

# PPST Summer Report

## The Formulation of DMORPH and its Applications

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### 1 Introduction: Costs and Observables

The primary goal of DMORPH, diffeomorphic modulation of observable response preserving homotopy, is to provide a systematic way of searching for alternative models to ODE-modeled problems that have some cost or goal to satisfy. In many situations there exist a number of models that account for the physical phenomena involved; DMORPH provides a means of exploring these different models. By differentially morphing the form of the differential equation in a controlled way, we can not only assemble a whole ensemble of potential models, but we can also identify certain elements of the set of models that minimize some cost or possess some other desirable quality. DMORPH has the potential to be applied to a tremendous breadth of systems, including plasma models, energy allocation schemes, and many others.

Given a differential equation  $\dot{x} = f(x, t, \vec{a})$  where  $\vec{a} \in \mathbb{R}^N$  is a vector of control parameters, so long as  $f$  is Lipschitz continuous in some region  $\Omega$  ( $|f(x_1, t, \vec{a}) - f(x_2, t, \vec{a})| \leq K|x_1 - x_2|$ ,  $\forall x_1, x_2 \in \Omega$ ) we can integrate numerically to obtain a unique solution curve  $\varphi(t)$ . Moreover we may parametrize  $\vec{a}$  with a function  $\mathcal{A} : \mathbb{R}^1 \rightarrow \mathbb{R}^N$  such that  $\mathcal{A}(s) = \vec{a}(s)$ ,  $s \in [0, 1]$ . In physical processes situations sometimes arise in which there is a cost associated with the control vector  $\vec{a}(s)$ . In such a case we may wish to control these costs, so we define a cost function  $J(\vec{a}(s)) : \mathbb{R}^N \rightarrow \mathbb{R}^1$ . In other situations, the actual solution curve  $\varphi(t)$  may give rise to some physical observable. In these cases, we may desire to control the observable, so we define a scalar-valued functional  $J(x(\cdot), \vec{a}(s)) : L^2 \rightarrow \mathbb{R}$ . We are capable of controlling up to  $N - 1$  costs and/or observables exactly, while in the event that our number of costs/observables exceeds our number of controls, our system is overdetermined and we can use the method of least squares. Moreover if we seek to control  $M$  different costs/observables, instead of a scalar-valued function  $J$ , we may specify a vector-valued  $\vec{J} : \mathbb{R}^N \rightarrow \mathbb{R}^M$ .

It should be noted that our control vector may actually be a function that evolves with time, yielding  $\vec{a}(s, t) : \mathbb{R}^2 \rightarrow \mathbb{R}^N$ . This changes the nature of the problem slightly (each time point can be conceived of as a control), but the underlying formulation is still analogous to that of the vector case.

## 2 The Preservation of $\vec{J}$ over $s$ : Moving Along Level Sets

In using DMORPH to scan for alternative models to some physical system, it is reasonable to assume that each acceptable model preserves some set of observables and/or costs. The set of observables/ costs that we would like our models to preserve serve as the basis for which we define  $\vec{J}$ , as each component represents one of these features. Our construction changes considerably depending on how we define  $\vec{J}$ , and additionally, the formulation changes depending on whether  $\vec{a}$ , our control vector, is time dependent. The cases that will be discussed are listed below, and an example function or functional is provided:

$$\begin{array}{ll}
 J \text{ is a function of } \vec{a}(s) & J(\vec{a}(s)) = \sum_{n=1}^N a_n(s)^2 \\
 J \text{ is a functional of } \vec{a}(t, s) & J[\vec{a}(\cdot, s)] = \sum_{n=1}^N \int_0^T a_n(t, s)^2 dt \\
 J \text{ is a functional of } x(\vec{a}(s)) & J[x(\cdot, \vec{a}(s))] = \int_0^T h(x) dt \\
 J \text{ is a functional of } x(t, [\vec{a}(t, s)]) & J[x(\cdot, [\vec{a}(\cdot, s)])] = \int_0^T h(x) dt
 \end{array}$$

The above examples in no way represent all the potential costs and observables that could be used as components of our  $\vec{J}$ . Indeed, for example, we could define some  $J_i$  to be some composition of the above functions.

In order to preserve the value of  $\vec{J}$  as we scan across potential alternative models, we require that  $\vec{J} = \vec{c} \in \mathbb{R}^M$ , a constant. Qualitatively, each  $\vec{c}$  represents a different state of our system, and by choosing  $\vec{c}$  to correspond with the observed behavior of the system, we guarantee that each of our alternative models will also preserve this behavior.

### 2.1 The Cost Function Case: $\vec{J}$ as a Function or Functional of $\vec{a}$

The first two cases described above involve a  $\vec{J}$  that is directly dependent on the control vector  $\vec{a}$ . They will be considered separately. One case in which we may choose to define a cost that is directly dependent upon  $\vec{a}$  is a system in which we use a Fourier basis to construct  $f$ . If each component of  $\vec{a}$  serves as the coefficient to each corresponding basis function, then it may be possible to control the degree to which certain frequencies are expressed.

#### 2.1.1 $\vec{J}(\vec{a}(s))$

By parametrizing  $\vec{a}$  by  $s$ , we are free to specify a trajectory of  $\vec{J}(\vec{a}(s))$  over  $s$  by imposing the condition that  $\vec{J}(\vec{a}(s)) = \mathbf{c} \in \mathbb{R}^M$ , a constant. Each  $i$ th component of  $\mathbf{c}$  corresponds to the fixed value of the  $i$ th component of  $\vec{J}$ . Differentiating by  $s$ , we find that:

$$\frac{\partial \vec{J}}{\partial s}(s) = \vec{0} \tag{1}$$

The control vector  $\vec{a}(s)$  does not exhibit time dependence, so  $\partial\vec{J}/\partial s$  will be a function of  $s$  alone:

$$\frac{\partial\vec{J}}{\partial s}(s) = \frac{d\vec{J}}{d\vec{a}} \cdot \frac{d\vec{a}}{ds} = \underbrace{\begin{pmatrix} | & | & | \\ \frac{\partial\vec{J}}{\partial a_1} & \cdots & \frac{\partial\vec{J}}{\partial a_N} \\ | & | & | \end{pmatrix}}_{=\mathbf{A}(s)} \cdot \begin{pmatrix} \frac{da_1}{ds} \\ \vdots \\ \frac{da_N}{ds} \end{pmatrix} = \vec{0} \quad (2)$$

Note that in this case, the dimension of  $\mathbf{A}$  will be  $M \times N$ , where  $N > M$ . The condition that  $\mathbf{A} \cdot d\vec{a}/ds = 0$  is equivalent to requiring  $d\vec{a}/ds \in \text{null}(\mathbf{A})$ . Before proceeding, a comment on notation should be made. (2) essentially says that the inner product of each row vector of  $\mathbf{A}$  with  $d\vec{a}/ds$  equals zero. In general inner products are supposed to return scalars, but it is convenient here for us to allow them to return vectors. Thus, I will use the notation that

$$\langle \mathbf{M}, \vec{f} \rangle = \mathbf{M}^T \vec{f} \quad (3)$$

where  $\mathbf{M}$  is some  $M \times N$  matrix, and  $\vec{f}$  is some  $M \times 1$  column vector. Thus, returning to our problem, we can rewrite (2) as

$$\left\langle \mathbf{A}^T(s), \frac{d\vec{a}}{ds}(s) \right\rangle = 0 \quad (4)$$

To satisfy (4), we project a free vector valued function  $\vec{g}(s) : \mathbb{R}^1 \rightarrow \mathbb{R}^N$  into the null space of  $\mathbf{A}$ . Observe that if we let

$$\frac{d\vec{a}}{ds}(s) = \vec{g}(s) - \mathbf{A}^T(s) \left( \left\langle \mathbf{A}^T(s), \mathbf{A}^T(s) \right\rangle \right)^{-1} \left\langle \mathbf{A}^T(s), \vec{g}(s) \right\rangle \quad (5)$$

we can verify that

$$\left\langle \mathbf{A}^T(s), \frac{d\vec{a}}{ds}(s) \right\rangle = \vec{0} \quad (6)$$

Thus, from the above we can see that our projector  $\tilde{\mathbf{P}}(s)$  will be given by:

$$\tilde{\mathbf{P}}(s) = \mathbf{I}_N - \mathbf{A}^T(s) \left( \mathbf{A}(s) \mathbf{A}^T(s) \right)^{-1} \mathbf{A}(s) \quad (7)$$

### 2.1.2 $\vec{J}[\vec{a}(\cdot, s)]$

The case in which our cost function  $\vec{J}$  is functionally dependent upon  $\vec{a}(t, s)$ , we have  $\vec{J}(\vec{a}(\cdot, s))$ . For example,  $\vec{J}$  could be a real-valued integral function evaluated over the interval  $[0, T]$ . In this case  $\partial\vec{J}/\partial s$  would be a function of  $s$  alone and we would have

$$\frac{\partial\vec{J}[\vec{a}]}{\partial s}(s) = \int_0^T \frac{\delta\vec{J}}{\delta\vec{a}(t, s)} \cdot \frac{\partial\vec{a}(t, s)}{\partial s} dt = 0 \quad (8)$$

In order to construct our projector  $\tilde{\mathbf{P}}$  we define a function  $\mathbf{A}(t, s)$  such that

$$\mathbf{A}(t, s) = \frac{\delta\vec{J}[\vec{a}(t, s)]}{\delta\vec{a}} \quad (9)$$

$\mathbf{A}(t, s)$  will be a matrix because it is the derivative of a vector by another vector. The construction of the projector in this case will vary slightly from that defined in (7). Again, before proceeding, a comment on notation is necessary. If we are working in function space, then

$$\left\langle \mathbf{M}(t, s), \vec{f}(t, s) \right\rangle = \int_0^T \mathbf{M}^T(t, s) \vec{f}(t, s) dt \quad (10)$$

where  $\mathbf{M}(t, s)$  is some  $M \times N$  matrix, and  $\vec{f}(t, s)$  is some  $M \times 1$  column vector. Thus, we can see that (8) can alternatively be written as

$$\left\langle \mathbf{A}^T(t, s), \frac{\partial \vec{a}(t, s)}{\partial s} \right\rangle = \vec{0} \quad (11)$$

We can guarantee this to be the case by letting

$$\frac{\partial \vec{a}(t, s)}{\partial s} = \vec{g}(t, s) - \mathbf{A}^T(t, s) \left\langle \mathbf{A}^T(t, s), \mathbf{A}^T(t, s) \right\rangle^{-1} \left\langle \mathbf{A}(t, s)^T, \vec{g}(t, s) \right\rangle \quad (12)$$

for some free vector valued function  $\vec{g}(t, s)$  that is the same dimension as  $\vec{a}(t, s)$ ,  $N \times 1$ . We can verify that (12) will satisfy (11) by checking

$$\left\langle \mathbf{A}^T(t, s), \frac{d\vec{a}(t, s)}{ds} \right\rangle = \int_0^T \mathbf{A}(t, s) \vec{g}(t, s) dt - \int_0^T \mathbf{A}(t, s) \vec{g}(t, s) dt = \vec{0} \quad (13)$$

so (11) will be satisfied, and our projector acting on a free function  $\vec{g}(t, s)$  will be given by

$$\frac{\partial \vec{a}(t, s)}{\partial s} = \left( \tilde{\mathbf{P}}(t, s) \vec{g}(t, s) \right) = \vec{g}(t, s) - \mathbf{A}^T(t, s) \left( \int_0^T \mathbf{A}(t, s) \mathbf{A}^T(t, s) dt \right)^{-1} \left( \int_0^T \mathbf{A}(t, s) \vec{g}(t, s) dt \right) \quad (14)$$

## 2.2 The Observable Case: $\vec{J}$ as a Functional of $x$

It is possible that we desire our model to preserve some feature that is functionally dependent on the solution curve. One example of such a functional is the energy, which is given by  $\int_0^T |x(t)|^2 dt$ . These aspects of the model will be incorporated as components of  $\vec{J}$  defined as functionals of  $x$ . Again the formulation changes depending on whether our control field is time dependent, and the cases will be considered separately:

### 2.2.1 $\vec{J}[x(\cdot, \vec{a}(s))]$

In the case that  $\vec{J}$  is a real-valued integral functional of  $x(t, \vec{a}(s))$  we again are free to specify a trajectory of  $\vec{J}(x(\cdot, \vec{a}(s)))$  over  $s$  by imposing the condition that  $\vec{J}(x(\cdot, \vec{a}(s))) = \tau(s)$ , where  $\tau(s) : \mathbb{R}^1 \rightarrow \mathbb{R}^M$ . As before, there remains the possibility that  $\vec{a}$  may be a function of time as well, in which case we impose the condition  $\vec{J}(x(\cdot, \vec{a}(\cdot, s))) = \tau(s)$ , where  $\tau(s) : \mathbb{R}^1 \rightarrow \mathbb{R}^M$ .

Analogously to the case of the cost function  $\vec{J}(\vec{a}(s))$ , in order to preserve the value of  $\vec{J}(x(\cdot, \vec{a}))$  over  $s$ , we require that:

$$\frac{\partial \vec{J}(x(t, \vec{a}(s)))}{\partial s} = \vec{0} \quad (15)$$

Evaluating the l.h.s. of (15) we get

$$\frac{\partial \vec{J}[x(\cdot, \vec{a}(s))]}{\partial s}(s) = \int_0^T \underbrace{\left( \begin{array}{c|c|c|c} \frac{\delta \vec{J}[x]}{\delta x(t, \vec{a}(s))} & \frac{\partial x(t, \vec{a}(s))}{\partial a_1(s)} & \cdots & \frac{\delta \vec{J}[x]}{\delta x(t, \vec{a}(s))} & \frac{\partial x(t, \vec{a}(s))}{\partial a_N(s)} \end{array} \right)}_{=\mathbf{A}(s)} dt \cdot \begin{pmatrix} \frac{da_1}{ds} \\ \vdots \\ \frac{da_N}{ds} \end{pmatrix}$$

Again, in this case the dimension of  $\mathbf{A}(s)$  will be  $M \times N$ . The condition that  $\mathbf{A}(s) \cdot d\vec{a}(s)/ds = 0$  implies  $d\vec{a}(s)/ds$  is in the nullspace of  $\mathbf{A}$ , and we construct the projector in the same way as in §2.1.1:

$$\tilde{\mathbf{P}} = \mathbf{I}_N - \mathbf{A}^T(s) \left( \mathbf{A}(s) \mathbf{A}^T(s) \right)^{-1} \mathbf{A}(s) \quad (16)$$

Finally, as before, we define a free vector-valued function  $\vec{g}(s) : \mathbb{R}^1 \rightarrow \mathbb{R}^N$  and let  $d\vec{a}(s)/ds = \tilde{\mathbf{P}}(s)\vec{g}(s)$ .

### 2.2.2 $\vec{J}[x(\cdot, \vec{a}(\cdot, s))]$

In the alternate case where  $\vec{a}(t, s)$  is a function of time as well, the evaluation of  $\partial \vec{J}/\partial s$  changes. In this situation,  $x(t, s)$  is a functional of  $\vec{a}(t', s)$ ,  $t' \in [0, t]$ . Thus, we have  $\vec{J}(x(\cdot, \vec{a}(\cdot, s)))$ , and

$$\frac{\partial \vec{J}[x]}{\partial s} = \int_0^T \frac{\delta \vec{J}[x(\cdot, \vec{a}(\cdot, s))]}{\delta x(t, s)} \left( \int_0^t \frac{\delta x[\vec{a}(\cdot, s)]}{\delta \vec{a}(t', s)} \frac{\partial \vec{a}(t', s)}{\partial s} dt' \right) dt \quad (17)$$

Where (17) captures the causality of  $J$  being a functional of  $x$ , which in turn is a functional of  $\vec{a}$ . Thus, in the above statement it is implicit that  $0 \leq t' \leq t \leq T$ .

The construction of the projector is slightly different in this case, as  $\partial \vec{a}/\partial s$  is not quite as accessible. We can reverse the order of integration, however, so that (17) reads

$$\frac{\partial \vec{J}}{\partial s} = \int_0^T \left( \int_{t'}^T \frac{\delta \vec{J}[x(\cdot, \vec{a}(\cdot, s))]}{\delta x} \frac{\delta x(t, \vec{a}(\cdot, s))}{\delta \vec{a}(t', s)} dt \right) \frac{\partial \vec{a}(t', s)}{\partial s} dt' = \vec{0} \quad (18)$$

Note than in (18) the term in parentheses gets integrated over  $t$ , so it is a function of  $t'$ . Thus, let

$$\mathbf{Q}(t', s) = \int_{t'}^T \frac{\delta \vec{J}[x(\cdot, \vec{a}(\cdot, s))]}{\delta x} \frac{\delta x(t, \vec{a}(\cdot, s))}{\delta \vec{a}(t', s)} dt \quad (19)$$

Thus, (18) can be rewritten as

$$\frac{\partial \vec{J}}{\partial s} = \int_0^T \mathbf{Q}(t', s) \frac{\partial \vec{a}(t', s)}{\partial s} dt' = \vec{0} \quad (20)$$

where  $\mathbf{Q}(t', s)$  is an  $M \times N$  time-dependent matrix. Using the notation established previously, we can rewrite (20) as

$$\int_0^T \mathbf{Q}(t, s) \frac{\partial \vec{a}(t, s)}{\partial s} dt = \left\langle \mathbf{Q}^T(t, s), \frac{\partial \vec{a}(t, s)}{\partial s} \right\rangle = \vec{0} \quad (21)$$

From here we can proceed exactly as we did in §2.1.2 and let

$$\frac{\partial \vec{a}}{\partial s}(t, s) = \vec{g}(t, s) - \mathbf{Q}^T(t, s) \left( \int_0^T \mathbf{Q}(t', s) \mathbf{Q}^T(t', s) dt' \right) \int_0^T \mathbf{Q}(t', s) \vec{g}(t', s) dt' \quad (22)$$

### 3 The Tracking Problem: Leaving Level Sets

It is also possible that, once we have accepted a model for our system, that we would like to alter the system in some way. For example, we may desire the features captured by  $\vec{J}$  to morph in some controlled way; this is equivalent to setting some trajectory for  $\vec{J}$  over  $s$ . We can use DMORPH to determine how  $\vec{a}$  must be changed over  $s$  in order to achieve this trajectory.

#### 3.1 Moving $J$ Along a Track

The above formulation, where we required  $\partial \vec{J} / \partial s = \vec{0}$ , amounted to exploring level sets where  $\vec{J}(\vec{a}(t, s))$  and  $\vec{J}[x(\vec{a}(t, s))]$  were set equal to some constant  $\mathbf{c} \in \mathbb{R}^M$ . We are not required, however, to remain on a level set; we are free to specify a non-preserving track for  $\vec{J}$  by requiring:

$$\frac{\partial \vec{J}}{\partial s} = \vec{\gamma}(s) \quad \vec{\gamma} : \mathbb{R}^1 \rightarrow \mathbb{R}^M \quad (23)$$

In §2 we had  $\vec{\gamma}(s) = 0 \forall s$ . In this section, however,  $\vec{\gamma}$  can be any continuous vector-valued function. Thus we can see that (23) represents an inhomogeneous equation to which we have found the corresponding homogeneous solution in §2. We previously found in §2.1 with a time-independent control field that:

$$\frac{\partial \vec{J}(\vec{a}(s))}{\partial s} = \mathbf{A}(s) \frac{d\vec{a}(s)}{ds} = \vec{\gamma}(s) \quad (24)$$

Recall that  $\mathbf{A}$  is non-square, so it is non-invertible. In general, however, it will have an  $N \times M$  pseudoinverse  $\mathbf{A}^+$ , which can be found with the Moore-Penrose pseudoinverse, which is given by:

$$\mathbf{A}^+ = \mathbf{A}^T (\mathbf{A} \mathbf{A}^T)^{-1} \quad (25)$$

Multiplying through from the left by  $\mathbf{A}^+$ , we can see that the solution

$$\frac{d\vec{a}(s)}{ds} = \mathbf{A}^+ \vec{\gamma}(s) \quad (26)$$

satisfies (24). Thus, using the principle of superposition to sum the homogeneous and inhomogeneous solutions, we can see that letting

$$\frac{d\vec{a}(s)}{ds} = \tilde{\mathbf{P}}(s) \vec{g}(s) + \mathbf{A}^+ \vec{\gamma}(s) \quad (27)$$

satisfies (23), where  $\tilde{\mathbf{P}}(s)$  is the projector matrix defined in (7) and  $\vec{g}(s)$  is our free function.

In the event that we have a cost function  $\vec{J}$  that is a functional of  $\vec{a}(t, s)$ , the tracking solution will be

somewhat different. In this case, we found in (8) that

$$\frac{\partial \vec{J}[\vec{a}]}{\partial s}(s) = \int_0^T \frac{\delta \vec{J}}{\delta \vec{a}(t, s)} \cdot \frac{\partial \vec{a}(t, s)}{\partial s} dt = \vec{\gamma}(s) \quad (28)$$

or alternatively,

$$\left\langle \mathbf{A}^T(t, s), \frac{\partial \vec{a}}{\partial s}(t, s) \right\rangle \quad (29)$$

where  $\mathbf{A}(t, s)$  is the  $M \times N$  matrix  $\delta \vec{J} / \delta \vec{a}$ . Observe that if we let

$$\frac{\partial \vec{a}}{\partial s}(t, s) = \underbrace{\mathbf{A}^T(t, s) \left( \left\langle \mathbf{A}^T(t, s), \mathbf{A}^T(t, s) \right\rangle \right)^{-1}}_{=\tilde{\mathbf{R}}(t, s)} \vec{\gamma}(t, s) \quad (30)$$

then we can see that

$$\left\langle \mathbf{A}^T(t, s), \left( \mathbf{A}^T(t, s) \left( \left\langle \mathbf{A}^T(t, s), \mathbf{A}^T(t, s) \right\rangle \right)^{-1} \vec{\gamma}(t, s) \right) \right\rangle = \vec{\gamma}(t, s) \quad (31)$$

Using the principle of superposition and summing our homogeneous and inhomogeneous equations, we have

$$\frac{\partial \vec{a}}{\partial s}(t, s) = \tilde{\mathbf{P}}(t, s) \vec{g}(t, s) + \tilde{\mathbf{R}}(t, s) \vec{\gamma}(t, s) \quad (32)$$

The cases in which  $\vec{J}$  is an observable functional have very similar formulations to those described above. With a time-independent control field  $\vec{a}(s)$ , our solution is analogous to that presented in (27). With a time-dependent control field, our solution is analogous to that presented in (32)

### 3.2 Maximizing and Minimizing $\vec{J}$

Less demanding than tracking  $\vec{J}$ , we may also wish to extremize  $\vec{J}$ . If we wish to maximize the value of  $\vec{J}$ , we can accomplish this by requiring  $\partial \vec{J} / \partial s \geq 0 \forall s$ . Drawing on the material from §3.1, this can be accomplished by choose a track  $\vec{\gamma}(s)$  where each entry  $\gamma_i(s) \geq 0 \forall s$ . Conversely, if we want to minimize the value of  $\vec{J}$ , we can choose a function  $\vec{\gamma}(s)$  such that each component  $\gamma_i(s) \leq 0 \forall s$ . Thus, by defining  $\vec{\gamma}$  appropriately we can guarantee that  $\vec{J}$  will increase or decrease monotonically.

## 4 Choosing the Free Function

While we are largely free to choose any continuous free function  $\vec{g}(s)$ , different functions will ultimately give rise to different tracks  $d\vec{a}(s)/ds$ . There are many tracks  $\vec{a}(s)$  that will satisfy our original equation, but some may be particularly costly, while others may be more desirable. One way to control these costs is through the free function.

Consider the following example. If we seek to preserve the value of  $\vec{J}(\vec{a}(s))$  over  $s$ , we would follow the construction established in §2.1. It is possible, however, that one of the controls  $a_1$  is particularly costly to use. Thus, we may wish to minimize the norm of  $a_1$  while still preserving  $\vec{J}(\vec{a}(s))$ . In this case we define a

cost  $K : \mathbb{R}^N \rightarrow \mathbb{R}^1$

$$K(\vec{a}(s)) = a_1^2 \quad (33)$$

where our cost is directly proportional to the square of  $a_1$ . Differentiating  $K$  by  $s$ , we have:

$$\frac{\partial K}{\partial s} = \underbrace{\begin{pmatrix} 2a_1 & 0 & 0 & \dots & 0 \end{pmatrix}}_{=\vec{B}^T(s)} \begin{pmatrix} \frac{da_1}{ds} \\ \frac{da_2}{ds} \\ \vdots \\ \frac{da_N}{ds} \end{pmatrix} \quad (34)$$

It has also been shown that the projector is semi-definite, which implies that  $\forall \vec{x} \in \mathbb{R}^N$ , we have  $\vec{x}^T \tilde{\mathbf{P}} \vec{x} \geq 0$ . Returning to (34) we can rewrite this as

$$\frac{\partial K}{\partial s} = \vec{B}^T(s) \tilde{\mathbf{P}}(s) \vec{g}(s) \quad (35)$$

If we want to minimize our cost  $K$ , then we require  $\partial K / \partial s \leq 0 \forall s$ . By using the fact that  $\tilde{\mathbf{P}}$  is positive semi-definite, we let  $\vec{g}(s) = -\vec{B}(s)$  and this will be accomplished. Analogously, if we wanted the value of  $K$  to increase, we would let  $\vec{g}(s) = \vec{B}(s)$ .

In another example, we could have a cost function  $K$  that is a functional of the solution curve  $x(\cdot)$ . For instance, we can define a cost:

$$K[x(\cdot)] = \int_0^T x(t) dt \quad (36)$$

Differentiating by  $s$ , we have:

$$\frac{\partial K}{\partial s} = \int_0^T \frac{\delta K}{\delta x(t)} \cdot \frac{\partial x(t)}{\partial \vec{a}(s)} dt \begin{pmatrix} d\vec{a} \\ ds \end{pmatrix} \quad (37)$$

or alternatively,

$$\frac{\partial K}{\partial s} = \underbrace{\left( \int_0^T \frac{\delta K}{\delta x(t)} \cdot \frac{\partial x(t)}{\partial a_1(s)} dt \quad \dots \quad \int_0^T \frac{\delta K}{\delta x(t)} \cdot \frac{\partial x(t)}{\partial a_N(s)} dt \right)}_{=\mathbf{B}^T(s)} \begin{pmatrix} \frac{da_1}{ds} \\ \vdots \\ \frac{da_N}{ds} \end{pmatrix} \quad (38)$$

As before, we can take advantage of the fact that the projector is positive semi-definite and define  $\vec{g}(s) = -\vec{B}(s)$ . Thus we will find the path for  $\vec{a}(s)$  that minimizes our cost  $K$  and still preserves  $\vec{J}$  (or follows some track  $\vec{\gamma}(s)$ ).

As a final example, consider a situation in which we have some observable or cost that we wish to preserve. At the same time, however, we can use the free function to control our trajectories  $x_s(t)$ . If we have some ideal trajectory  $x_*(t)$ , then we can define a cost function  $K : L^2 \rightarrow \mathbb{R}^1$

$$K[x(\cdot)] = \int_0^T (x(t) - x_*(t))^2 dt \quad (39)$$

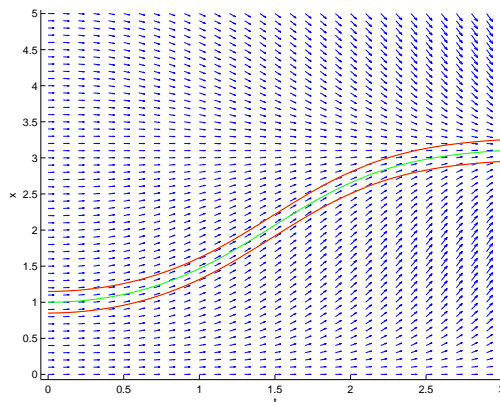
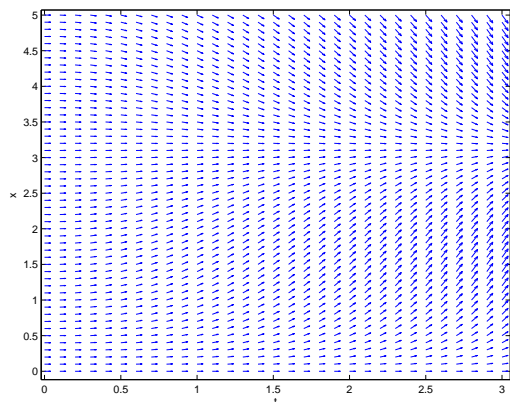
We can then use the formulation of (38) to find the appropriate free function  $\vec{g}(s)$  that will find the solution



that most closely approximates  $x_*(t)$ .

## 5 A Kinematic Approach

In our original construction of DMORPH, we make global differential changes in the vector field  $\dot{x}$  and then, given an initial condition  $x_0$ , our solution curves  $\varphi(t)$  continuously change accordingly. For example, the picture below on the left may represent the state of our vector field  $f$  at some particular  $s$ .



As we move across  $s$ , each arrow in the left picture above experiences a differential change, and the entire field is altered. It has been proposed, however, that a more direct approach may be to introduce a differential change only to that part of the field  $f$  that intersects some epsilon neighborhood of our solution curves  $\varphi(t)$ . Consider the picture on the right. As we move across  $s$ , we could leave everything outside of the red lines untouched. Then, we could introduce a differential change to our solution curve  $\varphi(t, s)$  (note that now we're directly changing the curve  $\varphi$  rather than the whole field  $f$ ). Because  $f = \dot{x}$ , the new field  $f(x(t, s + \epsilon), t, s + \epsilon)$  along the new curve would be entirely determined by our new solution curve. Then, in the epsilon neighborhood, we could arbitrarily define  $f$  such that a smooth transition occurs from outside the neighborhood up to the solution curve  $\varphi$ .

Consider a differential equation of the form

$$\dot{x}(t) = f(x(t), t) \tag{40}$$

Assuming  $f$  is Lipschitz continuous, the above equation has a unique solution curve  $\varphi(t)$  such that  $\dot{\varphi}(t) = f(\varphi(t), t)$ . Based on this solution curve, we can define an observable  $J : L^2 \rightarrow \mathbb{R}^1$  such that

$$J(\varphi) = \int_0^T h(\varphi(t)) dt \tag{41}$$

We can parametrize (40) and its corresponding solution curve  $\varphi(t)$  by some scalar  $s$ . We can then morph the solution curve  $\varphi(t, s)$  such that the observable  $J(\varphi)$  is preserved and see locally how  $f$  will respond with no consideration given to the behavior of  $f$  away from the solution curve  $\varphi(t, s)$ . The requirement that

$J(\varphi(t, s))$  be preserved is equivalent to requiring

$$\frac{\partial J(\varphi)}{\partial s} = \int_0^T \frac{\delta J}{\delta \varphi(t, s)} \cdot \frac{\partial \varphi(t, s)}{\partial s} dt = 0 \quad (42)$$

Equation (48) can alternatively be written as

$$\left\langle \frac{\delta J}{\delta \varphi(t, s)}, \frac{\partial \varphi(t, s)}{\partial s} \right\rangle = 0 \forall s \quad (43)$$

For the sake of notation, let  $a(t, s) = \delta J / \delta \varphi(t, s)$ . As previously described, we can satisfy (49) by letting

$$\frac{\partial \varphi(t, s)}{\partial s} = \tilde{\mathbf{P}}(t, s)g(t, s) = g(t, s) - a(t, s) \frac{\langle a(t, s), g(t, s) \rangle}{\langle a(t, s), a(t, s) \rangle} = g(t, s) - a(t, s) \frac{\int_0^T a(t', s)g(t', s)dt'}{\int_0^T a(t', s)^2 dt'} \quad (44)$$

where  $\tilde{\mathbf{P}}(t, s)$  is a projector and  $g(t, s)$  is some continuous free scalar function. We can calculate the derivative with respect to  $t$  at any given point along  $\varphi(t, s)$ . Bear in mind that we do not know how  $f$  will behave away from the solution curves  $\varphi(t, s)$ , but this information is of little consequence to us anyway.

One question that arises is how should we construct the free function  $g(t, s)$ ? We can approach this similarly to our original approach, whereby we define a cost function  $K : L^2 \rightarrow \mathbb{R}^1$ . For example, if we sought to preserve  $J$  while minimizing the integral over  $[0, T]$ , we could define

$$K(\varphi) = \int_0^T \varphi(t) dt \quad (45)$$

In order to minimize  $K$  over  $s$ , we require that  $\partial K / \partial s \leq 0$ , so

$$\frac{\partial K(\varphi)}{\partial s} = \int_0^T \frac{\delta K}{\delta \varphi(t, s)} \cdot \frac{\partial \varphi(t, s)}{\partial s} dt = \left\langle \frac{\delta K}{\delta \varphi(t, s)}, \tilde{\mathbf{P}}(t, s)g(t, s) \right\rangle \quad (46)$$

Note that in this case  $\delta K / \delta \varphi(t, s) = 1$ . Recalling from the previous notes that the projector  $\tilde{\mathbf{P}}(t, s)$  is positive semi-definite, we let our free function  $g(t, s) = -\delta K / \delta \varphi(t, s)$ , and  $K$  will decrease over  $s$ . Results of a numerical simulation are shown below in which the energy  $J$  was preserved over  $s$  and the area integral  $K$  was sought to be minimized. Also note that we were able to prescribe a track  $dx_0(s)/ds$ , a track for the initial conditions over  $s$ .

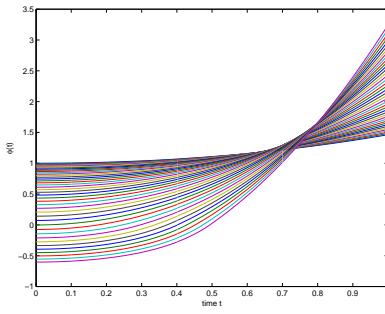


Figure 1: The successive solution curves  $\varphi(t, s)$ . Each curve corresponds to a value of  $s$ . In this simulation the energy was preserved and the area integral was minimized.

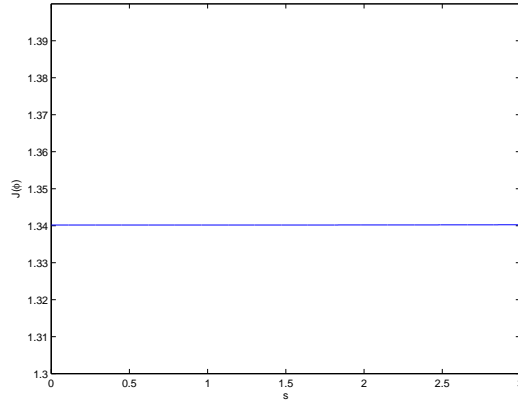


Figure 2: The observable  $J(\varphi)$  is preserved over  $s$ .

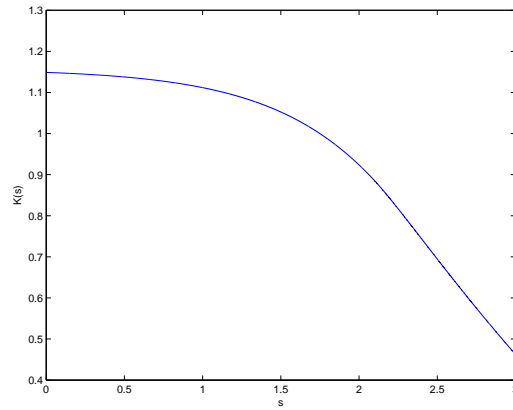


Figure 3: The cost function  $K(\varphi)$  decreases over  $s$ .

## 6 DMORPH as a Means of Decoupling Systems

In constructing models of physical phenomena, one question that regularly arises is *are the dynamics coupled or decoupled?* By looking at the Jacobian of the system, not only can we determine whether or not the dynamics are coupled, but we can also use DMORPH to control this coupling.

We begin by considering some path  $\vec{\varphi}(t)$  through  $\mathbb{R}^N$ . In the event that  $\dot{\vec{\varphi}}(t)$  is a function of time in addition to being a function of  $\vec{\varphi}(t)$ , the system is said to be *nonautonomous*. That is,

$$\frac{d}{dt}\vec{\varphi}(t) = \vec{f}(\vec{\varphi}(t), t) \quad (47)$$

where  $\dim(f) = N$ . Notice that time appears explicitly in the argument of  $\vec{f}$ . Regardless of how  $\vec{\varphi}(\cdot)$  was generated in the first place, the explicit appearance of  $t$  in the r.h.s. of (47) allows us to construct a system of *decoupled nonautonomous* equations to which  $\vec{\varphi}(t)$  is a solution. That is given  $\vec{\varphi}(t)$ , we could plot  $\varphi_i(t)$ , calculate its derivative as a function of both  $\varphi_i(t)$  and  $t$ , and then define a corresponding  $f_i(\varphi_i(t), t)$  such that

$$\frac{d}{dt}\varphi_i(t) = f_i(\varphi_i(t), t) \quad (48)$$

A system in which the derivative with respect to time at each point is independent of time is said to be *autonomous*. That is,

$$\frac{d}{dt}\vec{\varphi}(t) = \vec{f}(\vec{\varphi}(t)) \quad (49)$$

Notice that  $t$  does not appear explicitly in the r.h.s. of (49). In general, it will only be possible to construct a system of *decoupled autonomous* equations to which  $\varphi(\cdot)$  is a solution if each component  $\varphi_i$  of  $\vec{\varphi}$  is monotonic with respect to time. If one component  $\varphi_j$  is non-monotonic with respect to time, then  $\dot{\varphi}_j(t)$  cannot be a function of  $x_j$  alone. It must either exhibit time dependence, or it must be coupled to another component of  $\vec{x}$ . The figure below illustrates why non-monotonic behavior cannot be the result of an autonomous system.

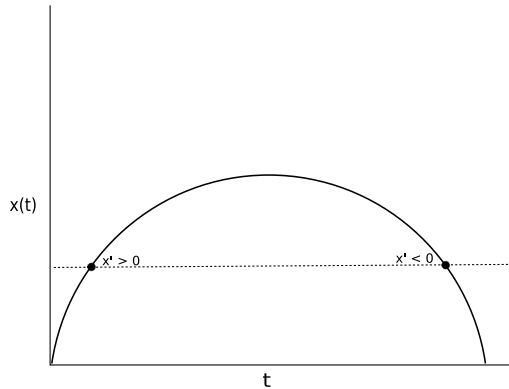


Figure 4: The value of the derivative at some particular  $x$  clearly changes over time

Returning to non-autonomous systems, the information provided by a single integral curve is quite limited, for we really have no idea whether or not the system is coupled (as mentioned before,  $\varphi(\cdot)$  could be the

result of  $N$  non-autonomous decoupled equations). To determine whether or not the dynamics of the system are coupled, we need more information. On the other extreme, we could look at the flow over the entire space on which the system is defined; this however, is numerically expensive and impractical, considering many systems are defined on all of  $\mathbb{R}^N$ .

As a sort of compromise, we could define some connected open set of initial conditions and flow these forward in time, defining a sort of "flow tube." We can define  $S(0)$  to be this set of initial conditions, and  $S(t)$  to be the state of  $S(0)$  after being flowed forward to time  $t$ . We can differentiate all of  $S(\cdot)$  by  $t$  to determine precisely the  $\vec{f}(t, x)$  for all  $t$  and  $x$  contained in our flow tube. Next, to determine whether the behavior is coupled, we need to answer the question *for a given time  $t$ , does each component  $f_i(t, \cdot)$  of  $\vec{f}$  only change as we vary the corresponding  $x_i$ ?* If  $f_i(t, \cdot)$  changes as we alter the other components of  $\vec{x}$ , then the dynamics must be coupled. We can answer the above question by determining the Jacobian of  $\vec{f}$  at each point within the flow tube. This will be given by:

$$J(\vec{f}) = \begin{pmatrix} \frac{\partial f_1(t, \vec{x})}{\partial x_1} & \cdots & \frac{\partial f_1(t, \vec{x})}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_N(t, \vec{x})}{\partial x_1} & \cdots & \frac{\partial f_N(t, \vec{x})}{\partial x_N} \end{pmatrix} \quad (50)$$

Note that the Jacobian will be defined for each time  $t$  and point  $\vec{x}$  in the flow tube, and we can differentiate numerically. This would involve looking at one particularly curve within the flow tube, and at each point  $\varphi_i(t)$  we could differentiate by  $t$  using finite differences to determine  $d\varphi/dt = \vec{f}(\vec{x}, t)$  at each point in the flow tube. Once  $\vec{f}$  has been defined everywhere in the tube, we will essentially have a grid of  $\vec{f}$ 's defined in the tube, although we may need to interpolate if the points aren't sufficiently dense. Following this, we can differentiate  $\vec{f}$  at each point by each component  $x_i$  of  $\vec{x}$  by looking at  $\frac{\vec{f}(\vec{x} + \delta \hat{x}_i) - \vec{f}(\vec{x})}{\delta}$  for small  $\delta$ . We can do this for each component of  $\vec{x}$  at each point in the tube to define the Jacobian everywhere.

If the dynamics are truly decoupled within the flow tube, then based on the above discussion, the Jacobian must be diagonal at each point in the flow tube.

Because the Jacobian provides us with a quantitative measure of the degree of coupling in the system, we can use DMORPH as a means of controlling this coupling. If we wished to decouple the system entirely, then we could place a cost  $K$  on each of the off-diagonal terms in the Jacobian. A less-demanding request may be to decouple only certain variables, in which case we could use DMORPH to drive down only the appropriate off-diagonal terms. The problem that follows then is *how do we define the cost function  $K$ ?* We could begin by defining a  $L : L^2 \rightarrow \mathbb{R}$  such that

$$K \left( \frac{\partial f_i(t, \vec{x})}{\partial x_j} \right) = \int_0^T \left| \frac{\partial f_i(t, \vec{x})}{\partial x_j} \right|^2 dt \quad i \neq j \quad (51)$$

The above, however, is defined for each  $\vec{x}$  in the flow tube, so in order to decouple the behavior of that off-diagonal term everywhere in the flow tube, we should integrate over the whole space as well. Thus a more appropriate  $K$  could be defined as:

$$K\left(\frac{\partial f_i(t, \vec{x})}{\partial x_j}\right) = \int_0^T \int_{\Omega} \left| \frac{\partial f_i(t, \vec{x})}{\partial x_j} \right|^2 d\vec{x} dt \quad (52)$$

Where  $\Omega$  is defined to be our set of initial conditions. Note that the above  $K$  only places a cost on one of the off-diagonal terms of the Jacobian. If we wanted to decouple each variable everywhere in the flow tube, then we could define an  $N^2 - N$  dimensional cost vector  $\vec{K}$ , each component of which could refer to a specific off-diagonal entry.

After parametrizing the vector field  $\vec{f}$  by  $s$ , we could differentiate (52) by  $s$ . The actual differentiation of (52) has posed problems, however, as a delta function arises and things become unclear. Before constructing an alternate cost function, it may be helpful to clarify some notation. We define our set of initial conditions by  $x_{0_i}$ . That is to say that  $S(0) = \{x_{0_n}\}_n$ . Next, we define some arbitrary point in our flow tube to be given by  $\varphi(x_{0_n}, t)$ . That is, given some initial condition, and given a time  $t$ , we can identify a unique point in our flow tube. Next note that given some arbitrary point  $\varphi(x_{0_n}, t)$  of our flow tube, we can differentiate by  $t$  to obtain  $\vec{f}$  at that point. In order to obtain  $f_i$ , however, we dot  $\vec{f}$  with the unit vector  $\hat{x}_i$ . Next, we can take the derivative of this with respect to  $x_j$  in order to obtain  $df_i/dx_j$ . Thus,

$$\frac{\partial f_i(\vec{x}, t, x_{0_n})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{d\vec{\varphi}(x_{0_n}, t)}{dt} \cdot \hat{x}_i \right) \quad (53)$$

It is important to observe that the above equation is defined for each point within the flow tube. Thus, we integrate over both time and the set of initial conditions  $S(0)$  to obtain a cost functional  $K$  that is a functional of the whole flow tube  $\varphi(\cdot, \cdot)$ :

$$K(\varphi(\cdot, \cdot)) = \int_0^T \left( \int_{S(0)} \left| \frac{d}{dx_j} \left( \frac{d\vec{\varphi}(\vec{x}_{0_n}, t) \cdot \hat{x}_i}{dt} \right) \right|^2 d\vec{x}_{0_n} \right) dt \quad (54)$$

With  $K$  defined in this way, it is easier to differentiate by  $s$  and use the kinematic approach, whereby we specify  $d\varphi(x_{0_n}, t)/ds$  for each point in the flow tube  $S(\cdot)$ . That is,

$$\frac{\partial K(\varphi(\cdot, \cdot))}{\partial s} = \int_0^T \left( \int_{S(0)} \frac{\partial K}{\partial \varphi(\cdot, \cdot)} \cdot \frac{\partial \varphi(x_{0_n}, t)}{\partial s} d\vec{x}_{0_n} \right) dt \quad (55)$$

I believe the above formulation is correct, but no numerical simulations have been run yet to verify this, so it is possible that I have defined  $K$  inappropriately.

## 7 Measure Preserving Flows

In order to truly decouple an  $N$  dimensional system in the manner presented above, we must impose  $N^2 - N$  costs on the system, which is quite costly. In fact it seems unlikely that we could use DMORPH to access a solution for which each one of these costs reaches zero. As a result, we considered other properties of physical systems that we may wish our model to reflect, and one of these such properties is the idea of a measure preserving flow. If we refer back to our flow tube  $S(\cdot)$  for reference, in a measure preserving flow the area of each slice of the flow tube remains constant for all  $t$  by definition. That is to say

$$\int_{S(0)} d\vec{x} = \int_{S(t)} d\vec{x} \forall t \in [0, T] \quad (56)$$

It can be shown that a flow to be measure-preserving if and only if  $\nabla \cdot \vec{f} = 0$ . However, this is true if and only if the trace of the Jacobian of  $\vec{f}$  is equal zero, so we could place a cost on the trace of the Jacobian and drive it to zero to obtain a model of a measure preserving flow. The primary attraction of the measure preserving flow is that it requires one cost, while the decoupling required  $N^2 - N$ .

## 8 Future Directions

While the basic approach to DMORPH has been well-formulated, more numerical simulations need to be run to verify some of our theoretical results. The idea of using DMORPH to obtain either decoupled or measure-preserving systems is relatively new for us as well, so the near future will be spent going over the formulation presented above and running numerical simulations. Moreover, it is necessary for us to devise more ways of characterizing physical systems in a quantitative way (e.g. measure preserving flows have  $\text{Tr}(f) = 0$ ). This would allow us to use DMORPH to search for solutions of increasingly fine quality.