

A List of Matrix Flows with Applications

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Abstract

Many mathematical problems, such as existence questions, are studied by using an appropriate realization process, either iteratively or continuously. This article is a collection of differential equations that have been proposed as special continuous realization processes. In some cases, there are remarkable connections between smooth flows and discrete numerical algorithms. In other cases, the flow approach seems advantageous in tackling very difficult problems. The flow approach has potential applications ranging from new development of numerical algorithms to the theoretical solution of open problems. Various aspects of the recent development and applications of the flow approach are reviewed in this article.

1 Introduction

A realization process, in a broad sense, means any deductive procedure that we use to comprehend and solve problems. In mathematics, especially for existence questions, a realization process often appears in the form of an iterative procedure or a differential equation. For years researchers have taken great effort to describe, analyze, and modify realization processes. Nowadays the success of this investigation is especially evident in discrete numerical algorithms. On the other hand, the use of differential equations to issues in computational mathematics has been found recently to afford fundamental insights into the structure and behavior of existing discrete methods and, sometimes, to suggest new and improved numerical methods.

This paper reflects upon a number of interesting continuous realization processes that have been proposed in the literature. Adopted from dynamical system terminology, each continuous realization process is referred to as a flow.

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Although the rich theory of differential equations can often be put to use, the dynamics of many of the proposed differential systems are not completely understood. The true impact on numerical algorithms also needs to be investigated further. The intention of this paper is to compile a list of flows with brief description of possible applications so as to stimulate further interest and advance in the flow approach for realizing a problem.

The basic idea of continuous realization methods is to connect two abstract problems by a mathematical bridge. Usually one of the abstract problems is a made-up problem whose solution is trivial while the other is the real problem whose solution is difficult to find. The bridge usually takes the form of an integral curve for a certain ordinary differential equation that describes how the problem data, including the answer to the problem, are transformed from the simple system to the more complicated system. This idea will become clear in the next section.

Obviously, the most important issue in the flow approach is the assurance that a bridge connecting the two abstract problems does exist. The construction of a bridge can be motivated in several different ways: Sometimes an existing discrete numerical method may be extended directly into a continuous model [32, 8]; Sometimes a differential equation arises naturally from a certain physical principles [40, 44]; More often a vector field is constructed with a specific task in mind [6, 11, 15, 16]. We shall report the material only descriptively. For more extensive discussion, readers should refer to the bibliography.

We present the flows on a case-by-case basis. For brevity, we encapsulate the circumstances under which the discussion is set forth by the following labels:

ORIGINAL PROBLEM: The underlying problem that is to be solved.

DISCRETE METHOD: Basic schemes of any existing discrete methods.

MOTIVATION: Motivation or idea for the construction of a bridge (flow).

FLOW: The description of the differential equation.

INITIAL CONDITIONS: The starting point of the flow (The simple system).

SPECIAL FEATURES: Special features of the flow approach.

EXAMPLE: Examples or applications.

GENERALIZATION: Possible generalizations or new numerical schemes.

2 List of Flows

2.1 Linear Stationary Flows

ORIGINAL PROBLEM: Solve the linear equation

$$Ax = b \tag{1}$$

where $A \in R^{n \times n}$ and $x, b \in R^n$.

DISCRETE METHOD: Most linear stationary methods assume the form [29]

$$x_{k+1} = Gx_k + c, \quad k = 0, 1, 2, \dots \quad (2)$$

where

$$\begin{aligned} G &= I - Q^{-1}A \\ c &= Q^{-1}b \end{aligned}$$

and Q is a splitting matrix of A .

MOTIVATION: Think of (2) as one Euler step with unit step size applied to a linear differential system.

FLOW:

$$\frac{dx}{dt} = -Q^{-1}Ax + c. \quad (3)$$

INITIAL CONDITIONS: $x(0)$ can be any point in R^n .

SPECIAL FEATURES: For global convergence of (3), only the inequalities

$$\Re \lambda_i(G) < 1 \quad (4)$$

for all eigenvalues λ_i of G are needed, which is much weaker than the would-be condition for the convergence of (2).

GENERALIZATION: Solving (3) by a numerical method amounts to a new iterative scheme, including highly complicated multistep iterative schemes [25, 8].

2.2 Homotopy Flows

ORIGINAL PROBLEM: Solve the nonlinear equation

$$f(x) = 0 \quad (5)$$

where $f : R^n \rightarrow R^n$ is continuously differentiable.

DISCRETE METHOD: A classical method is the Newton method [37]

$$x_{k+1} = x_k - \alpha_k (f'(x_k))^{-1} f(x_k). \quad (6)$$

MOTIVATION: At least two ways to motivate the continuous flows:

1. Think of (6) as one Euler step with step size α_k applied to the differential equation [32]

$$\frac{dx}{ds} = -(f'(x))^{-1} f(x). \quad (7)$$

2. Connect the system (5) to a trivial system by, for example,

$$H(x, t) = f(x) - tf(x_0) \tag{8}$$

where x_0 is an arbitrarily fixed point in R^n [1, 2]. Generically, the zero set $H^{-1}(0)$ is a one-dimensional smooth manifold.

FLOW: Either (7) or

$$\begin{bmatrix} f'(x) & -\frac{1}{t}f(x) \\ \frac{dx}{ds} & \frac{dt}{ds} \end{bmatrix} \begin{bmatrix} \frac{dx}{ds} \\ \frac{dt}{ds} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{9}$$

INITIAL CONDITIONS: For (7), $x(0)$ can be arbitrary. For (9), $x(0) = x_0$ and $t(0) = 1$.

SPECIAL FEATURES:

1. The flow of (7) satisfies $f(x(s)) = e^{-s}f(x(0))$. That is, the flow moves in the direction along which $\|f(x)\|$ is exponentially reduced.
2. Properties of f and the selection of x_0 must be taken into account in (9) in order that the bridge really makes the desired connection to $t = 0$ [1, 2].

EXAMPLE: Successful applications with specially formulated homotopy functions include eigenvalue problems [9, 34], nonlinear programming problem [27], physics applications and boundary value problems [38, 44], and polynomial systems [35, 36].

2.3 Scaled Toda Flows

ORIGINAL PROBLEM: Reduce a square matrix $A_0 \in R^{n \times n}$ to a certain canonical form [31], e.g., triangularization, so as to solve the eigenvalue problem

$$A_0x = \lambda x. \tag{10}$$

DISCRETE METHOD:

1. For triangularization, use the unshifted QR algorithm:

$$A_k = Q_k R_k \implies A_{k+1} = R_k Q_k \tag{11}$$

where $Q_k R_k$ is the QR decomposition of A_k ; or any other QR-type algorithms, e.g., the LU algorithm [28, 45].

2. For a general non-zero pattern which A_0 is reduced to, no discrete method is available.

FLOW:

1. The Toda flow

$$\frac{dX}{dt} = [X, \Pi_0(X)] \quad (12)$$

where $[A, B] = AB - BA$, $\Pi_0(X) = X^- - X^{-T}$ and X^- is the strictly lower triangular part of X .

2. The scaled Toda flow

$$\frac{dX}{dt} = [X, K \circ X] \quad (13)$$

where K is a constant matrix and \circ represent the Hadamard product.

INITIAL CONDITIONS: $X(0) = A_0$.

SPECIAL FEATURES:

1. The time-1 map of the Toda flow is equivalent to the QR algorithm [20, 40].
2. The time-1 map of the scaled Toda flow also enjoys a QR-like algorithm [18].
3. For symmetric X , K is necessarily skew-symmetric. Asymptotic behavior of (13) is completely known [18].

MOTIVATION: The Toda lattice originates as a description of a one-dimensional lattice of particles with exponential interaction. The connection between the Toda flow and the QR algorithm was discovered by Symes [40].

EXAMPLE: Different choices of the scaling matrix K give rise to different isospectral flows, including many already proposed in the literature [12, 18, 21, 41, 42]. In particular, (13) can be used to generate special canonical forms that no other methods can [10].

2.4 Projected Gradient Flows

ORIGINAL PROBLEM: Let $\mathcal{S}(n)$ and $\mathcal{O}(n)$ denote, respectively, the subspace of all symmetric matrices and the group of all orthogonal matrices in $R^{n \times n}$. Let $P(X)$ denote the projection of X onto a specified affine subspace of $\mathcal{S}(n)$. Then

$$\begin{aligned} \text{Minimize} \quad & F(X) := \frac{1}{2} \|X - P(X)\|^2 \\ \text{Subject to} \quad & X \in \mathcal{M}(X_0) \end{aligned} \quad (14)$$

where $\mathcal{M}(X_0) := \{X \in \mathcal{S}(n) | X = Q^T X_0 Q, Q \in \mathcal{O}(n)\}$ and $\|\cdot\|$ is the Frobenius norm.

DISCRETE METHOD: Depending upon the nature of the projection P , the problem may or may not have a discrete method [11]. The Jacobi method [28], for example, may be applied if $P(X) = \text{diag}(X)$.

FLOW:

$$\frac{dX}{dt} = [X, [X, P(X)]]. \quad (15)$$

MOTIVATION: The right hand side of (15) represents the negative of the gradient of F on the feasible set $\mathcal{M}(X_0)$.

INITIAL CONDITIONS: $X(0) = X_0$.

EXAMPLE:

1. The flow (15) may be employed to solve the least squares approximation problem subject to spectral constraints, the inverse eigenvalue problem and the eigenvalue problem [11]. For the latter, the flow (15) is a continuous analogue of the Jacobi method [24].
2. The flow (15) generalizes Brockett's double bracket flow [6, 7] which, in turn, has been found to have other applications in sorting, linear programming and total least squares problems [4, 5].

GENERALIZATION: The idea of projected gradient flow can be generalized to other types of approximation problems as will be seen below.

2.5 Simultaneous Reduction Flows

ORIGINAL PROBLEM: Simultaneous reduction by two kinds of transformations:

1. Reduction by orthogonal similarity transformations: Given matrices $A_i \in R^{n \times n}$, $i = 1, \dots, p$, and projection maps P_i onto specified subspaces,

$$\begin{aligned} \text{Minimize} \quad & F(Q) := \frac{1}{2} \sum_{i=1}^p \|\alpha_i(Q)\|^2 \\ \text{Subject to} \quad & Q \in \mathcal{O}(n) \end{aligned} \quad (16)$$

where $\alpha_i(Q) := Q^T A_i Q - P_i(Q^T A_i Q)$.

2. Reduction by orthogonal equivalence transformations: Given matrices $B_i \in R^{m \times n}$, $i = 1, \dots, p$, and projection maps R_i ,

$$\begin{aligned} \text{Minimize} \quad & G(Q, Z) := \frac{1}{2} \sum_{i=1}^p \|\beta_i(Q, Z)\|^2 \\ \text{Subject to} \quad & Q \in \mathcal{O}(m) \\ & Z \in \mathcal{O}(n) \end{aligned} \quad (17)$$

where $\beta_i(Q, Z) := Q^T B_i Z - R_i(Q^T B_i Z)$.

DISCRETE METHOD: Very few theoretical results or even numerical methods are available for simultaneous reduction problems [15, 31].

MOTIVATION: Compute the projected gradient of (16) and (17), respectively.

FLOW:

1. Orthogonal similar flow:

$$\frac{dX_i}{dt} = \left[X_i, \sum_{j=1}^p \frac{[X_j, P_j^T(X_j)] - [X_j, P_j^T(X_j)]^T}{2} \right]. \quad (18)$$

2. Orthogonal equivalence flow:

$$\frac{dY_i}{dt} = \sum_{j=1}^p \left\{ Y_i \frac{Y_j^T R_j(Y_j) - R_j^T(Y_j) Y_j}{2} + \frac{R_j(Y_j) Y_j^T - Y_j R_j^T(Y_j)}{2} Y_i \right\}. \quad (19)$$

INITIAL CONDITIONS: $X_i(0) = A_i$, $Y_i(0) = B_i$.

EXAMPLE: Here is a Jacobi flow for computing singular values of a single matrix:

$$\frac{dX}{dt} = X \frac{X^T \text{diag}(X) - (X^T \text{diag}(X))^T}{2} + \frac{\text{diag}(X) X^T - (\text{diag}(X) X^T)^T}{2} X. \quad (20)$$

GENERALIZATION: Two other related matrix flows (but not derived from projected gradient):

1. SVD flow:

$$\begin{aligned} \frac{dX}{dt} &= X \Pi_0(X X^T) - \Pi_0(X^T X) X, \\ X(0) &= A. \end{aligned} \quad (21)$$

2. QZ flow:

$$\begin{aligned} \frac{dX_1}{dt} &= X_1 \Pi_0(X_2^{-1} X_1) - \Pi_0(X_1 X_2^{-1}) X_1, \\ \frac{dX_2}{dt} &= X_2 \Pi_0(X_2^{-1} X_1) - \Pi_0(X_1 X_2^{-1}) X_2, \\ X_1(0) &= A_1, \\ X_2(0) &= A_2. \end{aligned} \quad (22)$$

SPECIAL FEATURES:

1. The continuous realization processes (18) or (19) have the advantages that the desired form to which matrices are reduced can be almost arbitrary, and that if a desired form is not attainable then the limit point of the differential system gives a way of measuring the distance from the best reduced matrices to the nearest matrices that have the desired form.

2. Just as the Toda lattice (12) models the QR algorithm, the system (21) models the SVD algorithm [14] for the $A \in R^{m \times n}$, and (22) models the QZ algorithm [13] for the matrix pencil $(A_1, A_2) \in R^{n \times n} \times R^{n \times n}$.

2.6 Inverse Eigenvalue Flows

ORIGINAL PROBLEM: Given a set of real numbers $\{\lambda_1, \dots, \lambda_n\}$, consider two kinds of inverse eigenvalue problems:

1. Given $A_0, \dots, A_n \in \mathcal{S}(n)$ that are mutually orthonormal, find $c = [c_1, \dots, c_n]$ such that

$$A(c) := A_0 + \sum_{i=1}^n c_i A_i \quad (23)$$

has the prescribed set as its spectrum. The special case is where $A(c)$ is a Toeplitz matrix which is known, thus far, to be an open problem [22].

2. Find a symmetric non-negative matrix P that has the prescribed set as its spectrum.

DISCRETE METHOD: A few locally convergent Newton-like algorithms are available for the first problem [26, 33]. Little is known for the non-negative matrix problem [3].

MOTIVATION: Minimize the distance between the isospectral surface and the set of matrices of desired form.

FLOW:

1. Inverse eigenvalue problem [11]:

$$\frac{dX}{dt} = [X, [X, A_0 + P(X)]] \quad (24)$$

where

$$P(X) = \sum_{i=1}^n \langle X, A_i \rangle A_i, \quad (25)$$

and $\langle \cdot, \cdot \rangle$ denotes the Frobenius inner product.

2. Inverse eigenvalue problem for non-negative matrices [16]:

$$\frac{dX}{dt} = [X, [X, Y]] \quad (26)$$

$$\frac{dY}{dt} = 4Y \circ (X - Y). \quad (27)$$

INITIAL CONDITIONS: For both (24) and (26), $X(0) = \text{diag}\{\lambda_1, \dots, \lambda_n\}$. For (27), $Y(0)$ can be any non-negative matrix.

GENERALIZATION:

1. For the inverse Toeplitz eigenvalue problem, the descent flow (24) may converge to a stationary point that is not Toeplitz. A new flow that seems to converge globally is [23].

$$\frac{dX}{dt} = [X, k(X)] \quad (28)$$

where

$$k_{ij}(X) := \begin{cases} x_{i+1,j} - x_{i,j-1} & \text{if } 1 \leq i < j \leq n \\ 0 & \text{if } 1 \leq i = j \leq n \\ x_{i,j-1} - x_{i+1,j} & \text{if } 1 \leq j < i \leq n \end{cases} \quad (29)$$

2. The idea of (24) can be generalized to inverse singular value problem:

$$\frac{dX}{dt} = X \frac{X^T(B_0 + R(X)) - (B_0 + R(X))^T X}{2} \quad (30)$$

$$- \frac{X(B_0 + R(X))^T - (B_0 + R(X))^T X}{2} X \quad (31)$$

where

$$R(X) = \sum_{k=1}^n \langle X, B_k \rangle B_k \quad (32)$$

and $B_0, B_1, \dots, B_n \in R^{m \times n}$ are prescribed mutually orthonormal matrices. Recently insights drawn from (30) give rise to new iterative methods [19].

2.7 Complex Flows

ORIGINAL PROBLEM: Most of the discussion hitherto can be generalized to the complex-valued cases. One such example is the nearest normal matrix problem [30, 39].

DISCRETE METHOD: The Jacobi algorithm [39] can be used.

MOTIVATION: The nearest normal matrix problem is equivalent to

$$\begin{aligned} \text{Minimize} \quad & H(U) := \frac{1}{2} \|U^*AU - \text{diag}(U^*AU)\|^2 \\ \text{Subject to} \quad & U \in \mathcal{U}(n) \end{aligned} \quad (33)$$

where $\mathcal{U}(n)$ is the group of all unitary matrices in $C^{n \times n}$.

FLOW:

$$\frac{dU}{dt} = U \frac{[W, \text{diag}(W^*)] - [W, \text{diag}(W^*)]^*}{2}, \quad (34)$$

$$\frac{dW}{dt} = \left[W, \frac{[W, \text{diag}(W^*)] - [W, \text{diag}(W^*)]^*}{2} \right]. \quad (35)$$

INITIAL CONDITIONS: $U(0) = I$ and $W(0) = A$.

SPECIAL FEATURES: The putative nearest normal matrix to A is given by $Z := U(\infty)\text{diag}(W(\infty))U(\infty)^*$ [15].

GENERALIZATION: Least square approximation by real normal matrices can also be done by a method described by Chu [17]

$$\frac{dX}{dt} = \left[X, \frac{[X, A^T] - [X, A^T]^T}{2} \right]. \quad (36)$$

3 Conclusion

Most matrix differential equations by nature are complicated, since the components are coupled into nonlinear terms. Nonetheless, as we have demonstrated, there have been substantial advances in understanding some of the dynamics. For the time being, the numerical implementation is still very primitive. But most important of all, we think there are many opportunities where new algorithms may be developed from the realization process. It is hoped that this paper has conveyed some values of this idea.

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