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A Geometric Interpretation of Optimal Iteration Strategies*

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The relationship between inner and outer iteration errors is extremely complex and even formal description of total error behavior is difficult. Inner and outer iteration error propagation is analyzed in a variational formalism for a reactor model describing multidimensional, one group theory. Generalizing the work of Akimov and Sabek,[1] the number of inner iterations performed during each outer serial that minimizes the total computation time is determined.[2] The generalized analysis admits a geometric interpretation of total error behavior. The results can be applied to both transport and diffusion theory computer methods.

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The optimization procedure is defined for a class of problems given by the binary iterative form:

$$Q_{n,i}(\underline{r}) = \Gamma Q_{n-1,i}(\underline{r}) + S_i(Q_i(\underline{r})) \qquad (1)$$

where $Q_{n,i}$ is the dependent variable (fission source) at the n^{th} inner and i^{th} outer iteration, Γ the inner iteration operator, and S_i the source term for the i^{th} outer. The inner and outer iteration errors are respectively given by

$$e_i(\underline{r}) = Q_{n,i}(\underline{r}) - Q_{\infty,i}(\underline{r}) \qquad (2a)$$

$$E_i(\underline{r}) = Q_{\infty,i}(\underline{r}) - Q_{\infty,\infty}(\underline{r}) \qquad (2b)$$

$Q_{\infty,i}(\underline{r})$ is the infinite inner iterated vector <u>at the i^{th} outer</u> and $Q_{\infty,\infty}(\underline{r})$ is the exact result. Both Eqs. (2a,b) can be reformulated in terms of the eigenfunctions of the outer iteration operator. Using the square summable norm, the total error vector is represented in Euclidean 2-space as

$$\epsilon^N = \| E_N \| \hat{i} + \| e_N \| \hat{j} \qquad (3)$$

where $\hat{i}$ and $\hat{j}$ are basis vectors. For an accuracy requirement, ε_o, the calculation is terminated when

$$\| \epsilon^N \|_p = \left[\| E_N \|^p + \| e_N \|^p \right]^{1/p} \le \varepsilon_o \qquad (4)$$

where p is determined from the variational procedure.

The overall computational time is expressed in terms of the total number of iterations. If $\alpha_i (0 \leq \alpha_i \leq 1)$ is the inner iteration error reduction at the i^{th} outer, ρ_o the spectral radius of the inner iteration operator, and τ the time required to calculate the source term $S_i(r)$, the total time function is given by

$$T(\underline{\alpha}) = \sum_{i=1}^{N} \left(\tau + \frac{\ln\alpha_i}{\ln\rho_o}\right) . \tag{5}$$

The ratio of logarithms above is an approximation for the number of inner iterations at the i^{th} outer. The number of inner iterations each outer sweep is the primary variable which controls the total time function above.

The minimization problem is to determine the set $\left\{\alpha_j\right\}_{j=1}^{N}$ which minimize (5) subject to the constraint (4). The p-norm can be interpreted as a "slack function"[3] which insures the optimum value of α is an admissible extremum. The results of the variational analysis are

$$\alpha_1 = \alpha_2 = \alpha_3 = \ldots = \alpha_{N-1} \equiv \alpha_I \tag{6a}$$

$$\alpha_N = \left\{\alpha_I^{\hat{\delta}p-1}\right\}^{1/p} \tag{6b}$$

where $\hat{\delta} = \sigma/(1 - \sigma)$. σ is the dominance ratio of the outer operator. The value of α_I is given by a transcendental equation obtained by minimization of (5) with respect to α. The value of p is chosen from (6b) to insure $\alpha_N < 1$. In E_2, the optimal iteration history of the total error vector corresponds to a series of points outlining a straight line trajectory directed towards the origin. The path stops when it intersects the "target set" defined by (4). A nonoptimal trajectory in general is not a straight line path. See Fig. 1.

The overall effect of this analysis is to "accelerate" convergence of the iterative scheme using only the inherent spectral properties of the numerical system. Standard acceleration techniques naturally complement the optimal procedure by effectively reducing the spectral radius of the inner iteration operator, ρ_0, and, σ, the dominance ratio of the outer procedure.

The generalized variational analysis provides a meaningful interpretation of the total error vector behavior for optimal iteration procedures, and yields improved results from the basic development of Akimov and Sabek. Based on the geometric construct, a priori estimates of the trajectory slope provide simple, explicit expressions of α_I and T_{min}. By varying the guess ±25% of the correct value, good estimates of α_I (< 8%) and excellent predictions for T_{min} (< 0.1%) are obtained. These estimates can be used to compare projected computational times for different error specifications. Furthermore the optimum number of inner iterations performed each outer serial can be simply calculated from the optimum inner error reduction values (α_I, α_N).

References

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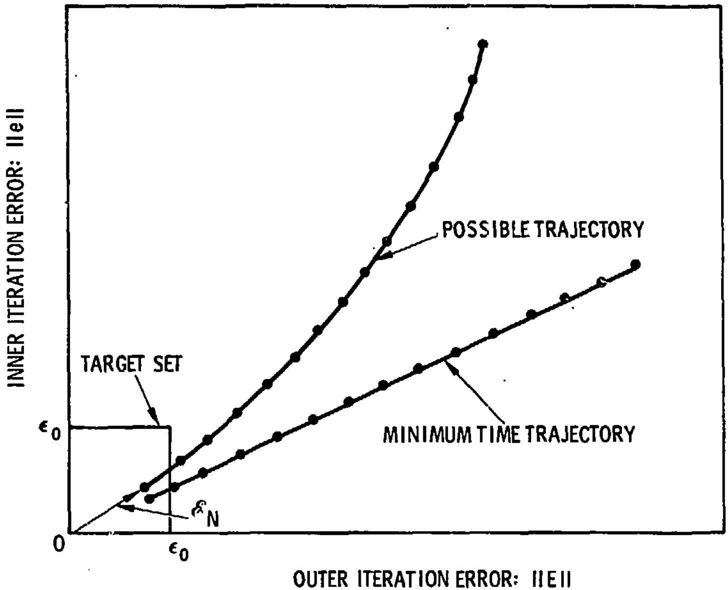

Fig. 1 Euclidean Representation of the Total Error Vector, $\underline{\varepsilon}$, Iteration History.