Equivalence Between the Combined Approximations Technique and Krylov Subspace Methods

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Nomenclature

$\boldsymbol{c} = \{c_1, c_2, \ldots, c_m\}$	=	vector of undetermined coefficients
$\boldsymbol{f}$	=	force vector
$\boldsymbol{K}, \boldsymbol{x}$	=	perturbed stiffness matrix and displacement vector
$\boldsymbol{K}_0, \Delta\boldsymbol{K}$	=	baseline stiffness matrix and its perturbation
$\mathcal{K}_m$	=	Krylov subspace of order m
m	=	number of basis vectors
n	=	number of degrees of freedom
p	=	rank of $\Delta\boldsymbol{K}$
q_j	=	index of the jth eigenvalue
$r(\boldsymbol{K})$	=	minimal polynomial of matrix $\boldsymbol{K}$
$\boldsymbol{r}_0$	=	residual error vector
s	=	number of distinct eigenvalues of $\boldsymbol{K}$
$\boldsymbol{x}_0, \Delta\boldsymbol{x}$	=	baseline displacement vector and its perturbation
λ_j	=	jth eigenvalue of $\boldsymbol{K}$
$\boldsymbol{\Psi} = [\psi_1, \psi_2, \ldots, \psi_m]$	=	matrix of basis vectors

Introduction

IN 1991 Kirsch[1] proposed a reduced basis technique for static reanalysis of structural systems. It was shown that the terms of a binomial series expansion (also referred to as the Neumann series) can be used as basis vectors for accurately approximating the static response for large changes in the design variables. The Neumann series can be interpreted as a local approximation method with a limited radius of convergence. Because the technique proposed by Kirsch combines this local approximation series with the global characteristics of the reduced basis method, it was dubbed as the *combined approximations* (CA) *technique*.

Over the last decade a number of studies on the application of the CA technique as well as its extensions have been reported in the literature. Examples include static sensitivity analysis,[2] reanalysis of structures subjected to topological modifications,[3,4] structural optimization,[5,6] and damage-tolerant design.[7] Further insights into the CA technique and orthogonalization procedures to improve its numerical stability have been presented by Kirsch[8,9] and Kirsch and Papalambros.[10]

Very few papers in the literature have rigorously examined why the CA technique gives high-quality approximations for large changes in the design variables. The only exception appears to be a recent study by Akgün et al.,[11] who examined the relationship between the Sherman–Morrison–Woodbury (SMW) formula and some static reanalysis techniques. It was shown that the CA technique is mathematically equivalent to the SMW formula for a particular choice of basis vectors.

The objective of this Note is to examine the equivalence between the CA technique and Krylov subspace methods. It is shown that the CA technique is a preconditioned Krylov subspace method. Based on this connection, it is briefly outlined why the CA technique will converge to the exact solution when the number of basis vectors is increased. The ramification of the present research on the practical issue of integrating static reanalysis techniques with structural optimization procedures is also discussed.

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Combined Approximations Technique

Consider the matrix system of equations for static equilibrium of a modified linear structural system

$$(\boldsymbol{K}_0 + \Delta\boldsymbol{K})(\boldsymbol{x}_0 + \Delta\boldsymbol{x}) = \boldsymbol{f} \tag{1}$$

where $\boldsymbol{K}_0$ and $\Delta\boldsymbol{K} \in \mathbb{R}^{n\times n}$ denote the baseline stiffness matrix and its perturbation, respectively; $\boldsymbol{x}_0 = \boldsymbol{K}_0^{-1}\boldsymbol{f} \in \mathbb{R}^n$ is the displacement of the baseline structure corresponding to the force vector $\boldsymbol{f} \in \mathbb{R}^n$; and $\Delta\boldsymbol{x} \in \mathbb{R}^n$ denotes the perturbation of the displacement vector.

The static reanalysis problem involves computing $\Delta\boldsymbol{x}$ using the data available from analysis of the baseline structure, without explicitly solving Eq. (1) in its exact form. Henceforth, the perturbed stiffness matrix and the corresponding perturbed displacement vector will be denoted as $\boldsymbol{K} = \boldsymbol{K}_0 + \Delta\boldsymbol{K}$ and $\boldsymbol{x} = \boldsymbol{x}_0 + \Delta\boldsymbol{x}$, respectively.

The Neumann series for the solution of Eq. (1) can be written as

$$\boldsymbol{x} = \sum_{i=0}^{\infty} (-1)^i \left(\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}\right)^i \boldsymbol{x}_0 \tag{2}$$

Note that the Neumann series will converge only when $\|\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}\| < 1$ or $\rho(\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}) < 1$, where ρ denotes the spectral radius. The CA technique attempts to improve the accuracy of Eq. (2) by approximating the perturbed displacement vector as

$$\hat{\boldsymbol{x}} = c_1\psi_1 + c_2\psi_2 + \cdots + c_m\psi_m = \boldsymbol{\Psi}\boldsymbol{c} \tag{3}$$

where $\psi_i = (\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K})^{i-1}\boldsymbol{x}_0 \in \mathbb{R}^n$ is the ith basis vector. $\boldsymbol{\Psi} = [\psi_1, \psi_2, \ldots, \psi_m] \in \mathbb{R}^{n\times m}$ and $\boldsymbol{c} = \{c_1, c_2, \ldots, c_m\}^T \in \mathbb{R}^m$ denote the matrix of basis vectors and the vector of undetermined coefficients, respectively.

An alternative choice of basis vectors was proposed by Kirsch and Liu[3] for cases when $\text{Rank}(\Delta\boldsymbol{K}) = p \ll n$. Here, the perturbed stiffness matrix can be written as $\boldsymbol{K} = \boldsymbol{K}_0 + \boldsymbol{K}_1 + \boldsymbol{K}_2 + \cdots + \boldsymbol{K}_p$, where $\boldsymbol{K}_i \in \mathbb{R}^{n\times n}$, $i = 1, 2, \ldots, p$ is a rank one matrix. The displacement of the baseline structure $\boldsymbol{x}_0$ is chosen as the first basis vector. The subsequent p basis vectors are computed as $\psi_i = \boldsymbol{K}_0^{-1}\boldsymbol{K}_{i-1}\boldsymbol{x}_0$, $i = 2, 3, \ldots, p+1$.

The undetermined constants in the reduced basis can be computed either using the Bubnov–Galerkin scheme or a residual error minimization approach. This involves imposition of any of the constraints shown here:

$$\boldsymbol{K}\boldsymbol{\Psi}\boldsymbol{c} - \boldsymbol{f} \perp \boldsymbol{\Psi} \tag{4a}$$

$$\boldsymbol{K}\boldsymbol{\Psi}\boldsymbol{c} - \boldsymbol{f} \perp \boldsymbol{K}\boldsymbol{\Psi} \tag{4b}$$

When the Bubnov–Galerkin scheme (4a) is used, the reduced-order $m \times m$ system of equations for the coefficient vector $\boldsymbol{c}$ is given by $\boldsymbol{\Psi}^T\boldsymbol{K}\boldsymbol{\Psi}\boldsymbol{c} = \boldsymbol{\Psi}^T\boldsymbol{f}$. Similarly, application of the residual error minimization condition (4b) leads to an $m \times m$ system of equations $\boldsymbol{\Psi}^T\boldsymbol{K}^T\boldsymbol{K}\boldsymbol{\Psi}\boldsymbol{c} = \boldsymbol{\Psi}^T\boldsymbol{K}^T\boldsymbol{f}$. Equation (4b) is equivalent to minimization of the $\mathcal{L}_2$ norm of the residual error vector $\boldsymbol{K}\boldsymbol{\Psi}\boldsymbol{c} - \boldsymbol{f}$. The coefficient vector $\boldsymbol{c}$ computed by solving the system of reduced-order equations can then be used in conjunction with Eq. (3) to approximate the static response.

If the alternative choice of basis vectors discussed earlier is used along with condition (4a), then it can be shown that the CA technique is equivalent to the SMW formula (see Akgün et al.[11] for details of the proof). Hence the perturbed displacement vector can be computed exactly. It will be shown next that, when the terms of the Neumann series are used as basis vectors, an equivalence can be shown with preconditioned Krylov subspace methods.

Preconditioned Krylov Subspace Connection

Krylov subspace methods for iterative solution of linear systems is an active area of research in numerical linear algebra, with a rich history spanning more than 50 years (see Saad and Van der Vorst[12] for an overview of progress made in the past century). The interested reader is referred to the text by Saad[13] for a detailed exposition. For a comprehensive overview an introductory paper by Ipsen and Meyer[14] is highly recommended. Some of the well-known methods in this class are Arnoldi's method, the Lanczos method, and the generalized minimal residual (GMRES) method.

In the context of solution of Eq. (1), Krylov methods seek to approximate the displacement vector $\boldsymbol{x}$ using the affine subspace $\boldsymbol{d} + \mathcal{K}_m(\boldsymbol{K}, \boldsymbol{r}_0)$, where

$$\mathcal{K}_m(\boldsymbol{K}, \boldsymbol{r}_0) = \text{span}\{\boldsymbol{r}_0, \boldsymbol{K}\boldsymbol{r}_0, \ldots, \boldsymbol{K}^{m-1}\boldsymbol{r}_0\} \tag{5}$$

denotes the Krylov subspace of order m, and $\boldsymbol{r}_0 = \boldsymbol{K}\boldsymbol{d} - \boldsymbol{f} \in \mathbb{R}^n$ is the residual error vector when $\boldsymbol{d} \in \mathbb{R}^n$ is used as an initial guess for the displacement vector. Clearly, a good initial guess for static reanalysis would be $\boldsymbol{d} = \boldsymbol{x}_0$. This implies that the displacement of the modified structure can be approximated using the terms $\boldsymbol{x}_0, \Delta\boldsymbol{K}\boldsymbol{x}_0, \boldsymbol{K}\Delta\boldsymbol{K}\boldsymbol{x}_0, \ldots, \boldsymbol{K}^{m-1}\Delta\boldsymbol{K}\boldsymbol{x}_0$ as basis vectors. As shown next, preconditioning schemes can be employed to improve the quality of these basis vectors.

Consider the case when the matrix $\boldsymbol{K}_0^{-1}$ is used as a left preconditioner for Eq. (1), which gives the transformed equation $\boldsymbol{K}_0^{-1}\boldsymbol{K}\boldsymbol{x} = \boldsymbol{K}_0^{-1}\boldsymbol{f}$. This preconditioning scheme assumes that the decomposed form of the baseline stiffness matrix is available. The preconditioned matrix system of equations for static equilibrium can be rewritten as

$$\left(\boldsymbol{I} + \boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}\right)\boldsymbol{x} = \boldsymbol{x}_0 \tag{6}$$

The solutions of Eqs. (1) and (6) are the same. If the zero vector is used as an initial guess for constructing a Krylov subspace for the solution of Eq. (6), then $\boldsymbol{r}_0 = \boldsymbol{x}_0$. The left preconditioned Krylov subspace can hence be written as

$$\mathcal{K}_m\left(\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}, \boldsymbol{x}_0\right) = \text{span}\left\{\boldsymbol{x}_0, \boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}\boldsymbol{x}_0, \left(\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}\right)^2\boldsymbol{x}_0, \ldots, \left(\boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}\right)^{m-1}\boldsymbol{x}_0\right\} \tag{7}$$

A comparison of Eqs. (2) and (7) clearly shows that the m terms of the Neumann series are identical to the left preconditioned Krylov subspace. Based on this observation, equivalence between the CA technique and various preconditioned Krylov subspace methods can be readily shown. This is possible because the CA technique and preconditioned Krylov methods use the same subspace for approximating the solution vector. Note that the equivalence suggested here assumes exact precision arithmetic because the implementation details of Krylov subspace methods and the CA technique are different.

For example, consider the case when the terms of the Neumann series are orthonormalized using the Gram–Schmidt algorithm, and the Bubnov–Galerkin scheme (4a) is employed to compute the undetermined coefficients in the reduced basis. Then the CA technique becomes equivalent to a preconditioned version of Arnoldi's method for linear systems,[15] when $\boldsymbol{K}$ is nonsymmetric. When $\boldsymbol{K}$ is symmetric, the CA technique becomes equivalent to the preconditioned Lanczos method for linear systems. If the residual error minimization condition (4b) is employed to compute the coefficients of the reduced basis, then the CA technique is equivalent to the popular GMRES algorithm.[16]

Convergence of the CA Technique

Based on the connections between the CA technique and Krylov subspace methods outlined in the preceding section, it can now be readily shown why the CA technique will converge to the exact solution when the number of basis vectors is increased. The analysis presented in this section follows that in Ipsen and Meyer.[14]

First, consider the notion of the minimal polynomial r of a square matrix $\boldsymbol{K}$, which can be defined as the unique monic polynomial of minimal degree such that $r(\boldsymbol{K}) = 0$. Let the s distinct eigenvalues of $\boldsymbol{K}$ be denoted by $\lambda_1, \lambda_2, \ldots, \lambda_s$, and let q_j denote the index of the jth eigenvalue. (For a general matrix $\boldsymbol{K}$, q_j is the size of the largest Jordan block associated with λ_j. When $\boldsymbol{K}$ is diagonalizable, then $q = \Sigma_{j=1}^{s} q_j$ is the total number of distinct eigenvalues of $\boldsymbol{K}$, that is, $q = s$.) Hence,

$$q = \sum_{j=1}^{s} q_j, \qquad r(t) = \prod_{j=1}^{s} (t - \lambda_j)^{q_j} \tag{8}$$

Using the preceding equations, $r(t)$ can be rewritten as a polynomial of the form

$$r(t) = \sum_{j=0}^{q} \alpha_j t^j \tag{9}$$

where the term

$$\alpha_0 = \prod_{j=1}^{s} (-\lambda_j)^{q_j}$$

is nonzero if the perturbed stiffness matrix is nonsingular.

The minimal polynomial of $\boldsymbol{K}$ hence becomes

$$r(\boldsymbol{K}) = \sum_{j=0}^{q} \alpha_j \boldsymbol{K}^j = 0 \tag{10}$$

Assuming $\alpha_0 \neq 0$, the inverse of $\boldsymbol{K}$ can be written as

$$\boldsymbol{K}^{-1} = -\frac{1}{\alpha_0} \sum_{j=1}^{q} \alpha_j \boldsymbol{K}^{j-1} \tag{11}$$

It can be clearly seen from Eq. (11) that the inverse of a nonsingular matrix lies in the space spanned by the terms of the minimal polynomial. Further, the desired solution vector $\boldsymbol{K}^{-1}\boldsymbol{f}$ can be computed using a linear combination of the terms of the Krylov subspace defined earlier in Eq. (5). The number of basis vectors required to compute the exact solution will depend on the degree of the minimal polynomial, that is, q. This observation can now be formally stated as follows[14]:

Theorem. If the minimal polynomial of a nonsingular matrix $\boldsymbol{K}$ has degree q, then the solution to $\boldsymbol{K}\boldsymbol{x} = \boldsymbol{f}$ lies in the Krylov subspace $\mathcal{K}_q(\boldsymbol{K}, \boldsymbol{f})$.

For a general matrix $\boldsymbol{K}$ the degree of the minimal polynomial could be rather high. To reduce the degree of the minimal polynomial, a preconditioning scheme becomes useful. A good preconditioning scheme will enable the computation of accurate approximations using a small number of basis vectors.

Consider the case when $\boldsymbol{K}_0^{-1}$ is used as the left preconditioning matrix. Here, the number of basis vectors required to compute the exact solution will depend on the eigenspectrum of the matrix $\boldsymbol{D} = \boldsymbol{K}_0^{-1}\boldsymbol{K} = \boldsymbol{I} + \boldsymbol{K}_0^{-1}\Delta\boldsymbol{K}$. If $\boldsymbol{D}$ has few distinct eigenvalues or the eigenvalues fall into k compact clusters, then high-quality approximations can be computed using around k basis vectors. This condition is clearly satisfied when the perturbation $\Delta\boldsymbol{K}$ is small because all of the eigenvalues of $\boldsymbol{D}$ will then tend to be clustered around unity, that is, from a numerical viewpoint $\boldsymbol{D}$ will tend to behave like a matrix with one distinct eigenvalue. As is well known from previous numerical studies,[1] two basis vectors will give good approximations for this case. For large perturbations it is difficult to determine a priori the number of basis vectors required to compute the exact solution. However, procedures exist in the literature[12] for adaptively increasing the number of basis vectors to compute the solution with desired accuracy.

Conclusions

It is shown that the combined approximations (CA) technique proposed by Kirsch[1] is a preconditioned Krylov subspace method. This connection enables a better understanding of why the CA technique will converge to the exact solution when the number of basis vectors is increased. Furthermore, research on issues such as error estimation, convergence rate, and termination criteria of the CA

technique can also benefit from existing and ongoing theoretical work on preconditioned Krylov subspace methods.[12,13]

The present study also has an important ramification on the practical issue of integrating static reanalysis techniques with numerical optimization algorithms. The success of the CA technique taken together with the observations made in the present research suggests that it might be worthwhile to invest computational effort in constructing a good preconditioner. Because a large number of repeated analyses will be carried out during the optimization iterations, a good preconditioning scheme can lead to a significant improvement in the overall efficiency of the optimization process. In practice, a direct method can be employed to construct a preconditioner by decomposing a baseline stiffness matrix. During the course of the optimization iterations, structural analysis can then be carried out using preconditioned Krylov solvers.

In this Note the issue of how to improve the CA technique was not considered. However, it is expected that by employing ideas from the conjugate gradient squared algorithm or its variants[13] accurate approximations can be computed using a smaller number of basis vectors. Detailed studies are required to fully explore such possibilities.

It also appears that the extension of the CA technique to static reanalysis of topologically modified structures can be better understood using the observations made here. Namely, the concept of modified initial stiffness matrix[3,4] can be interpreted as a preconditioning technique. It is expected that, by leveraging related work on constructing preconditioners for block-partitioned matrices arising in domain decomposition schemes, more efficient algorithms for reanalysis of topologically modified structures can be developed.

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Errata

Accurate Calibration of Low-Speed Wind Tunnels, Including Humidity and Compressibility

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EQUATION (6) should read:

$$U_\infty = \sqrt{\gamma RT_\infty}M_\infty = \sqrt{2RT_T\varepsilon}[1 - 0.45(\varepsilon/\gamma) + 0(\varepsilon^2/\gamma)]$$

AIAA regrets the error.