Generalized perturbation theory

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Content (week 9)

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Generalized perturbation theory (GPT) 1

- GPT permits to determine the sensibility of a reactor characteristic with respect to a variation of a state variable such as the exit burnup, fuel enrichment or poison load.
- The classical perturbation theory corresponds to the particular case where the reactor characteristic is the effective multiplication factor.
- A reactor characteristic is a functional $F\{\boldsymbol{\phi}(\boldsymbol{r})\}$ of the neutron flux $\boldsymbol{\phi}(\boldsymbol{r})$, retuning a single real value such as a zonal power, a fuel cost or a critical parameter.
- The perturbation of an eigenvalue equation leads to a fixed source eigenvalue equation, a type of problem with very specific and unusual characteristics.

We will limit ourself to the following situation:

- the reactor is at steady state and its neutron flux is the solution of the steady state diffusion equation;
- the reactor characteristics are homogeneous functionals of the neutron flux:

(1) $$F\{\boldsymbol{\phi}(\boldsymbol{r})\} = F\{\alpha\,\boldsymbol{\phi}(\boldsymbol{r})\} \;\; \forall \;\; \alpha \in \Re \;\; .$$

GPT techniques are powerful tools to compute the gradient in core optimisation studies involving continuous state variables.

Mathematical background 1

Definition 1

Let a vectorial space $\mathcal{S}$ defined over a field $\mathcal{K}$. A function F associating an element of $\mathcal{K}$ to each element $\boldsymbol{f}$ of $\mathcal{S}$ is called a functional.

We are considering a vectorial space $\mathcal{S}^*$ defined over the field $\Re$ of real numbers and containing G–component vectors $\boldsymbol{f}(\boldsymbol{r})$, so that

$$\boldsymbol{f}(\boldsymbol{r}) = \mathrm{col}\left[f_1(\boldsymbol{r}),\, f_2(\boldsymbol{r}),\, \ldots,\, f_G(\boldsymbol{r})\right] \tag{2}$$

$$\mathcal{S}^* = \left\{\boldsymbol{f}(\boldsymbol{r});\ f_g(\boldsymbol{r}) \in \mathcal{C}_0[V];\ g = 1, G\right\} \tag{3}$$

where V is the spatial domain of functions $f_g(\boldsymbol{r})$. A component $f_g(\boldsymbol{r})$ generally represents the neutron flux in group g and V represents the volume of the reactor.

Definition 2

The internal product, denoted as $\langle \boldsymbol{f}, \boldsymbol{h} \rangle$, of two vectors $\boldsymbol{f}(\boldsymbol{r})$ and $\boldsymbol{h}(\boldsymbol{r})$ taken in vectorial space $\mathcal{S}^*$ is defined as

$$\langle \boldsymbol{f}, \boldsymbol{h} \rangle = \sum_{g=1}^{G} \int_V d^3r\ f_g(\boldsymbol{r})\, h_g(\boldsymbol{r}) \quad . \tag{4}$$

Mathematical background 2

To illustrate this definition, we can define two examples of neutron flux functional. The first example is a reaction rate, defined as

(5) $$R\{\boldsymbol{\phi}(\boldsymbol{r})\} = \langle \boldsymbol{\Sigma}, \boldsymbol{\phi} \rangle$$

where $\boldsymbol{\Sigma}(\boldsymbol{r}) = \mathrm{col}\left[\Sigma_1(\boldsymbol{r})\,,\ \Sigma_2(\boldsymbol{r})\right]$ and $\boldsymbol{\phi}(\boldsymbol{r}) = \mathrm{col}\left[\phi_1(\boldsymbol{r})\,,\ \phi_2(\boldsymbol{r})\right]$.

The second example is a reaction rate ratio defined as

(6) $$P\{\boldsymbol{\phi}(\boldsymbol{r})\} = \frac{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi} \rangle}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi} \rangle}$$

where $\boldsymbol{\Sigma}_1(\boldsymbol{r}) = \mathrm{col}\left[\Sigma_{1,1}(\boldsymbol{r})\,,\ \Sigma_{1,2}(\boldsymbol{r})\right]$ and $\boldsymbol{\Sigma}_2(\boldsymbol{r}) = \mathrm{col}\left[\Sigma_{2,1}(\boldsymbol{r})\,,\ \Sigma_{2,2}(\boldsymbol{r})\right]$.

Definition 3

A functional $F\{\boldsymbol{f}(\boldsymbol{r})\}$ is homogeneous if Eq. (1) is met, i. e. if $F\{\boldsymbol{f}(\boldsymbol{r})\} = F\{\alpha\, \boldsymbol{f}(\boldsymbol{r})\}$ for all value of α element of field $\mathcal{K}$.

To illustrate this point, we observe that Eq. (6) is an homogeneous functional, but not Eq. (5). Only homogeneous functionals are independent of the flux normalization factor and can be used as reactor characteristics in the context of GPT.

Mathematical background 3

Definition 4

The gradient $\boldsymbol{\nabla} F\{\boldsymbol{f}(\boldsymbol{\zeta}); \boldsymbol{r}\}$ of functional $F\{\boldsymbol{f}(\boldsymbol{r})\}$ is a G–component function of $\boldsymbol{r}$ defined as

$$\nabla F_g\{\boldsymbol{f}(\boldsymbol{\zeta}); \boldsymbol{r}\} = \left[\frac{d}{d\epsilon} F\{\boldsymbol{f}(\boldsymbol{\zeta}) + \epsilon\, \boldsymbol{\delta}_g(\boldsymbol{\zeta} - \boldsymbol{r})\}\right]_{\epsilon=0} \quad ; \quad g = 1, G \tag{7}$$

where $\boldsymbol{\delta}_g(\boldsymbol{\zeta} - \boldsymbol{r})$ is a multidimensional Dirac delta distribution defined as

$$\boldsymbol{\delta}_g(\boldsymbol{\zeta} - \boldsymbol{r}) = \mathrm{col}\left[\delta_{g,h}\, \delta(\boldsymbol{\zeta} - \boldsymbol{r})\,,\, h = 1, G\right] \tag{8}$$

where $\delta_{g,h}$ is a Kronecker delta function and $\delta(\boldsymbol{\zeta} - \boldsymbol{r})$ is the classical Dirac delta distribution. Using Eq. (7), we can compute the gradient of functionals defined in Eqs. (5) and (6):

$$\boldsymbol{\nabla} R\{\boldsymbol{\phi}(\boldsymbol{\zeta}); \boldsymbol{r}\} = \boldsymbol{\Sigma}(\boldsymbol{r}) \tag{9}$$

$$\boldsymbol{\nabla} P\{\boldsymbol{\phi}(\boldsymbol{\zeta}); \boldsymbol{r}\} = P\{\boldsymbol{\phi}(\boldsymbol{r})\} \begin{bmatrix} \dfrac{\Sigma_{1,1}(\boldsymbol{r})}{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi}\rangle} - \dfrac{\Sigma_{2,1}(\boldsymbol{r})}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi}\rangle} \\ \dfrac{\Sigma_{1,2}(\boldsymbol{r})}{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi}\rangle} - \dfrac{\Sigma_{2,2}(\boldsymbol{r})}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi}\rangle} \end{bmatrix} \tag{10}$$

where $G = 2$, with $\boldsymbol{\Sigma}_1(\boldsymbol{r}) = \mathrm{col}(\Sigma_{1,1}(\boldsymbol{r}), \Sigma_{1,2}(\boldsymbol{r}))$ and $\boldsymbol{\Sigma}_2(\boldsymbol{r}) = \mathrm{col}(\Sigma_{2,1}(\boldsymbol{r}), \Sigma_{2,2}(\boldsymbol{r}))$.

Mathematical background

Definition 5

The variation of functional $F\{\boldsymbol{f}(\boldsymbol{r})\}$ with respect of an arbitrary variation $\boldsymbol{\delta f}(\boldsymbol{r})$ of its argument is denoted $\delta F_{\delta f}\{\boldsymbol{f}(\boldsymbol{r})\}$ and is an element of field $\mathcal{K}$ defined as

(11) $$\delta F_{\delta f}\{\boldsymbol{f}(\boldsymbol{r})\} = \left[\frac{d}{d\epsilon} F\{\boldsymbol{f}(\boldsymbol{r}) + \epsilon\, \boldsymbol{\delta f}(\boldsymbol{r})\}\right]_{\epsilon=0} \quad ; \quad \boldsymbol{\delta f}(\boldsymbol{r}) \in \mathcal{S}^* \quad .$$

It is possible to apply a limited Taylor expansion to a functional, by analogy with the Taylor expansion of a function with discrete variables. We write

(12) $$F\{\boldsymbol{f}(\boldsymbol{r}) + \epsilon\, \boldsymbol{\delta f}(\boldsymbol{r})\} = F\{\boldsymbol{f}(\boldsymbol{r})\} + \epsilon\, \langle \boldsymbol{\delta f}, \boldsymbol{\nabla} F\{\boldsymbol{f}(\boldsymbol{\zeta}); \boldsymbol{r}\}\rangle + \mathcal{O}(\epsilon^2)$$

where $\mathcal{O}(\epsilon^2)$ is a truncation term of order 2 in ϵ. Substituting Eq. (12) into Eq. (11) , we can show that

(13) $$\delta F_{\delta f}\{\boldsymbol{f}(\boldsymbol{r})\} = \langle \boldsymbol{\delta f}, \boldsymbol{\nabla} F\{\boldsymbol{f}(\boldsymbol{\zeta}); \boldsymbol{r}\}\rangle \quad .$$

Mathematical background

Theorem 1

The gradient of an homogeneous functional $F\{\boldsymbol{f}(\boldsymbol{r})\}$ is orthogonal to $\boldsymbol{f}(\boldsymbol{r})$.

Proof: Consider the variation of functional $F\{\boldsymbol{f}(\boldsymbol{r})\}$ with respect to its own argument $\boldsymbol{f}(\boldsymbol{r})$. Using Eqs. (11) and (13), we can write

(14) $$\delta F_f\{\boldsymbol{f}(\boldsymbol{r})\} = \langle \boldsymbol{f}, \boldsymbol{\nabla} F\{\boldsymbol{f}(\boldsymbol{\zeta}); \boldsymbol{r}\}\rangle = \left[\frac{d}{d\epsilon} F\{(1+\epsilon)\boldsymbol{f}(\boldsymbol{r})\}\right]_{\epsilon=0} .$$

Considering the fact that the functional is homogeneous, $F\{(1+\epsilon)\boldsymbol{f}(\boldsymbol{r})\} = F\{\boldsymbol{f}(\boldsymbol{r})\}$ and

(15) $$\delta F_f\{\boldsymbol{f}(\boldsymbol{r})\} = \left[\frac{d}{d\epsilon} F\{\boldsymbol{f}(\boldsymbol{r})\}\right]_{\epsilon=0} = 0$$

so that the gradient of $F\{\boldsymbol{f}(\boldsymbol{r})\}$ is orthogonal to $\boldsymbol{f}(\boldsymbol{r})$:

(16) $$\langle \boldsymbol{f}, \boldsymbol{\nabla} F\{\boldsymbol{f}(\boldsymbol{\zeta}); \boldsymbol{r}\}\rangle = 0 \ .$$

□

Mathematical background

Definition 6

A fixed source eigenvalue equation is an inhomogeneous equation of the form

(17) $$\mathbb{A}\left(\boldsymbol{r}\right)\boldsymbol{\Gamma}(\boldsymbol{r}) - \mu\ \mathbb{B}\left(\boldsymbol{r}\right)\boldsymbol{\Gamma}(\boldsymbol{r}) = \boldsymbol{S}(\boldsymbol{r})$$

where $\mathbb{A}(\boldsymbol{r})$ and $\mathbb{B}(\boldsymbol{r})$ are operator acting on unknown vector $\boldsymbol{\Gamma}(\boldsymbol{r})$ and where μ is an eigenvalue of the singular equation

(18) $$\mathbb{A}\left(\boldsymbol{r}\right)\boldsymbol{\phi}(\boldsymbol{r}) - \mu\ \mathbb{B}\left(\boldsymbol{r}\right)\boldsymbol{\phi}(\boldsymbol{r}) = \mathbf{0}\ .$$

A fixed source eigenvalue equation is always associated to an eigenvalue equation. Here, the fundamental eigenvalue μ is simply given as $\mu = 1/K_{\text{eff}}$.

In a similar way, we can define an adjoint fixed source eigenvalue equation as

(19) $$\mathbb{A}\left(\boldsymbol{r}\right)^{\top}\boldsymbol{\Gamma}^{*}(\boldsymbol{r}) - \mu\ \mathbb{B}\left(\boldsymbol{r}\right)^{\top}\boldsymbol{\Gamma}^{*}(\boldsymbol{r}) = \boldsymbol{S}^{*}(\boldsymbol{r})$$

assiociated to

(20) $$\mathbb{A}\left(\boldsymbol{r}\right)^{\top}\boldsymbol{\phi}^{*}(\boldsymbol{r}) - \mu\ \mathbb{B}\left(\boldsymbol{r}\right)^{\top}\boldsymbol{\phi}^{*}(\boldsymbol{r}) = \mathbf{0}\ .$$

Mathematical background

Theorem 2

A fixed source eigenvalue problem similar to Eq. (17) has a solution if and only if its fixed source $\boldsymbol{S}(\boldsymbol{r})$ is orthogonal to the solution of the adjoint eigenvalue Eq. (20).

Proof: Let us take the internal product of Eq. (17) with $\boldsymbol{\phi}^*(\boldsymbol{r})$. We write

$$\langle \boldsymbol{\phi}^*, \boldsymbol{S} \rangle = \langle \boldsymbol{\phi}^*, \mathbb{A}\,\boldsymbol{\Gamma} - \mu\ \mathbb{B}\,\boldsymbol{\Gamma} \rangle = \left\langle \mathbb{A}^\top \boldsymbol{\phi}^* - \mu\ \mathbb{B}^\top\ \boldsymbol{\phi}^*, \boldsymbol{\Gamma} \right\rangle = 0 \quad , \tag{21}$$

which prove the theorem. □

Theorem 3

If $\boldsymbol{\Gamma}(\boldsymbol{r})$ is a solution of the fixed source eigenvalue Eq. (17), then there exist an infinity of other solutions of the form

$$\boldsymbol{\Gamma}'(\boldsymbol{r}) = \boldsymbol{\Gamma}(\boldsymbol{r}) + k\,\boldsymbol{\phi}(\boldsymbol{r}) \tag{22}$$

where k is an arbitrary constant.

Proof: The proof involve substitution of Eq. (22) into Eq. (17) and use of Eq. (18) . □

A normalization relation is required to select a particular solution. We generally use the following condition:

$$\left\langle \boldsymbol{\Gamma}, \mathbb{B}^\top \boldsymbol{\phi}^* \right\rangle = 0 \quad . \tag{23}$$

State variables, reactor characteristics 1

- A state variable is a component of the state vector $\boldsymbol{X} = \{X_i \,;\; i = 1, I\}$ permitting the selection of all the nuclear properties of the reactor. For example, a state variable can be a number density, a burnup, a temperature, or any parameter having effect on the reactor physics.
- A reactor characteristic is an homogeneous functional of the neutron flux (and/or of its adjoint) and a function of the state variables. A zonal power ratio or the effective multiplication factor are examples of reactor characteristics.

The neutron flux and its adjoint are the solution of eigenvalues equations, similar to Eqs. (18) and (20), with state-variable–dependent operators. They are written

(24) $$\mathbb{A}\left(\boldsymbol{r}, \boldsymbol{X}\right) \boldsymbol{\phi}(\boldsymbol{r}) - \mu \; \mathbb{B}\left(\boldsymbol{r}, \boldsymbol{X}\right) \boldsymbol{\phi}(\boldsymbol{r}) = \mathbf{0} \quad .$$

and

(25) $$\mathbb{A}\left(\boldsymbol{r}, \boldsymbol{X}\right)^{\top} \boldsymbol{\phi}^{*}(\boldsymbol{r}) - \mu \; \mathbb{B}\left(\boldsymbol{r}, \boldsymbol{X}\right)^{\top} \boldsymbol{\phi}^{*}(\boldsymbol{r}) = \mathbf{0} \quad .$$

State variables, reactor characteristics 2

In the context of two–group diffusion theory, operators $\mathbb{A}(\boldsymbol{r}, \boldsymbol{X})$ and $\mathbb{B}(\boldsymbol{r}, \boldsymbol{X})$ are given by

$$\mathbb{A}\left(\boldsymbol{r}, \boldsymbol{X}\right) = \begin{bmatrix} -\nabla \cdot D_1(\boldsymbol{r}, \boldsymbol{X})\nabla + \Sigma_{\mathrm{r}1}(\boldsymbol{r}, \boldsymbol{X}) & 0 \\ -\Sigma_{2\leftarrow 1}(\boldsymbol{r}, \boldsymbol{X}) & -\nabla \cdot D_2(\boldsymbol{r}, \boldsymbol{X})\nabla + \Sigma_{\mathrm{r}2}(\boldsymbol{r}, \boldsymbol{X}) \end{bmatrix} \tag{26}$$

and

$$\mathbb{B}\left(\boldsymbol{r}, \boldsymbol{X}\right) = \begin{bmatrix} \nu\Sigma_{\mathrm{f}1}(\boldsymbol{r}, \boldsymbol{X}) & \nu\Sigma_{\mathrm{f}2}(\boldsymbol{r}, \boldsymbol{X}) \\ 0 & 0 \end{bmatrix} \quad . \tag{27}$$

Operators $\mathbb{A}(\boldsymbol{r}, \boldsymbol{X})^\top$ and $\mathbb{B}(\boldsymbol{r}, \boldsymbol{X})^\top$ in Eq. (25) are obtained by transposing the matrices in Eqs. (26) and (27).

The purpose of the GPT is to compute the sensibility of a reactor characteristics $F\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\}$ to a variation of the state variables. The first order GPT involves the calculation of the Jacobian vector $\boldsymbol{G}\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\}$ defined as

$$\boldsymbol{G}\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\} = \left\{ \frac{\partial}{\partial X_i} F\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\}\,;\; i = 1, I \right\} \quad . \tag{28}$$

State variables, reactor characteristics 1

We are now presenting the overview of the Jacobian vector calculation.

- As operators in Eqs. (26) and (27) are function of state variables, a perturbation calculation is required to evaluate the sensitivity of direct and adjoint neutron fluxes with respect to a variation in state variables.
- We write $\boldsymbol{\delta\phi}(\boldsymbol{r})$ and $\delta\mu$ the variations of the neutron flux and of the fundamental eigenvalue corresponding to variations $\delta\,\mathbb{A}\,(\boldsymbol{r},\boldsymbol{X})$ and $\delta\,\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X})$ of operators $\mathbb{A}$ and $\mathbb{B}$.

They are defined as

(29) $$\delta\,\mathbb{A}\,(\boldsymbol{r},\boldsymbol{X}) = \sum_{i=1}^{I} \frac{\partial}{\partial X_i}\,\mathbb{A}\,(\boldsymbol{r},\boldsymbol{X})\,\delta X_i$$

and

(30) $$\delta\,\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X}) = \sum_{i=1}^{I} \frac{\partial}{\partial X_i}\,\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X})\,\delta X_i \quad .$$

It is also possible to write the variation of the eigenvalue as

(31) $$\delta\mu = \sum_{i=1}^{I} \frac{\partial\mu}{\partial X_i}\,\delta X_i \quad .$$

State variables, reactor characteristics 2

The perturbed form of Eq. (24) is written

(32) $$\{[\mathbb{A}(\boldsymbol{r},\boldsymbol{X})+\delta\,\mathbb{A}\,(\boldsymbol{r},\boldsymbol{X})]-(\mu+\delta\mu)\,[\mathbb{B}(\boldsymbol{r},\boldsymbol{X})+\delta\,\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X})]\}\,[\boldsymbol{\phi}(\boldsymbol{r})+\boldsymbol{\delta\phi}(\boldsymbol{r})]=\mathbf{0}\quad .$$

We subtract the unperturbed Eq. (24) from Eq. (32) and get rid of all terms involving the product of two or three variations. After rearranging the terms, we obtain

(33) $$[\mathbb{A}(\boldsymbol{r},\boldsymbol{X})-\mu\;\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X})]\,\boldsymbol{\delta\phi}(\boldsymbol{r})=-\,[\delta\,\mathbb{A}\,(\boldsymbol{r},\boldsymbol{X})-\mu\,\delta\,\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X})-\delta\mu\;\mathbb{B}\,(\boldsymbol{r},\boldsymbol{X})]\,\boldsymbol{\phi}(\boldsymbol{r})\quad .$$

We observe that Eq. (33) is a fixed source eigenvalue equation with a singular left hand side and a fixed source. The variation of the eigenvalue is evaluated using the Rayleigh ratio, written as

(34) $$\mu=\frac{\langle\boldsymbol{\phi}^*,\mathbb{A}\boldsymbol{\phi}\rangle}{\langle\boldsymbol{\phi}^*,\mathbb{B}\boldsymbol{\phi}\rangle}\quad .$$

The Rayleigh ratio is stationary with respect to a first order variation of the neutron flux $\boldsymbol{\delta\phi}(\boldsymbol{r})$ and of its adjoint $\boldsymbol{\delta\phi}^*(\boldsymbol{r})$. The variation of the eigenvalue is therefore given as

(35) $$\delta\mu=\mu\left[\frac{\langle\boldsymbol{\phi}^*,\delta\,\mathbb{A}\,\boldsymbol{\phi}\rangle}{\langle\boldsymbol{\phi}^*,\mathbb{A}\boldsymbol{\phi}\rangle}-\frac{\langle\boldsymbol{\phi}^*,\delta\,\mathbb{B}\,\boldsymbol{\phi}\rangle}{\langle\boldsymbol{\phi}^*,\mathbb{B}\boldsymbol{\phi}\rangle}\right]\quad .$$

State variables, reactor characteristics 3

The remaining part of this section is dedicated to the evaluation of the Jacobian vector of an homogeneous functional similar to Eq. (6) and written

(36) $$P\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\} = \frac{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi} \rangle}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi} \rangle} \quad .$$

Two distinct evaluation techniques will be investigated: the implicit and explicit approaches.

The implicit approach

We take the internal product of Eq. (33) with an arbitrary element of the vectorial space $\mathcal{S}^*$ denoted as $\mathbf{\Gamma}^*(\boldsymbol{r})$. After rearranging the terms of the left hand side, we obtain

$$\left\langle \boldsymbol{\delta\phi}, \left[\mathbb{A}^\top - \mu\,\mathbb{B}^\top\right]\mathbf{\Gamma}^*\right\rangle = -\left\langle \left[\delta\,\mathbb{A} - \mu\,\delta\,\mathbb{B} - \delta\mu\,\mathbb{B}\right]\boldsymbol{\phi}, \mathbf{\Gamma}^*\right\rangle \quad . \tag{37}$$

The variation of the homogeneous functional defined in Eq. (36) is given by Eq. (13) as

$$\begin{aligned} \delta P_{\delta\phi}\{\boldsymbol{\phi}(\boldsymbol{r})\} &= \langle \boldsymbol{\delta\phi}, \boldsymbol{\nabla} P\{\boldsymbol{\phi}(\boldsymbol{\zeta}); \boldsymbol{r}\}\rangle \\ &= \left\langle \boldsymbol{\delta\phi}, \left[\mathbb{A}^\top - \mu\,\mathbb{B}^\top\right]\mathbf{\Gamma}^*\right\rangle \\ &= -\left\langle \left[\delta\,\mathbb{A} - \mu\,\delta\,\mathbb{B} - \delta\mu\,\mathbb{B}\right]\boldsymbol{\phi}, \mathbf{\Gamma}^*\right\rangle \\ &= -\left\langle \delta\left[\mathbb{A} - \mu\,\mathbb{B}\right]\boldsymbol{\phi}, \mathbf{\Gamma}^*\right\rangle \end{aligned} \tag{38}$$

using Eq. (37) and provided that $\mathbf{\Gamma}^*(\boldsymbol{r})$ is the solution of the following fixed source eigenvalue equation:

$$\left[\mathbb{A}(\boldsymbol{r}, \boldsymbol{X})^\top - \mu\ \mathbb{B}\,(\boldsymbol{r}, \boldsymbol{X})^\top\right]\mathbf{\Gamma}^*(\boldsymbol{r}) = \boldsymbol{\nabla} P\{\boldsymbol{\phi}(\boldsymbol{\zeta}); \boldsymbol{r}\} \quad . \tag{39}$$

The implicit approach

The components of the Jacobian vector are therefore written

$$\frac{\partial}{\partial X_i} P\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\} = P\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\} \left[\frac{\left\langle \frac{\partial \boldsymbol{\Sigma}_1}{\partial X_i}, \boldsymbol{\phi} \right\rangle}{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi} \rangle} - \frac{\left\langle \frac{\partial \boldsymbol{\Sigma}_2}{\partial X_i}, \boldsymbol{\phi} \right\rangle}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi} \rangle} \right] - \left\langle \frac{\partial}{\partial X_i} \left[\mathbb{A} - \mu \mathbb{B} \right] \boldsymbol{\phi}, \boldsymbol{\Gamma}^* \right\rangle \tag{40}$$

where $i = 1, I$.

- The evaluation of Jacobian using Eq. (40) requires the evaluation of one fixed source eigenvalue equation similar to Eq. (39) for each reactor characteristic, whatever the number of state variables.
- According to Theorem 2, a solution of Eq. (39) exists if and only if its right hand side is orthogonal to the direct neutron flux $\boldsymbol{\phi}(\boldsymbol{r})$. This condition is fulfilled, as Theorem 1 has proven that the gradient of an homogeneous functional of the flux is orthogonal to the flux.
- Theorem 3 states that an infinity of solutions exist for Eq. (40). It is necessary to prove that all these solutions are valid and can be used to compute the Jacobian.

The implicit approach

Theorem 4

The value of the Jacobian computed by Eq. (40) remains unchanged if $\boldsymbol{\Gamma}^*(\boldsymbol{r})$ is replaced by $\boldsymbol{\Gamma}^*(\boldsymbol{r}) + k\,\boldsymbol{\phi}^*(\boldsymbol{r})$, for all values of constant k.

□

- Theorem 4 also shows that the Rayleigh ratio of Eq. (34) is the correct definition of the eigenvalue to be used with the GPT.
- In order to select a particular solution of Eq. (39), the following normalization condition is generally used:

(41) $$\langle \boldsymbol{\Gamma}^*, \mathbb{B}\boldsymbol{\phi} \rangle = 0 \quad .$$

The explicit approach

With the explicit approach, neutron flux variations are computed explicitly. Let us first consider a first-order variation of the neutron flux. This variation is the solution of Eq. (33):

(42) $$\boldsymbol{\delta\phi}(\boldsymbol{r}) = \sum_{i=1}^{I} \frac{\partial \boldsymbol{\phi}(\boldsymbol{r})}{\partial X_i}\, \delta X_i \quad .$$

Substitution of Eqs. (29) to (31) and (42) into Eq. (33) leads to a set of I fixed source eigenvalue equations, each of them written as

(43) $$\left[\mathbb{A}(\boldsymbol{r},\boldsymbol{X}) - \mu\ \mathbb{B}\left(\boldsymbol{r},\boldsymbol{X}\right)\right] \frac{\partial \boldsymbol{\phi}(\boldsymbol{r})}{\partial X_i} = -\frac{\partial}{\partial X_i}\left[\mathbb{A}(\boldsymbol{r},\boldsymbol{X}) - \mu\ \mathbb{B}\left(\boldsymbol{r},\boldsymbol{X}\right)\right] \boldsymbol{\phi}(\boldsymbol{r})\ ;\ i = 1, I \quad .$$

Solutions of Eqs. (43) are used to compute the $\delta_{\delta\phi} P$ values using

(44) $$\begin{aligned} \delta_{\delta\phi} P\{\boldsymbol{\phi}(\boldsymbol{r}),\boldsymbol{X}\} &= P\{\boldsymbol{\phi}(\boldsymbol{r}),\boldsymbol{X}\} \\ &\times \sum_{i=1}^{I} \left[\frac{\left\langle \frac{\partial \boldsymbol{\Sigma}_1}{\partial X_i}, \boldsymbol{\phi} \right\rangle + \left\langle \boldsymbol{\Sigma}_1, \frac{\partial \boldsymbol{\phi}}{\partial X_i} \right\rangle}{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi} \rangle} - \frac{\left\langle \frac{\partial \boldsymbol{\Sigma}_2}{\partial X_i}, \boldsymbol{\phi} \right\rangle + \left\langle \boldsymbol{\Sigma}_2, \frac{\partial \boldsymbol{\phi}}{\partial X_i} \right\rangle}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi} \rangle} \right] \delta X_i \end{aligned}$$

where $i = 1, I$.

The explicit approach

Equation (40) can be replaced with the following explicit relation:

$$\frac{\partial}{\partial X_i} P\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\} = P\{\boldsymbol{\phi}(\boldsymbol{r}), \boldsymbol{X}\} \left[\frac{\left\langle \frac{\partial \boldsymbol{\Sigma}_1}{\partial X_i}, \boldsymbol{\phi} \right\rangle + \left\langle \boldsymbol{\Sigma}_1, \frac{\partial \boldsymbol{\phi}}{\partial X_i} \right\rangle}{\langle \boldsymbol{\Sigma}_1, \boldsymbol{\phi} \rangle} - \frac{\left\langle \frac{\partial \boldsymbol{\Sigma}_2}{\partial X_i}, \boldsymbol{\phi} \right\rangle + \left\langle \boldsymbol{\Sigma}_2, \frac{\partial \boldsymbol{\phi}}{\partial X_i} \right\rangle}{\langle \boldsymbol{\Sigma}_2, \boldsymbol{\phi} \rangle} \right]$$

(45)

where $i = 1, I$.

The evaluation of Jacobian using Eq. (45) requires the evaluation of one fixed source eigenvalue equation similar to Eq. (43) for each state variable, whatever the number of reactor characteristics.

According to Theorem 2, a solution of Eq. (43) exists if and only if its right hand side is orthogonal to the adjoint neutron flux $\boldsymbol{\phi}^*(\boldsymbol{r})$. This condition is fulfilled, as the inner product of this term with $\boldsymbol{\phi}^*(\boldsymbol{r})$ can be shown to vanish. Theorem 3 states that an infinity of solutions exist for Eq. (43). It is necessary to prove that all these solutions are valid and can be used to compute the Jacobian.

The explicit approach

Theorem 5

The value of the Jacobian computed by Eq. (45) remains unchanged if $\partial \boldsymbol{\phi}(\boldsymbol{r})/\partial X_i$ is replaced by $\partial \boldsymbol{\phi}(\boldsymbol{r})/\partial X_i + k\,\boldsymbol{\phi}(\boldsymbol{r})$, for all values of constant k. This proof is left to the reader.

Again, a particular solution can be set using the following normalization condition:

(46)
$$\left\langle \frac{\partial \boldsymbol{\phi}}{\partial X_i}, \mathbb{B}^{\top} \boldsymbol{\phi}^* \right\rangle = 0 \; ; \; i = 1, I \quad .$$

We observe that both Eqs. (40) and (45) allow to compute the same Jacobian of reactor characteristics, but require the solution of different fixed source eigenvalue equations. We generally choose the approach requiring the solution of the smallest number of fixed source eigenvalue equations.

- With the implicit approach, this number is equal to the number of reactor characteristics.
- With the explicit approach, this number is equal to the number of state variables.

The Matlab script `alfse` 1

This script `alfse` is called as

```
[iter,eval,delta]=alfse(a,b,evect,adect,sour,eps) ;
```

- This script find the solution of the fixed source eigenvalue equation

$$(\mathbb{A} - \mu_1 \mathbb{B})\, \mathbf{\Gamma} = \boldsymbol{S}$$

  using the inverse power method.

- Dummy variables are defined as follows:
  - variables a and b are the input matrices
  - `eps` is the convergence parameter of the inverse power method
  - arrays `evect` and `adect` are the direct and adjoint solutions of the corresponding eigenvalue problem
  - array `sour` is the fixed source. It must be orthogonal to `adect`.
- The script returns a list containing
  - the number of iterations
  - the fundamental eigenvalue μ_1 of the corresponding eigenvalue problem
  - the solution of the fixed source eigenvalue problem $\mathbf{\Gamma}$.