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Tabulating families of functions with symmetries

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Abstract

We propose a general algorithm which aims at optimizing the usage of computer resources for tabulating families of functions possessing known symmetries. The approach is based on the group theoretical description of symmetry relations among the functions and their parameters, where orbits play a crucial role.

1. Introduction

The problem of calculating complicated functions, or even whole families of functions, arises quite often in large scale calculations. It is a process which usually consumes a lot of computer memory and CPU time. In many cases, however, the functions can be related to each other by a kind of transformations, which lead to the very existence of a symmetry between the to-be-calculated values. This observation may be utilized to find the minimal number of required calculations and speeding up the whole process.

In this paper, a method based on the group theoretical approach is proposed to diminish the usage of computer resources. We start with some basic notions required for using the proposed method.

Let us consider a set of complex valued functions

$$\mathscr{F} \ni f : \mathbb{R} \to \mathbb{C} \tag{1}$$

and let $\boldsymbol{G}$ be a group of transformations of the set $\mathscr{F}$ into itself

$$\boldsymbol{G} \ni g : \mathscr{F} \to \mathscr{F}. \tag{2}$$

Throughout the paper we will assume, which is usually the case, that the group action on the set $\mathscr{F}$ may be written in the following way:

$$\boldsymbol{G}\mathscr{F}\ g\,f(x) = f(g^{-1}x). \tag{3}$$

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The group action defined above allows to decompose $\mathscr{F}$ into so-called *orbits* which classify the elements of $\mathscr{F}$ with respect to the group $\boldsymbol{G}$. By an orbit of $f \in \mathscr{F}$ we understand the following set:

$$O(f) = \boldsymbol{G} f = \{g f : g \in \boldsymbol{G}\}, \tag{4}$$

i.e., the orbit of the point f is the maximal set of points which can be obtained by all group transformations applied to f. This definition shows that it is sufficient to consider only a single element $f' \in O(f)$ to represent the full orbit. Such a point is called the *representative* of the orbit. The representative can be chosen in an arbitrary way, although the appropriate choice can greatly simplify further analysis.

On the basis of general theory one can prove the theorem, that orbits belonging to different elements are either identical or disjoint [1]. This implies that it is possible to decompose the set of functions $\mathscr{F}$ into disjoint orbits:

$$\mathscr{F} = \bigcup_i O(f'_i), \tag{5}$$

where the following condition holds: $O(f'_i) \cap O(f'_j) = \emptyset$ for $i \neq j$.

One of the basic features of orbits is that each orbit generated by the group $\boldsymbol{G}$ is isomorphic to one of the standard orbits of the form $\boldsymbol{G}/\boldsymbol{H}$, where $\boldsymbol{H} \subset \boldsymbol{G}$ is a subgroup of $\boldsymbol{G}$, and $\boldsymbol{G}/\boldsymbol{H}$ is the set of all left cosets of $\boldsymbol{H}$ in $\boldsymbol{G}$ [1,2]. The subgroup $\boldsymbol{H}$ is called the *stability* group (*isotropy* group) because it is the symmetry group of the representative f' of the orbit $O(f)$:

$$\boldsymbol{H} = \{h \in \boldsymbol{G} : h f' = f'\}. \tag{6}$$

The definition of the orbit $O(f\ )$ implies that all elements of the orbit have isomorphic isotropy groups; they can be obtained from $\boldsymbol{H}$ by the intrinsic automorphisms, *i.e.*, for every element $f' \in O(f)$ there exists an element $g \in \boldsymbol{G}$ such that $g \boldsymbol{H} g^{-1} f' = f'$.

The proper identification of orbits and stability groups allows to simplify the calculations of required functions.

2. Families of functions with symmetries

As mentioned above, in real life situations the families of functions we are dealing with often exhibit certain symmetries. We explain below what we mean by that.

Let us consider a family of functions $f(\lambda\,; x) \in \mathscr{F}$ parameterized by a set of parameters $\lambda = (\lambda_0, \lambda_1, \ldots, \lambda_N)$, which, in turn, can belong to a space $\wp$. We assume also the existence of a group $\boldsymbol{G}$ which acts on this family, as it was defined in Introduction.

By the *symmetry group* of the function $f(\lambda\,; x)$ we understand the maximal subgroup $\boldsymbol{H} \subset \boldsymbol{G}$ for which the action of its elements $h \in \boldsymbol{H}$ leaves the function $f(\lambda\,; x)$ invariant:

$$h\,f(\lambda\,;x) = f(\lambda\,;x). \tag{7}$$

In fact, the so-defined symmetry group coincides with the stability group and therefore determines an orbit in $\mathscr{F}$ which is isomorphic to the quotient space $\boldsymbol{G}/\boldsymbol{H}$. This observation suggests the possibility of constraining the domain of the function $f(\lambda\,;x)$. For this purpose one needs to factorize the elements g of the group $\boldsymbol{G}$ in the form of products $g = r\,h$, where $r \in \boldsymbol{G}/\boldsymbol{H}$ is an element of the orbit which parameterizes this orbit uniquely, and $h \in \boldsymbol{H}$. Using this decomposition one can rewrite the standard group action $g\,f(\lambda\,;x) = f(\lambda\,;g^{-1}x)$ as follows:

$$g\,f(\lambda\,;x) = r\,h\,f(\lambda\,;x) = r\,f(\lambda\,;x) = f(\lambda\,;r^{-1}x). \tag{8}$$

It is evident that the function $f(\lambda\,;r^{-1}x)$ has the same values for $g\,x$ and $r\,x$, which may be interpreted as a kind of periodic behaviour. Therefore it is sufficient to calculate values of the function $f(\lambda\,;x)$ only for arguments of the form $x = r\,x_0$, where x_0 is a fixed but an arbitrary point. This restricts the number of operations needed to tabulate the function. It is important to notice that a simpler parameterization of the orbit $\boldsymbol{G}/\boldsymbol{H}$ results in simpler numerical implementation of the calculations.

We conclude that for each λ it is sufficient to tabulate the function $f(\lambda\,;x)$ within a smaller effective domain D_x^f. Of course the higher the symmetry, the smaller the effective domain and we can save more computer resources.

On the other hand, we can reverse the situation and treat $f(\lambda\,;x)$ as a family of functions of variables λ, parameterized by x. It follows that, by repeating the just described procedure, one can find also the effective domain for λ, D_x^f. It is obvious that in general the group of transformations used in this case will be different from the previously chosen group $\boldsymbol{G}$.

The simplifications in the domains of x and λ are in general independent. It happens, however, that they both lead to equivalent narrowing of the domains.

It is interesting that in many cases there exists a third kind of symmetry relation between the action of the group $\boldsymbol{G}$ on the function space $\mathscr{F}$ and the action of this group on the parameter space $\wp$, namely:

$$g\,f(\lambda\,;x) = f(g^{-1}\lambda\,;x) \tag{9}$$

for all g $\in \boldsymbol{G}$. Keeping in mind the definition (3), the relation (9) allows to read (without further calculations) values of the function $f(\lambda\,;x)$ having calculated the function $f(\lambda_0\,;x)$, where $\lambda = g\,\lambda_0$. The systematic way of using this symmetry requires careful study of the orbits of $\boldsymbol{G}$ in both spaces $\mathscr{F}$ and $\wp$.

Notice first that h is an element of the stability group $\boldsymbol{H}\subset\boldsymbol{G}$ of the function $f(\lambda_0\,;x)$ if and only if $f(\lambda_0\,;h^{-1}x) = f(h^{-1}\lambda_0\,;x)$. This relation follows immediately from the symmetry property (9). It is also obvious that the invariance of the point λ_0 under a given transformation $k \in \boldsymbol{G}$, $k\,\lambda_0 = \lambda_0$ implies that the element k belongs to the stability group $\boldsymbol{H}$ of the function $f(\lambda_0\,;x)$.

Now, putting everything together, we can derive the main relation between different functions whose values can be read from the table of the representative function $f(\lambda_0\,; x)$. Let $\boldsymbol{K}$ be the stability group of the point λ_0 in the parameter space $\wp$. It means that this group has to be contained in the stability group $\boldsymbol{H}$ of the function $f(\lambda_0\,; x)$ belonging to the space $\mathscr{F}$. The orbits of the point λ_0 have to be isomorphic to the standard form of the orbit $\boldsymbol{G}/\boldsymbol{K}$ and can be constructed by factorization of an arbitrary element $g \in \boldsymbol{G}$ into two factors $g = r\,k$, where $r \in \boldsymbol{G}/\boldsymbol{K}$ and $k \in \boldsymbol{K}$. This factorization allows to write the relation between the representative function and the remaining members of the family,

$$f(g\,\lambda_0\,; x) = f(r\,k\,\lambda_0\,; x) = f(r\,\lambda_0\,; x) = f(\lambda_0\,; r^{-1}\,x), \tag{10}$$

where r labels the elements of the orbit.

Relation (10) shows the way how to find indpendent subsets of functions which have to be tabulated in order to cover all possible values for the whole family of functions in the space $\mathscr{F}$. Once the symmetry group $\boldsymbol{G}$ has been identified, or given *ad-hoc*, one proceeds as follows:

- decompose the parameter space $\wp$ into orbits with respect to the group $\boldsymbol{G}$;
- choose a representative λ_0 for each orbit;
- make the tables of functions $f(\lambda_0\,; x)$ for all representatives;
- values for other functions can be read from the tables using the relation (10).

In this section we have described three algorithms which can be used to optimize the process of tabulating functions with symmetries. The actual number of data we have to calculate and store is dependent on the group which acts on the function and/or parameter spaces $(\mathscr{F},\wp)$. Finding the maximal symmetry group for a given problem, which could lead to a maximal profit from the described procedure, is not an easy task. Our algorithm, however, works for an arbitrary group $\boldsymbol{G}$ for which we are able to define the group action on the spaces $(\mathscr{F},\wp)$.

3. An illustrative example

We start with a general scheme. Let $\boldsymbol{G}$ be a group which acts on a generic family of functions $f(x)$ in the usual way: $g\,f(x) = f(g^{-1}\,x)$. According to the Peter-Weyl theorem [3], the functions can be expanded in the series of the form:

$$f\left(x\right) = \sum_{R,n} \left(a_n^R\right)^* \boldsymbol{e}_n^R\left(x\right) \equiv \sum_R f_R\left(a_n^R; x\right) \tag{11}$$

where a_n^R are complex numerical coefficients, and $\boldsymbol{e}_n^R(x)$ is the n-*th* vector spanning the R-*th* irreducible representation of the group $\boldsymbol{G}$. The group action on f can now be rewritten in the following form:

$$\begin{aligned} gf(x) &= \sum_{R,n} \left(a_n^R\right)^* \boldsymbol{e}_n^R(x) = \sum_{R,n} \left(a_n^R\right)^* \sum_{n'} \Delta_{n'n}^R(g) \boldsymbol{e}_{n'}^R(x) \\ &= \sum_{R,n'} \left[\sum_n \left(a_n^R\right)^* \Delta_{n'n}^R(g) \right] \boldsymbol{e}_{n'}^R(x) \\ &= \sum_{R,n'} \left[\sum_n a_n^R \left(\Delta_{n'n}^R(g)\right)^* \right] \boldsymbol{e}_{n'}^R(x) = \sum_{R,n} \left[\sum_{n'} a_{n'}^R \left(\Delta_{nn'}^R\left(g^{-1}\right)\right)^* \right] \boldsymbol{e}_{n'}^R(x). \end{aligned} \tag{12}$$

In the last line we have assumed that we deal with a unitary transformation, which is usualy the case. As follows from (11) and (12) the group action may be applied to the variables x as well as to the parameters a_n^R,

$$gf_R\left(a_n^R;x\right) = f_R\left(a_n^R;g^{-1}x\right) = f_R\left(g^{-1}a_n^R;x\right). \tag{13}$$

To be more specific let us work out the example of the family of real functions defined by the following expansion:

$$f(\lambda;\varphi) = \sum_{m=-\infty}^{+\infty} \lambda_m \cdot e^{-im\varphi}, \quad \left(\lambda_{-m}\right)^* = \lambda_m \tag{14}$$

The symmetry in this case is described by the group ***SO(2)*** and the group action can be written as $g(\beta)f(\lambda;\varphi) = f(\lambda;g^{-1}(\beta)\varphi) = f(\lambda;\varphi-\beta)$. We notice first that for fixed m the functions $f_m = \lambda_m \exp(im\varphi) + (\lambda_m)^* \exp(-im\varphi)$ that span irreducible representations of ***SO(2)*** are invariant under the rotation about the angle $2\pi/m$:

$$g(2\pi/m) f_m = \lambda_m \mathrm{e}^{im\varphi} \mathrm{e}^{-i2\pi} + \left(\lambda_m\right)^* \mathrm{e}^{-im\varphi} \mathrm{e}^{-i2\pi} = f_m. \tag{15}$$

Such rotations form the discrete cyclic group $\boldsymbol{C_m} \subset \boldsymbol{SO(2)}$ and the quotients $\boldsymbol{SO(2)}/\boldsymbol{C_m}$ will define the sought orbits. This implies that the full space of φ parameters, $\varphi \in [0,2\pi)$, may be constrained for the functions f_m to the interval $[0,2\pi/m)$.

Using the general scheme we may also find constraints on the space of parameters λ by noticing that

$$\begin{aligned} g(\beta) f(\lambda;\varphi) &= \sum_{m=-\infty}^{+\infty} \left(\lambda_m\right)^* \mathrm{e}^{-im(\varphi-\beta)} = \sum_{m=-\infty}^{+\infty} \left(\lambda_m \mathrm{e}^{-im\beta}\right)^* \mathrm{e}^{-im\varphi} \\ &= f\left(g^{-1}(\beta)\lambda;\varphi\right). \end{aligned} \tag{16}$$

In this case, the group action allows us to consider only λ's with different absolute values |λ|.

To conclude this example, we have shown that the family of functions over which a group action may be defined, may be tabulated within constrained space of its argument (φ). The remaining values may be read from the table by proper shifting of φ. Alternatively, one may decide to keep the full range of arguments and to constrain the space of parameters (λ). In both cases the gain in speed, memory usage and CPU time is comparable.

References

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