Efficient Computation of Hessian Matrices in TensorFlow

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1 Introduction

The Hessian matrix has a number of important applications in a variety of different fields, such as optimization, image processing and statistics. Geometrically, the Hessian matrix describes the local curvature of scalar functions \( f : \mathbb{R}^p \rightarrow \mathbb{R} \), and is for this reason perhaps mostly known in the field of optimization \([5]\). Nevertheless, the Hessian matrix also has an important role in statistics, since its inverse is related to the powerful concept of uncertainty approximation \([6]\).

In this paper we mostly focus on the practical aspects of efficiently computing Hessian matrices in the context of deep learning \([4]\) using the Python \([7]\) scripting language and the TensorFlow \([1]\) library. We define a general feed-forward neural network model and show how to efficiently compute two quantities: the cost function’s exact Hessian matrix, and the cost function’s approximate Hessian matrix, known as the Outer Product of Gradients (OPG) matrix. Although we here use a feed-forward neural network architecture to introduce terminology, the theory and implementation presented is still directly applicable on more general neural network architectures using convolutional layers, pooling and regularization.

The paper is organized as follows: In Section 2 we give definitions which will be used throughout the paper. In Section 3 we present the problem statement, and discuss three complications which need to be dealt with in order to achieve a successful TensorFlow implementation: 1) \( \text{tf.hessians}() \) is fundamentally inadequate since it only calculates a subset of all the partial derivatives (Section 3.3), 2) computing Hessian matrices essentially requires per-example gradients of the cost function with respect to model parameters, and unfortunately, the differentiation functionality provided by TensorFlow does not support computing gradients with respect to individual examples efficiently \([2]\) (Section 3.1), and 3) when differentiating a function with respect to several variables represented by a
list of tensors, the result is also a list of
tensors (Section 3.2). In Section 4 we
show how to overcome the aforemen-
tioned complications and introduce our
Python module pyhessian [8] which is
released as open source licensed under
GNU GPL on GitHub. In Section 5
we summarize the paper and give some
concluding remarks.

2 Definitions

A feed-forward neural network is shown in Figure 1. There are L layers \( l = 1, 2, \ldots, L \) with \( T_l \) neurons in each layer. The input layer \( l = 1 \), is represented by the input vector \( x_n = [x_{n,1} \ x_{n,2} \ \ldots \ x_{n,T_1}]^T \) where \( n = 1, 2, \ldots, N \) is the input index. Furthermore, there are \( L - 2 \) dense hidden layers, \( l = 2, 3, \ldots, L - 1 \), and a dense output layer \( l = L \), all represented by weight matrices \( W^{(l-1)} \in \mathbb{R}^{T_{l} \times T_{l-1}} \), bias vectors \( b^{(l)} \in \mathbb{R}^{T_{l}} \) and vectorized activation functions \( \sigma^{(l)} \).

Let the cost function \( C \) coincide with TensorFlow’s built-in softmax cross-entropy function

\[
C = \frac{1}{N} \sum_{n=1}^{N} C_n(y_n, \hat{y}_n) = \frac{1}{N} \sum_{n=1}^{N} \left( -\sum_{m=1}^{T_1} y_{n,m} \log \hat{y}_{n,m} \right). \tag{1}
\]

It is defined as the average of \( N \) per-example cross-entropy cost functions \( C_n(y_n, \hat{y}_n) \), where \( y_n \) represents the one-hot target vector for the \( n \)th example, and where \( \hat{y}_n \) represents the corresponding prediction vector. The prediction vector is obtained by evaluating the model function \( \sigma^{(L)} \).

\[
1 \text{TensorFlow API r1.13: tf.losses.softmax_cross_entropy()}
\]
\[ y_n = f(x_n, \omega) = \sigma^{(L)}(W^{(L-1)}\sigma^{(L-1)}(\cdots \sigma^{(2)}(W^{(1)}x_n + b^{(2)}) + \cdots) + b^{(L)}) \]  

(3)

using the input vector \( x_n \) and a flat vector of model parameters \( \omega \in \mathbb{R}^P \) defined by

\[ \omega = [\omega_1 \ \omega_2 \ \ldots \ \omega_P]^T \quad (4) \]

The function flatten(\( \cdot \)) denotes a row-wise flattening operation to transform the collection of model parameters represented by the weight matrices \( W^{(l-1)} \) and bias vectors \( b^{(l)} \), \( l = 2, 3, \ldots, L \) into a flat column vector of dimension \( P = T_1T_2+T_2+\ldots+T_{L-1}T_L+T_L \). Finally, the activation function in the output layer is the vectorized softmax function

\[ \sigma^{(L)}(z) = \text{softmax}(z) \quad (6) \]

\[ = \frac{\exp(z)}{\sum_{m=1}^{T_L} \exp(z_m)}, \quad (7) \]

where \( z \in \mathbb{R}^{T_L} \), and where \( \exp(\cdot) \) denotes the vectorized exponential function.

3 Computing Hessian Matrices in TensorFlow

Given the cost function \( C \) defined in Section 2, the Hessian matrix \( H \in \mathbb{R}^{P \times P} \) is defined \(^2\)

\[ H = \frac{\partial^2 C}{\partial \omega \partial \omega^T} \quad (8) \]

\[ = \frac{1}{N} \sum_{n=1}^{N} \frac{\partial^2 C_n}{\partial \omega \partial \omega^T}, \quad (9) \]

The approximation to the Hessian matrix, known as the Outer Product of Gradients (OPG) matrix \( G \in \mathbb{R}^{P \times P} \), is defined

\[ G = \frac{1}{N} \sum_{n=1}^{N} \frac{\partial C_n}{\partial \omega} \frac{\partial C_n^T}{\partial \omega} \quad (10) \]

\[ = \frac{1}{N} \begin{bmatrix} \frac{\partial C_1}{\partial \omega} & \frac{\partial C_2}{\partial \omega} & \cdots & \frac{\partial C_N}{\partial \omega} \end{bmatrix} \]

\[ \begin{bmatrix} \frac{\partial C_1^T}{\partial \omega} & \frac{\partial C_2^T}{\partial \omega} & \cdots & \frac{\partial C_N^T}{\partial \omega} \end{bmatrix} \]

\[ = \frac{1}{N} \begin{bmatrix} \frac{\partial C}{\partial \omega} \frac{\partial C^T}{\partial \omega} \end{bmatrix}. \quad (11) \]

We notice that \( H \) in Equation (9) is formed by summing over \( N \) per-example Hessian matrices, and that \( G \) in Equation (10) is formed by summing over \( N \) per-example OPG matrices. We also note that \( H \) can be obtained by differentiating the cost function directly, whereas this property does not hold for \( G \) as seen by (12). Finally, we note that \( G \) can be written as a per-example cost Jacobian matrix product (11).

In order to proceed, we now need to consider three complications regarding gradients and Hessians in TensorFlow: the limitations of TensorFlow’s built-in tf.hessians() function is discussed in Section 3.3, per-example gradients will be discussed in Section 3.1, and gradient representation will be discussed in Section 3.2.

3.1 Per-Example Gradients

A per-example gradient of the cost function with respect to model parameters means to differentiate \( C_n \) in (9) and (10) with respect to model parameters

\(^2\)The notation used means that \( H_{i,j} = \frac{\partial^2 C}{\partial \omega_i \partial \omega_j} \).
for a single example \( n \). However, when TensorFlow computes gradients (e.g. \texttt{tf.gradients()}), it performs back propagation, which never actually computes the per-example gradients, but instead directly obtains the sum of per-example gradients. To see what this means, consider the following dummy multiple linear regression model (for simplicity with no bias term):

```python
In [1]: import tensorflow as tf
In [2]: import numpy as np
In [3]: W = tf.Variable([3., 4., 5., 2.])
In [4]: X = tf.placeholder('float32', shape=(None, 4))
In [5]: yhat = tf.tensordot(X, W, axes=1)
In [6]: init = tf.global_variables_initializer()
In [7]: sess = tf.InteractiveSession()
In [8]: sess.run(init)

We have model parameters represented by the variable tensor \( W \) (In [3]), and we use the placeholder tensor \( X \) (In [4]) as the model input. For simplicity, we do not define a cost function here, but instead conduct several differentiation experiments directly on the scalar model function \( yhat \) (In [5]) with \( N = 2 \):

```python
In [9]: sess.run(yhat, feed_dict={x: np.array([[1., 2., 3., 4.], [2., 3., 4., 5.]])})
```

Out [1]: array([34., 48.], dtype=float32)

We get back two values (Out [1]) corresponding to the two inner products as expected. We now take the gradient of the model function with respect to the model parameters for a single example:

```python
In [10]: sess.run(tf.gradients(yhat, W),
              feed_dict={x: np.array([[1., 2., 3., 4.]])})
```

Out [2]: [array([1., 2., 3., 4.], dtype=float32)]

We get back the per-example gradient as expected (Out [2]). We do the same for the second example:

```python
In [11]: sess.run(tf.gradients(yhat, W),
              feed_dict={x: np.array([[2., 3., 4., 5.]])})
```

Out [3]: [array([2., 3., 4., 5.], dtype=float32)]

But when we try to feed two examples:

```python
In [12]: sess.run(tf.gradients(yhat, W),
              feed_dict={x: np.array([[1., 2., 3., 4.],
                                     [2., 3., 4., 5.]])})
```

Out [4]: [array([3., 5., 7., 9.], dtype=float32)]

we notice that we do not get back two per-example gradients, but rather the sum of the two per-example gradients (Out [4]). The important observation is here that in order to obtain per-example gradients we seemingly need to run \texttt{tf.gradients()} once per example, which in turn is well known to be very inefficient when \( N \) grows large. We will get back to this and discuss solutions in Sections (4.1) and (4.2).
3.2 Gradient Representation

In practice, the $P$ model parameters are represented by a list of tensors (e.g. `[tf.Variable(),...]`) corresponding to the different layers of the model architecture. On the other hand, the Hessian matrix is only one $(P, P)$-shaped tensor (matrix) formed by every single variable element contained in the list of variable tensors.

When differentiating a function represented by a computational graph with respect to some variable(s) in that graph, the variable tensors we pass to the differentiation function (`tf.gradients()`) must be kept in their original form as upon defining the graph. One can still pass on the whole collection of variables as a list to get hold of the full gradient, but the result will not be a flat gradient vector – it will rather be a list of sub-gradients represented by multiple tensors. This means that in order to end up with the $(P, P)$-shaped Hessian matrix we want, we need to keep all the variables in a list during differentiation, and only afterwards reshape the result into the desired flat form.

3.2.1 Flattening of Gradients

To illustrate the concept of lists of sub-gradients vs. flat gradients, consider a dummy multinomial logistic regression model:

In [13]: `import tensorflow as tf`
In [14]: `T1 = 64`
In [15]: `T2 = 32`
In [16]: `P = T1*T2 + T2 # Total number of model parameters`
In [17]: `W = tf.Variable(tf.ones((T1, T2)), 'float32')`
In [18]: `b = tf.Variable(tf.ones((T2,)), 'float32')`
In [19]: `params = [W, b]`
In [20]: `params`  
Out [5]: [<tf.Variable 'Variable... shape=(64, 32) ...'>,
<tf.Variable 'Variable... shape=(32,) ...'>]
In [21]: `X = tf.placeholder(dtype='float32', shape=(None, T1))`
In [22]: `y = tf.placeholder(dtype='float32', shape=(None, T2))`
In [23]: `def model_fun(X, params):
               return tf.add(tf.matmul(X, params[0]), params[1])`
In [24]: `yhat_logits = model_fun(X, params)`
In [25]: `yhat = tf.nn.softmax(yhat_logits)`
In [26]: `def cost_fun(y, yhat_logits, params):
               return tf.losses.softmax_cross_entropy(y, yhat_logits)`
In [27]: `cost = cost_fun(y, yhat_logits, params)`

We thus have model parameters $W$ (In [17]) and $b$ (In [18]) with shapes $(T1, T2)$ and $(T2,)$, respectively. We can differentiate the cost function represented by the tensor `cost` (In [27]) with respect to the individual variables, or the full list `params` (In [19]):

In [28]: `tf.gradients(cost, W)`  
Out [6]: [<tf.Tensor 'gradients... shape=(64, 32) ...'>]
In [29]: `tf.gradients(cost, b)`  
Out [7]: [<tf.Tensor 'gradients... shape=(32,) ...'>]
In [30]: `tf.gradients(cost, params)`  
Out [8]: [<tf.Tensor 'gradients... shape=(64, 32) ...'>]
But if we try to reshape our parameters into a flat vector and then differentiate:

```python
In [31]: params_flat = tf.concat([tf.reshape(W, [-1]), b], axis=0)
In [32]: params_flat
Out [9]: <tf.Tensor 'concat...shape=(2080,)...'>
In [33]: tf.gradients(cost, params_flat)
Out [10]: [None]
```

We get [None] (Out [10]) because the new tensor `params_flat` (In [31]) is not part of the `cost` function graph (In [27]). We solve the issue by first differentiating with respect to the full list, and then flattening the resulting tensor:

```python
In [34]: grads = tf.gradients(cost, params)
In [35]: grads
Out [12]: [<tf.Tensor 'gradients...shape=(64, 32)...'>,
        <tf.Tensor 'gradients...shape=(32,)...'>]
In [36]: grads_flat = tf.concat([tf.reshape(grads[0], [-1]), grads[1]], axis=0)
In [37]: grads_flat
Out [13]: <tf.Tensor 'concat...shape=(2080,) dtype=float32'>
```

### 3.3 The built-in TensorFlow function `tf.hessians()`

The fundamental question is, why can we not simply use the built-in TensorFlow function `tf.hessians()`? To see why, consider the following:

```python
In [38]: tf.hessians(cost, params)
Out [14]: [<tf.Tensor 'Reshape...shape=(64, 32, 64, 32)...'>,
        <tf.Tensor 'Reshape...shape=(32, 32)...'>]
```

We observe that we get back two tensors (Out [14]). Let us name the two $H_U$ and $H_L$, respectively. Their respective shapes are $(T1, T2, T1, T2)$ and $(T2, T2)$. Firstly, if we reshape $H_U$ into a $(T1 \times T2, T1 \times T2)$-shaped tensor, it will correspond to the full Hessian’s upper block diagonal matrix $\in \mathbb{R}^{T1 \times T2 \times T1 \times T2}$. Secondly, the tensor $H_L$ corresponds to the full Hessian’s lower block diagonal matrix $\in \mathbb{R}^{T2 \times T1 \times T2 \times T1}$. In other words, we get no information about the full Hessian’s two off-diagonal block matrices $\in \mathbb{R}^{T1 \times T2 \times T2}$ and $\mathbb{R}^{T2 \times T1 \times T2}$. Equation (13) illustrates the concept.

\[
H = \begin{bmatrix}
H_U & ? \\
? & H_L
\end{bmatrix}
\in \mathbb{R}^{T1 \times T2 \times T1 \times T2} \quad \forall \in \mathbb{R}^{T2 \times T1 \times T2} \quad \forall \in \mathbb{R}^{T1 \times T2 \times T2}
\]  

The two missing off-diagonal block matrices represented by question marks in Equation (13) correspond to the partial derivatives involving variable entities from different tensors in the parameter list `params` (In [19]). The same principle applies for all `params` with `len(params) > 1`.

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3The two matrices are equal up to transposition, since $H$ is symmetric
4 Implementation

We will now address how to overcome the basic complications discussed in Sections 3.3, 3.1 and 3.2. The current section is divided into two parts: we first discuss how to compute the matrix $H$ in Equation (9), and afterwards move on to the matrix $G$ in Equation (10).

4.1 Computing $H$

We compute the matrix $H$ based on Hessian vector products [3]. A partial implementation of Equation (9) is essentially to form $P$ Hessian vector products using the full set of basis vectors in $\mathbb{R}^P$. As a bonus, the resulting implementation can easily be parallelized because the columns of the Hessian matrix can be computed independently.

In the following we describe the essential parts of this paper’s accompanying Python module `pyhessian` [8]. The Hessian vector product function `HessianEstimator.get Hv_op(v)` can be described as follows:

1. Differentiates the cost function with respect to the model parameters contained in the list `params` and flattens the result.
2. Performs elementwise multiplication of the flattened gradient and the vector $v$; `tf.stop_gradient()` ensures that $v$ is treated as a constant during differentiation.
3. Differentiates the resulting elementwise vector product with respect to the model parameters (to get second order derivatives) and flattens the result.

Note that the function `HessianEstimator.get Hv_op(v)` uses the function `HessianEstimator.flatten()` which is based on the insights from Section 3.2.1 and the mathematical operation defined in Equation (5). Furthermore, we have defined a parallelized function `HessianEstimator.get H_op()` to create the full Hessian matrix operation based on forming $P$ Hessian vector products using `HessianEstimator.get Hv_op(v)` for all $v$’s in $\mathbb{R}^P$. The function `HessianEstimator.get H_op()` sets up a parallelized operation using `tf.map_fn()` to get hold of all the $P$ columns of the full Hessian matrix as defined in Equation (9). It works by applying `Hv_op` on all basis vectors in $\mathbb{R}^P$ represented by `tf.eye(self.P, self.P)`, where $P$ is the total number of parameters in the model.

The important remark is now to realize that, by definition, the matrix $H$ in Equation (9) is the sum of per-example Hessian matrices. It means that we can directly leverage from the fact that `tf.gradients()` returns the sum of per-example gradients discussed in Section 3.1. In other words, when we run the resulting $H_{op}$ in a graph session, we get per-example Hessians (below In [43]) if we feed single examples, and the average of per-example Hessians if we feed more than one example. Thus, we can get a minibatch (below using size `batch_size`) Hessian matrix if we feed a minibatch (below In [45]), or we can obtain the full Hessian matrix directly by feeding the complete training set. However, to avoid excessive memory consumption for large $N$, we can sum over mini-batch Hessians and divide by the number of mini-batches (In [46] - In [57]):

In [39]: `from pyhessian import HessianEstimator`
In [40]: `hest = HessianEstimator(...)`
In [41]: H_op = hess.get_H_op()
In [42]: # Per-example
In [43]: H = sess.run(H_op, feed_dict={X: [X_train[0]],
   y: [y_train[0]]})
In [44]: # Mini-batch
In [45]: H = sess.run(H_op, feed_dict={X: X_train[:batch_size_H],
   y: y_train[:batch_size_H]})
In [46]: # Full
In [47]: B = int(N/batch_size_H)
In [48]: P = int(H_op.shape[0])
In [49]: H = np.zeros((P, P), dtype='float32')
In [50]: for b in range(B):
   ...:     feed_dict={
   ...:       X: X_train[(b+1)*batch_size_H:]
   ...:       (b+1)*batch_size_H],
   ...:       y: y_train[(b+1)*batch_size_H:]
   ...:       (b+1)*batch_size_H]})
In [51]: H = H/B

4.2 Computing $G$

Due to the inequality sign in Equation (12), the computation of $G$ (unlike $H$) cannot exploit the implicit sum of gradients as discussed in Section 3.1. Instead, we will pursue another efficient technique based on parallelized per-example gradients. Although the technique we present here has been reformulated and adapted to our needs, the original implementation idea is to our knowledge originating from the author of [2]. The OPG matrix operation function HessianEstimator.get_G_op() can be described as follows:

1. Creates `batch_size_G` copies of the model parameters
2. Splits the model input variable $X$, and the model output variable $y$ into respective lists of `batch_size_G` elements
3. Creates a list of `batch_size_G` elements holding model output tensors resulting from evaluating the model function using respective inputs and parameter copies
4. Creates a list of `batch_size_G` elements holding cost output tensors resulting from evaluating the cost using respective labels, model outputs and parameter copies
5. Stacks up a flat per-example gradient tensor by parallel differentiation of per-example costs with respect to the corresponding model parameter copy
6. Forms the OPG matrix operation by matrix multiplication of per-example cost Jacobians as in Equation (11)

Note that the function HessianEstimator.get_G_op() utilizes the function HessianEstimator.flatten() which is based on the insights from Section 3.2.1 and the mathematical operation defined in Equation (5).

Also note that the function HessianEstimator.get_G_op() requires itself to maintain redundant model parameter copies which size scale with `batch_size_G`. 

To avoid excessive memory consumption, we can sum over mini-batch OPGs and divide by the number of mini-batches (In [64] - In [70]):

In [58]: hest = HessianEstimator(..., batch_size=G)
In [59]: G_op = hest.get_G_op()

In [60]: # Per-example
In [61]: sess.run(G_op, feed_dict={X: X_train[0], y: y_train[0]})

In [62]: # Mini-batch
In [63]: sess.run(G_op, feed_dict={X: X_train[:batch_size,G], y: y_train[:batch_size,G]})

In [64]: # Full
In [65]: B = int(N/batch_size_G)
In [66]: P = int(G_op.shape[0])
In [67]: G = np.zeros((G, P), 'float32')
In [68]: for b in range(B):
   ...:     G = G + sess.run(G_op, feed_dict={
   ...:         X: X_train[b*batch_size_G: (b+1)*batch_size_G],
   ...:         y: y_train[b*batch_size_G: (b+1)*batch_size_G]})

In [70]: G = G/B

5 Summary and Concluding Remarks

We have presented a practical and efficient TensorFlow implementation for computing Hessian matrices in a deep learning context. The methods have a runtime of $O(NP^2)$ operations where $N$ is the number of examples in the training set and $P$ is the number of parameters in the model. The novelty of the methods presented in this paper prominently lies in the implementation technique rather than in the asymptotic bound analysis point of view. As noted by [2], a naive method running back propagation $N$ times with a mini-batch of size 1 is very inefficient because TensorFlow’s back propagation implementation will not be able to exploit the parallelism of mini-batch operations by efficient matrix operation implementations. An usage example of the pyhessian module [8] applied on a feed-forward neural network TensorFlow model can be found in the included file pyhessian_example.py.

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