

Use weighted loss function to solve imbalanced data classification problems



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Imbalanced datasets are a common problem in classification tasks, where number of instances in one class is significantly smaller than number of instances in another class. This will lead to biased models that perform poorly on minority class.



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A weighted loss function is a modification of standard loss function used in training a model. The weights are used to assign a higher penalty to misclassifications of minority class. The idea is to make model more sensitive to minority class by increasing cost of misclassification of that class.

The most common way to implement a weighted loss function is to assign higher weight to minority class and lower weight to majority class. The weights can be inversely proportional to frequency of classes, so that minority class gets higher weight and majority class gets lower weight.

In this post, I will show you how to add weights to pytorch's common loss functions

Binary Classification

`torch.nn.BCEWithLogitsLoss` function is a commonly used loss function for binary classification problems, where model output is a probability value between 0 and 1. It combines a sigmoid activation function with a binary cross-entropy loss.

$$\ell(x, y) = L = \{l_1, \dots, l_N\}^\top, \quad l_n = -w_n [y_n \cdot \log \sigma(x_n) + (1 - y_n) \cdot \log(1 - \sigma(x_n))]$$

For imbalanced datasets, where number of instances in one class is significantly smaller than other, `torch.nn.BCEWithLogitsLoss` function can be modified by adding a weight parameter to loss function. The weight parameter allows to assign different weights for the positive and negative classes.

The weight parameter is a tensor of size `[batch_size]` that contains weight value for each sample in the batch.

Here is an example:

```
import torch
import torch.nn as nn

# Define the BCEWithLogitsLoss function with weight parameter
weight = torch.tensor([0.1, 0.9]) # higher weight for positive class
criterion = nn.BCEWithLogitsLoss(weight=weight)

# Generate some random data for the binary classification problem
input = torch.randn(3, 1)
target = torch.tensor([[0.], [1.], [1.]])

# Compute the loss with the specified weight
loss = criterion(input, target)

print(loss)
```

we set weight of positive class to 0.9 and weight of negative class to 0.1. `input` tensor contains logits predicted by model. `target` tensor contains ground-truth labels for binary classification problem.

Note: Set weights manually to 0.1 and 0.9, based on assumption that positive class has only 10% of the samples.

To calculate weights, you can compute weight for each class as:

```
weight_for_class_i = total_samples / (num_samples_in_class_i * num_classes)
```

where `total_samples` is total number of samples in dataset, `num_samples_in_class_i` is number of samples in class `i`, and `num_classes` is total number of classes (in the case of binary classification, `num_classes` is 2).

If you have a binary classification problem with 1000 samples, where 900 samples belong to class 0 and 100 samples belong to class 1, calculate weights as:

```
weight_for_class_0 = 1000 / (900 * 2) = 0.5556  
weight_for_class_1 = 1000 / (100 * 2) = 5.0000
```

and the weight parameter of `torch.nn.BCEWithLogitsLoss` to a tensor of size 2 weights is:

```
import torch  
import torch.nn as nn  
  
weight = torch.tensor([0.5556, 5.0000]) # higher weight for class 1  
criterion = nn.BCEWithLogitsLoss(weight=weight)
```

Note: specific formula and method for calculating weights can depend on problem and dataset, and there may be other approaches to consider, such as using resampling techniques or other loss functions that are designed to handle class imbalance.

In addition to `weight` parameter, `torch.nn.BCEWithLogitsLoss` also has a `pos_weight` parameter, which is a simpler way to specify weight for positive class in a binary classification problem.

The `pos_weight` parameter is a scalar that represents weight for positive class. It is equivalent to setting `weight` parameter to `[1, pos_weight]`, where weight for negative class is 1.

```
import torch
import torch.nn as nn

# Define the BCEWithLogitsLoss function with pos_weight parameter
pos_weight = torch.tensor([3.0]) # higher weight for positive class
criterion = nn.BCEWithLogitsLoss(pos_weight=pos_weight)

# Generate some random data for the binary classification problem
input = torch.randn(3, 1)
target = torch.tensor([[0.], [1.], [1.]])

# Compute the loss with the specified pos_weight
loss = criterion(input, target)

print(loss)
```

Set `pos_weight` parameter to 3.0, means weight for positive class is 3 times of negative class. We compute loss using `criterion` function with specified `pos_weight`.

If you specify both `weight` and `pos_weight` parameters, `pos_weight` parameter takes precedence over `weight` for positive class.

If you set `pos_weight` to a value other than 1.0, weight for positive class in `weight` tensor will be ignored.

Multi-class Classification

Cross-Entropy Loss is commonly used in multi-class classification problems. It calculates negative log-likelihood of predicted class distribution compared to true class distribution. When dealing with imbalanced datasets, some classes might have more or fewer samples than others, and this can lead to a bias in model's predictions towards the more frequent classes.

$$\ell(x, y) = L = \{l_1, \dots, l_N\}^\top, \quad l_n = -w_{y_n} \log \frac{\exp(x_{n,y_n})}{\sum_{c=1}^C \exp(x_{n,c})} \cdot 1\{y_n \neq \text{ignore_index}\}$$

To address this issue, `weight` parameter in `torch.nn.CrossEntropyLoss` can be used to apply a weight to each class. The weights can be specified as a 1D Tensor or a list and should have same length as the number of classes. The loss is then calculated as follows:

$$\text{loss}(x, y) = -\text{weight}[y] * \log(\exp(x[y]) / \text{sum}(\exp(x)))$$

where x is model's output, y is target class, \exp is exponential function, and $\text{sum}(\exp(x))$ is sum of exponentials over all classes. The weight for true class is multiplied with negative log-likelihood of true class, so loss is up weighted for underrepresented classes.

Here's an example of using `weight` parameter in `torch.nn.CrossEntropyLoss` for a classification problem with three imbalanced classes.

Suppose we have a dataset with 1000 samples, and target variable has three classes: Class A, Class B, and Class C. The distribution of samples in dataset is as follows:

- Class A: 100 samples
- Class B: 800 samples
- Class C: 100 samples

To address class imbalance, we can assign a weight to each class that inversely proportional to its frequency. The weight of each class can be calculated as follows:

- Class A: $1000 / 100 = 10$
- Class B: $1000 / 800 = 1.25$
- Class C: $1000 / 100 = 10$

We can create a weight tensor that reflects these weights as follows:

```
import torch
```

```
weights = torch.tensor([10, 1.25, 10])
```

And use this weight tensor in `torch.nn.CrossEntropyLoss` as follows:

```
loss_fn = torch.nn.CrossEntropyLoss(weight=weights)
```

When we use this loss function to train a model, Classes A and C will contribute more to loss than Class B, due to up weighted effect of weight tensor. This helps to balance effect of different classes on model's training and can improve model's performance on the underrepresented classes.

In PyTorch's `torch.nn.CrossEntropyLoss`, `label_smoothing` parameter is used to smooth one-hot encoded target values to encourage model to be less confident in its predictions and prevent overfitting to training data.

This smoothing is achieved by adding a small value (i.e., smoothing factor) to off-diagonal elements of one-hot encoded target values and subtracting this same value from diagonal elements. This has effect of reducing confidence of model's predictions and encouraging it to explore a wider range of solutions.

`label_smoothing` parameter take a value between 0 and 1, 0 means no smoothing is applied, and 1 means maximum smoothing is applied. A typical value for `label_smoothing` is around 0.1. The loss is then calculated as follows:

```
loss(x, y) = -((1 - label_smoothing) * log(exp(x[y]) / sum(exp(x)))) + (label_sm
```

x is model's output, y is target class, \exp is exponential function, $\sum(\exp(x))$ is sum of exponentials over all classes, and K is number of classes. The smoothing factor is multiplied by a uniform prior probability for each class, which is equal to $1/K$, and achieve more generalized model.

Both `label_smoothing` and `weight` parameters can be used to address issues related to class imbalance and overfitting in multi-class classification problems. However, these two parameters work in different ways and have different use cases.

`weight` parameter is used to apply a weight to each class in loss calculation, which can be useful when dealing with imbalanced datasets. The weight for true class is multiplied with negative log-likelihood of true class, so loss is upweighted for underrepresented classes. `weight` parameter does not affect predicted probabilities or model's confidence in its predictions, but rather adjusts weight assigned to each class in loss calculation.

`label_smoothing` parameter is used to smooth one-hot encoded target values to encourage model to be less confident in its predictions and prevent overfitting to training data. Smoothing is achieved by adding a small value (i.e., smoothing factor) to off-diagonal elements of one-hot encoded target values and subtracting this same value from diagonal elements. This has effect of reducing confidence of the model's predictions and encouraging it to explore a wider range of solutions.

`label_smoothing` parameter does not affect weight assigned to each class in loss calculation, but rather adjusts the target values used in loss calculation.

In general, `weight` parameter is useful when dealing with imbalanced datasets, where the cost of misclassification is not same for all classes. On other hand,

`label_smoothing` parameter is useful when dealing with overfitting and highly confident predictions, where model is too confident in its predictions and is not exploring a wide range of solutions.

both `weight` and `label_smoothing` parameters can be used together to address both class imbalance and overfitting issues in multi-class classification problems.

However, two parameters may not always be used together and their use depends on specific characteristics of the dataset and problem at hand. It's important to experiment with different combinations of hyperparameters, including `label_smoothing` and `weight`, to determine best approach for a given problem.

Multilabel classification

Multilabel classification is a type of classification problem where an object or instance can belong to one or more classes simultaneously. In other words, instead of assigning a single label to each instance, multiple labels can be assigned to it.

This is in contrast to traditional classification problems, where each instance is assigned a single label.

Binary Cross-Entropy Loss commonly used in binary classification problems, but can also be used in multilabel classification by treating each label as a separate binary classification problem. It measures the difference between the predicted probabilities and actual labels for each class separately.

we can set the `weight` parameter, and `pos_weight` like Binary Classification do.

In summary

Imbalanced datasets are a common problem in machine learning, where one class of data may be significantly more prevalent than another. This can lead to issues when trying to train a classification model, as model may become biased towards more prevalent class. One solution to this problem is to use a weighted loss function during training. A weighted loss function assigns a higher weight to errors made on the minority class, thereby helping model to pay more attention to these samples. By using a weighted loss function, model can learn to better distinguish between the minority and majority classes, leading to improved performance on imbalanced datasets.

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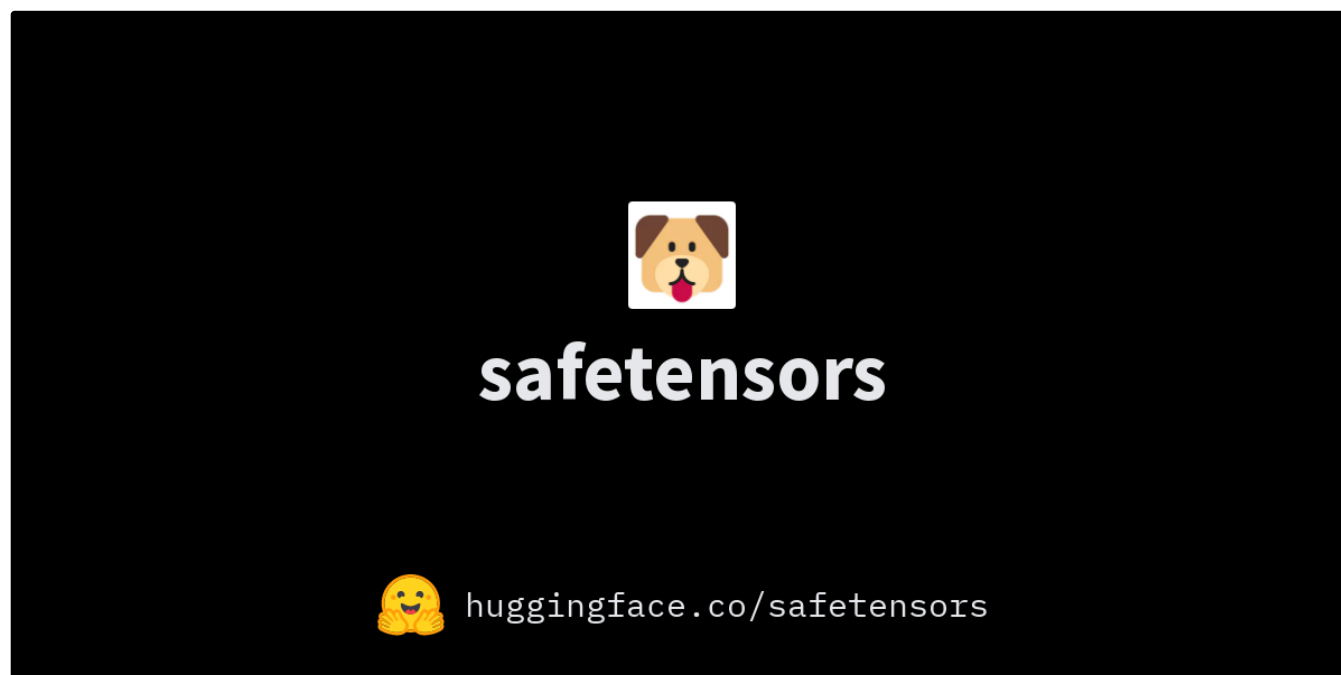


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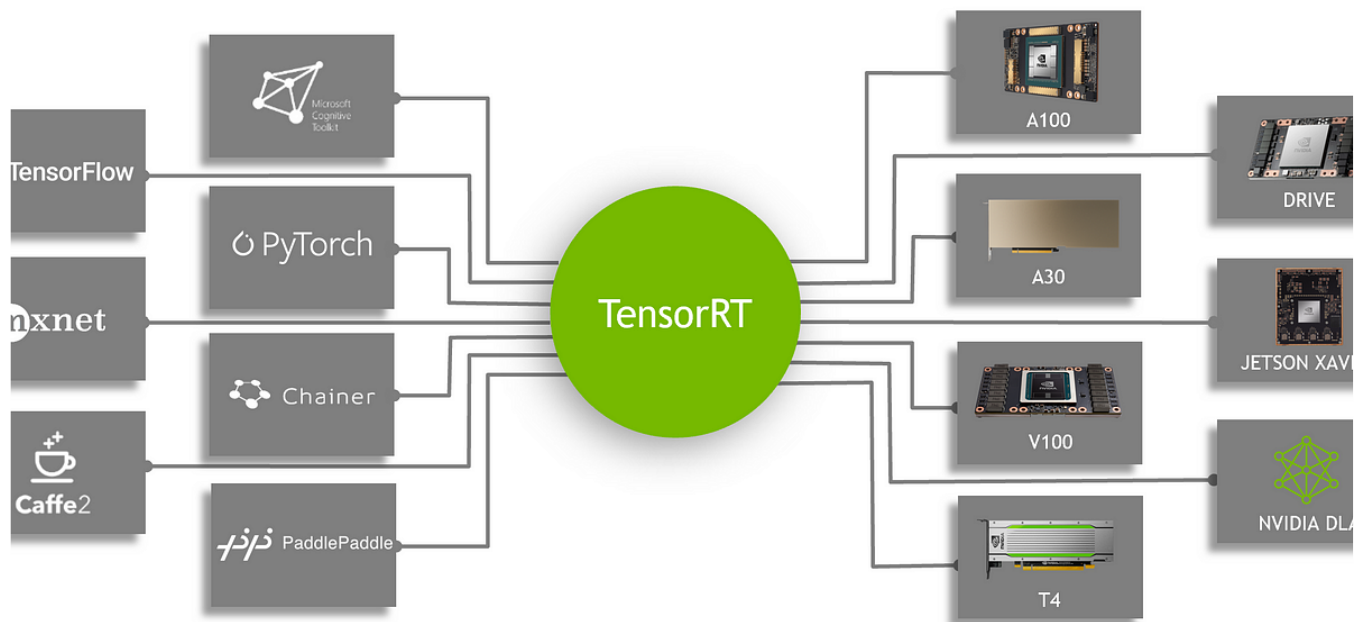
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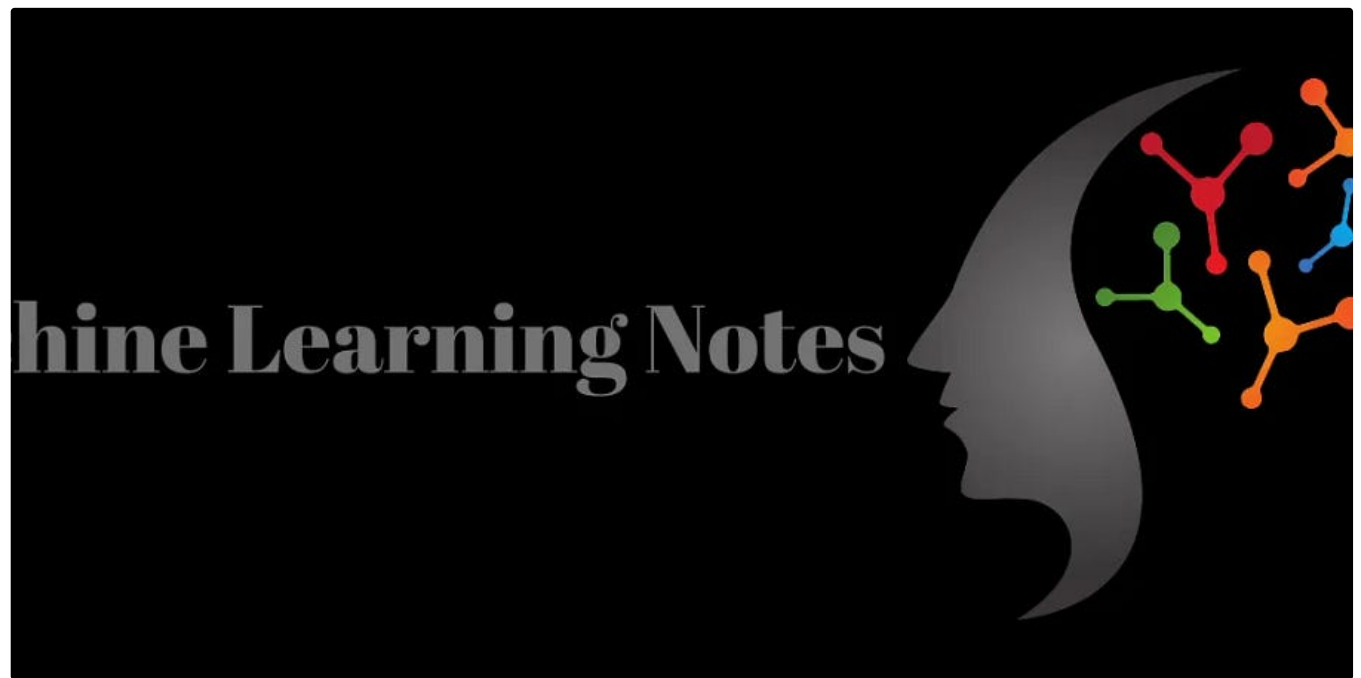
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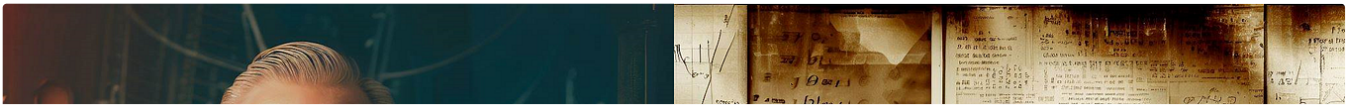
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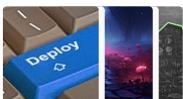
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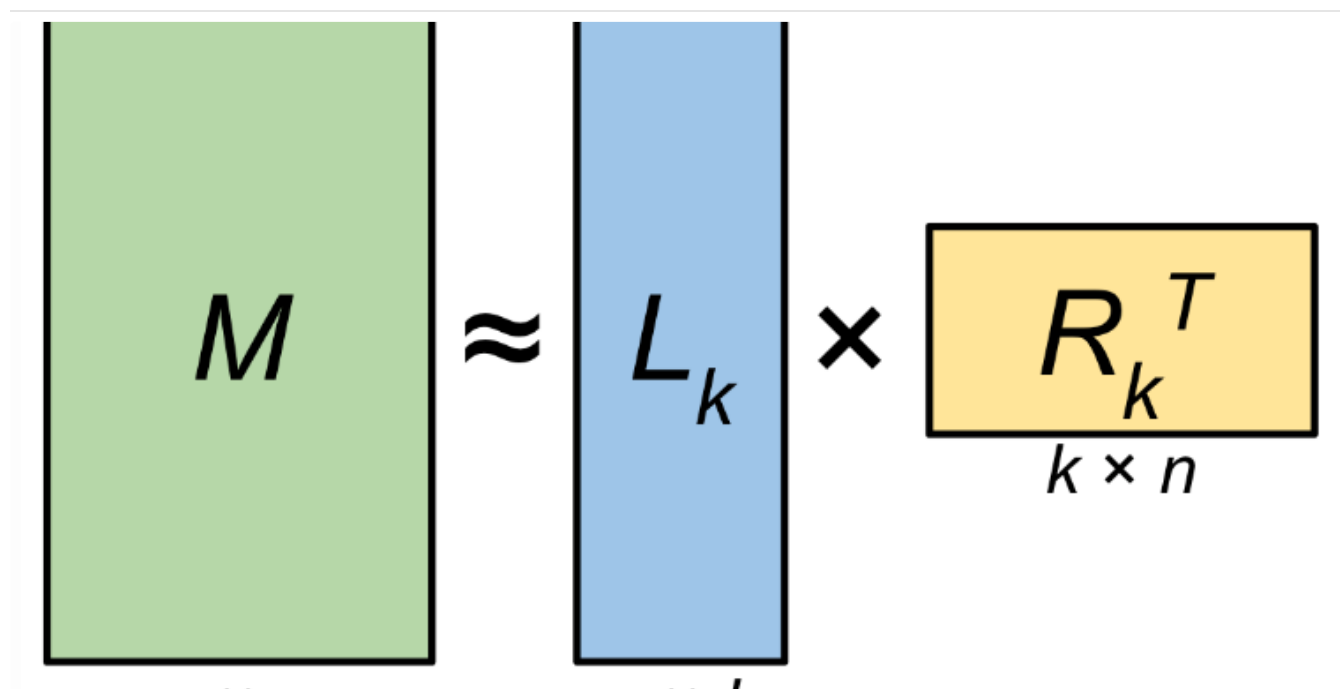
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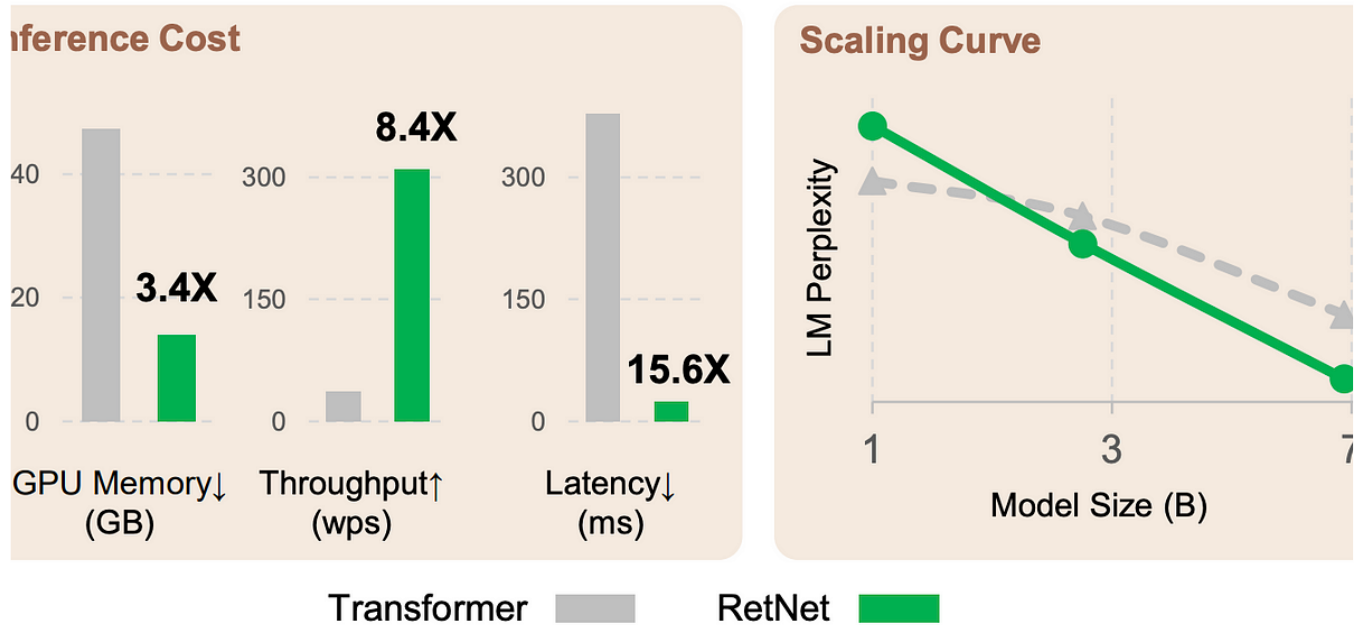
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