Algorithm 982: Explicit solutions of triangular systems of first-order linear initial-value ordinary differential equations with constant coefficients

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A method to compute explicit solutions of homogeneous triangular systems of first-order linear initial-value ordinary differential equations with constant coefficients is described. It is suitable for the limited case of well separated eigenvalues, or for multiple zero eigenvalues provided the entire column corresponding to a zero eigenvalue is zero. The solution for the case of constant inhomogeneity is described. The method requires only to compute a constant matrix using a simple recurrence. Computing the solutions of the system from that matrix, for values of the independent variable, requires to exponentiate only the diagonal of a matrix. It is not necessary to compute the exponential of a general triangular matrix. Although this work was motivated by a study of nuclear decay without fission or neutron absorption, which is used throughout as an example, it has wider applicability.

CCS Concepts: •**Mathematics of computing** →**Solvers; Ordinary differential equations;**

General Terms: Mathematics of computing, Mathematical software, Solvers, Mathematical analysis, Differential equations, Ordinary differential equations

Additional Key Words and Phrases: ordinary differential equations, initial value problem, first order, constant coefficient, triangular system, explicit solution

ACM Reference format:
W. Van Snyder. 2017. Algorithm 982: Explicit solutions of triangular systems of first-order linear initial-value ordinary differential equations with constant coefficients. *ACM Trans. Math. Softw.* 44, 2, Article 9 (November 2017), 4 pages.
DOI: 0000001.0000001

1 DEVELOPMENT OF THE SOLUTION

A system of first-order linear homogeneous initial-value ordinary differential equations

$$\frac{\mathrm{d}\mathbf{N}(t)}{\mathrm{d}t} = \mathbf{A}\mathbf{N}(t) \tag{1}$$

where $\mathbf{A}$ is a constant matrix, has a general solution of the form

$$\mathbf{N}(t) = \exp(\mathbf{A}t)\,\mathbf{N}(0)\,. \tag{2}$$

For the bidiagonal case with $N_i(0) = 0$ for $i > 1$, $a_{i+1,i} = -a_{ii}$, and other elements of $\mathbf{A}$ zero, Bateman [1] provided the solution

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DOI: 0000001.0000001

$$N_n(t) = \frac{N_1(0)}{a_{nn}} \sum_{i=1}^{n} a_{ii} \alpha_i \exp(a_{ii} t) \tag{3}$$

where

$$\alpha_i = \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{a_{jj}}{a_{jj} - a_{ii}} \,. \tag{4}$$

The structure of the case of a triangular matrix $\mathbf{A}$ is exploited below to produce a simple explicit solution that generalizes Bateman's result, and, like Bateman's result, requires computing the exponential of only a diagonal matrix. Other methods to solve such systems (e.g. [3]) either calculate the exponential of the entire matrix $\mathbf{A}$ or solve Equation (1) numerically.

Substituting from earlier equations into later ones to replace $N_1(t)$, $N_2(t)$, … by their derivatives results in a system of the form

$$\frac{\mathrm{d}\mathbf{N}(t)}{\mathrm{d}t} = \mathbf{C} \frac{\mathrm{d}\mathbf{N}(t)}{\mathrm{d}t} + \mathbf{D}\mathbf{N}(t)\,, \text{ where } \mathbf{D} = \operatorname{diag}(\mathbf{A}),\ \mathbf{C} = \mathbf{I} - \mathbf{D}\mathbf{A}^{-1} \tag{5}$$

and $\mathbf{C}$ is strictly lower triangular – its diagonal is zero. This substitution was chosen because Maple [4] produces the form of solution shown below in Equations (6–8), instead of one with indefinite integrals involving $\exp(a_{ii}\, t)$.

In decay equations without fission or neutron absorption, there is eventually a non-radioactive daughter, so $a_{nn} = 0$, the n^{th} column of $\mathbf{A}$ is zero, and $\mathbf{A}^{-1}$ does not exist. This isn't a problem because $\mathbf{C}$ is an intermediate matrix from which Equation (7) is derived formally under the assumption that $\mathbf{A}^{-1}$ exists. There is an explanation below Equation (8) concerning zero diagonal elements of $\mathbf{A}$.

The general solution of Equation (5) is

$$N_i(t) = N_i(0)\, e^{a_{ii} t} + \sum_{j=1}^{i-1} z_{ij} \left(N_j(t) - N_j(0)\, e^{a_{ii} t} \right) \tag{6}$$

where the constant coefficients z_{ij} are calculated from the recurrence

$$\begin{aligned} z_{ij} &= 0 \text{ if } i \leq j, \text{ and} \\ z_{ij} &= \frac{a_{ij} - \sum_{k=1}^{i-j-1} a_{i-k,j}\, z_{i,i-k}}{a_{jj} - a_{ii}} \text{ if } i > j\,. \end{aligned} \tag{7}$$

For the $n = 4$ case the coefficients z_{ij} are

$$\mathbf{Z} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \frac{a_{21}}{a_{11} - a_{22}} & \cdot & \cdot & \cdot \\ \frac{a_{31} - a_{21} z_{32}}{a_{11} - a_{33}} & \frac{a_{32}}{a_{22} - a_{33}} & \cdot & \cdot \\ \frac{a_{41} - a_{31} z_{43} - a_{21} z_{42}}{a_{11} - a_{44}} & \frac{a_{42} - a_{32} z_{43}}{a_{22} - a_{44}} & \frac{a_{43}}{a_{33} - a_{44}} & \cdot \end{bmatrix}. \tag{8}$$

The solutions Maple produced for Equation (5) were at first very complicated. The form of Equations (6–8) was obtained by solving the first solution for $\exp(a_{11}\, t)$ and substituting the result into the second solution, then solving the first two solutions for $\exp(a_{11}\, t)$ and $\exp(a_{22}\, t)$ and substituting the result into the third solution, etc.

Equation (7) assumes that $\mathbf{A}$ is not defective, i.e., that it has no duplicate eigenvalues. In decay equations, for example, it is possible but unlikely that two radioactive atoms in the same decay

chain will have identical or nearly-identical half lives, and therefore identical or nearly-identical diagonal elements of **A**. Cetnar [2] provides a method to deal with duplicate or near-duplicate eigenvalues, and also discusses the case of neutron absorption.

From Equation (7) it is clear that one zero eigenvalue does not cause a problem. Although the case of duplicate or near-duplicate nonzero eigenvalues is clearly problematic in Equation (7), duplicate zero eigenvalues do not cause a problem, at least when the entire column of **A** is zero if the diagonal element is zero, as is the case for nuclear decay equations. When there is more than one final stable decay product, $a_{ii} = a_{jj} = 0$. If $a_{ii} = 0$ then, assuming conservation of atoms, $a_{ki} = 0$ for $k > i$. The last condition is a statement of the physical fact that if isotope i does not decay, then it cannot contribute to an increase in the amount of isotope k. This does not lead to a problem to compute **Z**. For example, in Equation (8), if $a_{33} = a_{44} = 0$ then $a_{43} = 0$, and $z_{43} = 0$ is the correct interpretation of $a_{43}/(a_{33} - a_{44})$.

Because **A** is constant, the coefficients z_{ij} are constants. The only terms in the final solution that depend upon the independent variable are exponential functions of the diagonal elements of **A**. It is not necessary to compute $\exp(\mathbf{A}t)$. For the limited cases of well-separated eigenvalues, or multiple zero eigenvalues provided the entire column of **A** corresponding to each zero eigenvalue is zero, the simple method described here is effective and efficient. If the nonzero eigenvalues are not well separated, higher precision should be used to calculate z_{ij} to avoid cancellation, $\exp(\mathbf{A}t)$ should be calculated [5], or Equation (1) should be solved numerically. Since z_{ij} are constants, once their values are obtained, higher precision is not necessary to evaluate Equation (6).

2 INHOMOGENEOUS CASE

An inhogeneous equation of the form

$$\frac{\mathrm{d}\mathbf{N}(t)}{\mathrm{d}t} = \mathbf{A}(\mathbf{N}(t) + \mathbf{B}) \tag{9}$$

where **B** is constant, has a general solution of the form

$$\mathbf{N}(t) = \exp(\mathbf{A}t)\,\hat{\mathbf{N}}(0) - \mathbf{B} \tag{10}$$

where $\hat{\mathbf{N}}(0) = \mathbf{N}(0) + \mathbf{B}$. This solution can easily be obtained from the solution for the homogeneous case.

3 USAGE OF THE SOFTWARE

The software consists of two generic Fortran module subprograms, with interfaces

```
subroutine Compute_Z_Matrix ( A, Z )
  real(rk), intent(in) :: A(:,:)  ! Lower triangular activity matrix
  real(rk), intent(out) :: Z(:,:) ! Matrix of solution coefficients
end subroutine Compute_Z_Matrix
```

and

```
subroutine Compute_Solution ( T, A, Z, N0, N_T )
  real(rk), intent(in) :: T       ! Independent variable
  real(rk), intent(in) :: A(:,:)  ! Only the diagonal is needed
  real(rk), intent(in) :: Z(:,:)  ! Solution matrix
  real(rk), intent(in) :: N0(:)   ! Initial condition
  real(rk), intent(out) :: N_T(:) ! Solution N(T)
end subroutine Compute_Solution
```

In the specific subroutines for default real type and double precision type, the named constant RK has the values RK=kind(1.0e0) and RK=kind(1.0d0), respectively.

These subprograms might be used in the following way to solve Equation (1):

```
call Compute_Z_Matrix ( A, Z )
T = 0
do while ( T <= Final_T )
  call Compute_Solution ( T, A, Z, N0, N_T )
  print *, T, N_T
  T = T + Step
end do
```

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Received February 2017; revised March 2017 and April 2017; accepted June 2017