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Thesis

[Choose yours: Bachelor or Master's]

Learned Quantization Schemes for Data-centric ML Pipelines

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Hereby I declare that I wrote this thesis myself with the help of no more than the mentioned literature and auxiliary means.

Berlin, 01.01.2024

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Abstract

Machine learning (ML) models are notoriously resource-intensive. Given their widespread application across every-day edge devices, the need to reduce their memory and computing requirements is becoming ever more pressing. Despite the said resource-intensiveness of ML models, at the same time they offer the main ingredient for the remedy to the malady - redundancy - which can be exploited to reduce their memory usage. While the redundancy exploitation of ML models is already a common technique that comes in different forms, starting from weight pruning [8] and ending with knowledge distillation, quantization presents itself as an especially promising area especically in the sense of learned quantization - the process of making ML models learn their optimal quantization parameters on their own. Hence, the current work employs two techniques that bypass the main issue of learned quantization, that is, the non-differentiability of rounding operations. While the first technique involves custom loss functions that directly take into account quantization goals, the second, more novel approach incorporates a custom scaling factor gradient calculation that takes into account the gradient of the parameters that are being quantized. As a result of these two techniques, a memory usage reduction of up to ..x is obtained on MNIST, CIFAR10, and Imagenette.

Zusammenfassung

This is a placeholder for the german abstract (Kurzfassung) which should follow the same structure as the abstract. Just testing

Contents

1 Introduction

Such is the life of a modern human being that not a single day passes without a machine learning model toiling away in the background. From unlocking one's phone with Face ID in the morning to receiving a curated recommendation feed on Netflix in the evening — all is ML — but at what cost?

If we consider GPT-3 as an example, its 175 billion parameters need a whopping 700 gigabytes of storage in total - 4 bytes for each parameter represented in single-precision floating-point format (FP32). This costliness of modern ML models has revitalized interest in the research area of *quantization of Neural Networks* (NNs) which aims to reduce model size by developing methods that directly or indirectly decrease the amount of memory needed to store parameters numbering in the millions or billions. Going back to the GPT-3 example, by directly clamping its FP32 parameters to an 8-bit integer (INT8) representation, we can reduce its storage requirement from 700 to just 175 gigabytes.

But what costs does quantization itself entail? The natural answer to this question would be a reduction in model performance, as a decrease in precision logically implies a decrease in accuracy. However, there is a somewhat counterintuitive phenomenon where quantization improves accuracy by introducing noise, which act like a form of regularization, forcing the model to generalize better [2]. No matter whether quantization results in better or a slightly worse performance, the conclusion is that for each model there is an optimal way to quantize it within reasonable degradation ranges. And if the model is able to learn its optimal parameters, it is most likely also able to learn its optimal quantization parameters.

The fact that, indeed, models can learn their optimal quantization parameters has been proven many times in the past. But is there a way to make them do it better - is a question that will always remain and to which this thesis aims to contribute. In that sense, the current work will explore novel ways to tackle the two main problems that the process of learning optimal quantization parameters poses. First, how to overcome the issue of non-differentiability of rounding operations in the back-propagation. Second, how to guide the model to quantize selectively where necessary and adaptively relax the quantization when a certain threshold is reached.

While there is a number of methods dealing with the issue of non-differentiability of rounding operations in quantization, the most popular of them are the Straight-Through Estimator and other similar approaches that employ continuous relaxations of discrete functions to enable gradient-based optimization. Besides these approximation methods,

other more aggressive techniques — in a sense — avoid non-differentiability altogether and perform quantization based on strictly defined constraints. Binary Connect [2], for example, binarizes weights during both forward pass and backpropagation, with the real values of weights used only during parameter update. However, these aggressive methods, while effective in simpler scenarios, often struggle on more complex datasets. The more effective methods seem to combine both constraints and gradient approximations — just like XNOR-Net enhances BinaryConnect with a gradient computation formula designed for binary weights [20].

Despite the abundance of different methods, they do not seem to tackle the second problem mentioned earlier, namely, not only how to quantize but also where and when to do so. In this thesis, we try to bridge this gap by introducing a method that directly takes into account the gradient and value of the parameters that are being quantized and adjusts the quantization process using trainable scaling factors. These factors are guided by a threshold-like penalty mechanism that remains inactive when a certain parameter is too sensitive to quantization, encouraging selective quantization and adaptively relaxing it when it becomes too aggressive.

Paragraph about custom loss function term.

2 Background

This chapter addresses the theoretical and contextual background necessary to understand the key concepts and methodologies that form the foundation of the current research. The first section will discuss the basics of deep NNs, upon which the technical setup of this thesis is based. The next section aims to provide a broader context for the term quantization, followed by a final section that explains common techniques of *learned quantization*, as well as the trade-offs and challenges they present.

2.1 Fundamentals of Deep Learning

This section introduces the fundamental concepts of deep learning, beginning with the most basic NN architecture components 2.1.1 and progressing to loss functions with regularization 2.1.2. The concepts of the forward pass and backpropagation will be explained in the last subsection 2.1.3.

2.1.1 Dense and Convolutional Layers

NNs can be considered a mathematical abstraction of the human decision-making process. Consider a scenario where, given an image, you need to say aloud what you see. The two eyes can be regarded as input nodes that receive the initial data, the brain can be seen as a set of *hidden layers* that process this data, and your mouth — the output node that provides the final answer.

A hidden layer, which typically consists of many neurons, is where the magic — or the transformation of data — happens. In its simplest form, within the classic *Multilayer Perceptron* (MLP) model, each hidden layer neuron performs a weighted operation:

$$output = f(w \cdot input + b)$$

where:

- *input* refers to the outputs from the previous layer (or the initial data from input nodes) that are fed into a specific neuron in the hidden layer.
- w (weights) is a vector of parameters associated with that specific neuron, defining the importance of each input received by this neuron.
- b (bias) is an additional scalar parameter specific to the neuron, which shifts the result of the weighted sum, allowing for more flexibility.

- f is the *activation function*, a nonlinear function applied to the weighted sum of inputs and bias in that specific neuron, allowing for more complexity.
- *output* is the result produced by the neuron, which will then be passed on to the next hidden layer (or to the final output layer).

Hidden layers where each neuron is connected to every neuron in the previous layer and every neuron in the next layer are called *dense layers*.

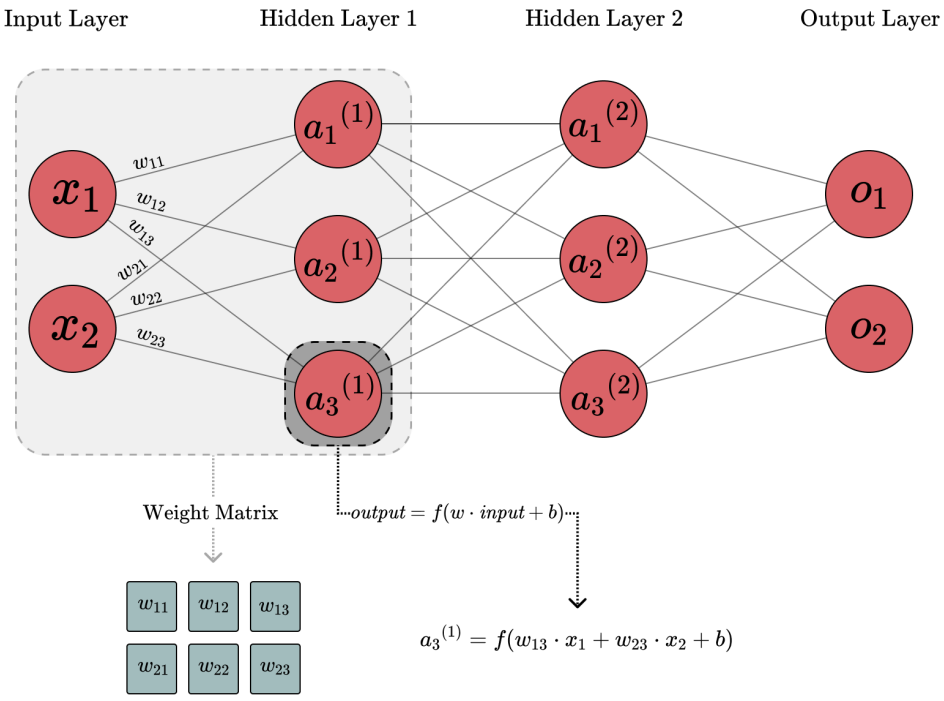


Figure 2.1: An example of a NN with two hidden dense layers, showing the connections between neurons in adjacent layers.

Mathematically, dense layers can be represented as:

$$a = f(W \cdot x + b)$$

where:

- x is the input vector, representing outputs from the previous layer (or initial input data for the first layer).
- W is the *weight matrix*, with each row corresponding to the weight vector w of a specific neuron.

- b represents the bias vector, where each scalar element corresponds to the bias of a specific neuron.
- f is the *activation function* that is applied element-wise.
- a refers to the output vector, representing the activations of all neurons.

This interconnectedness of dense layers introduces the inherent redundancy, or the over-parameterizedness of NNs [4]. It is particularly true in models with a large number of neurons, where W results in a vast number of parameters, which do not contribute to the model accuracy equally [10].

Convolutional layers are another type of hidden layers that involve a *convolution* operation on the input. Intuitively, a standard convolution is a process of sliding a small grid over an input to find patterns. The figure below, for example, shows the application of the Sobel kernel that detects edges on the input image.

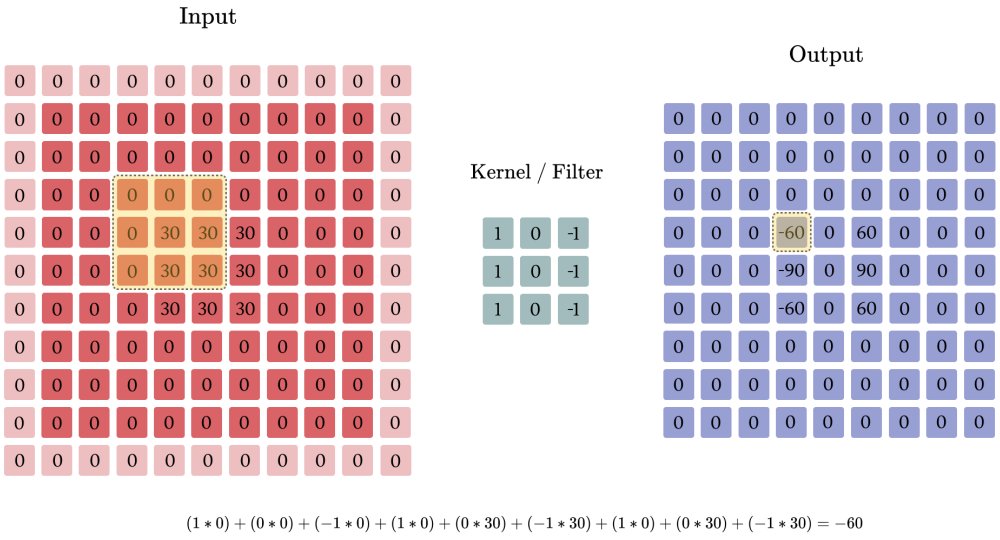


Figure 2.2: A 3×3 kernel (filter) sliding over a padded input matrix to compute the output feature map, demonstrating the interaction between the kernel weights and input values at a specific position.

For multi-channeled inputs, like RGB images, the convolution operation uses a multi-channeled kernel, as shown in Figure 2.3, producing a single-channeled feature map that combines weighted contributions from all input channels. A convolutional layer typically includes multiple such kernels, generating feature maps equal to the number of kernels. After the convolution operation generates the feature maps, a bias term is added to each map, and the activation function is applied element-wise — just like in dense layers.

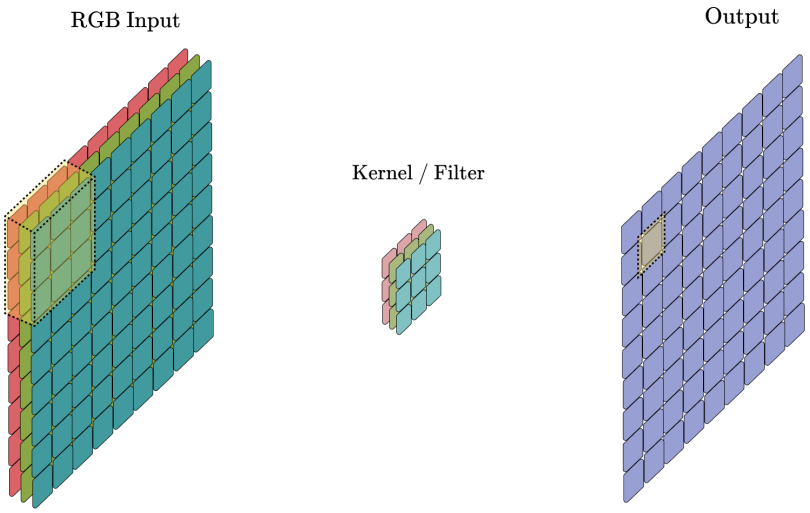


Figure 2.3: A 3×3x3 kernel (filter) sliding over an RGB input matrix to produce a single-channeled output feature map.

Mathematically, a convolutional layer can be represented as:

$$y_{i,j,k} = \phi\left(\sum_{m=1}^{M}\sum_{p=1}^{P}\sum_{q=1}^{Q} x_{i+p-1,j+q-1,m} \cdot w_{p,q,m,k} + b_k\right)$$

where:

- P, Q are the height and width of the filter, respectively.
- M is the number of input channels.
- $y_{i,j,k}$ denotes the output at position (i, j) for the k-th filter.
- $x_{i+p-1,j+q-1,m}$ is the input at position $(i + p - 1, j + q - 1)$ for the m-th input channel.
- $w_{p,q,m,k}$ represents the weight of the filter at position (p, q) for the m-th input channel and k-th filter.
- b_k is the bias for the k-th filter.
- $\phi(\cdot)$ is the activation function.

In simpler terms, a convolutional layer applies filter weights as it slides over rows (p), columns (q), and channels (m), sums the results, adds bias (b_k), and repeats this for all positions (i, j) and filters (k).

Although convolutional layers often have fewer weight parameters than dense layers in typical architectures, they still contain redundancies [9], presenting an opportunity for quantization. Thus, both dense and convolutional layers will be the focus of this work.

2.1.2 Loss Functions and Regularization

The weights and biases are usually *learnable parameters* that the model adjusts during *training*. The training process of NNs is similar to how our brains learn from mistakes. Given the ground truth, a NN adjusts its learnable parameters using a specific function that compares the ground truth with the output generated by the network, essentially measuring the magnitude of the network's errors.

This function is called a *loss function*, and depending on the type of question the network aims to answer, it can take many different forms. For example, for the MLP described in Figure 2.1 that generates a binary classification, we would use the *log loss* function. Since the datasets used in this thesis involve multi-class classification, the *sparse categorical cross-entropy* (SCCE) loss function will be used, which measures the difference between the predicted class probabilities and the true labels for each class in the dataset.

Often the loss function alone is not enough for a NN to perform well, as it may lead to overfitting or fail to capture desired generalization properties. This is why a *regularization term* that penalizes unwanted behaviours is added to the loss function.

A typical regularization term is L_2, which penalizes large weights by adding the sum of the squared weights to the loss. The modified loss function is then expressed as:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{data}} + \lambda \sum_i w_i^2$$

where:

- $\mathcal{L}_{\text{data}}$ is the original loss function (in our case, the SCCE loss function).
- λ is a scalar parameter that controls the strength of the regularization.
- w_i represents each individual weight value in the model.

The current work employs multiple custom regularization terms that encourage specific behaviors in the models while discouraging others. These terms will be discussed in detail in the Experimental Setup section 4.1.

2.1.3 Forward-Pass and Back-Propagation

The repetition of the mathematical operations described earlier in the Dense and Convolutional Layers subsection 2.1.1 during model training constitutes the *forward pass*. It is the process where input data is passed through the network layer by layer, with each layer applying its learned weights and biases to produce a final output.

As mentioned in the previous subsection, this output is then compared with the ground truth by the loss function that produces an error. This error is used to update the learnable parameters in W and b during a process called *back-propagation*.

In other words, back-propagation is the method by which the network adjusts its parameters to minimize the error. It calculates the gradient of the loss function with respect to each parameter using the chain rule. W and b are typically updated as follows:

$$W = W - \eta \frac{\partial L}{\partial W}, \quad b = b - \eta \frac{\partial L}{\partial b}$$

where L is the loss function, and η is the learning rate.
INSTEAD OF THIS WE NEED TO EXPLAIN HOW A CLASSICAL WEIGHT UPDATE LOOKS LIKE IN TENSORFLO ALSO ADD how the theory looks like in tensorflow so that it's easier to follow
For example, consider the weight $W_{I1,H1_1}$ represented as the line between *Input 1* and the hidden layer node $H1_1$ in Figure **??**. The gradient of this weight with respect to the loss is calculated using the chain rule:

$$\frac{\partial L}{\partial W_{I1,H1_1}} = \frac{\partial L}{\partial \text{Output 1}} \cdot \frac{\partial \text{Output 1}}{\partial H1_1} \cdot \frac{\partial H1_1}{\partial W_{I1,H1_1}}$$

Where:

- $\frac{\partial L}{\partial \text{Output 1}}$ is the gradient of the loss with respect to *Output 1*.
- $\frac{\partial \text{Output 1}}{\partial H1_1}$ is the gradient of *Output 1* with respect to the output of $H1_1$.
- $\frac{\partial H1_1}{\partial W_{I1,H11}}$ is the value of *Input 1*, since $H1_1$ is a weighted sum of the inputs.

This shows how each weight contributes to the final error during back-propagation.

2.2 Basics of Quantization

This section aims to answer the *why* question with respect to quantization and further provides a broader understanding of the term regarding its types.

2.2.1 Purpose and Definition

As we become increasingly dependent on deep learning models disguised as everyday tools, the need for these models to function in a resource- and time-efficient manner is more imperative than ever. The focus on resource efficiency is particularly important, with the research community expressing concerns regarding the environmental effects of large models, the exponential size growth of which continues to significantly outpace that of system hardware [22]. In this regard, studies have examined quantization within the context of Green AI as a method to reduce the carbon footprint of ML models [21].

Aside from the environmental considerations, the mere need to reduce the computational cost and speed of predictive models comes as an apparent business requirement. This requirement is essential when — quite ironically — embedded systems, famous for their compactness, meet ML models, infamous for their complexity. Microcontrollers, for instance, usually are not able to perform floating-point operations, which must therefore be emulated in software, introducing significant overhead. This is why quantization, the process which reduces the memory footprint of a model, is also extensively covered in the realm of embedded systems that inherently prefer integer arithmetic [1][17].

Another motivation for quantization — although somewhat controversial — is the fact that reducing the bit-width of ML models makes them robust to adversial attacks in certain cases [16]. This holds significant value in fields, such as autonomous driving, where model vulnerability may result in fatal outcomes. Interestingly enough, the use cases where such robustness is required also demand fast inference, as they rely on real-time predictions. Consider healthcare diagnostics needed for emergency scenarios or military defense mechanisms designed for immediate action.

The list of reasons why quantization is useful may go on for a while, but regardless of the motivation, the essence of the term itself — rooted in the early 20th century — remains unchanged: quantization refers to the division of a quantity into a discrete number of small parts [6]. With regard to ML models, it describes the process of dividing higher bit-width numbers into a discrete number of lower bit-width representations without causing significant degradation in performance [4].

Since ML models are generally considered redundant or over-parameterized, there are multiple points where quantization can be applied. Specifically, in this thesis, we apply quantization to the weights and biases of dense layers, as well as the kernels and biases of convolutional layers. Although not explicitly a part of a model, we also explore input data quantization. Other applications include, but are not limited to, layer activation and layer input quantization (two sides of the same coin), as well as gradient quantization. The bottom line is that wherever there is an opportunity for arithmetic or memory optimization, there is room for quantization.

2.2.2 Common Quantization Approaches

There is a multitude of ways to classify NN quantization methods, a broader overview of which will be covered in the Related Work chapter 5. For now, we will focus on a few selected approaches from the general categories of both *data-driven* and *data-free* methods [23] to provide a basic understanding of the NN quantization process.

The simplest form of data-free quantization, or *post-training quantization* [12], involves converting already trained parameters from FP32 to a lower bit-width format without using the initial training data. A common approach is to apply *uniform quantization* that maps real values to a set number of *bins*. The general formula can be written as:

$$Q(r) = round(\frac{r}{S})$$

Where:

- $Q(\cdot)$ denotes the quantization operation.
- r is the real value of a given model parameter in higher bit-width representation.
- $round(\cdot)$ is some rounding operation, such as a simple $floor(\cdot)$.
- S is a scaling factor.

As a result, we essentially end up with a discrete number of values in lower bit precision, instead of an almost continuous range of real numbers as shown in Figure 2.4.

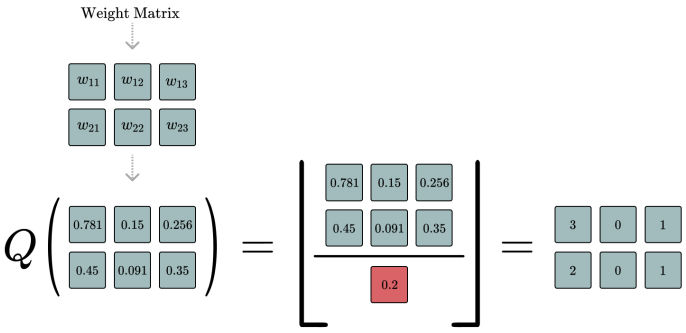
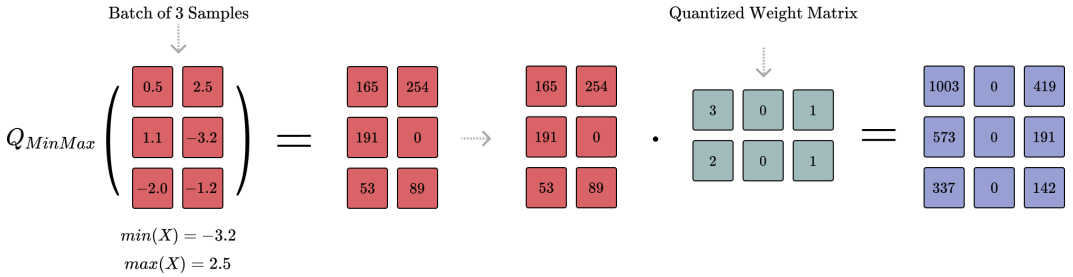


Figure 2.4: An example illustrating the quantization operation on the weight matrix from Figure 2.1, with arbitrary values for demonstration purposes.

Unlike data-free quantization — as the name suggests — data-driven quantization typically involves retraining the model using the initial data. An example of this approach is the Ristretto framework [7], which, similar to data-free methods, first analyzes the trained model to select suitable lower bit-width number formats for its weights. Then,

using a portion of the original dataset, the framework determines appropriate formats for layer inputs and outputs. As a next step, based on the validation data, Ristretto adjusts the quantization settings to achieve optimal performance under the given constraints. Finally, the quantized model is fine-tuned using the training data.

A much simpler example could be the min-max quantization on input data as shown in Figure 2.5. This method is used by Tensorflow Lite as part of its post-training quantization process.



$$Q_{MinMax}(x) = \lfloor \frac{x - min(X)}{s} \rfloor$$

$$s = \frac{max(X) - min(X)}{2^8 - 1} = \frac{2.5 - (-3.2)}{255} \approx 0.0224$$

Figure 2.5: An example illustrating min-max quantization of input data to 8 bits, followed by matrix multiplication with the quantized weight matrix from Figure 2.4. Input data has arbitrary values for demonstration purposes.

- In **static quantization**, quantization parameters are fixed before model inference, based on the data observed during training or calibration. This corresponds to Post-Training Quantization (PTQ), which directly quantizes the trained floating-point model [12], using various discretization approaches based on the range and distribution of the parameters being quantized, as well as the level of granularity at which the quantization values are applied.

- In **dynamic quantization**, the quantization parameters are calculated dynamically during inference. This typically applies to activations, as their range changes depending on the input data and, unlike that of the weights, cannot be precomputed with static quantization [14].

- In **learned quantization**, quantization parameters are learned as part of the model training process. This corresponds to Quantization Aware Training (QAT) [11], where quantization is integrated directly into training rather than applied

afterwards. Since learned quantization is central to this work, a detailed review of QAT and its applications is provided in the Related Work chapter.

2.3 Learned Quantization

Now that the fundamentals of quantization have been covered, this section introduces key concepts commonly encountered in learned quantization, including its challenges, trade-offs, and the popular techniques used to overcome them.

2.3.1 Strategies and Applications

This

2.3.2 Trade-offs and Challenges

THIS PART WILL GO TO THE NEXT SECTION:

An example approach is to define a regularization term that directly penalizes large differences between full-precision values and their quantized counterparts [25]. This can encourage the model to learn parameters that are easily quantizable without significant performance loss. If the values that are being quantized are W, then this regularization term could look like:

$$\mathcal{L}_{\text{quant}} = \lambda \sum_{i} \|W_i - q(W_i)\|^2$$

Where:

- λ is a scalar that controls the importance of the quantization penalty.
- W_i represents the full-precision weight value before quantization at index i.
- $q(W_i)$ represents the quantized version of W_i.

The current work uses multiple custom regularization terms that trigger the quantization process during training. These will be discussed in detail in the Experimental Setup section.

3 Learned Quantization

This chapter presents the custom methods of learned quantization developed to address the challenges posed by non-differentiability, while enabling the model to make informed decisions on whether to proceed with quantization or revert to preserve performance. The first section will discuss the *custom quantization layers* written in Tensorflow that can easily be integrated to existing workflows and directly deal with gradient calculation. The next section provides details on the *custom loss functions* as an alternative approach to learned quantization.

This chapter elaborates on the problem that this thesis tries to solve and explains the individual methods used for solving the problem.

3.1 Custom Quantization Layers

In this section, we introduce custom layers built upon Tensorflow's `tf.keras.Layer` class, which serves as the base for all Keras layers. Each custom layer also leverages Tensorflow's `tf.custom_gradient` decorator to define its own gradient computation. For clarity, the upcoming subsections start by showing how to define the corresponding standard, non-quantized layer using `tf.keras.Layer` and `tf.customg_gradient`, then move on to the specific quantized implementations.

3.1.1 Data Quantization Layer

3.1.2 Quantized Dense Layer

3.1.3 Quantized Convolutional Layer

3.2 Custom Loss Functions

3.2.1 Penalty for Inverse Scale Factor Magnitude

3.2.2 Constraint on Bin Count for Quantization

3.2.3 Deviation between Quantized and Original Values

4 Experiments

This chapter provides details about the experiments conducted within the context of this thesis.

You'll need these: there's a formula for precision requirement in [13]

4.1 Experimental Setup

All experiments are caried out on machine XYZ.

4.1.1 Software Setup

4.1.2 Hardware Setup

4.2 Hyperparamter Tuning

4.2.1 Learning Rate and Regularization Coefficients

4.2.2 Quantization Penalty Coefficient

4.3 Dataset-Specific Results

4.3.1 MNIST

4.3.2 CIFAR10

4.3.3 Imagenette

5 Related Work

A significant amount of scientific work has been done on QAT. This research can be categorized based on different characteristics, which are covered separately in the following paragraphs.
Model architecture.
RNN - [18]
CNN - [20]
CNN - [2] DNN - [5]
Quantization target parameters.
weights and activations - [15]
weights and activations - [10]
weights - [19]
weigths - [18]
binary weights and input activations - [20]
gradients - [24] layer inputs and weights - [23]
Granularity of quantization.
Handling of differentiability.
Quantization precision.
binary weights and input activations - [2]
binary weights and activations - [10]
binary weights and input activations - [20]
ternary weights - [18]
higher precision for more important parameters and lowe precision for less important ones - [13]
Integration with pruning & other techniques.
pruning and Huffman Codign - [8]
distillation - [19]
higher precision for more important parameters and lowe precision for less important ones or pruning - [13]
Modifications to loss functions. regularization term WaveQ - [3]
Other interesting approaches. k-means for parameters [5]

6 Conclusions

This chapter summarizes the contriubtions of the thesis and provides an outlook into future work.

List of Acronyms

ML	Machine Learning

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Appendix

Add additional experimental results that do not need to be directly included in the thesis body.