Adaptive Cross Approximation of Multivariate Functions

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In this article we present and analyze a new scheme for the approximation of multivariate functions ($d = 3, 4$) by sums of products of univariate functions. The method is based on the Adaptive Cross Approximation (ACA) initially designed for the approximation of bivariate functions. To demonstrate the linear complexity of the schemes we apply it to large-scale multidimensional arrays generated by the evaluation of functions.

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1 Introduction

Representations of functions κ of several variables by sums of functions of fever variables have been investigated in many publications; see [22] and the references therein. The best L^2-approximation of functions of two variables is shown in [23, 25] to be given by the truncated Hilbert-Schmidt decomposition. This result was extended by Pospelov [21] to the approximation of functions in d variables by sums of products of functions of one variable. For some classes of fuctions the approximation by specific function systems such as exponential functions might be advantageous; see [8, 9], [7]. One of the best known decompositions in statistics is the *analysis of variance* (ANOVA) decomposition [15]. Related to this field of research are *sparse grid* approximations; see [28, 10].

An important application of this kind of approximation is the approximation of multidimensional arrays generated by the evaluation of functions. In this case a d-dimensional tensor is approximated by the tensor product of a small number of vectors, which significantly improves the computational complexity. Multidimensional arrays of data appear in many different applications, e.g. statistics, chemometrics, and finance. While for $d = 2$ a result due to Eckart and Young [12] states that the optimal rank-k approximation can be computed via the singular value decomposition (SVD), the generalization of the SVD for tensors of order more than two is not clear; see the counterexample in [18]. In the *Tucker model* [27] a third order tensor is approximated by

$$\sum_{i=1}^{r_1}\sum_{j=1}^{r_2}\sum_{k=1}^{r_3} g_{ijk}\, x_i \otimes y_j \otimes z_k$$

with the so-called core array g and the Tucker vectors x_i, y_j, and z_k. The PARAFAC model [11] uses diagonal core arrays. A method for third order tensors is proposed in [16]. Multi-level decompositions

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are presented in [17]. The most popular method is based on alternating least squares minimization [19, 26]. In [29] an incremental method, i.e. the approximation is successively constructed from the respective remainder, is proposed. While our technique also is based on successive rank-1 approximations, in [29] the optimal rank-1 approximation is computed via a generalized Rayleigh quotient iteration. Since all previous methods require the whole matrix for constructing the respective approximation, they may be computationally still too expensive. We present a method having linear complexity using a small portion of the original matrix entries.

In [3] the *adaptive cross approximation* (ACA) was introduced. ACA approximates bivariate functions κ by sums of products of univariate functions. A characteristic property of ACA is that the approximation is constructed from restrictions of κ to lower dimensional domains of definition, i.e.

$$\kappa(x,y) \approx \sum_{i,j=1}^{k} \alpha_{ij}\kappa(x_i,y)\kappa(x,y_j)$$

with points x_i, y_j and coefficients α_{ij} which constitute the inverse of the matrix $\kappa(x_i,y_j)$, $i,j = 1,\dots,k$. The advantages of the fact that the restrictions $\kappa(x_i,y)$ and $\kappa(x,y_j)$, $i,j = 1,\dots,k$, are used, are manifold. First of all it can be seen that this kind of approximation allows to guarantee quasi-optimal accuracy, i.e. the quality of the approximation will (up to constants) be at least as good as the approximation in any other system of functions of the same cardinality. Furthermore, matrix versions of ACA are able to construct approximations without computing all the matrix entries in advance, only the entries corresponding to the restrictions have to be evaluated. Furthermore, the method is adaptive because it is able to find the required rank k in the course of the approximation.

In the present article the adaptive cross approximation will be extended to functions of three and four variables. The latter two classes of functions will be treated by algorithms which together with the bivariate ACA can be investigated in the general setting of what we call incremental approximation. These will be introduced and investigated in Sect. 2. The convergence analysis of the bivariate ACA can be obtained as a special case. Furthermore, in Sect. 3 we will show convergence also for singular functions. A principle difference appears if ACA is extended to more than two variables, because the dimension of the restricted domains of definition of the approximations are still more than one-dimensional. Hence, further approximation of these restrictions by an ACA of lower dimension is required. As a consequence, the influence of perturbation on the convergence has to be analyzed. In the trivariate case treated in Sect. 4 one additional approximation using bivariate ACA per step is sufficient. The approximation of functions of four variables is treated in Sect. 5 and requires two additional bivariate ACA approximations per step. To demonstrate the linear complexity of the presented techniques, our theoretical findings are accompanied by the application of the presented schemes to large-scale multidimensional arrays. A method that is similar to the kind of matrix approximation treated in this article (at least for the trivariate case) was presented in [20]. Although it is proved in [20] that low-rank approximations exist, the convergence of the actual scheme has not been analyzed.

As the need for techniques required to analyze the influence of perturbations on the convergence already appears in the cases of three and four variables, the results of this article are expected to be useful also for problems of more than four dimensions, because algorithms can be constructed by recursive bisection of the set of variables; see also [14]. In this sense this article lays ground to the adaptive cross approximation of high-dimensional functions.

2 Incremental Approximation

The approximation schemes considered in this article will be of the following form. Given a set X and a function $f : X \to \mathbb{C}$, define $r_0[f] := f$ and $r_k[f]$, $k = 1, 2, \dots,$ as

$$r_k[f] = r_{k-1}[f] - \frac{r_{k-1}[f](x_k)}{\ell_k(x_k)}\ell_k. \tag{1}$$

Here, x_k is chosen such that $\ell_k(x_k) \neq 0$. The choice of the functions $\ell_k : X \to \mathbb{C}$ defines the respective approximation scheme. Since the evaluation of functions at given points is central for our methods, we assume that f and ℓ_k are continuous on X. In the following lemmas properties of $r_k[f]$ will be investigated.

Lemma 1. *For $r_k[f]$ the non-recursive representation*

$$r_k[f] = f - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} \tag{2}$$

holds, where

$$U_k := \begin{bmatrix} \ell_1(x_1) & \dots & \dots & \ell_1(x_k) \\ 0 & \ell_2(x_2) & & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \ell_k(x_k) \end{bmatrix}.$$

Proof. The assertion is obviously true for $k = 1$. Assume that it is valid for $k - 1$. Then we obtain that

$$\begin{aligned} r_k &= r_{k-1} - \frac{r_{k-1}(x_k)}{\ell_k(x_k)}\ell_k \\ &= f - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_{k-1}) \end{bmatrix}^T U_{k-1}^{-1} \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_{k-1} \end{bmatrix} - \left(f(x_k) - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_{k-1}) \end{bmatrix}^T U_{k-1}^{-1} \begin{bmatrix} \ell_1(x_k) \\ \vdots \\ \ell_{k-1}(x_k) \end{bmatrix} \right) \frac{\ell_k}{\ell_k(x_k)}, \end{aligned}$$

which ends the proof, because

$$\begin{bmatrix} A & b \\ & \gamma \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} & -A^{-1}b/\gamma \\ & 1/\gamma \end{bmatrix}, \tag{3}$$

where A is a non-singular matrix and $0 \neq \gamma \in \mathbb{C}$. □

The previous lemma shows that the constructed approximation

$$s_k[f] := f - r_k[f]$$

is in the linear hull of the functions $\ell_1, \dots, \ell_k$. The following lemma shows an equivalent expression for the coefficients. In addition to the vector in (4) the quantities

$$\sigma_{i,k} := \sup_{x \in X} \sum_{\nu=i}^{k} |\xi_\nu^{(k)}(x)|$$

defined on the components of $\xi^{(k)} : X \to \mathbb{C}^k$,

$$\xi^{(k)} := U_k^{-1} \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix},$$

will play an important role in the stability analysis.

Lemma 2. *It holds that*

$$U_k^{-T} \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix} = \begin{bmatrix} \frac{r_0[f](x_1)}{\ell_1(x_1)} \\ \vdots \\ \frac{r_{k-1}[f](x_k)}{\ell_k(x_k)} \end{bmatrix}. \tag{4}$$

Hence,

$$s_k[f] = \sum_{i=1}^{k} r_{i-1}[f](x_i) \frac{\ell_i}{\ell_i(x_i)}.$$

Proof. Formula (4) is obviously true for $k = 1$. Assume that it is valid for $k - 1$, then using (3)

$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T \begin{bmatrix} U_{k-1}^{-1} & v_{k-1} \\ & \frac{1}{\ell_k(x_k)} \end{bmatrix},$$

where

$$v_{k-1} = -U_{k-1}^{-1} \begin{bmatrix} \ell_1(x_k) \\ \vdots \\ \ell_{k-1}(x_k) \end{bmatrix} / \ell_k(x_k).$$

From (2) together with the assumption, we obtain

$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} = \left[\frac{r_0(x_1)}{\ell_1(x_1)}, \ldots, \frac{r_{k-2}(x_{k-1})}{\ell_{k-1}(x_{k-1})}, \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_{k-1}) \end{bmatrix}^T v_{k-1} + \frac{f(x_k)}{\ell_k(x_k)} \right] = \left[\frac{r_0(x_1)}{\ell_1(x_1)}, \ldots, \frac{r_{k-1}(x_k)}{\ell_k(x_k)} \right].$$

□

In the following lemma we will investigate under which conditions on ℓ_k the function $s_k[f]$ interpolates f. Notice that $r_k[f](x_k) = 0$. However, $r_k[f](x_j)$ does not vanish for $j < k$ in general. The desired interpolation property will be characterized by the coincidence of the upper triangular matrix U_k with the $k \times k$ matrix

$$M_k := \begin{bmatrix} \ell_1(x_1) & \ldots & \ell_1(x_k) \\ \vdots & & \vdots \\ \ell_k(x_1) & \ldots & \ell_k(x_k) \end{bmatrix}$$

or equivalently by $\ell_i(x_j) = 0$ for $i > j$.

Lemma 3. *For $1 \leq j < k$ it holds that*

$$r_k[f](x_j) = - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \ell_{j+1}(x_j) \\ \vdots \\ \ell_k(x_j) \end{bmatrix}. \tag{5}$$

Hence, $s_k[f](x_j) = f(x_j)$, $1 \le j \le k$, if $M_k = U_k$. In the other case we have that $s_k[f](x_j) = (\tilde{f}_k)_j$, $1 \le j \le k$, where

$$\tilde{f}_k := (U_k^{-1} M_k)^T \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}.$$

Proof. Since $r_j(x_j) = 0$, we have that

$$f(x_j) = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_j) \end{bmatrix}^T U_j^{-1} \begin{bmatrix} \ell_1(x_j) \\ \vdots \\ \ell_j(x_j) \end{bmatrix}.$$

Formula (5) follows from

$$r_k(x_j) = f(x_j) - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \begin{bmatrix} \ell_1(x_j) \\ \vdots \\ \ell_k(x_j) \end{bmatrix} \tag{6}$$

and the upper triangular structure of U_k which contains U_j in the leading $j \times j$ subblock.

The second part

$$\begin{bmatrix} s_k(x_1) \\ \vdots \\ s_k(x_k) \end{bmatrix}^T = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} M_k$$

follows from $s_k = f - r_k$ and (6).

□

Remark 1. *Let M_k be non-singular. We denote by $M_k^{(i)}(x) \in \mathbb{C}^{k \times k}$ the matrix which arises from replacing the i-th column of M_k by the vector $v_k := [\ell_1(x), \ldots, \ell_k(x)]^T$. The functions*

$$L_i[f](x) := (M_k^{-1} v_k)_i = \frac{\det M_k^{(i)}(x)}{\det M_k} \in \operatorname{span}\{\ell_1, \ldots, \ell_k\}$$

are Lagrange functions for the points $x_1, \ldots, x_k$, i.e. $L_i[f](x_j) = \delta_{ij}$, $i, j = 1, \ldots, k$. As a consequence of Lemma 3, the approximation

$$s_k[f] = \sum_{i=1}^{k} (\tilde{f}_k)_i L_i[f]$$

is the uniquely defined Lagrangian interpolating function.

The following lemmas will help estimating the remainder r_k of the approximation. We first observe the following property.

Lemma 4. *Let $M_k = U_k$ and let functions $\hat{\ell}_1, \ldots, \hat{\ell}_k$ satisfy $\operatorname{span}\{\hat{\ell}_1, \ldots, \hat{\ell}_k\} = \operatorname{span}\{\ell_1, \ldots, \ell_k\}$. Then $\hat{M} \in \mathbb{C}^{k \times k}$ defined by $\hat{M}_{ij} = \hat{\ell}_i(x_j)$, $i, j = 1, \ldots, k$, is non-singular and*

$$r_k[f] = f - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T \hat{M}_k^{-1} \begin{bmatrix} \hat{\ell}_1 \\ \vdots \\ \hat{\ell}_k \end{bmatrix}.$$

Proof. Let $C \in \mathbb{C}^{k\times k}$ be an invertible matrix such that

$$\begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} = C \begin{bmatrix} \hat{\ell}_1 \\ \vdots \\ \hat{\ell}_k \end{bmatrix}.$$

Then it follows from $M_k = C\hat{M}_k$ that $\hat{M}_k$ is invertible and

$$M_k^{-1} \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} = \hat{M}_k^{-1} \begin{bmatrix} \hat{\ell}_1 \\ \vdots \\ \hat{\ell}_k \end{bmatrix}.$$

Lemma 1 gives the assertion. □

In the following lemma the remainder $r_k[f]$ is expressed as the error

$$\mathcal{E}_k[f](x) := f(x) - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T \Psi_k(x)$$

of a linear approximation in an arbitrary system $\{\psi_1, \ldots, \psi_k\} \subset C(X)$ of functions. Here, we set $\Psi_k := [\psi_1, \ldots, \psi_k]^T$.

Lemma 5. *It holds that*

$$r_k[f] = \mathcal{E}_k[f] - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1}(M_k - U_k)\Psi_k - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \begin{bmatrix} \mathcal{E}_k[\ell_1] \\ \vdots \\ \mathcal{E}_k[\ell_k] \end{bmatrix}.$$

In particular, if $M_k = U_k$, then

$$r_k[f] = \mathcal{E}_k[f] - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T \hat{M}_k^{-1} \begin{bmatrix} \mathcal{E}_k[\hat{\ell}_1] \\ \vdots \\ \mathcal{E}_k[\hat{\ell}_k] \end{bmatrix},$$

where $\hat{M}_k$ and $\hat{\ell}_1, \ldots, \hat{\ell}_k$ are as in Lemma 4.

Proof. The assertion follows from

$$\begin{aligned} r_k &= f - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} = f - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} M_k \Psi_k - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \left(\begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} - M_k \Psi_k \right) \\ &= f - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T \Psi_k - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \left(M_k - U_k \right) \Psi_k - \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \begin{bmatrix} \mathcal{E}_k[\ell_1] \\ \vdots \\ \mathcal{E}_k[\ell_k] \end{bmatrix}. \end{aligned}$$

The second part of the assertion follows from Lemma 4. □

Remark 2. *The previous lemma relates the remainder $r_k[f]$ to the error $\mathcal{E}_k[f]$ in the system Ψ_k. Assume that Ψ_k are Lagrange functions, i.e. $\psi_i(x_j) = \delta_{ij}$, $i, j = 1, \dots, k$. If $r_k[f]$ is to be estimated by the best approximation error in Ψ_k, then one can use the estimate*

$$\|\mathcal{E}_k[f]\|_\infty \le (1 + \|\mathcal{I}_k\|) \inf_{\psi \in \Psi_k} \|f - \psi\|_\infty, \tag{7}$$

where $\mathcal{I}_k : C(X) \to C(X)$ defined as $\mathcal{I}_k f = \sum_{i=1}^k f(x_i)\psi_i$ denotes the interpolation operator in Ψ_k and $\|\mathcal{I}_k\| := \sup\{\|\mathcal{I}_k f\|_\infty,\ f \in C(X),\ \|f\|_\infty = 1\}$. Estimate (7) is a consequence of

$$\|f - \mathcal{I}_k f\|_\infty \le \|f - \psi\|_\infty + \|\mathcal{I}_k(f - \psi)\|_\infty \le (1 + \|\mathcal{I}_k\|_\infty)\|f - \psi\|_\infty$$

for all $\psi \in \Psi_k$.

2.1 Perturbation analysis

The next question we are going to investigate is how approximations $\tilde{\ell}_k$ to the functions ℓ_k influence the approximation error $r_k[f]$, i.e., we will compare the remainder $r_k[f]$ with $\tilde{r}_k[f]$ defined by $\tilde{r}_0[f] = f$ and

$$\tilde{r}_k[f] = \tilde{r}_{k-1}[f] - \frac{\tilde{r}_{k-1}[f](x_k)}{\tilde{\ell}_k(x_k)}\tilde{\ell}_k, \quad k = 1, 2, \dots. \tag{8}$$

In (8) x_k is chosen such that $\tilde{\ell}_k(x_k) \neq 0$. Define $\tilde{U}_k$, $\tilde{\xi}^{(k)}$, and $\tilde{\sigma}_{i,k}$ by replacing ℓ_i in the respective definition with $\tilde{\ell}_i$. Notice that we use the same points x_k from the construction of $\tilde{r}_k[f]$ also for the construction of $r_k[f]$. Therefore, we have to make sure that U_k is invertible.

Lemma 6. *Let $\varepsilon_i := \|\tilde{\ell}_i - \ell_i\|_\infty$ such that $\varepsilon_i < |\tilde{\ell}_i(x_i)|$, $i = 1, \dots, k$. Then $\ell_i(x_i) \neq 0$ and*

$$\|\tilde{r}_k[f] - r_k[f]\|_\infty \le \sum_{i=1}^k \frac{|r_{i-1}[f](x_i)|}{|\ell_i(x_i)|}\,(\tilde{\sigma}_{i,k} + 1)\,\varepsilon_i.$$

Proof. From $|\ell_i(x_i)| \ge |\tilde{\ell}_i(x_i)| - \varepsilon_i > 0$ it follows that U_k is invertible. Setting

$$E_k = U_k - \tilde{U}_k \quad \text{and} \quad \delta^{(k)} = \begin{bmatrix} \tilde{\ell}_1 - \ell_1 \\ \vdots \\ \tilde{\ell}_k - \ell_k \end{bmatrix},$$

due to Lemma 1 and Lemma 2 we have that

$$\begin{aligned}
\tilde{r}_k - r_k &= \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T \left(\tilde{U}_k^{-1} \begin{bmatrix} \tilde{\ell}_1 \\ \vdots \\ \tilde{\ell}_k \end{bmatrix} - U_k^{-1} \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} \right) = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \left((\tilde{U}_k + E_k)\tilde{U}_k^{-1} \begin{bmatrix} \tilde{\ell}_1 \\ \vdots \\ \tilde{\ell}_k \end{bmatrix} - \begin{bmatrix} \ell_1 \\ \vdots \\ \ell_k \end{bmatrix} \right) \\
&= \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{bmatrix}^T U_k^{-1} \left(\delta^{(k)} + E_k \tilde{U}_k^{-1} \begin{bmatrix} \tilde{\ell}_1 \\ \vdots \\ \tilde{\ell}_k \end{bmatrix} \right) = \begin{bmatrix} \frac{r_0(x_1)}{\ell_1(x_1)} \\ \vdots \\ \frac{r_{k-1}(x_k)}{\ell_k(x_k)} \end{bmatrix}^T \left(\delta^{(k)} + E_k \tilde{\xi}^{(k)} \right).
\end{aligned}$$

The assertion follows from $\|\delta_i^{(k)}\|_\infty \le \varepsilon_i$, $\|(E_k)_{ij}\|_\infty \le \varepsilon_i$, and $(E_k)_{ij} = 0$ for $i > j$. □

In addition to (8) one may also consider the following scheme, in which $\tilde{r}_{k-1}[f](x_k)$ is replaced by some value $a_k \in \mathbb{C}$:

$$\tilde{\tilde{r}}_k[f] = \tilde{\tilde{r}}_{k-1}[f] - \frac{a_k}{\tilde{\ell}_k(x_k)}\tilde{\ell}_k. \tag{9}$$

Then $\tilde{\tilde{r}}_k[f]$ will usually neither vanish in the points x_j, $1 \le j < k$, nor a representation (2) will hold. However, the following lemma can be proved. We will make use of the recursive relation

$$\xi_i^{(k)} = \xi_i^{(k-1)} - \frac{\ell_k}{\ell_k(x_k)} \xi_i^{(k-1)}(x_k), \quad i = 1, \dots, k-1, \tag{10a}$$

$$\xi_k^{(k)} = \frac{\ell_k}{\ell_k(x_k)}, \tag{10b}$$

for the components of $\xi^{(k)}$, which follows from (3).

Lemma 7. *Let $\varepsilon_j := \tilde{\tilde{r}}_{j-1}[f](x_j) - a_j$ such that $|\varepsilon_j| \le \varepsilon$, $1 \le j \le k$. Then*

$$\tilde{\tilde{r}}_k[f] = \tilde{r}_k[f] + \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_k \end{bmatrix}^T \tilde{U}_k^{-1} \begin{bmatrix} \tilde{\ell}_1 \\ \vdots \\ \tilde{\ell}_k \end{bmatrix}.$$

Hence,

$$\|\tilde{r}_k[f] - \tilde{\tilde{r}}_k[f]\|_\infty \le \sup_{x \in X} \sum_{j=1}^{k} |\tilde{\xi}_j^{(k)}(x)|\, |\varepsilon_j| \le \tilde{\sigma}_{1,k} \varepsilon.$$

Proof. The assertion is proved by induction. It is obviously true for $k = 1$. Assume that it is valid for $k-1$. Then

$$\begin{aligned}
\tilde{\tilde{r}}_k &= \tilde{\tilde{r}}_{k-1} - \frac{\tilde{\tilde{r}}_{k-1}(x_k)}{\tilde{\ell}_k(x_k)} \tilde{\ell}_k + \frac{\tilde{\ell}_k}{\tilde{\ell}_k(x_k)} \varepsilon_k \\
&= \tilde{r}_{k-1} + \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_{k-1} \end{bmatrix}^T \tilde{\xi}^{(k-1)} - \frac{\tilde{\ell}_k}{\tilde{\ell}_k(x_k)} \left(\tilde{r}_{k-1}(x_k) + \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_{k-1} \end{bmatrix}^T \tilde{\xi}^{(k-1)}(x_k) \right) + \frac{\tilde{\ell}_k}{\tilde{\ell}_k(x_k)} \varepsilon_k \\
&= \tilde{r}_k + \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_{k-1} \end{bmatrix}^T \tilde{\xi}^{(k-1)} - \frac{\tilde{\ell}_k}{\tilde{\ell}_k(x_k)} \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_{k-1} \end{bmatrix}^T \tilde{\xi}^{(k-1)}(x_k) + \frac{\tilde{\ell}_k}{\tilde{\ell}_k(x_k)} \varepsilon_k.
\end{aligned}$$

Equation (10) finishes the proof. □

2.2 Estimating the amplification factors

As it can be seen from Lemma 6 and Lemma 7, for the perturbation analysis it is crucial to estimate the size of the amplification factors $\xi^{(k)}$. The following lemma is an obvious consequence of (10). Let $v_j : X \to \mathbb{C}$, $j = 1, \dots, k$, be given functions and set

$$\hat{\xi}^{(k)} := U_k^{-1} \begin{bmatrix} v_1 \\ \vdots \\ v_k \end{bmatrix}.$$

Lemma 8. *If there is $\mu \ge 1$ such that $\|v_i\|_\infty \le \mu |\ell_i(x_i)|$ for $i = 1, \dots, k$, then*

$$\|\hat{\xi}_i^{(k)}\|_\infty \le \mu \left(1 + \sum_{j=i}^{k-1} \|\xi_i^{(j)}\|_\infty \right).$$

Furthermore, $\|\xi_i^{(k)}\|_\infty \le \nu(1+\nu)^{k-i}$ provided that $\|\ell_i\|_\infty \le \nu |\ell_i(x_i)|$ for some $\nu \in \mathbb{R}$.

Proof. It readily follows from (10) that $\|\xi_i^{(k)}\|_\infty \le \nu(1+\nu)^{k-i}$. Similar to (10) we obtain the following recursion formula for the components of $\hat{\xi}^{(k)}$:

$$\begin{aligned}\hat{\xi}_i^{(k)} &= \hat{\xi}_i^{(k-1)} - \frac{v_k}{\ell_k(x_k)}\xi_i^{(k-1)}(x_k), \quad i = 1,\dots,k-1,\\ \hat{\xi}_k^{(k)} &= \frac{v_k}{\ell_k(x_k)},\end{aligned}$$

which shows $\|\hat{\xi}_i^{(i)}\|_\infty \le \mu$ and the recursive relation

$$\|\hat{\xi}_i^{(j+1)}\|_\infty \le \|\hat{\xi}_i^{(j)}\|_\infty + \mu\|\xi_i^{(j)}\|_\infty, \quad j = k-1,\dots,i.$$

Hence, we obtain that

$$\|\hat{\xi}_i^{(k)}\|_\infty \le \mu + \mu\sum_{j=i}^{k-1}\|\xi_i^{(j)}\|_\infty.$$

□

In particular the previous lemma shows that $\|\xi_i^{(k)}\|_\infty \le 2^{k-i}$ provided that x_i maximizes $|\ell_i|$. In this case we have

$$\sigma_{i,k} \le \sum_{\nu=i}^{k}\|\xi_\nu^{(k)}\|_\infty \le \sum_{\nu=i}^{k} 2^{k-\nu} = 2^{k-i+1} - 1.$$

If ℓ_i, $i = 1,\dots,k$, are smooth, i.e. if we may assume that

$$|\mathcal{E}_{k-i}[\ell_{i+\mu}](x)| \le \varepsilon|\ell_{i+\mu}(x_{i+\mu})|, \quad \mu = 0,\dots,k-i, \tag{11}$$

with some $\varepsilon > 0$ and if $\ell_i(x_j) = 0$, $i > j$, then significantly better bounds for $\|\xi_i^{(k)}\|_\infty$ can be derived. Due to (10) each $\xi_i^{(k)}$, $1 \le i \le k$, can be regarded as a remainder function of an approximation of type (1) with $f' := \xi_i^{(i)}$ and $\ell'_j := \xi_{i+j}^{(i+j)}$, because it follows from (10) that

$$\begin{aligned}\xi_i^{(i)}(x) &= \frac{\ell_i(x)}{\ell_i(x_i)},\\ \xi_i^{(i+j)}(x) &= \xi_i^{(i+j-1)}(x) - \frac{\ell_{i+j}(x)}{\ell_{i+j}(x_{i+j})}\xi_i^{(i+j-1)}(x_{i+j}), \quad j = 1,\dots,k-i.\end{aligned}$$

Since $\operatorname{span}\{\ell'_1,\dots,\ell'_{k-i}\} = \operatorname{span}\{\ell_{i+1},\dots,\ell_k\}$, Lemma 5 shows that

$$\xi_i^{(k)}(x) = \mathcal{E}_{k-i}[\xi_i^{(i)}](x) - \begin{bmatrix}\xi_i^{(i)}(x_{i+1})\\ \vdots\\ \xi_i^{(i)}(x_k)\end{bmatrix}^T (M'_{k-i})^{-1}\begin{bmatrix}\mathcal{E}_{k-i}[\ell_{i+1}](x)\\ \vdots\\ \mathcal{E}_{k-i}[\ell_k](x)\end{bmatrix},$$

where $(M'_{k-i})_{\mu\nu} = \ell_{i+\mu}(x_{i+\nu})$, $\mu,\nu = 1,\dots,k-i$. Hence, from (11) and Lemma 8 we obtain that

$$\|\xi_i^{(k)}\|_\infty \le \varepsilon + \varepsilon\sum_{\nu=1}^{k-i}|\xi_i^{(i)}(x_{i+\nu})|\left(1 + \sum_{j=\nu}^{k-i-1} 2^{j-\nu}\right) \le 2^{k-i}\varepsilon, \tag{12}$$

because $M'_{k-i} = U'_{k-i}$ and $|\xi_i^{(i)}(x_j)| \le 1$, $j = i+1,\dots,k$, provided that x_i maximizes $|\ell_i|$.

We will, however, see in the numerical examples that typically $\|\xi_i^{(k)}\|_\infty$ is significantly smaller than predicted by our worst-case estimates.

3 Adaptive Cross Approximation

The adaptive cross approximation (ACA) was introduced for Nyström matrices [3] and extended to collocation matrices [6]. A version with refined pivoting strategy and a generalization of the method to Galerkin matrices was presented in [5]. The following recursion is in the core of this method. Given $\kappa : X \times Y \to \mathbb{C}$, let $R_0(x, y) = \kappa(x, y)$ and

$$R_k(x, y) = R_{k-1}(x, y) - \frac{R_{k-1}(x, y_k)R_{k-1}(x_k, y)}{R_{k-1}(x_k, y_k)}, \quad k = 1, 2, \ldots. \tag{13}$$

The points x_k and y_k are chosen such that $R_{k-1}(x_k, y_k) \neq 0$. The previous recursion corresponds to the choice

$$f := \kappa_x, \quad \ell_i := R_{i-1}(x_i, \cdot)$$

in (1) if $x \in X$ is treated as a parameter. Then $R_k(x, y) = r_k[\kappa_x](y)$ holds, where κ_x is defined by $\kappa_x(y) = \kappa(x, y)$ for all $x \in X$, and $\ell_i(y_j) = 0$ for $i > j$ can be seen from inductively applying Lemma 3. Since

$$\operatorname{span}\{\ell_1, \ldots, \ell_k\} = \operatorname{span}\{\kappa(x_1, \cdot), \ldots, \kappa(x_k, \cdot)\},$$

we see that $\hat{\ell}_i := \kappa(x_i, \cdot)$ is a possible choice in Lemma 4. Hence, the degenerate approximation $S_k := \kappa - R_k$ of κ has the representation

$$S_k(x, y) = \begin{bmatrix} \kappa(x, y_1) \\ \vdots \\ \kappa(x, y_k) \end{bmatrix}^T \hat{M}_k^{-1} \begin{bmatrix} \kappa(x_1, y) \\ \vdots \\ \kappa(x_k, y) \end{bmatrix} = \sum_{i,j=1}^{k} (\hat{M}_k^{-1})_{ij} \kappa(x, y_i)\kappa(x_j, y)$$

with $(\hat{M}_k)_{ij} = \kappa(x_i, y_j)$, $i, j = 1, \ldots, k$.

In Lemma 5 we showed how the remainder R_k of the approximation can be estimated by relating the approximation to linear approximation in any system $\{\psi_1, \ldots, \psi_k\}$. In particular we obtain from the second part of Lemma 5 that

$$R_k(x, y) = \mathcal{E}_k[\kappa_x](y) - \begin{bmatrix} \mathcal{E}_k[\kappa_{x_1}](y) \\ \vdots \\ \mathcal{E}_k[\kappa_{x_k}](y) \end{bmatrix}^T \xi^{(k)}(x),$$

where

$$\xi^{(k)}(x) := \hat{M}_k^{-T} \begin{bmatrix} \kappa(x, y_1) \\ \vdots \\ \kappa(x, y_k) \end{bmatrix} \in \mathbb{C}^k$$

can be regarded as an amplification factor with respect to x. Therefore, we obtain

$$|R_k(x, y)| \leq (\sigma_{1,k} + 1) \max_{z \in \{x, x_1, \ldots, x_k\}} |\mathcal{E}_k[\kappa_z](y)|. \tag{14}$$

Similar to Remark 1 we denote by $\hat{M}_k^{(i)}(x)$ the matrix which arises from $\hat{M}_k$ by replacing the i-th row with the vector $[\kappa(x, y_1), \ldots, \kappa(x, y_k)]$. Then due to Cramer's rule we have that

$$\xi_i^{(k)}(x) = \frac{\det \hat{M}_k^{(i)}(x)}{\det \hat{M}_k}.$$

Hence, if the pivoting points x_i, $i = 1, \ldots, k$, are chosen such that

$$|\det \hat{M}_k^{(i)}(x)| \leq |\det \hat{M}_k| \quad \text{for all } x \in X \text{ and } i = 1, \ldots, k,$$

then $\|\xi_i^{(k)}\|_\infty = 1$, and we obtain

$$|R_k(x,y)| \le (k+1) \max_{z\in\{x,x_1,\dots,x_k\}} |\mathcal{E}_k[\kappa_z](y)|.$$

In this case of so-called matrices of maximum volume we also refer to the error estimates in [24] which are based on the technique of *exact anhilators*; see [2, 1]. In practice it is, however, difficult to find matrices of maximum volume. In Lemma 8 we observed that

$$\|\xi_i^{(k)}\|_\infty \le 2^{k-i}, \quad i = 1,\dots,k,$$

under the realistic condition

$$|R_{k-1}(x,y_k)| \le |R_{k-1}(x_k,y_k)| \quad \text{for all } x \in X. \tag{15}$$

In this case (14) becomes

$$|R_k(x,y)| \le 2^k \max_{z\in\{x,x_1,\dots,x_k\}} |\mathcal{E}_k[\kappa_z](y)|.$$

If κ is sufficiently smooth with respect to y and if the system Ψ_k is appropriately chosen, then it can be expected that for all $x \in X$

$$\|\mathcal{E}_k[\kappa_x]\|_\infty \sim \gamma^k \tag{16}$$

with some $0 < \gamma < 1$, which results in an approximation error of the order $(2\gamma)^k$. Hence, ACA convergences if $\gamma < 1/2$. Notice that the choice of y_k does not improve our estimates on the amplification factors $\xi^{(k)}$. However, it is important for obtaining a reasonable decay of the error $\mathcal{E}_k[\kappa_x]$; for details see [5].

Up to now we have exploited that κ is smooth only with respect to the second variable y. If κ is smooth also with respect to x, then the arguments from the end of Sect. 2.2 can be applied to improve the error estimate. Condition (11) is satisfied, because according to assumption (16) for $\mu = 0,\dots,k-i$ we have that

$$|\mathcal{E}_{k-i}[R_{i+\mu-1}(\cdot,y_{i+\mu})](x)| \le \varepsilon |R_{i+\mu-1}(x_{i+\mu},y_{i+\mu})|, \quad \varepsilon \sim \gamma^{k-i}.$$

Hence, if κ is smooth also with respect to x, then according to (12) we obtain $\|\xi_i^{(k)}\|_\infty \le 2^{k-i}\varepsilon$ and

$$|R_k(x,y)| \sim \gamma^k \sum_{i=1}^k 2^{k-i}\gamma^{k-i} \le 2^k\gamma^{2k} \sum_{i=1}^k \sqrt{2}^{-i}\gamma^{-i} \le \frac{2^k\gamma^{2k}}{1-\sqrt{2}\gamma},$$

which converges for $\gamma < 1/\sqrt{2}$.

Although the estimate has improved, the dependence of $\sigma_{1,k}$ on k is still exponential. The actual growth with respect to k seems to be significantly slower; see the following numerical examples.

3.1 Matrix approximation

The previous estimates can be applied when approximating function generated matrices

$$a_{ij} = \kappa(p_i,q_j), \quad i = 1,\dots,m,\ j = 1,\dots,n,$$

with $p_i \in X$ and $q_j \in Y$. In this case (13) becomes the following matrix iteration. Starting from $R_0 := A$, find a nonzero pivot (i_k,j_k) in R_k and subtract a scaled outer product of the i_k-th row and the j_k-th column:

$$R_{k+1} := R_k - [(R_k)_{i_kj_k}]^{-1}(R_k)_{1:m,j_k}(R_k)_{i_k,1:n},$$

where we use the notations $v_k := (R_{k-1})_{i_k,1:n}$ and $u_k := (R_{k-1})_{1:m,j_k}$ for the i_k-th row and the j_k-th column of R_{k-1}, respectively. We use (15) to select i_k. The choice of j_k is detailed in [5].

Since we are able to control the remainder R_k of the approximation by our estimates, it is sufficient to construct $S_k = A - R_k$, which requires the computation of only

$$u_k = (R_{k-1})_{1:m,j_k} = a_{1:m,j_k} - \sum_{\ell=1}^{k-1} \frac{(R_{\ell-1})_{i_\ell j_k}}{(R_{\ell-1})_{i_\ell j_\ell}} (R_{\ell-1})_{1:m,j_\ell} = a_{1:m,j_k} - \sum_{\ell=1}^{k-1} \frac{(v_\ell)_{j_k}}{(u_\ell)_{i_\ell}} u_\ell \tag{17}$$

and

$$v_k = (R_{k-1})_{i_k,1:n} = a_{i_k,1:n} - \sum_{\ell=1}^{k-1} \frac{(R_{\ell-1})_{i_k j_\ell}}{(R_{\ell-1})_{i_\ell j_\ell}} (R_{\ell-1})_{i_\ell,1:n} = a_{i_k,1:n} - \sum_{\ell=1}^{k-1} \frac{(u_\ell)_{i_k}}{(u_\ell)_{i_\ell}} v_\ell. \tag{18}$$

In particular this means that only $k(m+n)$ of the original entries of A have to be computed. The number of operations required for constructing $S_k = \sum_{\ell=1}^{k} u_\ell v_\ell^T$ is of the order $k^2(m+n)$, while the storage required for the approximation S_k is of the order $k(m+n)$. For further details see [4].

In the following example we consider the smooth function

$$\kappa(x,y) := \left(1 + x^2 + y^2\right)^{-1/2}, \quad x, y \in \mathbb{R},$$

and the points $p_i = q_i = \frac{1}{n}(i - \frac{1}{2})$, $i = 1, \ldots, n = m$. Table 1 shows the rank k required to satisfy

$$\|A - S_k\|_F \le \varepsilon \|A\|_F \tag{19}$$

and the CPU time in seconds on a single core of an Intel Core2 X5482 processor at 3.2 GHz. The

	$\varepsilon = 10^{-5}$				$\varepsilon = 10^{-6}$				$\varepsilon = 10^{-7}$			
	ACA		SVD		ACA		SVD		ACA		SVD	
n	k	time [s]	k	time [s]	k	time [s]	k	time [s]	k	time [s]	k	time [s]
1 250	4	0.00	3	4.2	4	0.00	4	4.2	5	0.00	4	4.2
2 500	4	0.00	3	43.1	4	0.00	4	43.1	5	0.00	4	43.1
5 000	4	0.00	3	381.7	4	0.00	4	381.7	5	0.00	4	381.7
10 000	4	0.00	–	–	4	0.00	–	–	5	0.00	–	–
20 000	4	0.00			4	0.01			5	0.01		
40 000	4	0.01			4	0.01			5	0.01		
80 000	4	0.02			4	0.03			5	0.03		
160 000	4	0.06			4	0.06			6	0.09		
320 000	4	0.13			4	0.13			6	0.21		
640 000	4	0.29			5	0.37			6	0.48		
1 280 000	4	0.61			5	0.81			6	1.01		

Table 1: Comparison of ACA and SVD.

approximation via SVD gives the best approximation but requires $\mathcal{O}(n^3)$ complexity. Notice that the CPU time for both methods includes the computation of the required matrix entries. For problem sizes larger than 5000 the SVD could not be computed within 30 minutes. ACA shows a linear complexity, and the approximation rank is insignificantly larger than the optimal one, which does not seem to depend on the problem size. Note that in order to guarantee linear complexity we replaced (19) with

$$\|u_{k+1}\|_2 \|v_{k+1}\|_F \le \varepsilon \|S_{k+1}\|_F, \tag{20}$$

because $\|A\|_F \approx \|S_{k+1}\|_F$ and $\|S_{k+1} - S_k\|_F \approx \|A - S_k\|_F$.

Table 2 shows the expression

$$\sigma_{1,k} = \max_{j=1,\ldots,n} \sum_{i=1}^{k} |\xi_i^{(k)}(q_j)|.$$

The amplification factors do not seem to grow exponentially with k.

$n\backslash k$	1	2	3	4	5	6
320 000	1.00	1.04	1.25	2.63	4.70	3.61
640 000	1.00	1.04	1.26	2.61	3.76	3.70
1 280 000	1.00	1.05	1.27	2.54	3.01	3.08

Table 2: Amplification factors $\sigma_{1,k}$ for the case $\varepsilon = 10^{-7}$.

3.2 Application to singular functions

In previous publications the adaptive cross approximation was applied to functions κ on domains $X \times Y$ which are well-separated from singular points of κ. The following lemma shows the rate of convergence in the case that $X \times Y$ approaches singular points. As an important prototype we consider

$$\kappa(x, y) := (|x|^q + |y|^q)^{-1/q} \tag{21}$$

with arbitrary $q \in \mathbb{N}$.

Theorem 1. *Let $\delta_1, \delta_2 > 0$ and $X \subset \{x \in \mathbb{R}^d : \|x\|_2 > \delta_1\}$, $Y \subset \{y \in \mathbb{R}^d : \|y\|_2 > \delta_2\}$. Then for R_k applied to κ from (21) there is a constant $c_k > 0$ such that*

$$|R_k(x, y)| \le c_k \frac{8 \cdot 2^{1/q}}{(\delta_1^q + \delta_2^q)^{1/q}} e^{-\pi\sqrt{k/q}}, \quad x \in X,\, y \in Y.$$

Proof. In [9] it is proved that for the approximation of the function $f(t) := t^{-1/q}$ by exponential sums

$$s_k(t) := \sum_{i=1}^{k} \omega_i e^{-\alpha_i t}, \quad \omega_i, \alpha_i \in \mathbb{R},$$

it holds that

$$\|f - \hat{s}_k\|_{[\varepsilon,\infty)} = \min_{\omega_i,\alpha_i} \|f - s_k\|_{[\varepsilon,\infty)} \le \frac{8 \cdot 2^{1/q}}{\varepsilon^{1/q}} e^{-\pi\sqrt{k/q}}.$$

Without loss of generality we may assume that the coefficients α_i are pairwise distinct.

Setting $\psi_i(y) := e^{-\alpha_i |y|^q}$, for $x \in X$ it holds that $\hat{s}_k(|x|^q + |\cdot|^q) \in \Psi_k$. Hence, for the approximation of κ on $X \times Y$ we obtain that

$$\begin{aligned}\sup_{x\in X} \inf_{\psi\in\Psi_k} \|\kappa(x,\cdot) - \psi\|_{\infty,Y} &\le \sup_{x\in X} \|f(|x|^q + |\cdot|^q) - \hat{s}_k(|x|^q + |\cdot|^q)\|_{\infty,Y} \\ &\le \|f - \hat{s}_k\|_{[\delta_1^q+\delta_2^q,\infty)} \le \frac{8 \cdot 2^{1/q}}{(\delta_1^q + \delta_2^q)^{1/q}} e^{-\pi\sqrt{k/q}}.\end{aligned}$$

The assertion follows from (14) and Remark 2 with $c_k := (1 + \|\mathcal{I}_k\|)(\sigma_{1,k} + 1)$. □

As a consequence, the rank k required to guarantee an error of order $\varepsilon > 0$ depends logarithmically on both ε and the maximum $\delta := \max\{\delta_1, \delta_2\}$ of the distances to the singularity provided that $c_k \lesssim e^{\frac{\pi}{2}\sqrt{k/q}}$:

$$\delta^{-1} 8 \cdot 2^{1/q} e^{-\frac{\pi}{2}\sqrt{k/q}} < \varepsilon \quad \Longleftrightarrow \quad k > \frac{4q}{\pi^2} \left[|\log\varepsilon| + |\log\delta| + (3 + 1/q)\log 2\right]^2. \tag{22}$$

We will now construct matrix approximations for matrices $A \in \mathbb{R}^{n\times n}$ generated by (21) for $q = 2, 5$ and $\varepsilon = 10^{-5}$. Table 3 shows that in contrast to Table 1 the rank increases with the problem size due to the singularity of κ. As predicted in (22) the dependence is logarithmic. The column labeled "factor" shows the compression ratio $2k/m$, i.e. the ratio of the number of units of memory required

	$q=2$					$q=5$				
	ACA			SVD		ACA			SVD	
n	k	factor	time [s]	k	time [s]	k	factor	time [s]	k	time [s]
1 250	18	$3 \cdot 10^{-2}$	0.00	16	4.2	31	$5 \cdot 10^{-2}$	0.00	29	4.2
2 500	19	$2 \cdot 10^{-2}$	0.00	18	43.1	35	$3 \cdot 10^{-2}$	0.01	32	43.1
5 000	21	$8 \cdot 10^{-3}$	0.00	19	381.7	38	$2 \cdot 10^{-2}$	0.03	35	381.7
10 000	22	$4 \cdot 10^{-3}$	0.02	–	–	41	$8 \cdot 10^{-3}$	0.06	–	–
20 000	24	$2 \cdot 10^{-3}$	0.06			44	$4 \cdot 10^{-3}$	0.25		
40 000	25	$1 \cdot 10^{-3}$	0.16			46	$2 \cdot 10^{-3}$	0.59		
80 000	27	$7 \cdot 10^{-4}$	0.41			49	$1 \cdot 10^{-3}$	1.36		
160 000	28	$4 \cdot 10^{-4}$	0.96			52	$7 \cdot 10^{-4}$	3.21		
320 000	28	$2 \cdot 10^{-4}$	2.41			55	$3 \cdot 10^{-4}$	8.93		
640 000	30	$9 \cdot 10^{-5}$	6.57			58	$2 \cdot 10^{-4}$	23.85		
1 280 000	31	$5 \cdot 10^{-5}$	14.12			61	$1 \cdot 10^{-4}$	52.91		

Table 3: Comparison of ACA and SVD for $\varepsilon = 10^{-5}$.

for the approximation and for the original matrix. Additionally, it is visible that q increases the approximation rank. However, the difference of the optimal rank and the one computed by ACA is still small.

Table 4 shows the corresponding amplification factors $\sigma_{1,k}$.

$n \backslash k$	1	2	3	4	5	6	7	8	9	10	15	20	25	30	31
320 000	1.0	1.0	1.2	2.6	2.5	1.9	2.5	3.3	2.7	2.8	3.0	3.3	8.3		
640 000	1.0	1.0	1.2	2.6	2.5	1.9	2.5	3.3	2.7	2.8	3.0	3.3	4.8	14.4	
1 280 000	1.0	1.0	1.2	2.6	2.5	1.9	2.5	3.3	2.7	2.8	3.0	3.3	4.2	11.0	10.1

Table 4: Amplification factors $\sigma_{1,k}$ for the case $q = 2$, $\varepsilon = 10^{-5}$.

4 Adaptive cross approximation of trivariate functions

In this section functions $\kappa : X \times Y \times Z \to \mathbb{C}$ in three variables will be considered. An obvious generalization of the bivariate method to such functions is the following recursion

$$R_k(x, y, z) = R_{k-1}(x, y, z) - \frac{R_{k-1}(x, y_k, z_k)}{R_{k-1}(x_k, y_k, z_k)} R_{k-1}(x_k, y, z)$$

for $k = 1, 2, \ldots$ and $R_0(x, y, z) = \kappa(x, y, z)$. The previous recursion still contains a function in two variables, which can be approximated using ACA. Instead of R_k we will therefore use the following recursion

$$\tilde{R}_k(x, y, z) = \tilde{R}_{k-1}(x, y, z) - \frac{\tilde{R}_{k-1}(x, y_k, z_k)}{\tilde{R}_{k-1}(x_k, y_k, z_k)} \mathcal{A}_{yz}[\tilde{R}_{k-1}|_{x_k}](y, z) \tag{23}$$

for $k = 1, 2, \ldots$ and $\tilde{R}_0(x, y, z) = \kappa(x, y, z)$. Here, $\mathcal{A}_{yz}[f]$ denotes the approximation of the bivariate function $f(y, z)$ as presented in Sect. 3. The number of ACA steps for the construction of $\mathcal{A}_{yz}[f]$ will be denoted by k'. The points x_k, y_k, and z_k are chosen such that $\tilde{R}_{k-1}(x_k, y_k, z_k) \neq 0$.

Before we analyze the decay of $|\tilde{R}_k|$ with k in the setting of incremental approximations, we show how the approximation $\tilde{S}_k := \kappa - \tilde{R}_k$ can be represented in terms of κ and $\tilde{R}_\ell$, $\ell = 1, \ldots, k-1$.

Lemma 9. *The function $\tilde{S}_k$ is of the form*

$$\tilde{S}_k(x,y,z) = \sum_{\ell=1}^{k} \frac{\tilde{R}_{\ell-1}(x,y_\ell,z_\ell)}{\tilde{R}_{\ell-1}(x_\ell,y_\ell,z_\ell)} \sum_{\mu,\nu=1}^{k'} \alpha_{\mu\nu}^{(\ell)} \tilde{R}_{\ell-1}(x_\ell,y,z_\mu^{(\ell)}) \tilde{R}_{\ell-1}(x_\ell,y_\nu^{(\ell)},z) \tag{24a}$$

$$= \sum_{\ell=1}^{k} \kappa(x,y_\ell,z_\ell) \sum_{i,j=1}^{k} \sum_{\mu,\nu=1}^{k'} \beta_{\mu\nu}^{(ij\ell)} \kappa(x_i,y,z_\mu^{(i)}) \kappa(x_j,y_\nu^{(j)},z). \tag{24b}$$

with points $y_\nu^{(j)}$, $z_\mu^{(i)}$ and suitable coefficients $\alpha_{\mu\nu}^{(\ell)}$, $\beta_{\mu\nu}^{(ij\ell)}$.

Proof. We have seen in Sect. 3 that

$$\mathcal{A}_{yz}[f](y,z) = \sum_{\mu,\nu=1}^{k'} \alpha_{\mu\nu} f(y,z'_\mu) f(y'_\nu,z)$$

with coefficients $\beta_{\mu\nu}$ and points y'_ν, z'_μ depending on f. Hence, it is easy to see that

$$\tilde{S}_1(x,y,z) = \kappa(x,y_1,z_1) \sum_{\mu,\nu=1}^{k'} \frac{\alpha_{\mu\nu}}{\kappa(x_1,y_1,z_1)} \kappa(x_1,y,z_\mu^{(1)}) \kappa(x_1,y_\nu^{(1)},z).$$

Assume that the assertion is valid for $k-1$. Since

$$\tilde{S}_{k-1}(x_k,y_\nu^{(k)},z) = \sum_{\nu'=1}^{k'} \sum_{j=1}^{k-1} \gamma_{\nu' j}^{(\nu)} \kappa(x_j,y_{\nu'}^{(j)},z) \quad \text{and} \quad \tilde{S}_{k-1}(x_k,y,z_\mu^{(k)}) = \sum_{\mu'=1}^{k'} \sum_{i=1}^{k-1} \tilde{\gamma}_{\mu' i}^{(\mu)} \kappa(x_i,y,z_{\mu'}^{(i)}),$$

where

$$\gamma_{\nu' j}^{(\nu)} = \sum_{i,\ell=1}^{k-1} \kappa(x_k,y_\ell,z_\ell) \sum_{\mu'=1}^{k'} \beta_{\mu'\nu'}^{(ij\ell)} \kappa(x_i,y_\nu^{(k)},z_{\mu'}^{(i)})$$

and

$$\tilde{\gamma}_{\mu' i}^{(\mu)} = \sum_{j,\ell=1}^{k-1} \kappa(x_k,y_\ell,z_\ell) \sum_{\nu'=1}^{k'} \beta_{\mu'\nu'}^{(ij\ell)} \kappa(x_j,y_{\nu'}^{(j)},z_\mu^{(k)}),$$

it follows that

$$\tilde{R}_{k-1}(x_k,y_\nu^{(k)},z) = \kappa(x_k,y_\nu^{(k)},z) - \tilde{S}_{k-1}(x_k,y_\nu^{(k)},z) = \sum_{\nu'=1}^{k'} \sum_{j=1}^{k} \zeta_{\nu' j}^{(\nu)} \kappa(x_j,y_{\nu'}^{(j)},z)$$

and similarly

$$\tilde{R}_{k-1}(x_k,y,z_\mu^{(k)}) = \sum_{\mu'=1}^{k'} \sum_{i=1}^{k} \tilde{\zeta}_{\mu' i}^{(\mu)} \kappa(x_i,y,z_{\mu'}^{(i)}).$$

Hence

$$\mathcal{A}_{yz}[\tilde{R}_{k-1}|_{x_k}](y,z) = \sum_{\mu,\nu=1}^{k'} \alpha_{\mu\nu}^{(k)} \tilde{R}_{k-1}(x_k,y,z_\mu^{(k)}) \tilde{R}_{k-1}(x_k,y_\nu^{(k)},z)$$

$$= \sum_{i,j=1}^{k} \sum_{\mu',\nu'=1}^{k'} \hat{\beta}_{\mu'\nu'}^{(ij)} \kappa(x_i,y,z_{\mu'}^{(i)}) \kappa(x_j,y_{\nu'}^{(j)},z),$$

where $\hat{\beta}^{(ij)}_{\mu'\nu'} := \sum_{\mu,\nu=1}^{k'} \alpha^{(k)}_{\mu\nu} \tilde{\zeta}^{(\mu)}_{\mu' i} \zeta^{(\nu)}_{\nu' j}$. Together with

$$\frac{\tilde{R}_{k-1}(x, y_k, z_k)}{\tilde{R}_{k-1}(x_k, y_k, z_k)} = \sum_{\ell=1}^{k} \gamma^{(k)}_{\ell} \kappa(x, y_\ell, z_\ell)$$

we obtain the assertion. □

Whereas in the bivariate case only the amplification factors $\sigma_{1,k}$ entered the error estimates, the perturbation introduced by $\mathcal{A}_{yz}[\tilde{R}_{k-1}|_{x_k}]$ is also amplified by the expression

$$c^{(k)}_{\text{piv}} := \max_{y\in Y,\, z\in Z} \frac{|\mathcal{A}_{yz}[\tilde{R}_{k-1}|_{x_k}](y,z)|}{|\tilde{R}_{k-1}(x_k, y_k, z_k)|}$$

as we shall see in the following theorem. Notice that the factor $c^{(k)}_{\text{piv}}$ can be evaluated easily in each step of the iteration to check its size.

Theorem 2. *Let $\varepsilon > 0$ be sufficiently small, and for $j = 1, \ldots, k$ assume that*

$$\sup_{y\in Y,\, z\in Z} |\tilde{R}_{j-1}(x_j, y, z) - \mathcal{A}_{yz}[\tilde{R}_{j-1}|_{x_j}](y,z)| \le \varepsilon.$$

Then for $x \in X$, $y \in Y$, and $z \in Z$

$$|\tilde{R}_k(x,y,z)| \le (\sigma_{1,k} + 1) \max_{\tau\in\{x,x_1,\ldots,x_k\}} \|\mathcal{E}_k[\kappa_\tau]\|_{\infty, Y\times Z} + c_k\varepsilon,$$

where $c_k := \tilde{\sigma}_{1,k} + 2\sum_{j=1}^{k} \tilde{\sigma}_{1,j-1} \prod_{i=j}^{k} (c^{(i)}_{\text{piv}} + 1)(\tilde{\sigma}_{i,k} + 1)$.

Proof. Notice that $|R_k(x,y,z)|$ was estimated in the last section if (y,z) is treated as a single variable; see (14). Hence,

$$|R_k(x,y,z)| \le (\sigma_{1,k} + 1) \max_{\tau\in\{x,x_1,\ldots,x_k\}} \|\mathcal{E}_k[\kappa_\tau]\|_{\infty, Y\times Z}.$$

Furthermore, for fixed y, z we have that $R_k = r_k[\kappa_{y,z}]$ is of type (1) if we choose $\ell_k := r_{k-1}[\kappa_{y_k,z_k}]$, while the recursion for $\tilde{R}_k$ is of type (9), i.e. $\tilde{R}_k(x,y,z) = \tilde{\tilde{r}}_k[\kappa_{y,z}](x)$ for the choice

$$\tilde{\ell}_k := \tilde{\tilde{r}}_{k-1}[\kappa_{y_k,z_k}] = \tilde{R}_{k-1}(\cdot, y_k, z_k), \qquad a_k := \mathcal{A}_{yz}[\tilde{R}_{k-1}|_{x_k}](y,z).$$

We obtain from Lemma 7 that

$$\|\tilde{\tilde{r}}_k[\kappa_{y,z}] - \tilde{r}_k[\kappa_{y,z}]\|_\infty \le \sum_{j=1}^{k} \|\tilde{\xi}^{(k)}_j\|_\infty |\tilde{\tilde{r}}_{j-1}[\kappa_{y,z}](x_j) - a_j| \le \tilde{\sigma}_{1,k}\varepsilon,$$

because

$$|\tilde{\tilde{r}}_{j-1}[\kappa_{y,z}](x_j) - a_j| = |\tilde{R}_{j-1}(x_j, y, z) - \mathcal{A}_{yz}[\tilde{R}_{j-1}|_{x_j}](y,z)| \le \varepsilon.$$

Let $F_k := \sup_{y,z} \|r_{k-1}[\kappa_{y,z}] - \tilde{r}_{k-1}[\kappa_{y,z}]\|_\infty$. Then it follows that

$$\begin{aligned}
\|\ell_k - \tilde{\ell}_k\|_\infty &= \|r_{k-1}[\kappa_{y_k,z_k}] - \tilde{\tilde{r}}_{k-1}[\kappa_{y_k,z_k}]\|_\infty \\
&\le \|r_{k-1}[\kappa_{y_k,z_k}] - \tilde{r}_{k-1}[\kappa_{y_k,z_k}]\|_\infty + \|\tilde{r}_{k-1}[\kappa_{y_k,z_k}] - \tilde{\tilde{r}}_{k-1}[\kappa_{y_k,z_k}]\|_\infty \\
&\le F_k + \tilde{\sigma}_{1,k-1}\varepsilon.
\end{aligned}$$

For sufficiently small ε we may assume that

$$F_k + (\tilde{\sigma}_{1,k-1} + 1)\varepsilon \le \frac{1}{2}|\tilde{\ell}_k(x_k)|. \tag{25}$$

Then Lemma 6 proves the estimate

$$F_{k+1} \le \sum_{i=1}^{k} \rho_i (F_i + \tilde{\sigma}_{1,i-1}\varepsilon) \tag{26}$$

with

$$\rho_i := \frac{\sup_{y,z} |r_{i-1}[\kappa_{y,z}](x_i)|}{|\ell_i(x_i)|}(\tilde{\sigma}_{i,k} + 1).$$

From $|r_{i-1}[\kappa_{y,z}](x_i) - \mathcal{A}_{yz}[\tilde{R}_{i-1}|_{x_i}](y,z)| \le F_i + (\tilde{\sigma}_{1,i-1} + 1)\varepsilon$ we obtain that

$$\frac{\sup_{y,z} |r_{i-1}[\kappa_{y,z}](x_i)|}{|\ell_i(x_i)|} \le \frac{\sup_{y,z} |\mathcal{A}_{yz}[\tilde{R}_{i-1}|_{x_i}](y,z)| + F_i + (\tilde{\sigma}_{1,i-1} + 1)\varepsilon}{|\tilde{\ell}_i(x_i)| - F_i - \tilde{\sigma}_{1,i-1}\varepsilon} \le 2c_{\text{piv}}^{(i)} + 1$$

due to (25).

Define $F_1' = 0$ and $F_{k+1}' = \sum_{i=1}^{k} \rho_i (F_i' + \tilde{\sigma}_{1,i-1}\varepsilon)$. We see that

$$F_{k+1}' = F_k' + \rho_k (F_k' + \tilde{\sigma}_{1,k-1}\varepsilon) = (\rho_k + 1)F_k' + \rho_k \tilde{\sigma}_{1,k-1}\varepsilon$$

and thus

$$F_k' = \varepsilon \sum_{j=1}^{k-1} \tilde{\sigma}_{1,j-1}\rho_j \prod_{i=j+1}^{k-1} (\rho_i + 1).$$

From $F_1 = 0$ and (26) we see that

$$F_k \le F_k' = \varepsilon \sum_{j=1}^{k-1} \tilde{\sigma}_{1,j-1}\rho_j \prod_{i=j+1}^{k-1} (\rho_i + 1) \le \varepsilon \sum_{j=1}^{k-1} \tilde{\sigma}_{1,j-1} \prod_{i=j}^{k-1} (\rho_i + 1).$$

It follows that

$$\begin{aligned} \|\tilde{\tilde{r}}_k\|_\infty &\le \|\tilde{\tilde{r}}_k - \tilde{r}_k\|_\infty + F_{k+1} + \|r_k\|_\infty \\ &\le \|r_k\|_\infty + \tilde{\sigma}_{1,k}\varepsilon + 2\varepsilon \sum_{j=1}^{k} \tilde{\sigma}_{1,j-1} \prod_{i=j}^{k} (c_{\text{piv}}^{(i)} + 1)(\tilde{\sigma}_{i,k} + 1). \end{aligned}$$

□

4.1 Matrix approximation

We apply the approximation (23) to the matrix $A \in \mathbb{R}^{n\times n\times n}$ with entries $a_{i_1 i_2 i_3} = \kappa(p_{i_1}, p_{i_2}, p_{i_3})$ and $p_i = \frac{1}{n}(i - \frac{1}{2})$, $i = 1, \ldots, n$, generated by evaluating the smooth function

$$\kappa(x, y, z) = (1 + x^2 + y^2 + z^2)^{-1/2}.$$

From (24a) we obtain the representation

$$(S_k)_{i_1 i_2 i_3} = \sum_{\ell=1}^{k} (w_\ell)_{i_1} \sum_{\nu=1}^{k_\ell} (u_{\ell\nu})_{i_2} (v_{\ell\nu})_{i_3}$$

with appropriate vectors $u_{\ell\nu}$, $v_{\ell\nu}$, and w_ℓ, $\nu = 1, \ldots, k_\ell$, $\ell = 1, \ldots, k$. Here, k_ℓ denotes the rank of the ℓ-th two-dimensinal approximation. Hence,

$$\|S_k\|_F^2 = \sum_{i_1,i_2,i_3=1}^{n} (S_k)_{i_1 i_2 i_3}^2 = \sum_{\ell,\ell'=1}^{k} (w_\ell, w_{\ell'})\alpha_{\ell\ell'},$$

where

$$\alpha_{\ell\ell'} := \sum_{\nu=1}^{k_\ell} \sum_{\nu'=1}^{k_{\ell'}} (u_{\ell\nu}, u_{\ell'\nu'})(v_{\ell\nu}, v_{\ell'\nu'}),$$

can be exploited to evaluate $\|S_k\|_F$ with linear complexity. Furthermore, we have that $\|S_{k+1} - S_k\|_F^2 = \|w_{k+1}\|_2^2 \alpha_{k+1,k+1}$, and condition (20) becomes

$$\|w_{r+1}\|_2 \sqrt{\alpha_{r+1,r+1}} \leq \varepsilon \|S_{k+1}\|_F$$

in the case of third order tensors. Notice that the computation of R_k can be avoided by tracing back the error as in (17) and (18).

The pivoting indices $(i_1^{(k)}, i_2^{(k)}, i_3^{(k)})$ can be obtained in many ways. The aim of this choice is to reduce the amplification factors $\tilde{\sigma}_{1,k}$ and $c_{\text{piv}}^{(k)}$. In the following numerical examples we have chosen $i_1^{(\ell)}$ as the index of the maximum entry of the vector $A_{1:n,i_2^{(\ell)},i_3^{(\ell)}}$, where $(i_2^{(\ell+1)}, i_3^{(\ell+1)})$ is the index of the maximum entry in modulus of the rank-k_ℓ matrix $U_\ell V_\ell^H$, $U_\ell \in \mathbb{C}^{n \times k_\ell}$ and $V_\ell \in \mathbb{C}^{n \times k_\ell}$. The maximum can be found with complexity $\mathcal{O}(k_\ell^2 n)$ via the following procedure. Let u_j and v_j denote the columns of U_ℓ and V_ℓ, respectively. In [13] it is pointed out that the $n^2 \times n^2$ matrix

$$C := \sum_{j=1}^{k} \operatorname{diag}(u_j) \otimes \operatorname{diag}(v_j)$$

has the eigenvalues $(U_\ell V_\ell^H)_{ij}$ for the eigenvectors $e_i \otimes e_j$, $i, j = 1, \ldots, n$. Hence, the maximum entry can be computed, for instance, by vector iteration. Here, the problem arises that

$$C(x \otimes y) = \sum_{j=1}^{k_\ell} (\operatorname{diag}(u_j)x) \otimes (\operatorname{diag}(v_j)y),$$

i.e. the rank increases from step to step. In order to avoid this, $C(x \otimes y) \in \mathbb{C}^{n \times n}$ is truncated to rank-1 via the singular value decomposition. The latter can be computed with $\mathcal{O}(k_\ell^2 n)$ operations; see [4].

Hence, the complexity of the matrix approximation algorithm is $\mathcal{O}(n \sum_{\ell=1}^{k} k_\ell^2)$, while the storage requirement is $\mathcal{O}(n k_S)$, where $k_S := \sum_{\ell=1}^{k} k_\ell$. Table 5 shows the number of steps k, the Kronecker rank k_S, and the CPU time required for constructing the approximation. The column labeled "factor" contains the compression ratio $(2k_S + 1)/n^2$.

	$\varepsilon = 10^{-3}$				$\varepsilon = 10^{-4}$				$\varepsilon = 10^{-5}$			
n	k	k_S	factor	time [s]	k	k_S	factor	time [s]	k	k_S	factor	time [s]
160 000	3	9	$7 \cdot 10^{-10}$	0.6	3	11	$9 \cdot 10^{-10}$	0.7	4	18	$1 \cdot 10^{-09}$	1.5
320 000	3	9	$2 \cdot 10^{-10}$	1.5	3	11	$2 \cdot 10^{-10}$	1.8	4	19	$4 \cdot 10^{-10}$	4.0
640 000	3	9	$5 \cdot 10^{-11}$	3.8	3	10	$5 \cdot 10^{-11}$	4.5	4	20	$1 \cdot 10^{-10}$	10.6
1 280 000	3	9	$1 \cdot 10^{-11}$	6.9	3	10	$1 \cdot 10^{-11}$	9.0	4	20	$3 \cdot 10^{-11}$	21.3

Table 5: ACA for third order tensors.

Table 6 shows the results obtained for the functions

$$\kappa(x, y, z) = (x^q + y^q + z^q)^{-1/q}$$

with $q = 1, 2$, which are singular for $x = y = z = 0$. The ranks increase compared with Table 5, but the complexity is still linear with respect to n.

	$q=1$				$q=2$			
n	k	k_S	factor	time [s]	k	k_S	factor	time [s]
160 000	21	308	$2 \cdot 10^{-08}$	127.1	32	706	$6 \cdot 10^{-08}$	597.7
320 000	17	214	$4 \cdot 10^{-09}$	190.8	30	660	$1 \cdot 10^{-08}$	1416.3
640 000	26	405	$2 \cdot 10^{-09}$	1426.2	31	667	$3 \cdot 10^{-09}$	3653.2
1 280 000	24	421	$5 \cdot 10^{-10}$	3102.5	28	574	$7 \cdot 10^{-10}$	5756.9

Table 6: ACA for third order tensors and $\varepsilon = 10^{-3}$.

5 Adaptive cross approximation of functions of four variables

The construction of approximations to functions

$$\kappa : W \times X \times Y \times Z \to \mathbb{C}$$

of four variables w, x, y, z can be done by applying ACA to the pairs (w, x) and (y, z):

$$R_k(w, x, y, z) = R_{k-1}(w, x, y, z) - \frac{R_{k-1}(w, x, y_k, z_k)\, R_{k-1}(w_k, x_k, y, z)}{R_{k-1}(w_k, x_k, y_k, z_k)}.$$

Since this leads to bivariate functions, we approximate them using ACA again. Hence, in this section we will investigate the recursion

$$\tilde{R}_k(w, x, y, z) = \tilde{R}_{k-1}(w, x, y, z) - \frac{\mathcal{A}_{wx}[\tilde{R}_{k-1}|_{y_k,z_k}](w, x)\, \mathcal{A}_{yz}[\tilde{R}_{k-1}|_{w_k,x_k}](y, z)}{\mathcal{A}_{wx}[\tilde{R}_{k-1}|_{y_k,z_k}](w_k, x_k)} \tag{27}$$

for $k = 1, 2, \ldots$ and $\tilde{R}_0 = \kappa$. The choice of (w_k, x_k, y_k, z_k) guarantees $\mathcal{A}_{wx}[\tilde{R}_{k-1}|_{y_k,z_k}](w_k, x_k) \neq 0$. Here, $\mathcal{A}_{wx}[f]$ and $\mathcal{A}_{yz}[g]$ denote ACA approximations of the bivariate functions f and g with rank k'.

Lemma 10. *The approximating function $\tilde{S}_k := \kappa - \tilde{R}_k$ is of the form*

$$\tilde{S}_k(w, x, y, z) = \sum_{\ell=1}^{k} u_\ell(w, x) v_\ell(y, z) = \sum_{|\boldsymbol{\mu}|=1}^{k} \sum_{|\boldsymbol{i}|=1}^{k'} \alpha_{\boldsymbol{\mu}\boldsymbol{i}} f_{\boldsymbol{\mu}\boldsymbol{i}}(w, x, y, z), \tag{28}$$

where $\boldsymbol{\mu}, \boldsymbol{i} \in \mathbb{N}^4$, $|\boldsymbol{\mu}| := \max_{j=1,\ldots,4} \mu_j$,

$$u_\ell(w, x) := \sum_{i,j=1}^{k'} \beta_{ij}^{(\ell)} \tilde{R}_{\ell-1}(w, x_i^{(\ell)}, y_\ell, z_\ell) \tilde{R}_{\ell-1}(w_j^{(\ell)}, x, y_\ell, z_\ell),$$

$$v_\ell(y, z) := \sum_{i,j=1}^{k'} \gamma_{ij}^{(\ell)} \tilde{R}_{\ell-1}(w_\ell, x_\ell, y, z_i^{(\ell)}) \tilde{R}_{\ell-1}(w_\ell, x_\ell, y_j^{(\ell)}, z),$$

and

$$f_{\boldsymbol{\mu}\boldsymbol{i}}(w, x, y, z) := \kappa(w, x_{i_1}^{(\mu_1)}, y_{\mu_1}, z_{\mu_1}) \kappa(w_{i_2}^{(\mu_2)}, x, y_{\mu_2}, z_{\mu_2}) \kappa(w_{\mu_3}, x_{\mu_3}, y, z_{i_3}^{(\mu_3)}) \kappa(w_{\mu_4}, x_{\mu_4}, y_{i_4}^{(\mu_4)}, z)$$

with points $x_{i_1}^{(\mu_1)}, y_{i_2}^{(\mu_2)}, z_{i_3}^{(\mu_3)}$, $y_{i_4}^{(\mu_4)}$ and coefficients $\alpha_{\boldsymbol{\mu}\boldsymbol{i}}$, $\beta_{ij}^{(\ell)}$, and $\gamma_{ij}^{(\ell)}$.

Proof. We already know that

$$\mathcal{A}_{wx}[f](w,x) = \sum_{i,j=1}^{k'} \beta_{ij} f(w,x_i')f(w_j',x)$$

with suitable coefficients β_{ij} and points x_i', w_j' depending on f. Hence, it is easy to see that $\tilde{S}_1$ is of the desired form. Assuming that the assertion is true for $k-1$, we obtain from

$$\tilde{S}_{k-1}(w_k,x_k,y_j^{(k)},z) = \sum_{\mu_4=1}^{k-1}\sum_{i_4=1}^{k'} \gamma_{j\mu_4 i_4}\kappa(w_{\mu_4},x_{\mu_4},y_{i_4}^{(\mu_4)},z),$$

where

$$\gamma_{j\mu_4 i_4} := \sum_{\mu_1,\mu_2,\mu_3=1}^{k-1}\sum_{i_1,i_2,i_3=1}^{k'} \alpha_{\boldsymbol{\mu i}}\kappa(w_k,x_{i_1}^{(\mu_1)},y_{\mu_1},z_{\mu_1})\kappa(w_{i_2}^{(\mu_2)},x_k,y_{\mu_2},z_{\mu_2})\kappa(w_{\mu_3},x_{\mu_3},y_j^{(k)},z_{i_3}^{(\mu_3)}),$$

that

$$\tilde{R}_{k-1}(w_k,x_k,y_j^{(k)},z) = \kappa(w_k,x_k,y_j^{(k)},z) - \tilde{S}_{k-1}(w_k,x_k,y_j^{(k)},z) = \sum_{\mu_4=1}^{k}\sum_{i_4=1}^{k'} \zeta_{j\mu_4 i_4}\kappa(w_{\mu_4},x_{\mu_4},y_{i_4}^{(\mu_4)},z)$$

and similarly

$$\tilde{R}_{k-1}(w_k,x_k,y,z_i^{(k)}) = \sum_{\mu_3=1}^{k}\sum_{i_3=1}^{k'} \hat{\zeta}_{i\mu_3 i_3}\kappa(w_{\mu_3},x_{\mu_3},y,z_{i_3}^{(\mu_3)}).$$

Hence

$$\begin{aligned}\mathcal{A}_{yz}[\tilde{R}_{k-1}|_{w_k,x_k}](y,z) &= \sum_{i,j=1}^{k'} \gamma_{ij}^{(k)}\tilde{R}_{k-1}(w_k,x_k,y,z_i^{(k)})\tilde{R}_{k-1}(w_k,x_k,y_j^{(k)},z)\\ &= \sum_{\mu_3,\mu_4=1}^{k}\sum_{i_3,i_4=1}^{k'} \tilde{\zeta}_{\mu_3\mu_4 i_3 i_4}\kappa(w_{\mu_3},x_{\mu_3},y,z_{i_3}^{(\mu_3)})\kappa(w_{\mu_4},x_{\mu_4},y_{i_4}^{(\mu_4)},z),\end{aligned}$$

where $\tilde{\zeta}_{\mu_3\mu_4 i_3 i_4} := \sum_{i,j=1}^{k'} \beta_{ij}^{(k)}\hat{\zeta}_{i\mu_3 i_3}\zeta_{j\mu_4 i_4}$. Similarly

$$\mathcal{A}_{wx}[\tilde{R}_{k-1}|_{y_k,z_k}](w,x) = \sum_{\mu_1,\mu_2=1}^{k}\sum_{i_1,i_2=1}^{k'} \tilde{\zeta}'_{\mu_1\mu_2 i_1 i_2}\kappa(w,x_{i_1}^{(\mu_1)},y_{\mu_1},z_{\mu_1})\kappa(w_{i_2}^{(\mu_2)},x,y_{\mu_2},z_{\mu_2}),$$

where $\tilde{\zeta}'_{\mu_1\mu_2 i_1 i_2} := \sum_{i,j=1}^{k'} \hat{\beta}_{ij}^{(k)}\hat{\zeta}'_{i\mu_1 i_1}\zeta'_{j\mu_2 i_2}$, from which the assertion follows. □

For four variables we obtain a similar result as Theorem 2 in the trivariate case. Here, in addition to the amplification factor $\tilde{\sigma}_{1,k}$ the expression

$$c_{\text{piv}}^{(k)} := \max_{y\in Y,\, z\in Z} \frac{|\mathcal{A}_{yz}[\tilde{R}_{k-1}|_{w_k,x_k}](y,z)|}{|\mathcal{A}_{wx}[\tilde{R}_{k-1}|_{y_k,z_k}](w_k,x_k)|}$$

will enter the estimates.

Theorem 3. *Let $\varepsilon > 0$ be sufficiently small, and for $j = 1, \dots, k$ let*

$$\sup_{y\in Y,\, z\in Z} |\tilde{R}_{j-1}(w_j, x_j, y, z) - \mathcal{A}_{yz}[\tilde{R}_{j-1}|_{w_j,x_j}](y, z)| \le \varepsilon, \tag{29a}$$

$$\sup_{w\in W,\, x\in X} |\tilde{R}_{j-1}(w, x, y_j, z_j) - \mathcal{A}_{wx}[\tilde{R}_{j-1}|_{y_j,z_j}](w, x)| \le \varepsilon. \tag{29b}$$

Then for $w \in W$, $x \in X$, $y \in Y$, and $z \in Z$

$$|\tilde{R}_k(w, x, y, z)| \le (1 + \sigma_{1,k}) \max_{(\sigma,\tau)\in\{(w,x),\,(w_i,x_i),\, i=1,\dots,k\}} \|\mathcal{E}_k[\kappa_{\sigma,\tau}]\|_{\infty,Y\times Z} + c_k\varepsilon,$$

where

$$c_k := \tilde{\sigma}_{1,k} + 2\sum_{j=1}^{k}(\tilde{\sigma}_{1,j-1} + 1)\prod_{i=j}^{k}(c_{\mathrm{piv}}^{(i)} + 1)(\tilde{\sigma}_{i,k} + 1).$$

Proof. For fixed parameters y, z the recursion for $\tilde{R}_k$ is of type (9), i.e. $\tilde{R}_k(w, x, y, z) = \tilde{\tilde{r}}_k[\kappa_{y,z}](w, x)$, if we choose

$$\tilde{\ell}_k(w, x) := \mathcal{A}_{wx}[\tilde{\tilde{r}}_{k-1}[\kappa_{y_k,z_k}]](w, x) = \mathcal{A}_{wx}[\tilde{R}_{k-1}|_{y_k,z_k}](w, x), \qquad a_k := \mathcal{A}_{yz}[\tilde{R}_{k-1}|_{w_k,x_k}](y, z).$$

Let r_k be defined as in (1) with $\ell_k(w, x) = r_{k-1}[\kappa_{y_k,z_k}](w, x)$. From Lemma 7 we obtain

$$\|\tilde{\tilde{r}}_k[\kappa_{y,z}] - \tilde{r}_k[\kappa_{y,z}]\|_{\infty,W\times X} \le \sum_{j=1}^{k} \|\tilde{\xi}_j^{(k)}\|_\infty |\tilde{\tilde{r}}_{j-1}[\kappa_{y,z}](w_j, x_j) - a_j| \le \tilde{\sigma}_{1,k}\varepsilon,$$

because

$$|\tilde{\tilde{r}}_{j-1}[\kappa_{y,z}](w_j, x_j) - a_j| = |\tilde{R}_{j-1}(w_j, x_j, y, z) - \mathcal{A}_{yz}[\tilde{R}_{j-1}|_{w_j,x_j}](y, z)| \le \varepsilon.$$

Let $F_k := \sup_{y,z} \|r_{k-1}[\kappa_{y,z}] - \tilde{r}_{k-1}[\kappa_{y,z}]\|_{\infty,W\times X}$. Then from assumption (29b) we have that

$$\begin{aligned}
\|\ell_k - \tilde{\ell}_k\|_{\infty,W\times X} &= \|r_{k-1}[\kappa_{y_k,z_k}] - \mathcal{A}_{wx}[\tilde{\tilde{r}}_{k-1}[\kappa_{y_k,z_k}]]\|_{\infty,W\times X} \\
&\le \|r_{k-1}[\kappa_{y_k,z_k}] - \tilde{r}_{k-1}[\kappa_{y_k,z_k}]\|_\infty + \|\tilde{r}_{k-1}[\kappa_{y_k,z_k}] - \tilde{\tilde{r}}_{k-1}[\kappa_{y_k,z_k}]\|_\infty + \varepsilon \\
&\le F_k + \delta_k,
\end{aligned}$$

where $\delta_k := \varepsilon(\tilde{\sigma}_{1,k-1} + 1)$. For small enough ε we may assume that

$$F_k + \delta_k \le \frac{1}{2}|\tilde{\ell}_k(w_k, x_k)|. \tag{30}$$

Then Lemma 6 proves the estimate

$$F_{k+1} \le \sum_{i=1}^{k} \rho_i(F_i + \delta_i) \tag{31}$$

with

$$\rho_i := \frac{\sup_{y,z} |r_{i-1}[\kappa_{y,z}](w_i, x_i)|}{|\ell_i(w_i, x_i)|}(\tilde{\sigma}_{i,k} + 1).$$

From $|r_{i-1}[\kappa_{y,z}](w_i, x_i) - \mathcal{A}_{yz}[\tilde{R}_{i-1}|_{w_i,x_i}](y, z)| \le F_i + \delta_i$ we obtain that

$$\frac{\sup_{y,z} |r_{i-1}[\kappa_{y,z}](w_i, x_i)|}{|\ell_i(w_i, x_i)|} \le \frac{\sup_{y,z} |\mathcal{A}_{yz}[\tilde{R}_{i-1}|_{w_i,x_i}](y, z)| + F_i + \delta_i}{|\tilde{\ell}_i(w_i, x_i)| - F_i - \delta_i} \le 2c_{\mathrm{piv}}^{(i)} + 1$$

due to (30). Similar to the proof of Theorem 2 from $F_1 = 0$ and (31) we see that

$$F_k \le \sum_{j=1}^{k-1} \delta_j \rho_j \prod_{i=j+1}^{k-1} (\rho_i + 1) \le \sum_{j=1}^{k-1} \delta_j \prod_{i=j}^{k-1} (\rho_i + 1).$$

It follows that

$$\begin{aligned} \|\tilde{\tilde{r}}_k\|_{\infty,W\times X} &\le \|\tilde{\tilde{r}}_k - \tilde{r}_k\|_{\infty,W\times X} + F_{k+1} + \|r_k\|_{\infty,W\times X} \\ &\le \|r_k\|_{\infty,W\times X} + \tilde{\sigma}_{1,k}\varepsilon + 2\sum_{j=1}^{k} \delta_j \prod_{i=j}^{k} (c_{\text{piv}}^{(i)} + 1)(\tilde{\sigma}_{i,k} + 1). \end{aligned}$$

Notice that that $\|r_k\|_\infty$ was estimated in Sect. 3. □

5.1 Matrix approximation

We apply the algorithm (27) to a matrix $A \in \mathbb{R}^{n\times n\times n\times n}$ with entries $a_{i_1 i_2 i_3 i_4} = \kappa(p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4})$ and $p_i = \frac{1}{n}(i - \frac{1}{2})$, $i = 1, \ldots, n$, generated by evaluating the smooth function

$$\kappa(w, x, y, z) = (1 + w + x + y + z)^{-1}.$$

The stopping criterion (see (20))

$$\|S_{k+1} - S_k\|_F \le \varepsilon \|S_{k+1}\|_F$$

can be evaluated with linear complexity, because from (28) we obtain the matrix representation

$$(S_k)_{i_1 i_2 i_3 i_4} = \sum_{\ell=1}^{k} \left(\sum_{\nu=1}^{k_\ell} (u_{\ell\nu})_{i_1} (v_{\ell\nu})_{i_2} \right) \left(\sum_{\mu=1}^{k'_\ell} (u'_{\ell\mu})_{i_3} (v'_{\ell\mu})_{i_4} \right)$$

with suitable vectors $u_{\ell\nu}$, $v_{\ell\nu}$, $u'_{\ell\mu}$, and $v'_{\ell\mu}$, which shows that

$$\|S_k\|_F^2 = \sum_{\ell,\ell'=1}^{k} \alpha_{\ell\ell'} \beta_{\ell\ell'},$$

where

$$\alpha_{\ell\ell'} := \sum_{\nu=1}^{k_\ell} \sum_{\mu=1}^{k_{\ell'}} (u_{\ell\nu}, u_{\ell'\mu})(v_{\ell\nu}, v_{\ell'\mu}) \quad \text{and} \quad \beta_{\ell\ell'} := \sum_{\nu=1}^{k'_\ell} \sum_{\mu=1}^{k'_{\ell'}} (u'_{\ell\nu}, u'_{\ell'\mu})(v'_{\ell\nu}, v'_{\ell'\mu}).$$

Furthermore, $\|S_{k+1} - S_k\|_F^2 = \alpha_{k+1,k+1}\, \beta_{k+1,k+1}$. Also in the case of four dimensional arrays the computation of R_k can be avoided by tracing back the error as in (17) and (18).

The pivots $(i_1^{(\ell)}, i_2^{(\ell)})$ are chosen as the indices of the entry of maximum modulus in the rank-k_ℓ matrix $U_\ell V_\ell^T$, while $(i_3^{(\ell+1)}, i_4^{(\ell+1)})$ corresponds to the maximum entry in the rank-k'_ℓ matrix $U'_\ell (V'_\ell)^T$, where U_ℓ, V_ℓ, U'_ℓ, and V'_ℓ consist of the columns $u_{\ell\nu}$, $v_{\ell\nu}$, $u'_{\ell\nu}$, and $v'_{\ell\nu}$, respectively. Both maxima can be found with linear complexity using the technique from Sect. 4.1.

Hence, the complexity of the matrix approximation algorithm is $\mathcal{O}(n \sum_{\ell=1}^{k} k_\ell^2 + (k'_\ell)^2)$ and the storage required by the approximation is $\mathcal{O}(n(k_S + k'_S))$, where $k_S := \sum_{\ell=1}^{k} k_\ell$ and $k'_S := \sum_{\ell=1}^{k} k'_\ell$.

Table 7 shows the number of steps k, the ranks k_S and k'_S, and the CPU time required for constructing the approximation. The column labeled "factor" contains the compression ratio $2(k_S + k'_S)/n^3$.

	$\varepsilon = 10^{-3}$					$\varepsilon = 10^{-4}$				$\varepsilon = 10^{-5}$			
n	k	k_S	k'_S	factor	time [s]	k	k_S	k'_S	time [s]	k	k_S	k'_S	time [s]
160 000	4	19	13	$2 \cdot 10^{-14}$	2.5	5	27	18	4.0	7	53	35	10.6
320 000	4	19	13	$2 \cdot 10^{-15}$	6.2	5	27	19	10.5	7	59	35	31.9
640 000	4	19	13	$2 \cdot 10^{-16}$	15.8	5	26	19	26.1	7	57	34	69.8
1 280 000	4	19	13	$3 \cdot 10^{-17}$	31.5	5	28	19	55.6	7	55	35	142.3

Table 7: ACA for fourth order tensors.

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