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Model Interpretation via Multivariate Padé-Approximant in Low-Rank Format

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Summary:

The aim of this paper is to present a computationally efficient method for approximation of a response function in several variables using a novel class of multivariate rational functions in low-rank format, constructed via power series summation. This method is well suited for high-dimensional problems where evaluating response function will take long time. In addition to sensitivity analysis, models based on the rational functions, are able to provide further insight into response of a man-made systems (or physical phenomena) under investigation; e.g. it is possible to reconstruct response hypersurfaces beyond region that was used to build the approximation, and certain types of singularities can be located with high accuracy.

The concept of Padé-approximants, which is the kernel of the proposed method, has been already generalized to multivariate function approximation [1]. It is well known that such approximants, applied in summation of power series, are useful for interpretation of models (i.e. parametrized response functions). "Magically", it is possible to deduce important properties of a model from a given power series. For example, local behavior near a singularity, characterized with parameter values for which a model is unbounded or not unique, can be analyzed. It is important to note that Padé approximation is the optimal technique in the construction of models that belong to the class of rational functions, and for more general class of algebraic-function models, the Hermite-Padé-approximants are more suitable [2]. In this paper, we propose the method that is able to reduce computational cost of constructing the multivariate Padé approximants [1]. Brief description of the method is presented in the sequel.

Consider power series expansion of a multivariate function,

$$f(z) = \sum_{\nu} f_{\nu}(z-c)^{\nu}, \tag{1}$$

where $\nu = (\nu_1, \dots, \nu_d) \in \mathbb{Z}_{\geq 0}^d$ is the multi-index ($\mathbb{Z}_{\geq 0}^d$ denotes the set of non-negative integers), $z = (z_1, \dots z_d) \in \mathbb{C}^d$ where $\mathbb{C}$ denotes the set of complex numbers, and $c = (c_1, \dots, c_d)$ is an approximation centre point. To each multi-index ν corresponds the product function $(z-c)^{\nu} = \prod_{k=1}^{d}(z_k - c_k)^{\nu_k}$.

The coefficients $f_{\nu} = f_{\nu_1,\dots,\nu_d}$ in (1) are computed by introducing the variable transformations $z_k = c_k + \rho_k \exp(i\theta_k), k = 1, \dots, d$, $i = \sqrt{-1}$, and rewriting (1) as

$$f(\theta) = \sum_{\nu} f_{\nu}\rho^{\nu}\exp(i\nu \cdot \theta), \tag{2}$$

where $\nu \cdot \theta$ denotes the dot product so $\exp(i\nu \cdot \theta) = \prod_{k=1}^{d}\exp(i\nu_k\theta_k)$, $\theta = (\theta_1, \dots, \theta_d) \in \mathbb{R}^d$ ($\mathbb{R}$ is the set of real numbers), $\rho = (\rho_1, \dots, \rho_d) \in \mathbb{R}^d$ is the radius vector, and $\rho^{\nu} = \prod_{k=1}^{d}\rho_k{}^{\nu_k}$. Radius vector ρ and centre point c are problem-dependent; values are selected so that function samples are generated within the region where $f(z)$ is analytic and where the power series (1) converges.

Discretisation points of the function $f(\theta)$ on a tensor product grid, defined on the hypercube domain $\{0 \leq \theta_k \leq 2\pi, 1 \leq k \leq d\}$, can be stored as a multidimensional data array (i.e. tensor) with elements

$$F(i_1, \dots, i_d) = f(\theta_1(i_1), \dots, \theta_d(i_d)). \tag{3}$$

Abbreviated expression of (3) would be: $F(i) = f\big(\theta(i)\big)$, where $i = (i_1, \dots, i_d) \in \mathbb{Z}_{>0}^d$ ($\mathbb{Z}_{>0}^d$ denotes the set of positive integers). Equidistant sampling points $\theta_k(i_k) = 2\pi(i_k - 1)/n_k$, $i_k = 1, \dots, n_k$, are used since $f(\theta)$ is a 2π-periodic function of θ. The expression (2) is the multivariate trigonometric series, therefore we use Discrete Fourier Transform (DFT) to compute the coefficients in (1):

$$f_{\nu} = \frac{1}{\rho^{\nu} N}\sum_{i} F(i)\exp[-i\nu \cdot \theta(i)], \tag{4}$$

where $N = \prod_{k=1}^{d} n_k$ and $\exp[-i\nu \cdot \theta(i)] = \prod_{k=1}^{d} \exp[-i\nu_k \theta_k(i_k)]$.

In many practical problems, multivariate functions can be well approximated using a sum of finitely many separable functions. Such functions belong to the class of semi-separable functions; the following notation is used to represent such functions: $f(\theta_1, \dots, \theta_d) = \mathbb{F}_1(\theta_1) \cdots \mathbb{F}_d(\theta_d)$, where $\mathbb{F}_k(\theta_k)$ are $r_{k-1} \times r_k$ arrays with univariate functions as elements. Therefore, after discretisation, the tensor representing a semi-separable function can be written in the following matrix-product form:

$$F(i_1, \dots, i_d) = \mathrm{F}_1(i_1) \cdots \mathrm{F}_d(i_d), \tag{5}$$

where $\mathrm{F}_k(i_k), k = 1, \dots, d$, are index i_k - dependent matrices of the sizes $r_{k-1} \times r_k$. By exploiting the semi-separable structure, it is possible to overcome curse of dimensionality occurring when sampling on a tensor product grid. Number of stored elements in (5) is $\mathcal{O}(dnr^2)$ compared to $\mathcal{O}(n^d)$ elements in tensor product grid (3), where $n = \max(n_1, \dots, n_d)$ and $r = \max(r_0, \dots, r_d)$. Therefore, when the rank r is low, we can achieve considerable savings compared to tensor product grid. When constructing (5), we have used the tensor cross interpolation algorithm [3]. This is similar to the strategy used for the Tensor Train (TT) decomposition based on sequential application of the Singular Value Decomposition (SVD) algorithm to construct low-rank approximations of unfolding matrices [4]. However, there are two major improvements which considerably reduce number of function evaluations: a) avoid to use complete unfolding matrices (contain all tensor elements), but rather their sub-matrices which size increases during iterative process; and b) replace the SVD algorithm with the matrix cross interpolation.

When the tensor $F(i)$ is available in the matrix-product form (5), the multivariate DFT (4) can be computed efficiently as the product of univariate DFTs,

$$f_{\nu_1,\dots,\nu_d} = \prod_{k=1}^{d} \mathcal{F}_k(\nu_k) = \prod_{k=1}^{d} \frac{1}{n_k \rho_k^{\nu_k}} \sum_{i_k=1}^{N_k} \mathrm{F}_k(i_k) \exp[-i\nu_k \theta_k(i_k)], \tag{6}$$

and then the power series expansion (1) is approximated as a product of $r_{k-1} \times r_k$ arrays storing univariate expansions,

$$f(z_1, \dots z_d) = \prod_{k=1}^{d} \sum_{\nu_k} \mathcal{F}_k(\nu_k)(z_k - c_k)^{\nu_k}. \tag{7}$$

Finally, the SVD-based univariate Padé approximation algorithm [5] is applied in the summation of each univariate series in (7), and the following low-rank structure of the multivariate Padé - approximant is obtained:

$$f(z_1, \dots z_d) = \prod_{k=1}^{d} \mathbb{P}_k(z_k), \tag{8}$$

where the elements of $r_{k-1} \times r_k$ arrays $\mathbb{P}_k(z_k), k = 1, \dots, d$, are univariate rational functions.

Numerical examples are devised to illustrate efficiency and accuracy of the proposed method. In addition, this paper presents a practical application of the method. We show how to reconstruct solution hypersurfaces and locate singularities in the non-linear power flow problem associated with investigation of steady-state voltage stability in electric power networks [6].

References:

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