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Fréchet Sensitivity Analysis for Partial Differential Equations with Distributed Parameters

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***Abstract*— This paper reviews Fréchet sensitivity analysis for partial differential equations with variations in distributed parameters. The Fréchet derivative provides a linear map between parametric variations and the linearized response of the solution. We propose a methodology based on representations of the Fréchet derivative operator to find those variations that lead to the largest changes to the solution (the *most significant variations*). This includes an algorithm for computing these variations that only requires the action of the Fréchet operator on a given direction (the Gateaux derivative) and its adjoint. This algorithm is applicable since it does not require an approximation of the entire Fréchet operator, but only typical sensitivity analysis software for partial differential equations. The proposed methodology can be utilized to find worst case distributed disturbances and is thus applicable to uncertainty quantification and the optimal placement of sensors and actuators.**

I. INTRODUCTION

The primary objective of this paper is to develop efficient algorithms for computing the most significant variations of distributed parameters in physical systems and discuss their utility in applications such as robust actuator/sensor placement and uncertainty quantification. Our interest is in physical systems modeled by partial differential equations (PDEs) with uncertain parameters. This research specifically targets infinite dimensional parameters such as spatially varying material properties, boundary conditions or initial conditions. In particular, we will develop a methodology to better model uncertainty in spatially distributed parameters when a precise characterization of the parametric uncertainty is not available. The methodology is derived directly from the mathematical model by considering the Fréchet derivative operator of the model outputs with respect to the spatially (and temporally) varying parameters, i.e. distributed parameters. A decomposition of this parameter-to-output map can illuminate those parametric variations that produce the greatest change to in the model solution (or state) and thus are those variations that are the most important to account for in actuator/sensor placement and uncertainty quantification.

A number of recent works have used the notion of "worst-case spatial distribution of disturbances" to address the actuator and sensor placement problem (see, e.g. Demetriou et al. [1], [2]). In these studies, the methodology was demonstrated by assuming the form of normalized distributions of disturbances, then demonstrating the superiority of sensor locations that minimize $\mathcal{H}^2$ and $\mathcal{H}^\infty$ norms of the disturbance to state estimate transfer function. A methodology based on optimization was proposed in [3] to calculate worst-case spatial disturbances. However, that approach often led to challenging optimization problems and is not practical for complex problems.

In this paper, we present a methodology for mathematically producing those spatial distribution functions that have the most influence on the state using Fréchet sensitivity analysis. We consider linear elliptic equations in this study. Since the Fréchet derivative of the state with respect to disturbance functions is often a Hilbert-Schmidt operator, we can apply spectral analysis to identify the most significant variations of disturbances. In other words, by computing the dominant Schmidt pairs, this approach identifies those variations that produce the largest changes in the state. By including these variations in the design of controlled systems, we complement the aforementioned developments to produce robust state estimators. We provide a range of algorithms to compute these Schmidt pairs, including one appropriate for fine discretizations of the linear operator based on iteratively computing sensitivity and adjoint solutions.

II. MODEL AND CONTROL DESIGN PROBLEM

Although the emphasis of our approach is finding worst-case distributions in control problems, we introduce a model problem to simplify the technical discussion and to illustrate our ideas with preliminary results. Consider weak solutions to the elliptic boundary value problem

$$-\nabla \cdot (p \nabla w) = f, \qquad w \in H^1_0(\Omega) \tag{1}$$

where $f \in H^{-1}(\Omega)$, Ω is an open set with compact closure, and

$$p \in \mathcal{P} \equiv \{ p \in H^1(\Omega) |\ p(x) \in (p_{min}, p_{max}), \\ \|\nabla p(x)\|_\infty < d_{max},\ \text{a.e. in } \Omega \}.$$

As a physical motivation for this problem, we can identify w as the temperature, p as the material conductivity, and f as a given heat source term. The analysis problem is well understood, cf. [4], with more regularity of the solution w with improved regularity of the data p and f. However, if our interest was to quantify the uncertainty in solutions to the analysis problem as part of the overarching goal of quantifying the uncertainty in the simulation, we require quantitative information on how w changes with changes in p and f. If these changes are not prescribed, knowledge of which variations in p and f produce the largest changes to w (with additional knowledge of how likely these particular variations are) would be useful in determining how well the model output can be trusted.

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III. SENSITIVITY ANALYSIS

Loosely, the *sensitivity* of the state is the derivative of a model solution or output with respect to parameters of interest. Thus, we introduce the following definition.

Definition [Gateaux Derivative, Sensitivity Derivative]: *For any given $p \in \mathcal{P}$, let $w(\cdot;p) \in H_0^1(\Omega)$ be defined as the solution to (1) and let h be an admissible variation of p (i.e. $p+\epsilon h \in \mathcal{P}$ for ϵ sufficiently small). Then the sensitivity of w with respect to the variation h at the parameter p is defined as*

$$s_h(x;p) = \lim_{\epsilon \to 0} \frac{w(x;p+\epsilon h) - w(x;p)}{\epsilon} \qquad \text{for } x \in \Omega. \quad (2)$$

We use the terminology: s_h is the sensitivity *of w to the variation h.*

By viewing (1) as a mapping from $\mathcal{P} \times H_0^1 \to H^{-1}$ we can apply the implicit function theorem to derive a *sensitivity equation* that describes s_h. In particular, through implicit differentiation of (1, with $p \to p + \epsilon h$) with respect to ϵ and assuming equality of mixed partial derivatives we have

$$-\nabla \cdot (p \nabla s_h) = \nabla \cdot (h \nabla w), \qquad s_h \in H_0^1(\Omega), \quad (3)$$

where f is independent of h. We point out that

- Regardless of the application, the *sensitivity equation* is always linear in the sensitivity s_h, regardless of whether or not the partial differential equation model is. Moreover, it shares the same Newton linearization as the model equation. Thus, sensitivity equations can often be approximated for a fraction of the cost of computing approximations of the model equations.
- For parametric constants ($p \in \mathbb{R}$), the scaled sensitivity is defined as $s_p p_0$ where p_0 is a nominal value of the parameter p. Comparing magnitudes of scaled sensitivity variables provides a means of determining which parameters are important in the model [5]. When comparing parametric variations, it is important that the sizes of the variations are comparable: $\|h_1\| = \|h_2\|$, then $\|s_{h_1}\| \gg \|s_{h_2}\|$ implies that the variation h_1 has a more significant influence on the solution.
- Equation (2) with small values of ϵ can be used to estimate the solution at nearby parameter values by using truncated Taylor series expansions [6], [7], [8].

A. Fréchet Sensitivity Analysis

A stronger notion than the (Gateaux) sensitivity derivative above is the Fréchet derivative (cf. [9], [10] for a more generic definition). Let $\mathcal{P}_0$ be a ball in $W^{1,\infty} \cap H^1$.

Definition [Fréchet Derivative]: *For any $p \in \mathcal{P}$ consider the solution $w(\cdot;p)$ of (1) as a mapping from $\mathcal{P} \to H_0^1$. Then the solution operator is* Fréchet differentiable *at p if there exists a bounded linear operator $[D_p w] : \mathcal{P}_0 \to H_0^1$ such that*

$$\lim_{\|h\| \to 0} \frac{\|w(\cdot;p+h) - w(\cdot;p) - ([D_p w]\, h)(\cdot)\|}{\|h\|} = 0.$$

Then $[D_p w]$ is the Fréchet differential *at p.*

Note that if the solution map is Fréchet differentiable, then it is also Gateaux differentiable. This implies the following useful result

$$w(x;p+\tilde{h}) \approx w(x;p) + \left([D_p w]\, \tilde{h}\right)(x), \qquad x \in \Omega,$$

holds for every small $\tilde{h}$. Replacing $\tilde{h}$ by ϵh in the expression above gives the estimate that

$$w(x;p+\epsilon h) \approx w(x;p) + \epsilon\left([D_p w] h\right)(x)$$

and motivates the role of sensitivity analysis in uncertainty quantification. In fact,

$$s_h \equiv [D_p w]\, h. \quad (4)$$

As above for the Gateaux derivative, we can derive an equation for the Fréchet derivative operator. To simplify the exposition, we will use the notation $\mathcal{H}_1 = H_0^1$ and $\mathcal{H}_2 = H^{-1}$ and define $\mathcal{A}(p) : \mathcal{H}_1 \to \mathcal{H}_2$ for the (p dependent) elliptic operator in (1) as $\mathcal{A}(p)w = -\nabla \cdot (p \nabla w)$ (using weak derivatives). Then, if $f \in \mathcal{H}_2$, the unique solution to the equation $\mathcal{A}(p)w = f$ is

$$w = [\mathcal{A}(p)]^{-1} f.$$

We can derive the expression for $[D_p w]$ acting on any h as

$$[D_p w]\, h = -[\mathcal{A}(p)]^{-1} \mathcal{A}(h) [\mathcal{A}(p)]^{-1} f \quad (5)$$

or

$$[D_p w]\, h = -[\mathcal{A}(p)]^{-1} \mathcal{A}(h) w \quad (6)$$

This expression can be derived directly from the sensitivity equation for (1),

$$[\mathcal{A}(p)]\, s_h = -\mathcal{A}(h) w \quad \text{or} \quad -\nabla \cdot (p \nabla s_h) = \nabla \cdot (h \nabla w)$$

which can be manipulated using (4) to give the expression (6).

We now justify the formalism above by proving the Fréchet differentiability of w with respect to p.

Theorem [Fréchet Differentiability of Solutions to (1)] Suppose $w \in H_0^1(\Omega)$ is the solution to (1) where $f \in H^{-1}(\Omega)$ and $p \in \mathcal{P}$. Then w is Fréchet differentiable with respect to p.

Proof: For any variation h satisfying $p + h \in \mathcal{P}$, let w_h be the unique solution to

$$-\nabla \cdot ((p+h) \nabla w_h) = f. \quad (7)$$

Thus, using (1) and rearranging terms

$$-\nabla \cdot (p \nabla (w_h - w)) = \nabla \cdot (h \nabla w_h). \quad (8)$$

Multiplying both sides by $(w_h - w)$, integrating by parts, and using the bounds on p leads to

$$p_{\min} \|\nabla (w_h - w)\|^2 \leq -\int_\Omega h \nabla w_h \cdot \nabla (w_h - w).$$

Using the fact that h is bounded and Hölders inequality,

$$p_{\min} \|\nabla (w_h - w)\| \leq \|h\|_\infty \|\nabla w_h\|. \quad (9)$$

Similarly, multiplication of (7) by w_h and integrating by parts yields

$$\int_\Omega (p+h)\|\nabla w_h\|^2_{\mathbb{R}^d} = \int_\Omega f w_h.$$

Since $p+h \in \mathcal{P}$ and using the duality pairing

$$p_{\min}\|\nabla w_h\|^2 \le \|f\|_{-1}\|w_h\|_1 \le C\|f\|_{-1}\|\nabla w_h\| \qquad (10)$$

by Poincaré's inequality. Combining (9) and (10),

$$\|\nabla(w_h - w)\| \le C\|h\|_\infty \|f\|_{-1}. \qquad (11)$$

Let $v_h \equiv [D_p w]h$ be the solution to (6), then subtracting $-\nabla\cdot(p\nabla v_h) = \nabla\cdot(h\nabla w)$ from (8) leads to

$$-\nabla\cdot(p\nabla(w_h - w - v_h)) = \nabla\cdot(h\nabla(w_h - w)).$$

Multiplying both sides by $(w_h - w - v_h)$, integrating by parts and applying similar arguments as above,

$$\begin{aligned}\|w_h - w - v_h\|_1 &\le C'\|h\|_\infty\|\nabla(w_h - w)\| \\ &\le C''\|h\|^2_\infty\|f\|_{-1}\end{aligned}$$

using (11), where the constants C' and C'' depend on $p_{\min}$ and Ω, but are independent of h. Using (4) and substitution for v_h, we see that

$$\begin{aligned}\lim_{\|h\|_\infty\to 0}\frac{\|w_h - w - [D_p w]h\|_1}{\|h\|_\infty} &\le \lim_{\|h\|_\infty\to 0} C''\|h\|_\infty\|f\|_{-1} \\ &= 0.\end{aligned}$$

Thus, the solution to (1) is Fréchet differentiable with respect to p. ■

Note that the use of Fréchet derivatives for inverse problems is well known in geosciences, cf. [11]. Their use in characterizing a first order relationship between (a finite set of) model parameters and discrepancies between the model and measured data is similar to the spirit of the uncertainty quantification applications we have in mind. However, the role of the Fréchet derivative in those applications is closely tied to identifying parameters and the inversion of the derivative is equivalent to a root finding problem for identifying the parameters. As geophysical models become more complicated, and analytic expressions for the Fréchet operator are no longer available, geoscientists turn toward sophisticated optimization algorithms for the inversion problem.

We present a few of the approaches for finding approximations to the linear operator $[D_p w]$ in the sections below. These approaches illuminate the need to avoid direct calculation of the operator for partial differential equations of interest and motivate our methodology of using the formalism of the Fréchet derivative operator to compute only a few of the most significant variations. Note that if we have access to an approximation of $[D_p w]$, it would lead to fast calculation of s_h at the point p. However, our interest is to estimate the dominant spectra and Schmidt vectors (defined below) of the Fréchet derivative operator.

B. Direct Finite Element Approximation

Although considerably more expensive, we can compute an approximation to $[D_p w]$ in one monolithic calculation. If we consider (6), and operate on both sides with $\mathcal{A}(p)$, we have

$$\mathcal{A}(p)\,[D_p w]\,h = -\mathcal{A}(h)w.$$

We introduce finite element approximations to solve for the action of the Fréchet operator on approximating subspaces. Define $a_p(w,v) = (p\nabla w, \nabla v)$, then a weak form of the Fréchet sensitivity equation has the form

$$a_p([D_p w]\,h, v) = -a_h(w,v) \qquad \forall v \in H^1_0(\Omega).$$

Writing $h = \sum_{j=1}^n \phi_j(x)h_j$, $w = \sum_{j=1}^n \phi_j(x)w_j$, etc., in $S^n \subset H^1_0(\Omega)$ and choosing $v = \phi_i$ leads to the Galerkin finite element approximations of the Fréchet derivative

$$a_h(w,v) = \int_\Omega h\nabla w\cdot\nabla v = \int_\Omega \sum_{j=1}^n \phi_j h_j \sum_{k=1}^n w_k \nabla\phi_k\cdot\nabla\phi_i$$

$$[\mathbf{A}_h]_{ij} = \int_\Omega \left(\sum_{k=1}^n w_k\nabla\phi_k\right)\cdot\nabla\phi_i\phi_j$$

and thus, $[\mathbf{A}_h\mathbf{h}]_i = a_h(w,\phi_i)$ when $w \in S^n$. The computation of $a_p(\phi_j,\phi_i) = [\mathbf{A}_p]_{ij}$ follows standard finite element procedures, leading to a direct calculation for a finite dimensional representation of $[D_p w]$ as $-\mathbf{A}_p^{-1}\mathbf{A}_h$. Furthermore, $\mathbf{s}_h = -\mathbf{A}_p^{-1}\mathbf{A}_h\mathbf{h}$ is the representation of s_h in the finite element basis.

C. Action on a Basis

Since $[D_p w]$ is a linear operator, we can consider its action on a (local, finite element) basis. Thus, if $h \in \text{span}\{\phi_1,\ldots,\phi_n\} \equiv S^n \in \mathcal{P}$, then

$$h = [\phi_1\cdots\phi_n]\,\mathbf{h} \quad \text{and} \quad [D_p w]h = [s_{\phi_1}\cdots s_{\phi_n}]\,\mathbf{h}$$

where $\mathbf{h} \in \mathbb{R}^n$ is the representation of h in S^n, and s_{ϕ_i} is the (Gateaux) sensitivity derivative of w with respect to variation ϕ_i. Thus, the matrix $[\mathbf{s}_{\phi_1}\cdots\mathbf{s}_{\phi_n}]$ provides the finite dimensional representation of $[D_p w]$ in S^n. Here we directly see that direct computation of $[D_p w]$ will not be feasible except in demonstration problems, since we essentially need to compute sensitivity variables for every function in the basis.

D. Adjoint Methods

Rather than solving a sensitivity equation for each parameter, we could resort to adjoint methods (cf. [12]), as the computational tradeoffs typically favor adjoint methods as the number of "input variables" increases. This would be the case if we are interested in output functionals but all computational advantages of this approach vanishes when there is an infinite dimensional output as well. If applicable, the adjoint variables themselves would provide the desired information on how variations would influence functionals of interest.

Therefore, our interest in the formalism of the Fréchet derivative operator is simply to motivate an approximate spectral decomposition that gives us a means to feasibly compute a number of the *most significant variations*. As we shall see, this methodology combines a solution algorithm for solving sensitivity equations as well as the approximation of adjoint operators.

E. Hilbert-Schmidt Operators and Their Decompositions

The fact that computing approximations to Fréchet derivative operators is intractable can be overcome for our purposes by utilizing the following (cf. [9])

Theorem [Hilbert-Schmidt Decomposition] *If* $\mathcal{F} = [D_p w]$ *is a compact operator from* $\mathcal{H}_1 \to \mathcal{H}_2$*, then it has the representation*

$$s_h = [D_p w]\, h = \sum_{i=1}^{\infty} \xi_i \sigma_i \langle \psi_i, h \rangle$$

where $\{\psi_i\}$ and $\{\xi_i\}$ are eigenvectors of $\mathcal{F}^*\mathcal{F}$ and $\mathcal{F}\mathcal{F}^*$, respectively, and $\sigma_i \geq 0$ are the square roots of the corresponding eigenvalues. The *Schmidt functions* $\{\psi_i\}$ and $\{\xi_i\}$ form orthogonal bases for $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

Thus, compact operators have a decomposition that is analogous to the singular value decomposition for matrices. We can then seek the dominant Schmidt functions $\{\psi_1, \psi_2, \ldots, \psi_r\}$ that describe the parameter variations leading to the most significant changes in the solution (measured by the values of $\sigma_1, \ldots, \sigma_r$, respectively). Therefore, we refer to these as the *most significant variations*. Our proposed methodology is to utilize a subspace iteration algorithm that approximates dominant eigenvectors for the operator $\mathcal{F}^*\mathcal{F}$.

For the elliptic boundary value problem (1), we can show that the Fréchet derivative operator is compact and thus has a Hilbert-Schmidt decomposition.

Theorem [Compactness of the Fréchet derivative operator] The Fréchet derivative operator, $[D_p w]$, defined in Section III A, is compact.

A sketch of the proof follows.

Proof: Let $\eta_n = \sqrt{2}\sin(n\pi x)/(\sqrt{1+n^2\pi^2})$, then $\{\eta_n\}$ is an orthonormal basis for $\mathcal{P}_0$ (in the H^1-inner product). Then $s_n = [D_q w]\eta_n$ solves (6). Multiplying both sides by s_n, integrating by parts and applying Hölder's inequality, we find

$$p_{\min} \|\nabla s_n\|^2 \leq \|\eta_n \nabla w\| \|\nabla s_n\|.$$

Applying the Poincaré inequality, we have the estimate that

$$\|s_n\| \leq c \|\nabla w\| \|\eta_n\|_\infty.$$

Since each basis function is bounded ($\|\eta_n\|_\infty \leq \sqrt{2}/(n\pi)$) and w is fixed, $\{\|[D_p w]\eta_n\|\}$ is an ℓ^2 sequence implying the compactness of $[D_p w]$. ■

IV. NUMERICAL RESULTS

In a preliminary study, we will use our model problem to show the utility of the *most significant variations*. In this problem, we show that one particular variation leads to large solution sensitivity. Thus, if this variation is accounted for in determining uncertainty quantification, we account for a dominant portion of the solution sensitivity.

We now present *most significant variations* for one instance of our Model Problem given in (1). We arbitrarily chose functions $p(x) = (1+x)^2$ and $f(x) = 27x^4 - 72x^3 - 21x^2 + 21x + 6$ over $\Omega = (0, 1)$. The finite element solution is shown in Fig. 1.

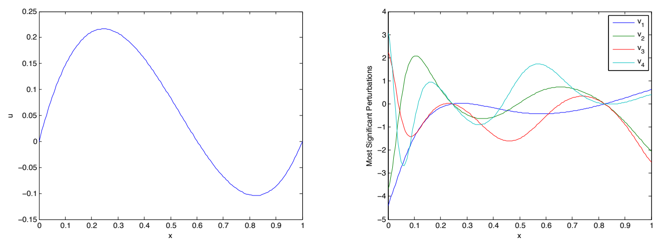

Fig. 1. Solution to (1) on left, first four *most significant variations*

For this problem we can easily compute finite dimensional approximations to $[D_p w]$ that can be used to find the *most significant variations* to the parameter $p(x)$. These are also plotted in Fig. 1. Note that these variations are all normalized so that $\|\psi_i\| = 1$. The dominant variation indicates that the largest change in the solution would be realized if p were varied somewhat sharply towards the left end. This is the location where p is the smallest, but one would not necessarily expect the solution to vary this dramatically (and any intuition would have to weigh the values of $f(x)$ and the influence of the boundary conditions). Note that the dominant singular values are $0.01488, 0.00394, 0.003284, 0.00233, \ldots$ indicating a substantial drop off from σ_1 to σ_2.

In Fig. 2, we compare the sensitivity of the solution w with respect to a variation ψ_1 (dashed) with sensitivities of w with respect to a typical Fourier basis (scaled to have unit L_2-norm). We see that there is a dramatic difference between the two sets and that a similar perturbation leads to a larger variation in the solution if ψ_1 is used. For comparison purposes, we also compare sensitivities of the solution to each of the first six *most significant variations*. Note that the sensitivity of w to ψ_1 is $s_{\psi_1} = \sigma_1 \xi_1$.

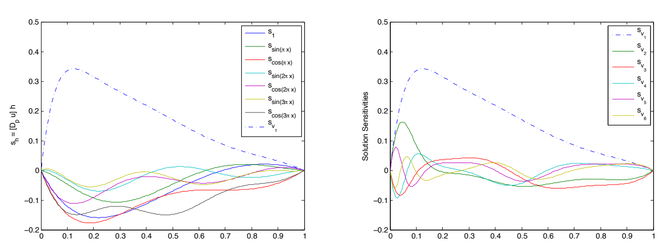

Fig. 2. Sensitivity of solution w with respect to Fourier basis compared to the *most significant variation* ψ_1 (left); and the sensitivity of w with respect to the four *most significant variations* (right). Note the substantial sensitivity the solution exhibits to ψ_1 over any of the Fourier basis functions even though all variations are scaled to have L_2-norm one.

Note that the decay of the singular values can lead to important conclusions about the uncertainty analysis. For example, small values changes of σ_i would lead to small changes in w. Thus, there is no need to investigate the contribution to the uncertainty intervals from components ψ_i associated with these small values.

A. Proposed Algorithm for Approximating Most Significant Variations

In this section, we will exploit the operator theoretic properties of the Fréchet derivative to create an algorithm for approximating the most significant/worst case parametric variations. As outlined below, we develop a variant of the power method for computing the dominant eigenfunctions of the $\mathcal{F}^*\mathcal{F}$ operator. As will be shown below, this can be implemented by iterating between solutions to sensitivity equations and adjoint equations.

It is, of course, not feasible to compute the Fréchet derivative operator in practical distributed parameter problems. With the knowledge that the operator is Hilbert-Schmidt, it makes sense to seek finite dimensional approximations of the *most significant variations* and their associated influence on the model solution. At the same time, we want to design an algorithm that avoids the explicit formulation of $\mathcal{F}$. This leads us to the following natural first algorithm

Algorithm [Power Method] *For the uncertainty quantification problem, we are most interested in the dominant eigenspaces of the operator $\mathcal{F}^*\mathcal{F} = [D_p w]^*[D_p w]$. It is then natural to apply a power method to approximate the desired eigenfunctions. Note that the application of $\mathcal{F}$ to a variation h can simply be carried out by solving a linear sensitivity equation. Similarly, it is straightforward to build the adjoint equations associated with the linear sensitivity equations. We outline the power method applied to one function below as implemented for our model problem*

1) *Let h^0 be a given function*
2) *for $n = 1, \dots$ until convergence*
   - $\tilde{h}^n = [D_p w]\, h^{n-1}$*: In other words, let $\tilde{h}^n$ be the solution to*

$$-\nabla \cdot \left(p \nabla \tilde{h}^n\right) = \nabla \cdot \left(h^{n-1} \nabla w\right)$$

   - $h^n = [D_p w]^*\, \tilde{h}^n$*: In other words, let h^n be the solution to the system*

$$\begin{aligned} -\nabla \cdot (p \nabla r) &= \tilde{h}^n \\ h^n &= -\nabla w \cdot \nabla r \end{aligned}$$

   - $h^n := h^n / \|h^n\|$*. This step is for numerical stability. Note that we can also keep track of*

$$\begin{aligned} \lambda^{n-1} &= \langle h^{n-1}, [D_p w]^*\, [D_p w]\, h^{n-1} \rangle \\ &= \langle [D_p w]\, h^{n-1}, [D_p w]\, h^{n-1} \rangle \\ &= \langle \tilde{h}^n, \tilde{h}^n \rangle \end{aligned}$$

   as an approximation to the dominant eigenvalue.
3) $\psi_1 = h^n$
4) $s_{\psi_1} = \tilde{h}^n$
5) $\sigma_1 \approx \sqrt{\lambda^{n-1}}$

This algorithm converged to the values in Fig. 1 for our simple model problem. The extension of the above algorithm to multiple variations based on subspace iteration is natural.

V. CONCLUSIONS AND FUTURE WORK

As we see, there is a substantial difference in the output of the solution with unit perturbations in the *most significant variations* compared with other "natural" functions that could be used. Thus, when applying the methodology in [1], [2], accounting for the *most significant variations* could make a dramatic difference in actuator/sensor locations.

A future study will be concerned with justifying the theoretical properties of the Fréchet derivative for a wider class of problem settings. This includes cases where the parametric dependence occurs through boundary variations as well as extensions to nonlinear and parabolic problems. A first step towards the justification for time dependent problems recently appeared in the literature [13]. However, the predominant effort of the ongoing work will be in the development and implementation of efficient software for computing these *most significant variations*.

Note that in principle, the adjoint of the Fréchet derivative operator needs to be worked out to implement our proposed algorithm. It is possible that discretized adjoints would work for this algorithm if their use could be justified. This would allow the introduction of automatic differentiation methods and allow for more reusable software. Therefore, the consistency of the discrete adjoint is important for easy applicability to a wide range of applications.

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