sparseHessianFD: An R Package for Estimating Sparse Hessian Matrices

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Abstract

Sparse Hessian matrices occur often in statistics, and their fast and accurate estimation can improve efficiency of numerical optimization and sampling algorithms. By exploiting the known sparsity pattern of a Hessian, methods in the sparseHessianFD package require many fewer function or gradient evaluations than would be required if the Hessian were treated as dense. The package implements established graph coloring and linear substitution algorithms that were previously unavailable to R users, and is most useful when other numerical, symbolic or algorithmic methods are impractical, inefficient or unavailable.

Keywords: sparse Hessians, sparsity, computation of Hessians, graph coloring, finite differences, differentiation, complex step.

The Hessian matrix of a log likelihood function or log posterior density function plays an important role in statistics. From a frequentist point of view, the inverse of the negative Hessian is the asymptotic covariance of the sampling distribution of a maximum likelihood estimator. In Bayesian analysis, when evaluated at the posterior mode, it is the covariance of a Gaussian approximation to the posterior distribution. More broadly, many numerical optimization algorithms require repeated computation, estimation or approximation of the Hessian or its inverse; see Nocedal and Wright (2006).

The Hessian of an objective function with M variables has M^2 elements, of which $M(M+1)/2$ are unique. Thus, the storage requirements of the Hessian, and computational cost of many linear algebra operations on it, grow quadratically with the number of decision variables. For applications with hundreds of thousands of variables, computing the Hessian even once might not be practical under time, storage or processor constraints. Hierarchical models, in which each additional heterogeneous unit is associated with its own subset of variables, are particularly vulnerable to this curse of dimensionality

However, for many problems, the Hessian is *sparse*, meaning that the proportion of "structural" zeros (matrix elements that are always zero, regardless of the value at which function is estimated) is high. Consider a log posterior density in a Bayesian hierarchical model. If the outcomes across units are conditionally independent, the cross-partial derivatives of heterogeneous variables across units are zero. As the number of units increases, the size of the Hessian still grows quadratically, but the number of *non-zero* elements grows only linearly; the Hessian becomes increasingly sparse. The row and column indices of the non-zero elements comprise the *sparsity pattern* of the Hessian, and are typically known in advance, before computing the values of those elements. R packages such as **trustOptim** (Braun 2014), **sparseMVN** (Braun

2015) and **ipoptr** (Wächter and Biegler 2006) have the capability to accept Hessians in a compressed sparse format.

The **sparseHessianFD** package is a tool for estimating sparse Hessians numerically, using either finite differences or complex perturbations of gradients. Section 1.1 will cover the specifics, but the basic idea is as follows. Consider a real-valued function $f(x)$, its gradient $\nabla f(x)$, and its Hessian $\mathsf{H}f(x)$, for $x \in \mathbb{R}^M$. Define the derivative vector as the transpose of the gradient, and a vector of partial derivatives, so $\mathsf{D}f(x) = \nabla f(x)^\top = (\mathsf{D}_1, \ldots, \mathsf{D}_M)$. (Throughout the paper, we will try to reduce notational clutter by referring to the derivative and Hessian as D and H, respectively, without the $f(x)$ symbol). Let e_m be a vector of zeros, except with a 1 in the mth element, and let δ be a sufficiently small scalar constant. A "finite difference" linear approximation to the mth column of the Hessian is $\mathsf{H}_m \approx (\nabla f(x + \delta e_m) - \nabla f(x))/\delta$. Estimating a dense Hessian in this way involves at least $M + 1$ calculations of the gradient: one for the gradient at x, and one after perturbing each of the M elements of x, one at a time. Under certain conditions, a more accurate approximation is the "complex step" method: $\mathsf{H}_m \approx \mathrm{Im}(\nabla f(x + i\delta e_m))/\delta$, where $i = \sqrt{-1}$ and Im returns the imaginary part of a complex number (Squire and Trapp 1998). Regardless of the approximation method used, if the Hessian is sparse, most of the elements are constrained to zero. Depending on the sparsity pattern of the Hessian, those constraints may let us recover the Hessian with fewer gradient evaluations by perturbing multiple elements of x together. For some sparsity patterns, estimating a Hessian in this way can be profoundly efficient. In fact, for the hierarchical models that we consider in this paper, the number of gradient evaluations does not increase with the number of additional heterogeneous units.

The package defines the *sparseHessianFD* class, whose initializer requires the user to provide functions that compute an objective function, its gradient (as accurately as possible, to machine precision), and the sparsity pattern of its Hessian matrix. The sparsity pattern (e.g., location of structural zeros) must be known in advance, and cannot vary across the domain of the objective function. The only functions and methods of the class that the end user should need to use are the initializer, methods that return the Hessian in a sparse compressed format, and perhaps some utility functions that simplify the construction of the sparsity pattern. The class also defines methods that partition the variables into groups that can be perturbed together in a finite differencing step, and recovers the elements of the Hessian via linear substitution. Those methods perform most of the work, but should be invisible to the user.

As with any computing method or algorithm, there are boundaries around the space of applications for which **sparseHessianFD** is the right tool for the job. In general, numerical approximations are not "first choice" methods because the result is not exact, so **sparseHessianFD** should not be used when the application cannot tolerate any error, no matter how small. Also, we admit that some users might balk at having to provide an exact gradient, even though the Hessian will be estimated numerically.[1] However, deriving a vector of first derivatives, and writing R functions to compute them, is a lot easier than doing the same for a matrix of second derivatives, and more accurate than computing second-order approximations from the objective function. Even when we have derived the Hessian symbolically, in practice it may still be faster to estimate the Hessian using **sparseHessianFD** than coding it directly. These are the situations in which **sparseHessianFD** adds the most value to the statistician's

[1] It is possible that a gradient that is approximated using a complex step method would be precise enough to be useful. A further investigation is beyond the scope of this paper.

toolbox.

This article proceeds as follows. First, we present some background information about numerical differentiation, and sparse matrices in R, in Section 1. In Section 2, we explain how to use the package. Section 3 explains the underlying algorithms, and Section 4 demonstrates the scalability of those algorithms.

1. Background

Before describing how to use the package, we present two short background notes. The first note is an informal mathematical explanation of numerical estimation of the Hessian matrix, with an illustration of how the number of gradient estimates can be reduced by exploiting the sparsity pattern and symmetric structure. This note borrows heavily from, and uses the notation in, Magnus and Neudecker (2007, Chapter 6). The second note is a summary of some of the sparse matrix classes that are defined in the **Matrix** package (Bates and Maechler 2015), which are used extensively in **sparseHessianFD**.

1.1. Numerical differentiation of sparse Hessians

The partial derivative of a real scalar-valued function $f(x)$ with respect to x_j (the jth component of $x \in \mathbb{R}^M$) is defined as

$$\mathsf{D}_j f(x) = \lim_{\delta \to 0} \frac{f(x + \delta e_j) - f(x)}{\delta} \tag{1}$$

For a sufficiently small δ, this definition allows for a linear approximation to $\mathsf{D}_j f(x)$. The derivative of $f(x)$ is the vector of all M partial derivatives.

$$\mathsf{D} f(x) = (\mathsf{D}_1 f(x), \ldots, \mathsf{D}_M f(x)) \tag{2}$$

The *gradient* is defined as $\nabla f(x) = \mathsf{D} f(x)^\top$.

We define the second-order partial derivative as

$$\mathsf{D}^2_{jk} = \lim_{\delta \to 0} \frac{\mathsf{D}_j f(x + \delta e_k) - \mathsf{D}_j f(x)}{\delta} \tag{3}$$

and the Hessian as

$$\mathsf{H} f(x) = \begin{pmatrix} \mathsf{D}^2_{11} & \mathsf{D}^2_{12} & \ldots & \mathsf{D}^2_{1M} \\ \mathsf{D}^2_{21} & \mathsf{D}^2_{22} & \ldots & \mathsf{D}^2_{2M} \\ \vdots & \vdots & & \vdots \\ \mathsf{D}^2_{M1} & \mathsf{D}^2_{M2} & \ldots & \mathsf{D}^2_{MM} \end{pmatrix} \tag{4}$$

The Hessian is symmetric, so $\mathsf{D}^2_{ij} = \mathsf{D}^2_{ji}$.

Approximation using finite differences

To estimate the mth column of H using finite differences, we choose a sufficiently small δ, and compute

$$\mathsf{H}_m f(x) \approx \frac{\mathsf{D} f(x + \delta e_m) - \mathsf{D} f(x)}{\delta} \tag{5}$$

For $M = 2$, our estimate of a general $\mathsf{H}f(x)$ would be

$$\mathsf{H}f(x) \approx \begin{pmatrix} \mathsf{D}_1 f(x_1 + \delta, x_2) - \mathsf{D}_1 f(x_1, x_2) & \mathsf{D}_1 f(x_1, x_2 + \delta) - \mathsf{D}_1 f(x_1, x_2) \\ \mathsf{D}_2 f(x_1 + \delta, x_2) - \mathsf{D}_2 f(x_1, x_2) & \mathsf{D}_2 f(x_1, x_2 + \delta) - \mathsf{D}_2 f(x_1, x_2) \end{pmatrix} / \delta \tag{6}$$

This estimate requires three evaluations of the gradient to get $\mathsf{D}f(x_1, x_2)$, $\mathsf{D}f(x_1 + \delta, x_2)$, and $\mathsf{D}f(x_1, x_2 + \delta)$.

Now suppose that the Hessian is sparse, and that the off-diagonal elements are zero. That means that

$$\mathsf{D}_1 f(x_1, x_2 + \delta) - \mathsf{D}_1 f(x_1, x_2) = 0 \tag{7}$$
$$\mathsf{D}_2 f(x_1 + \delta, x_2) - \mathsf{D}_2 f(x_1, x_2) = 0 \tag{8}$$

If the identity in Equation 7 holds for x_1, it must also hold for $x_1 + \delta$, and if Equation 8 holds for x_2, it must also hold for $x_2 + \delta$. Therefore,

$$\mathsf{H}f(x) \approx \begin{pmatrix} \mathsf{D}_1 f(x_1 + \delta, x_2 + \delta) - \mathsf{D}_1 f(x_1, x_2) & 0 \\ 0 & \mathsf{D}_2 f(x_1 + \delta, x_2 + \delta) - \mathsf{D}_2 f(x_1, x_2) \end{pmatrix} / \delta \tag{9}$$

Only two gradients, $\mathsf{D}f(x_1, x_2)$ and $\mathsf{D}f(x_1 + \delta, x_2 + \delta)$, are needed. Being able to reduce the number of gradient evaluations from 3 to 2 depends on knowing that the cross-partial derivatives are zero.

Approximation using complex steps

If $f(x)$ is defined over a complex domain and is holomorphic, then we can we can approximate $\mathsf{D}f(x)$ and $\mathsf{H}f(x)$ at real values of x using the complex step method. This method comes from a Taylor series expansion of $f(x)$ in the imaginary direction of the complex plane (Squire and Trapp 1998). After rearranging terms, and taking the imaginary parts of both sides,

$$f(x + i\delta) = f(x) + i\delta \mathsf{D}f(x) + \mathcal{O}(\delta^2) \tag{10}$$
$$\mathsf{D}f(x) \approx \frac{\mathrm{Im}(f(x + i\delta))}{\delta} \tag{11}$$

Estimating a first derivative using the complex step method does not require a differencing operation, so there is no subtraction operation that might generate roundoff errors. Thus, the approximation can be made arbitrarily precise as $\delta \to 0$ (Lai and Crassidis 2008). This is not the case for second-order approximations of the Hessian (Abreu, Stich, and Morales 2013). However, when the gradient can be computed exactly, we can compute a first-order approximation to Hessian by treating it as the Jacobian of a vector-valued function (Lai and Crassidis 2008).

$$\mathsf{H}f(x) \approx \begin{pmatrix} \mathrm{Im}(\mathsf{D}_1 f(x_1 + i\delta, x_2)) & \mathrm{Im}(\mathsf{D}_1 f(x_1, x_2 + i\delta)) \\ \mathrm{Im}(\mathsf{D}_2 f(x_1 + i\delta, x_2)) & \mathrm{Im}(\mathsf{D}_2 f(x_1, x_2 + i\delta)) \end{pmatrix} / \delta \tag{12}$$

If this matrix were dense, we would need two evaluations of the $\mathsf{D}f(x)$ to estimate it. If the matrix were sparse, with the same sparsity pattern as the Hessian in Equation 9, and

we assume that structural zeros remain zero for all complex $x \in \mathbb{Z}^M$, then we need only one evaluation. Suppose we were to subtract $\text{Im}(\mathsf{D}f(x_1, x_2))$ from each column of $\mathsf{H}f(x)$. When x is real, the imaginary part of the gradient is zero, so this operation has no effect on the value of the Hessian. But the sparsity constraints ensure that the following identities hold all complex x.

$$\text{Im}(\mathsf{D}_1 f(x_1, x_2 + i\delta)) - \text{Im}(\mathsf{D}_1 f(x_1, x_2)) = 0 \tag{13}$$
$$\text{Im}(\mathsf{D}_2 f(x_1 + i\delta, x_2)) - \text{Im}(\mathsf{D}_2 f(x_1, x_2)) = 0 \tag{14}$$

As with the finite difference method, because Equation 13 holds for x_1, it must also hold for $x_1 + i\delta$, and because Equation 14 holds for x_2, it must also hold for $x_2 + i\delta$. Thus,

$$\mathsf{H}f(x) \approx \begin{pmatrix} \text{Im}(\mathsf{D}_1 f(x_1 + i\delta, x_2 + i\delta)) & 0 \\ 0 & \text{Im}(\mathsf{D}_2 f(x_1 + i\delta, x_2 + i\delta)) \end{pmatrix} / \delta \tag{15}$$

for real x. Only one evaluation of the gradient is required.

Perturbing groups of variables

Curtis, Powell, and Reid (1974) describe a method of estimating sparse Jacobian matrices by perturbing groups of variables together. Powell and Toint (1979) extend this idea to the general case of sparse Hessians. This method partitions the decision variables into C mutually exclusive groups so that the number of gradient evaluations is reduced. Define $\mathbf{G} \in \mathbb{R}^{M \times C}$ where $\mathbf{G}_{mc} = \delta$ if variable m belongs to group c, and zero otherwise. Define $\mathbf{G}_c \in \mathbb{R}^M$ as the cth column of $\mathbf{G}$.

Next, define $\mathbf{Y} \in \mathbb{R}^{M \times C}$ such that each column is either a difference in gradients, or the imaginary part of a complex-valued gradient, depending on the chosen method.

$$\mathbf{Y}_c = \begin{cases} \nabla f(x + G_c) - \nabla f(x) & \text{finite difference method} \\ \text{Im}(\nabla f(x + iG_c)) & \text{complex step method} \end{cases} \tag{16}$$

If $C = M$, then $\mathbf{G}$ is a diagonal matrix with δ in each diagonal element. The matrix equation $\mathsf{H}\mathbf{G} = \mathbf{Y}$ represents the linear approximation $\mathsf{H}_{im}\delta \approx y_{im}$, and we can solve for all elements of H just by computing $\mathbf{Y}$. But if $C < M$, there must be at least one $\mathbf{G}_c$ with δ in at least two rows. The corresponding column $\mathbf{Y}_c$ is computed by perturbing multiple variables at once, so we cannot solve for any H_{im} without further constraints.

These constraints come from the sparsity pattern and symmetry of the Hessian. Consider an example with the following values and sparsity pattern.

$$\mathsf{H}f(x) = \begin{pmatrix} h_{11} & 0 & h_{31} & 0 & 0 \\ 0 & h_{22} & 0 & h_{42} & 0 \\ h_{31} & 0 & h_{33} & 0 & h_{53} \\ 0 & h_{42} & 0 & h_{44} & 0 \\ 0 & 0 & h_{53} & 0 & h_{55} \end{pmatrix} \tag{17}$$

Suppose $C = 2$, and define group membership of the five variables through the following $\mathbf{G}$ matrix.

$$\mathbf{G}^\top = \begin{pmatrix} \delta & \delta & 0 & 0 & \delta \\ 0 & 0 & \delta & \delta & 0 \end{pmatrix} \tag{18}$$

Variables 1, 2 and 5 are in group 1, while variables 3 and 4 are in group 2.

Next, compute the columns of $\mathbf{Y}$ using Equation 16. We now have the following system of linear equations from $\mathsf{H}\mathbf{G} = \mathbf{Y}$.

$$\begin{aligned} h_{11} &= y_{11} & h_{31} &= y_{12} \\ h_{22} &= y_{21} & h_{42} &= y_{22} \\ h_{31} + h_{53} &= y_{31} & h_{33} &= y_{32} \\ h_{42} &= y_{41} & h_{44} &= y_{42} \\ h_{55} &= y_{51} & h_{53} &= y_{52} \end{aligned} \tag{19}$$

Note that this system is overdetermined. Both $h_{31} = y_{12}$ and $h_{53} = y_{52}$ can be determined directly, but $h_{31} + h_{53} = y_{31}$ may not necessarily hold, and h_{42} could be either y_{41} or y_{22}. Powell and Toint (1979) prove that it is sufficient to solve $\mathsf{L}\mathbf{G} = \mathbf{Y}$ instead via a substitution method, where L is the lower triangular part of H. This has the effect of removing the equations $h_{42} = y_{22}$ and $h_{31} = y_{12}$ from the system, but retaining $h_{53} = y_{52}$. We can then solve for $h_{31} = y_{31} - y_{52}$. Thus, we have determined a 5×5 Hessian with only three gradient evaluations, in contrast with the six that would have been needed had H been treated as dense.

The **sparseHessianFD** algorithms assign variables to groups before computing the values of the Hessian. This is why the sparsity pattern needs to be provided in advance. If a non-zero element is omitted from the sparsity pattern, the resulting estimate of the Hessian will be incorrect. The only problems with erroneously including a zero element in the sparsity pattern are a possible lack of efficiency (e.g., an increase in the number of gradient evaluations), and that the estimated value might be close to, but not exactly, zero. The algorithms for assigning decision variables to groups, and for extracting nonzero Hessian elements via substitution, are described in Section 3.

1.2. Sparse matrices and the Matrix package

The **sparseHessianFD** package uses the sparse matrix classes that are defined in the **Matrix** package (Bates and Maechler 2015). All of these classes are subclasses of *sparseMatrix*. Only the row and column indices (or pointers to them), the non-zero values, and some meta-data, are stored; unreferenced elements are assumed to be zero. Class names, summarized in Table 1, depend on the data type, matrix structure, and storage format. Values in numeric and logical matrices correspond to the R data types of the same names. Pattern matrices contain row and column information for the non-zero elements, but no values. The storage format refers to the internal ordering of the indices and values, and the layout defines a matrix as symmetric (so duplicated values are stored only once), triangular, or general. The levels of these three factors determine the prefix of letters in each class name. For example, a triangular sparse matrix of numeric (double precision) data, stored in column-compressed format, has a class *dtCMatrix*.

Storage	Layout	Data type		
		numeric	logical	pattern
Triplet	general	*dgTMatrix*	*lgTMatrix*	*ngTMatrix*
	triangular	*dtTMatrix*	*ltTMatrix*	*ntTMatrix*
	symmetric	*dsTMatrix*	*lsTMatrix*	*nsTMatrix*
Row-compressed	general	*dgRMatrix*	*lgRMatrix*	*ngRMatrix*
	triangular	*dtRMatrix*	*ltRMatrix*	*ntRMatrix*
	symmetric	*dsRMatrix*	*lsRMatrix*	*nsRMatrix*
Column-compressed	general	*dgCMatrix*	*lgCMatrix*	*ngCMatrix*
	triangular	*dtCMatrix*	*ltCMatrix*	*ntCMatrix*
	symmetric	*dsCMatrix*	*lsCMatrix*	*nsCMatrix*

Table 1: Class names for sparse matrices, as defined in the Matrix package.

Matrix also defines some other classes of sparse and dense matrices that we will not discuss here. The **Matrix** package uses the `as` function to convert sparse matrices from one format to another, and to convert a **base** R matrix to one of the **Matrix** classes.

The distinctions among sparse matrix classes is important because **sparseHessianFD**'s `hessian` method returns a *dgCMatrix*, even though the Hessian is symmetric. Depending on how the Hessian is used, it might be useful to coerce the Hessian into a *dsCMatrix* object. Also, the utility functions in Table 2 expect or return certain classes of matrices, so some degree of coercion of input and output might be necessary. Another useful **Matrix** function is `tril`, which extracts the lower triangle of a general or symmetric matrix.

2. Using the package

In this section, we demonstrate how to use the **sparseHessianFD**, using a hierarchical binary choice model as an example. Then, we discuss the sparsity pattern of the Hessian, and estimate the Hessian values.

2.1. Example model: hierarchical binary choice

Suppose we have a dataset of N households, each with T opportunities to purchase a particular product. Let y_i be the number of times household i purchases the product, out of the T purchase opportunities, and let p_i be the probability of purchase. The heterogeneous parameter p_i is the same for all T opportunities, so y_i is a binomial random variable.

Let $\beta_i \in \mathbb{R}^k$ be a heterogeneous coefficient vector that is specific to household i, such that $\beta_i = (\beta_{i1}, \ldots, \beta_{ik})$. Similarly, $z_i \in \mathbb{R}^k$ is a vector of household-specific covariates. Define each p_i such that the log odds of p_i is a linear function of β_i and z_i, but does not depend directly on β_j and z_j for another household $j \neq i$.

$$p_i = \frac{\exp(z_i'\beta_i)}{1 + \exp(z_i'\beta_i)}, \ i = 1...N \tag{20}$$

The coefficient vectors β_i are distributed across the population of households following a

multivariate normal distribution with mean $\mu \in \mathbb{R}^k$ and covariance $\mathbf{\Sigma} \in \mathbb{R}^{k \times k}$. Assume that we know $\mathbf{\Sigma}$, but not μ, so we place a multivariate normal prior on μ, with mean 0 and covariance $\mathbf{\Omega} \in \mathbb{R}^{k \times k}$. Thus, the parameter vector $x \in \mathbb{R}^{(N+1)k}$ consists of the Nk elements in the N β_i vectors, and the k elements in μ.

The log posterior density, ignoring any normalization constants, is

$$\log \pi(\beta_{1:N}, \mu | \mathbf{Y}, \mathbf{Z}, \mathbf{\Sigma}, \mathbf{\Omega}) = \sum_{i=1}^{N} \left(p_i^{y_i} (1 - p_i)^{T - y_i} - \frac{1}{2} (\beta_i - \mu)^\top \mathbf{\Sigma}^{-1} (\beta_i - \mu) \right) - \frac{1}{2} \mu^\top \mathbf{\Omega}^{-1} \mu \tag{21}$$

2.2. Sparsity patterns

Let x_1 and x_2 be two subsets of elements of x. Define $\mathsf{D}^2_{x_1, x_2}$ as the product set of cross-partial derivatives between all elements in x_1 and all elements in x_2. From the log posterior density in Equation 21, we can see that $\mathsf{D}^2_{\beta_i, \beta_i} \neq 0$ (one element of β_i could be correlated with another element of β_i), and that, for all i, $\mathsf{D}^2_{\beta_i, \mu} \neq 0$ (because μ is the prior mean of each β_i). However, since the β_i and β_j are independently distributed, and the y_i are conditionally independent, the cross-partial derivatives $\mathsf{D}^2_{\beta_i, \beta_j} = 0$ for all $i \neq j$. When N is much greater than k, there will be many more zero cross-partial derivatives than non-zero. Each D^2 is mapped to a submatrix of H, most of which with be zero. The resulting Hessian of the log posterior density will be sparse.

The sparsity pattern depends on the indexing function; that is, on how the variables are ordered in x. One such ordering is to group all of the coefficients in the β_i for each unit together.

$$\beta_{11}, \ldots, \beta_{1k}, \beta_{21}, \ldots, \beta_{2k}, \ \ldots \ , \beta_{N1}, \ldots, \beta_{Nk}, \mu_1, \ldots, \mu_k \tag{22}$$

In this case, the Hessian has a "block-arrow" structure. For example, if $N = 5$ and $k = 2$, then there are 12 total variables, and the Hessian will have the pattern in Figure 1a.

Another possibility is to group coefficients for each covariate together.

$$\beta_{11}, \ldots, \beta_{N1}, \beta_{12}, \ldots, \beta_{N2}, \ \ldots \ , \beta_{1k}, \ldots, \beta_{Nk}, \mu_1, \ldots, \mu_k \tag{23}$$

Now the Hessian has an "banded" sparsity pattern, as in Figure 1b.

In both cases, the number of non-zeros is the same. There are 144 elements in this symmetric matrix, but only 64 are non-zero, and only 38 values are unique. Although the reduction in RAM from using a sparse matrix structure for the Hessian may be modest, consider what would happen if $N = 1,000$ instead. In that case, there are 2,002 variables in the problem, and more than 4 million elements in the Hessian. However, only $12,004$ of those elements are non-zero. If we work with only the lower triangle of the Hessian, then we need to work with only 7,003 values.

The sparsity pattern required by **sparseHessianFD** consists of the row and column indices of the non-zero elements in the *lower triangle* the Hessian, and it is the responsibility of the user to ensure that the pattern is correct. In practice, rather than trying to keep track of the row and column indices directly, it might be easier to construct a pattern matrix first, check visually that the matrix has the right pattern, and then extract the indices. The package

```
 [1,] | | . . . . . . . . . | |
 [2,] | | . . . . . . . . . | |
 [3,] . . | | . . . . . . . | |
 [4,] . . | | . . . . . . . | |
 [5,] . . . . | | . . . . . | |
 [6,] . . . . | | . . . . . | |
 [7,] . . . . . | | . . . | |
 [8,] . . . . . | | . . . | |
 [9,] . . . . . | | | | |
[10,] . . . . . | | | | |
[11,] | | | | | | | | | | |
[12,] | | | | | | | | | | |
```

(a) A "block-arrow" sparsity pattern.

```
 [1,] | . . . . | . . . . | |
 [2,] . | . . . . | . . . | |
 [3,] . . | . . . . | . . | |
 [4,] . . . | . . . . | . | |
 [5,] . . . . | . . . . | | |
 [6,] | . . . . | . . . . | |
 [7,] . | . . . . | . . . | |
 [8,] . . | . . . . | . . | |
 [9,] . . . | . . . . | . | |
[10,] . . . . | . . . . | | |
[11,] | | | | | | | | | | |
[12,] | | | | | | | | | | |
```

(b) A "banded" sparsity pattern.

Figure 1: Two examples of sparsity patterns for a hierarchical model.

`Matrix.to.Coord`	Returns a list of vectors containing row and column indices of the non-zero elements of a matrix.
`Matrix.to.Pointers`	Returns indices and pointers from a sparse matrix.
`Coord.to.Pointers`	Converts list of row and column indices (triplet format) to a list of indices and pointers (compressed format).

Table 2: sparseHessianFD matrix conversion functions.

defines utility functions (Table 2) to convert between sparse matrices, and the vectors of row and column indices required by the *sparseHessianFD* initializer.

The `Matrix.to.Coord` function extracts row and column indices from a sparse matrix. The following code constructs a logical block diagonal matrix, converts it to a sparse matrix, and prints the sparsity pattern of its lower triangle.

```
R> library("sparseHessianFD")
R> bd <- kronecker(diag(3), matrix(TRUE, 2, 2))
R> Mat <- as(bd, "nMatrix")
R> printSpMatrix(tril(Mat))


[1,] | . . . . .
[2,] | | . . . .
[3,] . . | . . .
[4,] . . | | . .
[5,] . . . . | .
[6,] . . . . | |

R> mc <- Matrix.to.Coord(tril(Mat))
R> mc

$rows
[1] 1 2 2 3 4 4 5 6 6

$cols
[1] 1 1 2 3 3 4 5 5 6
```

To check that a proposed sparsity pattern represents the intended matrix visually, use the **Matrix** `sparseMatrix` constructor.

```
R> pattern <- sparseMatrix(i=mc$rows, j=mc$cols)
R> printSpMatrix(pattern)


[1,] | . . . . .
[2,] | | . . . .
[3,] . . | . . .
[4,] . . | | . .
[5,] . . . . | .
[6,] . . . . | |
```

If there is uncertainty about whether an element is a structural zero or not, one should err on the side of it being non-zero, and include that element in the sparsity pattern. There might be a loss of efficiency if the element really is a structural zero, but the result will still be correct. All that would happen is that the numerical estimate for that element would be zero (within machine precision). On the other hand, excluding a non-zero element from the sparsity pattern will likely lead to an incorrect estimate of the Hessian.

x	A numeric vector, with length M at which the object will be initialized and tested.
fn,gr	R Functions that return the value of the objective function, and its gradient. The first argument is the numeric variable vector. Other named arguments can be passed to `fn` and gr as well (see the `...` argument below).
rows, cols	Sparsity pattern: integer vectors of the row and column indices of the non-zero elements in the *lower triangle* of the Hessian.
delta	The perturbation amount for finite differencing of the gradient to compute the Hessian (the δ in Section 1.1). Defaults to `sqrt(.Machine$double.eps)`.
index1	If `TRUE` (the default), `row` and `col` use one-based indexing. If `FALSE`, zero-based indexing is used.
complex	If `TRUE`, the complex step method is used. If `FALSE` (the default), a simple finite differencing of gradients is used.
...	Additional arguments to be passed to `fn` and `gr`.

Table 3: Arguments to the sparseHessianFD initializer.

2.3. The *sparseHessianFD* class

The function `sparseHessianFD` is an initializer that returns a reference to a *sparseHessianFD* object. The initializer determines an appropriate permutation and partitioning of the variables, and performs some additional validation tests. The arguments to the initializer are described in Table 3.

To create a *sparseHessianFD* object, just call `sparseHessianFD`. Applying the default values for the optional arguments, the usage syntax to create a *sparseHessianFD* object is

```
obj <- sparseHessianFD(x, fn, gr, rows, cols, ...)
```

where `...` represents all other arguments that are passed to `fn` and `gr`.

The `fn`, `gr` and `hessian` methods respectively evaluate the function, gradient and Hessian at a variable vector x. The `fngr` method returns the function and gradient as a list. The `fngrhs` method includes the Hessian as well.

```
R> f <- obj$fn(x)
R> df <- obj$gr(x)
R> hess <- obj$hessian(x)
R> fngr <- obj$fngr(x)
R> fngrhs <- obj$fngrhs(x)
```

2.4. An example

Now we can estimate the Hessian for the log posterior density of the model from Section 2.1. For demonstration purposes, **sparseHessianFD** includes functions that compute the value (`binary.f`), the gradient (`binary.grad`) and the Hessian (`binary.hess`) of this model. We

will treat the result from `binary.hess` as a "true" value against which we will compare the numerical estimates.

To start, we load the data, set some dimension parameters, set prior values for $\mathbf{\Sigma}^{-1}$ and $\mathbf{\Omega}^{-1}$, and simulate a vector of variables at which to evaluate the function. The `binary.f` and `binary.grad` functions take the data and priors as lists. The `data(binary)` call adds the appropriate data list to the environment, but we need to construct the prior list ourselves.

```
R> set.seed(123)
R> data("binary")
R> str(binary)

List of 3
 $ Y: int [1:50] 13 1 18 18 19 6 16 6 5 8 ...
 $ X: num [1:4, 1:50] -0.07926 -0.23018 1.55871 0.00997 0.01828 ...
 $ T: num 20

R> N <- length(binary[["Y"]])
R> k <- NROW(binary[["X"]])
R> T <- binary[["T"]]
R> nvars <- as.integer(N * k + k)
R> priors <- list(inv.Sigma = rWishart(1, k + 5, diag(k))[,,1],
+    inv.Omega = diag(k))
```

This dataset represents the simulated choices for $N = 50$ customers over $T = 20$ purchase opportunties, where the probability of purchase is influenced by $k = 4$ covariates.

The next code chunk evaluates the "true" value, gradient and Hessian. The `order.row` argument tells the function whether the variables are ordered by household (`TRUE`) or by covariate (`FALSE`). If `order.row` is `TRUE`, then the Hessian will have a banded pattern. If `order.row` is `FALSE`, then the Hessian will have a block-arrow pattern.

```
R> P <- rnorm(nvars)
R> order.row <- FALSE
R> true.f <- binary.f(P, binary, priors, order.row=order.row)
R> true.grad <- binary.grad(P, binary, priors, order.row=order.row)
R> true.hess <- binary.hess(P, binary, priors, order.row=order.row)
```

The sparsity pattern of the Hessian is specified by two integer vectors: one each for the row and column indices of the non-zero elements of the lower triangule of the Hessian. For this example, we happen to have a matrix with the same sparsity pattern of the Hessian we are trying to compute, so we can use the `Matrix.to.Coord` function to extract the appropriate index vectors. In practice, it is more likely that we would need to determine the row and column indices directly, through our knowledge of the structure of the problem. For a hierarchical model, we can create a block-arrow pattern matrix using either the `Matrix::bdiag` or `kronecker` functions to create a block diagonal matrix, and concatenate dense rows and columns to the margins.

```
R> pattern <- Matrix.to.Coord(tril(true.hess))
R> str(pattern)

List of 2
 $ rows: int [1:1310] 1 2 3 4 201 202 203 204 2 3 ...
 $ cols: int [1:1310] 1 1 1 1 1 1 1 1 2 2 ...
```

Finally, we create an instance of a *sparseHessianFD* object. Evaluations of the function and gradient using the `fn` and `gr` methods will always give the same results as the true values because they are computed using the same functions.

```
R> obj <- sparseHessianFD(P, fn=binary.f, gr=binary.grad,
+    rows=pattern[["rows"]], cols=pattern[["cols"]],
+    data=binary, priors=priors, order.row=order.row)
R> f <- obj$fn(P)
R> identical(f, true.f)

[1] TRUE

R> gr <- obj$gr(P)
R> identical(gr, true.grad)

[1] TRUE
```

The default choice of method is `complex=FALSE`, so the evaluation of the Hessian is a finite differenced approximation, so it is very close to, but not identical to, the true value, in terms of mean relative difference.

```
R> hs <- obj$hessian(P)
R> mean(abs(hs-true.hess))/mean(abs(hs))

[1] 2.33571e-09
```

If `complex=TRUE` in the initializer, the call to the `hessian` method will apply the complex step method. To use this method, the functions passed as `fn` and `gr` must both accept a complex argument, and return a complex result, even though we are differentiating a real-valued function. Although **base** R supports complex arguments for most basic mathematical functions, many common functions (e.g., `gamma`, `log1p`, `expm1`, and the probability distribution functions) do not have complex implementations. Furthermore, the complex step method is valid only if the function is holomorphic. The methods in *sparseHessianFD* do *not* check that this is the case for the function at hand. We convey the following warning from the documentation of the **numDeriv** package (Gilbert and Varadhan 2012), which also implements the complex step method: "avoid this method if you do not know that your function is suitable. Your mistake may not be caught and the results will be spurious."

Fortunately for demonstration purposes, the log posterior density in Equation 21 is holomorphic, so we can estimate its Hessian using the complex step method, and compute the mean relative difference from the true Hessian.

```
R> obj2 <- sparseHessianFD(P, fn=binary.f, gr=binary.grad,
+    rows=pattern[["rows"]], cols=pattern[["cols"]],
+    complex=TRUE,
+    data=binary, priors=priors, order.row=order.row)
R> hs2 <- obj2$hessian(P)
R> mean(abs(hs2-true.hess))/mean(abs(hs2))

[1] 8.055502e-17
```

In short, the complex step method can be more accurate than finite differencing, but it comes with theoretical and implementation restrictions that may limit its universality.

3. Algorithms

In this section, we explain how **sparseHessianFD** works. The algorithms are adapted from Coleman, Garbow, and Moré (1985b), who provided Fortran implementations as Coleman, Garbow, and Moré (1985a). Earlier versions of **sparseHessianFD** included licensed copies of the Coleman *et al.* (1985a) code, on which the current version no longer depends. Although newer partitioning algorithms have been proposed (e.g., Gebremedhin, Manne, and Pothen 2005; Gebremedhin, Tarafdar, Pothen, and Walther 2009), mainly in the context of automatic differentiation, we have chosen to implement established algorithms that are known to work well, and are likely optimal for the hierarchical models that many statisticians will encounter.

3.1. Partitioning the variables

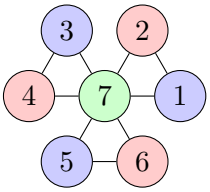
Finding consistent, efficient partitions can be characterized as a vertex coloring problem from graph theory (Coleman and Moré 1984). In this sense, each variable is a vertex in an undirected graph, and an edge connects two vertices i and j if and only if $\mathsf{H}_{ij} f(x) \neq 0$. The sparsity pattern of the Hessian is the adjacency matrix of the graph. By "color," we mean nothing more than group assignment; if a variable is in a group, then its vertex has the color associated with that group. A "proper" coloring of a graph is one in which two vertices with a common edge do not have the same color. Coleman and Moré (1984) define a "triangular coloring" as a proper coloring with the additional condition that common neighbors of a vertex do not have the same color. A triangular coloring is a special case of an "cyclic coloring," in which any cycle in the graph uses at least three colors (Gebremedhin, Tarafdar, Manne, and Pothen 2007).

An "intersection set" contains characteristics that are common to two vertices, and an "intersection graph" connects vertices whose intersection set is not empty. In our context, the set in question is the row indices of the non-zero elements in each column of L. In the intersection graph, two vertices are connected if the corresponding columns in L have at least one non-zero element in a common row.

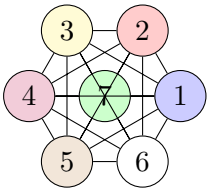
Powell and Toint (1979) write that a partitioning is consistent with a substitution method if and only if no columns of the of lower triangle of the Hessian that are in the same group have a non-zero element in the same row. An equivalent statement is that no two adjacent vertices in the intersection graph can have the same color. Thus, we can partition the variables by creating a proper coloring of the intersection graph of L.

	1	2	3	4	5	6	7
1	1						
2	1	1					
3	0	0	1				
4	0	0	1	1			
5	0	0	0	0	1		
6	0	0	0	0	1	1	
7	1	1	1	1	1	1	1

(a) Adjacency matrix.



(b) Sparsity graph.

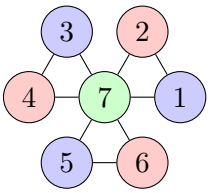


(c) Intersection graph.

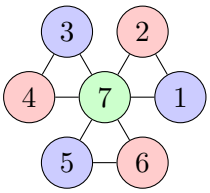
Figure 2: Unpermuted matrix.

	7	1	2	3	4	5	6
7	1						
1	1	1					
2	1	1	1				
3	1	0	0	1			
4	1	0	0	1	1		
5	1	0	0	0	0	1	
6	1	0	0	0	0	1	1

(a) Adjacency matrix.



(b) Sparsity graph.



(c) Intersection graph.

Figure 3: Permuted matrix.

This intersection graph, and the number of colors needed to color it, are not invariant to permutation of the rows and columns of H. Let π represent such a permutation, and let L_π be the lower triangle of $\pi\mathsf{H}\pi^\top$. Coleman and Moré (1984, Theorem 6.1) show that a coloring is triangular if and only if it is also a proper coloring of the intersection graph of L_π. Furthermore, Coleman and Cai (1986) prove that a partitioning is consistent with a substitution method if and only if it is an acyclic coloring of the graph of the sparsity pattern of the Hessian. Therefore, finding an optimal partitioning of the variables involves finding an optimal combination of a permutation π, and coloring algorithm for the intersection graph of L_π.

These ideas are illustrated in Figures 2 and 3. Figure 2a shows the sparsity pattern of the lower triangle of a Hessian as an adjacency matrix, and Figure 2b is the associated graph with a proper vertex coloring. Every column (and thus, every pair of columns) in Figure 2a has a non-zero element in row 7, so there are no non-empty intersection sets across the columns. All vertices are connected to each other in the intersection graph (Figure 2c), which requires seven colors for a proper coloring. Estimating a sparse Hessian with this partitioning scheme would be no more efficient than treating the Hessian as if it were dense.

Now suppose we were to rearrange H so the last row and and column were moved to the front. In Figure 3a, all columns share at least one non-zero row with the column for variable 7, but variable groups $\{2, 4, 6\}$ and $\{1, 3, 5\}$ have empty intersection sets. The intersection graph in Figure 3c has fewer edges than Figure 2c, and can be colored with only three colors.

The practical implication of all of this is that by permuting the rows and columns of the

Hessian, we may be able to reduce the number of colors needed for a cyclic coloring of the graph of the sparsity pattern. Fewer colors means fewer partitions of the variables, and that means fewer gradient evaluations to estimate the Hessian.

The *sparseHessianFD* class finds a permutation, and partitions the variables, when it is initialized. The problem of finding a cyclic coloring of the graph of the sparsity pattern is NP-complete (Coleman and Cai 1986), so the partitioning may not be truly optimal. Fortunately, we just need the partitioning to be reasonably good, to make the effort worth our while. A plethora of vertex coloring heuristics have been proposed, and we make no claims that any of the algorithms in **sparseHessianFD** are even "best available" for all situations.

The first step is to permute the rows and columns of the Hessian. A reasonable choice is the "smallest-last" ordering that sorts the rows and columns in decreasing order of the number of elements (Coleman and Moré 1984, Theorem 6.2). To justify this permutation, suppose non-zeros within a row are randomly distributed across columns. If the row is near the top of the matrix, there is a higher probability that any non-zero element is in the upper triangle, not in the lower. By putting sparser rows near the bottom, we do not change the number of non-zeros in the lower triangle, but we should come close to minimizing the number of non-zeros in each row. Thus, we would expect the number of columns with non-zero elements in common rows to be smaller, and the intersection graph to be sparser (Gebremedhin *et al.* 2007).

The adjacency matrix of the intersection graph of the permuted matrix is the Boolean crossproduct, $\mathsf{L}_\pi^\top \mathsf{L}_\pi$. Algorithm 1 is a "greedy" vertex coloring algorithm, in which vertices are colored sequentially. The result is a cyclic coloring on the sparsity graph, which in turn is a consistent partitioning of the variables.

3.2. Computing the Hessian by substitution

The cycling coloring of the sparsity graph defines the $\mathbf{G}$ matrix from Section 1.1. We then estimate $\mathbf{Y}$ using Equation 16. Let C_m be the assigned color to variable m. The substitution method is defined in Coleman and Moré (1984, Equation 6.1).

$$\mathsf{H}_{ij} f(x) = \mathbf{Y}_{i,C_j}/\delta - \sum_{l>i, l\in C_j} \mathsf{H}_{li} f(x) \tag{24}$$

We implement the substitution method using Algorithm 2. This algorithm completes the bottom row of the lower triangle, copies values to the corresponding column in the upper triangle, and advances upwards.

3.3. Software libraries

The coloring and substitution algorithms use the **Eigen** numerical library (Guennebaud, Jacob *et al.* 2010), and the **Rcpp** (Eddelbuettel and François 2011) and **RcppEigen** (Bates and Eddelbuettel 2013) R packages. The **testthat** (Wickham 2011), **scales** (Wickham 2016) and **knitr** (Xie 2016) packages were used for testing, and to prepare this article.

4. Speed and scalability

Algorithm 1 Consistent partitioning of variables for a triangular substitution method.

Require: $P[i], i = 1, \ldots, M$: sets of column indices of non-zero elements in row i.
Require: $F[i], i = 1, \ldots, M$: sets of "forbidden" colors for vertex i (initially empty)
Require: U: set of used colors (initially empty)
Require: $C[i], i = 1, \ldots, M$: vector to store output of assigned colors (initially all zero).
  $k \leftarrow 0$ {Largest color index used}
  Insert 0 in U
  for $i = 1$ **to** M **do**
    if $F[i]$ is empty (no forbidden colors) **then**
      $C[i] \leftarrow 0$
    else
      $V \leftarrow U - F[i]$ {Used colors that are not forbidden}
      if V is empty **then**
        $k \leftarrow k + 1$
        Insert k into U
        $C[i] \leftarrow k$
      else
        $C[i] \leftarrow \min(V)$ {Assign smallest existing non-forbidden color to i}
      end if
    end if
  end for
  for j in $P[i]$ **do**
    Insert $C[i]$ into $F[j]$ {Make i's color forbidden to all of its uncolored neighbors}
  end for
  return C

Algorithm 2 Triangular substitution method.

Require: $P[i], i = 1, \ldots, M$: sets of column indices of non-zero elements in row i.
Require: $C[i], i = 1, \ldots, M$: vector of assigned colors
Require: $\mathbf{H}$, an $M \times M$ Hessian (initialized to zero)
Require: $\mathbf{B}$, a $\max(C) \times M$ matrix (initialized to zero)
Require: $\mathbf{Y}$, a matrix of finite differences
Require: δ, the small constant used to estimate $\mathbf{Y}$
  for $i = M$ **to** 1 **do**
    for All j in P_i **do**
      $z \leftarrow Y[i, C[j]]/\delta - B[C[j], i]$
      $\mathbf{B}[C[i], j] \leftarrow \mathbf{B}[C[i], j] + z$
      $H[i, j] \leftarrow z$
      $H[j, i] \leftarrow H[i, j]$
    end for
  end for

			Finite differencing				Complex step			
			numDeriv		sparseHessianFD		numDeriv		sparseHessianFD	
N	k	M	mean	sd	mean	sd	mean	sd	mean	sd
15	2	32	12.7	0.9	2.4	0.1	13.2	0.7	2.0	0.1
15	5	80	32.2	0.9	5.0	0.5	36.1	10.1	5.2	0.8
50	2	102	51.3	9.8	3.0	0.4	54.5	1.0	2.7	0.6
15	8	128	53.6	0.9	7.8	0.6	62.5	16.7	8.2	0.8
100	2	202	131.7	16.9	3.7	0.3	147.6	24.1	3.4	0.5
50	5	255	144.0	27.1	6.6	0.6	162.8	29.2	6.7	0.7
50	8	408	256.2	43.5	12.5	12.9	291.1	39.0	11.7	0.7
100	5	505	495.7	129.5	9.8	3.1	559.8	125.9	11.8	10.4
100	8	808	850.0	171.4	20.9	20.4	999.2	217.5	23.6	17.3
500	2	1002	1953.4	321.7	10.8	3.7	2156.2	339.7	9.5	3.4
500	5	2505	5444.0	951.0	27.1	10.6	6159.3	1009.2	26.5	4.6
500	8	4008	9533.1	190.9	54.5	12.8	14059.4	3797.9	62.5	21.8

Table 4: Computation times (milliseconds) for computing Hessians using the **numDeriv** and **sparseHessianFD** packages, and the finite difference and complex step methods, across 500 replications. Rows are ordered by the number of variables.

As far as we know, **numDeriv** (Gilbert and Varadhan 2012) is the only other R package that computes numerical approximations to derivatives. Like **sparseHessianFD** it includes functions to compute Hessians from user-supplied gradients (through the `jacobian` function), and implements both the finite differencing and complex step methods. Its most important distinction from **sparseHessianFD** is that it treats all Hessians as dense. Thus, we will use **numDeriv** as the baseline against which we can compare the performance of **sparseHessianFD**.

To prepare Table 4, we estimated Hessians of the log posterior density in Equation 21 with different numbers of heterogeneous units (N) and within-unit parameters (k). The total number of variables is $M = (N + 1)k$. Table 4 shows the mean and standard deviations (across 500 replications) for the time (in milliseconds) to compute a Hessian using functions for both the finite difference and complex step methods from each package. Times were generated on a compute node running Scientific Linux 6 (64-bit) with an 8-core Intel Xeon X5560 processor (2.80 GHz) with 24 GB of RAM, and collected using the **microbenchmark** package (Mersmann 2014). Code to replicate Table 4 is available in the `doc/` directory of the installed package, and the `vignettes/` directory of the source package. In Table 4 we see that computation times using **sparseHessianFD** and considerably shorter than those using **numDeriv**.

To help us understand just how scalable **sparseHessianFD** is, we ran another set of simulations, for the same hierarchical model, for different values of N and k. We then recorded the run times for different steps in the sparse Hessian estimation, across 200 replications. The steps are summarized in Table 5. The times were generated on an Apple Mac Pro with a 12-core Intel Xeon E5-2697 processor (2.7 GHz) with 64 GB of RAM.

In the plots in Figure 4, the number of heterogeneous units (N) is on the x-axis, and median run time, in milliseconds, is on the y-axis. Each panel shows the relationship between N and run time for a different step in the algorithm, and each curve in a panel represents a different

Measure	Description
Function	estimating the objective function
Gradient	estimating the gradient
Hessian	computing the Hessian (not including initialization or partitioning time)
Partitioning	finding a consistent partitioning of the variables (the vertex coloring problem)
Initialization	total setup time (including the partitioning time)

Table 5: Summary of timing tests (see Figure 4).

number of within-unit parameters (k).

Computation times for the function and gradient, as well as the setup and partitioning times for the *sparseHessianFD* object, grow linearly with the number of heterogenous units. The time for the Hessian grows linearly as well, and that might be partially surprising. We saw in Section 3.1 that adding additional heterogeneous units in a hierarchical model does not increase the number of required gradient evaluations. So we might think that the time to compute a Hessian should not increase with N *at all*. The reason it does is that each gradient evaluation takes longer. Nevertheless, we can conclude that the **sparseHessianFD** algorithms are quite efficient and scalable for hierarchical models.

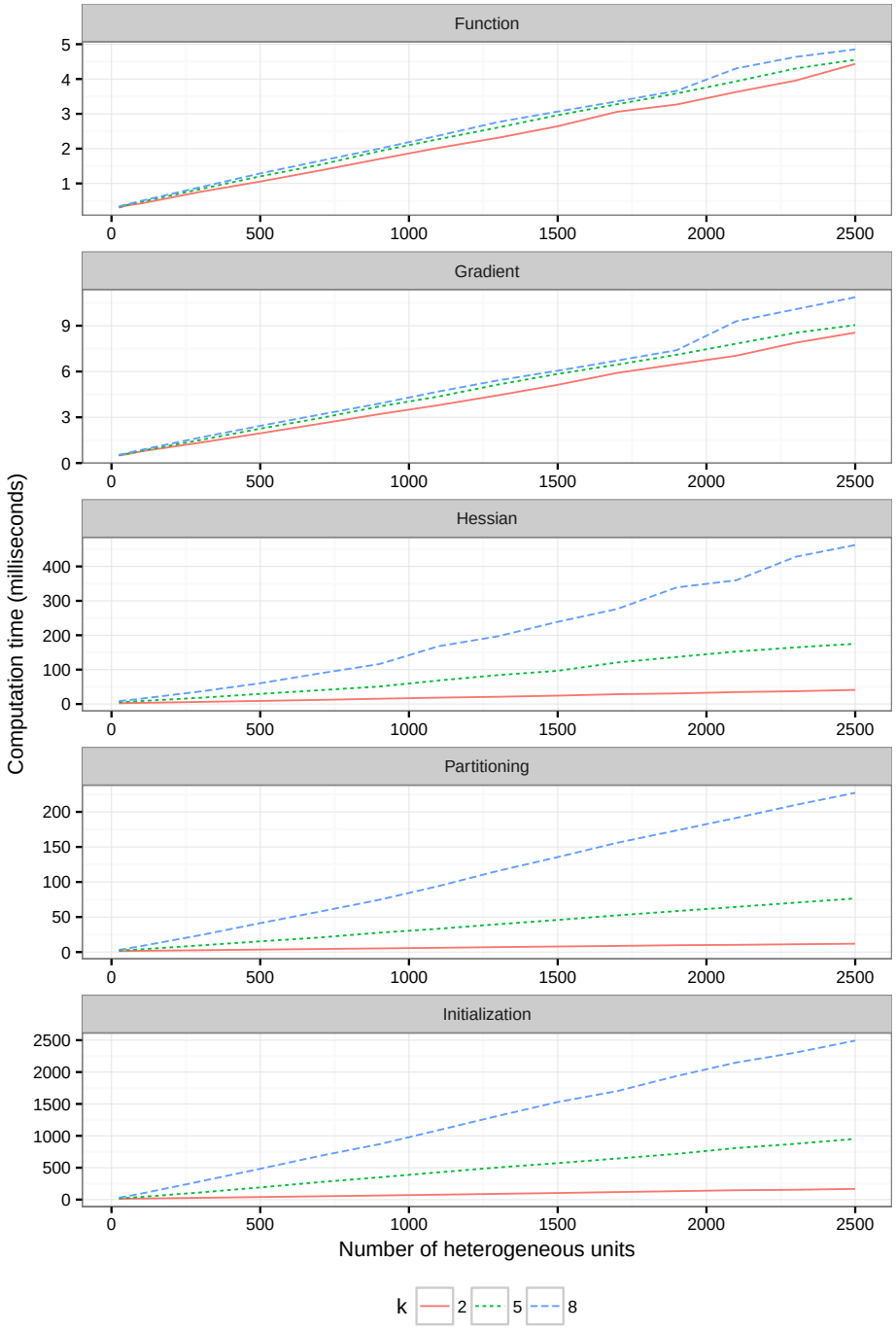


Figure 4: Run times for sparse Hessian computation.

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