1 Introduction

In some use cases of automatic differentiation, it is desired to differentiate a code list which contains calls to an ODE integration routine, as for example the \texttt{ode23} solver in MATLAB or GNU Octave. This function is one of a family of similar builtins, which all have the same interface, such as for example \texttt{ode15s} or \texttt{ode45}.

In ADiMat \cite{1, 9} this will currently throw an error as the derivative of the builtin function \texttt{ode23} is not yet specified. On the other hand some users have use cases where this situation occurs and hence it is desirable that a method is developed for handling such cases.

This paper is organised as follows: in Section 2 we describe the mathematical methods for computing the derivatives of the solution of an ODE w.r.t. some parameters. In Section 3 we introduce a simple ODE system that serves as an illustrating example, the well-known Lotka-Volterra equations, and show the analytic derivatives for it. In Section 4 we explain how the derivatives can be computed with ADiMat, in particular when the use code uses the ODE integration function \texttt{ode23}. We show how to construct working substitution functions to propagate the derivative in both forward and reverse mode, and also how support was added to ADiMat to compute the Hessian of such user code in forward-over-reverse mode. Finally in Section 5 we provide a set of conclusions.

2 Derivatives of ODE solutions

Consider a simple ODE system of the form

\[ Y' = f(t, Y) \]
which describes the behaviour of $M$ time-dependent quantities $Y(t) \in \mathbb{R}^M$ given an initial state $Y(t_0)$ at initial time $t_0 = 0$.

The most simple way to determine $Y(t,P)$ for times $t > t_0$ is by integrating forward from the initial state using the well-known explicit Euler method using small discrete time steps $\delta t$:

$$Y(t_k) = Y(t_{k-1}) + \delta t Y'(t_{k-1})$$

with $t_k = k\delta t$ for $k = 1, \ldots, N$. In practice such ODE systems are routinely solved with more powerful methods such as the Runge-Kutta schemes of various orders.

Now it is often the case that the derivative of the ODE depends on a set of parameters $P \in \mathbb{R}^K$.

$$Y' = f(t, Y, P),$$

and thus its solution can also be seen as a function of $P$, that is $Y = Y(t, P)$. Then let us further assume that the derivatives of $Y$ w.r.t. the parameters $P$ are of interest, i.e. the quantity $\frac{dY}{dP} \in \mathbb{R}^{M \times P}$. The general method to obtain the derivatives of an ODE solution w.r.t. some parameters or the initial condition is described in [4], which we will restate in the following for our problem setup.

Since

$$\frac{d}{dt} \frac{dY}{dP} = \frac{df(t, Y, P)}{dP},$$

we get

$$\frac{d}{dt} \frac{dY}{dP} = \frac{df(t, Y, P)}{dY} \frac{dY}{dP} + \frac{df(t, Y, P)}{dP}$$

and by setting $V = \frac{dY}{dP}$ see that we obtain an augmented ODE system

$$Y' = f(t, Y, P) \quad (1)$$
$$V' = f_Y(t, Y, P) \cdot V + f_P(t, Y, P) \quad (2)$$

which can be integrated in the same manner as the original system. Assuming that the initial values $Y(t_0)$ do not depend on the parameters, the initial values $V(t_0)$ are set to zero.

When the derivatives of the solution $Y(t)$ w.r.t. the initial values $Y(t_0)$ are of interest we get with a very similar reasoning for $W = \frac{dY(t_0)}{dY}$ the additional equation

$$W' = f_Y(t, Y, P) \cdot W. \quad (3)$$

In this case the initial values $W(t_0)$ are set to the identity matrix.

### 3 Example: Differentiating the Lotka-Volterra ODE system

As an example we consider the Lotka-Volterra ODE system in Subsection 3.1, derive the analytical derivatives for it in Subsection 3.2 and compute the derivatives with several different approaches, including automatic differentiation and numerical methods in Subsection 3.3.

#### 3.1 The Lotka-Volterra ODE system

We consider a system of two ODEs describing the population numbers of two interdependent species, for example rabbits $Y_1$ and foxes $Y_2$; the well-known Lotka-Volterra equations given by

$$Y_1' = (\epsilon_1 - \gamma_1 Y_2) \cdot Y_1 \quad (4)$$
$$Y_2' = -(\epsilon_2 - \gamma_2 Y_1) \cdot Y_2 \quad (5)$$

with $P = [\epsilon_1, \gamma_1, \epsilon_2, \gamma_2]$ a set of four positive real parameters [3, 6, 8].

For our example we choose the parameters $P$ as given in the following table
and set the initial conditions as follows:

\[
Y_1(t_0) = 1000 \quad Y_2(t_0) = 20
\]

When we integrate the ODE in the time span \( T = [t_0, t_{\text{end}}] = [0, 10^3] \) with the explicit Euler method with fixed time steps \( \delta t = 0.1 \) we obtain the result shown in Figure 1.

![Figure 1: An example solution of the Lotka-Volterra equations integrated with explicit Euler.](image)

3.2 The derivatives of the Lotka-Volterra ODE system

Now we apply the equations (1)–(3) to our example problem. The derivative \( f_Y \) is given by

\[
f_Y = \frac{df}{dY} = \begin{pmatrix}
\epsilon_1 - \gamma_1 Y_2 & -\gamma_1 Y_1 \\
\gamma_2 Y_2 & -\gamma_2 Y_1 - \epsilon_2 + \gamma_1 Y_1
\end{pmatrix},
\]

the derivative \( f_P \) is

\[
f_P = \frac{df}{dP} = \begin{pmatrix}
Y_1 & -Y_1 \cdot Y_2 & 0 & 0 \\
0 & 0 & -Y_2 \cdot Y_1 & 0
\end{pmatrix},
\]

we set the initial state \( V(t_0) \) to zero

\[
V(t_0) = \frac{dY(t_0)}{dP} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]
and the initial state \( W(t_0) \) to the identity matrix

\[
W(t_0) = \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}.
\]

Applying the explicit Euler method to the augmented system yields the derivatives of the population numbers w.r.t. the four parameters over time, as shown in Figures 2 and 3, and the derivatives w.r.t. the initial population numbers shown in Figure 4. Note that in order to use the \texttt{ode23} solver the augmented ODE system has to be cast into a single column vector, that is, the system is then solved by integrating a composite state \( x = \begin{pmatrix} Y^T & [V]^T & [W]^T \end{pmatrix}^T \) from the initial state \( x(t_0) \) using the composite derivative

\[
x' = \begin{pmatrix}
Y' \\
V' \\
W'
\end{pmatrix} = \begin{pmatrix}
f(t, Y, P) \\
\frac{df}{dY} V + \frac{df}{dP} \\
\frac{df}{dY} W
\end{pmatrix},
\]

where \( \lfloor \cdot \rfloor \) shall denote the cast to a column vector.

Figure 2: The derivatives of the Lotka-Volterra equations w.r.t. the parameters \( \epsilon_1 \) and \( \gamma_1 \)

We show the function \texttt{dfode} in Listing 1. This function defines the composite ODE system as defined in (8). Note how the vector \( x \), which corresponds to \( x \), is split into the three parts corresponding to \( Y \), \( V \), and \( W \), and how the latter two are reshaped to the correct shapes so that the matrix expressions \( f_Y \cdot V + f_P \) and \( f_Y \cdot W \) can be evaluated correctly. The functions \texttt{fodep}, \texttt{fodep_y} and \texttt{fodep_p} are not shown, they correspond exactly to \( f \) from (4)-(5) and the partial derivatives \( f_Y \) from (6) and \( f_P \) from (7), resp.

Listing 1: Function defining the augmented ODE system for the Lotka-Volterra equations

\begin{verbatim}
function dyp = dfode(t, x, p)
    % dfode defines the composite ODE system
    % for the Lotka-Volterra equations w.r.t. the parameters
    % \epsilon_1 and \gamma_1.
    % \( x = \begin{pmatrix} Y^T & [V]^T & [W]^T \end{pmatrix}^T \)
    % is integrated from the initial state \( x(t_0) \).
    % \( f(t, Y, P) \), \( \frac{df}{dY} V + \frac{df}{dP} \), and
    % \( \frac{df}{dY} W \) are evaluated correctly.
    % \texttt{fodep}, \texttt{fodep_y}, and \texttt{fodep_p}
    % are not shown, they correspond exactly to \( f \) from
    % (4)-(5) and the partial derivatives \( f_Y \) from (6) and
    % \( f_P \) from (7), resp.

    % ... implementation ...
end
\end{verbatim}
Figure 3: The derivatives of the Lotka-Volterra equations w.r.t. the parameters $\epsilon_2$ and $\gamma_2$

\[
y = x(1:2);
dydp = \text{reshape}(x(3:10), [2,4]);
dydy0 = \text{reshape}(x(11:end), [2,2]);
dy = \text{fodep}(t, y(1:2), p);
ddydp = \text{fodep}_y(t, y, p) \ast dydp + \text{fodep}_p(t, y, p);
ddydy0 = \text{fodep}_y(t, y, p) \ast dydy0;
dyp = [\]
  dy(:)
ddydp(:)
ddydy0(:)
\]

Obviously we could also use automatic differentiation of the MATLAB code implementing $f$ to obtain $f_Y$ and $f_P$. This approach yields exactly the same results as the analytic derivatives. Here we could of course use the ADiMat driver \texttt{admDiffFor}, cf. \cite{9}, but for such a small derivative being computed many times in a hot loop the overhead of this convenience driver is just too large. This driver can be made a little bit faster by setting the option nochecks. This option has the effect that neither will the source transformation be done nor the transformed file be checked for conformity. Thus, the user must first run the \texttt{admDiffFor} once exactly as intended to let ADiMat produce the differentiated code correctly. Then in the ODE function the option nochecks is added. However, the overall expense of the driver is still much too high for this approach to be competitive here. Instead, the user just take the time to code the appropriate manual invocations of the differentiated code. In our test this results in a reduction of the overall runtime by a factor of 10. We show the function \texttt{adfode} in Listing 2, including a branch to select one of the two variants.
Listing 2: The augmented ODE function using automatic differentiation with ADiMat

```matlab
function dyp = adfode(t, x, p)
    y = x(1:2);
    dydp = reshape(x(3:10), [2, 4]);
    dydy0 = reshape(x(11:end), [2, 2]);
    useDriver = false;
    if useDriver
        [J, dy] = admDiffFor(@fodep, 1, t, y, p, admOptions('i', [2, 3], 'nochecks', 1));
        dfdy = J(:,1:2);
        dfdp = J(:,3:end);
    else
        dfdy = zeros(2, 2);
        dfdp = zeros(2, 4);
        g_y = zeros(2, 1);
        g_p = zeros(4, 1);
        for k=1:2
            g_y(k) = 1;
            [g_dy, dy] = g_fodep(t, g_y, y, g_p, p);
            dfdy(:,k) = g_dy;
            g_y = zeros(2, 1);
        end
        for k=1:4
            g_p(k) = 1;
            [g_dy, dy] = g_fodep(t, g_y, y, g_p, p);
            dfdp(:,k) = g_dy;
            g_p = zeros(4, 1);
    end
end
```
end
end
ddydp = dfdy * dydp + dfdp;
ddydy0 = dfdy * dydy0;
dyp = [
    dy(:),
    ddydp(:),
    ddydy0(:)
];

Another completely different approach is to numerically differentiate the entire ODE integration, using either the finite difference approximation (FD) method [7] or the complex step (CS) method [5]. The latter method is well-known to yield accurate derivatives of real analytic computations while the typical accuracy of finite differences is at best half the machine precision. Since both \( f \) and the explicit Euler method are real analytic we get the expected relative errors when comparing the four different ways to evaluate these derivatives, as shown in the all-vs-all comparison shown in Table 1.

Table 1: The relative error of the derivatives, computed with the four different methods, of the ODE integrated with the explicit Euler scheme, each compared against all the others

|                | vs. AD  | vs. FD  | vs. CS  |
|----------------|---------|---------|---------|
| Analytic       | 0       | 1.55324(-06) | 3.3805(-15) |
| AD             | 1.55324(-06) | 3.3805(-15) |         |
| FD             |         | 1.55324(-06) |         |

Integration of the augmented ODE system with either analytic or AD derivatives yields exactly the same result, while using the CS method to differentiate through the integration of the original ODE system yields very nearly the same result. The relative error in the divided differences is a little more than the square root of the machine precision, as expected.

3.3 Integration of the original and augmented Lotka-Volterra ODE system with the Runge-Kutta method

Things become a little more interesting when we use the more sophisticated Runge-Kutta method with adaptive timesteps as it is implemented in MATLAB or GNU Octave by the ode23 builtin function.

The first thing to note is that when integrating the augmented system the ODE integrator will generally choose different time step sizes than for the original system. Hence it will yield result vectors of different lengths, which makes it difficult to compare the different differentiation methods. This can be circumvented by prescribing a vector of time points to the integrator, instead of the tuple of start and end points \( T \), forcing it to return the solution at exactly the given points. This is in particular also required when using finite differences to approximate the derivative, because otherwise the results are completely spurious. Apparently the perturbations in the parameters are small enough to result in the same number of time steps, but the output time points themselves do change.

The results of the augmented system with either analytic or AD derivatives are visually very similar to those with the explicit Euler method, shown in the previous subsection. We show the AD derivative w.r.t. the first two parameters in Figure 5, we show the FD approximation w.r.t. the first two parameters in the Figure 6, and the CS method derivative w.r.t. the same parameters in Figure 7.

However, the relative error all-vs-all relative error comparison shown in Table 2 reveals that the FD and CS methods are apparently yielding results which are substantially different from the analytic and AD derivatives in this case.
Figure 5: The results of the complex step method applied to the integration of the Lotka-Volterra equations with the ode23 solver, w.r.t. the parameters $\epsilon_2$ and $\gamma_2$

Table 2: The relative error of the derivatives w.r.t. $P$, computed with the four different methods, of the ODE integrated with the ode23 solver, each compared against all the others

|       | vs. AD   | vs. FD   | vs. CS   |
|-------|----------|----------|----------|
| Analytic | 0   | 0.0398952 | 0.0411807 |
| AD     | 0.0398952 | 0.0411807 |          |
| FD     |          | 0.0112255 |          |

The runtimes with all four methods, using explicit Euler or ode23 are given in Table 3. While using AD with the manually written invocations of the differentiated code is slightly slower than using analytic derivatives, it is about twice as fast as using the FD or CS method.

Table 3: Runtimes of the augmented ODE equations with the four different methods to compute the derivatives, in seconds

|       | Analytic | AD   | FD   | CS   |
|-------|----------|------|------|------|
| Expl. Euler | 0.845753 | 1.86251 | 3.04297 | 2.76348 |
| ode23  | 0.208587 | 0.318961 | 0.635216 | 0.600115 |

4 Computing derivatives of ODE integrations with ADiMat

Although ADiMat is a relatively mature AD tool which supports a substantial set of MATLAB built-in functions, due to the sheer number of these it often occurs that a particular user code makes use of a builtin that is not yet supported. An example for this is the ode23 ODE solver
which we use here to solve the Lotka-Volterra equations. In this section we want to show how to insert a manually derived derivative into a larger piece of differentiated code.

Consider as an example the function \texttt{fmain} shown in Listing 3. In order to facilitate this task it is most convenient to place the call to \texttt{ode23} into a separate function, so as to isolate it as much as possible. For this purpose we define the function \texttt{calcode}, which is shown in Listing 4.

Listing 3: Main function to be differentiated with ADiMat, which makes indirect use of the unsupported builtin \texttt{ode23}, via the sub function \texttt{calcode}

\begin{verbatim}
function z = fmain(y0, p, ts)
  %ADiMat BMFUNC [$$1$$, $$2$$]=calcode($$1$$,$$2$$) DIFFTO [$$@1$$,$$1$$, $$@2$$,$$2$$]=g_calcode($$@1$$,$$1$$,$$@2$$,$$2$$,$$3$$)
  p2 = p ./ 2;
  [t1, y1] = calcode(y0, p, ts);
  [t2, y2] = calcode(y0, p2, ts);
  z = sum(y1(end,:), + y2(end,:));
end
\end{verbatim}

Listing 4: Function \texttt{calcode} is used to isolate the call to the unsupported builtin \texttt{ode23}, via the sub function \texttt{calcode}

\begin{verbatim}
function [t, yt] = calcode(y0, p, ts)
  [t, yt] = eeuler(@(t, y) fodep(t, y, p), ts, y0);
end
\end{verbatim}

Then we differentiate the function \texttt{fmain} as normally in forward mode. ADiMat will differentiate \texttt{calcode} as well and complain about the unsupported builtin \texttt{ode23}. As a result the generated function \texttt{g_calcode} will be invalid. However, by looking at the signature of \texttt{g_calcode} we know how a manually created replacement function should look like, as shown in Listing 5.

Listing 5: Signature of the invalid differentiated function for \texttt{calcode} generated by ADiMat

\begin{verbatim}
function [t, g_y, y] = g_calcode(y0, g_p, p, ts)
end
\end{verbatim}
For the reverse mode, the approach is a little bit trickier. We delete the file `calcode.m` before launching the differentiation. This will lead ADiMat to creating a generic call to an adjoint function. Of course we restore `calcode.m` afterwards. For this to work we have to declare the identifier `calcode` to ADiMat using the `BMFUNC` directive [2].

Next we prepare two functions which compute the correct derivatives when called from the differentiated code of `fmain`. This requires a little bit of insight into how ADiMat works, so a few comments are in order. The general approach is to obtain in any conceivable way the local Jacobian $J$ or partial derivative of the function `calcode`. To this end we can set up the augmented ODE system (1)–(2) using either analytic or AD derivatives. In the latter case we would effectively use ADiMat in a hierarchical, two-tier fashion.

Then, in forward mode, we reshape in incoming derivative to a column vector and multiply it from the left with $J$. Afterwards we reshape it to the same shape as the function result of `calcode`. This is code is placed in a file `fn_calcode.m` which is shown in Listing 6. Note one particularity: since `g_calcode` also returns the function results of `calcode` we can replace these by extracting the corresponding bits of the augmented ODE system. Remember however that the result vectors have different lengths when solving the augmented ODE. In this case, due what is actually done with these results in `fmain` or `g_fmain` we get way with this substitution. In other cases this may not be the case. We will see how to handle that when we consider the reverse mode.

Listing 6: FM substitution function for `calcode`, using the augmented ODE system with analytic derivatives to compute the derivative

```matlab
function [t, g_y, y] = g_calcode(g_y0, y0, g_p, p, ts)
dydp_0 = zeros(2, 4);
dydy0_0 = eye(2);
yp0 = [y0(:);
```
dydp_0(:)
dydy0_0(:,:]);
[t, ypt] = ode23(@(t, yp) dfode(t, yp, p), ts, yp0);
no = length(t);
y = ypt(:,1:2);
Jp = reshape(ypt(:,3:10), [2.*no, 4]);
Jy0 = reshape(ypt(:,11:end), [2.*no, 2]);
g_y = Jy0 * g_y0(:) + Jp * g_p(:);
g_y = reshape(g_y, size(y));

In reverse mode, we reshape in incoming adjoint to a row vector and multiply it from the right
with \( J \). Then we reshape the result to the same shape as the function parameter of which we
require the adjoint, in this case \( p \). This is code is placed in a file \( \text{rm_calcode.m} \) which shown in
Listing 7. Here we run into the problem of the changing number of integrations steps that we
mentioned. The function \( \text{rm_calcode.m} \) receives the adjoint of \( y \), and so we are stuck with its size
and need to create a Jacobian of conforming size. To this end, we have to run the original ODE
system first, simply to get the vector of time steps. Of course this is only necessary when the time
argument \( ts \) to the \( \text{calcode} \) function is really a time span, i.e. a vector of length two, and not a
vector of time points already. Obviously the second variant is preferable.

Listing 7: RM substitution function for \( \text{calcode} \), using the augmented ODE system with analytic
derivatives to compute the derivative

\[
\begin{align*}
\text{function} & \quad [a_y0, a_p] = \text{a_calcode}_110(y0, p, ts, a_y) \\
\text{if} & \quad \text{length}(ts) == 2 \\
& \% \text{timespan given: run ODE integration to get resulting time points} \\
& \quad [t, yt] = \text{calcode}(y0, p, ts); \\
\text{else} & \\
& \quad t = ts; \\
\text{end} \\
& \quad dydp_0 = \text{zeros}(2, 4); \\
& \quad dydy0_0 = \text{eye}(2); \\
& \quad yp0 = [y0(:), dydp_0(:), dydy0_0(:)]; \\
& \% \text{run augmented ODE integration with same time points as} \\
& \% \text{non-augmented integration} \\
& \quad [t_{alt}, ypt] = \text{ode23}(@(t, yp) \text{dfode}(t, yp, p), t, yp0); \\
& \quad no = \text{length}(t); \\
& \quad assert(no == \text{length}(t_{alt})); \\
& \quad y = ypt(:,1:2); \\
& \quad Jp = \text{reshape}(ypt(:,3:10), [2.*no, 4]); \\
& \quad Jy0 = \text{reshape}(ypt(:,11:end), [2.*no, 2]); \\
& \quad a_p = a_y(:,') * Jp; \\
& \quad a_y0 = a_y(:,') * Jy0; \\
& \quad a_p = \text{reshape}(a_p, \text{size}(p)); \\
& \quad a_y0 = \text{reshape}(a_y0, \text{size}(y0)); \\
\end{align*}
\]

The entire process to produce and then run a valid function \( g_{fmain} \) which calls the manually
prepared code in Listing 6 can be expressed with the following MATLAB commands:

\[
\begin{align*}
r_f = \text{admTransform}(@fmain, \text{admOptions('i', [1,2], 'mode', 'F'))} \\
copyfile('fm_calcode.m', 'g_calcode.m'); \\
J_f = \text{admDiffFor(@fmain, 1, y0, p, ts, admOptions('i', [1,2], 'nochecks', 1))} \\
\end{align*}
\]

For the reverse mode, the following MATLAB commands will produce and then run a valid function
\( a_{fmain} \) which calls the manually prepared code in Listing 7:

\[
\begin{align*}
r_f = \text{admTransform}(@fmain, \text{admOptions('i', [1,2], 'mode', 'F'))} \\
copyfile('fm_calcode.m', 'g_calcode.m'); \\
J_f = \text{admDiffFor(@fmain, 1, y0, p, ts, admOptions('i', [1,2], 'nochecks', 1))} \\
\end{align*}
\]
if exist('calcode')
    movefile('calcode.m', '_calcode.m');
clear calcode
end

r_r = admTransform(@fmain, admOptions('i', [1,2], 'mode', 'r'))
movefile('_calcode.m', 'calcode.m');
copyfile('rm_calcode_110.m', 'a_calcode_110.m');
J_r = admDiffRev(@fmain, 1, y0, p, ts, admOptions('i', [1,2], 'nochecks',1))

The runtimes of derivative evaluations with AD in FM and RM are compared to those with the FD and CS methods in Table 4.

Table 4: Runtimes of the example function differentiated with ADiMat in FM, RM and with the FD and CS methods, in seconds

|            | FM       | RM       | FD       | CS       |
|------------|----------|----------|----------|----------|
| Expl. Euler| 1.85121  | 2.39589  | 5.76037  | 5.35389  |
| ode23      | 2.06182  | 0.571279 | 1.11894  | 0.734798 |

4.1 Evaluating the Hessian in forward-over-reverse mode

ADiMat can compute the Hessian matrix of a function using forward-over-reverse mode, through its driver function admHessian. In this case the code differentiated in reverse mode, which is exactly the same function a_fmain that we created in the previous section, is being run with arguments that are of a special class tseries2 with overloaded operators (OO) which propagate derivatives – more precisely, truncated Taylor coefficients – in forward mode. Assuming to use this to differentiate fmain will fail however, with an error being thrown by ode23. It appears it is not allowed to run the ode23 solver with any other type than single or double floats in MATLAB. This is the case even when the OO type enters the picture only via the additional parameter p used by the function handle given to the solver as the first argument, that is, when we differentiate w.r.t. P only, but not w.r.t. Y(t0).

Hence it is required to add a method ode23 to the OO class and ensure that the call is dispatched to it. This would will only happen when one of the immediate arguments to the call is of the OO type. That means, one must compute the derivative w.r.t. y0. Then it is possible, albeit by means of some quite advanced MATLAB hacking, to analyse the function handle passed, extract the OO value p from its closure, or workspace, and construct a new one which, firstly, does not have an OO type in the closure and, secondly, represents the augmented ODE system which can be used to calculate the derivatives.

This derivative can then be used to propagate the derivatives to the output OO value, just as in the FM example shown before. This approach will only yield the first order derivatives, which is a limitation for the class tseries2, which in general can propagate Taylor coefficients truncated at a finite but arbitrary order. However, computing the first derivative in tseries2 is enough to evaluate the Hessian since the second order derivative is obtained by virtue of the reverse mode code.

The runtime of the Hessian evaluation with admHessian is compared to those with the second order FD method in Table 5.

Table 5: Runtimes of the evaluation of the Hessian of example function with ADiMat and with the method, in seconds

|            | FM-over-RM | FD     |
|------------|------------|--------|
| Expl. Euler| 21.398     | 3.89455|
| ode23      | 2.80302    | 7.81168|
5 Conclusion

In this report we showed several methods to calculate the derivatives of an ODE integration. In particular we showed how to use ADiMat to differentiate a larger code that calls the MATLAB ODE solver `ode23` in some sub function as part of its overall computations. This works with both the forward and reverse mode of ADiMat but currently requires some manual intervention. Obviously a continuation of these results would look into discerning a method that automates the entire process. To get this done correctly, however, will probably require that ADiMat first supports lambda expressions, which is most likely still a substantial development effort.

Another result that we obtain is that both the FD and CS methods can be used to calculate the derivatives of a simple explicit Euler scheme, however both fail when attempting to differentiate the `ode23` solver. The exact reason should be investigated further, since it is not usual that AD and FD derivatives deviate by more than the to-be-expected inaccuracy. However, it is possible to give examples where FD approximation can fare almost arbitrarily bad. Also, the fact that we apparently get the correct derivatives when using the simple explicit Euler scheme seems to show that we are indeed doing the correct thing when setting up the augmented ODE system.

The Hessian matrix can also be computed by means of the forward-over-reverse mode using the operated overloading Taylor propagation class in ADiMat. The implementation of the `ode23` method added to the class for this purpose shows the way to go for a full support for the differentiation of ODE integration builtins with ADiMat.

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