Lecture Notes for the Course on
NUMERICAL METHODS FOR NUCLEAR REACTORS

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Unit 2 – Eigenvalue Problems and Solution Strategies Outer Iterations

MULTIGROUP CRITICALITY PROBLEMS
Existence of the Fundamental Eigenvalue

- **The multi-group steady-state equation can be written in vector form making use of the differential operators in matrix form**

$$\left(\mathbf{A}+\mathbf{R}\right)\boldsymbol{\phi}+\frac{1}{k}\mathbf{M}\boldsymbol{\phi}=0$$

$$\mathbf{A}=\begin{bmatrix} div\,D_1(\vec{r})\,grad_{\vec{r}}\cdot-\Sigma_{r,1}(\vec{r}) & 0 & 0 & \circ & 0 \\ 0 & div\,D_2(\vec{r})\,grad_{\vec{r}}\cdot-\Sigma_{r,2}(\vec{r}) & 0 & \circ & 0 \\ 0 & 0 & 0 & \circ & 0 \\ \circ & \circ & \circ & \circ & \circ \\ 0 & 0 & 0 & \circ & div\,D_G(\vec{r})\,grad_{\vec{r}}\cdot-\Sigma_{r,G}(\vec{r}) \end{bmatrix}$$

$$\mathbf{R}=\begin{bmatrix} 0 & 0 & 0 & \circ & 0 \\ \Sigma_{s,1\to2}(\vec{r}) & 0 & 0 & \circ & 0 \\ \Sigma_{s,1\to3}(\vec{r}) & \Sigma_{s,2\to3}(\vec{r}) & 0 & \circ & 0 \\ \circ & \circ & \circ & \circ & \circ \\ \Sigma_{s,1\to G}(\vec{r}) & \Sigma_{s,2\to G}(\vec{r}) & \Sigma_{s,3\to G}(\vec{r}) & \circ & 0 \end{bmatrix} \qquad \boldsymbol{\phi}=\begin{bmatrix} \phi_1(\vec{r}) \\ \phi_2(\vec{r}) \\ \phi_3(\vec{r}) \\ \circ \\ \phi_G(\vec{r}) \end{bmatrix}$$

$$\mathbf{M}=\begin{bmatrix} \chi_1(\nu\Sigma_f)_1(\vec{r}) & \chi_1(\nu\Sigma_f)_2(\vec{r}) & \chi_1(\nu\Sigma_f)_3(\vec{r}) & \circ & \chi_1(\nu\Sigma_f)_G(\vec{r}) \\ \chi_2(\nu\Sigma_f)_1(\vec{r}) & \chi_2(\nu\Sigma_f)_2(\vec{r}) & \chi_2(\nu\Sigma_f)_3(\vec{r}) & \circ & \chi_2(\nu\Sigma_f)_G(\vec{r}) \\ \chi_3(\nu\Sigma_f)_1(\vec{r}) & \chi_3(\nu\Sigma_f)_2(\vec{r}) & \chi_3(\nu\Sigma_f)_3(\vec{r}) & \circ & \chi_3(\nu\Sigma_f)_G(\vec{r}) \\ \circ & \circ & \circ & \circ & \circ \\ \chi_G(\nu\Sigma_f)_1(\vec{r}) & \chi_G(\nu\Sigma_f)_2(\vec{r}) & \chi_G(\nu\Sigma_f)_3(\vec{r}) & \circ & \chi_G(\nu\Sigma_f)_G(\vec{r}) \end{bmatrix}$$

- **Putting**

$$\mathbf{A}=diag_{g}\left\{A_g\right\} \qquad\qquad \mathbf{L}=\mathbf{A}+\mathbf{R}$$

$$\mathbf{L}=\begin{bmatrix} A_1 & 0 & 0 & \circ & 0 \\ \Sigma_{s,1\to2}(\vec{r}) & A_2 & 0 & \circ & 0 \\ \Sigma_{s,1\to3}(\vec{r}) & \Sigma_{s,2\to3}(\vec{r}) & A_3 & \circ & 0 \\ \circ & \circ & \circ & \circ & \circ \\ \Sigma_{s,1\to G}(\vec{r}) & \Sigma_{s,2\to G}(\vec{r}) & \Sigma_{s,3\to G}(\vec{r}) & \circ & A_G \end{bmatrix}$$

it is $\qquad\qquad -\mathbf{L}\boldsymbol{\phi}=\dfrac{1}{k}\mathbf{M}\,\boldsymbol{\phi}$

- **By introducing the inverse operator of $-\mathbf{L}$, identified by $\mathbf{H}$, it is**

$$\boxed{\phi = \frac{1}{k}\mathbf{H}\mathbf{M}\,\phi}$$ (°)

  with

$$\mathbf{H} = \begin{bmatrix} H_{11} & 0 & 0 & \circ & 0 \\ H_{21} & H_{22} & 0 & \circ & 0 \\ H_{31} & H_{32} & H_{33} & \circ & 0 \\ \circ & \circ & \circ & \circ & \circ \\ H_{G1} & H_{G2} & H_{G3} & \circ & H_{GG} \end{bmatrix}$$

- **From the condition $\mathbf{H} = -\mathbf{L}^{-1} \Rightarrow -\mathbf{L}\cdot\mathbf{H} = \mathbf{I}$ it is possible to obtain indication on the components of the integral matrix operator $\mathbf{H}$**

$$-A_1 H_{11} = 1 \Rightarrow H_{11} = -A_1^{-1} = G_1 \qquad\qquad -A_2 H_{22} = 1 \Rightarrow H_{22} = -A_2^{-1} = G_2$$

$$-\Sigma_{s,1\to2} H_{11} - A_2 H_{21} = 0 \Rightarrow H_{21} = -A_2^{-1}\Sigma_{s,1\to2} H_{11} = G_2 \Sigma_{s,1\to2} G_1$$

  where the G_g's are the integral Green operators

$$G\cdot_g = \int_V G_g(\vec{r}' \to \vec{r})\cdot dV'$$

  For instance, putting

$$\mathbf{M}\phi = <\nu\Sigma_f, \phi> \chi = \psi(\vec{r})\chi$$

with

$$\psi(\vec{r}) = <\nu\Sigma_f, \phi> = \sum_{g=1}^{G} \nu\Sigma_{f,g}(\vec{r})\,\phi_g(\vec{r}) \qquad\qquad \chi \equiv \{\chi_1, \chi_2, \cdots, \chi_G\}$$

the first two equations of the system (°) take the form

$$\phi_1(\vec{r}) = \underbrace{G_1\chi_1\psi(\vec{r})/k}_{\substack{\textit{contribution from fission} \\ \textit{source in the 1st group}}}$$

$$\phi_2(\vec{r}) = \underbrace{G_2\Sigma_{s,1\to2}G_1\chi_1\psi(\vec{r})/k}_{\substack{\textit{contribution from fission} \\ \textit{source in the 1st group}}} + \underbrace{G_2\chi_2\psi(\vec{r})/k}_{\substack{\textit{contribution from fission} \\ \textit{source in the 2nd group}}}$$

etc..

It is important to point out the "positivity" of the operator H

- **In fact, Green integral operators are "positive", i.e., they transform positive sources in positive fluxes: therefore, also the H_{ij} are positive in this regard**

- **Putting**

$$\mathbf{HM = K}$$

the criticality problem can be put in the eigenvalue problem form

$$\boxed{\mathbf{K}\phi = k\phi} \qquad (^{\circ\circ})$$

where $\mathbf{K}$ is a matrix integral operator which, actually, *transforms non negative fluxes into non negative fluxes ; so it is not exactly a "positive" operator*

- **In fact, non-zero distributions of neutron flux only in non multiplicating regions of the reactor could be transformed into zero flux distributions**

- **In order to find an eigenvalue problem expressed in terms of a "positive" operator, the relationship ($^{\circ\circ}$) can be scalarly multiplied at both sides by the vector $\nu\Sigma_f$**

$$< \nu\Sigma_f, \mathbf{K}\phi >= k < \nu\Sigma_f, \phi > \qquad \text{with}$$

$$< \nu\Sigma_f, \mathbf{K}\phi > =< \nu\Sigma_f, \mathbf{HM}\phi > =< \nu\Sigma_f, \mathbf{H}\chi\psi(\vec{r}) > = \hat{K}\psi(\vec{r})$$

Putting

$$\boxed{\hat{K}\psi(\vec{r}) = k\psi(\vec{r})} \qquad (\vec{r} \in active\ core) \qquad (^{\circ\circ\circ})$$

the operator $\hat{K}\circ =< \nu\Sigma_f, \mathbf{H}\chi\circ >$ is a positive operator, if at least the following requirements are satisfied:

$$\boxed{\chi_1 > 0 \qquad\qquad \left(\nu\Sigma_f\right)_G(\vec{r}) > 0 \qquad\qquad \Sigma_{s,g-1\to g} > 0}$$

This allows to apply the *Jentsch's Theorem* stating that ($^{\circ\circ\circ}$):

- ◆ *a positive fundamental eigenvalue (i.e., $k = k_1 > k_2 \geq...$) exists*

- ◆ *in relation to this eigenvalue, a single positive eigenfunction exists*

- **Since the eigenvalue problems ($^{\circ\circ}$) e ($^{\circ\circ\circ}$) are equivalent, we have the proof of the existence and uniqueness of the fundamental eigenvalue ($^{\circ\circ}$)**

MULTIGROUP CRITICALITY PROBLEMS
Discretised Form

- **Once the diffusion equations are discretised in space, matrix integral operators become just matrices. It is**

$$\boxed{\mathbf{K}\ \phi = k\phi}$$

   where it is meant that

$$\mathbf{K} = square\ matrix\ (N \times G) \times (N \times G)$$

$$\phi = N \times G - vector$$

$$N = number\ of\ spatial\ nodes$$

- **The results obtained for the problem in the continuum space can be extended to the case of the discretised problem by the:**

   Perron Theorem. Assigned a matrix M having all positive entries (a "positive" matrix), it is:
   a) **M has a simple and positive eigenvalue μ_1 such that for any other eigenvalue μ_n it is $\mu_1 > |\mu_n|$. This is termed the fundamental eigenvalue**
   b) **a single eigenvector φ_1 is related to the eigenvalue μ_1, having all positive components: this is the single one having this "positivity" property and is said fundamental eigenvector**
   c) **μ_1 increases by increasing any entry of M.**

   Frobenius Thorem. If M is a matrix with non-negative entries and irreducible, it is:
   a) **M has a simple and positive eigenvalue μ_1 such that for any other eigenvalue μ_n it is $\mu_1 \geq |\mu_n|$.**
   b) **and c) as for Perron theorem.**

> *In our purposes this means that*
> *in order to estimate the fundamental eigenvalue of a criticality problem*
> *it is possible to make use of the "power method"*

THE POWER METHOD

- **This is the method adopted to calculate** *the fundamentaleigenvalue and eigenvector*

- **If we assume that M has a fundamental eigenvalue, the sequence**
$$\mathbf{q}, \ \mathbf{M}\mathbf{q}, \ \mathbf{M}^2\mathbf{q}, \ ...$$
converges to the related eigenvector

 Limiting the illustration to the case in which:

$$\mathbf{q} = \sum_h c_h \boldsymbol{\varphi}_h$$

where the $\boldsymbol{\varphi}_h$ are the eigenvectors of M, it is:

$$\mathbf{M}^m\mathbf{q} = \sum_h c_h \mathbf{M}^m \boldsymbol{\varphi}_h = \sum_h c_h \mu_h^m \boldsymbol{\varphi}_h = \mu_1^m \left[c_1 \boldsymbol{\varphi}_1 + \boxed{\sum_{h \geq 2} c_h \frac{\mu_h^m}{\mu_1^m} \boldsymbol{\varphi}_h} \right] \to \mu_1^m c_1 \boldsymbol{\varphi}_1$$

- **In order to evaluate the eigenvalue, it must be considered that**
$$\mathbf{M}^{m+1}\mathbf{q} \to \mu_1^{m+1} c_1 \boldsymbol{\varphi}_1$$
adopting one of the following estimates

$$\mu_1 \approx \frac{\left\{ \mathbf{M}^{m+1}\mathbf{q} \right\}_i}{\left\{ \mathbf{M}^m\mathbf{q} \right\}_i} \left(for \ any \ i \right)$$

$$\mu_1 \approx \frac{\sum_{i=1}^n \left\{ \mathbf{M}^{m+1}\mathbf{q} \right\}_i}{\sum_{i=1}^n \left\{ \mathbf{M}^m\mathbf{q} \right\}_i} \qquad \left| \mu_1 \right| \approx \frac{\left\| \mathbf{M}^{m+1}\mathbf{q} \right\|}{\left\| \mathbf{M}^{m+1}\mathbf{q} \right\|}$$

OUTER ITERATIONS
WITH THE POWER METHOD

- **The solution of a criticality problem involves solving the iterative scheme**

$$-\mathbf{L}\,\boldsymbol{\phi}^{(n+1)} = \frac{1}{k^{(n)}}\mathbf{M}\,\boldsymbol{\phi}^{(n)}$$

  with *"inner iterations"*, for the solution of the discretised group equations, and updating the eigenvalue and the fission source (at the RHS of the equation) with *"outer iterations"*

- **As already suggested, this process is equivalent to the iteration process**

$$\boldsymbol{\phi}^{(n+1)} = \frac{1}{k^{(n)}}\mathbf{K}\,\boldsymbol{\phi}^{(n)}$$

$$k^{(n+1)} = \frac{\left[\boldsymbol{\phi}^{(n+1)}, \mathbf{v}\Sigma_f\right]}{\dfrac{1}{k^{(n)}}\left[\boldsymbol{\phi}^{(n)}, \mathbf{v}\Sigma_f\right]} = k^{(n)}\frac{\left[\boldsymbol{\phi}^{(n+1)}, \mathbf{v}\Sigma_f\right]}{\left[\underline{\boldsymbol{\phi}}^{(n)}, \mathbf{v}\Sigma_f\right]}$$

  where the inner product [a,b] is specified as follows

$$\left[\boldsymbol{\phi}^{(n)}, \mathbf{v}\Sigma_f\right] = \sum_{g=1}^{G}\sum_{h=1}^{N}\phi_g\left(\vec{r}_h\right)v\Sigma_{f,g}\left(\vec{r}_h\right)$$

  Considering the definition of $\boldsymbol{\phi}^{(n+1)}$ it is therefore

$$k^{(n+1)} = \frac{\left[\mathbf{K}\boldsymbol{\phi}^{(n)}, \mathbf{v}\Sigma_f\right]}{\left[\boldsymbol{\phi}^{(n)}, \mathbf{v}\Sigma_f\right]}$$

- **The adopted process is therefore the following:**
  - ◆ **An estimate $k^{(0)}$ and an admissible $\psi^{(0)}$ will provide a spatial distribution of the group neutron fluxes $\boldsymbol{\phi}^{(1)}$ such that**

$$\boldsymbol{\phi}^{(1)} = \boxed{c\boldsymbol{\varphi}} + \sum_{h\geq 2}c_h\boldsymbol{\varphi}_h$$

    where $\boldsymbol{\varphi}$ is the fundamental eigenvector and $\boldsymbol{\varphi}_h$ are the higher harmonics

♦ **Iterations are the carried on, obtaining:**

$$\phi^{(2)} = \frac{1}{k^{(1)}} \mathbf{K}\phi^{(1)}$$

$$\phi^{(3)} = \frac{1}{k^{(2)}} \mathbf{K}\phi^{(2)} = \frac{1}{k^{(2)}k^{(1)}} \mathbf{K}^2\phi^{(1)}$$

………..

$$\phi^{(n)} = \frac{1}{k^{(n-1)}...k^{(2)}k^{(1)}} \mathbf{K}^{n-1}\phi^{(1)} = \frac{1}{k^{(n-1)}...k^{(2)}k^{(1)}} \mathbf{K}^{n-1}\left(c\varphi + \sum_{h\geq 2} c_h \varphi_h \right)$$

$$= \frac{k^{n-1}}{k^{(n-1)}...k^{(2)}k^{(1)}} \left[c\varphi + \sum_{h\geq 2} c_h \left(\frac{k_h}{k}\right)^{n-1} \varphi_h \right]$$

then $$\mathbf{K}\phi^{(n)} = \frac{k^n}{k^{(n-1)}...k^{(2)}k^{(1)}} \left[c\varphi + \sum_{h\geq 2} c_h \left(\frac{k_h}{k}\right)^{n} \varphi_h \right]$$

By substituting the relationship $$k^{(n+1)} = \frac{\left[\mathbf{K}\phi^{(n)}, \mathbf{v}\Sigma_f \right]}{\left[\phi^{(n)}, \mathbf{v}\Sigma_f \right]}$$

it is $$k^{(n+1)} = k \frac{\left[c\varphi, \mathbf{v}\Sigma_f \right] + \sum_{h\geq 2} c_h \left(\frac{k_h}{k}\right)^{n} \left[\varphi_h, \mathbf{v}\Sigma_f \right]}{\left[c\varphi, \mathbf{v}\Sigma_f \right] + \sum_{h\geq 2} c_h \left(\frac{k_h}{k}\right)^{n-1} \left[\varphi_h, \mathbf{v}\Sigma_f \right]} \rightarrow k$$

♦ **We also note that**

$$\phi^{(n)} = \frac{k^{n-1}}{k^{(n-1)}...k^{(2)}k^{(1)}} \left[c\varphi + \sum_{h\geq 2} c_h \left(\frac{k_h}{k}\right)^{n-1} \varphi_h \right] \rightarrow C\varphi$$

therefore, an appropriate normalization provides the eigenvector in the required form.

ACCELERATION
OF OUTER ITERATIONS

In many cases of practical interest, the *dominance ratio* $\sigma = \dfrac{k_2}{k}$ is too close to unity to result in an efficient convergence of the power method. Acceleration schemes are then adopted.

a) Wielandt Method
The idea at the basis of the method is to introduce a "spectral shift" in the eigenvalues in order to increase the separation between the first and the second one.

In principle, *a good estimate "in excess"* of k, identified as k^*, is needed, calculating the eigenvalues of the matrix

$$\left(k^* \mathbf{I} - \mathbf{K}\right)^{-1}$$

having the same eigenvectors of $\mathbf{K}$, with eigenvalues given by

$$\lambda_h = \frac{1}{k^* - k_h}$$

In such a way, it is

$$\lambda_1 = \frac{1}{k^* - k} \qquad\qquad \lambda_2 = \frac{1}{k^* - k_2} = \frac{1}{k^* - \sigma k}$$

and, being $k^* \approx k$ (and $k^* > k$), the difference between the first and the second eigenvalues is amplified, granting a faster convergence.

A practical way of implementing something similar to the above is the following. From the relation:

$$\left(\mathbf{A} + \mathbf{R}\right)\phi + \frac{1}{k}\mathbf{M}\phi = 0$$

we can write

$$-\left(\mathbf{A} + \mathbf{R}\right)\phi - \frac{1}{k^*}\mathbf{M}\phi = \left(\frac{1}{k} - \frac{1}{k^*}\right)\mathbf{M}\phi$$

and then

$$-\left(\mathbf{A} + \mathbf{R} + \frac{1}{k^*}\mathbf{M}\right)\phi = \left(\frac{1}{k} - \frac{1}{k^*}\right)\mathbf{M}\phi$$

or

$$\phi = -\left(\frac{1}{k} - \frac{1}{k^*}\right)\left(\mathbf{A} + \mathbf{R} + \frac{1}{k^*}\mathbf{M}\right)^{-1}\mathbf{M}\,\phi$$

and then we have the new eigenvalue problem

$$\phi^{(n+1)} = \frac{1}{\lambda}\hat{\mathbf{K}}\,\phi^{(n)}$$

where

$$\hat{\mathbf{K}} = -\left(\mathbf{A} + \mathbf{R} + \frac{1}{k^*}\mathbf{M}\right)^{-1}\mathbf{M} \quad \textbf{and} \quad \lambda = \left(\frac{1}{k} - \frac{1}{k^*}\right)^{-1}$$

The new dominance ratio in this case is:

$$\frac{\lambda_2}{\lambda_1} = \left(\frac{1}{k_1} - \frac{1}{k^*}\right)\Big/\left(\frac{1}{k_2} - \frac{1}{k^*}\right) = \left(\frac{k^* - k_1}{k_1 k^*}\right)\Big/\left(\frac{k^* - k_2}{k_2 k^*}\right) = \left(\frac{k^* - k_1}{k^* - k_2}\right)\boxed{\frac{k_2}{k_1}} = \underbrace{\left(\frac{k^* - k_1}{k^* - k_2}\right)}_{\ll 1}\sigma \ll \sigma$$

and convergence is faster.

It must be noted that:
- **this method can be applied to any eigenvalue problem, to be used also for transport or Monte Carlo calculations;**
- **in the case of deterministic methods (diffusion and transport) the lower triangular structure of the matrix A+R is not preserved in the matrix $\mathbf{A} + \mathbf{R} - \frac{1}{k_e}\mathbf{M}$, limiting the use of this technique to few-energy cases.**

b) Method of Chebyshev polynomials

After performing a sufficient number n^* of iterations by the power method, as to obtain *a good estimate* of k, identified as k^*, for the subsequent iterations the process could be adopted

$$\phi^{(n^*+n)} = \left(\frac{1}{k^*}\mathbf{K}\right)^n\phi^{(n^*)}$$

in other words, the source is normalised by k^*, instead for a new value of k.

This iteration scheme can be considered a special case of a more general method in which a full matrix polynomial is adopted for iteration advancement

$$\phi^{(n^*+n)} = p_n\left(\frac{1}{k^*}\mathbf{K}\right)\phi^{(n^*)} = \left[a_0\mathbf{I} + a_1\left(\frac{1}{k^*}\mathbf{K}\right) + \ldots + a_n\left(\frac{1}{k^*}\mathbf{K}\right)^n\right]\phi^{(n^*)}$$

The basic idea is therefore to choose the coefficients of the polynomial $p_n(x)$ in order to obtain the fastest convergence of the process. Assuming as usual that

$$\phi^{(n^*)} = c\varphi + \sum_{h\geq 2} c_h \varphi_h$$

it is

$$\phi^{(n^*+n)} = p_n\left(\frac{1}{k^*}\mathbf{K}\right)\phi^{(n^*)} = p_n\left(\frac{1}{k^*}\mathbf{K}\right)\left[c\varphi + \sum_{h\geq 2} c_h \varphi_h\right]$$

$$= c\,p_n\left(\frac{k}{k^*}\right)\varphi + \sum_{h\geq 2} c_h p_n\left(\frac{k_h}{k^*}\right)\varphi$$

Therefore, the most efficient choices would be the one of a polynomial such that

$$p_n\left(\frac{k}{k^*}\right) \approx p_n(1) = 1 \qquad\qquad p_n\left(\frac{k_h}{k^*}\right) = 0 \qquad (h = 2,\ldots,n)$$

In fact, after such process, it would be

$$\phi^{(n^*+n)} \approx c\varphi$$

Such an ideal objective would anyway require the knowledge of all the k_h $(h = 2,\ldots,n)$, which is hardly achievable in practical terms. However, assuming the knowledge of the dominance ratio, it is possible to define an interval separating the k_h

$$0 \leq \frac{k_h}{k^*} \leq \frac{k_2}{k^*} = \sigma < 1$$

searching for a polynomial p_n having its coefficients satisfying the condition

$$p_n(1) = 1 \qquad\qquad \min_{a_0,a_1,\ldots,a_n} \max_{0\leq x\leq\sigma}\left|p_n(x)\right|$$

The solution of this problem is known to be

$$p_n(x) = C_n\left(\frac{2x}{\sigma} - 1\right)\Big/ C_n\left(\frac{2}{\sigma} - 1\right)$$

where $C_n(t)$ is the n-th *Chebyshev polynomial* to be obtained by the recurrence relationship

$$C_0(t) = 1 \qquad C_1(t) = t \qquad C_{n+1}(t) = 2tC_n(t) - C_{n-1}(t) \quad (n \geq 1)$$

It must be noted that to advance the calculation, it is not necessary to construct the matrix polynomial, because the recurrence relation reduces the problem to an iterative advancement, starting with *n=0*

$$\hat{\phi}^{(n^*+n+1)} = \frac{1}{k^*} \mathbf{K} \phi^{(n^*+n)}$$

$$\phi^{(n^*+n+1)} = \phi^{(n^*+n)} + \alpha_n\left(\hat{\phi}^{(n^*+n+1)} - \phi^{(n^*+n)}\right) + \beta_n\left(\phi^{(n^*+n)} - \phi^{(n^*+n-1)}\right)$$

where $\quad \alpha_0 = \dfrac{2}{2-\sigma} \qquad \alpha_1 = \dfrac{2}{2-\sigma-\sigma^2\dfrac{\alpha_0}{4}} \qquad \alpha_n = \dfrac{2}{2-\sigma-\sigma^2\dfrac{\alpha_{n-1}}{8}} \quad (n \geq 2)$

$$\beta_n = \left(1 - \frac{\sigma}{2}\right)\alpha_n - 1$$

It is necessary to clarify that:

- it is advisable to apply the acceleration method after a convenient number of iterations by the power method in order to obtain an estimate of k^* and because the acceleration method is very effective to suppress the harmonics with $k_h \approx 1$, but it is not so for higher order ones (see the figure);

- in order to apply the Chebyshev acceleration scheme, it is needed to know the dominance ratio; this can be achieved by iterating with the power method as explained in the following.
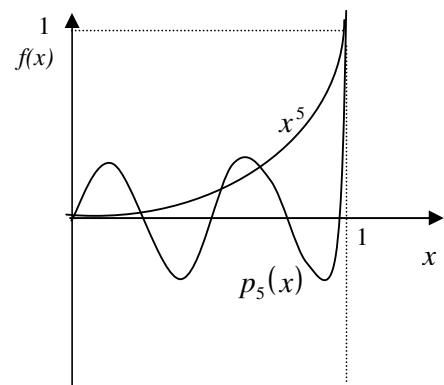
In fact, assuming that a sufficient number of iterations was made to suppress all the higher harmonics but the second one, it is

$$\boxed{\phi^{\left(n^*\right)}} = c\,\varphi + c_2 \varphi_2$$

By defining the increment vector as

$$\delta^{(n)} = \phi^{(n)} - \phi^{(n-1)}$$

it is

$$\boxed{\delta^{\left(n^*+1\right)}} = \phi^{\left(n^*+1\right)} - \phi^{\left(n^*\right)} = \frac{1}{k^*}\mathbf{K}\,\phi^{\left(n^*\right)} - \phi^{\left(n^*\right)} = \frac{1}{k^*}\mathbf{K}\left[c\varphi + c_2\varphi_2\right] - c\varphi - c_2\varphi_2$$

$$\approx c\varphi + c_2\frac{k_2}{k^*}\varphi_2 - c\varphi - c_2\varphi_2 = \boxed{c_2\left(\sigma - 1\right)\varphi_2}$$

Similarly, it is:

$$\boxed{\delta^{\left(n^*+2\right)}} = \phi^{\left(n^*+2\right)} - \phi^{\left(n^*+1\right)} = \left(\frac{1}{k^*}\mathbf{K}\right)^2 \phi^{\left(n^*\right)} - \frac{1}{k^*}\mathbf{K}\,\phi^{\left(n^*\right)}$$

$$= \left[\left(\frac{1}{k^*}\mathbf{K}\right)^2 - \frac{1}{k^*}\mathbf{K}\right]\left[c\varphi + c_2\varphi_2\right] = c_2\left(\sigma^2 - \sigma\right)\varphi_2 = \boxed{c_2\sigma\left(\sigma - 1\right)\varphi_2}$$

It is therefore:

$$\sigma \approx \frac{\left\|\delta^{\left(n^*+2\right)}\right\|}{\left\|\delta^{\left(n^*+1\right)}\right\|}$$

- **More refined formulations are available when the range separating the eigenvalues is better estimated (e.g., knowing a lower bound of it greater than zero).**