Sensitivity analysis of thermo-acoustic eigenproblems with adjoint methods

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This paper outlines two new applications of adjoint methods in the study of thermo-acoustic instability. The first is to calculate gradients for the active subspace method, which is used in uncertainty quantification. The second is to calculate gradients in a non-linear thermo-acoustic Helmholtz solver. Two methods are presented. The first, which uses the discrete adjoint approach, is specifically for nonlinear Helmholtz eigenvalue problems that are solved iteratively. The second, which uses a hybrid adjoint approach, is more general and can be applied to both problems.

1. Introduction

Thermo-acoustic oscillations involve the interaction of heat release (e.g., from a flame) and sound. In rocket and aircraft engines, heat release fluctuations can synchronize with the natural acoustic modes in the combustion chamber. This can cause loud vibrations that sometimes lead to catastrophic failure. It is one of the biggest and most persistent problems facing rocket and aircraft engine manufacturers (Lieuwen & Yang 2005).

In situations that are susceptible to these oscillations, often only a handful of oscillation modes are unstable. Existing techniques examine how a change in one parameter affects all oscillation modes, whether unstable or not. Adjoint techniques turn this around. In a single calculation, they examine how each oscillation mode is affected by changes in all parameters. In other words, they provide gradient information about the variation of an eigenvalue with respect to all the parameters in the model. In a system with a thousand parameters, they calculate gradients a thousand times faster than finite difference methods. When combined with gradient-based optimization methods, they hold great promise for the practical control of thermo-acoustic oscillations.

This paper outlines two new applications of adjoints to the study of thermo-acoustic instabilities. The first is to calculate gradients for the active subspace method, which is used in uncertainty quantification. The second is to calculate gradients in a nonlinear Helmholtz solver. Two different sensitivity methods and algorithms are derived. The first method works on the Helmholtz eigenproblem and exploits a purely discrete adjoint method. The second method works on general nonlinear eigenproblems and exploits a hybrid adjoint approach.

2. Thermo-acoustics framework

Many studies have demonstrated the ability of Large-Eddy Simulations (LES) to represent flame dynamics (Pierce & Moin 2004; Wolf *et al.* 2012; Poinsot 2013, among many

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others). However, even when LES simulations confirm that a combustor is unstable, they do not suggest how to control the instability. Moreover, LES is computationally expensive. Methods of lower complexity allowing an extensive use for pre-design, optimization, control, and uncertainty-quantification are therefore also developed.

2.1. *Low-order methods*

Two low-order methods are considered here: network models and Helmholtz solvers. Network models simulate the combustor as a network of homogeneous (constant density) 1D or 2D axisymmetric acoustic elements, in which the acoustic problem can be solved analytically (Stow & Dowling 2003; Evesque *et al.* 2003; Morgans & Stow 2007). Jump relations connect these elements, enforcing pressure continuity and mass conservation while accounting for the dilatation caused by flames. The acoustic quantities in each segment are related to the amplitudes of the forward and backward acoustic waves, which are determined such that all the jump relations and the boundary conditions are satisfied. This can only be achieved for discrete values of the angular frequency, ω. In general, the number of degrees of freedom is twice the number of 1D acoustic elements, which is typically a few dozen in the case of an industrial geometry.

Helmholtz solvers assume that the base flow is at rest, in which case an approximate linear wave equation for the small pressure perturbations $p_1(\mathbf{x},t)$ can be derived from the compressible Navier–Stokes equations (Poinsot & Veynante 2005)

$$\nabla\cdot\left(\frac{1}{\rho_0}\nabla p_1\right)-\frac{1}{\gamma p_0}\frac{\partial^2 p_1}{\partial t^2}=-\frac{\gamma-1}{\gamma p_0}\frac{\partial q_1}{\partial t}, \tag{2.1}$$

where p_0 is the uniform thermodynamic pressure, ρ_0 is the density of the baseline flow, and $q_1(\mathbf{x},t)$ is the heat release fluctuation. This is a linear equation in p_1 and q_1, so we can examine the superposition of wavy solutions of the form $p_1=\hat{p}(\mathbf{x})\exp(-\mathrm{i}\omega t)$, $q_1=\hat{q}(\mathbf{x})\exp(-\mathrm{i}\omega t)$, which gives

$$\nabla\cdot\left(\frac{1}{\rho_0}\nabla\hat{p}\right)+\frac{\omega^2}{\gamma p_0}\hat{p}=\mathrm{i}\omega\frac{\gamma-1}{\gamma p_0}\hat{q}. \tag{2.2}$$

In order to close the problem, the flame is often modeled as a purely acoustic element whose response is linear with respect to the acoustic field:

$$\hat{q}(\mathbf{x})=\hat{\mathcal{G}}\left[\nabla\hat{p}\right]+\hat{\mathcal{L}}\left[\hat{p}\right], \tag{2.3}$$

where $\hat{\mathcal{L}}$ and $\hat{\mathcal{G}}$ are two linear operators acting on $\hat{p}$ and $\nabla\hat{p}$ respectively. The general formulation Eq. (2.3) can include many physical effects. It allows the unsteady heat release to be related to the acoustic velocity at a reference position $\mathbf{x}_{\mathrm{ref}}$ as suggested by the classical $n-\tau$ model, $\hat{q}\propto n\exp(\mathrm{i}\omega\tau)\nabla_{\mathbf{n}_{\mathrm{ref}}}\hat{p}(\mathbf{x}_{\mathrm{ref}})$, where $\nabla_{\mathbf{n}_{\mathrm{ref}}}$ stands for the gradient in the direction $\mathbf{n}_{\mathrm{ref}}$. Alternatively, it allows the flame response to be related to both the acoustic velocity and pressure consistently with the matrix identification approach for flame modeling (Polifke *et al.* 2001). Once properly discretized (for example, by a convenient finite-element formulation), Eq. (2.2) and its boundary conditions lead to a nonlinear eigenvalue problem, which can be solved efficiently (Nicoud *et al.* 2007).

Both the network-based model and the Helmholtz approach eventually lead to an eigenvalue problem that is nonlinear in the angular frequency of the acoustic fluctuations

$$\mathbf{N}\left\{\omega,\mathbf{p}\right\}\hat{p}=0, \tag{2.4}$$

where $\mathbf{N}\{\}$ is a matrix acting on the eigenfunction $\hat{p}$ and depends nonlinearly on the

complex-valued pulsation, ω. $\mathbf{p}$ is a vector containing the system's parameters. The size of the matrix is either equal to 4, in the case of a factorized network-based model, or to the number of nodes in the finite-element mesh in the case of the Helmholtz approach, typically of order $10^5 - 10^6$ for industrial geometries. An important source of nonlinearity is the model of the flame, which necessarily introduces a characteristic time delay τ appearing as $\exp(\mathrm{i}\omega\tau)$ in the frequency space. Other nonlinearities in ω may appear because of the boundary impedances. The eigenvalue problem Eq. (2.4) is, however, linear in the mode shape $\hat{p}$ as long as the nonlinear response of the flame is not accounted for.

2.2. *Dealing with uncertainties*

The output of any frequency-based low-order tool is typically a map of the thermo-acoustic eigenvalues in the complex plane. Each eigenfunction is either stable or unstable, depending on the input parameters, $\mathbf{p}$, of the thermo-acoustic analysis. Each unstable mode must be controlled (e.g., by including acoustic dampers) for the combustor to be stable. The design process is even more complex because of the uncertainty in the input parameters $\mathbf{p}$ of the low-order model Eq. (2.4). For example, the speed of sound, c_0, the boundary impedances, and the flame forcing, $\hat{q}$, are sensitive to partly-unknown physical parameters such as the flow regime, manufacturing tolerances, fuel changes, acoustic losses, and heat losses. As a consequence, each mode actually belongs to an uncertain region of the complex plane (see Figure 1a in Bauerheim *et al.* (2014*a*)).

Since low-order methods are fast, they are suitable for studying how the uncertainties in the input parameters propagate and affect the uncertainties in the eigenvalues. This was done by Bauerheim *et al.* (2014*a*), who applied a standard Monte Carlo analysis to a 19-burner annular configuration represented by a network-based model made of 76 acoustic elements and subsequently reduced to a 4×4 matrix through annular network reduction (Bauerheim *et al.* 2014*b*). Assuming that only the amplitude and phase of the 19 flame responses were uncertain (38 uncertain parameters), they found that approximately 10,000 computations were necessary to assess the risk factor, which is the probability of the mode being unstable. If more accuracy is required, a Helmholtz-based strategy should be used. In this case, each computation would require a few tens of minutes or hours, making the generation of a 10,000-sample database CPU-demanding.

In order to avoid expensive Monte Carlo methods and speed up the uncertainty evaluation, a UQ (uncertainty quantification) approach called active subspace (Constantine *et al.* 2013) was tested in Bauerheim *et al.* (2014*a*). The objective is to reduce the dimension of the parameter space (38 dimensions in Bauerheim *et al.* (2014*a*)) to just a few. Denoting the actual surface response $\omega_i = \omega_i(\mathbf{p})$, where $\omega_i = \mathrm{Im}(\omega)$ is the growth rate of the thermo-acoustic mode of interest and $\mathbf{p} = \{n_i, \tau_i\}_{i=1..19}$ is the vector containing the 38 uncertain inputs (19 flame response amplitude n_i and 19 time delays τ_i), the idea is to seek a set of active variables, $\mathbf{W} = W_k, \;\; k = 1, 2, ..., K$, which can describe the surface response. Of course, this dimension reduction is interesting only if the number of active variables is small compared to the dimension of the parameter space. For the particular case of the annular combustor investigated by Bauerheim *et al.* (2014*a*), only 3 active variables are sufficient to represent the 38-dimensional surface response. This gives rise to a two-step strategy to propagate the uncertainties at lower cost: (i) approximate the surface response by a linear regression model $\tilde{\omega}_i = \alpha_0 + \alpha_1 W_1 + \alpha_2 W_2 + \alpha_3 W_3$, where the α's coefficients must be tuned from a few samples belonging to the actual surface response; (ii) use the linear regression model to perform a Monte Carlo analysis at lower cost, thus producing an assessment of the risk factor of the mode of interest. This strategy was successfully applied in Bauerheim *et al.* (2014*a*), where the α's coefficients and thus

the risk factor of the first azimuthal mode of the chamber were computed with only 100 computations, instead of the 10,000 computations required by a classical Monte Carlo analysis.

Note that in order to define the active variables, $\mathbf{W}$, the active subspace method detects which directions (or linear combination of directions) in the parameter space lead to strong variations of the growth rate. Other directions leading to flat response surfaces are not useful for describing the combustor stability and are disregarded, thus reducing the dimension of the surface response. In Bauerheim *et al.* (2014*a*), 35 out of the 38 initial dimensions were disregarded, giving a 3D surface response that was linearly approximated with 100 samples. The computational gain is, however, not as big as it may seem at first sight. Indeed, computing the active variables requires a singular value analysis of the gradient of the surface response, which is to be performed with respect to all the 38 dimensions. The latter was computed in Bauerheim *et al.* (2014*a*) by finite differences for each of the 100 samples required to build the active variables $\mathbf{W} = (W_1, W_2, W_3)$ and to find the coefficients of the linear regression model $\tilde{\omega}_i = \alpha_0 + \alpha_1 W_1 + \alpha_2 W_2 + \alpha_3 W_3$. In the end, the total number of computations was $100 + 100\times38 = 3900$, not significantly less than the 10,000 computations required to perform a classical Monte Carlo analysis. Being able to assess the gradient of the growth rate $\omega_i(\mathbf{p})$ at much lower cost than by performing finite differences is therefore necessary to achieve an efficient UQ analysis. This can be achieved with the adjoint methods described in the following sections.

{sec:MPJhelmh}

3. Eigenvalue sensitivity of a nonlinear Helmholtz eigenproblem

The first adjoint method is designed for a non-degenerate nonlinear Helmholtz eigenproblem Eq. (2.2) that is solved by iteration. It uses the discrete adjoint (DA) approach, meaning that it derives the adjoint of the discretized iteration process. The eigenvalue of the adjoint problem is, to machine precision, the same as that of the direct problem, which is useful for debugging. We define an inner product between two column vectors $\mathbf{f}$ and $\mathbf{g}$ to be $\langle \mathbf{f}, \mathbf{g} \rangle \equiv \mathbf{f}^H \mathbf{M} \mathbf{g}$, where $\mathbf{M}$ is a positive-definite mass matrix, which is defined later. For a generalized matrix eigenvalue problem, $\mathbf{A}\hat{p} = \sigma \mathbf{B}\hat{p}$, there is an associated adjoint matrix eigenvalue problem, $\mathbf{A}^+\hat{p}^+ = \sigma^* \mathbf{B}^+\hat{p}^+$. The relationship between $\mathbf{A}$ and $\mathbf{A}^+$ is given by $\langle \mathbf{A}\mathbf{f}, \mathbf{g} \rangle = \langle \mathbf{f}, \mathbf{A}^+\mathbf{g} \rangle$, from which one obtains $\mathbf{A}^+ = \mathbf{M}^{-1}\mathbf{A}^H\mathbf{M}$. The same relation holds for $\mathbf{B}$ and $\mathbf{B}^+$. When matrix $\mathbf{A}$ is perturbed by $\delta\mathbf{A}$, in which $||\delta\mathbf{A}|| \sim \epsilon \sim o(1)$, the eigenvalue drift is given by

$$\delta\sigma = \frac{\langle \hat{p}^+, \delta\mathbf{A}\hat{p} \rangle}{\langle \hat{p}^+, \mathbf{B}\hat{p} \rangle} \equiv \langle\langle \hat{p}, \delta\mathbf{A} \rangle\rangle, \tag{3.1}$$

where the right-hand term is a convenient abbreviation of the middle term.

For simplicity, we examine a model that has variations in one spatial dimension only, x, for which the eigenvalue problem becomes

$$\frac{\partial}{\partial x}\left(\frac{1}{\rho_0}\frac{\partial}{\partial x}\right)\hat{p} + \frac{\omega^2}{\gamma p_0}\hat{p} = \frac{\gamma - 1}{\gamma p_0}\mathcal{F}(x)\mathrm{e}^{\mathrm{i}\omega\tau_u(x)}\frac{\partial}{\partial x}\hat{p}(x_{ref}), \tag{3.2}$$

where $\mathcal{F}(x)$ is a real valued function of x and is related to amplitude of the flame response (see Nicoud *et al.* (2007) for more details), $\tau_u(x)$ is the time delay between heat release fluctuations at x and earlier velocity fluctuations at x_{ref}. Note that Eq. (3.2) is the 1D version of the general formalism Eq. (2.2) where the RHS was modeled with Eq. (2.3) setting $\hat{\mathcal{L}} \equiv 0$ and $\hat{\mathcal{G}}[\frac{\partial}{\partial x}\hat{p}] \equiv -\frac{\mathrm{i}}{\omega}\mathcal{F}(x)\mathrm{e}^{\mathrm{i}\omega\tau_u(x)}\frac{\partial}{\partial x}\hat{p}(x_{ref})$. This equation is linear in $\hat{p}$ but

nonlinear in ω. It is solved by discretizing in space and then solving a sequence of linear eigenvalue problems until ω converges.

When discretized in space, the eigenvalue problem Eq. (3.2) becomes a matrix eigenvalue problem:

$$\big(\mathbf{DRD} + \mathbf{C}\Phi\mathbf{F}\big)\hat{p} = \sigma\mathbf{B}\hat{p}. \tag{3.3}$$

In Eq. (3.3), $\mathbf{D}$ is the differentiation matrix; $\mathbf{R}$ is a matrix whose diagonal contains the value of $1/\rho$ at each gridpoint; $\mathbf{C}$ is a matrix whose diagonal contains $\mathcal{F}(x)$ at each gridpoint; $\mathbf{F}$ is a matrix whose rows all extract the value of $\partial\hat{p}/\partial x$ at the reference point x_{ref}; $\sigma = \omega^2$; $\mathbf{B}$ is $-\mathbf{I}/(\gamma p_0)$ when the acoustic boundaries are perfectly reflective or is a function of ω when frequency-dependent acoustic boundaries are considered. Finally, Φ is the matrix exponential $\Phi = -\exp(\mathrm{i}\omega\mathbf{T}) = -\exp(\mathrm{i}\sigma^{1/2}\mathbf{T})$, where $\mathbf{T}$ is the matrix whose diagonal contains $\tau(x_1), \tau(x_2), \ldots, \tau(x_{Ndisc})$. $Ndisc$ is the number of discretization points. The leading diagonal of Φ therefore contains $\exp(\mathrm{i}\omega\tau_n(x_1))$, $\exp(\mathrm{i}\omega\tau_n(x_2))$, …, $\exp(\mathrm{i}\omega\tau_n(x_{N_{disc}}))$. Consequently, $\partial\Phi/\partial\omega = \mathrm{i}\mathbf{T}\Phi\sigma^{-1/2}/2$. For simplicity, we define $\mathbf{A}_0 \equiv \mathbf{DRD}$.

The iteration process is described below. (i) Solve $\mathbf{A}_0\hat{p}_0 = \sigma_0\mathbf{B}_0\hat{p}_0$ for a chosen eigenmode σ_0, $\hat{p}_0$. This is a natural acoustic mode of the system in the absence of heat release and is the starting point for the iteration. (ii) Find the corresponding adjoint eigenmode $\hat{p}_0^+$ by solving the adjoint eigenvalue problem $\mathbf{A}_0^+\hat{p}_0^+ = \sigma_0^*\mathbf{B}_0^+\hat{p}_0^+$, where $\mathbf{A}^+ = \mathbf{M}^{-1}\mathbf{A}^H\mathbf{M}$ and $\mathbf{B}^+ = \mathbf{M}^{-1}\mathbf{B}^H\mathbf{M}$, in which the mass matrix $\mathbf{M}$ contains the values of δx along the leading diagonal. (iii) Calculate $\omega = \sigma_0^{1/2}$. (iv) Calculate $\Phi(\omega_0)$ from ω_0. (v) Calculate $\mathbf{B}(\omega_0)$ from ω_0 if using frequency-dependent boundary conditions. (vi) Calculate $\mathbf{A}_1 = \mathbf{A}_0 + \mathbf{C}\Phi(\omega_0)\mathbf{F}$. (vii) Solve $\mathbf{A}_1\hat{p}_1 = \sigma_1\mathbf{B}_1\hat{p}_1$ for σ_1, $\hat{p}_1$. (viii) Solve the corresponding adjoint eigenproblem for $\hat{p}_1^+$. (ix) Calculate $\omega_1 = \sigma_1^{1/2}$. (x) Repeat this process N times until ω_N has converged sufficiently.

In this paper, we will present only the influence of changes to matrix $\mathbf{A}$. Similar techniques can be used to examine the influences of changes to $\mathbf{C}$ and Φ and to the acoustic boundary conditions. Our aim is to calculate $\partial\sigma_N/\partial A_0$ – i.e., to calculate how the converged eigenvalue is affected by changes to the acoustics – as cheaply as possible. We can work backwards from Eq. (3.1) at the final iteration:

$$\delta\sigma_N = \langle\langle\hat{p}_N, \delta\mathbf{A}_N\rangle\rangle. \tag{3.4}$$

Now, in general,

$$\mathbf{A}_n = \mathbf{A}_0 + \mathbf{C}\Phi(\sigma_{n-1})\mathbf{F}, \tag{3.5}$$

which means that

$$\delta\mathbf{A}_n = \delta\mathbf{A}_0 + \frac{\mathrm{i}}{2}\sigma_{n-1}^{-1/2}\mathbf{C}\mathbf{T}\Phi(\sigma_{n-1})\mathbf{F}\delta\sigma_{n-1}. \tag{3.6}$$

We substitute Eq. (3.6) into Eq. (3.4) and, for convenience, define $\xi_n \equiv \frac{\mathrm{i}}{2}\sigma_{n-1}^{-1/2}\langle\langle\hat{p}_n, \mathbf{C}\mathbf{T}\Phi(\sigma_{n-1})\mathbf{F}\rangle\rangle$ which leads to

$$\delta\sigma_N = \langle\langle\hat{p}_N, \delta\mathbf{A}_N\rangle\rangle, \tag{3.7}$$

$$= \langle\langle\hat{p}_N, \delta\mathbf{A}_0\rangle\rangle + \xi_N\delta\sigma_{N-1}. \tag{3.8}$$

And we repeat this until the right-hand side contains $\delta\sigma_{N-N}$, which is known to be zero. This can be written as $\delta\sigma_N = \sum_{n=0}^{N}\chi_n\langle\langle\hat{p}_n, \delta\mathbf{A}_0\rangle\rangle$, where $\chi_N = 1$ and $\chi_{n-1} = \xi_n\chi_n$. This has been verified for the 1D Helmholtz solver by checking the result against that

found by a finite-difference method. The rate of convergence shows that it is correct to first order, as expected.

In summary, a change in $\mathbf{A}_0$ causes a change in all the eigenvalues σ_0 to σ_N calculated during the iteration. We store the direct and adjoint eigenvectors at each stage of the iteration and this allows us to quickly calculate how all the eigenvalues will shift when $\mathbf{A}_0$ changes. The only eigenvalue that concerns us is the final one: σ_N. The computational cost of calculating each adjoint eigenfunction is less than that of each direct eigenfunction because the eigenvalue is already known. The memory requirement is for two eigenfunctions at each stage of the iteration. Even for large 3D Helmholtz solvers, these requirements are easily met.

4. Eigenvalue and singular-value sensitivity in nonlinear eigenproblems

The second adjoint method is designed for general nonlinear eigenproblems. We show how to compute the eigenvalue and singular value sensitivity via a hybrid approach. This approach assumes that the problems are governed by continuous operators (the continuous adjoint approach) but without explicitly deriving the continuous adjoint equations. The final sensitivity formulae can be applied by using a discrete adjoint philosophy, which is more accurate and easier to implement. The proposed procedure requires fewer calculations than the purely discrete adjoint approach described in the previous section. The formalism introduced is meant to be general. Mathematical details of functional analysis will be left out for brevity.

The direct eigenproblem can be conveniently expressed as

$$\mathcal{N}\left\{\omega, \mathbf{p}\right\}\hat{\mathbf{q}} = 0, \tag{4.1}$$

where $\mathcal{N}\{\}$ is the compact linear operator; ω is the nonlinear complex eigenvalue; $\mathbf{p}$ is the vector of the system's parameters (geometry, $n-\tau$ parameters, area expansions; etc); and $\hat{\mathbf{q}}$ is the eigenfunction paired with ω. Note that if $\mathcal{N}$ represents the Helmholtz problem Eq. (2.2), then the eigenfunction is the acoustic pressure, $\hat{\mathbf{q}} = \hat{p}$.

First, we solve the nonlinear direct eigenproblem iteratively. Starting from an initial guess for the eigenvalue, we assume that at the N-th iteration $|\omega_N - \omega_{N-1}|<$ tol, where $N = 1, 2, ...$ and 'tol' is the tolerance desired. The eigenvalue ω is such that

$$\det\left(\mathcal{N}\left\{\omega, \mathbf{p}\right\}\right) = 0, \tag{4.2}$$

where 'det' is the determinant. The corresponding eigenfunction $\hat{\mathbf{q}}$ is calculated from the linear system

$$\left(\mathcal{N}\left\{\omega_N, \mathbf{p}\right\}\right)\hat{\mathbf{q}} = 0. \tag{4.3}$$

Note that, in the continuous formulation, the operator $\mathcal{N}$ depends only on the final converged eigenvalue, ω_N, whereas, in the discrete formulation Eq. (3.5), the equivalent operator, $\mathbf{A}$, depends on the previous eigenvalue, σ_{N-1}. The non-trivial solutions of Eq. (4.3) can be found by computing the eigenfunction (or singular vector) associated with the eigenvalue (or singular value) $0 + \mathrm{i}0$.

Second, defining the adjoint eigenfunction and operator through a Hermitian inner product in an appropriate Hilbert space

$$\left\langle \hat{\mathbf{q}}^{+}, \left(\mathcal{N}\left\{\omega_N, \mathbf{p}\right\}\right)\hat{\mathbf{q}}\right\rangle = \left\langle \left(\mathcal{N}\left\{\omega_N, \mathbf{p}\right\}\right)^{+}\hat{\mathbf{q}}^{+}, \hat{\mathbf{q}}\right\rangle, \tag{4.4}$$

we solve for the adjoint eigenfunction associated with the converged eigenvalue ω_N

$$\left(\mathcal{N}\left\{\omega_N, \mathbf{p}\right\}\right)^H \hat{\mathbf{q}}^+ = 0. \tag{4.5}$$

If we were to follow a purely continuous adjoint approach (Magri & Juniper 2013, 2014), we would need to derive explicitly the hermitian operator $\mathcal{N}^H$ and the continuous adjoint equations. However, we will not derive these equations explicitly and proceed only with the abstract expression of the hermitian operator. Through this, we will be able to apply the discrete adjoint method directly to the final sensitivity formulae, as explained subsequently. We label this the hybrid adjoint method. In Eq. (4.5), the adjoint eigenfunction can be found with the same procedure as Eq. (4.3) because it uses ω_N, not ω_{N-1}. Therefore, we do not need to iterate ω to find the adjoint eigenfunction, as we did for the discrete adjoint in the previous section.

Third, we perturb the parameters' vector such that

$$\mathbf{p} = \mathbf{p}_0 + \epsilon\mathbf{p}_1 \implies \omega = \omega_0 + \epsilon\omega_1 + \epsilon^2\omega_2 \text{ and } \hat{\mathbf{q}} = \hat{\mathbf{q}}_0 + \epsilon\hat{\mathbf{q}}_1 + \epsilon^2\hat{\mathbf{q}}_2, \tag{4.6}$$

where the perturbation parameter is $\epsilon = o(1)$. Note that we relabel ω_N as ω_0. Substituting Eq. (4.6) into the nonlinear eigenproblem Eq. (4.1) and using a Taylor expansion around the unperturbed eigenvalue ω_0 and parameters' vector $\mathbf{p}$, yields

$$\mathcal{N}\left\{\omega_0 + \epsilon\omega_1 + \epsilon^2\omega_2, \mathbf{p}_0 + \epsilon\mathbf{p}_1\right\}\left(\hat{\mathbf{q}}_0 + \epsilon\hat{\mathbf{q}}_1 + \epsilon^2\hat{\mathbf{q}}_2\right) = 0, \tag{4.7}$$

$$\implies \mathcal{N}\left\{\omega_0, \mathbf{p}_0\right\}\hat{\mathbf{q}}_0 \ldots \tag{4.8}$$

$$+ \epsilon\left[\mathcal{N}\left\{\omega_0, \mathbf{p}_0\right\}\hat{\mathbf{q}}_1 + \frac{\partial\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega}\Big|_{\omega_0}\omega_1\hat{\mathbf{q}}_0 + \frac{\partial\mathcal{N}\left\{\omega_0, \mathbf{p}\right\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{q}}_0\right] + \ldots \tag{4.9}$$

$$+ \epsilon^2\left[\mathcal{N}\left\{\omega_0, \mathbf{p}_0\right\}\hat{\mathbf{q}}_2 + \frac{\partial\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega}\Big|_{\omega_0}\omega_1\hat{\mathbf{q}}_1 + \frac{\partial\mathcal{N}\left\{\omega_0, \mathbf{p}\right\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{q}}_1\right] + \ldots \tag{4.10}$$

$$+ \frac{\epsilon^2}{2}\left[\frac{\partial^2\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega^2}\Big|_{\omega_0}\omega_2 + 2\frac{\partial^2\mathcal{N}\left\{\omega, \mathbf{p}\right\}}{\partial\omega\partial\mathbf{p}}\Big|_{\omega_0,\mathbf{p}_0}\omega_1\mathbf{p}_1\right]\hat{\mathbf{q}}_0 + o(\epsilon^2) = 0. \tag{4.11}$$

The unperturbed term of order $\sim O(\epsilon^0)$ in Eq. (4.7) is trivially zero because of Eq. (4.1). Higher-order terms $\sim o(\epsilon^2)$ are neglected. The equation at first order $\sim O(\epsilon^1)$ is

$$\mathcal{N}\left\{\omega_0, \mathbf{p}_0\right\}\hat{\mathbf{q}}_1 = -\left(\frac{\partial\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega}\Big|_{\omega_0}\omega_1\hat{\mathbf{q}}_0 + \frac{\partial\mathcal{N}\left\{\omega_0, \mathbf{p}\right\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{q}}_0\right). \tag{4.12}$$

The equation at second-order is

$$\mathcal{N}\left\{\omega_0, \mathbf{p}_0\right\}\hat{\mathbf{q}}_2 = -\left(\frac{\partial\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega}\Big|_{\omega_0}\omega_1\hat{\mathbf{q}}_1 + \frac{\partial\mathcal{N}\left\{\omega_0, \mathbf{p}\right\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{q}}_1\right) + \ldots \tag{4.13}$$

$$- \frac{1}{2}\left[\frac{\partial^2\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega^2}\Big|_{\omega_0}\omega_2 + 2\frac{\partial^2\mathcal{N}\left\{\omega, \mathbf{p}\right\}}{\partial\omega\partial\mathbf{p}}\Big|_{\omega_0,\mathbf{p}_0}\omega_1\mathbf{p}_1\right]\hat{\mathbf{q}}_0 = 0.$$

The objective is to find the eigenvalue drifts ω_1 and ω_2 due to the perturbation $\mathbf{p}_1$. The adjoint eigenfunction provides a solvability condition for the non-homogenous system Eqs. (4.12) and (4.13), fulfilling the Fredholm alternative. The left-hand side operator range is equal to the kernel of the orthogonal complement of its adjoint operator. Mathematically, this is achieved by projecting Eq. (4.12) onto the adjoint eigenfunction

$$\left\langle\hat{\mathbf{q}}^+, \mathcal{N}\left\{\omega_0, \mathbf{p}_0\right\}\hat{\mathbf{q}}_1\right\rangle = -\left\langle\hat{\mathbf{q}}^+, \left(\frac{\partial\mathcal{N}\left\{\omega, \mathbf{p}_0\right\}}{\partial\omega}\Big|_{\omega_0}\omega_1\hat{\mathbf{q}}_0 + \frac{\partial\mathcal{N}\left\{\omega_0, \mathbf{p}\right\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{q}}_0\right)\right\rangle. \tag{4.14}$$

Using Eq. (4.5), the definition of the inner product Eq. (4.4) and its linearity, yields a

formula for the first-order eigenvalue drift

$$\omega_1 = \frac{-\left\langle \hat{\mathbf{q}}^+, \frac{\partial \mathcal{N}\{\omega_0,\mathbf{p}\}}{\partial \mathbf{p}}\Big|_{\mathbf{p}_0} \mathbf{p}_1 \hat{\mathbf{q}}_0 \right\rangle}{\left\langle \hat{\mathbf{q}}^+, \frac{\partial \mathcal{N}\{\omega,\mathbf{p}_0\}}{\partial \omega}\Big|_{\omega_0} \hat{\mathbf{q}}_0 \right\rangle}. \tag{4.15}$$

Assuming that $\partial \mathcal{N}\{\omega, \mathbf{p}_0\}/\partial\omega \neq 0$, the denominator is different from zero because of the bi-orthogonality condition. If the number of components of $\mathbf{p}$ is M, and we are interested in the first-order sensitivity for each, formula Eq. (4.15) enables us to reduce the number of computations by MQ, where Q is the average of the number of iterations needed to obtain ω_1 by iteratively solving the nonlinear eigenproblem perturbed via finite difference. If the unperturbed eigenvalue ω_0 is N-fold degenerate, the eigenfunction expansion becomes $\hat{\mathbf{q}} = \sum_{i=1}^{N} \alpha_i \hat{\mathbf{e}}_i + \epsilon \hat{\mathbf{q}}_1 + \epsilon^2 \hat{\mathbf{q}}_2$, where α_i are complex numbers and $\hat{\mathbf{e}}_i$ are the N independent eigenfunctions associated with ω_0. By requiring the right-hand side of the degenerate case of Eq. (4.14) to have no component along the independent directions, $\hat{\mathbf{e}}_i$ (Fredholm alternative), we obtain an eigenproblem in α_i and the eigenvalue ω_1 (Hinch 1991) as

$$\omega_1 \alpha_j = -\frac{\left\langle \hat{\mathbf{e}}_j^+, \frac{\partial \mathcal{N}\{\omega_0,\mathbf{p}\}}{\partial \mathbf{p}}\Big|_{\mathbf{p}_0} \mathbf{p}_1 \sum_{i=1}^{N} \alpha_i \hat{\mathbf{e}}_i \right\rangle}{\left\langle \hat{\mathbf{e}}_j^+, \frac{\partial \mathcal{N}\{\omega,\mathbf{p}_0\}}{\partial \omega}\Big|_{\omega_0} \hat{\mathbf{e}}_j \right\rangle}, \tag{4.16}$$

for $j = 1, 2, ..., N$ (repeated indices not to be summed). The degenerate case is relevant to annular combustors in which azimuthal modes have twofold degeneracy. The projection of Eq. (4.13) onto the adjoint eigenfunction gives

$$\langle \hat{\mathbf{q}}^+, \mathcal{N}\{\omega_0, \mathbf{p}_0\}\hat{\mathbf{q}}_2 \rangle = \left\langle \hat{\mathbf{q}}^+, -\left(\frac{\partial \mathcal{N}\{\omega, \mathbf{p}_0\}}{\partial \omega}\Big|_{\omega_0} \omega_1 \hat{\mathbf{q}}_1 + \frac{\partial \mathcal{N}\{\omega_0, \mathbf{p}\}}{\partial \mathbf{p}}\Big|_{\mathbf{p}_0} \mathbf{p}_1 \hat{\mathbf{q}}_1 \right) \right\rangle + \dots \tag{4.17}$$

$$\left\langle \hat{\mathbf{q}}^+, -\frac{1}{2}\left[\frac{\partial^2 \mathcal{N}(\omega, \mathbf{p}_0)}{\partial \omega^2}\Big|_{\omega_0} \omega_2 + 2\frac{\partial^2 \mathcal{N}(\omega, \mathbf{p})}{\partial \omega \partial \mathbf{p}}\Big|_{\omega_0, \mathbf{p}_0} \omega_1 \mathbf{p}_1 \right] \hat{\mathbf{q}}_0 \right\rangle. \tag{4.18}$$

The calculation of the perturbed eigenfunction $\hat{\mathbf{q}}_1$ is obtained via the restricted inversion of the singular operator on the left-hand side of Eq. (4.12). Likewise, using Eqs. (4.5) and (4.4) yields a formula for the second-order eigenvalue drift

$$\begin{aligned} \omega_2 = {} & 2\frac{\left\langle \hat{\mathbf{q}}^+, \left(\frac{\partial \mathcal{N}\{\omega,\mathbf{p}_0\}}{\partial \omega}\Big|_{\omega_0} \omega_1 \hat{\mathbf{q}}_1 + \frac{\partial \mathcal{N}\{\omega_0,\mathbf{p}\}}{\partial \mathbf{p}}\Big|_{\mathbf{p}_0} \mathbf{p}_1 \hat{\mathbf{q}}_1 \right) \right\rangle}{\left\langle \hat{\mathbf{q}}^+, \frac{\partial^2 \mathcal{N}\{\omega,\mathbf{p}_0\}}{\partial \omega^2}\Big|_{\omega_0} \hat{\mathbf{q}}_0 \right\rangle} + \dots \\ & + 4\frac{\left\langle \hat{\mathbf{q}}^+, \frac{\partial^2 \mathcal{N}(\omega,\mathbf{p})}{\partial \omega \partial \mathbf{p}}\Big|_{\omega_0,\mathbf{p}_0} \omega_1 \mathbf{p}_1 \hat{\mathbf{q}}_0 \right\rangle}{\left\langle \hat{\mathbf{q}}^+, \frac{\partial^2 \mathcal{N}\{\omega,\mathbf{p}_0\}}{\partial \omega^2}\Big|_{\omega_0} \hat{\mathbf{q}}_0 \right\rangle}, \end{aligned} \tag{4.19}$$

assuming that the denominator is different from zero.

4.1. *Singular value drift*

The singular value s is the solution of the nonlinear eigenproblem $\mathcal{H}\{s,\mathbf{p}\}\,\hat{\mathbf{u}}=0$, where $\mathcal{H}=\mathcal{N}^{+}\mathcal{N}$ and $\hat{\mathbf{u}}$ is the right singular function. The first- and second- order singular value drifts read, respectively,

$$s_1=\frac{-\left\langle \hat{\mathbf{u}}^{+},\,\frac{\partial\mathcal{Q}\{\omega_0,\mathbf{p}\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{u}}_0\right\rangle}{\left\langle \hat{\mathbf{u}}^{+},\,\frac{\partial\mathcal{Q}\{\omega,\mathbf{p}_0\}}{\partial\omega}\Big|_{\omega_0}\hat{\mathbf{u}}_0\right\rangle}, \tag{4.20}$$

$$s_2=2\frac{\left\langle \hat{\mathbf{u}}^{+},\left(\frac{\partial\mathcal{Q}\{\omega,\mathbf{p}_0\}}{\partial\omega}\Big|_{\omega_0}\omega_1\hat{\mathbf{u}}_1+\frac{\partial\mathcal{Q}\{\omega_0,\mathbf{p}\}}{\partial\mathbf{p}}\Big|_{\mathbf{p}_0}\mathbf{p}_1\hat{\mathbf{u}}_1\right)\right\rangle}{\left\langle \hat{\mathbf{u}}^{+},\,\frac{\partial^2\mathcal{Q}\{\omega,\mathbf{p}_0\}}{\partial\omega^2}\Big|_{\omega_0}\hat{\mathbf{u}}_0\right\rangle}+\ldots$$
$$+4\frac{\left\langle \hat{\mathbf{u}}^{+},\,\frac{\partial^2\mathcal{Q}(\omega,\mathbf{p})}{\partial\omega\partial\mathbf{p}}\Big|_{\omega_0,\mathbf{p}_0}\omega_1\mathbf{p}_1\hat{\mathbf{u}}_0\right\rangle}{\left\langle \hat{\mathbf{u}}^{+},\,\frac{\partial^2\mathcal{Q}\{\omega,\mathbf{p}_0\}}{\partial\omega^2}\Big|_{\omega_0}\hat{\mathbf{u}}_0\right\rangle}, \tag{4.21}$$

in which $\partial\mathcal{Q}/\partial\omega=\mathcal{N}(\partial\mathcal{N}^{+}/\partial\omega)+\mathcal{N}^{+}(\partial\mathcal{N}/\partial\omega)$ and $\partial^2\mathcal{Q}/\partial\omega^2=\mathcal{N}(\partial^2\mathcal{N}^{+}/\partial\omega^2)+\mathcal{N}^{+}(\partial^2\mathcal{N}/\partial\omega^2)+2(\partial\mathcal{N}^{+}/\partial\omega)(\partial\mathcal{N}/\partial\omega)$. When an unperturbed singular value is degenerate, the singular value drift can be calculate as described in the previous subsection. Eqs. (4.14), (4.19), (4.20), and (4.21) can be applied to Helmholtz solvers as well as to network models whenever gradient information is needed. This is the case in uncertainty quantification and active subspace identification (Bauerheim *et al.* 2014*a*). In these analyses, the gradient information has so far been evaluated via finite difference, which is prone to cancellation errors and requires the perturbed nonlinear eigenproblem to be solved. When these linear operators are numerically discretized, they can be expressed as matrices. In order to use these formulae in a discrete adjoint approach, which gives the same eigenvalue as the direct problem to machine precision, we have to (i) derive the analytical expressions for the linearized operators $\partial\mathcal{N}\{\omega,\mathbf{p}_0\}/\partial\omega$, $\partial^2\mathcal{N}\{\omega,\mathbf{p}_0\}/\partial\omega^2$, $\partial\mathcal{Q}\{\omega,\mathbf{p}_0\}/\partial\omega$, $\partial^2\mathcal{Q}\{\omega,\mathbf{p}_0\}/\partial\omega^2$, and the cross-derivatives and discretize them; (ii) compute the perturbation matrices, for example, $\partial\mathcal{N}\{\omega_0,\mathbf{p}\}/\partial\mathbf{p}\cdot\mathbf{p1}$, to the i^{th} unperturbed system's parameter $p_0^{(i)}$ by setting $p_1^{(i)}$ to a small value and setting the remaining parameters to zero; (iii) compute the adjoint matrix as the Hermitian transpose of the discretized operator $\mathcal{N}\{\omega_0,\mathbf{p}_0\}$; (iv) compute the direct and adjoint eigenfunctions $\hat{\mathbf{q}_0}$ and $\hat{\mathbf{q}}^{+}$; (v) solve for the perturbed eigenvector $\hat{\mathbf{q}}_1$; (vi) combine the above matrices and vectors in the discretized inner products, defined in section 3; (vii) calculate the eigenvalue/singular value sensitivities to $p_1^{(i)}$ by dividing the drifts by the perturbation, for example, $\omega_1/p_1^{(i)}$; (viii) repeat for all the remaining parameters $p_0^{(i)}$.

5. Conclusion

Adjoint methods have the potential to greatly speed up calculations for the optimization and uncertainty quantification of thermo-acoustic instability. This report presents two methods. The first, which uses the discrete adjoint approach, is specifically for nonlinear Helmholtz eigenvalue problems that are solved iteratively. The second, which uses a hybrid adjoint approach, is more general and can be applied to both problems.

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