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A new method for reconstruction of cross-sections using Tucker decomposition

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ABSTRACT

The full representation of a d-variate function requires exponentially storage size as a function of dimension d and high computational cost. In order to reduce these complexities, function approximation methods (called *reconstruction* in our context) are proposed, such as: interpolation, approximation, etc. The traditional interpolation model like the multilinear one, has this dimensionality problem. To deal with this problem, we propose a new model based on the Tucker format – a low-rank tensor approximation method, called here *the Tucker decomposition*. The Tucker decomposition is built as a tensor product of one-dimensional spaces where their one-variate basis functions are constructed by an extension of the Karhunen–Loève decomposition into high-dimensional space. Using this technique, we can acquire, direction by direction, the most important information of the function and convert it into a small number of basis functions. Hence, the approximation for a given function needs less data than that of the multilinear model. Results of a test case on the neutron cross-section reconstruction demonstrate that the Tucker decomposition achieves a better accuracy while using less data than the multilinear interpolation.

1. Introduction

The concept of "function approximation" is widely used in many branches of applied mathematics and computer science to apprehend quantities of interest, or a function depends on input parameters, such as spatial position, time evolution or any other type of input quantity. The a priori knowledge of the quantity of interest may either be "explicit", as coming out from measurements, or "implicit" as solution of a modeling equation. There is a third way that is relevant to this paper. Cross-sections that feed the neutron flux solver cannot be directly measured in an environment such as a nuclear reactor core. They neither can be computed using a single equation since there is an interaction between many physics (neutronics, hydraulic, thermic, ...). The way to solve this situation is through a simplified "experimental simulation" and we will call later on this process a "calculation scheme". Since cross-sections depend continuously on many parameters, a parametrized calculation scheme is also very useful to emulate many different "experiments" with different configurations. Therefore, one calculation point corresponds to one experiment for a given configuration. That explains why, although cross-sections are computed and not measured, we will consider them as "explicit" data acquired through "experimental simulation".

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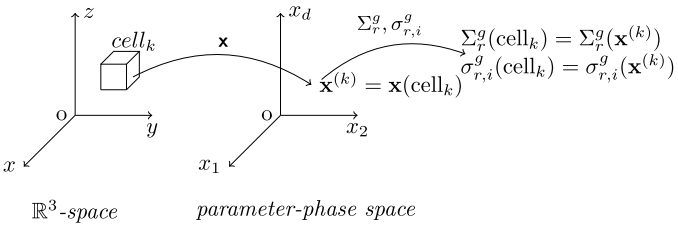

Fig. 1. Dependence of cross-sections on parameters.

Multipurpose/universal approaches such as global or piecewise polynomial approximations are general approximation methods that are valid for a large variety of functions: depending on the hypothesis/knowledge we have on the function such as regularity in terms of existence of a certain number of derivatives, we may prefer to use global polynomial versus piecewise ones. This step of the approximation requires some know-how that is now rather well understood. Once the approximation basis set is chosen, the coefficients or components of the function that we want to approximate in this basis set, will be determined in order to fit with the "input" that are explicitly available and have been acquired by some series of measurements. The stability of the mapping from the input to the coefficients or components that is an important feature for the quality of the approximation also depends on the chosen basis set. Once this is done, a second step in the approximation is the reconstruction (or evaluation) of the function we are interested in, on other points than those that have been used to construct the approximation.

All this framework involves four different concepts: i) data acquisition, ii) storage of these data, iii) reconstruction of the function we are interested in, iv) further evaluation, that all have their particular complexity and cost, that, of course depend on the number of the inputs that are used to define the function of interest. These complexity and cost suffer from what is known as the curse of dimension that leads to an exponential explosion of the complexity and cost with respect to the number of inputs.

In order to face this particular problem, different ad hoc strategies have been proposed and leave away the notion of linear approximation in multipurpose/universal representation spaces for preferring nonlinear, adapted representations. This enters in the concept of model reduction approaches.

In this paper, we are interested in the research coming from the particular application, which is the *reconstruction of cross-sections in neutronics*.

In neutronics, cross-sections are used to represent the probability of interaction between an incident neutron and a given target nuclei ([1]). These cross-sections are inputs for the Boltzmann equation ([2]) that describes the neutron population in the core. They depend on various parameters which characterize the local material behavior. Among the parameters stand for instance: *i) burnup, ii) fuel temperature, iii) moderator density, iv) boron concentration, v) xenon level, ...* These are 5 parameters that we are interested in in this paper but there may be many more, leading to larger values of d. They are denoted by $\mathbf{x} = (x_1, \ldots, x_d)$, where here $d = 5$ and they vary in a space called *parameter-phase space*; hence cross-sections are multivariate functions of $\mathbf{x}$, $\mathbf{x} \in$ *parameter-phase space*.

There are different cross-section kinds that represent different aspects of the physics involved (fission, absorption, scattering ...). These different kinds of *reaction* are indexed by *" r"*.

The cross-sections also depend on the energy of the incident neutron, this energy is discretized through "groups" and we designate by the exponent *"g"* the incident discretized energy group. *Microscopic cross-sections* (σ) depend also on the target nuclei (or isotope), designated by *"i"*. Therefore, $\{\sigma_{r,i}^g\}$ stands for these microscopic cross-sections.

Macroscopic cross-sections (Σ) that feed the neutron flux solver are related to above quoted microscopic ones using a formula such as:

$$\Sigma_r^g = \sum_{i=1}^{I} c_i \sigma_{r,i}^g \tag{1}$$

where c_i is the concentration of isotope i.

For EDF's applications, $I \sim 50$ isotopes, $g = 2$ energy groups and $r \sim 10$ reactions, we obtain already one thousand types of microscopic cross-sections, i.e. one thousand multivariate functions to approximate.

In the current core simulations, the core is described as a full three-dimensional object $\subset \mathbb{R}^3$. At each different position P in the core, we have specific thermo-hydraulic-state conditions, leading to a corresponding value of $\mathbf{x} = (x_1, \ldots, x_d)$ in the parameter-phase space. It means that the cross-sections $\{\sigma_{r,i}^g\}$, $\{\Sigma_r^g\}$ that are functions of $\mathbf{x}$ thus depend (implicitly) on the position P in the core since $\mathbf{x}$ is a function of P: $P \in \mathbb{R}^3 \mapsto \mathbf{x}(P)$.

In practice, the core is discretized into cells. Therefore, $\mathbf{x}$ depends now on the position k of a cell, $\mathbf{x} = \mathbf{x}(\text{cell}_k)$. Hence, cross-sections need to be determined cell per cell (see Fig. 1).

In the core simulation, we need accurate values for the various cross-sections at all cells (about 200,000 cells for industrial cases and 10 times more for "reference" cases). This leads to a number of cross-section values needed for the simulation which scales in billions.