Fast Evaluation and Approximation of the Gauss-Newton Hessian Matrix for the Multilayer Perceptron

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Abstract. We introduce a fast algorithm for entry-wise evaluation of the Gauss-Newton Hessian (GNH) matrix for the multilayer perceptron. The algorithm has a precomputation step and a sampling step. While it generally requires $O(Nn)$ work to compute an entry (and the entire column) in the GNH matrix for a neural network with $N$ parameters and $n$ data points, our fast sampling algorithm reduces the cost to $O(n + d/\epsilon^2)$ work, where $d$ is the output dimension of the network and $\epsilon$ is a prescribed accuracy (independent of $N$). One application of our algorithm is constructing the hierarchical-matrix ($\mathcal{H}$-matrix) approximation of the GNH matrix for solving linear systems and eigenvalue problems. While it generally requires $O(N^2)$ memory and $O(N^3)$ work to store and factorize the GNH matrix, respectively. The $\mathcal{H}$-matrix approximation requires only $O(Nr_o)$ memory footprint and $O(Nr_o^2)$ work to be factorized, where $r_o \ll N$ is the maximum rank of off-diagonal blocks in the GNH matrix. We demonstrate the performance of our fast algorithm and the $\mathcal{H}$-matrix approximation on classification and autoencoder neural networks.

Key words. Gauss-Newton Hessian, Fast Monte Carlo Sampling, Hierarchical Matrix, Second-order Optimization, Multilayer Perceptron

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1. Introduction. Consider a multilayer perceptron (MLP) with $L$ fully connected layers and $n$ data pairs $\{(x_i^0, y_i)\}_{i=1}^n$, where $y_i$ is the label of $x_i^0$. Given input data point $x_i^0 \in \mathbb{R}^{d_0}$, the output of the MLP is computed via the forward pass:

$$x_i^\ell = s(W_\ell x_i^{\ell-1}), \quad \ell = 1, \ldots, L$$

where $x_i^\ell \in \mathbb{R}^{d_\ell}$, $W_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$ and $s$ is a nonlinear activation function. Without loss of generality, Eq. (1.1) does not have bias parameters. Otherwise, bias can be included in the weight matrix $W_\ell$, and vector $x_i^\ell$ is appended with an additional homogeneous coordinate of value one. For ease of presentation, we assume constant layer size, i.e., $d_\ell \equiv d$, for $\ell = 1, 2, \ldots, L$. Define the weight vector consisting of all weight parameters concatenated together as $w = [\text{vec}(W_1), \text{vec}(W_2), \ldots, \text{vec}(W_L)] \in \mathbb{R}^N$, where $N = d^2L$ and vec is the operator vectorizing matrices.

Given a loss function $f(x_i^\ell, y_i)$, which measures the misfit between the network output and the true label, we define $F(w) = \frac{1}{n} \sum_{i=1}^n f(x_i^L, y_i)$ as the total loss of the MLP with respect to the weight vector $w$. Note $x_i^L$ is a function of the weights $w$.

Definition 1.1 ((Generalized) Gauss-Newton Hessian). Let $Q_i = \frac{1}{n} \partial_{xx}^2 f(x_i^L, y_i) \in \mathbb{R}^{d \times d}$ be the Hessian of the loss function $f(x_i^L, y_i)$, and $Q \in \mathbb{R}^{dn \times dn}$ be a block diagonal matrix with $Q_i$ being the $i$th block. Let $J_i = \partial_w x_i^L \in \mathbb{R}^{d \times N}$ be the Jacobian of $x_i^L$ with respect to the weights $w$.

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\( w, \) and \( J \in \mathbb{R}^{dn \times N} \) be the vertical concatenation of all \( J_i. \) The (generalized) Gauss-Newton Hessian (GNH) matrix \( H \in \mathbb{R}^{N \times N} \) associated with the total loss \( F \) with respect to the weights \( w \) is defined as

\[
H = J^T Q J = \sum_{i=1}^{n} J_i^T Q_i J_i.
\] (1.2)

The GNH matrix is closely related to the Hessian matrix and, importantly, it is always (symmetric) positive semi-definite when the loss function \( f(x_i^L, y_i) \) is convex in \( x_i^L \) (\( Q_i \) is positive semi-definite), a useful property in many applications. For several standard choices of the loss function, the GNH matrix is mathematically equivalent to the Fisher matrix as used in the natural gradient method. The GNH matrix is also equivalent to the Hessian matrix of a particular approximation of \( F(w) \) constructed by replacing \( x_i^L \) with its first-order approximation with respect to the weights \( w \) [30].

This paper is concerned with fast entry-wise evaluation of the GNH matrix. Such an algorithmic primitive can be used in constructing approximations of the GNH matrix for solving linear systems and eigenvalue problems, which are useful for training and analyzing neural networks [6, 30, 5, 34], for selecting training data to minimize the inference variance [9], for estimating learning rates [25], for network pruning [19], for robust training [41], for probabilistic inference [20], for designing fast solvers [7, 38, 15] and so on.

1.1. Previous work. We classify related work into two groups. One group avoids entry-wise evaluation of the GNH matrix and relies on the matrix-vector multiplication (matvec) with the Hessian or the GNH that is matrix-free [28, 32, 30]. For example, the matrix-free matvec can be used to construct low-rank approximations of the GNH matrix through the randomized singular value decomposition (RSVD) [18], but the numerical rank may not be small [43, 11]. Other examples are the following: [10] introduces a low-rank approximation using the Lanczos algorithm to tackle saddle points; [36] maintains a low-rank approximation of the inverse of the Hessian based on rank-one updates at each optimization step; [15] uses a quasi-Newton-like construction of the low-rank approximation; [42, 40] study the convergence of stochastic Newton methods combined with a randomized low-rank approximation; [41] uses a matrix-free method with only the layers near the output layer.

The other group of methods are based on evaluating or approximating entries on or close to the diagonal of the GNH matrix [24]. For example, [47] introduces a recursive fast algorithm to construct block-diagonal approximations. As another example, [31, 30] introduce the K-FAC algorithm, which is based on an entry-wise approximation of the Fisher matrix (mathematically equivalent to the GNH for several standard choices of the loss function). The Fisher matrix is given by \( \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_y g_i(y) g_i(y)^T \), where \( g_i \) is the gradient evaluated for the \( i \)th training point \( x_i^0 \), and \( y \) is sampled from the network’s predictive distribution \( \propto \exp(-f(x_i^L, y)). \) In practice, an extra step of block-diagonal approximation or block-tridiagonal approximation is used for fast inversion purpose. The method has been tested within optimization frameworks on modern supercomputers and has been shown to perform well [35]. However, the sampling in the K-FAC algorithm converges slowly, and block-diagonal approximations do not account for off-diagonal information.
1.2. Contributions. In this paper, we introduce a fast algorithm for entry-wise evaluation of the GNH matrix $H$, i.e., computing

$$H_{km} = e_k^T H e_m,$$

where $e_k$ and $e_m$ are two canonical bases. With the fast evaluation, we propose the hierarchical-matrix ($\mathcal{H}$-matrix) approximation [4, 17] of the GNH matrix for the MLP network, which has applications in autoencoders, long-short memory networks, and is often used to study the potential of second-order training methods. Notice if the matrix-free matvec is used to evaluate $H_{km}$, the computational cost would be $O(Nn)$.

Our fast algorithm includes a precomputation step and a sampling step, which reduces the cost to $O(n + d)$ work (independent of $N$), where $d$ is the output dimension of the network. Specifically, suppose the network employs the mean squared loss ($Q_i$ is the identity), and therefore, the GNH matrix is $H = \frac{1}{n} JJ^T$, where $J \in \mathbb{R}^{dn \times N}$ is the Jacobian of the network output with respect to the weights. Then $H_{km} = \frac{1}{n} (Je_k)^T (Je_m)$, and only columns in the Jacobian are required to be computed. Our precomputation algorithm exploits the structure of a feed-forward neural network, where the gradient is back propagated layer by layer, so the intermediate results effectively form a compressed format of the Jacobian with $O(Nn)$ memory. As a result, every column can be retrieved in only $O(nd)$ time (note every column has $O(nd)$ entries).

To accelerate the computation of $H_{km}$, we introduce a fast Monte Carlo sampling algorithm. Let $v_k(i)$ denote the sub-vector in the Jacobian’s $k$th column corresponding to the $i$th data point, and therefore, $H_{km} = \frac{1}{n} \sum_{i=1}^{n} v_k(i)^T v_m(i)$. In the sampling, we draw $c$ (independent of $n$) independent samples $t_1, t_2, \ldots, t_c$ from $\{1, 2, \ldots, n\}$ with a carefully designed probability distribution $P_{km}$ and compute an estimator

$$\tilde{H}_{km} = \frac{1}{nc} \sum_{j=1}^{c} \frac{v_k(t_j)^T v_m(t_j)}{P_{km}(t_j)}.$$

We prove $|H - \tilde{H}_{km}| = O(1/\sqrt{c})$ with high probability. Note it requires only $O(n + dc)$ work to compute $\tilde{H}_{km}$ as an approximation, where $d$ is the output dimension of the network.

With the fast evaluation algorithm, we are able to take advantage of the existing GOFMM method [44, 45, 46] to construct the $\mathcal{H}$-matrix approximation of the GNH matrix through evaluating $O(N)$ entries in the matrix. The $\mathcal{H}$-matrix approximation is a multi-level scheme that stores diagonal blocks and employs low-rank approximations for off-diagonal blocks in the input matrix. So suppose work on the (global) low-rank approximation and the block-diagonal approximation can be viewed as the two extremes in the spectrum of our $\mathcal{H}$-matrix approximation, which effectively works for a broader range of problems. $\mathcal{H}$-matrices are algebraic generalizations of the well-known fast $n$-body calculation algorithms [3, 16] in computational physics, and they have been applied to kernel methods in machine learning [26, 27]. An $\mathcal{H}$-matrix can be formulated as

$$H = D + S + UV^T$$

where $U$ and $V$ are tall-and-skinny matrices, $S$ is a block-sparse matrix, and $D$ is a block-diagonal matrix with the blocks being either smaller $\mathcal{H}$-matrices at the next level or dense
blocks at the last level. Figure 1 shows the structure of a low-rank matrix and the hierarchically
low-rank structure of $H$-matrices.

Figure 1: (a) A low-rank matrix $H = U V^T$, where $U$ and $V$ are tall-and-skinny matrices; (b) a three-level $H$-matrix, where blue represents dense diagonal blocks, and green, red and orange represent off-diagonal low-rank blocks at level 1, 2 and 3, respectively; (c) ranks of diagonal and off-diagonal blocks in an $H$-matrix, where every block has size 2-by-2.

Given an $H$-matrix approximation, the memory footprint is $O(N r_o^1)$, where $N$ is the
matrix size or the number of weights in a network and $r_o$ is the maximum off-diagonal rank.
Compared to the $O(N^2)$ storage for the entire matrix, an $H$-matrix approximation leads
to significant memory savings. Once constructed, an $H$-matrix can be factorized with only
$O(N r_o^2)$ work, and there exists an entire class of well-established numerical techniques [33, 39,
21, 12, 1, 8, 37]. The factorization can be applied to a vector with $O(N r_o)$ work and be used
as either a fast direct solver or a preconditioner depending on the approximation accuracy.

To summarize, our work makes the following two major contributions:

- a fast algorithm that requires $O(N n)$ storage and requires $O(n + d/\epsilon^2)$ work to evaluate
  an arbitrary entry in the GNH matrix, where $N$ and $d$ are the number of parameters
  and the output dimension of the MLP, respectively, $n$ is the data size, and $\epsilon$ is a
  prescribed accuracy.
- a framework to construct the $H$-matrix approximation of the GNH matrix, analysis
  and demonstration of the corresponding accuracy and the cost, as well as comparison
  with the RSVD and the K-FAC methods.

Outline. In §2 we review the background material. In §3 we present our fast algorithm
for evaluating entries in the GNH matrix. In §4 we show how to construct the $H$-matrix
approximation of the GNH matrix. In §5 we show numerical results, and in §6 we conclude
with further extensions.

2. Background. In this section, we review the importance of the GNH matrix and the
associated computational challenge.

2.1. Neural network training. The GNH matrix is useful in training and analyzing neural
networks, selecting training data, estimating learning rate, and so on. Here we focus on its use
in second-order optimization to show the challenge that is common in other applications. In
the MLP, the weight vector $w$ is obtained via solving the following constrained optimization

\[ \min_{w \in \mathbb{R}^d} \frac{1}{2} \| y - f(x, w) \|^2 + \frac{\lambda}{2} \| w \|^2 \]

subject to $g(w) = 0$, where $y$ is the target output, $f(x, w)$ is the output of the MLP
for input $x$, and $\lambda$ is a regularization parameter.

\[ \begin{bmatrix} \frac{\partial f(x, w)}{\partial w} \end{bmatrix} \begin{bmatrix} \Delta w \end{bmatrix} = \begin{bmatrix} \nabla f(x, w) \end{bmatrix} \]

where $\frac{\partial f(x, w)}{\partial w}$ is the gradient of $f$ with respect to $w$. The GNH matrix
is defined as $H = \begin{bmatrix} \frac{\partial f(x, w)}{\partial w} \end{bmatrix} \begin{bmatrix} \frac{\partial f(x, w)}{\partial w} \end{bmatrix}^T$. It captures
the curvature of the loss function and is used in second-order optimization methods.

\[ H^{-1} \begin{bmatrix} \nabla f(x, w) \end{bmatrix} = \begin{bmatrix} \Delta w \end{bmatrix} \]

The factorization of $H$ allows for efficient computation of $H^{-1}$, and hence the gradient
update in second-order methods.

\[ H = UV^T \]

where $U$ and $V$ are orthogonal matrices. The low-rank structure of $H$ allows for
memory savings and efficient computation.

\[ O(N r_o) \]

\[ O(n + d/\epsilon^2) \]

\[ \log(N) \] or $\log^2(N)$ prefactor
problem (regularization on \( w \) could be added):

\[
(2.1) \quad \min F(w) \quad \text{subject to Eq. (1.1)}.
\]

Recall that \( F(w) = \frac{1}{n} \sum_{i=1}^{n} f(x_i^T, y_i) \), where \( f \) is the loss function, \( x_i^T \) is the network output corresponding to input \( x_i^T \), which has label \( y_i \).

To solve for \( w \) in problem (2.1), a second-order optimization method solves a sequence of local quadratic approximations of \( F(w) \), which requires solving the following linear systems repeatedly:

\[
(2.2) \quad Hp = -g,
\]

where \( H \) is the curvature matrix (the Hessian of \( F(w) \) in the standard Newton’s method), \( g = \partial_w F \) is the gradient, and \( p \) is the update direction. Generally speaking, second-order optimization methods are highly concurrent and could require much less number of iterations to converge than first-order methods, which imply potentially significant speedup on modern distributed computing platforms.

In the Gauss-Newton method, a popular second-order method, the GNH matrix is employed (with a small regularization) as the curvature matrix in Eq. (2.2), which can be solved using the Conjugate Gradient method. Since the GNH is mathematically equivalent to the Fisher matrix for several standard choices of the loss, and then the solution of Eq. (2.2) becomes the natural gradient, a efficient steepest descent direction in the space of probability distribution with an appropriately defined distance measure [29].

Table 1: Gradient evaluation and matrix-free matvec with the GNH matrix. Notations: \( \hat{w} = [\text{vec}(\hat{W}_1), \ldots, \text{vec}(\hat{W}_L)] \) is the input of the matvec, \( \hat{x}_i^0 = 0, \ M_i^\ell = \text{diag} \left( \hat{s}(W_{\ell} \hat{x}_{i}^{\ell-1}) \right) \), where \( \hat{s} \) is the derivative of the activation function \( s \). Equations in the table can be derived by introducing Lagrange multipliers \( z_i^\ell \) (and \( \hat{z}_i^\ell \)) for the \( \ell \)-th-layer weights [13, 14]. Step (a) of gradient evaluation is known as the forward pass, and step (b) and (c) are the back-propagation. Correspondingly, step (a) in the matvec is known as the linearized forward.

| Evaluate gradient \( g \) | Matvec with GNH: \( H\hat{w} = J^TQJ\hat{w} \) |
|--------------------------|-------------------------------------|
| (a) \( x_i^\ell = s(W_{\ell}x_{i}^{\ell-1}) \) | (a) \( \hat{x}_i^\ell = M_i^\ell(W_{\ell}\hat{x}_{i}^{\ell-1} + \hat{W}_{\ell}\hat{x}_{i}^{\ell-1}) \) \( \forall i, \ell \) (Compute \( J\hat{w} \)) |
| (b) \( z_i^\ell = q_i \) | (b) \( \hat{z}_i^\ell = Q_i\hat{x}_i^\ell \) \( \forall i \) |
| (c) \( z_i^{\ell-1} = W_{\ell}^T M_i^\ell \hat{z}_i^\ell \) | (c) \( \hat{z}_i^{\ell-1} = W_{\ell}^T M_i^\ell \hat{z}_i^\ell \) \( \forall i, \ell \) |
| (d) \( g^\ell = \sum_{i=1}^{n} (M_i^\ell \hat{z}_i^\ell) (x_{i}^{\ell-1})^T \forall \ell \) | (d) \( (H\hat{w})^\ell = \sum_{i=1}^{n} (M_i^\ell \hat{z}_i^\ell) (x_{i}^{\ell-1})^T \) \( \forall \ell \) |

**2.2. Back-propagation & matrix-free matvec.** Table 1 shows the back-propagation algorithm for evaluating the gradient \( g = \partial_w F \) in Eq. (2.2) and the matrix-free matvec with the GNH matrix, both of which have complexity \( \mathcal{O}(Nn) \). Note a direct matvec with the full GNH matrix would require \( \mathcal{O}(N^2) \) work.

Based on the two basic ingredients, iterative solvers such as Krylov methods can be used to solve Eq. (2.2) as in Hessian-free methods [28, 32]. However, the iteration count for con-
verge can grow rapidly in the presence of ill-conditioning, in which case fast solvers or preconditioners for Eq. (2.2) are necessary [2, 23, 30].

3. Fast computation of entries in GNH. This section presents a precomputation algorithm and a fast Monte Carlo algorithm for fast computation of arbitrary entries in the GNH matrix of an MLP network.

A naive method. Consider a GNH matrix $H \in \mathbb{R}^{N \times N}$, where an entry $H_{km}$ can be written as

$$H_{km} = e_k^T H e_m,$$

where $e_k$ and $e_m$ are the $k_{th}$ and the $m_{th}$ columns in the $N$-dimensional identity matrix. We can take advantage of the matrix-free matvec with the GNH matrix in Table 1 to compute $H_{km} = e_k^T (H e_m)$, which costs the same as one pass of forward propagation plus one pass of backward propagation, i.e., $O(Nn) = O(d^2Ln)$ work.

In the following, we introduce a precomputation algorithm that reduces the cost of evaluating an entry in the GNH to $O(dn)$ work with $O(Nn)$ memory, and a fast Monte Carlo algorithm that further reduces the cost to $O(d + n)$ work.

3.1. Precomputation algorithm. The motivation of our precomputation algorithm is to exploit the sparsity of $e_k$ and $e_m$ plus the symmetry of $H$ in Eq. (3.1). Recall the definition of $H$ in Eq. (1.2), and let $Q_i = R_i^T R_i$ be a symmetric factorization, which can be computed via, e.g., the eigen-decomposition or the LDLT factorization with pivoting. We have

$$H_{km} = e_k^T (\sum_{i=1}^n J_i^T R_i^T R_i J_i) e_m = \sum_{i=1}^n (R_i J_i e_k)^T (R_i J_i e_m) := \sum_{i=1}^n v_k(i)^T v_m(i)$$

where $v_k(i)$ and $v_m(i)$ are two $d$-dimensional vectors:

$$v_k(i) = R_i J_i e_k, \quad v_m(i) = R_i J_i e_m,$$

for $k, m = 1, 2, \ldots, N$ and $i = 1, 2, \ldots, n$.

Theorem 3.1. For an MLP network that has $L$ fully connected layers with constant layer size $d$ (by-d weight matrices), every entry $H_{km}$ in the GNH matrix can be computed in $O(dn)$ time with a precomputation that requires $O(nN)$ storage and $O(dnN)$ work.

Proof. We precompute and store

$$C_i^\ell = R_i M_i^\ell W_{L-1} \cdots W_1 W_{L-1} \cdots W_1, \quad i = 1, 2, \ldots, n; \quad \ell = 1, 2, \ldots, L$$

where $M_i^\ell = \text{diag}(s(W_i x_i^{\ell-1}))$ and $s$ is the derivative of the activation function. Notice that computing the symmetric factorizations for $Q_i$ cost $O(d^3n)$, which is negligible compared to other parts of the computation. Moreover, a forward pass of the network (step (a) of gradient evaluation in Table 1) computes $M_i^\ell$ with $O(nN)$ work.

Since every $C_i^\ell$ is a $d \times d$ matrix, the total storage cost is $O(d^2nL) = O(nN)$, where $N = d^2L$ is the total number of weights. In addition, notice that $C_i^{\ell-1} = C_i^\ell \left(W_\ell M_i^{\ell-1}\right)$, so they can be computed from $\ell = L$ to $\ell = 1$ iteratively, which requires $O(d^3Ln) = O(dnN)$ work in total.
To complete the proof we show how to compute \( v_k(i) \) as defined in Eq. (3.3) with \( \mathcal{O}(d) \) work. Recall that \( J_e k \) can be computed using linearized forward, i.e., step (a) of the matvec in Table 1, as follows.

1. Let \( \tau = \lceil k/d^2 \rceil, \mu = k \mod d, \) and \( \nu = \lceil (k \mod d^2)/d \rceil. \) Since \( e_k \) has only one nonzero entry, \( \hat{x}_{\ell i}^\tau = 0 \) for \( \ell = 1, 2, \ldots, \tau - 1 \) because \( \hat{W}_{\ell} \) are all zeros except for \( \ell = \tau. \) The matrix \( \hat{W}_{\tau} \) has only one nonzero at position \( (\mu, \nu) \) (column-major ordering) as the following:

\[
\begin{bmatrix}
\nu & \ldots \\
\mu & \ldots \\
1 & \ldots \\
\vdots & \\
\end{bmatrix}
= \hat{W}_{\tau}.
\]

2. Following step (a) of the matvec in Table 1, we have \( \hat{x}_{\tau i}^\tau = M_{\tau i}^\tau \hat{W}_{\tau} x_{\tau - 1 i}^\tau \) at layer \( \tau. \) Denote \( a_{\tau i}^\tau = \hat{W}_{\tau} \hat{x}_{\tau - 1 i}^\tau, \) and we have

\[
\begin{align*}
\hat{x}_{\tau i}^\tau &= M_{\tau i}^\tau a_{\tau i}^\tau \\
\hat{x}_{\tau i}^{\tau + 1} &= M_{\tau i}^{\tau + 1} W_{\tau + 1} \hat{x}_{\tau i}^\tau \\
&= M_{\tau i}^{\tau + 1} W_{\tau + 1} M_{\tau i}^\tau a_{\tau i}^\tau \\
&\cdots \\
\hat{x}_{\tau i}^L &= M_{\tau i}^L W_L M_{\tau i}^{L - 1} W_{L - 1} \cdots M_{\tau i}^\tau a_{\tau i}^\tau
\end{align*}
\]

3. Notice that the only nonzero entry in \( a_{\tau i}^\tau \) is the \( \mu_{th} \) element, which equals to the \( \nu_{th} \) element in \( x_{\tau - 1 i}^\tau, \) Therefore,

\[(3.5) \quad v_k(i) = R_i J_i e_k = R_i \hat{x}_{\tau i}^L = C_{\tau i} a_{\tau i}^\tau,
\]

where \( C_{\tau i} a_{\tau i}^\tau \) should be interpreted as a scaling of the \( \mu_{th} \) column in \( C_{\tau i} \) by the \( \nu_{th} \) element in \( x_{\tau - 1 i}^\tau, \) which costs \( \mathcal{O}(d) \) work.

3.2. Fast Monte Carlo algorithm. Recall Eq. (3.2), which sums over a large number of data points, and the idea is to sample a subset with judiciously chosen probability distribution and scale the (partial) sum appropriately to approximate \( H_{km}. \) It is important to note that the computation of the probabilities is fast based on the previous precomputation. The fast sampling algorithm is given in Algorithm 3.1.

Define \( v_k = [v_k(1), \ldots, v_k(n)] \) and \( v_m = [v_m(1), \ldots, v_m(n)] \) as two vectors in \( \mathbb{R}^{dn}, \) and Eq. (3.2) can be written as the inner product of the two vectors:

\[ H_{km} = v_k^T v_m. \]

The following theorem shows that our sampling algorithm returns a good estimator of \( H_{km}, \) where the error is measured using \( \|v_k\| \|v_m\|, \) an upper bound on \( |H_{km}|. \)

**Theorem 3.2 (Sampling error).** Consider an MLP network that has \( L \) fully connected layers with constant layer size \( d \) (\( d \)-by-\( d \) weight matrices). For every entry \( H_{km} \) in the GNH matrix, Algorithm 3.1 returns an estimator \( \hat{H}_{km} \) that
Algorithm 3.1 Fast Monte Carlo Algorithm

1: **Input:** $\|v_k(i)\|$ and $\|v_m(i)\|$ for $i = 1, 2, \ldots, n$.
2: Compute sampling probabilities for $t = 1, 2, \ldots, n$:

$$P_{km}(t) = \frac{\|v_k(t)\| \|v_m(t)\|}{\sum_{j=1}^{n} \|v_k(j)\| \|v_m(j)\|}.$$  

3: Draw $c$ independent random samples $t_j$ from $\{1, 2, \ldots, n\}$ with replacement.

4: **Output:**

$$\tilde{H}_{km} = \frac{1}{c} \sum_{j=1}^{c} \frac{v_k(t_j)^T v_m(t_j)}{P_{km}(t_j)}.$$  

- is an unbiased estimator of $H_{km}$, i.e., $E[\tilde{H}_{km}] = H_{km}$.
- its variance or mean squared error (MSE) satisfies

$$\text{Var}[H_{km}] = \mathbb{E} \left[ |H_{km} - \tilde{H}_{km}|^2 \right] \leq \frac{1}{c} \|v_k\|^2 \|v_m\|^2$$

where $c$ is the number of random samples.
- with probability at least $1 - \delta$, where $\delta \in (0, 1)$, its absolute error satisfies

$$|H_{km} - \tilde{H}_{km}| \leq \frac{\eta}{\sqrt{c}} \|v_k\| \|v_m\|$$

where $\eta = 1 + \sqrt{8 \log(1/\delta)}$ and $c$ is the number of random samples.

**Proof.** Our proof consists of the following three parts.

**Unbiased estimator.** Define a random variable

$$X_t = \frac{v_k(t)^T v_m(t)}{P(t)}$$

where $t$ is a random sample from $\{1, 2, \ldots, n\}$ according to the distribution in Eq. (3.6). Observe that $\tilde{H}_{km}$ is the mean of $c$ independent identically distributed variables, and thus

$$\mathbb{E}[\tilde{H}_{km}] = \mathbb{E}[X_t] = \sum_{t=1}^{n} \frac{v_k(t)^T v_m(t)}{P(t)} P(t) = H_{km}.$$
**Variance/MSE error.** The variance or MSE error of the estimator is the following:

\[
E\left[|H_{km} - \tilde{H}_{km}|^2\right] = \text{Var}[\tilde{H}_{km}] = \frac{1}{c}\text{Var}[X_i]
\]

\[
= \frac{1}{c}(E[X_i^2] - E^2[X_i])
\]

\[
= \frac{1}{c} \sum_{t=1}^{n} \left(\frac{v_k(t)^T v_m(t)}{P(t)}\right)^2 P(t) - \frac{H_{km}^2}{c}
\]

\[
\leq \sum_{t=1}^{n} \left(\frac{v_k(t)^T v_m(t)}{c P(t)}\right)^2
\]

\[
\leq \sum_{t=1}^{n} \|v_k(t)\|^2 \|v_m(t)\|^2 \left(\frac{1}{c P(t)}\right)
\]

\[
= \frac{1}{c} \left(\sum_{t=1}^{n} \|v_k(t)\| \|v_m(t)\|\right)^2
\]  \hspace{1cm} (Cauchy-Schwarz)

\[
\leq \frac{1}{c} \left(\sum_{t=1}^{n} \|v_k(t)\|^2\right) \left(\sum_{t=1}^{n} \|v_m(t)\|^2\right)
\]  \hspace{1cm} (Eq. (3.6))

\[
\leq \frac{1}{c} \|v_k\|^2 \|v_m\|^2.
\]

Notice that with Jensen’s inequality, we also obtain a bound of the absolute error in expectation:

\[
E\left[|H_{km} - \tilde{H}_{km}|\right] \leq \frac{1}{\sqrt{c}} \|v_k\| \|v_m\|.
\]  \hspace{1cm} (3.10)

**Concentration result.** We will use the McDiarmid’s (a.k.a., Hoeffding-Azuma or Bounded Differences) inequality to obtain Eq. (3.9). Define function \(F(t_1, t_2, \ldots, t_c) = |H_{km} - \hat{H}_{km}|\), where \(t_1, t_2, \ldots, t_c\) are random samples, and we show that changing one sample \(t_i\) at a time does not affect \(F\) too much. Consider changing a sample \(t_i\) to \(t_i'\) while keeping others the same. The new estimator \(\hat{H}_{km}\) differs from \(H_{km}\) by only one term. Thus,

\[
|\hat{H}_{km} - H_{km}| = \left|\frac{v_k(t_i)^T v_m(t_i)}{c P(t_i)} - \frac{v_k(t_i')^T v_m(t_i')}{c P(t_i')}\right|
\]

\[
\leq \left|\frac{v_k(t_i)^T v_m(t_i)}{c P(t_i)}\right| + \left|\frac{v_k(t_i')^T v_m(t_i')}{c P(t_i')}\right|
\]

\[
\leq \frac{\|v_k(t_i)\| \|v_m(t_i)\|}{c P(t_i)} + \frac{\|v_k(t_i')\| \|v_m(t_i')\|}{c P(t_i')}
\]

\[
= \frac{2}{c} \sum_{j=1}^{n} \|v_k(j)\| \|v_m(j)\|
\]

\[
\leq \frac{2}{c} \|v_k\| \|v_m\|.
\]
where we have used Cauchy-Schwarz inequality twice. Then, define \( \Delta = \frac{2}{c} \|v_k\|_2 \|v_m\|_2 \); using the triangle inequality we see

\[
|F(\ldots, t_i, \ldots) - F(\ldots, t'_i, \ldots)| \leq \Delta.
\]

Finally, let \( \gamma = \sqrt{2c \log(1/\delta)} \Delta \), and we use the McDiarmid’s inequality to obtain Eq. (3.9) as follows

\[
\Pr \left[ |H_{km} - \tilde{H}_{km}| \geq \frac{\eta}{\sqrt{c}} \|v_k\|_2 \|v_m\|_2 \right] \leq \exp \left( -\frac{\gamma^2}{2c \Delta^2} \right) = \delta \quad \text{(McDiarmid’s inequality)}.
\]

**Remark 3.3.** The error \( \epsilon \) in the approximation of \( H_{km} \) depends on only the number of random samples \( c \) (but not \( n \)) and can be made arbitrarily small as needed. In particular, if \( c \geq 1/\epsilon^2 \), we have

\[
\text{Var}[H_{km}] = \mathbb{E} \left[ |H_{km} - \tilde{H}_{km}|^2 \right] \leq \epsilon \|v_k\|_2^2 \|v_m\|_2^2
\]

and if \( c \geq \eta^2/\epsilon^2 \), then with probability at least \( 1 - \delta \), where \( \delta \in (0, 1) \)

\[
|H_{km} - \tilde{H}_{km}| \leq \epsilon \|v_k\|_2 \|v_m\|_2.
\]

Furthermore, the error of the entire matrix in the Frobenius norm is

\[
\|H - \tilde{H}\|_F \leq \epsilon \sqrt{\sum_k \sum_m \|v_k\|_2^2 \|v_m\|_2^2} = \epsilon \sum_k \|v_k\|_2^2 = \epsilon \text{trace}(H) \leq \epsilon \sqrt{N} \|H\|_F.
\]

**Remark 3.4.** The estimator \( \tilde{H}_{km} \) is exact using at most one sample when \( k = m \). The (trivial) case \( H_{kk} = 0 \) is implied by the situation that \( v_{kk}(i) = 0 \) for all \( i \); otherwise, we have \( H_{kk} = \|v_k\|_2^2 \), and the sampling probability becomes

\[
P_{kk}(t) = \frac{\|v_k(t)\|^2}{\sum_{j=1}^n \|v_k(j)\|^2} = \frac{\|v_k(t)\|^2}{\|v_k\|^2}.
\]

Therefore, \( \tilde{H}_{kk} = \|v_k(t)\|^2 / P_{kk}(t) = H_{kk} \) with any random sample \( t \).

**Theorem 3.5 (Computational cost of sampling).** Given the precomputation in Theorem 3.1, it requires \( \mathcal{O}(nN) \) work to compute \( \|v_k(i)\|_2 \) for all \( i \) and \( k \) as the input of Algorithm 3.1, and it requires \( \mathcal{O}(n + d/\epsilon^2) \) work to compute every estimator, where \( \epsilon \) is a prescribed accuracy that does not depend on \( n \).

**Proof.** Recall Eq. (3.5) that \( \|v_k(i)\|_2 \) is proportional to the norm of a column in \( C_{i}^t \). Since every \( C_{i}^t \) is a \( d \)-by-\( d \) matrix, computing all the norms requires \( \mathcal{O}(d^2 n L) = \mathcal{O}(nN) \) work. Once all \( \|v_k(i)\|_2 \) have been computed, the sampling probabilities in Eq. (3.6) and the estimator in Eq. (3.7) requires \( \mathcal{O}(n) \) and \( \mathcal{O}(d/\epsilon^2) \) work, respectively. 

\( \blacksquare \)
4. \( \mathcal{H} \)-matrix approximation.\ This section introduces the \( \mathcal{H} \)-matrix approximation of the GNH matrix for the MLP. While the low-rank and the block-diagonal approximations focus on the global and the local structure of the problem, respectively. The \( \mathcal{H} \)-matrix approximation handles both as they may be equally important.

4.1. Overall algorithm.\ Here we take advantage of the existing \textsc{GOFMM} method \[44, 45, 46\], which evaluates \( \mathcal{O}(N) \) entries in a symmetric positive definite (SPD) matrix \( H \in \mathbb{R}^{N \times N} \) to construct the \( \mathcal{H} \)-matrix approximation \( H_{\text{GOFMM}} \) such that
\[
\|H - H_{\text{GOFMM}}\| \leq \epsilon \|H\|,
\]
where \( \epsilon \) is a prescribed tolerance.

Since \textsc{GOFMM} requires only entry-wise evaluation of the input matrix, we apply it with our fast evaluation algorithm to the regularized GNH matrix (note the GNH matrix is symmetric positive semi-definite, so we always add a small regularization of \( \lambda \) times the identity matrix, where \( \lambda^2 \) is the unit roundoff). The overall algorithm that computes the \( \mathcal{H} \)-matrix approximation (and approximate factorization) of the GNH matrix using the \textsc{GOFMM} method is shown in Algorithm 4.1.

The error analysis of Algorithm 4.1 is the following. Let \( \tilde{H}_\lambda = \tilde{H} + \lambda I \) be computed by Algorithm 3.1 and \( \lambda > 0 \) is a regularization, and \( \tilde{H}_{\text{GOFMM}} \) be the approximation of \( \tilde{H}_\lambda \) computed by \textsc{GOFMM}. Then the error between the output \( \tilde{H}_{\text{GOFMM}} \) from Algorithm 4.1 and the (regularized) GNH matrix \( H_\lambda = H + \lambda I \) is
\[
\|H_\lambda - \tilde{H}_{\text{GOFMM}}\| = \|H_\lambda - \tilde{H}_\lambda + \tilde{H}_\lambda - \tilde{H}_{\text{GOFMM}}\| \leq \|H - \tilde{H}\| + \|\tilde{H}_\lambda - \tilde{H}_{\text{GOFMM}}\|,
\]
where the first term is the sampling error from Algorithm 3.1 and the second term is the \textsc{GOFMM} approximation error. For simplicity, we drop the regularization parameter for the rest of this paper.

4.2. \textsc{GOFMM} overview.\ Given an SPD matrix \( H \), the \textsc{GOFMM} takes two steps to construct the \( \mathcal{H} \)-matrix approximation as follows. First of all, a permutation matrix \( P \) is computed to reorder the original matrix, which often corresponds to a hierarchical domain decomposition for applications in two- or three-dimensional physical spaces. The recursive domain partitioning is often associated with a tree data structure \( T \). Unlike methods targeting applications in physical spaces, the \textsc{GOFMM} does not require the use of geometric information (thus its name “geometry-oblivious fast multipole method”), which does not exist for neural networks.
Instead of relying on geometric information, the GOFMM exploits the algebraic distance measure that is implicitly defined by the input matrix $H$. As a matter of fact, any SPD matrix $H \in \mathbb{R}^{N \times N}$ is the Gram matrix of $N$ unknown Gram vectors $\{\phi_i\}_{i=1}^N$ [22]. Therefore, the distance between two row/column indices $i$ and $j$ can be defined as

$$d_{ij} = \|\phi_i - \phi_j\| = \sqrt{H_{ii} - 2H_{ij} + H_{jj}},$$

or

$$d_{ij} = \sin^2(\angle(\phi_i, \phi_j)) = 1 - \frac{H_{ij}^2}{(H_{ii}H_{jj})}.$$

With either definition, the GOFMM is able to construct the permutation $P$ and a balanced binary tree $T$.

The second step is to approximate the reordered matrix $P^T HP$ by

$$H_{\text{GOFMM}} = \begin{bmatrix} H_{11} & 0 & 0 \\ 0 & H_{rr} \\ 0 & S_{r1} & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ S_{r1} \\ 0 \end{bmatrix} + U_{r1} V_{r1}^T,$$

where $H_{11}$ and $H_{rr}$ are two diagonal blocks that have the same structure as $H_{\text{GOFMM}}$ unless their sizes are small enough to be treated as dense blocks, which occurs at the leaf level of the tree $T$; $S_{r1}$ and $S_{r2}$ are block-sparse matrices, and $U_{r1} V_{r1}^T$ and $U_{r2} V_{r2}^T$ are low-rank approximations of the remaining off-diagonal blocks in $H$. These bases are computed recursively with a post-order traversal of $T$ using the interpolative decomposition [18] and a nearest neighbor-based fast sampling scheme. There is a trade-off here: while the so-called weak-admissibility criteria sets $S_{r1}$ and $S_{r2}$ to zero and obtains relatively large ranks, the so-called strong-admissibility criteria selects $S_{r1}$ and $S_{r2}$ to be certain subblocks in $H$ corresponding to a few nearest neighbors/indices of every leaf node in $T$ and achieves smaller (usually constant) ranks.

Here we focus on the hierarchical semi-separable (HSS) format among other types of hierarchical matrices. Technically speaking, the HSS format means $S_{r1}$ and $S_{r2}$ are both zero and the bases $U_{r1} V_{r1}$ and $U_{r2} V_{r2}$ of a node in $T$ are recursively defined through the bases of the node’s children, i.e., the so-called nested bases.

### 4.3. Summary & comparison of complexity

We summarize the storage and computational complexity of our $H$-matrix approximation method (HM), and compare HM with three reference methods, namely, the Hessian-free method (HF) [28, 32], the Kronecker-factorization (K-FAC) [30, 31] and the randomized singular value decomposition (RSVD, Algorithm 5.1 in [18]). As before, we assume the MLP network has $L$ layers of constant layer sizes $d$, so the number of weights is $N = d^2 L$. We also assume the number of data points is $n$. The four algorithms of interest are as follows.

**HM.** The algorithm is given in Algorithm 4.1. Suppose the rank is $r_o$ in the $H$-matrix approximation; The GOFMM needs to call Algorithm 3.1 $O(N r_o)$ times ($O((d + n) N r_o)$ work), and it requires $O(N r_o^2)$ work to compute the approximation and its factorization, which has $O(N r_o)$ storage and can be applied to a vector with $O(N r_o)$ work. These are standard results in the HSS literature [33, 39, 21].

**MF.** The (iterative) Hessian-free methods [28, 32] combine the conjugate gradient (CG) method and the matrix-free matvec for solving linear systems and eigenvalue problems. The method is based on the two primitives in Table 1, where every iteration costs $O(Nn)$ work.
and storage. The number of CG iteration is generally upper bounded by \( \log(\frac{1}{\epsilon}) \sqrt{\kappa} \), where \( \epsilon \) is a prescribed accuracy and \( \kappa \) is the condition number of the (regularized) GNH matrix.

**RSVD [18].** Recall the definition \( H = J^T Q J \) in Eq. (1.2). Assume \( Q \) is an identity to simplify the presentation. The algorithm is to compute an approximate SVD of \( J \), which leads to an approximate eigenvalue decomposition of \( H \). The algorithm is the following.

First, we apply the back-propagation in Table 1 with a random Gaussian matrix as input. Second, the QR decomposition of the result is used to estimate the row space of \( J \). Third, the linearized forward is applied to project \( J \) onto the approximate row space, and finally, the SVD is computed on the projection. Overall, the storage is \( O(Nr) \), and the work required is \( \mathcal{O}(Nnr + Nr^2 + dnr^2) \), where \( r \) is the numerical rank from the QR decomposition.

**K-FAC [31, 30].** The algorithm computes an approximation of the Fisher matrix \( F \). Let a column vector \( g = [\text{vec}(g^1), \ldots, \text{vec}(g^L)] \in \mathbb{R}^N \) (\( g^i \) defined in Table 1) be the network gradient, and \( F = \mathbb{E}[gg^T] \) be a \( L \)-by-\( L \) block matrix with block size \( d^2 \)-by-\( d^2 \). Note the expectation here is taken with respect to both the empirical input data distribution \( \hat{Q}_{x,0} \) and the network’s predictive distribution \( P_{y|x} \). In particular, the \((\ell_1, \ell_2)\)-th block \((\ell_1, \ell_2 = 1, 2, \ldots, L)\) is given by

\[
F_{\text{block}}(\ell_1, \ell_2) = \mathbb{E}[\text{vec}(g^{\ell_1})\text{vec}(g^{\ell_2})^T]
\]

\[
= \mathbb{E}[M^{\ell_1} z^{\ell_1}(x^{\ell_1-1})^T \left( M^{\ell_2} z^{\ell_2}(x^{\ell_2-1})^T \right)^T]
\]

\[
= \mathbb{E}[\left( M^{\ell_1} z^{\ell_1} \otimes x^{\ell_1-1} \right) \left( M^{\ell_2} z^{\ell_2} \otimes x^{\ell_2-1} \right)^T]
\]

\[
= \mathbb{E}[\left( M^{\ell_1} z^{\ell_1} \otimes x^{\ell_1-1} \right) \left( (M^{\ell_2} z^{\ell_2})^T \otimes (x^{\ell_2-1})^T \right)]
\]

\[
= \mathbb{E}[M^{\ell_1} z^{\ell_1} (M^{\ell_2} z^{\ell_2})^T \otimes x^{\ell_1-1}(x^{\ell_2-1})^T]
\]

\[
\approx \mathbb{E}[M^{\ell_1} z^{\ell_1} (M^{\ell_2} z^{\ell_2})^T] \otimes \mathbb{E}[x^{\ell_1-1}(x^{\ell_2-1})^T]
\]

where Eq. (4.1) uses the definition of the network gradient in Table 1, Eq. (4.2) uses the definition of Kronecker product, Eq. (4.3) and Eq. (4.4) use the properties of Kronecker product, and Eq. (4.5) assumes certain statistical independence (see Section 6.3.1 in [30]). In Eq. (4.5), the expectation in the first term is taken with respect to both \( \hat{Q}_{x,0} \) and \( P_{y|x} \), and in the second term is taken with respect to \( \hat{Q}_{x,0} \). To compute the first expectation, \( k \) samples are drawn from the distribution \( P_{y|x} \propto \exp(-f(x^L_t, y)) \), where \( x^L_t \) is the network’s output corresponding to input \( x^0_t \). In practice, an additional block diagonal \((\ell_1 = \ell_2)\) or block tri-diagonal \(|\. -- 1| \leq 1 \) approximation is used for fast inversion purposes. The main cost of the algorithm is constructing, updating and inverting \( \mathcal{O}(L) \) matrices of size \( d \)-by-\( d \), which requires \( \mathcal{O}(d^2 L) = \mathcal{O}(N) \) storage and \( \mathcal{O}(nk + dN) \) work.

We summarize the above results in Table 2, where we further assume \( r, r_o \) and \( d \) are smaller than \( n \). Notice that the construction cost of the three methods: the RSVD, the K-FAC and the HM are \( r, k \) and \( r_o \) times the cost of the matrix-free matvec, respectively.

**5. Experimental Results.** In this section, we show (1) the cost and the accuracy of our \( \mathcal{H} \)-matrix approximations, (2) the memory savings from using the precomputation algorithm \( (\mathcal{O}(N^2) \rightarrow \mathcal{O}(Nn)) \), and (3) the efficiency of the fast sampling algorithm.
Table 2: Comparison of asymptotic complexities among four methods for the GNH matrix: the MF is based on the CG and the matrix-free matvec; the RSVD computes the low-rank approximation; the K-FAC assumes certain statistical independence (Eq. (4.5)) and uses the block-diagonal or block-tridiagonal approximation; the HM uses the $\mathcal{H}$-matrix approximation.

| Method | MF | RSVD | K-FAC | HM |
|--------|----|------|-------|----|
| matvec | $O(Nn)$ | $O(Nr)$ | $O(Nd)$ | $O(Nr_o)$ |
| construction | - | $O(Nnr)$ | $O(Nnk)$ | $O(Nnr_o)$ |
| storage | $O(Nn)$ | $O(Nr)$ | $O(Nd)$ | $O(Nr_o)$ |
| solve | $O(Nn\sqrt{\kappa})$ | $O(Nr)$ | $O(Nd)$ | $O(Nr_o)$ |

MF: $\sqrt{\kappa}$ iteration generally, where $\kappa$ is the condition number.
HM: the precomputation requires $O(Nn)$ storage and $O(Nnd)$ work.

**Machine.** All experiments were performed using single precision on a single node from the Texas Advanced Computing Center “Stampede 2” system, which has two sockets with 48 cores of Intel Xeon Platinum 8160 (“Skylake”) and 192 GB of RAM.

**Networks and datasets.** We focus on classification networks and autoencoder networks with the MNIST and CIFAR-10 datasets. In the following, we denote networks’ layer sizes as $d_1 \rightarrow d_2 \rightarrow \ldots \rightarrow d_L$ from the input layer to the output layer. Every network has been trained using the stochastic gradient descent for a few steps, so the weights are not completely random.

1. “classifier”: classification networks with the ReLU activation and the cross-entropy loss.
   (a) $N=15,910$; MNIST dataset; layer sizes: 784 $\rightarrow$ 20 $\rightarrow$ 10.
   (b) $N=61,670$; CIFAR-10 dataset; layer sizes: 3072 $\rightarrow$ 20 $\rightarrow$ 10.
   (c) $N=203,530$; MNIST dataset; layer sizes: 784 $\rightarrow$ 256 $\rightarrow$ 10.
   (d) $N=789,258$; CIFAR-10 dataset; layer sizes: 3072 $\rightarrow$ 256 $\rightarrow$ 10.

2. “AE”: autoencoder networks with the softplus activation (sigmoid activation at the last layer) and the mean-squared loss.
   (a) $N=16,474$; MNIST dataset; layer sizes: 784 $\rightarrow$ 10 $\rightarrow$ 784.
   (b) $N=64,522$; CIFAR-10 dataset; layer sizes: 3072 $\rightarrow$ 10 $\rightarrow$ 3072.
   (c) $N=125,972$; CIFAR-10 dataset; layer sizes: 3072 $\rightarrow$ 20 $\rightarrow$ 3072.
   (d) $N=248,872$; CIFAR-10 dataset; layer sizes: 3072 $\rightarrow$ 40 $\rightarrow$ 3072.

**GOFMM parameters.** We focus on three parameters in the GOFMM that control the accuracy of the $\mathcal{H}$-matrix approximation: (1) the leaf node size $m$ of the hierarchical partitioning $T$ (equivalent to setting the number of tree levels), (2) the maximum rank $r_o$ of off-diagonal blocks, and (3) the accuracy $\tau$ of low-rank approximations. In particular, we test two levels of accuracies: “low” and “high”, where “low” stands for $m=128$, $r_o=128$, $\tau=5E-2$, and “high” stands for $m=1024$, $r_o=1024$, $\tau=1E-5$.

**Notations.** We report the following results for our experiments.
- $t_{\text{build}}$: time of constructing the $\mathcal{H}$-matrix approximation of the GNH matrix.
- $t_{\text{matv}}$: time of applying the $\mathcal{H}$-matrix approximation to 128 random vectors.
- $\%K$: compression rate of the $\mathcal{H}$-matrix approximation, i.e., ratio between the $\mathcal{H}$-matrix storage and the GNH matrix storage.
• $\epsilon_F$: relative error of the $H$-matrix approximation measured in Frobenius norm, estimated by $\|Hx - H_{GOFMM}x\|_F / \|Hx\|_F$, where $x \in \mathbb{R}^{N \times 128}$ is a Gaussian random matrix.

5.1. Cost and accuracy of $H$-matrix approximation. Table 3 shows results of our $H$-matrix approximations for networks that have relatively small numbers of parameters. The GNH matrices are computed and fully stored in memory.

As Table 3 shows, the approximation can achieve four digits’ accuracy except for one network (two digits) when the accuracy of low-rank approximations is 1E-5. Since we have enforced the maximum rank $r$, the runtime of constructing $H$-matrix approximations ($t_{\text{build}}$) increases roughly proportionally to the number of network parameters, and the compression rate scales inverse proportionally to the number of parameters. As a result, applying the $H$-matrix approximations to 128 random vectors took less than one second for the five networks. These $H$-matrix approximations can be factorized in linear time for solving linear systems and eigenvalue problems.

### Table 3: Timing ($t_{\text{build}}$ and $t_{\text{matv}}$), compression rate ($%K$) and accuracy ($\epsilon_F$) of $H$-matrix approximations corresponding to low- and high-accuracy settings, respectively. $t_{\text{build}}$ is the time of applying the GOFMM on the GNH matrices, which were computed with 1000 data points ($n = 1000$ in Eq. (1.2)).

| # | network | $N$ | accuracy | $t_{\text{build}}$ | $t_{\text{matv}}$ | %K          | $\epsilon_F$ |
|---|---------|-----|----------|---------------------|-------------------|-------------|--------------|
| 1 | classifier (a) | 16k | low      | 0.24                | 0.03              | 1.80%       | 1.5E-1       |
| 2 |         |     | high     | 5.74                | 0.11              | 13.59%      | 4.4E-4       |
| 3 | classifier (b) | 61k | low      | 0.42                | 0.08              | 0.57%       | 4.7E-1       |
| 4 |         |     | high     | 13.28               | 0.33              | 4.78%       | 4.0E-2       |
| 5 | AE (a)   | 16k | low      | 0.27                | 0.03              | 1.25%       | 1.2E-1       |
| 6 |         |     | high     | 5.67                | 0.10              | 11.38%      | 6.5E-4       |
| 7 | AE (b)   | 64k | low      | 0.43                | 0.08              | 0.53%       | 5.5E-3       |
| 8 |         |     | high     | 13.26               | 0.38              | 4.62%       | 6.6E-4       |
| 9 | AE (c)   | 126k| low      | 0.87                | 0.17              | 0.28%       | 4.1E-3       |
|10 |         |     | high     | 24.10               | 0.94              | 2.32%       | 5.2E-4       |

Comparison with RSVD and K-FAC. Table 4 shows the accuracies of our method (HM), the RSVD and the K-FAC under about the same compression rate for the low- and high-accuracy settings, respectively. For the RSVD, the storage is $rN$ entries, where $r$ is the numerical rank of the (symmetric) GNH matrix, so the compression rate is $r/N$. For the K-FAC, we use the relatively more accurate block tri-diagonal version. The compression rate of the K-FAC is defined as $k/N$, and the reason is that the construction of the RSVD and the K-FAC requires the same number of back-propagation if $k = r$ (recall Table 2). So we choose $k$ and $r$ to be the same value such that the corresponding compression rate of the RSVD and the K-FAC are slightly higher than the HM.

As Table 4 shows, the $H$-matrix approximation achieved higher accuracy than the RSVD and the K-FAC for most cases, especially for the high accuracy setting. For the RSVD, suppose
Table 4: Comparison of accuracies ($\epsilon_F$) among the $H$-matrix approximation (HM), the RSVD and the K-FAC with about the same compression rate ($\%K$) for the low- and high-accuracy settings, respectively. For the RSVD and the K-FAC, the compression rate means $r/N$ and $k/N$, respectively, where $r$ is the rank and $k$ is the number of random samples. For all cases, the GNH matrices correspond to 10,000 data points ($n = 10,000$ in Eq. (1.2)).

|       | HM-low | HM-high | RSVD-low | RSVD-high | KFAC-low | KFAC-high |
|-------|--------|---------|----------|-----------|----------|-----------|
| AE (a)| %K     | $\epsilon_F$ | 1.23%    | 11.77%    | 1.40%    | 12.14%    |
|       |        |         |        | 12.14%    | 1.40%    | 12.14%    |
| AE (b)| %K     | $\epsilon_F$ | 0.53%    | 4.62%     | 0.62%    | 4.65%     |
|       |        |         |        | 4.65%     | 0.62%    | 4.65%     |
| AE (c)| %K     | $\epsilon_F$ | 0.28%    | 2.31%     | 0.32%    | 2.38%     |
|       |        |         |        | 2.38%     | 0.32%    | 2.38%     |

the eigenvalues of the GHN matrix are $\{\sigma_i\}$, and the error of the rank-$k$ approximation measured in the Frobenius norm is proportional to $(\sum_{i>k} \sigma_i^2)^{1/2}$. For autoencoder (b) and (c), the spectrums of the GNH matrices decay slowly, so the RSVD is not efficient. For the K-FAC, the approximation that the expectation of a Kronecker product equals to the Kronecker product of expectations (Eq. (4.5)) is, in general, not exact. As a result, the convergence is slow.

5.2. Memory savings. Table 5 shows the memory footprint between our precomputation Eq. (3.4) and the full GNH matrix, i.e., $O(N^2)$. Recall Theorem 3.1 that the storage of our precomputation is $O(nN)$, where $n$ is the number of data points.

As Table 5 shows, our precomputation has a much smaller memory footprint compared with storing the full GNH matrix. This allows using the GOFMM method for networks that have a large number of parameters. For example, the storage of the GNH matrix for classifier (d) network requires more than 2 TB! But we were able to run GOFMM with the compressed storage (at the price of spending $O(dn)$ work for the evaluation of every entry).

5.3. Fast Monte Carlo sampling. Table 6 shows the accuracy of our fast Monte Carlo sampling scheme for a sequence of increasingly large data sizes for classifier (d) network. The relative error measured in the Frobenius norm is between the exact GNH matrix $H$ and the approximation $\tilde{H}$ computed using Algorithm 3.1 with a prescribed number of random samples. For reference, we also run the same sampling scheme but with a uniform probability distribution.

As Table 6 shows, when the number of random samples increases by $100 \times$, the accuracy improves by $10 \times$, which confirms the convergence rate in Theorem 3.2. Importantly, the error bound and the convergence rate do not depend on the problem size $n$, which is verified by results in the same column. Last, our sampling scheme outperforms the uniform sampling by more than an order of magnitude. In other words, the uniform sampling requires $10 \times$ more random samples to achieve the same accuracy as our sampling scheme.
Table 5: Comparison of memory footprint (in single-precision) between our precomputation (Eq. (3.4)) and the full GNH (same size as the Hessian). For every network, we show the compression rate and accuracy of $\mathcal{H}$-matrix approximations for two levels of accuracies. For all cases, the GNH matrices correspond to 100 data points.

|        | $N$ | $M_{ours}$ | $M_{GNH}$ | accuracy | $\%K$ | $\epsilon_F$ |
|--------|-----|------------|-----------|----------|-------|--------------|
| classifier (c) | 203k | 14 MB | 165 GB | low | 0.065% | 1.3E−1 |
|          |     |           |           | high  | 0.429% | 6.7E−5 |
| classifier (d) | 789k | 2 MB | 2491 GB | low  | 0.029% | 3.1E−1 |
|          |     |           |           | high  | 0.104% | 2.3E−4 |
| AE (d)  | 248k | 3.8 GB | 247 GB | low  | 0.299% | 2.7E−2 |
|          |     |           |           | high  | 1.21%  | 1.6E−3 |

Table 6: Accuracy of our fast Monte Carlo (FMC) sampling scheme for increasing sizes of data points. The error $\epsilon_K = \| H - \tilde{H}\|_F / \| H\|_F$, where $H$ and $\tilde{H}$ are the exact GNH matrix of classifier (d) and the approximation computed using $K$ random samples in Algorithm 3.1, respectively. The reference uniform sampling scheme uses a uniform sampling probability instead of Eq. (3.6) in Algorithm 3.1.

| $n$   | scheme | $\epsilon_{10}$ | $\epsilon_{100}$ | $\epsilon_{1000}$ | $\epsilon_{10,000}$ |
|-------|--------|------------------|------------------|------------------|------------------|
| 100   | uniform | 1.51E-0          | 3.94E-1          | 1.32E-1          | 3.85E-2          |
|       | FMC    | 3.70E-1          | 1.17E-1          | 3.70E-2          | 1.18E-2          |
| 1000  | uniform | 1.05E-0          | 3.08E-1          | 9.58E-2          | 3.57E-2          |
|       | FMC    | 2.50E-1          | 7.95E-2          | 2.48E-2          | 7.89E-3          |
| 10,000| uniform | 1.52E-0          | 4.85E-1          | 2.38E-1          | 4.87E-2          |
|       | FMC    | 4.56E-1          | 1.45E-1          | 4.59E-2          | 1.45E-2          |

$\mathcal{H}$-matrix approximation with sampling. Table 7 shows the error of Algorithm 4.1 for a sequence of increasingly large number of random samples. Recall that Algorithm 4.1 computes the $\mathcal{H}$-matrix approximation $\tilde{H}_{GOFMM}$ for the (inexact) GNH matrix, namely $\tilde{H}$ from Algorithm 3.1. The error between the $\mathcal{H}$-matrix approximation $\tilde{H}_{GOFMM}$ and the exact GNH matrix, namely $H$ is

$$\| H - \tilde{H}_{GOFMM}\| = \| H - \tilde{H} + \tilde{H} - \tilde{H}_{GOFMM}\| \leq \| H - \tilde{H}\| + \| \tilde{H} - \tilde{H}_{GOFMM}\|,$$

where the first term is the sampling error, and the second term is the $\mathcal{H}$-matrix approximation error. As Table 6 shows, the former converges to zero and is independent of the data size. Table 7 shows that the latter also converges as the sampling becomes increasingly accurate, which justifies the overall approach.

6. Conclusions. We have presented a fast method to evaluate entries in the GNH matrix of the MLP network, and our method is consisted of two parts: a precomputation algorithm and
Table 7: $\mathcal{H}$-matrix approximation with and without sampling. Without sampling, the GNH matrix is computed exactly using 100 data points for classifier (a) network. The compression rate and the accuracy are shown for low- and high-accuracy settings, respectively. The error of our sampling algorithm is $\epsilon_K = \| H - \tilde{H} \|_F / \| H \|_F$, where $H$ and $\tilde{H}$ are the exact GNH matrix and approximated GNH computed using $K$ random sampling in Algorithm 3.1, respectively. With 100 samples, $\epsilon_{100}^{100} = 0.074$; with 1000 samples, $\epsilon_{1000}^{1000} = 0.024$; with 10,000 samples, $\epsilon_{10,000} = 0.0074$.

|        | no sampling/exact | 100 samples | 1000 samples | 10,000 samples |
|--------|-------------------|-------------|--------------|---------------|
| accuracy | %K | $\epsilon_F$ | %K | $\epsilon_F$ | %K | $\epsilon_F$ |
| low    | 0.70% | 5.5E−2 | 1.56% | 1.5E−1 | 0.95% | 7.5E−2 | 0.74% | 9.6E−3 |
| high   | 5.60% | 4.1E−5 | 17.43% | 6.0E−2 | 17.43% | 1.9E−2 | 17.43% | 1.1E−3 |

a fast Monte Carlo algorithm. While the precomputation allows evaluating entries in the GNH matrix exactly with reduced storage, the random sampling is based on the precomputation and further accelerates the evaluation. With the new method, we can apply GOFMM to construct the $\mathcal{H}$-matrix approximation for the GNH matrix. As a result, we obtain an $\mathcal{H}$-matrix (and its factorization) that can be used for solving linear systems and eigenvalue problems with the GNH in linear complexity.

Extensions of the proposed framework to multi-core, many-core and distributed-memory parallel platforms are straightforward. GOFMM already supports corresponding parallel capabilities [44, 45, 46]. The precomputation algorithm can be parallelized using a parallel-scan type of algorithm, and it can be done in a data parallel fashion over different partitions of the dataset. The sampling algorithm is also straightforward to parallel using data parallelism.

Two important directions for future research are (1) extending our method to other types of networks such as convolutional networks, where weight matrices are highly structured, (preliminary experiments on the VGG network show similar results as those in Table 3) and (2) incorporating our method in the context of a learning task, which would also require several algorithmic choices related to optimization, such as initialization, damping and adding momentum.

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