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Sensitivity analysis of finite element-based equilibrium problems using Padé approximants

Soon Ki Kwon
Iowa State University

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Sensitivity analysis of finite element-based equilibrium problems using Padé approximants

Kwon, Soon Ki, Ph.D.

Iowa State University, 1990
Sensitivity analysis of finite element-based equilibrium problems using Padé approximants

by

Soon Ki Kwon

A Dissertation Submitted to the Graduate Faculty in Partial Fulfillment of the Requirements for the Degree of DOCTOR OF PHILOSOPHY

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For the Graduate College

Iowa State University
Ames, Iowa
1990

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CHAPTER 1. INTRODUCTION

The finite element method is routinely used for the solution of static and dynamic structural problems. The solution takes on the order of $n^3$ calculations. Since $n$ can be very large, the solution can be very time consuming.

Design optimization typically requires many re-solutions to the finite element problem. For large problems, this procedure is very costly in time and computer resources. This has led analysts to use approximations to the finite element solution which are valid in some neighborhood of the original solution. The use of these approximations, which typically require the order of $n^2$ rather than $n^3$ calculations, is called sensitivity analysis.

This thesis presents a sensitivity analysis based on Padé approximants. The method is illustrated with a straightforward example concerning a clamped plate and a much more complicated example concerning the design optimization of a plastic bumper endcap.

Chapter 2 presents a review of some recent literature in structural optimization and design sensitivity analysis. Chapter 3 presents a definition of Padé approximants and a numerical procedure for implementing their use. The use of Padé approximants requires higher order derivatives of the stiffness matrix with respect to the design variable. Chapter 4 presents a method to determine these derivatives numerically.
Chapter 5 presents an example using design optimization based on Padé expansions. The example illustrates the design optimization of a plastic bumper endcap modeled using MSC/NASTRAN. The solutions for the deflection and stress are key parts of the objective function. Chapter 6 presents conclusions and recommendations for the extension of this research.
CHAPTER 2. LITERATURE REVIEW

The mathematical model of structures is typically described by a matrix equation of the form

\[ Kx = f \]  \hspace{1cm} (2.1)

for the statics problem and, in the absence of damping

\[ M\ddot{x} + Kx = f \]  \hspace{1cm} (2.2)

for the dynamics problem, where M and K are \( n \times n \) mass and stiffness matrices of the structure. The \( n \times 1 \) vectors \( \ddot{x}, x \) and \( f \) represent the acceleration, displacement and external forces, respectively.

These two equations are used to calculate displacements, natural frequencies and mode shapes of the structure under load. If the displacements or natural frequencies are objectionable, the original structure should be changed, so solutions to equations (2.1) and (2.2) need to be calculated again. Since it takes on the order of \( n^3 \) calculations to solve these two equations, the solution can be very time consuming when \( n \) is very large.

This has led to the desire to approximate the solution of equations (2.1) and (2.2) with less burdensome equations which yield approximate solutions as a function of perturbations about an original solution, so called sensitivity analysis. By easing the
computational burden associated with re-solution of the problem, sensitivity analysis facilitates design optimization. The success of this procedure depends on the range of validity of the sensitivity based approximations.

This review gives a brief overview of the literature of structural optimization and discusses some details of sensitivity analysis.

**Structural Optimization**

Structural optimization searches for designs which achieve objectives, usually minimum weight or cost, while satisfying a set of design requirements called constraints.

As early as 1960, Schmit [1] presented work which approached structural optimization numerically. Since that time, significant developments have included the growth of computing power, the routine availability of finite element software, and the development of sensitivity analysis. Schmit [2] reviewed the various developments in structural optimization stressing nonlinear programing techniques and optimality criteria techniques from 1960 to 1980. Arora and Belegundu [3], and Shanno [4] developed mathematical programming methods to apply to structural optimization. The efficient and improved optimality criteria were proposed by Khot [5], Levy and Parzynski [6], and Pappas [7]. In 1979, Haug and Arora presented an overview of numerical optimization [8]. The contribution of numerical techniques to the development of structural optimization was discussed by Vanderplaats [9]. Levy and Lev [10] present a recent developments in the area of numerical structural optimization.

This body of literature, which is too large for an in depth review here, typically
deals with optimization in the following sense; the designer supplies the original structure, design goals in the form of an objective function, and design parameters subject to change. The optimal solution is then found numerically.

Another point of view on the optimization process holds that the experienced designer carries a great deal of valuable knowledge not easily captured in the form required by objective functions, knowledge that would be lost in traditional, numerically intensive design optimization. Furthermore, design constraints are often not amenable to the usual inequality constraints. In fact, the constraints are often "fuzzy" and an experienced designer recognizes that tradeoffs among constraints are an important intuitively-based part of the design process.

Work with the objective on capturing the designer's capability to work interactively in the optimization process was presented by Starkey and Bernard [11], who proposed a technique to shift the natural frequencies of the existing design away from the undesirable frequency bands. This procedure, which can be contrasted to optimization with equality constraints on frequency, seeks to minimize a penalty function which becomes smaller as the design improves. They suggested a penalty function $P(\omega, e)$ is of the form

$$P(\omega, e) = \sum_{i=1}^{m} A_i F_i(\omega_i) + \sum_{j=1}^{r} S_j(e_j)$$  

(2.3)

where $\omega$ is an $(m \times 1)$ vector of natural frequencies of the modified system, $e$ is the $(r \times 1)$ vector of design variables, the $F_i(\omega_i)$ are scalar functions which are large when natural frequencies lie in the undesirable bands, and $S_j(e_j)$ are scalar functions which become large when the design changes become large. The $A_i$ are positive scalars which weight the importance of each frequency band relative to each others and the size-of-change constraint. By interactively choosing the $A_i$ and $S_j$, the designer participated
in the optimization process.

Figures 2.1 and 2.2 show the shapes of the frequency and size-of-change constraint functions respectively. Minimizing of this penalty function gives the optimal design vector e.

Somayajula and Bernard extended Starkey's technique to develop a design optimization process for large problems having several displacement, stress, combination and frequency constraints [12-14]. This work was presented in a finite element context in which the designer interactively alters penalty functions to achieve the desired optimum.

Design Sensitivity

Our interest here is in large problems which are computationally burdensome. Thus successful optimization, particularly when it involves interactivity on the part of the designer, involves approximate solutions which are easy to compute. The use of these approximate solutions is referred to as design sensitivity analysis.

There is a wide-ranging literature on this topic. Wittrick [15] presented the rates of change of eigenvalues in the field of buckling and vibration. Fox and Kapoor [16] used the first derivative of eigenvalues to approximate the eigenvalues with respect to several design variables for symmetric mass and stiffness matrices. They also presented two methods for determining n eigenvector derivatives. Rogers [17] generalized the second approach in reference [16] to include nonsymmetric matrices.
Figure 2.1: Frequency constraint function
Figure 2.2: Size-of-change constraint function
Storaasli and Sobieszczanski [18], and Starkey and Bernard [11] proposed the use of linear Taylor expansion for modifications involving a small number of structural members. Rudisill and Bhatia used second derivatives of eigenvalues to find the role of change of the flutter velocity of aircraft structure with respect to structural parameters [19]. For the determination of the derivative of eigenvectors of nth order algebraic eigensystems, Nelson [20] presented an alternative procedure which is applicable to symmetric or nonsymmetric systems. To improve the quality of the approximations, Kirsch [21] presented a modified nonpolynomial series from a simple iteration procedure. Adelman and Haftka [22] surveyed methods for calculating sensitivity derivatives for discrete structural systems. These methods concern calculation of derivatives of static displacements and stresses, eigenvalues and eigenvectors, transient structural response, and derivatives of optimum structural designs with respect to problem parameters.

The first order expansion of the solution to equations (2.1) and (2.2) requires only the product of a matrix and a vector, at most \( O(n^2) \) calculations. This can easily be done for several design variables. Higher order terms present a more difficult problems. First of all, cross derivatives are important. Extension of the expansion to even the third or fourth order leads to so many terms in the series that the method becomes impractical. Secondly, some methods of expanding the eigenvalue problem of equation (2.2) require \( O(n^3) \) calculations.

In 1980, Whitesell presented a method to expand the eigenvalue problem in one variable based on only \( O(n^2) \) calculations [23]. Based on this work Rizai and Bernard [24] used higher order Taylor series expansion in a finite element context to expand the range of the approximations for natural frequencies. Although the
work illustrated the potential of higher order expansions, recurring problems were numerical calculation of higher order derivatives of mass and stiffness matrices, which are required constituents in the calculations of the coefficients of the Taylor series, and occasional divergence of the series.

In 1984, Whitesell [25] presented a design reanalysis method based on rational approximation techniques which overcomes the convergence limitations of Taylor series. Whitesell's work, which is based on Padé approximants, makes possible the expansion of the solution of equation (2.1) and (2.2) across a very wide range of a single design variable.

This thesis uses Whitesell's work as the cornerstone for design optimization of the statics problem, equation (2.1). The next chapters presents some details of Padé approximants and indicates how they apply in the solution of equation (2.1). This is followed by presentation of a stable solution of the required higher order derivatives of the stiffness matrix and by example problems illustrating the technique.
CHAPTER 3. APPLICATION OF HIGH ORDER SENSITIVITY

Consider again equation (2.1)

\[ K(e)x(e) = f(e) \]

We consider one design change \( e \), which may involve geometry or material properties. We wish to expand the solution for the displacement \( x \) about the original design value \( e_0 \).

For the first derivative, we have

\[ Kx' = -K'x + f' \] (3.1)

where the prime indicates differentiation with respect to \( e \). The solution for \( x' \) is analogous to the solution to \( Kx = f \) for another load, in this case \(-K'x + f'\), and is thus easily determined in \( O(n^2) \) calculations based on the already-calculated solution to \( Kx = f \).

Differentiating again yields

\[ Kx'' = -K''x - 2K'x' + f'' \] (3.2)

and we can find \( x'' \) with an additional \( O(n^2) \) calculation. The process can be repeated \( m \) times to yield

\[ Kx^{(m)} = -\sum_{r=1}^{m} \frac{m!}{r!(m-r)!} K^{(r)}x^{(m-r)} + f^{(m)} \] (3.3)
and \( x^{(m)} \) is available in \( O(n^2) \) as well. The Taylor polynomial for displacement is then

\[
x(e) = \sum_{i=0}^{\infty} \frac{x^{(i)}(e_0)}{i!} (e - e_0)^i
\]

(3.4)

where \( e_0 \) is the initial design value.

Although the series for \( x \) appears to be straightforward calculation, there are two difficulties in its implementation. First of all, the required high order derivatives of the stiffness matrix can present numerical problems. This is discussed in more detail in Chapter 4. A second difficulty is the potentially frequent recurrence of lack of convergence of the Taylor series. We illustrate this difficulty here with a simple example.

Consider the simple spring displaced by force \( f \) as shown in Figure 3.1. Assume, for the purpose of this example that we have the solution for \( K = 1, f = 1 \). We wish to expand this solution about \( K = 1 \) to determine the displacement, \( x \), for other values of the design variable \( K \). The governing equation is

\[
Kx = f
\]

(3.5)

Differentiating equation (3.5) with respect to \( K \) yields

\[
Kx' = -K'x,
\]

(3.6)

but, since \( K' = 1 \) and \( K'', K''', \ldots = 0 \), continuing to differentiate yields,

\[
\frac{d^m x}{dK^m} = -mx^{m-1}
\]

(3.7)

Assume our interest is in the range \( 1 \leq K \leq 6 \). Figure 3.2 presents the solution for \( x \) computed using Taylor series. Note that the Taylor series diverges at \( K = 2 \), an expected result of the singularity at \( K = 0 \).
Figure 3.1: One degree of freedom spring mass system
Figure 3.2: Prediction of displacement using Taylor series
The appropriate procedure to follow here would be to detect the divergence of the series, perhaps by comparing the \( m+1 \) terms with the \( m \) terms. When divergence becomes a problem, recompute the solution to equation (3.5) for a new initial \( K \) and re-do the approximation as in [24]. Assume the resolution must occur for \( K \leq 2 \). It is obvious then that the new expansion will again have convergence problems at \( K \leq 2 \) due to the singularity at \( K = 0 \). Thus the procedure will need to be repeated at least three times to find an approximated solution valid across the range \( 1 \leq K \leq 6 \).

It is this challenge, the recurrence of convergence problems, that leads us to Padé approximants.

**Padé Approximants**

Assume that

\[
G(x) = \sum_{n=0}^{\infty} a_n x^n
\]  

(3.8)

is analytic at \( x = 0 \) with \( a_0 \neq 0 \). (More generally, \( G \) may be regarded as a formal power series.) The Padé approximant \( R_{l,m} \) for \( G \) is a rational function \( P/Q_m \) with degree \( P \leq l \), degree \( Q \leq m \), and

\[
\frac{P}{Q} - G = O(x^k)
\]  

(3.9)

as \( x \to 0 \) with \( k \) maximal. Clearly for \( m=0 \), \( P/Q \) is the Taylor polynomial of degree \( l \). In any case, the rational function \( P/Q \) is uniquely determined, and if we normalize by requiring that \( P \) and \( Q \) have no common first degree factors and \( Q(0) = 1 \), then \( P \) and \( Q \) are also uniquely determined.
Example 1

Let \( G(x) = e^x \) and expand this using Taylor series, then

\[
G(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \cdots \quad (3.10)
\]

\[
R_{0,0} = \frac{p_0}{q_0}, \text{ where } Q_0 = Q(0) = 1. \quad \text{From equation (3.11), } R_{0,0} = 1. \quad \text{So, } P_0 = 1.
\]

Thus \( p_0 = q_0 = 1 \).

\[
R_{0,1} = \frac{p_0}{q_1}, \text{ where } Q_1 = 1 + q_1 x. \quad \text{Expanding this equation}
\]

\[
R_{0,1} = \frac{p_0}{1 - (-q_1 x)} = p_0(1 - q_1 x + - \cdots)
\]

So, \( p_0 = 1, q_1 = -1 \).

\[
R_{1,1} = \frac{P_1}{Q_1}, \text{ where } P_1 = p_0 + p_1 x \text{ and } Q_1 = 1 + q_1 x. \quad \text{Expanding this equation}
\]

\[
R_{1,1} = \frac{P_0 + P_1 x}{1 - (-q_1 x)} = \frac{(p_0 + p_1 x)(1 - q_1 x + q_1^2 x^2 - + \cdots)}{\text{ }}
\]

\[
= p_0 + (p_1 - p_0 q_1)x + (p_0 q_1^2 - p_1 q_1)x^2
\]

So, \( p_0 = 1, p_1 = 1/2 \) and \( q_1 = -1/2 \).

An equivalent characterization of the Padé approximant \( P/Q \) is that \( Q \neq 0, \) degree \( P \leq l, \) degree \( Q \leq m, \) and

\[
P - QG = O(x^{l+m+1}) \quad (3.12)
\]

as \( x \to 0. \) Again, suitable polynomials \( P \) and \( Q \) always exist, and the quotient \( R_{l,m} \) is the same uniquely determined rational function. Here, however, we may not require
Q(0) = 1, since all solutions to equation (3.12) may have Q(0) = 0.

Example 2

Let \( G(x) = \cos x \) and expand this equation

\[
\cos x = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n)!} \quad (3.13)
\]

\[
= 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - + \cdots \quad (3.14)
\]

\( R_{1,1} = P_1/Q_1 \), where \( P_1 = p_0 + p_1 x \) and \( Q_1 = q_0 + q_1 x \). Substituting these into equation (3.12) yields

\[
p_0 + p_1 x - (q_0 + q_1 x)(1 - \frac{x^2}{2!} + - \cdots) = O(x^3)
\]

\[
p_0 + q_0 + (p_1 - q_1)x - \frac{q_0}{2!} x^2 + - \cdots = O(x^3)
\]

So, \( Q(0) = q_0 = 0 \), \( p_0 = 0 \) and \( p_1 = q_1 \). Therefore, \( R_{1,1} = 1 \) and equation (3.12) is satisfied with \( P(x) = Q(x) = cx \), where \( c \) is any constant.

There is a standard formula giving the polynomials \( P \) and \( Q \) exclusively in terms of the coefficients of \( G \) and powers of \( x \). It is not completely general, since it assumes that equation (3.12) has a solution with \( Q(0) = 1 \), and that the linear system which arises in the calculation which follows is nonsingular. Set \( P = \sum_{i=0}^{l} p_i x^i \) and \( Q = 1 + \sum_{j=1}^{m} q_j x^j \). The coefficient of \( x^i \) in equation (3.12) is

\[
p_i - \sum_{j=0}^{m} q_j a_{i-j} = 0 \quad (3.15)
\]

for \( i = 0, 1, \ldots, l + m \), where \( a_r = 0 \) for \( r < 0 \). For \( i = 0, 1, \ldots, l \),

\[
p_i = \sum_{j=0}^{l} q_j a_{i-j} \quad (3.16)
\]
So, the \( p_i \) can be found once the \( q_j \) are found. For \( i = l + 1, l + 2, \ldots, l + m \)

\[
\sum_{j=0}^{m} q_j a_{i-j} = 0 \tag{3.17}
\]

i.e. \( q_1 a_{i-1} + q_2 a_{i-2} + \cdots + q_m a_{i-m} = -a_i \), and we have \( m \) equations in \( m \) unknowns.

\[
\begin{bmatrix}
    a_l & a_{l-1} & \ldots & a_{l-m+1} \\
    a_{l+1} & a_l & \ldots & a_{l-m} \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{l+m-1} & a_{l+m-2} & \ldots & a_l
\end{bmatrix}
\begin{bmatrix}
    q_1 \\
    q_2 \\
    \vdots \\
    q_m
\end{bmatrix}
= \begin{bmatrix}
    -a_{l+1} \\
    -a_{l+2} \\
    \vdots \\
    -a_{l+m}
\end{bmatrix} \tag{3.18}
\]

Assuming

\[
\Delta_{l,m} = \begin{vmatrix}
    a_l & a_{l-1} & \ldots & a_{l-m+1} \\
    a_{l+1} & a_l & \ldots & a_{l-m} \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{l+m-1} & a_{l+m-2} & \ldots & a_l
\end{vmatrix} \neq 0 \tag{3.19}
\]

Then, unique solution for \( q_1, q_2, \ldots, q_m \) is given by Cramer's rule:

\[
q_j = \frac{1}{\Delta_{l,m}} \begin{vmatrix}
    a_l & a_{l-1} & \ldots & -a_{l+1} & \ldots & a_{l-m+1} \\
    a_{l+1} & a_l & \ldots & -a_{l+2} & \ldots & a_{l-m+2} \\
    \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
    a_{l+m-1} & a_{l+m-2} & \ldots & -a_{l+m} & \ldots & a_l
\end{vmatrix} \tag{3.20}
\]

\[
= \frac{1}{\Delta_{l,m}} \begin{vmatrix}
    0 & 0 & \ldots & 0 & \overset{(j+1)th \ column}{1} & \ldots & 0 \\
    a_{l+1} & a_l & \ldots & a_{l-j+2} & a_{l-j+1} & \ldots & a_{l-m+1} \\
    a_{l+2} & a_{l+1} & \ldots & a_{l-j+3} & a_{l-j+2} & \ldots & a_{l-m+2} \\
    a_{l+m} & a_{l+m-1} & \ldots & a_{l+m-j} & a_{l+m-j} & \ldots & a_l
\end{vmatrix} \tag{3.21}
\]
The numerator in equation (3.21) is an \((m + 1) \times (m + 1)\) determinant. Using these \(q'\)'s, we can write \(Q\) as a determinant.

\[
Q = \sum_{j=0}^{m} q_j x^j
\]

\[
= \begin{vmatrix}
1 & x & \ldots & x^m \\
a_{l+1} & a_l & \ldots & a_{l-m+1} \\
\vdots & \vdots & \ddots & \vdots \\
a_{l+m} & a_{l+m-1} & \ldots & a_l
\end{vmatrix} / \Delta_{l,m} \tag{3.23}
\]

\(p_i\) also can be written in a determinant form from equation (3.16)

\[
p_i = \begin{vmatrix}
a_i & a_{i-1} & \ldots & a_{i-m} \\
a_{l+1} & a_l & \ldots & a_{l-m+1} \\
\vdots & \vdots & \ddots & \vdots \\
a_{l+m} & a_{l+m-1} & \ldots & a_l
\end{vmatrix} / \Delta_{l,m} \tag{3.24}
\]

So,

\[
P = \sum_{i=0}^{l} p_i x^i
\]

\[
= \frac{1}{\Delta_{l,m}} \sum_{i=0}^{l} \begin{vmatrix}
a_i x^i & x(a_{i-1}x^{i-1}) & \ldots & x^m(a_{i-m}x^{l-m}) \\
a_{l+1} & a_l & \ldots & a_{l-m+1} \\
\vdots & \vdots & \ddots & \vdots \\
a_{l+m} & a_{l+m-1} & \ldots & a_l
\end{vmatrix} \tag{3.26}
\]

\[
= \frac{1}{\Delta_{l,m}} \begin{vmatrix}
G_l & xG_{l-1} & \ldots & x^mG_{l-m} \\
a_{l+1} & a_l & \ldots & a_{l-m+1} \\
\vdots & \vdots & \ddots & \vdots \\
a_{l+m} & a_{l+m-1} & \ldots & a_l
\end{vmatrix} \tag{3.27}
\]
For a standard normalization of $P, Q$, take $q_0 = \Delta_{l,m}$. Then

$$Q = \begin{bmatrix} 1 & x & \ldots & x^m \\ a_{l+1} & a_l & \ldots & a_{l-m+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{l+m} & a_{l+m-1} & \ldots & a_l \end{bmatrix}$$

(3.28)

and

$$P = \begin{bmatrix} G_l & xG_{l-1} & \ldots & x^m G_{l-m} \\ a_{l+1} & a_l & \ldots & a_{l-m+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{l+m} & a_{l+m-1} & \ldots & a_l \end{bmatrix}$$

(3.29)

Calculating Padé approximants can be done from recurrence relations [26]. We assume the $a_i$'s are given. There are then two different calculation problems. One is calculating coefficients of $P$ and $Q$, the other is calculating $R_{l,m}(x)$, for given $x$, directly using recurrence relations.

Whitesell [25] introduced a numerical procedure for determining $R_{l,m}(x)$, $x \neq 0$ and $l \geq m$, from the values of the Taylor polynomials $G_k(x) = \sum_{i=0}^{k} a_i x^i$, $k = l - m, l - m + 1, \ldots, l + m$. In fact, the methods is equally applicable when $m > l$, if we interpret $G_k(x)$ as 0 for $k < 0$. The procedure solves the equations

$$\begin{bmatrix} G_{l-m}(x) & G_{l-m+1}(x) & \ldots & G_l(x) \\ G_{l-m+1}(x) & G_{l-m+2}(x) & \ldots & G_{l+1}(x) \\ \vdots & \vdots & \ddots & \vdots \\ G_l(x) & G_{l+1}(x) & \ldots & G_{l+m}(x) \end{bmatrix} \begin{bmatrix} \eta_m \\ \eta_{m-1} \\ \vdots \\ \eta_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

(3.30)
and then sets $R_{l,m}(x) = (\eta_0 + \eta_1 + \cdots + \eta_m)^{-1}$. $R_{l,m}(x) = \infty$ if $\eta_0 + \eta_1 + \cdots + \eta_m = 0$.

Singular systems are handled by perturbing zero pivots. If we ignore exceptional cases, this result can be derived easily from equation (3.12). By using all terms of equation (3.12) with exponent less than or equal to $l + r$, we get

$$
\sum_{j=0}^{m} G_{l+r-j}(x)(q_j x^j) = P(x)
$$

for $r = 0, 1, 2, \ldots, m$. At least if $P(x) \neq 0$,

$$
\sum_{j=0}^{m} G_{l+r-j}(x) \left( \frac{q_j x^j}{P(x)} \right) = 1
$$

Solve

$$
\sum_{j=0}^{m} G_{l+r-j}(x) \eta_j = 1
$$

where $\eta_j = q_j x^j / P(x)$. Add $\eta_j$ for $j = 0, 1, \ldots, m$

$$
\sum_{j=0}^{m} \eta_j = \frac{1}{P(x)} (q_0 + q_1 x + q_2 x^2 + \cdots + q_m x^m)
$$

$$
= \frac{Q(x)}{P(x)}
$$

$$
= \frac{1}{R_{l,m}(x)}
$$

then

$$
R_{l,m}(x) = \frac{1}{\eta_0 + \eta_1 + \cdots + \eta_m}
$$

This method is easily implemented in an algorithm and is efficient for the calculation of Padé approximants if $m$ is not large.
Application of Padé Approximants

Now consider again our example from equation (3.5). Substituting Taylor polynomials from equation (3.4) with the Taylor series coefficients from equation (3.7) into equation (3.30), we can calculate Padé approximants $R_{l,m}(K)$, of $x$ as a function of the design variable $K$. Obviously the solution of equation (3.30) is $O((l + m)^3)$, but $l + m$ is small and the calculation is not computationally burdensome.

Figure 3.3 presents the solution for $x$ computed using Taylor series and Padé approximants. Note that the Padé approximants give good results across the entire range of interest, where 11 terms of the Taylor series ($x, x', x'', ..., x^{(10)}$) are used to calculate the Padé approximant, $R_{5,5}$.

This simple example illustrates the power of the Padé approximants to converge to the desired solution over a very wide range of the design variable. The next chapter continues this line of discussion in a finite element context.
Figure 3.3: Prediction of displacement
CHAPTER 4. APPLICATION OF PADÉ APPROXIMANTS IN A
FINITE ELEMENT CONTEXT

Approximate Method for High Derivatives

The use of high order terms in either Taylor series or a Padé approximation requires high order derivatives of the stiffness matrix, $K$.

If the stiffness matrix is simply related to the design variable $e$, it will be straightforward to calculate $K^{(m)}$ analytically. However, complicated relationships between $K$ and $e$, which will be typical of any but the most simple changes, do not lead to analytical solutions for $K^{(m)}$. Finite difference calculations, which are increasingly subject to error as $m$ gets large, should be expected to be of little use for large $m$.

This chapter presents an approximate method for the calculation of $K^{(m)}$. The method, presented by Bernard, Kwon and Wilson [27], requires only the ability to compute $K$, $K'$ and $K''$ at the initial configuration, which we refer to here as $e_0$, and evaluation of $K$ at an $e$ value at the far range of our interest, which we refer to here as $e_f$.

Assume each element $k_{ij}$ of $K$ may be written as a cubic polynomial

$$ k_{ij} = \sum_{p=0}^{3} a_{ijp} (e - e_0)^p $$

(4.1)

The values of the $a_{ij}$ are chosen so that $k_{ij}$, $k'_{ij}$ and $k''_{ij}$ matches the required values at
\( e_0 \) and \( k_{ij} \) match the required value at \( e_i \). Differentiating equation (4.1) and matching coefficients yields

\[
\begin{align*}
  a_{ij0} &= k_{ij}(e_0) \\
  a_{ij1} &= k'_{ij}(e_0) \\
  a_{ij2} &= k''_{ij}(e_0) \\
  a_{ij3} &= \frac{1}{L^3}(k_{ij}(e_i) - a_{ij0} - a_{ij1}L - a_{ij2}L^2)
\end{align*}
\]  

where \( L = e_i - e_0 \).

It is important to note that we are not restricting ourselves to \( k_{ij} \) which are cubic polynomials in the design change \( e \). Rather, we are replacing the \( k \) matrix with an alternate formulation. To the extent that the cubic of equation (4.1) closely fits the \( k_{ij} \) values which would have been computed by the finite element preprocessor in the range \( e_0 \) to \( e_i \), the alternate formulation will be the basis for a good approximation to the finite element calculations. This is illustrated in the next section through an example.

**Example**

Figure 4.1 presents a plate with fixed boundaries which has been modeled with twenty-four plate finite elements using MSC/NASTRAN finite element preprocessor. The plate elements each have four nodes and each node has three degrees of freedom.

For this example, the thickness of the hatched elements in Figure 4.1 is the design variable. The solution we focus on here is the deflection \( \delta \) of the plate directly under the force \( f \) which is applied at the center of the plate. The initial plate thickness is
Figure 4.1: Plate with fixed boundaries
0.1 in, and our interest is in the range \(0.1 \leq t \leq 0.6\) in.

Our goal is to expand the solution for \(\delta\) in a Padé approximation based on the plate thickness \(t\) in the hatched area. The formulation for the Padé approximants \(R_{l,m}\), given in the Chapter 3, requires the calculation of the first \(l+m\) derivatives of \(K\).

To facilitate calculation of these derivatives, we first fit each term of the \(K\) matrix as explained in equations (4.1) through (4.5) over the range \(t = 0.1\) in to \(t = 0.6\) in. This requires an additional run of the preprocessor at \(t = 0.6\), and calculation, either analytically or through finite differences, of \(K'\) and \(K''\) at \(t = 0.1\).

Figure 4.2 presents the results of this exercise for one element of the \(K\) matrix. The figure indicates that the fit is very good indeed. This is not surprising in view of our expectation that the affected terms in the stiffness matrix will vary with the cube of the plate thickness.

Since the stiffness elements are now assumed to be cubic polynomials, there are only three nonzero derivatives of \(K\). Thus equation (3.3) can be rewritten as:

\[
Kx^{(m)} = -\sum_{r=1}^{3} \frac{m!}{r!(m-r)!} \cdot K^{(r)}x^{(m-r)} + f^{(m)}
\]  

(4.6)

Based on \(m\) derivatives of \(x\) as calculated in equation (4.6), we can now compute \(\delta\) as a function of \(t\). Figure 4.3 presents results. The figure indicates that a linear approximation is reasonably good to perhaps \(t = 0.125\), and the quadratic approximation is reasonably good to perhaps \(t = 0.18\). Note that the Taylor series diverges at \(t = 0.2\), an expected result of the singularity at \(t = 0\). A Padé approximation was computed for two \([l,m]\) values, where \(l = m\), to illustrate convergence. The Padé approximant \(R_{a,b}\) gives good results across the entire range of interest. Note that
Figure 4.2: Cubic approximation for stiffness
Figure 4.3: Prediction of displacement
both the 17-term Taylor series and the Padé approximant $R_{8,8}$ require 16 derivatives of the stiffness matrix.

This illustration of the procedure should be expected to lead to good results since we expect the elements of the $K$ matrix to be cubic functions of the plate thickness $t$. To illustrate for a less-likely but more difficult-to-fit candidate for a design variable, consider re-solving the problem with the variable $e = t^{1/2}$.

Figure 4.4 presents a fit of a term in $K$ by a cubic in the design variable $t^{1/2}$. The comparison is to the "correct" data, where the fit based on $K$ vs. $t$ as shown in Figure 4.2. Note the good match near $t = 0.1$, a consequence of agreement of first and second derivatives. This ensures a good approximation to the displacement near $t = 0.1$. Only the points match at $t = 0.6$ in the cubic fit to the stiffness matrix.

Figure 4.5 presents the solution for $\delta$ vs. $t$. The figure compares the correct solution, as indicated by the solid line taken from Figure 4.3, with the 17-term Taylor series and the Padé approximation $R_{8,8}$ solution based on $t^{1/2}$. Since the difference between the fit illustrated in Figure 4.4 and the preprocessor-generated values of $K$ are small, it is not surprising that the solution based on the design variable $t^{1/2}$ closely approximates the correct solution.
Figure 4.4: Cubic approximation for stiffness (In this case, the fit is a cubic in $\sqrt{t}$.)
Figure 4.5: Changing variable $t$ to $\sqrt{t}$ (displacement)
CHAPTER 5. OPTIMIZATION USING PADÉ APPROXIMANTS

We plan to use Padé approximants to facilitate the calculation of the objective function for purposes of design optimization. Since the optimization problem typically involves several design variables and the Padé approximants as presented here deal in one design variable, we will first use linear sensitivity-based optimization to find the direction of search followed by nonlinear sensitivity-based optimization along the indicated direction. This follows a methodology presented by Rizai and Bernard [24].

This method can be explained in two steps. First, we compute the optimization based on linear sensitivity. In particular, the objective function is based on a linear approximation of the displacements and stresses of interest in terms of the design variables. The solution of this linear sensitivity-based optimization problem indicates the direction of search for nonlinear sensitivity-based optimization. For the second step, the ratios of the design variables with respect to each other are kept constant and a new design variable, \( \bar{\varepsilon} \), scales the magnitude of the variables is determined.

\[
\begin{align*}
\mathbf{p} &= \mathbf{e}^* - \mathbf{e}^0 \\
\mathbf{e} &= \mathbf{e}^0 + \bar{\varepsilon} \mathbf{p}
\end{align*}
\]  

where \( \mathbf{p} \) is \( r \)-vector of the direction of search,  

\( \mathbf{e}^* \) is \( r \)-vector of the optimum design variables from linear sensitivity-based
optimization,
e\(0\) is \(r\)-vector of the initial design variables,
e is \(r\)-vector of the design variables from Padé approximants.
\(\tilde{e}\) is the stepsize.

The optimal solution is \(e^{**}\)

\[
e^{**} = e^0 + \tilde{e}^* p
\]  

(5.3)

where \(e^{**}\) is \(r\)-vector of the optimum design variables from Padé approximants,
\(\tilde{e}^*\) is the optimal stepsize.

Note if \(\tilde{e}^* = 1\), the optimum design variables, \(e^{**}\), agree with the linear sensitivity-based solution.

To verify that the nonlinear line search has converged to a local optimum, it is necessary to rerun the finite element analysis at \(e^{**}\). If local linearization verifies the optimum, \(e^{**}\) is the optimal design, otherwise the search is re-done in the new direction indicated by linear sensitivity-based optimization at \(e^{**}\). The remainder of this chapter present details and an example to illustrate the method.

Linear Approximation and Optimization

Linear Approximation

The approximations of the displacement and stress are based on a linear expansion. The approximation for displacement is

\[
x = x_0 + \sum_{i=1}^{r} \frac{\partial x}{\partial e_i} e_i
\]  

(5.4)
where \( x \) and \( x_0 \) are the modified and original displacement vectors respectively, and
\[
\frac{\partial x}{\partial e_i}
\]
is the rate of change of displacement vector with respect to the \( i \)th design variable. The derivative of displacement vector can be calculated under the assumption that applied load, \( f \), is dependent of the design variables.

\[
K \frac{\partial x}{\partial e_i} = -\frac{\partial K}{\partial e_i} x + \frac{\partial f}{\partial e_i}
\]

The computation of stress approximation is straightforward once the displacement approximation is done. The element stresses and the displacement are simply related in finite element analysis.

\[
\sigma = Bx
\]

where \( \sigma \) is the element stress vector, \( B \) is the stress-displacement matrix and \( x \) is the nodal displacement vector. For the linear approximation, the derivative of stress vector can be computed by

\[
\frac{\partial \sigma}{\partial e_i} = B \frac{\partial x}{\partial e_i} + \frac{\partial B}{\partial e_i} x
\]

For the nonlinear approximation, we compute the stress directly from equation (5.6) by reformulating \( B \) for any \( x \) value of interest.

**Optimization**

To compute the linear sensitivity-based optimization, First Order Structure Design and Optimization developed by Somayajula and Mikaili [28, 29] is used. This software is based on the cost function, presented by Starkey and Bernard [11] and Somayajula and Bernard [12] to determine the optimum design changes. This method uses constraint function technique. The constraint functions are smooth curves or
surfaces which assign a cost to design changes. The penalties become larger as the
design produces less desirable structural behavior or when it becomes heavier. Using
these constraint functions, the individual performance requirements are transformed
into a number of objective functions. The objective function for the scalar optimi­
mization problem, which is called cost function, is the sum of the weighted objective
functions. The global cost function $C(x, s, e)$ for displacement, stress and change of
design variables is expressed as:

$$C(x, s, e) = P \sum_{i=0}^{p} X_i(x_i) + Q \sum_{j=0}^{q} S_j(s_j) + R \sum_{k=0}^{r} E_k(e_k)$$  \hspace{1cm} (5.8)$$

where $x$ is a $p$-vector of desired nodal displacements,

$s$ is a $q$-vector of desired element stresses,

$e$ is a $r$-vector of design variables,

$X_i$ is the displacement constraint function,

$S_j$ is the stress constraint function,

$E_k$ is the change of design variable constraint function,

$P, Q$ and $R$ are scalar weighting factors.

We choose simple penalty functions:

$$X_i(x_i) = \begin{cases} 
0 & \text{for } x_i \leq \bar{x}_i \\
\left( \frac{x_i - \bar{x}_i}{\bar{x}_i} \right)^2 & \text{for } x_i > \bar{x}_i 
\end{cases}$$  \hspace{1cm} (5.9)$$

where $\bar{x}_i$ is a nominal limit on the displacement value.

$$S_j(s_j) = \begin{cases} 
0 & \text{for } s_j \leq \bar{s}_j \\
\left( \frac{s_j - \bar{s}_j}{\bar{s}_j} \right)^2 & \text{for } s_j > \bar{s}_j 
\end{cases}$$  \hspace{1cm} (5.10)$$
where $\bar{s}_j$ is a nominal limit on the stress value.

\[
E_k(\varepsilon_k) = \begin{cases} 
\frac{\left(\varepsilon_k - \varepsilon_k^l\right)^2}{\varepsilon_k^u - \varepsilon_k^l} & \text{for } \varepsilon_k \geq \varepsilon_k^0 \\
\frac{\left(\varepsilon_k^0 - \varepsilon_k\right)^2}{\varepsilon_k^u - \varepsilon_k^0} & \text{for } \varepsilon_k < \varepsilon_k^0
\end{cases}
\]  

(5.11)

where $\varepsilon_k^l$ and $\varepsilon_k^u$ are nominal limit of lower and upper design variables respectively, and $\varepsilon_k^0$ is the initial value of the design variable.

The functions $X_i(x_i)$ and $S_j(s_j)$ become large when the displacements and stresses violate prescribed conditions. $E_k(\varepsilon_k)$ increases as the design change gets larger. The coefficients $P, Q$ and $R$ are positive scalars which weight the relative importance of the displacement, stress, and change of design variables respectively. The choice for these coefficients determines the relative importance of each constituent of the objective function.

The problem statement of the minimization of the global cost function is expressed as:

\[
\begin{align*}
\text{Minimize} & : C(x, s, e) \\
\text{Subject to} & : e_k^l < \varepsilon_k < e_k^u \quad k = 1, 2, \cdots, r
\end{align*}
\]

(5.12, 5.13)

where $e_k$ is the design variables and $e_k^l$ and $e_k^u$ are lower and upper limit of the design variables respectively. The solution to this problem provides an improvement in the design with reference to the designer's choice of the importance of the constraints. In particular, the designer chooses the global cost function by interactively choosing weighting constants $P, Q$ and $R$ in equation (5.8). Thus the process facilitates the selection of the global cost function, $C$, whose minimum yields, in the designer's judgement, an optimal design.
Padé Approximants and Optimization

If design variables have a linear relationship with the displacements and stresses of the structure, the linear approximation will provide the correct solution. However, since the displacements and stresses are, in fact, nonlinear functions of the design variables, the linear sensitivity-based results have a limited range of validity. The use of Padé approximants can lead to accuracy over a much wider range of changes.

Padé approximants

The stiffness matrix and displacement vector can be expressed as a function of a single design variable, \( \bar{\epsilon} \), which was introduced in equation (5.2). The change along the path is scaled by \( \bar{\epsilon} \), with \( \bar{\epsilon} = 1 \) indicating the solution of the linear sensitivity-based optimization.

Following the analysis presented in Chapter 4, we assume the stiffness elements are cubic polynomials, thus equation (4.6) can be written as:

\[
\mathbf{K}(\bar{\epsilon})\mathbf{x}^{(m)}(\bar{\epsilon}) = -\sum_{r=1}^{3} \frac{m!}{r!(m-r)!} \mathbf{K}^{(r)}(\bar{\epsilon})\mathbf{x}^{(m-r)}(\bar{\epsilon}) + \mathbf{f}^{(m)}(\bar{\epsilon}) \tag{5.14}
\]

where \( (\cdot)^{(m)} \) means \( \frac{d^m(\cdot)}{d\bar{\epsilon}^m} \). So, we can expand the displacement of interest using Padé approximants as a function of \( \bar{\epsilon} \), \( R_{i,m}(\bar{\epsilon}) \). The stress approximation is directly calculated from equation (5.6) with the approximated displacement vector of interest.

Optimization

To decide the optimum stepsize, \( \bar{\epsilon}^* \), IMSL math library subroutine NCONF [30] is used. This subroutine solves a general nonlinear programming problem using the successive quadratic programming algorithm and a finite difference gradient. The
problem is stated as follows:

\[
\text{Minimize} \quad \hat{C}(\tilde{e}) \quad (5.15)
\]

\[
\text{Subject to} \quad \hat{X}_i(x_i) \geq 0, \quad \text{for} \quad i = 1, \ldots, p \quad (5.16)
\]

\[
\hat{S}_j(s_j) \geq 0, \quad \text{for} \quad j = 1, \ldots, q \quad (5.17)
\]

\[
\tilde{e}' \leq \tilde{e} \leq \tilde{e}^{u} \quad (5.18)
\]

choosing functions:

\[
\hat{X}_i(x_i) = \bar{x}_i - x_i \quad (5.19)
\]

\[
\hat{S}_j(s_j) = \bar{s}_j - s_j \quad (5.20)
\]

where \(x_i\) and \(s_j\) are function of \(\tilde{e}\).

Example

This section presents example which illustrates optimization procedure using linear sensitivity-based optimization followed by a line search using Padé approximants. The example concerns a plastic bumper endcap which is to be redesigned for displacement and stress. The load case of interest is a 120 mph wind load (2 trucks passing while travelling 60 mph in opposite directions) plus the weight of bumper endcap.

Figure 5.1 presents the finite element model of the initial design of the bumper. The model, which was set up using MSC/NASTRAN finite element preprocessor, has 741 elements and 793 nodes. The plate elements each have four nodes and each node has six degrees of freedom.
Figure 5.1: Finite element model of the bumper endcap
MSC/NASTRAN was used to obtain the finite element analysis for displacements and stresses. The finite element analysis indicated that the largest displacement of the original design is 0.3335 in, and the largest stress is 725.23 psi. The location of the largest displacement is given by N1112 and the location of the largest stress is given by E2041y in Figure 5.1. The bumper is divided into five sections (Figure 5.2).

The goal of this example is to redesign the bumper to have the Translation-Z component of displacement vector of N1112 is less than or equal to 0.25 in and Normal-Y component of stress of E2041y is less than or equal to 500 psi by changing the thicknesses of T1 and T2. We refer to these design variables as e1 and e2. Table 5.1 lists the thickness of five sections. Table 5.2 lists the structural characteristics of the original design.

An optimal design for this example is sought according the following procedure.

1. Calculate the optimal design variables, e*, from linear sensitivity-based optimization.

2. Calculate the direction of search, p.

3. Compute mth order displacement derivatives and set up Padé approximants.

4. Calculate the optimum stepsize, ê*.

5. Extract the optimum design variables using the optimum stepsize, e**

6. Verify the results by solving finite element problem for the modified model with the proposed design change, e**.

7. Restart the procedure and repeat the linear sensitivity-based optimization.
Figure 5.2: Five sections of the bumper endcap
Table 5.1: Thickness of bumper

<table>
<thead>
<tr>
<th>Section</th>
<th>Thickness (in)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_1$</td>
<td>0.250</td>
</tr>
<tr>
<td>$T_2$</td>
<td>0.250</td>
</tr>
<tr>
<td>$T_3$</td>
<td>0.250</td>
</tr>
<tr>
<td>$T_4$</td>
<td>0.237</td>
</tr>
<tr>
<td>$T_5$</td>
<td>0.213</td>
</tr>
</tbody>
</table>

Table 5.2: Structural characteristics of the initial design

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e^0_1$</td>
<td>0.2500 in</td>
</tr>
<tr>
<td>$e^0_2$</td>
<td>0.2500 in</td>
</tr>
<tr>
<td>$N_{111z}$</td>
<td>0.3335 in</td>
</tr>
<tr>
<td>$E_{2041y}$</td>
<td>725.23 psi</td>
</tr>
</tbody>
</table>
8. If the linear sensitivity-based optimization indicates $e^{**}$ is not optimum, return to step 1.

Table 5.3 presents the results of linear sensitivity-based optimization. Although linear sensitivity-based optimization results satisfy the goal of this example, we are not sure yet if they are correct or not since the change of the design variables is large.

The next step is to use Padé approximants to improve the results of the linear sensitivity-based optimization. This requires higher order derivatives of the stiffness matrix.

Noting that $\bar{e} = 1$ indicates linear sensitivity-based solution and that we as yet do not know the nonlinear sensitivity-based solution, we choose a wide range of $\bar{e}$ for the the cubic approximation to the stiffness matrix.

For this example, the range of the cubic approximations for the stiffness matrix is $0 \leq \bar{e} \leq 2.0$.

Table 5.3 indicates that the direction of search, $p$ is

\[ p_1 = 0.1394 \quad (5.21) \]
\[ p_2 = 0.0228 \quad (5.22) \]

Table 5.4 shows the results of the optimization using Padé approximants. Note that the linear sensitivity-based solution is not close to the nonlinear sensitivity-based solution. In particular, $\bar{e}^* = 1.9963$ indicates that the nonlinear sensitivity-based design changes are 1.9963 times larger than the linear sensitivity-based design changes.

Figure 5.3 and Figure 5.4 present the Padé approximants $R_{a,b}(\bar{e})$ for $N111z$ and $E2041y$. (The finite element solutions, indicated by the boxes, were computed after
### Table 5.3: Linear sensitivity-based optimization
(1st iteration)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_1^*$</td>
<td>0.3894 in</td>
</tr>
<tr>
<td>$e_2^*$</td>
<td>0.2728 in</td>
</tr>
<tr>
<td>$N111Z$</td>
<td>0.2499 in</td>
</tr>
<tr>
<td>$E2041Y$</td>
<td>420.80 psi</td>
</tr>
</tbody>
</table>

### Table 5.4: Nonlinear sensitivity-based optimization

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Padé</th>
<th>FEA @ $e^{**}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e^*$</td>
<td>1.9963</td>
<td></td>
</tr>
<tr>
<td>$e_1^{**}$</td>
<td>0.5283 in</td>
<td></td>
</tr>
<tr>
<td>$e_2^{**}$</td>
<td>0.2955 in</td>
<td></td>
</tr>
<tr>
<td>$N111Z$</td>
<td>0.2500 in</td>
<td>0.2500 in</td>
</tr>
<tr>
<td>$E2041Y$</td>
<td>363.54 psi</td>
<td>363.50 psi</td>
</tr>
</tbody>
</table>
Figure 5.3: Padé approximants of $N_{111_2}$
Figure 5.4: Padé approximants of $E_{2041_Y}$
the fact, and in themselves have no use in the solution procedure.)

At this stage, it is necessary to rerun the finite element analysis at $e^{**}$. Table 5.4 indicates that these results are essentially identical to the Padé approximation.

The next step is to verify that the line search retained the appropriate direction, i.e., to restart the linear sensitivity-based optimization to determine if $e^{**}$ indicates a local minimum. The result of the linear sensitivity-based optimization, presented in Table 5.5, indicate that $e^{**}$ is a minimum.
Table 5.5: Structural characteristics of the linear sensitivity-based optimization (2nd iteration)

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_1$</td>
<td>0.5283 in</td>
</tr>
<tr>
<td>$e_2$</td>
<td>0.2955 in</td>
</tr>
<tr>
<td>$N_{111y}$</td>
<td>0.2500 in</td>
</tr>
<tr>
<td>$E_{2041y}$</td>
<td>363.50 psi</td>
</tr>
</tbody>
</table>
Discussion

There are two related important issues which bear brief discussion. These are the convergence of the Padé approximation and a comparison of CPU time required for finite element analysis and time required for the various approximations.

Convergence

Figure 5.3 illustrates excellent convergence, yet Figure 4.3 showed less impressive convergence for lower order approximants. The work in this thesis was done using $R_{8,8}$ which provided very satisfactory results for the problems herein. For the bumper endcap, $R_{8,8}$ required numbers as large as $D+12$ to compute $x^{(16)}$. Since these calculations were done on a VAX 11/785 which can handle up to $D+32$, it seems clear that several terms could be added without overflow problems. To test this hypothesis, $x^{(22)}$ was calculated. That value required $D+22$.

Benchmarking the methodology

The goal of this thesis is to provide an approximation to finite element solutions which is valid for large design changes. Implicit in the method is the idea that the approximation is much less computationally burdensome than re-doing several finite element solutions.

This section presents CPU time for the bumper endcap example. Although the example does not give a definitive picture, it does give a reasonable basis for comparison. All calculations were performed using a VAX 11/785 with 16 megabytes of memory. The MSC/NASTRAN solution for the statics finite element problem (4734 degrees of freedom) took about 24 CPU minutes. The linear sensitivity analysis
for the linear sensitivity-based optimization took about 2 CPU minutes.

Nonlinear sensitivity-based analysis starts with creating a cubic fit to the stiffness matrix. The preprocessor needs to be run three times to supply $k_{ij}$ values for the cubic fit (two at near initial design value, one at far end of interest). Each preprocessor run took about 6 CPU minutes. Not counting time for the LU decomposition of the stiffness matrix, the calculation of the coefficients for Taylor series ($x, ..., x^{(16)}$) took about 10 CPU minutes. (Our inability to transfer the original LU decomposition out of MSC/NASTRAN led to the need for one additional LU run. This is a software problem unrelated to the methodology of this thesis.) The CPU time for the calculation of the optimum stepsize, $\bar{\varepsilon}^*$, was 43 seconds. These results are summarized in Table 5.6.

In summary, the linear sensitivity-based optimization and nonlinear line search using Padé approximants took about 31 CPU minutes compared to about 24 CPU minutes for a finite element solution.
Table 5.6: Comparison of CPU time

<table>
<thead>
<tr>
<th>Description</th>
<th>CPU Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>statics problem</td>
<td>24 CPU min.</td>
</tr>
<tr>
<td>linear sensitivity</td>
<td>2 CPU min.</td>
</tr>
<tr>
<td>preprocessing of K</td>
<td>18 CPU min.</td>
</tr>
<tr>
<td>derivatives of $x$</td>
<td>10 CPU min.</td>
</tr>
<tr>
<td>optimum stepsize</td>
<td>43 CPU sec.</td>
</tr>
</tbody>
</table>
CHAPTER 6. CONCLUSIONS

This thesis has illustrated the use of Padé approximants to expand the solution of finite element-based equilibrium problems. The use of the procedure for multiple design variables demands a linear expansion followed by a line search in the direction indicated by the linear solution. Examples showed that the procedure provided excellent results for very large changes in the design variables.

Finite element preprocessing, which is necessary to compute the derivatives of the stiffness matrix, is currently a time-consuming part of this optimization process. Future work should improve this procedure by recomputing only those elements of the stiffness matrix which are altered by changing design variables. Additional work is needed to apply these methods in a dynamic context.
BIBLIOGRAPHY


