the script "TrainLeNet.py".

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2 Recurrent Layer

Many prediction problems require memorization capabilities along a particular dimension. Typical examples are time series prediction problems. A common method to address those are Recurrent Neural Networks (RNNs). To implement RNNs we can reuse most algorithms of our framework. The only necessary new components are new layers implementing the specific RNN cells.

2.1 Activation functions

Two common activation functions which we didn't implement so far will come in handy: The hyperbolic tangent (Tangens Hyperbolicus) and the Sigmoid.

Task:

Implement two <u>classes</u> **TanH** and **Sigmoid** in files: "TanH.py" and "Sigmoid.py" in the folder "Layers".

- Implement the operations forward(input_tensor), backward(error_tensor) for the TanH and the Sigmoid activation function.
- Specifically store *activations* for the dynamic programming component, instead of the **input_tensor**. This is possible because the gradient involves only activations instead of the input (see slides).

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2.2 Elman Recurrent Neural Network (RNN) (optional)

The type of recursive neural networks known as Elman network consists of the simplest RNN cells. They can be modularly implemented as layers. The respective Unittests are deactivated per default. To activate them set the boolean flag **TEST_RNN** in line 12 of the unittests to **True**.

Task:

Implement a <u>class</u> **RNN** in the file: "RNN.py" in folder "Layers". This <u>class</u> has to provide all the methods required by a trainable layer for our framework.

- Write a <u>constructor</u>, receiving the <u>arguments</u> (input_size, hidden_size, output_size). Here input_size denotes the dimension of the *input vector* while hidden_size denotes the dimension of the hidden state. Initialize the hidden state with all zeros.
- Add a <u>property</u> memorize which sets the <u>boolean</u> state representing whether the RNN regards subsequent sequences as a belonging to the same long sequence. In the constructor, initialize this member with False.
- Implement a <u>method</u> **forward(input_tensor)** which returns the **input_tensor** for the next layer. Consider the "batch" dimension as the "time" dimension of a sequence over which the recurrence is performed. The first **hidden_state** for this iteration is all zero if the boolean member variable is **False**, otherwise restore the hidden state from the last iteration. You can choose to <u>compose</u> parts of the RNN from other *layers* you already implemented.
- Implement a <u>method</u> backward(error_tensor) which updates the parameters and returns the error_tensor for the next layer. Remember that optimizers are decoupled from our *layers*.
- Implement the accessor <u>property</u> **gradient_weights**. Here the **weights** are defined as the weights which are involved in calculating the **hidden_state** as a stacked tensor. E.g. if the **hidden_state** is computed with a single Fully Connected layer, which receives a stack of the **hidden_state** and the **input_tensor**, the weights of this particular Fully Connected Layer, are the weights considered to be weights for the whole class. In order to provide access to the **weights** of the RNN layer, implement a getter and a setter with a property for the **weights** member.
- To be able to reuse all regularizers, add the <u>property</u> to add an optimizer as **optimizer** and to calculate the loss caused by *regularization* as **calculate_regularization_loss()** as introduced in the regularization exercise. Finally add the <u>method</u> **initialize(weights_initializer, bias_initializer)** to use our *initializers*.

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2.3 Long Short-Term Memory (LSTM)

Elman networks severely suffer from the vanishing gradient problem. A common method to remedy this is to use more complicated RNN cells. The classical example is the LSTM cell.

Task:

Implement a <u>class</u> **LSTM** in the file: "LSTM.py" in folder "Layers". This <u>class</u> has to provide all the <u>methods</u> required by a trainable layer for our framework.

- Write a <u>constructor</u>, receiving the <u>arguments</u> (input_size, hidden_size, output_size). Here input_size denotes the dimension of the *input vector* while hidden_size denotes the dimension of the *hidden state*. Initialize the hidden state with all zeros.
- Add a <u>property</u> memorize which sets the <u>boolean</u> state representing whether the RNN regards subsequent sequences as a belonging to the same long sequence. In the constructor, initialize this member with False. That means if this state is True, the *hidden_state* of one sequence processed in one forward call is carried over to next forward call as an initial state for the *hidden_state*. Otherwise the *hidden_state* is initialized with zeros every time a new sequence is processed. This is required to switch form BPTT to TBPTT.
- Implement a <u>method</u> **forward(input_tensor)** which returns the **input_tensor** for the next layer. Consider the *batch* dimension as the *time* dimension of a sequence over which the recurrence is performed. The first *hidden_state* for this iteration is all zero if the boolean member variable is **False**, otherwise restore the hidden state from the last iteration. You can choose to <u>compose</u> parts of the LSTM from other *layers* you already implemented.
- Implement a <u>method</u> backward(error_tensor) which updates the parameters and returns the error_tensor for the next layer. Remember that optimizers are decoupled from our *layers*.
- Implement the accessor <u>property</u> **gradient_weights**. Here the **weights** are defined as the weights which are involved in calculating the **hidden_state** as a stacked tensor. E.g. if the **hidden_state** is computed with a single Fully Connected layer, which receives a stack of the **hidden_state** and the **input_tensor**, the weights of this particular Fully Connected Layer, are the weights considered to be weights for the whole class. In order to provide access to the **weights** of the LSTM layer, implement a getter and a setter with a property decorator for the **weights** member.
- To be able to reuse all regularizers, add the <u>property</u> to add an optimizer as **optimizer** and to calculate the loss caused by <u>regularization</u> as **calculate_regularization_loss()**

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as introduced in the regularization exercise. Finally add the <u>method</u> initialize(weights_initializer, bias_initializer) to use our *intializers*.

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3 Test, Debug and Finish

Now we implemented everything.

Task:

Debug your implementation until every test in the suite passes. You can run all tests by providing no commandline parameter.