A VARIATIONAL FRAMEWORK FOR FLOW OPTIMIZATION USING SEMI-NORM CONSTRAINTS

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Summary When considering a general system of equations describing the space-time evolution (flow) of one or several variables, the problem of the optimization over a finite period of time of a measure of the state variable at the final time is of great interest in many fields. Methods already exist in order to solve this kind of optimization problem, but sometimes fail when the constraint bounding the state vector at the initial time is not a norm, meaning that some part of the state vector remains unbounded and might cause the optimization procedure to diverge. In order to regularize this problem, we propose a general method which extends the existing optimization framework in a self-consistent manner to consider such problems. We will demonstrate the utility of this framework with a fluid dynamics problem of interest.

GOVERNING EQUATIONS

We consider an arbitrary state vector $\mathbf{q}$ from a vector space Ω, defined on the time interval $[0, T]$. We choose $\mathbf{q} \in H^2(\Omega)$, a Sobolev space of order 2. We choose this space so that $\mathbf{q}$ and its gradient on Ω are both in $L^2(\Omega)$ (space of square integrable functions on Ω), which means that the state vectors are appropriately well-behaved for the types of differential operations we wish to consider. We will assume that $\mathbf{q}$ satisfies a partial differential equation associated with an initial conditions. For simplicity and clarity, we will focus on linear homogeneous equations of the type:

$$\partial_t \mathbf{q} - \mathbf{L}\mathbf{q} = 0, \quad \text{with} \quad \mathbf{q}(\mathbf{x}, 0) - \mathbf{q}_0 = 0 \;\; \forall\, \mathbf{x} \in \Omega, \tag{1}$$

where $\mathbf{L}$ is a linear operator. We also require the state vector to satisfy boundary conditions defined on $\partial\Omega$ and for all t.

OBJECTIVE FUNCTIONAL

Depending on the particular problem studied, we will define "the objective functional" $\mathcal{J}(\mathbf{q})$ (unique to any problem) which takes as its input the state vector $\mathbf{q}$ and will yield a real number (quantity of interest), which we want to be optimal with respect to an optimized variable of our choice (such as the initial condition for example). In order to demonstrate the framework, we will focus on the case of the identification of optimal perturbations, i.e. finding the optimal initial condition $\mathbf{q}_0$ which maximizes (the output of) an objective functional. We will in this work consider the following generic objective functional:

$$\mathcal{J}(\mathbf{q}) = \|\mathbf{q}(T)\|_O^2\,, \quad \|\mathbf{q}(T)\|_O^2 = \frac{1}{2}\int_\Omega \mathbf{q}(T)^\top \mathbf{W}_O \mathbf{q}(T)\, d\Omega, \tag{2}$$

which defines a quantity of interest at the target time T. This expression defines a norm if $\mathbf{W}_O$ is invertible. If this is not the case, it defines a semi-norm which has a non-trivial null space or kernel, defined as the set of state vectors $\mathbf{q}$ such that $\|\cdot\|_O$ returns a zero value (for a "true" norm the kernel is trivial, containing only the zero state vector). We then define the complementary space to this kernel (henceforth called cokernel) which is the restriction of the space $H^2(\Omega)$ for which the semi-norm $\|\cdot\|$ (on $H^2(\Omega)$) becomes a norm. This space will be denoted as $\ker^*(\|\cdot\|)$.

SEMI-NORM CONSTRAINTS

The Lagrangian variational method is a way to perform an optimization under constraints. By adding extra degrees of freedom to consider these, we are then able to investigate the impact of variations of the constraints on the returned value of the objective functional. In addition to the natural constraints (1), in order to avoid the final state vector amplitude becoming arbitrarily large during the optimization process, we have to impose a normalization (and hence scalar) constraint on the initial condition, i.e.

$$\|\mathbf{q}_0\|_N^2 - N_0 = 0, \quad \|\mathbf{q}_0\|_N^2 = \frac{1}{2}\int_\Omega \mathbf{q}_0^\top \mathbf{W}_N \mathbf{q}_0\, d\Omega, \tag{3}$$

where the subscript N stands for normalization and emphasizes the fact that this norm is used for a normalization purpose. This norm is defined in an analogous way to $\|\cdot\|_O$ defined in (2) but is in general defined by a weight matrix $\mathbf{W}_N$ different from the energy weight matrix $\mathbf{W}_O$. The normalization constraint has to act on the totality of the state vector $\mathbf{q}$ in order to have a well-posed optimization problem. In particular, imposing constraint (3) with a singular matrix $\mathbf{W}_N$ is not an appropriate constraint, as this constraint will not affect any vector which is part of the kernel of the semi-norm involved in the definition of the objective functional, and will as a consequence remain unbounded. Although such an optimization can still be conducted, and an optimal $\mathbf{q}_0$ can in principle be identified, it is very likely that the objective functional will diverge with the magnitude of the non-constrained part of the state vector, a typically undesired and unrealistic behavior.

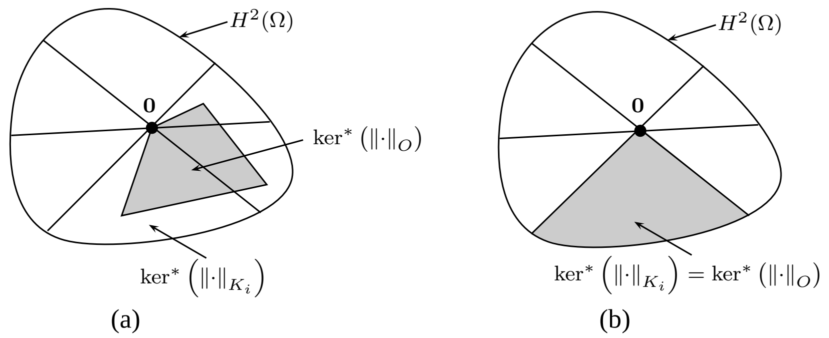

Figure 1. Schematic representation of the partition of the space $H^2(\Omega)$ through the choice of $n_c + 1$ (here $n_c = 5$) semi-norm constraints. (a) Schematic representation of the case of final value optimization, where the objective semi-norm is different from all the constraint semi-norms. (b) Schematic representation of the special case of gain optimization, where the objective semi-norm coincides with one of the constraint semi-norm.

As a consequence, to define a well-posed problem we have to add further constraints on the part of the state vector which is in the kernel of the semi-norm. A natural way to do this is to appreciate that we can define several normalization constraints. In a general way, we will consider multiple constraints associated with semi norms $\|\cdot\|_{K_i}$ which have to span the full space $H^2(\Omega)$ without interfering with each other, meaning we have the following property:

$$\left\{ \begin{array}{l} \|\mathbf{q}_0\|^2_{K_i} - K_{0_i} = 0, \quad \text{for } i \text{ from } 0 \text{ to } n_c, \\ \displaystyle\bigoplus_{i=0}^{n_c} \ker^*\left(\|.\|_{K_i}\right) = H^2(\Omega), \end{array} \right. \tag{4}$$

where the symbol $\oplus$ denotes the direct sum[1], and where the number of complementary constraints is n_c+1, with implicitly $n_c + 1$ different complementary semi-norms which satisfy

$$\sum_{i=0}^{n_c} \|\mathbf{q}_0\|^2_{K_i} = \sum_{i=0}^{n_c} K_{0_i} = \|\mathbf{q}_0\|^2_N = N_0, \tag{5}$$

Consequently, a set of n_c (because the problem is linear) independent (and adjustable) parameter arises which quantifies the relative size of the initial magnitude given by a semi-norm of interest to the total normalization norm

$$R_{0_i} = \frac{K_{0_i}}{N_0},\ i = 1 \dots n_c. \tag{6}$$

This general situation is shown in figure (1a), making it explicit that the semi-norm used to define the objective functional does not need to correspond to any of these constraint semi-norms.
The situation where we wish to optimize a gain requires that one of the constraint semi-norms has to coincide with the objective semi-norm, and so without loss of generality, we define $\|\cdot\|_{K_0} = \|\cdot\|_O$ (see figure (1b)).
One attractive possibility of this method is then to optimize semi-norm gain then naturally defined as:

$$G_O(T) = \frac{\|\mathbf{q}(T)\|_O}{O_0}, \tag{7}$$

which will be optimized through a variational method, and over all possible ratios R_{0_i}.
We demonstrate the utility of this framework by considering optimization under various aspects of fluid flows.

References

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[1] The direct sum is a regular ensemble sum for which the two terms have no intersection but the null vector of the space.