# Approximating Large-Scale Hessian Matrices Using Secant Equations

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Consider the optimization problem

$$\min_x f(x),$$

where $f(x)$ is twice differentiable function of $n$ variables.

Gradient

$$g(x) := \nabla f(x)$$

Hessian matrix

$$H(x) := \nabla^2 f(x)$$

Our interest is $n$ large and $H(x)$ sparse

# Summary

- Large-scale optimization algorithms frequently require large sparse Hessian matrices $H(x)$
  For example, in a trust region method.
- How can we obtain good approximations to $H(x)$?
- We want fast and efficient approximation algorithm with scope to exploit parallelism.
- We propose a novel approach that seeks to satisfy as many componentwise secant equations as is necessary to define each row of the Hessian matrix.

# Why do we need an approximation?

In optimisation algorithms, there are both theoretical and practical benefits of having $H(x)$.

In practice, $H(x)$ is generally not readily available.

- Analytic expression unlikely.
- Backward mode of automatic differentiation, $g(x)$ costs small multiple of evaluating $f(x)$
- BUT $H(x)$ costs $\mathcal{O}(n)$ times that of $f(x)$.

**Key issue:** $n$ is LARGE

# Challenge

Build approximations $B^{(k)} = \{b_{ij}^{(k)}\}$ of $H(x)$ at a sequence of iterates $x^{(k)}$.

- Interest in approximating $H(x)$ dates back to 1960s.
- Focus was on $n$ small and $H(x)$ dense.
- Extensions to sparse case unsuccessful because either the formulae used generated dense matrices (impractical for large problems), or imposing sparsity led to numerical instability in the approximation algorithms.
- In 1990s, limited-memory strategy proposed (Fletcher, Grothey and Leyffer) that incorporated the curvature observed at a number of previous iterates. But no attempt to impose sparsity.

# Secant equations

Let $H^{(k)} = H(x^{(k)})$

Properties: $H^{(k)}$ is $n \times n$ symmetric matrix with known sparsity pattern.

**Aim:** use previously accumulated information to estimate $B^{(k)} \approx H^{(k)}$.

Define $s^{(l)} := x^{(l)} - x^{(l-1)}$ and $y^{(l)} := g(x^{(l)}) - g(x^{(l-1)})$

Construct $B^{(k)}$ that best satisfies the multiple *secant conditions*

$$B^{(k)} s^{(l)} = y^{(l)}, \qquad l = k - m + 1, \ldots, k$$

where $m$ is the number of past (known) data pairs $\{s^{(l)}, y^{(l)}\}$

# Secant equations

Construct $B^{(k)}$ that best satisfies the multiple *secant conditions*

$$B^{(k)}s^{(l)} = y^{(l)}, \qquad l = k - m + 1, \ldots, k.$$

For each $k$, solve convex quadratic programming problem

$$\min_{B^{(k)}} \sum_{l=k-m+1}^{k} \|B^{(k)}s^{(l)} - y^{(l)}\|_F^2$$

such that

$$B^{(k)} = (B^{(k)})^T \quad \text{and} \quad \mathcal{S}(B^{(k)}) = \mathcal{S}(H^{(k)}).$$

Here $\mathcal{S}(B) := \{(i,j) : b_{ij} \neq 0\}$ denotes sparsity pattern of $B$.

Prohibitively expensive for large $n$ within optimization code.

# New approach

Start with the case that all rows of $H^{(k)}$ are sparse.

Instead of imposing full secant conditions for each row $i$, we will satisfy as many *componentwise* equations

$$e_i^T B^{(k)} s^{(l)} = e_i^T y^{(l)}, \quad l = k, k-1, \ldots,$$

as are necessary to define the row.

Set $\mathcal{S}_i^{(k)} := \{j : h_{ij}^{(k)} \neq 0\}$ and $nz_i := |\mathcal{S}_i^{(k)}|$

Then for $l = k, k-1, \ldots, k - nz_i + 1$ we require

$$\sum_{j \in \mathcal{S}_i^{(k)}} b_{ij}^{(k)} s_j^{(l)} = y_i^{(l)}$$

Let $z_i^{(k)}$ denote the vector of entries in row $i$

Rewriting, $z_i^{(k)}$ is the solution of $nz_i \times nz_i$ dense linear system

$$A_i^{(k)} z_i^{(k)} = c_i^{(k)} \qquad (1)$$

where $(A_i^{(k)})_{lj} = s_j^{(l)}$ and $(c_i^{(k)})_l = y_i^{(l)}$.

**Example 1** Consider the $3 \times 3$ approximate Hessian matrix

$$B^{(k)} = \begin{pmatrix} b_{11}^{(k)} & b_{12}^{(k)} & 0 \\ b_{21}^{(k)} & 0 & b_{23}^{(k)} \\ 0 & b_{32}^{(k)} & b_{33}^{(k)} \end{pmatrix}, \quad \text{with } b_{12}^{(k)} = b_{21}^{(k)} \text{ and } b_{23}^{(k)} = b_{32}^{(k)}.$$

For row $i = 2$, $\mathcal{S}_2^{(k)} = \{1, 3\}$, $nz_2 = 2$ and system (1) is

$$\underbrace{\begin{pmatrix} s_1^{(k)} & s_3^{(k)} \\ s_1^{(k-1)} & s_3^{(k-1)} \end{pmatrix}}_{A_2^{(k)}} \underbrace{\begin{pmatrix} b_{21}^{(k)} \\ b_{23}^{(k)} \end{pmatrix}}_{z_2^{(k)}} = \underbrace{\begin{pmatrix} y_2^{(k)} \\ y_2^{(k-1)} \end{pmatrix}}_{c_2^{(k)}}.$$

## Algorithm 1: Sparse Hessian approximation (row-wise independent)

1: **for** $i = 1, \ldots, n$ **do**
2: Compute row $i$ by constructing and solving system (1).
3: **end for**
4: Symmetrise $B^{(k)} := (B^{(k)} + (B^{(k)})^T)/2$.

Important: the rows can be computed in parallel in any order.

But averaging the off-diagonal entries does not truly take symmetry into account.

Also, only one triangle of $B^{(k)}$ may be available.

Rewrite the system

$$A_i^{(k)} z_i^{(k)} = c_i^{(k)} \qquad (1)$$

$$U_i^{(k)} \tilde{z}_i^{(k)} = c_i^{(k)} - K_i^{(k)} w_i^{(k)}, \qquad (2)$$

where

- $w_i^{(k)}$ holds the entries in row $i$ of $B^{(k)}$ that are already known.
- $\tilde{z}_i^{(k)}$ holds the $nu_i$ unknown entries in row $i$.
- $U_i^{(k)}$ is a square matrix of order $nu_i \leq nz_i$.

**Example 2** Consider the $5 \times 5$ approximate Hessian matrix

$$B^{(k)} = \begin{pmatrix} b_{11}^{(k)} & 0 & 0 & b_{14}^{(k)} & 0 \\ 0 & b_{22}^{(k)} & 0 & b_{24}^{(k)} & 0 \\ 0 & 0 & 0 & b_{34}^{(k)} & 0 \\ b_{41}^{(k)} & b_{42}^{(k)} & b_{43}^{(k)} & b_{44}^{(k)} & b_{45}^{(k)} \\ 0 & 0 & 0 & b_{54}^{(k)} & b_{55}^{(k)} \end{pmatrix}.$$

Assume rows are computed in the natural order $1, 2, 3, 4, 5$.

In row 4, $b_{41}^{(k)}, b_{42}^{(k)}, b_{43}^{(k)}$ are already known by symmetry. Hence $nu_4 = 2$.

$$\underbrace{\begin{pmatrix} s_4^{(k)} & s_5^{(k)} \\ s_4^{(k-1)} & s_5^{(k-1)} \end{pmatrix}}_{U_4^{(k)}} \underbrace{\begin{pmatrix} b_{44}^{(k)} \\ b_{45}^{(k)} \end{pmatrix}}_{\tilde{z}_4^{(k)}} = \underbrace{\begin{pmatrix} y_4^{(k)} \\ y_4^{(k-1)} \end{pmatrix}}_{c_4^{(k)}} - \underbrace{\begin{pmatrix} s_1^{(k)} & s_2^{(k)} & s_3^{(k)} \\ s_1^{(k-1)} & s_2^{(k-1)} & s_3^{(k-1)} \end{pmatrix}}_{K_4^{(k)}} \underbrace{\begin{pmatrix} b_{14}^{(k)} \\ b_{24}^{(k)} \\ b_{34}^{(k)} \end{pmatrix}}_{w_4^{(k)}}.$$

The order in which the rows are processed is now important.

## Algorithm 2: Sparse Hessian approximation (row-wise dependent)

1: Compute adjacency graph $\mathcal{G}(B^{(k)})$ and degree* of each vertex.
2: **for** $i = 1, \ldots, n$ **do**
3: Select vertex $v$ of minimum degree; let corresponding row be $row_i$.
4: Compute the $nu_i$ unknown entries in $row_i$ by solving a linear system of order $nu_i$.
5: Remove $v$; decrement degree of each remaining neighbour by 1.
6: **end for**

* initially the degree is the number of entries in the corresponding row

Problems:

- serial approach;
- inaccurate estimates from earlier steps can be magnified when solving for current row, leading to large error growth, particularly if some rows have a large number of entries. This happens in practice!

## Numerical experiments to illustrate the issues

- Examples from CUTEst test set
- Results for fixed Hessian $H(x^{(k)}) = H$ for all $k$.
- Randomly generate $s^{(l)} \in (-1, 1)$ and then compute $y^{(l)} = Hs^{(l)}$ for $l = 1, \ldots, m$.
- If the linear system to be solved for the unknowns in a row is under or over determined then compute the linear least squares solution (using an SVD decomposition).

Check results using maximum and median relative componentwise error

$$max\_rel\_err = \max_{(i,\, j)\in\mathcal{S}(H)} |b_{ij} - h_{ij}|/\max(1, |h_{ij}|),$$

$$med\_rel\_err = \operatorname{median}_{(i,\, j)\in\mathcal{S}(H)} |b_{ij} - h_{ij}|/\max(1, |h_{ij}|),$$

## Results with $m = 100$

| identifier | $nnz(row)$ | Algorithm 1 | | Algorithm 2 | |
|---|---|---|---|---|---|
| | | *max_rel_err* | *med_rel_err* | *max_rel_err* | *med_rel_err* |
| CURLY30 | 61 | 8.83E-10 | 9.69E-15 | 6.00E-06 | 9.29E-12 |
| NCVXBQP1 | 9 | 1.41E-09 | 1.22E-15 | ‡ | 2.59E+01 |
| SINQUAD | 5000 | 9.77E-01 | 2.30E-16 | 3.66E-11 | 2.30E-16 |
| SPARSQUR | 56 | 3.24E-09 | 1.69E-14 | ‡ | ‡ |
| LUKVLE12 | 2502 | 9.55E-01 | 6.33E-16 | 3.22E-09 | 1.63E-15 |
| MSQRTA | 64 | 3.69E-12 | 4.66E-15 | ‡ | ‡ |
| YATP1SQ | 352 | 2.10 | 9.44E-16 | 2.41E-09 | 9.44E-16 |

$nnz(row)$ denotes max number of entries in a row of $H$

‡ indicates error exceeds $10^{15}$

Conclude:

- Algorithm 1 has problems if rows are "dense".
- Algorithm 2 is unstable.

## How to overcome problems of simple approach?

Suppose $B^{(k)}$ has been permuted to form

$$\begin{pmatrix} B_{11}^{(k)} & B_{12}^{(k)} \\ B_{21}^{(k)} & B_{22}^{(k)} \end{pmatrix}, \quad \text{with} \quad B_{21}^{(k)} = (B_{12}^{(k)})^T.$$

- $B_{11}^{(k)}$ and $B_{22}^{(k)}$ are square symmetric matrices
- the $n_1 < n$ rows of $(B_{11}^{(k)} \; B_{12}^{(k)})$ are sparse
- remaining $n_2 = n - n_1 \ll n_1$ rows of $(B_{21}^{(k)} \; B_{22}^{(k)})$ considered "dense"

## Algorithm 3: Sparse-dense block parallel approach

- Use Algorithm 1 to compute sparse rows $(B_{11}^{(k)} \; B_{12}^{(k)})$ (parallel)
- Set $B_{21}^{(k)}$ by symmetry
- Use Algorithm 1 for small $n_2 \times n_2$ block $B_{22}^{(k)}$ (parallel)

## Example 3

$$B^{(k)} = \left(\begin{array}{cc|cc} b_{11}^{(k)} & 0 & b_{13}^{(k)} & b_{14}^{(k)} \\ 0 & 0 & b_{23}^{(k)} & b_{24}^{(k)} \\ \hline b_{31}^{(k)} & b_{32}^{(k)} & b_{33}^{(k)} & b_{34}^{(k)} \\ b_{41}^{(k)} & b_{42}^{(k)} & b_{43}^{(k)} & b_{44}^{(k)} \end{array}\right)$$

Rows 1 and 2 are sparse and rows 3 and 4 dense.
Linear system for dense row 3 is

$$\begin{pmatrix} s_3^{(k)} & s_4^{(k)} \\ s_3^{(k-1)} & s_4^{(k-1)} \end{pmatrix} \begin{pmatrix} b_{33}^{(k)} \\ b_{34}^{(k)} \end{pmatrix} = \begin{pmatrix} y_3^{(k)} \\ y_3^{(k-1)} \end{pmatrix} - \begin{pmatrix} s_1^{(k)} & s_2^{(k)} \\ s_1^{(k-1)} & s_2^{(k-1)} \end{pmatrix} \begin{pmatrix} b_{13}^{(k)} \\ b_{23}^{(k)} \end{pmatrix}$$

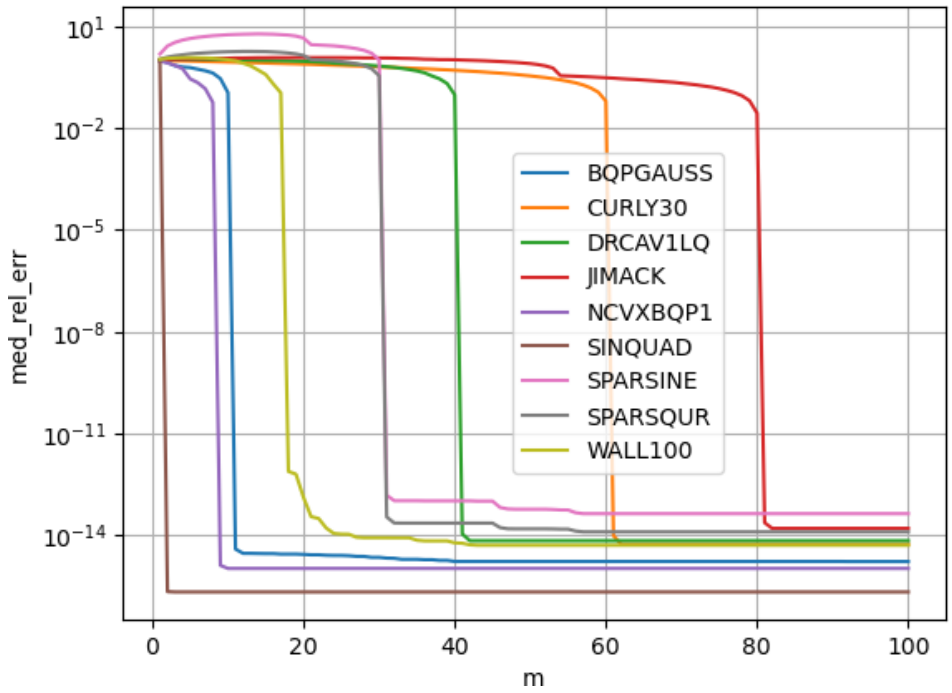
Similar expression for dense row 4.
Final value of entries (3,4) and (4,3) of $B^{(k)}$ is $(b_{34}^{(k)} + b_{43}^{(k)})/2$ (symmetrisation).

## Does this work? ($m = 100$)

| identifier | *max_rel_err* | *med_rel_err* | *serial* | *parallel* | *speedup* |
|---|---|---|---|---|---|
| CURLY30 | 5.41E-11 | 5.56E-15 | 4.55 | 0.34 | 13.23 |
| NCVXBQP1 | 3.15E-11 | 1.07E-15 | 0.53 | 0.05 | 10.06 |
| SINQUAD | 1.99E-11 | 2.17E-16 | 0.01 | 0.01 | 2.17 |
| SPARSQUR | 7.63E-10 | 1.28E-14 | 1.40 | 0.12 | 11.38 |
| LUKVLE12 | 4.48E-13 | 6.66E-16 | 0.04 | 0.01 | 4.78 |
| MSQRTA | 9.47E-13 | 2.66E-15 | 0.51 | 0.06 | 8.10 |
| YATP1SQ | 1.36E-11 | 9.17E-16 | 0.49 | 0.07 | 7.17 |

Times in seconds are on single core and 28 cores of a dedicated machine with 32 AMD Epyc 7502 CPUs clocked at 2.5GHz with 256 GB of RAM

Now vary number $m$ of past iterates. Plot is median relative error.




- If insufficient past data ($m$ too small) do not get accurate $H$
- Once $m$ sufficiently large, sharp transition to accurate $H$
- e.g, CURLY30 has a banded Hessian (bandwidth 61)

Can we do better?

## Algorithm 4: Recursive block parallel approach

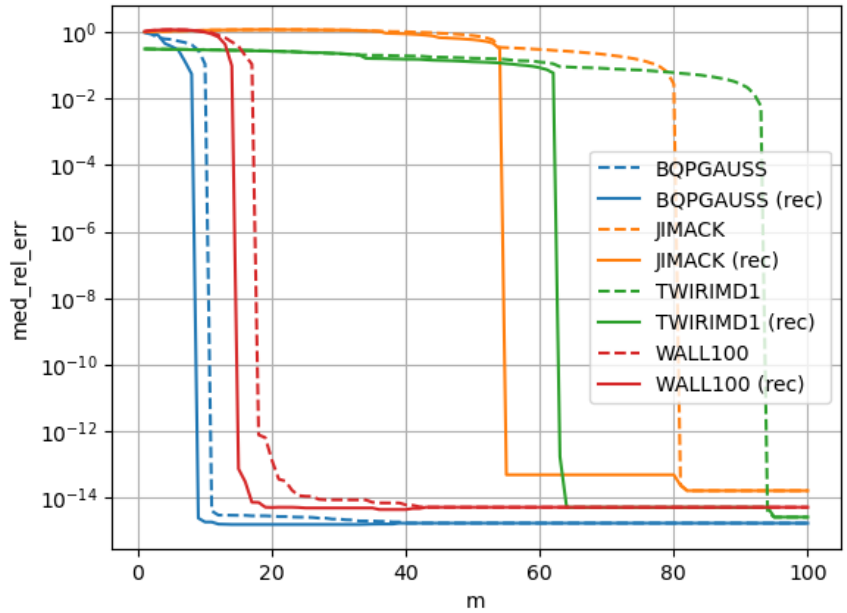
Apply block approach recursively.

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{12}^T & B_{22} \end{pmatrix} \implies B_{22} = \begin{pmatrix} B_{11}^{(1)} & B_{12}^{(1)} \\ (B_{12}^{(1)})^T & B_{22}^{(1)} \end{pmatrix} \implies B_{22}^{(1)} = \begin{pmatrix} B_{11}^{(2)} & B_{12}^{(2)} \\ (B_{12}^{(2)})^T & B_{22}^{(2)} \end{pmatrix}$$

Rows in $(B_{11}\ B_{12})$ are sparse. Compute with Algorithm 1.

Then set $B_{12}^T$. Repeat process on $B_{22}$ (split it into sparse and dense rows).

Problems for which recursion is beneficial.




- Can get good improvment with smaller $m$
- e.g, JIMACK ($nnz(row) = 81$)

## Concluding remarks

- We have addressed the problem of approximating large sparse Hessian matrices.
- We have proposed new algorithms and derived one that is efficient in parallel and stable.
- We obtain accurate approximate Hessians provided there is sufficient past data.
- The methods are available in the Fortran module `sha`, with a C interface, as part of the open-source GALAHAD library.

# Thank you for listening.

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