The hypersecant Jacobian approximation for quasi-Newton solves of sparse nonlinear systems

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Abstract
A new Jacobian approximation is developed for use in quasi-Newton methods for solving systems of nonlinear equations. The new hypersecant Jacobian approximation is intended for the special case where the evaluation of the functions whose roots are sought dominates the computation time, and additionally the Jacobian is sparse. One example of such a case is the solution of the discretized transport equation to calculate particle and energy fluxes in a fusion plasma. The hypersecant approximation of the Jacobian is calculated using function values from previous Newton iterations, similarly to the Broyden approximation. Unlike Broyden, the hypersecant Jacobian converges to the finite-difference approximation of the Jacobian. The calculation of the hypersecant Jacobian elements requires solving small, dense linear systems, where the coefficient matrices can be ill-conditioned or even exactly singular. Singular-value decomposition (SVD) is therefore used. Convergence comparisons of the hypersecant method, the standard Broyden method, and the colored finite differencing of the PETSc SNES solver are presented.

Key words: quasi-Newton method, Broyden’s method, singular-value decomposition

1. Introduction
The Newton-Raphson method can provide solutions to systems of nonlinear equations. It works by finding a linear approximation to the residual vector (the vector whose root is desired), and then solving the resulting linear system to obtain an approximate solution. Iteration of this process, if it converges, gives a numerical solution to the nonlinear equations. Thus, there are three parts to each iteration. The first is to obtain the linear approximation, i.e., the Jacobian, the matrix of the derivatives of the residual vector components with respect to the parameters. The second is solving the resulting linear system. The third is to correct a change that makes the solution worse (e.g., by using a line search along the direction of the change). Here we concentrate on the first two parts.
Generally, calculating the Jacobian is the most computationally intensive part of the problem because the Jacobian has \(N^2\) terms for \(N\) variables (and \(N\) residuals). In many cases of interest it cannot be calculated directly, as the residuals are not known as simple analytic functions. Hence, the Jacobian is found by the finite difference approximation. However, when the number of variables is large, this becomes prohibitive, hence the development of quasi-Newton methods, such as the Broyden method \([\text{1}]\). In the Broyden method, the Jacobian is updated by adding a term to it so that it accurately predicts the change in the residuals of the previous iteration. However, the Broyden method can be problematic; it is often found not to converge, in large part due to this update not converging to the true Jacobian.

Our motivating application is the time advance of systems of nonlinear partial differential equations. In such cases there are a number of variables associated with each cell upon discretization, and the residual is the change of those variables in a given time step that gives one a stable advance. Since the continuum equations are local, the residuals for a cell depend on the values of the variables in that cell and some nearby cells. Hence, the Jacobian is sparse with \(O(N)\) terms, and so it is reasonable to find the Jacobian through finite differences. In particular, one can use *coloring*, as is done in the PETSc SNES solver \([\text{2}]\) to ensure that the minimal number of evaluations are carried out to obtain those finite differences.

We combine ideas from both these two approaches. We recognize that the Jacobian is sparse, and so there are only a small number of derivatives to be calculated for each residual. However, rather than explicitly computing all the finite differences at each step, we use the results from the last several solver iterations to solve for an approximation to the Jacobian. This may not be enough information for a precise solution, as either there may be an insufficient number of equations, or some of the equations may be degenerate (as can happen when successive steps are in the same direction). In the former case, which occurs for the first few iterations of a quasi-Newton solve, we use Broyden until sufficient state has been generated to calculate the hypersecant Jacobian. In the latter case we use singular-value decomposition (SVD) to determine the Jacobian. Finally, because the resulting Jacobian may in general itself be ill-conditioned, we solve for the linear approximation for the change in the parameters again through SVD.

We compare our method, the Broyden method, and the (colored) PETSc SNES solver to three problems. The first is a three-variable linear system, which illustrates how the Broyden Jacobian does not correctly converge. In contrast, our hypersecant method does provide the converged Jacobian. For linear problems, once the Jacobian is correct, the problem is solved in the next step. Thus, for this case there is no need to apply the PETSc SNES solver as the results are known. The second problem is a three-variable nonlinear system. There we find that the Broyden and hypersecant methods are competitive, with the finite-difference approximation taking more function evaluations. This is perhaps not surprising, as with only three variables, the Jacobian is nearly dense. Finally, we apply the methods to our motivating application, a nonlinear trans-
port equation of a kind that arises in certain problems in plasma physics. Here we find that the hypersecant method takes roughly half the number of function evaluations to converge compared with the finite difference approximation. The Broyden convergence is much slower still.

The organization of this paper is as follows. In the next section we discuss the Broyden method for updating the Jacobian. In the subsequent section we develop our hypersecant method. Next we compare the methods in application to the simple three-variable linear and nonlinear problems. Subsequently we compare them in application to our motivating problem, a discretized transport equation. Finally we summarize.

2. Quasi-Newton methods and the Broyden approximation

The goal of any Newton-like method is to solve a system of \(N\) nonlinear equations

\[
F(x) = 0
\]

of \(N\) variables, \(x\). Given a current best guess \(x^k\) for the solution, one Taylor expands in its vicinity to obtain the linear equation,

\[
F(x^k + \delta x^k) = F(x^k) + J(x^k) \cdot \delta x^k + O(\delta x^k \cdot \delta x^k) = 0,
\]

(1)

where \(J\) is the Jacobian

\[
J(x) = \frac{\partial F}{\partial x},
\]

which implies that a better approximation \(x^{k+1}\) to the root is found by solving for the linearized change \(\delta x^k\),

\[
J(x^k) \cdot \delta x^k = -F(x^k),
\]

from which one obtains the improved guess for the root,

\[
x^{k+1} = x^k + \delta x^k.
\]

Iterating this process then gives the root, if the process converges.

In the standard Newton-Raphson method the true, analytic Jacobian is used. If the true Jacobian is not known, a finite-difference approximation can be used, making the scheme a quasi-Newton method. However, if \(F(x)\) is numerically expensive to evaluate, the finite-difference Jacobian can become inefficient due to the number of function evaluations needed to compute it.

The Broyden method [1] is a common quasi-Newton method where the Jacobian is approximated as:

\[
J^{k+1} = J^k + \frac{F^{k+1} - F^k - J^k \cdot \delta x^k}{\delta x^k \cdot \delta x^k} \otimes \delta x^k,
\]

(2)

where we have introduced the shorthand notation \(F^k = F(x^k)\) and \(J^k = J(x^k)\), and where \(\otimes\) is the dyadic (or outer) product. The above approximation comes
from demanding that the new Jacobian \( J^{k+1} \) predict the change in the residuals for the most recent step,

\[
F^{k+1} - F^k = J^{k+1} \cdot (x^{k+1} - x^k).
\]

(3)

The initial approximation \( J^0 \) is typically set to either the finite-difference Jacobian (good, but numerically expensive) or the unit matrix (free).

The obvious advantage of the Broyden Jacobian is that it is free in the sense that it requires no extra evaluations of \( F \). The disadvantage of the Broyden Jacobian is that it is not guaranteed to converge toward the true Jacobian; in fact error can accumulate until the increment \( \delta x \) found by inverting it is not even in the descent direction, i.e. \( x + \delta x \) is not closer to the root than \( x \). This occurs because Eq. (3) is underdetermined, so the update (2) is only one of many possible. In a solver using the Broyden approximation one must intercept this occurrence and reinitialize the Jacobian. Indeed, in our experience from using the Broyden method to solve a discretized fusion transport equation [3], optimal performance, i.e. the minimal number of function evaluations, required the Broyden Jacobian to be reinitialized as often as every 5–10 Newton iterations.

3. The hypersecant approximation of the Jacobian

Our hypersecant approximation is like the Broyden method in that the Jacobian comes with no additional function evaluations, but unlike Broyden, the approximate Jacobian will approach the true Jacobian after sufficiently many iterations as one approaches the solution, provided the directions of the steps span the relevant space. The primary difference is that instead of requiring only Eq. (3) we require that this hold for several previous steps,

\[
F(x^{k+1}) - F(x^{k-\ell}) = J^{k+1} \cdot (x^{k+1} - x^{k-\ell}), \quad \ell = 0, \ldots, L-1.
\]

(4)

For the fully dense Jacobian, one obtains a full set of equations after \( N \) linear independent steps. For large systems, this is not practical in general. However, it can be very good when the Jacobian is sparse, such as occurs in the implicit advance of discretized partial differential equations. In particular, the above system of equations is determining when the sparsity is such that any residual depends on only \( L \) variables. For example, in a finite difference discretization of a one-dimensional, single-variable, second-order PDE, each residual depends at most on three variables, and so after three linearly independent steps one has a good approximation to the Jacobian.

One issue is that the above approach cannot alone be used to find a new Jacobian via Eq. (4) until one has taken a number of steps equal to the maximum number of nonzero elements in a row of the Jacobian. This is clearly the case for the first few iterations. The Broyden update can then be used to reduce the number of unknowns to make the system well determined, see Section 4.1, until a sufficient number of steps have been taken. Even if a sufficient number of steps have been taken, the system of equations (4) can be underdetermined,
e.g. because several successive steps are in nearly the same direction. This case is handled by using singular-value decomposition (SVD) to solve for the hypersecant Jacobian elements, see Section 4.1.

4. Comparison of hypersecant, Broyden and PETSc colored FD Jacobian for few-variable systems

In this section we compare the application of two approaches (hypersecant and Broyden) to a linear three-variable system, and then we compare the application of three approaches (hypersecant, Broyden, and finite-difference Jacobian) to a nonlinear three-variable system. Our solvers did not attempt to correct for an increment that takes the solution further away from the true root.

4.1. Linear system

The linear system is defined by the equations,

\[
\begin{align*}
f_1(x_1, x_2) &= x_1 + \frac{x_2}{2} - \frac{3}{2} = 0 \\
f_2(x_1, x_2, x_3) &= \frac{x_1}{2} + x_2 + \frac{x_3}{2} - \frac{2}{2} = 0 \\
f_3(x_2, x_3) &= \frac{x_1}{2} + x_3 - \frac{3}{2} = 0.
\end{align*}
\]

This system has the true solution \( x = (x_1, x_2, x_3) = (1, 1, 1), \) and the Jacobian is

\[
J = \frac{df}{dx} = \begin{bmatrix} 1 & 1/2 & 0 \\ 1/2 & 1 & 1/2 \\ 0 & 1/2 & 1 \end{bmatrix}. \tag{5}
\]

A simple quasi-Newton solver was implemented using the LAPACK [4] implementation ATLAS [5] version 3.8.3. This simple linear system could of course have been solved in a more direct manner, but the purpose of the test is primarily to compare the Broyden and hypersecant Jacobian approximations.

We initialize the Jacobian as the unit matrix, \( J^0 = 1 \) and use the initial guess \( x = (1/2, 1/2, 1/2) \). It takes 14 Newton iterations using the Broyden approximate Jacobian to calculate the root to 12 significant digits. The reason for the poor convergence is that the Broyden Jacobian does not converge toward the true Jacobian. At the final iteration, the Broyden Jacobian is

\[
B^{k=14} = \begin{bmatrix} 1.124366 & 0.599240 & 0 \\ 0.397825 & 0.823632 & 0.397825 \\ 0 & 0.599240 & 1.124366 \end{bmatrix},
\]

which is far from the exact Jacobian (5).

For the hypersecant solve, we initialized the Jacobian with the identity and used the Broyden update for the first two iterations, but after the third iteration we used Eqs. (4). As an example, for the middle row, the system of equations to solve is:

\[
\begin{bmatrix}
  x^k_1 - x^{k-3}_1 \\
  x^k_1 - x^{k-2}_1 \\
  x^k_1 - x^{k-1}_1 \\
  x^k_2 - x^{k-3}_2 \\
  x^k_2 - x^{k-2}_2 \\
  x^k_2 - x^{k-1}_2 \\
  x^k_3 - x^{k-3}_3 \\
  x^k_3 - x^{k-2}_3 \\
  x^k_3 - x^{k-1}_3 \\
\end{bmatrix}
\begin{bmatrix}
  H^k_{2,1} \\
  H^k_{2,2} \\
  H^k_{2,3}
\end{bmatrix}
= \begin{bmatrix}
  f^k_2 - f^{k-3}_2 \\
  f^k_2 - f^{k-2}_2 \\
  f^k_2 - f^{k-1}_2
\end{bmatrix}. \tag{6}
\]
Thus, at the third step we obtain the hypersecant Jacobian,

\[
H^{k=3} = \begin{bmatrix}
1.000000 & 0.500000 & 0 \\
0.500000 & 1.000000 & 0.500000 \\
0 & 0.500000 & 1.000000
\end{bmatrix},
\]

It is seen to equal the finite-difference approximation of the Jacobian (which in turn equals the true Jacobian for the linear system used in this case). This simple example thus clearly illustrates how the hypersecan t Jacobian avoids the major disadvantage of the Broyden approximation, while maintaining the greatest advantage: the fact that it is calculated without making any extra evaluations of the function \( f(x) \).

This linear example also illustrates how singular-value decomposition (SVD) is used to solve for the hypersecan t Jacobian elements. The variables \( x_1 \) and \( x_3 \) are interchangeable. So if they are given the same initial values, they will follow exactly the same trajectory. The linear system to solve, Eqs. (4) for the hypersecan t Jacobian elements on row 1, therefore becomes singular:

\[
\begin{bmatrix}
-4.143137616670 \times 10^{-2} & -1.429236794928 \times 10^{-1} & -4.143137616670 \times 10^{-2} \\
-3.254780687737 \times 10^{-1} & -3.617952748235 \times 10^{-1} & -3.254780687737 \times 10^{-1} \\
+4.245219312263 \times 10^{-1} & +6.382047251765 \times 10^{-1} & +4.245219312263 \times 10^{-1}
\end{bmatrix}
\times
\begin{bmatrix}
H_{1,1}^3 \\
H_{1,2}^3 \\
H_{1,3}^3
\end{bmatrix} = 0.
\]

Column 1 and 3 are identical and LAPACK \texttt{dgesvx()} fails with error code \textsc{info} = 4 signifying a coefficient matrix singular to within machine precision. The inverse condition number \textsc{rcond} = \( 7.426728596992e-17 \) confirms this. The implementation of the hypersecan t solver used here handles situations like this by switching to SVD when \texttt{dgesvx()} fails. LAPACK \texttt{dgesvd()} informs us that the singular values of the coefficient matrix are

\[
(w_1, w_2, w_3) = (1.060808064514, 9.516998001847 \times 10^{-2}, 4.162068222172 \times 10^{-17}).
\]

Following the usual SVD prescription to solve linear systems, our hypersecan t solver implementation treats \( w_3 \) as approximately zero and sets \( 1/w_3 = 0 \) when it calculates the hypersecan t Jacobian elements

\[
(H_{1,1}^3, H_{1,2}^3, H_{1,3}^3) = (0.500000000000, 1.000000000000, 0.500000000000)
\]

which equals the true Jacobian to within machine precision, exactly the answer we want. The fact that Eqs. (4) can be ill-conditioned or even exactly singular therefore does not mean that their solutions, the hypersecan t Jacobian elements, are a poor approximation. As shown here, by using SVD, hypersecan t Jacobian elements can be extracted, exact to within machine precision, even from a very ill-conditioned system.
4.2. Nonlinear system

The next test is for the system of nonlinear equations

\[
\begin{align*}
\begin{cases}
f_1(x_1, x_2) &= \frac{x_1^2}{x_2} + \frac{x_2^2}{x_2^2} + \frac{x_2^2}{x_1} - \frac{3}{4} = 0 \\
f_2(x_1, x_2, x_3) &= \frac{x_1^4}{x_2} + \frac{x_2^4}{x_2} + \frac{x_3^4}{x_3} - 1 = 0 \\
f_3(x_2, x_3) &= x_2^2 + x_3^2 - \frac{3}{4} = 0
\end{cases}
\end{align*}
\]

This system also has the root \( x = (x_1, x_2, x_3) = (1, 1, 1) \), and the Jacobian at the root is

\[
J(1, 1, 1) = \begin{bmatrix} 1 & 1/2 & 0 \\ 1/2 & 1 & 1/2 \\ 0 & 1/2 & 1 \end{bmatrix}.
\]

To be able to compare not only the hypersecant and Broyden Jacobians, but also a finite-difference (FD) Jacobian, a quasi-Newton solver was implemented using the PETSc SNES nonlinear solver toolkit. PETSc can do colored finite differencing, i.e. take full advantage of the sparsity of the Jacobian to minimize the number of function evaluations used to calculate the FD Jacobian. We only specify the sparsity pattern of the Jacobian and let PETSc determine how to do the colored finite differencing.

For the hypersecant Jacobian, we take advantage of the fact that the first and last rows of the Jacobian have only two non-zero elements. For the first row, the hypersecant Jacobian elements are given as the solution to the linear system

\[
\begin{bmatrix} x_k^1 - x_0^1 \\ x_k^1 - x_1^1 \\ x_k^2 - x_1^2 \\ x_k^2 - x_2^2 \end{bmatrix} \begin{bmatrix} \tilde{H}^k_{1,1} \\ \tilde{H}^k_{1,2} \end{bmatrix} = \begin{bmatrix} f_1^k - f_1^0 \\ f_2^k - f_2^0 \end{bmatrix}.
\]

For the first and the last rows of the Jacobian, the hypersecant approximation can thus be used already after two iterations (the hypersecant Jacobian elements can be calculated from the available state at the end of the second iteration, and is thus first available for use during the third iteration).

When the iteration number is too small to calculate the hypersecant Jacobian elements \( k = 1 \) for row 1 and 3, and \( k = 1, 2 \) for row 2), we first do a Broyden update of the old Jacobian. Elements of this updated Jacobian are then used to replace sufficiently many unknowns in Eq. (4) to reduce the number of unknowns to equal the number of iterations, thereby making the system well determined.

For example, for the first iteration we get for the first row of the Jacobian

\[
\tilde{H}^1_{1,1} (x_1^1 - x_1^0) + B^1_{1,2} (x_2^1 - x_2^0) = f_1^1 - f_1^0,
\]

which only has the single unknown \( \tilde{H}^1_{1,1} \), where the tilde is used to indicate that this is only an approximate hypersecant Jacobian element. This equation can be trivially solved,

\[
\tilde{H}^1_{1,1} = \frac{f_1^1 - f_1^0 - B^1_{1,2} (x_2^1 - x_2^0)}{(x_1^1 - x_1^0)}.
\]
Figure 1: Accuracy as a function of the number of function evaluations when doing quasi-
Newton solve of Eq. (7). For the triangles, the Broyden approximation of the Jacobian was
used. For the diamonds, the hypersecant Jacobian. For the squares, the PETSc colored
finite-difference Jacobian.

Because the diagonal elements have larger values, we somewhat arbitrarily
choose to use $B_{1,2}^1$ to calculate $\tilde{H}_{1,1}^1$, instead of $B_{1,1}^1$ to calculate $\tilde{H}_{1,2}^1$. Sim-
ilarly, for the middle row we get

$$\tilde{H}_{2,2}^1 = \frac{f_2^1 - f_2^0 - B_{2,1}^1(x_1^1 - x_1^0) - B_{2,3}^1(x_3^1 - x_3^0)}{(x_2^1 - x_2^0)},$$

etc. For $k \geq 3$, the full hypersecant Jacobian is calculated (and subsequently
used for $k \geq 4$).

As usual, we initialize the Jacobian as the unit matrix and use the initial
guess $x = (1/2, 1/2, 3/2)$. As can be seen in Fig. 1 the quasi-Newton solve converges
to the default SNES accuracy in eleven iterations when either the
hypersecant or Broyden Jacobians are used. Using the SNES colored FD app-
proximation of the Jacobian, the solve converges in just five iterations. However,
because the colored FD approximation requires three extra function evaluations
(for a Jacobian with this particular sparsity pattern), the total number of func-
tion evaluations is 21 vs. the 11 needed by hypersecant/Broyden.

Even if the final Broyden Jacobian is a much poorer approximation of the
true Jacobian than the final hypersecant Jacobian is, the performance of the
Broyden and hypersecant methods in this case is very similar. However, the
hypersecant Jacobian gives more rapid convergence for the last few iterations,
as it becomes a more accurate approximation to the true Jacobian.
5. Application to a nonlinear transport equation

As noted in the introduction, our motivation for this research is to develop methods for solving nonlinear transport equations. Our particular example comes from cross-flux-surface transport in a fusion confinement device, where the transport equation is a radial continuity equation [6]:

$$\frac{\partial u}{\partial t} + \frac{1}{V'(r)} \frac{\partial}{\partial r} V'(r) \Gamma = S,$$

where the highly nonlinear flux is given by $\Gamma = \Gamma(r, u, u')$ and $u' = \partial u/\partial r$. The volume element, the differential volume in the radial variable $r$, is denoted by $V'(r)$. The components of $u(r)$ are typically the temperatures and densities of the plasma particle species, but they could also include momenta. In the cases where it is difficult to advance this partial differential equation, the dominant contribution to the flux comes from turbulent transport, which is triggered when a critical gradient is exceeded. This creates a sensitive dependence on $u'$. The stiffness of the transport equation makes it necessary to use implicit time discretization.

Time-implicit, spatially second-order finite-difference discretization on an equidistant mesh $r_j = j \Delta r, j = 0, \ldots, N$ gives the discretized system of nonlinear equations:

$$F_j(\Delta u_{j-1}, \Delta u_j, \Delta u_{j+1}) = \Delta u_j + \theta \left( \frac{1}{W'(r_j)} \frac{W'(r_{j+1/2})}{\Delta r} I_{j+1/2} - \frac{w'(r_{j-1/2})}{\Delta r} I_{j-1/2} - S_j^{n+1} \right) \Delta t + (1 - \theta) \left( \frac{1}{W'(r_j)} \frac{W'(r_{j+1/2})}{\Delta r} I_{j+1/2} - \frac{W'(r_{j-1/2})}{\Delta r} I_{j-1/2} - S_j^n \right) \Delta t = 0,$$

where subscript denotes spatial location and superscript time level, e.g. $S^n = S(r_j, n \Delta t)$ is the source at radius $r = r_j$ and time $t = n \Delta t$. The independent variables $\Delta u_j = u_j^{n+1} - u_j^n$ and $I_j = I(r_j, u_j, u'_{j+1/2})$, with $u_{j+1/2} = (u_j + u_{j+1})/2$ and $u'_{j+1/2} = (u_{j+1} - u_j)/\Delta r$. The implicitness parameter $\theta = 0$ gives fully explicit (FE) equations, $\theta = 1$ fully implicit (FI) and $\theta = \frac{1}{2}$ time-centered implicit (CI), with second-order temporal accuracy.

We next compare the three Jacobian approximations for this transport equation (10) with a single profile evolved [e.g. the ion temperature $T_i(r)$]. For the nonlinear flux we use the linear critical gradient model, which assumes the flux $\Gamma = -\chi u'$ and diffusivity

$$\chi = \max\{(1/L - 1/L_c)/L, \chi_{\text{min}}\},$$

where $L = u/|u'|$ and $L_c$ and $\chi_{\text{min}}$ are parameters. We also use a source term $S(r) = 1 - r^\alpha$. We somewhat arbitrarily choose the parameters $L = 1/2$, $\chi_{\text{min}} = 1/10$ and $\alpha = 2$. With fully implicit time discretization we get the
system of nonlinear equations

\[ F_j(\Delta u_{j-1}, \Delta u_j, \Delta u_{j+1}) = \Delta u_j + \left( \frac{1}{W'(r_j)} \frac{W'(r_{j+1/2})^{n+1} \Gamma_{j+1/2}^{n+1} - W'(r_{j-1/2})^{n+1} \Gamma_{j-1/2}^{n+1}}{\Delta r} - S_j^{n+1} \right) \Delta t = 0, \quad (11) \]

\( j = 1, \ldots, N - 1. \) To determine the appropriate on-axis \((r_0 = 0)\) boundary condition, we take one step back and write the flux term as an undiscretized divergence term:

\[ W'(r_0) F_0 = W'(r_0) \Delta u_0 + \left( \frac{\partial}{\partial r} W'(r_0) \right)_0 \Delta t - W'(r_0) S_0^{n+1} \Delta t = 0, \]

where we have also multiplied the equation with \( W'(r_0). \) In the limit \( r_0 \to 0, \) in which \( W'(r_0) \to 0, \) we get

\[ \left( \frac{\partial}{\partial r} W'(r_0) \Gamma \right)_0 \Delta t = 0. \]

Discretizing this equation with second-order error gives

\[ 3 \Gamma_{1/2}^{n+1} - \Gamma_{3/2}^{n+1} = 0, \quad (12) \]

which is a nonlinear on-axis boundary condition. The first term depends on \( \Delta u_0 \) and \( \Delta u_1, \) and the second term on \( \Delta u_1 \) and \( \Delta u_2. \) The first row of the Jacobian will thus have non-zero elements in the first three columns. The Jacobian is then tri-diagonal, but with \( J_{0,2} \neq 0, \) due to the nonlinear BC.

The hypersecant Jacobian is calculated in the way described above in Section 4.2, but both hypersecant and Broyden Jacobians are initialized as the unit matrix with the first row replaced by \( J_{0,0} = 3/10 \times N, \) \( J_{0,1} = -4/10 \times N \) and \( J_{0,2} = 1/10 \times N \) (the values given by the nonlinear BC at steady state).

Taking a single time step of 0.1 ms, the PETSc SNES quasi-Newton solve converges as shown in Fig. 5 for the three different Jacobian approximations. With the hypersecant Jacobian, the solve converges using 9 function evaluations. With PETSc colored FD 16, and with Broyden 20 function evaluations. With PETSc colored FD, only three quasi-Newton iterations are needed, but during each iteration, four extra functions calls are used to calculate the colored-FD Jacobian. With hypersecant Jacobian, the convergence is poor until the fourth iteration, the first iteration where the full hypersecant Jacobian is used. After that it takes five more iterations until convergence (for a total of nine), but each iteration only requires a single function evaluation. With the Broyden Jacobian the convergence is much poorer.

For larger time steps, a problem with using the hypersecant Jacobian approximation for PETSc SNES quasi-Newton solves becomes evident. The hypersecant Jacobian is a poor approximation of the true Jacobian for the first few iterations. To use hypersecant quasi-Newton solves for the transport equation with large time steps, one probably even needs to accept that the accuracy gets
Figure 2: Accuracy as a function of the number of function evaluations when doing quasi-Newton solve of Eq. (11). For the triangles, the Broyden approximation of the Jacobian was used. For the diamonds, the hypersecant Jacobian. For the squares, the PETSc colored finite-difference Jacobian.

worse for the first few iteration. The purpose of the first few iterations is not primarily to get closer to the root, but to sample enough function values to make Eq. (4) well determined to allow the calculation of the full hypersecant Jacobian. PETSc SNES tries to improve the accuracy for every iteration by doing a line search for the minimum accuracy along the direction of the increment. This typically fails for a poor approximation of the Jacobian. We are currently investigating some promising ways to solve these problems and plan to report on our findings in a future publication.

6. Conclusions

We have introduced the hypersecant Jacobian approximation, which has improved characteristics for solving systems of nonlinear equations with sparse Jacobians, such as occurs in the implicit advance of nonlinear PDEs. The basic idea behind this approximation is to keep several historical values – sufficient to be able to solve uniquely for an approximate Jacobian generically, but with use of Singular Value Decomposition to find a best solution when the equations are degenerate. Like the Broyden Jacobian approximation, the hypersecant Jacobian is calculated without making any additional function evaluations. Unlike the Broyden Jacobian it converges toward the finite-difference approximation of the Jacobian.
Multiple examples (linear and nonlinear systems of three independent variables and the 1D transport equation with linear-critical-gradient diffusivity) were solved using these different methods. The new hypersecent method was shown to lead to a convergent Jacobian. Improved overall convergence with respect to number of function evaluations was observed.

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