Matrix Analysis of Tracer Transport

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Abstract

We review matrix methods as applied to tracer transport. Because tracer transport is linear, matrix methods are an ideal fit for the problem. In particular, solutions of linear, first-order systems of ordinary differential equations (ODEs) are reviewed as well as special properties of these solutions. Detailed derivations are included.

Keywords

tracer dynamics, Eulerian transport, numerical analysis, matrix methods, partial differential equations, ordinary differential equations, advection
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1 Introduction

Mills (2012) introduces a method of dynamical tracer interpolation in which the tracer dynamics are represented as a matrix and the largest principal components correlated with a series of sparse measurements. The method is called “principal component proxy tracer analysis”.

Because the processes of tracer advection as well as the related ones of local stretching and diffusion are linear, matrix methods represent a powerful and general set of techniques to apply to these problems. This review summarizes some of these techniques as well as special properties of the matrices as used to represent transport processes. In particular, we review methods of solving systems of linear ordinary differential equations (ODEs) of the form:

\[
\frac{d\vec{r}(t)}{dt} = A(t) \cdot \vec{r}(t)
\]  

(1)

where \(A\) is the instantaneous dynamics, while \(\vec{r}\) is either the tracer, the stretching of an infinitesimal area in Lagrangian space or the tracer gradient at a single point in Lagrangian space.

The solution can be represented in the form:

\[
\vec{r}(t) = R \cdot \vec{r}(t_0)
\]

(2)

The solution matrix, \(R\), can be broken down in a number of useful ways and may possess important properties depending upon those of \(A\).

It is hoped that this compilation can help improve understanding of fluid transport and in particular improve both understanding and implementation of principal component proxy and similar techniques.

## 2 Fundamentals

A trajectory is the motion in time of an infinitesimal packet of fluid as it is carried along by the flow:

\[
\frac{d\vec{x}}{dt} = \vec{v}(\vec{x}, t)
\]

(3)

where \(\vec{x}\) is position, \(t\) is time and \(\vec{v}\) is the flow field. If we integrate this in time, starting at \(t_0\) and ending at \(t = t_0 + \Delta t\), we get a vector function, call it, \(\Phi\):

\[
\vec{x} = \Phi(\vec{x}_0, t_0, \Delta t)
\]

(4)

where \(x_0 = x(t_0)\) is the Lagrangian or starting coordinate. Unlike in Ottino (1989), we specify the starting time explicitly instead of assuming that \(t_0 = 0\). This convention will become useful later on, e.g., when chaining functions:

\[
\vec{x} = \Phi(\vec{x}_0, \Delta t_1 + \Delta t_2) = \Phi[\Phi(\vec{x}_0, t_0, \Delta t_1), t_0 + \Delta t_1, \Delta t_2]
\]

(5)

A flow tracer is a scalar field that follows the flow, typically a dissolved trace substance, but could also comprise a suspension or in fact any property of the fluid such as temperature or the velocity field itself.
The change in the total amount of tracer in a fixed volume, \( \delta V \), is given by the flux plus the source term:

\[
\frac{\partial}{\partial t} \int_{\delta V} \rho d\vec{x} = - \int_A \rho \vec{v} \cdot \hat{n} dA + \int_{\delta V} \sigma d\vec{x}
\]

(6)

where \( \rho \) is the density of the tracer, \( A \) is the area enclosing \( \delta V \) and \( \sigma \) is the source term, which for the moment, we will take to be zero but in later analysis will be needed both for the diffusion term and for explicit generation and loss terms.

From divergence theorem:

\[
\int_{\delta V} \frac{\partial \rho}{\partial t} d\vec{x} = - \int_{\delta V} \nabla \cdot (\rho \vec{v}) d\vec{x}
\]

(7)

Removing the integrals and expanding the first term on the right side:

\[
\frac{\partial \rho}{\partial t} = - \vec{v} \cdot \nabla \rho - \rho \nabla \cdot \vec{v}
\]

(8)

The first term is the advection term while the second term is the mass conservation term and is governed by the expansion and contraction of the fluid. In an incompressible fluid (that is, \( \nabla \cdot \vec{v} = 0 \)), this term will be zero.

To go from the Lagrangian to the Eulerian formulation, we use the following equation for the total derivative:

\[
\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho
\]

(9)

Combining this with Equation (8):

\[
\frac{d\rho}{dt} = - \rho \nabla \cdot \vec{v}
\]

(10)

This is the Lagrangian equation for conservation of mass and governs the total density of the fluid, that is, fluid density is itself a flow tracer.

Suppose we use a mixing ratio instead of density to track the tracer:

\[
q = \frac{\rho}{\rho_t}
\]

(11)

where \( \rho_t \) is the total density of the fluid. Differentiating this wrt \( t \) and then substituting Equation (10) produces the following:

\[
\frac{dq}{dt} = \frac{1}{\rho_t} \frac{d\rho}{dt} - \frac{\rho}{\rho_t^2} \frac{d\rho_t}{dt}
\]

(12)

\[
= 0
\]

(13)
or, in Eulerian form:

\[
\frac{\partial q}{\partial t} = -\vec{v} \cdot \nabla q
\]  

(14)

This is the advection equation.

3 Volume deformation

Most of this analysis can be found in Pattanayak (2001) and Mills (2004). The instantaneous rate of stretching of Lagrangian space is given by the gradient, or Jacobi matrix, of the velocity, \( \nabla \vec{v} \). Suppose we perturb a trajectory by a minute amount, \( \delta \vec{x} \). The Taylor expansion of the time derivative is, to first order:

\[
\frac{d}{dt}(\vec{x} + \delta \vec{x}) \approx \vec{v} + \nabla \vec{v} \cdot \delta \vec{x}
\]  

(15)

or:

\[
\frac{d}{dt}\delta \vec{x} \approx \nabla \vec{v} \cdot \delta \vec{x}
\]  

(16)

Whether we left multiply or right multiply depends on which convention we adopt for the application of the gradient or nabla operator, \( \nabla \), to a vector, therefore we write it out component-by-component:

\[
\nabla \vec{v} = \begin{bmatrix}
\frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} & \frac{\partial v_x}{\partial z} \\
\frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial y} & \frac{\partial v_y}{\partial z} \\
\frac{\partial v_z}{\partial x} & \frac{\partial v_z}{\partial y} & \frac{\partial v_z}{\partial z}
\end{bmatrix}
\]  

(17)

where \( \vec{x} = [x_1, x_2, x_3] = [x, y, z] \).

We define \( H(\vec{x}_0, t_0, \Delta t) \) as follows:

\[
\frac{dH}{dt}(\vec{x}_0, t_0, 0) = \nabla \vec{v} \cdot H
\]  

(18)

\[
H(\vec{x}_0, t_0, 0) = I
\]  

(19)

where \( I \) is the identity matrix. This is known as the tangent model of a dynamical system and applied to a trajectory is the total stretching of Lagrangian space.

We can relate \( H \) to the integrated trajectory, \( \Phi \), as follows:

\[
\frac{d\Phi}{dt} = v(\Phi, t)
\]  

(20)

\[
\frac{d}{dt} \nabla_{\vec{x}_0} \Phi = \nabla \vec{v} \cdot \nabla_{\vec{x}_0} \Phi
\]  

(21)
or,

\[ \nabla \vec{x}_0 \Phi = H \quad (22) \]

Note that:

\[ \delta \vec{x} = H \cdot \delta \vec{x}_0 \quad (23) \]

where \( \delta \vec{x}_0 = \delta \vec{x}(t = t_0) \).

In conjunction with the equations for the evolution of error vectors, above, we can derive a set of corresponding equations for the evolution of the tracer gradient. Taking the gradient of Equation (14):

\[ \frac{\partial}{\partial t} \nabla q = -\nabla q \cdot \nabla \vec{v} - \vec{v} \cdot \nabla \nabla q \quad (24) \]

Meanwhile, using the total derivative:

\[ \frac{d}{dt} \nabla q = \vec{v} \cdot \nabla \nabla q + \frac{\partial}{\partial t} \nabla q \quad (25) \]

and combining the two:

\[ \frac{d}{dt} \nabla q = -\nabla q \cdot \nabla \vec{v} \quad (26) \]

In parallel with \( H \), we define \( H' \):

\[ \frac{dH'}{dt} = -H' \cdot \nabla \vec{v} \quad (27) \]

\[ H' (\vec{x}_0, t_0, 0) = I \quad (28) \]

It is easy to show that:

\[ H^{-1} = H' \quad (29) \]

by taking the time derivative of \( H' \cdot H \):

\[ \frac{d}{dt} H' \cdot H = H' \cdot \frac{dH}{dt} + \frac{dH'}{dt} \cdot H \quad (30) \]

\[ = H' \cdot \nabla \vec{v} \cdot H - H' \cdot \nabla \vec{v} \cdot H \quad (31) \]

\[ = 0 \quad (32) \]

and that:

\[ \nabla q = \nabla q_0 \cdot H' \quad (33) \]

Also, by defining \( \Phi^{-1}(\vec{x}, t, \Delta t) \) as,

\[ \Phi^{-1}[\Phi(\vec{x}_0, t_0, \Delta t), t_0, \Delta t] = \vec{x}_0 \quad (34) \]

we can show:

\[ H' = \nabla \Phi^{-1} \quad (35) \]
4 Transport map

The dynamics of the tracer, \(q\), can be summarized using a linear transport map, \(Q\):

\[
q(\vec{x}, t) = \int_V Q(\vec{x}_0, \vec{x}, t_0, \Delta t)q(\vec{x}_0, t_0)d\vec{x}_0
\]  

(36)

where \(V\) here represents the total volume. In the absence of diffusion or source terms, this map can be calculated in at least two ways, by a differential equation:

\[
\frac{\partial}{\partial t} Q = (\vec{v} \cdot \nabla) Q
\]  

(37)

\[
Q(\vec{x}_0, \vec{x}, t_0, 0) = \delta(\vec{x} - \vec{x}_0)
\]  

(38)

where \(\delta\) is the delta function, and using the trajectory function:

\[
Q(\vec{x}_0, \vec{x}, t_0, \Delta t) = \delta[\Phi(\vec{x}_0, t_0, \Delta t) - \vec{x}]
\]  

(39)

In the latter case, combination with (36) produces the Frobenius-Perron equation. (Ott, 1993)

The transport map can be approximated by a matrix:

\[
\vec{q}(t) = R \cdot \vec{q}(t_0)
\]  

(40)

where \(\vec{q}\) is a discrete approximation of the tracer configuration: \(q_i = q(\vec{x}_i)\).

Tracer transport is fully linear and the time evolution of \(R\) is governed by the same mathematics as \(H\) and \(H'\):

\[
\frac{dR}{dt} = A \cdot R
\]  

(41)

There are a number of ways to calculate \(A\), the most obvious being from an Eulerian finite difference scheme, which, in one dimension, would look something like this:

\[
\frac{dr_{ij}}{dt} = \frac{v(x_j, t)}{\Delta x_{j-1} + \Delta x_j}(r_{i,j+1} - r_{i,j-1})
\]  

(42)

or,

\[
a_{i-1,i} = -\frac{v(x_i, t)}{\Delta x_{i-1} + \Delta x_i}
\]  

(43)

\[
a_{i+1,i} = \frac{v(x_i, t)}{\Delta x_{i-1} + \Delta x_i}
\]  

(44)
Neither representation shows the boundary conditions. Typically, \( A \) will be either band diagonal or, as in the case of a semi-Lagrangian scheme, quite close.

For simplicity, we will analyze both this system and the pair of systems discussed in the previous section using matrix algebra. A more thorough treatment would use abstract algebra and operator theory, especially for the transport map.

## 5 Matrix solution of systems of linear ODEs

### 5.1 Analytic solution of the stationary case

We wish to solve the system of linear ordinary differential equations (ODEs):

\[
\frac{d\vec{r}}{dt} = A \cdot \vec{r}
\]  

(45)

Supposing \( A \) has no time dependence, we perform an eigenvector decomposition:

\[
A = T \cdot \Lambda \cdot T^{-1}
\]  

(46)

where \( T \) is a matrix of right eigenvectors, and \( \Lambda \) is a diagonal matrix of eigenvalues, \( \lambda_{ii} = \lambda_i \geq \lambda_{i-1} \). The left eigenvectors are contained in \( T^{-1} \).

Thus,

\[
\frac{d}{dt}T^{-1} \cdot \vec{r} = \Lambda \cdot T^{-1} \cdot \vec{r}
\]  

(47)

By performing the linear coordinate transformation,

\[
\vec{r}' = T^{-1} \cdot \vec{r}
\]  

(48)

the equation is easily solved:

\[
r'_i = e^{\lambda_i \Delta t} r'_i(t = t_0)
\]  

(49)

or, in the un-transformed system:

\[
\vec{r}' = [T \cdot \exp(\Delta t \Lambda) \cdot T^{-1}] \cdot \vec{r}_0
\]  

\( \equiv \exp(\Delta t A) \cdot \vec{r}_0 \)  

(50)

(51)

where \( \vec{r}_0 = \vec{r}(t_0) \).
5.2 Solving the time-dependent case

The stationary case is interesting, but what can it tell us about the more general case in which $A$, which we’ll call the evolution matrix, is time-dependent? We can generalize the problem further as in (19) and (28) so that a matrix, $R$, is used in place of the vector, $\vec{r}$:

$$\frac{dR}{dt} = A(t) \cdot R$$  \hspace{1cm} (52)

One of the most important properties of the solution is that it is decomposable as follows:

$$R(t_0, t_n - t_0) = R(t_n, \Delta t_n) \cdot R(t_{n-1}, \Delta t_{n-1}) \cdot R(t_{n-2}, \Delta t_{n-2}) \cdot \ldots \cdot R(t_0, \Delta t_0)$$  \hspace{1cm} (53)

where,

$$t_n = t_0 + \sum_{i=0}^{n} \Delta t_i$$  \hspace{1cm} (54)

and we have used the convention, begun in Equation (4) of making $R$ a function both of the initial time and of the subsequent time interval. It follows that $R(t, 0) = I$.

Going back to Equation (45), we can see that the vector solution is given by a product of the initial vector with the matrix solution:

$$\vec{r}(t_0 + \Delta t) = R(t_0, \Delta t) \cdot \vec{r}(t_0)$$  \hspace{1cm} (55)

It stands to reason that each element in the decomposition in (53) may be approximated by the stationary solution in the limit as the time step approaches zero:

$$R(t, \Delta t \to 0) = \exp[A(t)\Delta t]$$  \hspace{1cm} (56)

5.3 Negative and left-multiplied cases

Consider the case in which the order of the factors on the R.H.S of Equation (45) are reversed (left-multiply vs. right-multiply):

$$\frac{d\vec{r}}{dt} = \vec{r} \cdot A$$  \hspace{1cm} (57)

This case is particularly important, since Equation (16) when rearranged in this way becomes the vorticity equation (Acheson, 1990).
We start with the analytic solution of the stationary case:

\[
A = T \cdot \Lambda \cdot T^{-1}
\]  
\[
\frac{d\vec{r}}{dt} = \vec{r} \cdot T \cdot \Lambda \cdot T^{-1}
\]  
\[
\frac{d}{dt}(\vec{r} \cdot T) = (\vec{r} \cdot T) \cdot \Lambda
\]  
\[
\vec{r} \cdot T = \vec{r}_0 \cdot T \cdot \exp(\Lambda t)
\]  
\[
\vec{r} = \vec{r}_0 \cdot T \cdot \exp(\Lambda t) \cdot T^{-1}
\]

In other words, the solution is the same, but the initial conditions are left-multiplied instead of right multiplied, or equivalently, the whole thing could be transposed.

In the time-dependent case each element of the solution is in reverse order, not just the initial conditions:

\[
\vec{r}(t_n) = \vec{r}_0 \cdot R^*(t_0, \Delta t_0) \cdot R^*(t_1, \Delta t_1) \cdot R^*(t_2, \Delta t_2) \cdots R^*(t_n, \Delta t_n)
\]

where \( R^* \) is a solution to the equation:

\[
\frac{d}{dt} R^*(t_0, t) = R^*(t_0, t) \cdot A(t)
\]  
\[
R^*(t_0, 0) = I
\]

and,

\[
R^*(t, \Delta t \to 0) = R(t, \Delta t) = \exp[A(t)\Delta t]
\]

For the case of a negative R.H.S.:

\[
\frac{d\vec{r}}{dt} = -A \cdot \vec{r}
\]

it is easy to show that the stationary solution is simply inverted:

\[
\vec{r} = T \cdot \exp(-\Delta t) \cdot T^{-1} \cdot \vec{r}
\]  
\[
= T \cdot [\exp(\Lambda t)]^{-1} \cdot T^{-1} \cdot \vec{r}
\]  
\[
= [T \cdot \exp(\Lambda t) \cdot T^{-1}]^{-1} \cdot \vec{r}
\]

while for the time-dependent case, we have:

\[
\vec{r} \approx R^{-1}(t_n, \Delta t_n) \cdot R^{-1}(t_{n-1}, \Delta t_{n-1}) \cdot R^{-1}(t_{n-2}, \Delta t_{n-2}) \cdots R^{-1}(t_0, \Delta t_0) \cdot \vec{r}_0
\]
assuming that each $\Delta t_i$ is small enough that $R$ approximates the stationary case. This provides an alternative derivation for the solution of the negative, transposed (left-multiplied) case which we saw already in (26):

$$\frac{dR}{dt} = -\vec{r} \cdot A$$

which is given by:

$$\vec{r}(t_n) \approx \vec{r}_0 \cdot R^{-1}(t_0, \Delta t_0) \cdot R^{-1}(t_1, \Delta t_1) \cdot ... \cdot R^{-1}(t_{n-1}, \Delta t_{n-1}) \cdot R^{-1}(t_n, \Delta t_n)$$

(73)

$$= \vec{r}_0 \cdot R^{-1}(t_0, t_n - t_0)$$

(74)

Where $R$ is the solution to Equation (52).

6 SVD and the Lyapunov spectrum

The singular value decomposition of a matrix is given as:

$$R = U \cdot S \cdot V^T$$

(75)

where $R$ is an $[m \times n]$ matrix, $U$ is an $[m \times n]$ ortho-normal matrix, $S$ is an $[n \times n]$ diagonal matrix of singular values ($s_{ii} = s_i > s_{i+1}$) and $V$ is an $[n \times n]$ ortho-normal matrix.

$U$ and $V^T$ are also termed the left and right singular vectors, respectively and are normally calculated through eigenvalue analysis:

$$R \cdot R^T \cdot U = U \cdot S^2$$

(76)

$$R^T \cdot R \cdot V = V \cdot S^2$$

(77)

Typically, only one of $U$ or $V$ is calculated and then the other by projection onto $R$. Which one is calculated first is best determined by whether $m$ is greater than or less than $n$. Equation (75) assumes that $m > n$. For all the problems discussed in this review, $m = n$.

Because both $R^T \cdot R$ and $R \cdot R^T$ are symmetric the singular values, $\{s_i\}$, are always real. Moreover, the eigenvectors in $U$ and $V$ form an orthogonal set spanning the space and by convention are normalized so that, $U^T \cdot U = V^T \cdot V = I$.

Assuming that $R$ is an integrated tangent model as in (19), (28) and (41), the Lyapunov exponents are defined as the time averages of the logarithms of the singular values in the limit as time goes to infinity:

$$h_i = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \log s_i$$

(78)
If there is any significant difference between the largest and next largest Lyapunov exponents, the largest singular value will come to dominate the matrix as it evolves forward in time. Thus:

\[ r_i(t \to \infty) = u_is_1 \sum_j v_j r_j(t_0) \]  

and:

\[ |\vec{r}(t \to \infty)| = |\vec{r}_0|e^{h_1\Delta t} \]  

The Lyapunov exponent is often somewhat incorrectly defined as (80) above.

7 Special properties

Since each element in (53) approaches the non-time-dependent solution given by the first factor of (50) in the limit as \( \Delta t_i \to 0 \), we can use the properties of the non-time-dependent solution to reason about those of the time-dependent one. In many cases of the problems discussed in Section 3 and Section 4, the evolution matrix, \( A \), will have special properties that will affect the solution.

7.1 Volume conservation

In the solution of (19) for instance, \( A = \nabla \vec{v} \), while the velocity field, \( \vec{v} \), is frequently non-divergent, that is \( \nabla \cdot \vec{v} = 0 \) or \( \text{Tr}(A) = 0 \). It can be shown that if the trace of a matrix is zero, then the eigenvalues sum to zero. We provide a brief outline of the proof.

We begin by writing the characteristic polynomial as follows:

\[ \lambda^n + k_1\lambda^{n-1} + k_2\lambda^{n-2} + ... + k_{n-2}\lambda + k_{n-1}\lambda + k_n = 0 \]  

The first coefficient, \( k_1 \), is always given as:

\[ k_1 = a_{11} + a_{22} + a_{33} + ... = \text{Tr}(A) \]  

We can rewrite the characteristic polynomial in terms of the roots:

\[ (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3) ... \]

\[ = \lambda^n + (\lambda_1 + \lambda_2 + \lambda_3 + ...)\lambda^{n-1} + ... \]

Thus:

\[ k_1 = \text{Tr}(A) = \sum_i \lambda_i = 0 \]
The determinant of the stationary solution matrix, $R = T \cdot \exp(\Delta t\Lambda) \cdot T^{-1}$, in (50) is:

$$|R| = |T||\exp(\Delta t\Lambda)||T^{-1}| = |T| \prod_i \exp(\Delta t\lambda_i) \frac{1}{|T|}$$ (86)

$$= \exp\left(\Delta t \sum \lambda_i\right)$$ (88)

$$= 1$$ (89)

In other words, the solution, in this case, is \textit{volume-conserving}: volumes in the space, e.g. as calculated by the determinant of a set of solution vectors spanning the space, are conserved. This is known as Liouville Theorem (Thornton, 2003).

The result generalizes to the time-dependent case since the solution can always be decomposed as an infinite product of infinitessimally small stationary integrations. Like the eigenvalues, the Lyapunov exponents will also sum to zero:

$$|R| = |U||S||V^T| = 1$$ (90)

$$\prod_i s_i = 1$$ (91)

$$\prod_i \exp(\Delta t h_i) = 1$$ (92)

$$\sum_i h_i = 0$$ (93)

### 7.2 Mass and length conservation

Suppose $R$ has the property that it preserves lengths when applied to a vector:

$$|R \cdot \vec{q}| = |\vec{q}|$$ (94)

thus the rate of change of the vector will always be perpendicular:

$$\frac{d}{dt}|\vec{q}| = \nabla|\vec{q}| \cdot \frac{d\vec{q}}{dt}$$ (95)

$$= \frac{\vec{q}}{|\vec{q}|} \cdot A \cdot \vec{q}$$ (96)

$$= 0$$ (97)

$$\vec{q} \cdot A \cdot \vec{q} = 0$$ (98)
A is what we shall call an “orthogonality transform”. By separating the diagonal and off-diagonal components in the last expression,

$$\sum_i \sum_j a_{ij} q_i q_j = \sum_{i=1}^n a_{ii} q_i^2 + \sum_{i=1}^n \sum_{j=i+1}^n (a_{ij} q_i q_j + a_{ji} q_i q_j) = 0 \quad (99)$$

we can show that it has the following properties:

$$a_{ii} = 0 \quad (100)$$

$$a_{ij} + a_{ji} = 0 \quad (101)$$

Meanwhile, $R$ is a rotation. All the singular values of $R$ will be 1:

$$\vec{q} \cdot R^T \cdot R \cdot \vec{q} = \vec{q} \cdot \vec{q} \quad (102)$$

This implies:

$$R^T \cdot R \cdot \vec{v} = s^2 \vec{v}$$

$$s = 1 \quad (103)$$

or perhaps more simply:

$$R^T \cdot R \cdot \vec{v} = I \vec{v} = s^2 \vec{v} \quad (104)$$

Because it is a rotation, it will be orthonormal with a determinant of 1.

The tracer mapping, $Q$, as defined in (37) and (38), that is, without diffusion, will fulfill these properties. Discrete mappings can only approximate them and by necessity always include some diffusion.

A more important property of tracer advection is that the total substance remains constant, thus:

$$\sum_i q_i = \text{const.} \quad (105)$$

$$\frac{d}{dt} \sum_i q_i = 0 \quad (106)$$

This will be true even if $q$ is measured as a mixing ratio, provided that the flow is non-divergent. It also assumes, of course, an equal-volume grid. Most flows in real fluids are approximately non-divergent, especially when considered over long time scales. Continuing the derivation:

$$\sum_i \sum_j r_{ij} q_j = \sum_j q_j \quad (107)$$

$$\sum_j q_j \left( \sum_i r_{ij} - 1 \right) = 0 \quad (108)$$
and:

\[ \sum_i \frac{dq_i}{dt} = 0 \]  \hspace{1cm} (109)  
\[ \sum_i \sum_j a_{ij}q_j = 0 \]  \hspace{1cm} (110)  
\[ \sum_j q_j \sum_i a_{ij} = 0 \]  \hspace{1cm} (111)  

Therefore:

\[ \sum_i r_{ij} = 1 \]  \hspace{1cm} (112)  
\[ \sum_i a_{ij} = 0 \]  \hspace{1cm} (113)  
\[ \sum_j a_{ij} = 0 \]  \hspace{1cm} (114)  

For grids that aren’t equal-volume, we apply the following transformations:

\[ \tilde{q}_i = w_i q_i \]  \hspace{1cm} (115)  

where \( w_i \) is a weight accounting for the relative differences in volume at the \( i \)th grid point. The relevant matrices will also need to be transformed:

\[ \tilde{r}_{ij} = \frac{w_i}{w_j} r_{ij} \]  \hspace{1cm} (116)  
\[ \tilde{a}_{ij} = \frac{w_i}{w_j} a_{ij} \]  \hspace{1cm} (117)  

The same constraints in (112) and (113) now apply to the transformed matrices, \( \tilde{R} = \{\tilde{r}_{ij}\} \) and \( \tilde{A} = \{\tilde{a}_{ij}\} \). If the weights are given time dependence, a similar method can be applied to account for local changes in density in non-divergent flows.

As pointed out already, a discrete tracer mapping will always require some amount of diffusion. This means that the tracer configuration will tend towards a uniform distribution over time, that is, it will “flatten out.” We can show that, given the above constraint, a tracer field with all the same values has the smallest magnitude. Suppose there are only two elements in the tracer vector, \( \tilde{q} = \{q, q\} \). The magnitude of the vector is:

\[ |\tilde{q}| = \sqrt{q^2 + q^2} = \sqrt{2q} \]  \hspace{1cm} (118)  

Now we introduce a separation between the elements, $2\Delta q$, that nonetheless keeps the sum of the elements constant:

$$|q + \Delta q, q - \Delta q| = \sqrt{(q + \Delta q)^2 + (q - \Delta q)^2}$$  \hspace{1cm} (119)

$$= \sqrt{2q^2 + (\Delta q)^2} \geq \sqrt{2q} \hspace{1cm} (120)$$

This will generalize to higher-dimensional vectors. In general, we can say that:

$$\vec{q} \cdot R^T \cdot R \cdot \vec{q} \leq \vec{q} \cdot \vec{q} \hspace{1cm} (121)$$

Implying that for the eigenvalue problem,

$$R^T \cdot R \cdot \vec{v} = s^2 \vec{v}$$

$$s^2 \leq 1 \hspace{1cm} (122)$$

This further shows that the Lyapunov exponents are all either zero or negative with the largest equal to 0. This has been shown numerically in Mills (2012). Note however that this does not constitute a proof; the actual proof is more involved.

To prove (122) from (121), we first expand $\vec{q}$ in terms of the right singular values, $\{\vec{v}_i\}$:

$$\vec{q} = \sum_{i} c_i \vec{v}_i \hspace{1cm} (123)$$

where $\{c_i\}$ are a set of coefficients. Substituting this into the left-hand-side of (121):

$$\vec{q} \cdot R^T \cdot R \cdot \vec{q} = \left( \sum_{i} c_i \vec{v}_i \right) \cdot \left( \sum_{i} c_i s_i^2 \vec{v}_i \right) \hspace{1cm} (124)$$

$$= \sum_{i} \sum_{j} c_i c_j s_i^2 \vec{v}_i \cdot \vec{v}_j \hspace{1cm} (125)$$

$$= \sum_{i} \sum_{j} c_i c_j s_i^2 \delta_{ij} \hspace{1cm} (126)$$

$$= \sum_{i} c_i^2 s_i^2 \hspace{1cm} (127)$$

where $\delta$ is the Kronecker delta. Similarly, we can show that:

$$\vec{q} \cdot \vec{q} = \sum_{i} c_i^2 \hspace{1cm} (128)$$
If we assume that \( s_i \leq 1 \) for every \( i \), then:

\[
\sum_i c_i^2 s_i^2 \leq \sum_i c_i^2
\]

(129)
since each term on the left side is less-than-or-equal-to the corresponding term on the right side. Note that in order for the inequality in (129) to be broken, at least one singular value must be greater-than one. Therefore (121) is true for every \( \vec{q} \) if-and-only-if (122) is true for every \( s \). In the language of set theory and first-order logic:

\[
\forall \vec{q} \in \mathbb{R}^n (\vec{q} \cdot R^T \cdot R \cdot \vec{q} \leq \vec{q} \cdot \vec{q}) \iff \forall s \in \mathbb{R} | R^T \cdot R = s^2 \vec{v} (s \leq 1)
\]

(130)
A similar argument will prove (102) iff (103).

8 Volume deformation versus the transport map

Since the volume deformation matrices, \( H \) and \( H' \), and the transport map, \( Q \), are all derived from the transport equations, and their time evolution has the same mathematical form, we would expect them to be closely related. The \( H \) matrices describe the local deformation of Lagrangian space while \( Q \) describes the global deformation. Since \( \delta [\Phi(\vec{x}_0) - \vec{x}] = \delta [\vec{x}_0 - \Phi^{-1}(\vec{x})] \), we can derive (28) from (36) and (39) by taking the gradient of \( q \):

\[
\nabla_{\vec{x}}q = -\int_V \delta^T [\vec{x}_0 - \Phi^{-1}(\vec{x})] q_0(\vec{x}_0)d\vec{x}_0 \cdot \nabla_{\vec{x}}\Phi^{-1} = -\nabla_{\vec{x}_0}q_0 \cdot H'
\]

(131)

(132)
where \( \delta^T \) is the generalized vector derivative of the Dirac delta function.

Once we admit diffusion, the final tracer gradient is no longer locally dependent on the gradient at the starting point, but rather depends on the whole initial tracer configuration:

\[
\nabla_{\vec{x}}q = \int_V \nabla_{\vec{x}}Q(\vec{x}_0, \vec{x})q_0(\vec{x}_0)d\vec{x}_0
\]

(133)

As with \( \Phi \) and \( \Phi' \), there will exist an inverse transport map, \( Q^{-1} \), from which we can derive \( H \). In the absence of diffusion, the mathematics will be identical whether we move forward or backward in time. That is, for every \( q_0 \):

\[
\int_V Q^{-1}(\vec{x}, \vec{x}_0, t_0 + \Delta t, \Delta t) \int_V Q(\vec{x}_0', \vec{x}, t_0, \Delta t)q_0(\vec{x}_0', t_0)d\vec{x}_0'd\vec{x} = q_0(\vec{x}_0, t_0)
\]

(134)
or:

\[
\int_V Q^{-1}(\vec{x}', \vec{x}, t_0 + \Delta t, \Delta t)Q(\vec{x}_2, \vec{x}', t_0, \Delta t)\,d\vec{x}'
\]

(135)

\[
= \int_V Q^{-1}(\vec{x}', \vec{x}, t_0 + \Delta t, \Delta t)Q(\vec{x}_2, \vec{x}', t_0, \Delta t)\,d\vec{x}'
\]

(136)

\[
= \delta(\vec{x}_1 - \vec{x}_2)
\]

(137)

For the non-diffusive case, \(Q\) is a rotation and therefore orthogonal. We construct the inverse by simply reversing the roles of the variables: \(Q^{-1}(\vec{x}, \vec{x}_0) = Q(\vec{x}_0, \vec{x})\), the equivalent of the matrix transpose in the discrete case.

Of particular interest is what happens to these maps in the limit as time goes to infinity, \(\Delta t \to \infty\). By SVD:

\[
\lim_{\Delta \to \infty} H' = s_{h'1} \vec{R}_f' \otimes \vec{R}_0'
\]

(138)

where \(\otimes\) is the outer product and \(s_{h'1}\) is the largest singular value. The tracer gradient becomes:

\[
\nabla_{\vec{x}}q = s_{h'1} \vec{R}_f' \nabla_{\vec{x}_0} q_0 \cdot \vec{R}_0'
\]

(139)

Once we generalize SVD to continuous distributions, a similar thing will be seen to happen with the transport map:

\[
\lim_{\Delta \to \infty} Q(\vec{x}_0, \vec{x}) = Q_f(\vec{x})Q_0(\vec{x}_0)
\]

(140)

In other words, it has become separable and:

\[
\nabla_{\vec{x}}q = \nabla_{\vec{x}}Q_f \int_V Q_0(\vec{x}_0)q_0(\vec{x}_0)\,d\vec{x}_0
\]

(141)

Note that no singular value has been included since we saw from (122) that it should be close to unity.

In other words:

\[
\vec{R}_f' \approx \frac{k}{s_{h'1}} \nabla_{\vec{x}}Q_f
\]

(142)

where

\[
k \approx \frac{\int_V Q_0(\vec{x}')q(\vec{x}')\,d\vec{x}'}{\nabla_{\vec{x}_0} q_0 \cdot \vec{R}_0'}
\]

(143)

is a constant of proportionality. Because (140) is only true when diffusion is present, the relationships will only be approximate.
9 Practical considerations

The traditional method of testing Eulerian tracer simulations for stability is von Neumann analysis. Equation (42) provides a simple, finite difference method for calculating the evolution matrix, $A$, for an Eulerian tracer simulation. Assuming we’ve obeyed the Courant-Friedrichs-Lewy (CFL) criterion for choosing the time-step (which itself is derived from von Neumann analysis), von Neumann analysis shows this method to be unconditionally stable.

In fact the method is quite naive and if applied to any real fluid flow would quickly overflow. This is because shear flows and mixing cause the tracer gradient to grow without bound. To fix this, some amount of diffusion must be added. Here is the advection-diffusion equation:

$$\frac{\partial q}{\partial t} = -\vec{v} \cdot \nabla q + \nabla \cdot D \cdot \nabla q$$  \hspace{1cm} (144)

where $D$ is the diffusivity tensor. Here is its translation, in one dimension, to a second-order, centred, finite-difference equation with uniform spatial grids:

$$\frac{\partial q_i}{\partial t} = \frac{v(q_{i+1} - q_{i-1})}{2\Delta x} + \frac{d(q_{i-1} + q_{i+1} - 2q_i)}{\Delta x^2}$$  \hspace{1cm} (145)

$$= \left( -\frac{v}{2\Delta x} + \frac{d}{\Delta x^2} \right) q_{i-1} - \frac{2d}{\Delta x^2} q_i + \left( \frac{v}{2\Delta x} + \frac{d}{\Delta x^2} \right) q_{i+1}$$  \hspace{1cm} (146)

where $d$ is a scalar diffusion coefficient. Expressed as elements of a matrix:

$$a_{i,i-1} = \left( -\frac{v}{2\Delta x} + \frac{d}{\Delta x^2} \right)$$  \hspace{1cm} (147)

$$a_{i,i} = \frac{2d}{\Delta x^2}$$  \hspace{1cm} (148)

$$a_{i,i+1} = \left( \frac{v}{2\Delta x} + \frac{d}{\Delta x^2} \right)$$  \hspace{1cm} (149)

In order to prevent the simulation from overflowing, $d$ will have to be tuned. Generalization to two or more dimensions is straightforward. Since the simulation is discrete, the actual order of points in the vector or matrix is arbitrary.

Semi-Lagrangian methods perform a back-trajectory from each of the Eulerian points in the simulation, then interpolate the new value. Rather than directly integrating the tracer values, the interpolation coefficients are
stored immediately in the transport matrix, \( R(t_i, \Delta t_i) \), skipping the integration step. Each Eulerian time-step produces one element in the decomposition of the larger transport matrix \( R(t_0, t_n - t_0) \).

Semi-Lagrangian methods are unconditionally stable and not subject to the CFL criterion. Both the final transport map, and each member of its decomposition normally have the following properties:

- every element is between 0 and 1:
  \[ 0 \leq r_{ij} \leq 1 \]  \hspace{1cm} (150)

- rows sum to 1:
  \[ \sum_j r_{ij} = 1 \]  \hspace{1cm} (151)

The first condition holds for linear interpolation methods which will have a maximum of \( 2^N \) non-zero elements per row, where \( N \) is the number of dimensions. Some kernel-smoothing methods include negative coefficients.

In addition, we can approximate the evolution matrix to second order:

\[
A(t_i + \Delta t/2) \approx \frac{1}{\Delta t} [R(t_i, \Delta t) - I]
\]  \hspace{1cm} (152)

### 9.1 Criteria for stability

If the transport map, \( R \), satisfies both Equation (112) and the inequality in (150) then it is mathematically equivalent to a conditional probability. In addition, if we normalize the tracer such that \( \sum_i q_i = 1 \) then it too is equivalent to a probability.

By translating Equation (141) into an inequality, we arrive at a pair of criteria for the evolution matrix:

\[
a_{ii} \leq 0
\]  \hspace{1cm} (153)

\[
a_{ij} + a_{ji} \leq 0
\]  \hspace{1cm} (154)

in agreement with our definition of a strictly diffusive transport map in (121).

### 10 Adding sources and sinks

We wish to add a source term, \( \vec{\sigma} \), to the matrix tracer model described in the previous sections:

\[
\frac{d\vec{q}}{dt} = A(t) \cdot \vec{q} + \vec{\sigma}(t)
\]  \hspace{1cm} (155)
Integrating to a discrete, first order approximation:

\[ \vec{q}(t_n) \approx \Delta t_{n-1}\sigma(t_{n-1}) + \\
R(t_{n-1}, \Delta t_{n-1}) \cdot [(\Delta t_{n-2}\bar{\sigma}(t_{n-2}) + \\
R(t_{n-2}, \Delta t_{n-2}) \cdot [\Delta t_{n-3}\bar{\sigma}(t_{n-3}) + \\
\vdots + \\
R(t_2, \Delta t_2) \cdot [\Delta t_1\bar{\sigma}(t_1) + \\
R(t_1, \Delta t_1) \cdot [\Delta t_0\bar{\sigma}(t_0) + \\
R(t_0, \Delta t_0) \cdot q(t_0)]]]] \] (156)

and multiplying through:

\[ \vec{q}(t_n) \approx R(t_0, t_n - t_0) \cdot \vec{q}(t_0) + \\
\Delta t_0 R(t_1, t_n - t_1) \cdot \bar{\sigma}(t_0) + \\
\Delta t_1 R(t_2, t_n - t_2) \cdot \sigma(t_1) + \\
\vdots + \\
\Delta t_{n-3} R(t_{n-2}, t_n - t_{n-2}) \cdot \bar{\sigma}(t_{n-3}) + \\
\Delta t_{n-2} R(t_{n-1}, \Delta t_{n-1}) \cdot \bar{\sigma}(t_{n-2}) + \\
\Delta t_{n-1}\sigma(t_{n-1}) \] (157)

\[ = R(t_0, t_n - t_0) \cdot \vec{q}(t_0) + \sum_{i=1}^{n} \Delta t_{i-1} R(t_i, t_n - t_i) \cdot \bar{\sigma}(t_{i-1}) \] (158)

### 10.1 Diffusion

Unlike external sources and sinks, we can add diffusion to the matrix model without fundamentally changing it or its linearity. Consider the diffusion equation in one dimension:

\[ \frac{\partial q}{\partial t} = d\frac{\partial^2 q}{\partial x^2} \] (159)

where \( d \) is the diffusion coefficient. Solving by separation of variables:

\[ q = q_0 e^{-d\omega^2 t} e^{i\omega x} \] (160)

where \( \omega \) is the angular frequency of a stationary wave and \( q_0 \) is its initial amplitude. In other words, if we decompose a function using Fourier analysis, the speed with which each component will decay is proportional to the square of the angular frequency times the diffusion coefficient.

Now consider a point distribution centred at the origin which will be evenly spread in frequency space, leaving only the first factor in Equation
This is a Gaussian function and transformed back into regular ($x$) space returns another Gaussian:

$$\frac{1}{2\pi} \int e^{-\text{d} \omega^2 t} e^{i\omega x} \text{d}\omega = \frac{e^{-\frac{x^2}{4dt}}}{2\sqrt{\pi dt}} \quad (161)$$

Thus applying diffusion to a function for time $t$ is equivalent to convolution with a Gaussian of width $\sqrt{2dt}$.

A convenient property of Gaussian functions is that they are dimensionally separable making results easy to generalize from one to multiple dimensions:

$$(2\pi)^{-N/2} e^{-\frac{|\vec{x}|^2}{2}} = (2\pi)^{-N/2} \exp \left( \frac{1}{2} \sum_{i=1}^{N} x_i^2 \right) \quad (162)$$

$$= \prod_{i=1}^{N} e^{\frac{x_i^2}{2}} \sqrt{2\pi} \quad (163)$$

where $N$ is the number of dimensions.

There are a number of different approaches to adding diffusion. If the transport matrix, $R$, is integrated from an “evolution matrix”, $A$, as in Equation (52), then a diffusion term can be included in it directly, as in the finite difference example in (146).

In a semi-Lagrangian scheme, the transport matrix is generated directly by gathering the interpolation coefficients, so diffusion must be added separately. Since interpolation of back-trajectories provides a small amount of implicit diffusion, we should first calculate how much that is before adding it in more explicitly. For a linearly-interpolated semi-Lagrangian scheme in one dimension, if we assume the back-trajectory falls directly in the centre of the grid, then the coefficients form a truncated kernel each at half-maximum of the Gaussian in (161):

$$e^{-\frac{\Delta x^2}{4d_0\Delta t}} = 1/2 \quad (164)$$

where $\Delta x$ is the grid spacing and $\Delta t$ is the Eulerian time step, and $d_0$ is the “implicit” diffusion. Since the series is truncated and the normalization is the sum of the interpolation coefficients, the normalization coefficient in the denominator of (161) has been left off. Solving for the approximate diffusion coefficient:

$$d_0 = \frac{\Delta x^2}{16 \ln 2 \Delta t} \quad (165)$$

$$= \frac{\Delta x^2}{11.09\Delta t} \quad (166)$$
Because of the dimensional separability of the normal distribution, and because of how the number of points used per interpolate scales, the result generalizes to higher dimensions. If the desired diffusion is not too large, the diffusion coefficient can be set by varying the time step.

The convolution of a Gaussian with another Gaussian is a third Gaussian whose variance is the sum of the variances of the other two:

$$\frac{1}{2\pi \sigma_1 \sigma_2} \int e^{-\frac{x'^2}{2\sigma_1^2}} e^{-\frac{(x'-x)^2}{2\sigma_2^2}} dx' = \frac{e^{-\frac{x^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}}$$

(167)

Thus, if we wish to add diffusion through a smoothing matrix, applied after each time step, we calculate the diffusion coefficient, $d_s$, to use for the Gaussian kernel from the desired diffusion coefficient, $d$, less the implicit diffusion coefficient, $d_0$:

$$d_s = d - \frac{\Delta x^2}{11.09 \Delta t}$$

(168)

The advantage to this scheme is that varying amounts of diffusion can be added as needed after integrating the transport matrix. Alternatively, rather than linear interpolation, the interpolation coefficients can be calculated in the same way as each row of the smoothing matrix: based on a Gaussian kernel according to (161).

### 11 Conclusions

Any Eulerian tracer simulation can be expressed as the product between a matrix, which captures the tracer dynamics, and a vector, which represents the tracer configuration. If the matrix is considered as a multi-dimensional function taking as parameters the start time in addition to the integration time, then it may be decomposed in terms of itself by splitting the integration into shorter intervals. By considering the tracer in this manner we can take advantage of the rich assortment of mathematical techniques for analysing matrices and linear systems.

The same mathematics can be applied to the local deformation of space produced by the flow. In this case the mathematics is exact and the size of the matrices always equal to the dimension of the flow field.

When tracer transport is treated using matrix methods, there are many special properties that can be derived for the solutions. Matrix methods are also helpful in understanding and improving the stability of solutions.
List of symbols

| Symbol | Description                  | First used |
|--------|------------------------------|------------|
| $\vec{x}$ | spatial position             | (3)        |
| $\vec{v}$ | velocity                     | (3)        |
| $t$ | time                         | (3)        |
| $\Phi$ | integrated trajectory        | (4)        |
| $\Delta t$ | change in time; time step    | (4)        |
| $\delta V$ | volume of integration        | (6)        |
| $A$ | surface area of integration enclosing $\delta V$ | (6)        |
| $\rho$ | tracer density               | (6)        |
| $\sigma$ | source term                  | (6)        |
| $q$ | tracer mixing ratio          | (11)       |
| $\rho_t$ | fluid density                | (11)       |
| $\delta \vec{x}$ | positional error             | (15)       |
| $H$ | volume deformation matrix    | (19)       |
| $\vec{x}_0$ | initial position; Lagrangian coordinate | (23) |
| $H'$ | inverse volume deformation matrix | (28) |
| $Q$ | continuous transport map     | (36)       |
| $V$ | volume of integration (whole space) | (36) |
| $R = \{r_{ij}\}$ | discrete transport map; matrix solution of a system of lODEs | (40) |
| $A = \{a_{ij}\}$ | matrix of coefficients in a system of linear ODEs | (41) |
| $\Delta x$ | grid size in Eulerian tracer simulation | (42) |
| $\Lambda = \{\lambda_i\}$ | diagonal matrix of eigenvalues | (46) |
| $T$ | matrix of eigenvectors       | (46)       |
| $\vec{r}$ | vector solution of a system of linear ODEs | (45) |
| $U$ | matrix of left singular vectors | (75) |
| $S = \{s_i\}$ | diagonal matrix of singular values | (75) |
| $V = \{v_{ij}\}$ | matrix of right singular vectors | (75) |
| $m$ | number of rows in matrix     | (75)       |
| $n$ | number of columns; size/dimension of problem | (75) |
| $\{h_i\}$ | Lyapunov spectrum            | (78)       |
| $D$ | diffusivity tensor           | (144)      |
| $d$ | diffusion coefficient        | (146)      |
| $N$ | number of spatial dimensions | (83)       |

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