Appendix: Expressive Power of Tensor Decompositions

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Tensor decompositions represent multidimensional objects like mathematical functions or data sets over regular grids as sums and products of a limited number of coefficients (the decomposition's *weights* or *parameters*). Such formats are convenient because the decomposition algorithms that produce them are numerically stable, scalable, and build upon long-standing mathematical theory [KB09, OT10]. More recently, tensor decompositions have been identified as a particular case of deep neural networks, namely architectures whose activation functions are all linear [NPOV15], and have been also connected with graphical models [RS18].

A decisive advantage of such representations is their intrinsic multilinearity. Multidimensional integration, a challenging task in mathematical modeling and numerical methods, can be performed inexpensively using tensor decompositions. In this paper, we have expressed set functions as compressed tensor trains (TT). This is one of the most recently proposed decompositions and it has enjoyed great popularity over the last decade. Its main strength is the straightforward in which it lays out the input dimensions: each dimension is mapped to a *tensor core*, which is essentially a collection of matrices. It can be seamlessly applied to set functions, whereby for every n, the n-th core consists of exactly two matrices that represent the absence or the presence of the n-th item in the set, respectively.

In TT tensors, multilinearity means that all usual set operations (unions, intersections, set complements, etc.s) can be performed in the compressed domain by simple linear combinations of some coefficients. For instance, set unions translate to summing matrices together, whereas set intersections translate to subtracting matrices from one another [BRPP19]. For example, if $n \notin \boldsymbol{\alpha}$, then the cardinality of $\boldsymbol{\alpha}$ *and maybe* n is $\mathcal{T}_{\boldsymbol{\alpha}} + \mathcal{T}_{\boldsymbol{\alpha} \cup \{n\}}$ and is decompressed as we would decompress $\boldsymbol{\alpha} \cup \{n\}$, after summing together both matrices of the n-th core. This kind of matrix-wise operations in the TT cores is instrumental to obtaining derivations of Sobol indices in real time. For example, let $\mathcal{T}$ with cores $[[\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(N)}]]$ be a TT representation of all the Sobol indices of some model. Let us create a new tensor $\widehat{\mathcal{T}}$ with cores $[[\widehat{\mathcal{G}}^{(1)}, \dots, \widehat{\mathcal{G}}^{(N)}]]$ defined as:

$$\begin{cases} \widehat{\mathcal{G}}^{(n)}[:, 0, :] := \mathcal{G}^{(n)}[:, 0, :] \\ \widehat{\mathcal{G}}^{(n)}[:, 1, :] := \mathcal{G}^{(n)}[:, 0, :] + \mathcal{G}^{(n)}[:, 1, :] \end{cases}$$

for $n = 1, \dots, N$, where we are using NumPy-like notation to index our tensors. After this manipulation, the entries of $\mathcal{T}$ now contain all *closed indices* of the original model. Similar operations can yield the total or superset indices, instead.

We can also perform other more advanced transformations via the so-called TT *cross-approximation* algorithm (CA), which is able to apply any element-wise function to a tensor (for example, square its elements). CA can be also used to find global extrema of a tensor, which is in turn useful to find, for instance, the largest Sobol index (or any related quantity covered in this paper) of a model. For more details on these and other operations that can be performed in the TT compressed domain, we refer the interested reader to [Ose11, OT10].

References

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