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KILLING – An algebraic computational package for Lie algebras

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Abstract

The KILLING package is a set of algebraic computational procedures to manipulate elements of representation theory for classical, exceptional and deformed Lie algebras. It is divided in two major parts: (1) The Roots & Weights formalism to classify all semisimple Lie algebras and their irreducible representations, and (2) The Gelfand–Tsetlin method to construct explicitly the irreducible representations of classical Lie algebras, including the deformed unitary Lie algebras.

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CPC Program Library index: Computer languages; Hardware and software; Software including parallel algorithms

Keywords: Symmetry; Lie algebras; Representation; Symbolic; Algebraic; Computation

PROGRAM SUMMARY

Title of program: Killing

Catalogue identifier: ADLX

Program Summary URL: http://cpc.cs.qub.ac.uk/summaries/ADLX

Program obtainable from: http://pages.prodigy.net/bernardes; CPC Program Library, Queen's University of Belfast, N. Ireland

Computers: any one

Operating systems: any one

Programming languages: Maple V (Release 5); Mathematica (Release 3)

No. of bytes in distributed program, including test data, etc.: 213 657 bytes

Distribution format: Compressed Windows ZIP file; compressed Unix tar zip file; default ASCII files

Keywords: Lie algebra, representation, symbolic, algebraic, symmetry, computation

Nature of the physical problem
Symmetry has been a very important fundamental principle underlying human knowledge about our physical world. Among several mathematical formulations of symmetry, the Lie algebras and their corresponding Lie groups are probably the ones most explored. They were discovered by Sophus Lie and Wilhelm Killing during the last two decades of the 19th century. Lie's work on Lie groups was inspired by Galois' work in 1832 in which he discovered the finite groups. Independently, Killing had started a classification of Lie groups which was the starting point to the Élie Cartan's doctoral thesis in the beginning at the 20th century. Cartan was able to make a complete classification of Lie groups. Since Cartan's classification, the theory of Lie groups has been utilized in many branches of physics, including molecular physics, atomic physics, nuclear physics and particle physics.

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Method of solution
In spite of the high level of knowledge about the representation theory of semisimple Lie algebras, the manipulation of elements such as roots, weights and matrices is very difficult for the non-trivial cases. The goal in writing this package is to make possible the handling of several elements of the theory of representation of Lie algebras in a very convenient way in which the user can easily modify and augment every code. A great deal of flexibility is achieved by choosing the algebraic programming scenario in which huge sets of weights and complicated algebraic matrix elements can be handled in an interactive way.

Restrictions on the complexity of the problem
Until now, the Gelfand–Tsetlin method has been restricted to classical orthogonal algebras, and to classical and deformed unitary algebras, and to the classical symplectic algebra of rank two.

Typical running time
Under one minute for each procedure except for the multiplicities determination procedures.

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1. Introduction

Symmetry has been a very important fundamental principle underlying human knowledge about our physical world. Among several mathematical formulations of symmetry, the Lie algebras and their corresponding Lie groups are probably the ones most explored [1–5]. They were discovered by Sophus Lie and Wilhelm Killing during the last two decades of the 19th century. Lie's work on Lie groups was inspired by Galois' work in 1832 in which he discovered the finite groups. Independently, Killing had started a classification of Lie groups, which was the starting point for Élie Cartan's doctoral thesis at the beginning of the 20th century [6]. Cartan was able to make a complete classification of Lie groups. Since Cartan's classification, the theory of Lie groups has been utilized in many branches of physics, including molecular physics [7–9], atomic physics [10], nuclear physics [11,8], particle physics [12,13], dynamical systems [14–16] and molecular genetics [17–19].

In regard to physical applications, roots and weights play a special role in the classification of the Lie algebras and their irreducible representations, respectively. The typical use of representations in physics can be summarized as follows [20]. In general, each vector in an irreducible representation of a Lie algebra is identified by one set of weight vectors. When the physically observable operators of a given physical quantum system can be constructed from the elements of the algebra, the components of the weight vectors can be identified with the physical quantum numbers.

Therefore, one very important task is to know how to write the matrix elements of all elements in a given algebra explicitly in terms of the components of the weight vectors in a given irreducible representation. While there is a general program to calculate roots and weights for all semisimple Lie algebras [2,5], there are only partial methods to obtain the matrix elements. One very important method is the Gelfand–Tsetlin method for orthogonal [21,4] and unitary [22,4] Lie algebras. Unfortunately, there is not an equivalent method for the exceptional and symplectic algebras in general [23,24].

In spite of the high level of knowledge about the representation theory of semisimple Lie algebras, the manipulation of elements such as roots, weights and matrix elements by hand is very difficult for non-trivial cases. The goal in writing the KILLING package is to make possible the handling of several elements of the theory of representation of Lie algebras in a convenient way. This package is intended to be helpful to students, teachers and researchers using Lie algebras. It grew out of several algebraic routines developed at The Institute of Physics of São Carlos, University of São Paulo, as computational tools to understand and apply Lie algebras in physical systems. Now, the first part of the KILLING package (Roots & Weights Formalism) covers the analytical results in the first 15 chapters of Wybourne's book [2], the first chapter of Barut and Raczka's book [4], and Chapter 5 of Chen's [5] book on which some of the codes are based. The second part, the Gelfand–Tsetlin method, covers Chapters 9–10 of Barut and Raczka's book [4] on which the other codes are based.

The KILLING package is an extension and a complement to the existing packages written in Maple V [25] (www.maplesoft.com) and Mathematica [26] (www.wolfram.com) symbolic languages. The following Maple V packages, Coxeter/Weyl by John R. Stembridge, and Crystal by David Joyner, Roland Martin and Michael Foute, and Dynkin by David Joyner, all described in the Maple V share library, can be used to compute roots and weights (including multiplicities), to draw Dynkin diagrams, to plot weight systems and to write the structure constants and the defining matrices. They also can be used to decompose the tensor product of fundamental irreducible representations. General algebraic properties of the theory of representation of Lie groups can be handled by routines written by Feinsilver and Schott [27].

The GAP algebraic language is an important free software devoted to group theory in general. It is maintained by The GAP Group at Lehrstuhl D für Mathematik, Rheinisch-Westfälische Technische Hochschule Aachen (LDFM/ RWTHA), Germany (www.math.rwth-aachen.de/~gap/), and by The School of Mathematical and Computational Sciences, University of St. Andrews, Scotland (www-history.mcs.st-and.ac.uk/~gap/). It has a set of routines dedicated to algebraic properties of Lie algebras. There are also two other packages which extend the capabilities of the GAP functions on Lie algebras: (1) the LAG package by Richard Rossmanith, documented in the GAP share library; and (2) the CHEVIE package developed at LDFM/RWTHA (www.math.rwth-aachen.de/ldfm/homes/chevie/). The Chevie package also has a Maple V version dedicated to the construction of character tables. These GAP routines can also be used to compute roots and weights and character tables.

There are at least four other interactive systems written specially to perform computations on analytical results in the theory of representations of Lie algebras. There is the Symmetrica package developed at The Mathematics Department, University of Bayreuth, Germany (www.math2.uni-bayreuth.de). It is a collection of C routines which can be used as basic structures for more specific programs. The SimpLie software (www.crm.umontreal.ca/~rand/simplie) by Moody, Patera [28,29] and Rand [30] and the LiE software by van Leeuwen [31] (wallis.univ-poiliers.fr/~maavl/lie/) can be used to compute branching rules, weight multiplicities and tensor product decompositions very efficiently. The LiE software is also an algebraic software. They are free softwares. The commercial software Schur, by Wybourne [32] (www.phys.uni-torun.pl/~bgw/schur), adds the properties of symmetric functions to the capabilities of the former packages.

The KILLING package brings most of the analytical capabilities of the existing packages concerning roots and weights to Maple V and Mathematica users. It also adds some enhancements or complements to the roots and weights formalism by allowing basis exchanges in the weight space [5], and it adds the explicit construction of irreducible matrices through the Gelfand–Tsetlin method [4].

2. Elements of the representation theory of Lie algebras

Although the theory of Lie algebras is well explained in many excellent text books, we reproduce here a few definitions and theorems concerning the representation theory in order to make it a readable text. Refs. [1–5] can be used for further information. The classification of Lie algebras and their irreducible representations is presented in Section 2.1 and the explicit construction of the irreducible matrices is presented in Section 2.2.

2.1. Roots and weights

We recall a non-associative algebra as just a vector space L in which the bilinear composition (internal product) $xy \equiv [x, y] \to z,\ \ x, y, z \in L$, can be defined. A Lie algebra is a non-associative algebra L in which the internal product (or Lie product) satisfies

$$[x, y] = -[y, x], \tag{1}$$

$$\big[x, [y, z]\big] + \big[z, [x, y]\big] + \big[y, [z, x]\big] = 0, \tag{2}$$

where $x, y, z \in L$. The last condition is known as Jacobi identity. The Lie product can assume more than one form. For example, when the elements x, y of L can be represented by matrices then the Lie product can be defined as the usual commutator $[x, y] = xy - yx$.

An algebra is said to be Abelian if (symbolically) $[L, L] = 0$. A subspace I of L is an ideal of L if $[L, I] \subseteq I$. An ideal is an invariant subspace. An algebra L is solvable if $L^{(n)} = 0$ for some integer n in the series $L = L^{(0)} \supseteq L^{(1)} \supseteq L^{(2)} \supseteq \cdots$ where $L^{(k)} = [L^{(k-1)}, L^{(k-1)}]$. Each new subalgebra $L^{(k)}$ is an ideal of L. A radical of L is the solvable ideal of maximum dimensionality of L. If L has no non-zero radical, then it is called semisimple. When the non-Abelian algebra L has no ideals, besides 0 and L itself, it is called simple. There is a complete classification for all semisimple and simple Lie algebras as well for their irreducible representations.

In general, a finite Lie algebra L can be defined by giving all commutation relations among the elements of a chosen basis x_i:

$$[x_i, x_j] = c_{ijk} x_k, \tag{3}$$

where the numbers c_{ijk} are known as the structure constants. A canonical form for the commutation relations and matrices representing the elements of a Lie algebra, that is, matrices satisfying the defining commutation relations, can be found. The possibility of determining these matrices means that a vector space with a finite basis and a set of linear operators acting on it, representing the abstract elements of a Lie algebra, can always be found. The simplest example is given when the elements X and Y of a Lie algebra can simultaneously be seen as vectors in an abstract vector space and as the linear operators acting on it. The action of an operator X in a vector Y is defined by

$$XY \equiv [X, Y]. \tag{4}$$

This particular representation is called the adjoint representation. It is irreducible, that is, there is no linear transformation that can simultaneously bring all matrices in this representation to a block diagonal form (there is no invariant subspace). From the adjoint representation, it can be shown that a canonical form (the Cartan–Weyl canonical form) for the commutation relations can be written as follows:

$$\begin{aligned} &[H_i, H_j] = 0, \\ &[H_i, E_{\alpha_j}] = (\alpha_j)_i E_{\alpha_j}, \\ &[E_{\alpha_i}, E_{-\alpha_i}] = \sum_{k=1}^{r} (\alpha_i)_k H_k, \\ &[E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta}, \end{aligned} \tag{5}$$

where

$$\begin{aligned} &N_{\alpha\beta} = \begin{cases} 0 & \text{if } \beta = -\alpha, \\ 0 & \text{if } \alpha + \beta \notin \Sigma, \\ \pm\{q(p+1)/N_\alpha\}^{1/2} & \alpha + \beta \in \Sigma, \end{cases} \\ &N_\alpha = \frac{2}{|\alpha|^2}, \\ &p = m,\ m > 0,\ \beta - m\alpha \in \Sigma,\ \beta - (m+1)\alpha \notin \Sigma, \\ &q = m,\ m > 0,\ \beta + m\alpha \in \Sigma,\ \beta + (m+1)\alpha \notin \Sigma, \end{aligned} \tag{6}$$

The numbers $(\alpha_i)_k$ are the eigenvalues of the operators H_k, as it can be seen from (4) and (5). These numbers form an r-dimensional vector $\alpha = [(\alpha)_1, \ldots, (\alpha)_r]$ called a root or a weight of the adjoint representation, and they form a vector space called root space. The notation $\alpha = [(\alpha)_1, \ldots, (\alpha)_r]$ using square brackets is called Cartan–Weyl labeling, and the root α is said to be in the Fundamental Weight System (FWS) basis. The geometrical meaning of the FWS basis will be clear later in this subsection. Since the roots label the eigenvectors of the adjoint representation, one root corresponds to each element in the algebra. The Abelian algebra formed by the elements H_i, corresponding to the null roots, is called Cartan subalgebra. There are only r null roots and they are only associated with the operators H_i. The set of all roots is called root system Σ, and each Lie algebra has its own root system. Two algebras with the same root system are said to be isomorphics. The dimension of the adjoint representation is the dimension of the algebra itself, and the degeneracy of degree r of the null root is the rank of the algebra.

In the commutation relations (5), there are only r linearly independent roots (α_i) called simple roots Π. They spawn a root space of dimension r. This natural basis is called Simple Root System (SRS) basis. An arbitrary root α in the SRS basis is denoted by using braces: $\alpha = \{(\alpha)_1, \ldots, (\alpha)_r\}$. The root space is very restrictive. For example, (1) There are only roots of two lengths; (2) The multiples of a root α are only $\pm\alpha$; (3) The angles between two arbitrary roots are only 90°, 120°, 135°, 150°, or 180°. One root is said to be positive (negative) if its first non-zero component is positive (negative) in some given basis. The set of all positive roots is denoted by Σ^+.

Another useful canonical form for the commutation relations of Lie algebras is the Chevalley form. It can be written as follows:

$$\begin{aligned}
&[h_i, h_k] = 0, \quad i \leqslant k \leqslant r,\\
&[h_i, e_k] = +A_{ik} e_k,\\
&[h_i, f_k] = -A_{ik} f_k,\\
&[e_i, f_k] = \delta_{ik} h_i,\\
&[e_\alpha, e_\beta] = \pm(p+1) e_{\alpha+\beta},\\
&\quad p = m,\ m > 0,\ \beta - m\alpha \in \Sigma,\ \beta - (m+1)\alpha \notin \Sigma,
\end{aligned} \tag{7}$$

where A is the Cartan matrix whose elements are

$$A_{ij} \equiv N_i \alpha_i \cdot \alpha_j, \quad N_i = \frac{2}{|\alpha_i|^2}, \quad i \leqslant j \leqslant r, \tag{8}$$

and $\alpha_i \cdot \alpha_j$ is the scalar product. From (7) and (8), we have another basis for the root space: the Dynkin (DYN) basis. The component $(\alpha)_i$ of an arbitrary root α in the DYN basis is given by

$$(\alpha)_i \equiv N_i \alpha_i \cdot \alpha, \quad N_i = \frac{2}{|\alpha_i|^2}, \tag{9}$$

where α_i is a simple root. An arbitrary root α in the DYN basis is denoted by using parentheses: $\alpha = ((\alpha)_1, \ldots, (\alpha)_r)$. In particular, the simple roots are the columns of the Cartan matrix. The geometrical meaning of the DYN basis will be clear later in this subsection. The half sum of the positive roots (Weyl vector) in the DYN basis, for every Lie algebra, is:

$$\rho = \sum_{\alpha>0} \alpha = (1, 1, \ldots, 1). \tag{10}$$

Every Lie algebra can be defined by its Cartan matrix or by its Dynkin diagrams, which can be constructed from the Cartan matrix and vice-versa. The Dynkin diagrams constitute a useful graphical way to classify simple Lie algebras. In a Dynkin diagram, each pair of simple roots making angles of 90°, 120°, 135° or 150° are joined by 0, 1, 2, and 3 straight lines, respectively. The number of lines joining the simple roots α_i and α_j in the Cartan matrix A is given by

$$\text{number of lines} = A_{ij} A_{ji}. \tag{11}$$

There are only two lengths for roots: the longer ones (represented by open circles) are double the length of the shorter ones (filled circles). The ratio between their lengths is given by

$$\frac{|\alpha_i|^2}{|\alpha_j|^2} = \frac{A_{ji}}{A_{ij}}. \tag{12}$$

The Dynkin diagrams play a special role in the classification of all possible finite Lie algebras. There are four major families of rank r finite complex simple Lie algebras. They are denoted by A_r, of dimension $(r+1)^2 - 1$; B_r, of dimension $r(2r+1)$; C_r, of dimension $r(2r+1)$; and D_r, of dimension $r(2r-1)$. Besides these four types, there are only five other (exceptional) finite complex simple Lie algebras: F_4, of dimension 52; E_6, of dimension 78; E_7, of dimension 133; E_8, of dimension 248; and G_2 of dimension 14. The A_r algebra is isomorphic to the complex algebra of the $n \times n$ traceless matrices, $sl(n, C)$, $n = r + 1$. Two well-known (real) subalgebras are $sl(n, R)$ and the special unitary algebra $su(n)$ consisting of anti-Hermitian traceless matrices. The B_r and D_r algebras are isomorphics to the complex algebra formed by anti-symmetric traceless matrices of order $2r+1$ and $2r$, $so(2r+1, C)$ and $so(2r, C)$, respectively. They are called orthogonal algebras. The C_r algebra is isomorphic to the complex symplectic algebra $sp(2r, C)$.

The basic ideas from the adjoint representation can be generalized in order to classify the irreducible representations. Suppose $|\lambda\rangle$ are vectors of an arbitrary irreducible representation. Then they can be labeled by the eigenvalues λ_i of the commuting elements H_i of the Cartan subalgebra:

$$H_i|\lambda\rangle = \lambda_i|\lambda\rangle, \quad i \leqslant r. \tag{13}$$

The eigenvalues λ_i are the components of a vector λ, called the weight vector, corresponding to the eigenvector $|\lambda\rangle$. At least one weight corresponds to each vector of the representation. The non-degenerate weights are called simple. The positiveness (negativeness) of a weight is defined in the same way it was defined for roots. A weight λ_1 is said to be higher than λ_2, when $\lambda_1 - \lambda_2$ is positive. There is one, and only one, simple highest weight for each irreducible representation. This means that two irreducible representations with the same highest weights are isomorphic. The components of a highest weight in the DYN basis are all non-negative integers. Weights can also be used to give the general shape of the matrices of an arbitrary irreducible representation. Let $\Delta(\Lambda)$ denote the system of weights λ of an irreducible representation given by the simple highest weight Λ. Then,

$$\begin{aligned} &E_\alpha|\lambda\rangle \propto |\lambda + \alpha\rangle, && \text{if } \lambda + \alpha \in \Delta(\Lambda), \\ &E_\alpha|\lambda\rangle = 0, && \text{if } \lambda + \alpha \notin \Delta(\Lambda), \end{aligned} \tag{14}$$

where α is a root. The elements E_α are known as step (or ladder) operators. Weights, as roots, spawn an r-dimensional vector space. The same three bases for roots can be used for weights. The DYN basis is formed by the basic irreducible representations $M_1 = (1, 0, \ldots, 0), \ldots, M_r = (0, 0, \ldots, 1)$. It is non-orthogonal and dual to the SRS basis. The DYN and SRS bases can be defined for all classical and exceptional Lie algebras. The FWS basis is formed by the positive weights of the defining fundamental representation (the lowest-dimensional basic irreducible representation). It is orthonormal for the classical A–D algebras and unique for the classical B–D algebras. The exchange of bases among the DYN, SRS and FWS bases can be summarized as follows [5, Ch. 5]:

$$(u)_{\mathrm{DYN}} = A\,\{v\}_{\mathrm{SRS}}, \tag{15}$$

$$(u)_{\mathrm{DYN}} = W\,[v]_{\mathrm{FWS}}, \tag{16}$$

$$[u]_{\mathrm{FWS}} = R\,\{v\}_{\mathrm{SRS}}, \tag{17}$$

where A are the Cartan matrices, whose columns are the simple roots in the DYN basis; W are the weights matrices, whose columns are the positive weights of the fundamental representation in the DYN basis; and R are the root matrices, whose columns are the simple roots in the FWS basis. While the Cartan matrices are unique for any Lie algebra, the weight and root matrices are not unique for the exceptional algebras [33] and A_r algebras [5, Ch. 5].

The FWS basis for A_r deserves some comment [5, Ch. 5]. The components v_i of any weight v in the FWS basis for A_r algebras are not linearly independent and they can be negative integers or fractions. This means that there are more vectors among the weights λ_i of the fundamental representation $\mathbf{M}_1$ than necessary. In fact, there are $r+1$ vectors λ_i. The usual condition to ensure uniqueness of the FWS basis is

$$\sum_{i=1}^{r+1} \lambda_i = 0. \tag{18}$$

Therefore we have another basis for the weights of A_r algebras: the modified-FWS basis, or FWS′, whose basis vectors are $\lambda_1, \ldots, \lambda_r$. The components in these two bases are related by:

$$v_i^{\mathrm{FWS}'} = v_i^{\mathrm{FWS}} - v_{r+1}^{\mathrm{FWS}}. \tag{19}$$

The transformation relations for the DYN and SRS bases are [5, Ch. 5]:

$$(u)_{\mathrm{DYN}} = W'[v]_{\mathrm{FWS}'}, \quad W' = W^{C_r}, \tag{20}$$

$$\{u\}_{\mathrm{SRS}} = R'^{-1}[v]_{\mathrm{FWS}'}, \quad R'^{-1} = R^{-1}W'. \tag{21}$$

An equivalence relation can be defined for weights in such a way to be useful in determining the weight multiplicities. Two weights λ_1 and λ_2 are said to be equivalents if

$$\lambda_2 = \lambda_1 - N_\alpha\,(\lambda_1 \cdot \alpha)\alpha, \qquad N_\alpha = \frac{2}{|\alpha|^2}, \tag{22}$$

where α is an arbitrary root. The weight λ_2 is the image of the weight λ_1 with respect to the (Weyl) reflection plane perpendicular the root α through the origin. The set of Weyl reflections associated with the simple roots forms a finite group called the Weyl or Weyl–Coxeter reflection group. Equivalent weights belong to the same representation and have the same multiplicity. The highest weight in a set of equivalent weights is called the dominant weight.

Another interesting feature of weights is that they can be grouped into layers. Let λ be a weight of the representation Λ, then the layer index $L(\lambda)$ of λ is

$$L(\lambda) = \tfrac{1}{2}\big[\delta(\Lambda) - \delta(\lambda)\big], \tag{23}$$

where $\delta(\lambda)$ is the power (or level) of λ

$$\delta(\lambda) = 2\sum_{i=1}^{r}\{\lambda\}_i, \tag{24}$$

and $\{\lambda\}_i$ represents the components of λ in the SRS basis. The number of layers is called the height of the representation, and it is given by $\delta(\Lambda)+1$. The layer index $L(\lambda)$ represents the number of simple roots that have to be subtracted from the highest weight Λ in order to have λ.

The multiplicity η_λ of a weight λ in a representation Λ can be calculated recursively by the Freudenthal formula:

$$(C_\Lambda - C_\lambda)\eta_\lambda = 2\sum_{\alpha>0}\sum_{k=1,2,\ldots}(\lambda + k\alpha)\cdot\alpha\,\eta_{\lambda+k\alpha}, \tag{25}$$

where

$$C_\lambda = \lambda\cdot(\lambda + 2\rho). \tag{26}$$

In (25) the sum in k stops when $\lambda + k\alpha > \Lambda$. Despite a numerical factor, C_Λ is the eigenvalue of the second order invariant operators or the Casimir operators.

The dimension of an irreducible representation Λ can be calculated by the Weyl formula:

$$\dim(\Lambda) = \sum_{\alpha>0} \frac{\alpha \cdot (\Lambda + \rho)}{\alpha \cdot \rho}, \tag{27}$$

where α is a positive root and ρ is the Weyl vector (half the sum of the positive roots) given in (10).

2.2. *Irreducible matrices*

While the roots and weights formalism is a powerful tool to classify Lie algebras and their irreducible representations, it does not provide us enough information to perform the explicit construction of the irreducible matrices. Theorem (14), for example, tells us when the matrix elements must be zero (selection rules), but it does not tell us about the value of the non-zero matrix elements. This means that we have to look for the weight systems of the subalgebras L_i of a Lie algebra L, $L \supset L_1 \supset L_2 \supset \cdots$, in order to complete the information needed to construct the irreducible matrices of L.

One very important problem is to know how to compute the weight systems of the irreducible representations of the subalgebras L_i from the highest weight of an arbitrary irreducible representation of L. The solution to this problem is known as the branching rules. In general, an irreducible representation of a given subalgebra can be degenerate, that is, it can be present several times in an irreducible representation of L. When the irreducible representations of all subalgebras L_i in a given chain $L \supset L_1 \supset L_2 \supset \cdots$ have no degeneracy, that is, they are multiplicity free, the chain is said to be canonical. The chains $A_r \supset A_{r-1} \supset \cdots$ and $B_r \supset D_r \supset B_{r-1} \supset D_{r-1} \supset \cdots$ are canonical chains and their branching rules are known analytically [4]. For the symplectic algebras, the branching rules for the non-canonical chain $C_r \supset C_{r-1} \oplus C_1 \supset \cdots$ are known analytically [34]. The branching rules for many other chains can be found numerically [28,30].

In general, each Lie algebra of rank r has r invariant operators. These operators commute with any element of the algebra. They are polynomials in the elements of the algebra and, therefore, they do not belong to the algebra itself. Their eigenvalues can be calculated from the highest weight components of an arbitrary irreducible representation for any Lie algebra. The physical meaning of these invariants is that the observables in a quantum system can be functions of invariants. In that way, physical quantum numbers can be made to correspond with weights [20].

2.2.1. *The Gelfand–Tsetlin method*

We reproduce here the basic results from the Gelfand–Tsetlin formalism for unitary and orthogonal algebras [4, Chs. 9–10] as well partial results for symplectic algebras [34,24].

Unitary algebras

Let $gl(n, R)$ be the general (linear) Lie algebra formed by all matrices of order n. This algebra can be decomposed as $gl(n, R) = I \oplus sl(n, R)$, where I is the Abelian algebra formed by the matrices proportional to the identity and $sl(n, R)$ is the (special linear) Lie algebra formed by the traceless matrices. The special linear algebra $sl(n, R)$ and the special unitary algebra $su(n)$ are both real forms of A_r, $n = r + 1$. One important fact to be used in the construction of the matrix elements for the unitary algebras is that one arbitrary irreducible representation of $gl(n, R)$ induces one irreducible representation of $sl(n, R)$ and $su(n)$.

The n defining matrices of $gl(n)$ are given by the Weyl matrices A_{ij}:

$$(A_{ij})_{kl} = \delta_{ik}\delta_{jl}, \qquad (A_{ij})^{\mathrm{t}} = A_{ji}. \tag{28}$$

They obey the following commutation relation:

$$[A_{ij}, A_{kl}] = \delta_{jk}A_{il} - \delta_{il}A_{kj}. \tag{29}$$

The commuting A_{ii} matrices are associated with the null roots, and the matrices A_{ij} (A_{ji}) with $j > i$ are associated with the positive (negative) roots. In general, because of

$$A_{k-h\,k} = [A_{k-h\,k-1}, A_{k-1\,k}], \tag{30}$$

we do not need to construct the matrix elements of all non-diagonal elements A_{ij}, but for $A_{i\,i+1}$ only.

The algebra $sl(n,R)$ can be formed by A_{ij}, A_{ji}, and by $H_{ii} = A_{i\,i} - A_{i+1\,i+1}$ or

$$H_{ii} = A_{ii} - \frac{1}{n}\sum_{k=1}^{n} A_{kk}, \tag{31}$$

with the highest weight $\Lambda = [m_{1n}, m_{2n}, \ldots, m_{nn}]$ changed to

$$\Lambda_i' = \Lambda_i - \frac{1}{n}\sum_{k=1}^{n} \Lambda_k. \tag{32}$$

The unitary algebra $su(n)$ is given by H_{ii}, $A_{ij} - A_{ji}$ and $\mathrm{i}(A_{ij} + A_{ji})$.

Each finite-dimensional irreducible representation of $gl(n,R)$, and also of A_{n-1}, is given by a highest weight Λ which, in the FWS basis, can always assume the form

$$\begin{aligned}\Lambda &= [m_{1n}' + w, m_{2n}' + w, \ldots, m_{nn}' + w] \\ &= [m_{1n}, m_{2n}, \ldots, m_{nn}], \quad m_{i,n} \geqslant m_{i+1,n} \geqslant 0,\ n = r+1,\end{aligned} \tag{33}$$

where w is an arbitrary constant and the components m_{in} are non-negative integers. Each vector of the irreducible representation (33) in the canonical chain $gl(n) \supset gl(n-1) \supset \cdots \supset gl(1)$ or, equivalently, $sl(n) \supset sl(n-1) \supset \cdots \supset sl(1)$, is given by the following Gelfand–Tsetlin pattern:

$$|m\rangle = \left|\begin{array}{ccccccc} m_{1n} & & m_{2n} & \ldots & m_{n-1\,n} & & m_{nn} \\ & m_{1\,n-1} & & \ldots & & m_{n-1\,n-1} & \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ & & m_{12} & & m_{22} & & \\ & & & m_{11} & & & \end{array}\right|, \qquad m_{in} \geqslant m_{i\,n-1} \geqslant m_{i+1\,n}. \tag{34}$$

Each line of (34) characterizes one irreducible representation of a subalgebra. The matrix elements of A_{ij} are given by

$$\begin{aligned} A_{kk}|m\rangle &= (r_k - r_{k-1})|m\rangle, \\ A_{k-1\,k}|m\rangle &= \sum_{i=1}^{k-1} b_{k-1}^{i}(m)|m_{i\,k-1}+1\rangle, \\ A_{k\,k-1}|m\rangle &= \sum_{i=1}^{k-1} a_{k-1}^{i}(m)|m_{i\,k-1}-1\rangle, \end{aligned} \tag{35}$$

where

$$\begin{aligned} r_k &= \sum_{i=1}^{k} m_{ik},\ r_0 = 0, \quad 1 \leqslant k \leqslant n, \\ a_{k-1}^{j}(m) &= \left\{-\frac{\prod_{i=1}^{k}(l_{ik} - l_{j\,k-1}+1)\prod_{i=1}^{k-2}(l_{i\,k-2} - l_{j\,k-1})}{\prod_{i\neq j}^{k}(l_{ik} - l_{j\,k-1}+1)(l_{ik} - l_{j\,k-1})}\right\}^{1/2}, \\ b_{k-1}^{j}(m) &= \left\{-\frac{\prod_{i=1}^{k}(l_{ik} - l_{j\,k-1})\prod_{i=1}^{k-2}(l_{i\,k-2} - l_{j\,k-1}-1)}{\prod_{i\neq j}^{k}(l_{ik} - l_{j\,k-1})(l_{ik} - l_{j\,k-1}-1)}\right\}^{1/2}, \\ l_{ik} &= m_{ik} - i. \end{aligned} \tag{36}$$

The matrix elements a and b in (36) are all real numbers and $(A_{ij})^{\mathrm{t}} = A_{ji}$.

The generators of the q-deformed (or “quantum group”) $sl_q(n)$ algebra satisfy the following commutation relations [35,36]:

$$[H_i, H_j] = 0,$$
$$[A_{i\,i+1}, A_{i+1\,i}] = [H_i]_q, \tag{37}$$

where

$$H_i = A_{ii} - A_{i+1\,i+1}, \tag{38}$$

and

$$[x]_q \equiv \frac{q^x - q^{-x}}{q - q^{-1}} = \frac{\sinh(zx)}{\sinh(z)}, \quad q = \exp(z). \tag{39}$$

Note that the deformation defined above has the following properties:

$$\begin{aligned}
&[-x]_q = -[x]_q,\\
&[x]_{1/q} = [x]_q,\\
&[0]_q = 0,\\
&[1]_q = 1,\\
&\lim_{q\to 1}[x]_q = x.
\end{aligned} \tag{40}$$

When $|q| \neq 1$ then the irreducible representations of the deformed algebras are classified by the roots and weights formalism as well. The irreducible q-deformed matrix elements for $sl_q(n)$ are given by the same formulae (35) with q-deformed terms [35,37]:

$$\begin{aligned}
a^j_{k-1} &= \left\{-\frac{\prod_{i=1}^{k}[(l_{ik} - l_{j\,k-1} + 1)]_q \prod_{i=1}^{k-2}[(l_{i\,k-2} - l_{j\,k-1})]_q}{\prod_{i\neq j}^{k}[(l_{ik} - l_{j\,k-1} + 1)]_q[(l_{ik} - l_{j\,k-1})]_q}\right\}^{1/2},\\
b^j_{k-1} &= \left\{-\frac{\prod_{i=1}^{k}[(l_{ik} - l_{j\,k-1})]_q \prod_{i=1}^{k-2}[(l_{i\,k-2} - l_{j\,k-1} - 1)]_q}{\prod_{i\neq j}^{k}[(l_{ik} - l_{j\,k-1})]_q[(l_{ik} - l_{j\,k-1} - 1)]_q}\right\}^{1/2}.
\end{aligned} \tag{41}$$

Orthogonal algebras

The orthogonal algebras $so(n)$ formed by anti-symmetric matrices are real forms of B_r, $n = 2r + 1$, and D_r, $n = 2r$. An element X_{ij} of an orthogonal algebra can be written as

$$X_{ij} = A_{ij} - A_{ji}, \qquad (X_{ij})^{\mathrm{t}} = -X_{ij}, \tag{42}$$

where A_{ij} are the Weyl matrices given in (28). Their commutation relations are:

$$[X_{ik}, X_{lm}] = \delta_{kl}X_{im} + \delta_{im}X_{kl} - \delta_{km}X_{il} - \delta_{il}X_{km}. \tag{43}$$

Unfortunately, these commutation relations are not in the Cartan–Weyl canonical form.

The irreducible representations of $so(n)$ can be given by the following highest weights with integral or half-integral components:

$$\begin{aligned}
&\Lambda = [m_{1\,2k}, \ldots, m_{k\,2k}], \quad n = 2k+1,\ B_k,\\
&\quad m_{1\,2k} \geqslant m_{2\,2k} \geqslant \cdots \geqslant m_{k\,2k} \geqslant 0,\\
&\Lambda = [m_{1\,2k+2}, \ldots, m_{k+1\,2k+2}], \quad n = 2(k+1),\ D_{k+1},\\
&\quad m_{1\,2k+2} \geqslant m_{2\,2k+2} \geqslant \cdots \geqslant |m_{k+1\,2k+2}|.
\end{aligned} \tag{44}$$

Each basis vector in the canonical chain $so(n) \supset so(n-1) \supset \cdots \supset so(2)$ is given by the Gelfand–Tsetlin pattern

$$|m\rangle = \left|\begin{array}{ccccccc} m_{1\,2k} & & m_{2\,2k} & \ldots & m_{k-1\,2k} & & m_{k\,2k} \\ m_{1\,2k-1} & & m_{2\,2k-1} & \ldots & m_{k-1\,2k-1} & & m_{k\,2k-1} \\ & m_{1\,2k-2} & & \ldots & & m_{k-1\,2k-2} & \\ & m_{1\,2k-3} & & \ldots & & m_{k-1\,2k-3} & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & m_{14} & & m_{24} & & \\ & & m_{13} & & m_{23} & & \\ & & & m_{12} & & & \\ & & & m_{11} & & & \end{array}\right|, \tag{45}$$

$$m_{1\,2k} \geqslant m_{1\,2k-1} \geqslant m_{2\,2k} \geqslant m_{2\,2k-1} \geqslant \cdots \geqslant m_{k-1\,2k} \geqslant m_{k-1\,2k-1} \geqslant m_{k\,2k} \geqslant m_{k\,2k-1} \geqslant -m_{k\,2k},$$
$$m_{1\,2k-1} \geqslant m_{1\,2k-2} \geqslant m_{2\,2k-1} \geqslant \cdots \geqslant m_{k-1\,2k-1} \geqslant m_{k-1\,2k-2} \geqslant |m_{k\,2k-1}|,$$

for $n = 2k+1$, and

$$|m\rangle = \left|\begin{array}{ccccccc} m_{1\,2k+1} & & m_{2\,2k+1} & \ldots & m_{k\,2k+1} & & m_{k+1\,2k+1} \\ & m_{1\,2k} & & \ldots & & m_{k\,2k} & \\ & m_{1\,2k-1} & & \ldots & & m_{k\,2k-1} & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & m_{15} & & m_{25} & & m_{34} & \\ & & m_{14} & & m_{24} & & \\ & & m_{13} & & m_{23} & & \\ & & & m_{12} & & & \\ & & & m_{11} & & & \end{array}\right|, \tag{46}$$

$$m_{1\,2k+1} \geqslant m_{1\,2k} \geqslant m_{2\,2k+1} \geqslant \cdots \geqslant m_{k\,2k+1} \geqslant m_{k\,2k} \geqslant |m_{k+1\,2k+1}|,$$
$$m_{1\,2k} \geqslant m_{1\,2k-1} \geqslant m_{2\,2k} \geqslant \cdots \geqslant m_{k\,2k} \geqslant m_{k\,2k-1} \geqslant -m_{k\,2k},$$

for $n = 2(k+1)$. The matrix elements of any X_{ij} can be found using (43) if the matrix elements of $X_{2p+1\,2p}$, $p = 1, 2, \ldots, [(n-1)/2]$, and $X_{2p+2\,2p+1}$, $p = 0, 1, \ldots, [(n-2)/2]$, are known:

$$\begin{aligned} X_{2k+2,2k+1}|m\rangle &= \sum_{j=1}^{k} b_{2k}^{j}(m)|m_{j\,2k}+1\rangle \\ &\quad - \sum_{j=1}^{k} b_{2k}^{j}(m_{j\,2k})|m_{j\,2k}-1\rangle + \mathrm{i}c_{2k}|m\rangle, \\ X_{2k+1,2k}|m\rangle &= \sum_{j=1}^{k} a_{2k-1}^{j}(m)|m_{j\,2k-1}+1\rangle \\ &\quad - \sum_{j=1}^{k} a_{2k-1}^{j}(m_{j\,2k-1})\,|m_{j\,2k-1}-1\rangle, \end{aligned} \tag{47}$$

where

$$
\begin{aligned}
a^{j}_{2k-1}(m) &= \frac{1}{2}\left\{\frac{\prod_{r=1}^{k-1}(l_{r\,2k-2}-l_{j\,2k-1}-1)(l_{r\,2k-2}+l_{j\,2k-1})}{\prod_{r\neq j}^{k}(l^2_{r\,2k-1}-l^2_{j\,2k-1})(l^2_{r\,2k-1}-(l_{j\,2k-1}+1)^2)}\right\}^{1/2} \\
&\quad\times\left\{\prod_{r=1}^{k}(l_{r\,2k}-l_{j\,2k-1}-1)(l_{r\,2k}+l_{j\,2k-1})\right\}^{1/2}, \\
b^{j}_{2k}(m) &= \frac{1}{2}\left\{\frac{\prod_{r=1}^{k}(l^2_{r\,2k-1}-l^2_{j\,2k})\prod_{r=1}^{k+1}(l^2_{r\,2k+1}-l^2_{j\,2k})}{l^2_{j\,2k}(4l^2_{j\,2k}-1)\prod_{r\neq j}^{k}(l^2_{r\,2k}-l^2_{j\,2k})((l_{r\,2k}-1)^2-l^2_{j\,2k})}\right\}^{1/2}, \\
c_{2k}(m) &= \frac{\prod_{r=1}^{k}l_{r\,2k-1}\prod_{r=1}^{k+1}l_{r\,2k+1}}{\prod_{r=1}^{k}l_{r\,2k}(l_{r\,2k}-1)}, \\
&l_{r\,2k}=m_{r\,2k}+k-r+1,\ l_{r\,2k-1}=m_{r\,2k-1}+k-r.
\end{aligned}
\tag{48}
$$

Symplectic algebras

The finite irreducible representations of C_r (or $sp(2r)$) are given by the integral components of the highest weight

$$
\Lambda=[\omega_{1r},\omega_{2r},\ldots,\omega_{rr}],\quad \omega_{1r}\geqslant\omega_{2r}\geqslant\cdots\geqslant\omega_{rr}\geqslant 0. \tag{49}
$$

Each basis vector in the non-canonical chain $C_r\supset C_{r-1}\oplus C_1\supset\cdots$ is given by the Gelfand–Tsetlin–Cerkaski pattern [34]:

$$
|\omega\rangle=\left|\begin{array}{ccccccccc}
\omega_{1\,r} & & \omega_{2\,r} & \ldots & \omega_{r-1\,r} & & \omega_{r\,r} & & \\
& \gamma_{1\,r} & & \gamma_{2\,r} & \ldots & \gamma_{r-1\,r} & & & h_r \\
& & \omega_{1\,r-1} & & \omega_{2\,r-1} & \ldots & \omega_{r-1\,r-1} & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
& & \omega_{12} & & \omega_{22} & & & & \\
& & & \gamma_{12} & & & & & h_2 \\
& & & & \omega_{11} & & & & \\
& & & & & & & & h_1
\end{array}\right|,
\tag{50}
$$

$$
\omega_{ik}\geqslant\gamma_{ik}\geqslant\omega_{i+1\,k},\quad \gamma_{k\,k+1}\geqslant\omega_{kk}\geqslant\rho_k,
$$

$$
h_k=\sigma_k,\sigma_k-2,\ldots,-\sigma_k,
$$

where

$$
\begin{aligned}
\rho_k &= \gamma_{k\,k+1}-\omega_{k+1\,k+1}+\sum_{i=1}^{k}(2\gamma_{i+1\,k+1}-\omega_{i+1\,k+1}-\omega_{ik}), \\
\sigma_k &= \omega_{kk}+\sum_{i=1}^{k-1}(\omega_{ik}+\omega_{i\,k-1}-2\gamma_{ik}).
\end{aligned}
\tag{51}
$$

In (50), $\omega_{i\,r-h}$ are the components of the highest weight of C_{r-h} and $[h_1,\ldots,h_r]$ are the weights of the weight system $\Delta(\Lambda)$ in the FWS basis. The highest weights of the C_1 algebras are given by σ_k in (51).

Unfortunately, there are no general formulae for the matrix elements of C_r algebras [38,34,39,24]. The following notation

$$
\begin{aligned}
&E_{i\,0}\to \text{null roots},\quad i\leqslant r, \\
&E_{i\,+}\to \text{positive roots}, \\
&E_{i\,-}\to \text{negative roots},
\end{aligned}
\tag{52}
$$

Table 1
Independent invariants $\mathcal{C}_p$ for classical Lie algebras

	p	α	β	r_i	i
A_r	$2, 3, \ldots, r$	$r/2$	0	$(r+2)/2 - i$	$1, 2, \ldots, r+1$
B_r	$2, 4, \ldots, 2(r-1), r$	$r - 1/2$	1	$(r+1/2)\varepsilon_i - i$	$1, \ldots, r, 0, -r, \ldots, -1$
C_r	$2, 4, \ldots, 2r$	r	-1	$(r+1)\varepsilon_i - i$	$1, \ldots, r, -r, \ldots, -1$
D_r	$2, 4, \ldots, 2r$	$r - 1$	1	$r\varepsilon_i - i$	$1, \ldots, r, -r, \ldots, -1$

for the generators E_{it} of C_r, comes from [24] where the matrix elements of C_2 and C_1 were calculated directly in the chain $C_2 \subset C_1 \oplus C_1$ satisfying the Cartan–Weyl commutation relations.

Invariant operators

In general, there is a set of r linearly independent self-commuting invariant operators $\mathcal{C}_p$ for each Lie algebra of rank r. They are polynomials of degree r in the algebra elements and commute with all elements of a Lie algebra L:

$$[\mathcal{C}_p, L] = 0. \tag{53}$$

Therefore, they must be multiples of the identity operator $\mathcal{I}$ in a given irreducible representation:

$$\mathcal{C}_p = C_p \mathcal{I}, \tag{54}$$

where C_p is the eigenvalue of $\mathcal{C}_p$. The set of independent invariants of classical algebras are given in Table 1. Their corresponding eigenvalues, in terms of the components of the highest weight (in the FWS basis),

$$\begin{aligned} &\Lambda = [m_1, \ldots, m_{r+1}], \qquad m_i \geqslant m_{i+1} \geqslant 0, \quad \text{for } A_r, \\ &\Lambda = [m_1, \ldots, m_r] \quad \text{for } B_r,\ C_r \text{ and } D_r, \end{aligned} \tag{55}$$

are given by [4, Ch. 9]:

$$C_p(\Lambda) = \mathrm{Tr}(K^p E), \tag{56}$$

where

$$\begin{aligned} &E_{ij} = 1, \\ &K_{ij} = (l_i + \alpha)\delta_{ij} - \theta_{ji} + \tfrac{1}{2}\beta(1 + \varepsilon_i)\delta_{i,-j}, \\ &l_i = m_i + r_i, \end{aligned} \tag{57}$$

and

$$\theta_{ij} = \begin{cases} 1 & \text{for } j < i, \\ 0 & \text{for } j \geqslant i, \end{cases} \qquad \varepsilon_i = \begin{cases} 0 & \text{for } i = 0, \\ 1 & \text{for } i > 0, \\ 1 & \text{for } i < 0. \end{cases} \tag{58}$$

The constants α, β and r_i are given in Table 1.

3. Structure of the KILLING package

Every algebraic procedure in the KILLING package has the same name and the same arguments in the Maple V [25] and Mathematica [26] environments. The only difference in the syntax is that parentheses are used in Maple V to specify the arguments of a function instead of the brackets used in Mathematica. For example, in Maple V we have rs(A,3) whereas in Mathematica it is written rs[A,3].

In both environments, the name X of each family of Lie algebras is a string and must be surrounded by double quotes: {″A″, ″B″, ″C″, ″D″, ″E″, ″F″, ″G″}. The corresponding rank is designated by r. An irreducible representation is indicated by Λ and a weight (or root) by λ. The root system is indicated by Σ, the positive roots by Σ^+, and the simple roots by Π.

In the first part (The Roots & Weights formalism), all input and output weights (and roots) are in the DYN basis, unless it is clear from the context that they are not. In the second part (The Gelfand–Tsetlin method), all input and output weights (and roots) are in the FWS basis.

3.1. The Roots & Weights formalism

3.1.1. Computing weights and roots

- **bi**(r) → basic irreducible representations **M**
- **irrdim**(Λ, X) → irreducible representation dimensions
- **ws**(Λ, X) → weight system $\Delta(\Lambda)$
- **wsm**(Λ, X) → multiplicities in $\Delta(\Lambda)$
- **power**(Λ, X) → power (or level) $\delta(\Lambda)$
- **layer**(λ, Λ, X) → layer index $L(\lambda)$ in $\Delta(\Lambda)$
- **rs**(X, r) → root system Σ
- **sr**(X, r) → simple roots Π
- **check**(Σ) → ρ, Σ^+ (ρ is the half sum of Σ^+)
- **algdim**(X, r) → algebra dimension

3.1.2. Exchanging bases in the weight space

- **dyn2srs**(λ, X) → $\lambda_{\text{DYN}} \to \lambda_{\text{SRS}}$
- **dyn2fws**(λ, X) → $\lambda_{\text{DYN}} \to \lambda_{\text{FWS}}$ (classical algebras only)
- **dyn2fwsm**(λ, X) → $\lambda_{\text{DYN}} \to \lambda_{\text{FWS}'}$ (A_r algebras only)
- **fws2dyn**(λ, X) → $\lambda_{\text{FWS}} \to \lambda_{\text{DYN}}$ (classical algebras only)
- **fws2srs**(λ, X) → $\lambda_{\text{FWS}} \to \lambda_{\text{SRS}}$ (classical algebras only)
- **fws2fws**(λ) → $\lambda_{\text{FWS}} \to \lambda_{\text{FWS}}$ (A_r algebras only)
- **fws2fwsm**(λ) → $\lambda_{\text{FWS}} \to \lambda_{\text{FWS}'}$ (A_r algebras only)
- **srs2dyn**(λ, X) → $\lambda_{\text{SRS}} \to \lambda_{\text{DYN}}$
- **srs2fws**(λ, X) → $\lambda_{\text{SRS}} \to \lambda_{\text{FWS}}$ (classical algebras only)
- **srs2fwsm**(λ, X) → $\lambda_{\text{SRS}} \to \lambda_{\text{FWS}'}$ (A_r algebras only)
- **Cm**(X, r) → Cartan matrices A
- **Wm**(X, r) → Weight matrices W (classical algebras only)
- **Rm**(X, r) → Root matrices R (classical algebras only)
- **Cm**(X, r, ″inv″) → inverse Cartan matrices
- **Wm**(X, r, ″inv″) → inverse Weight matrices (classical algebras only)
- **Rm**(X, r, ″inv″) → inverse Root matrices R (classical algebras only)

3.1.3. Operations in the weight space

- **kronecker**(Λ', Λ'', X) → Kronecker product $\Lambda' \times \Lambda''$
- **sprod**(λ', λ'', X) → scalar product $\lambda' \cdot \lambda''$
- **angle**(λ', λ'', X) → angle between two weights
- **casimir**(Λ, X) → eigenvalue of the Casimir operators
- **dominant**(hwts, X) → sorts highest weights in descending order

- **sortwts**(wts) → sorts weights in descending order
- **weyl**(i, λ, X) → Weyl reflection of λ through the simple root α_i
- **weyl**(λ', λ, X) → Weyl reflection of λ through the weight λ
- **t2l**(wts) → converts a table of weights into a flat list of weights (Maple V) or flattens a list of lists of weights (Mathematica)

3.2. The Gelfand–Tsetlin method

In the following procedures, $|m\rangle$ is a generic Gelfand–Tsetlin vector and M is a specific Gelfand–Tsetlin basis. The optional argument z is the deformation parameter $q = \exp(z)$.

3.2.1. Eigenvectors

- **patterns**(X, r) → Gelfand–Tsetlin basis M

3.2.2. Matrix elements

- **Ame**($i, k, |m\rangle$) → matrix elements of the generator A_{ik} for A_r algebras
- **Ame**($i, k, |m\rangle, z$) → q-deformed matrix elements of the generator ${}_qA_{ik}$ for deformed A_r algebras
- **Ome**($i, k, |m\rangle$) → matrix elements of the generator X_{ik} for B_r and D_r algebras
- **Cme**($i, t, |m\rangle$) → matrix elements of the generator E_{it} for C_1 and C_2 algebras
- **Aim**(i, k, M) → irreducible matrix A_{ik} for A_r algebras
- **Aim**(i, k, M, z) → q-deformed irreducible matrix ${}_qA_{ik}$ for deformed A_r algebras
- **Oim**(i, k, M) → irreducible matrix X_{ik} for B_r and D_r algebras
- **Cim**(i, t, M) → irreducible matrix of E_{it} for C_1 and C_2 algebras

3.2.3. Eigenvalues

- **spectra**(n, Λ, X) → eigenvalue of the invariant $\mathcal{C}_n(\Lambda)$

3.2.4. Auxiliary routines

- **m_jk**(m, j, k, p) → $m_{jk} \to m_{jk} + p$ (m is a Gelfand–Tsetlin vector)
- **qdeform**(x, q) → q-deformation of x
- **commute**(a, b) → commutator $[a, b] = ab - ba$
- **commute**(a, b, q) → q-commutator $[a, b]_q = ab - qba$

4. Detailed description of the KILLING package

In this section, we present a detailed description of each routine in the KILLING package, including comments on the codes, examples and comments on the basic theorems about the representation theory of finite semisimple Lie algebras.

Every algebraic procedure in the KILLING package has the same name and arguments in the Maple V [25] and Mathematica [26] environments. The only difference in the syntax is that parentheses are used in Maple V to specify the arguments of a function instead of the brackets used in Mathematica. For example, in Maple V we have rs(A,3) whereas in Mathematica it is written rs[A,3]. It must be observed that weights are represented by lists in both algebraic languages and that lists are only represented by brackets [] in Maple V and by braces {} in Mathematica. Therefore, we do not have any way, other than the context, to differentiate the DYN, SRS and FWS bases in either symbolic computational softwares.

In this section, the name of each family of Lie algebras is a string X which must be surrounded by double quotation marks in both environments: {″A″, ″B″, ″C″, ″D″, ″E″, ″F″, ″G″}. The corresponding rank is designated by r. An irreducible representation is indicated by Λ, a weight by λ, and a simple root by α_i. The weight system is indicated by $\Delta(\Lambda)$ and the root system by Σ. The positive roots are denoted by Σ^+, and the simple roots by Π.

In the first part (The Roots & Weights formalism), all input and output weights (and roots) are in the DYN basis, unless it is clear from the context that they are not. In the second part (The Gelfand–Tsetlin method), all input and output weights (and roots) are in the FWS basis.

4.1. The Roots & Weights formalism

Weights and roots are represented by lists in the Maple V and Mathematica algebraic programming languages. Therefore, the weight Λ, whose components are Λ_i, written as $\Lambda = (\Lambda_1, \ldots, \Lambda_r)$ in the DYN basis for an algebra of rank r, must be typed

$$\Lambda := [\Lambda_1, \ldots, \Lambda_r] \to \text{in Maple V},$$
$$\Lambda = \{\Lambda_1, \ldots, \Lambda_r\} \to \text{in Mathematica}.$$

4.1.1. Computing roots and weights

The procedure **bi**(r) writes the basic irreducible representations (irreps) $\mathbf{M}_i$, $i \leqslant r$, in the DYN basis for any Lie algebra of rank r. Its output is a list of highest weights:

$$\text{bi}(r) \to [\mathbf{M}_1, \ldots, \mathbf{M}_r] \quad \text{Maple V},$$
$$\text{bi}[r] \to \{\mathbf{M}_1, \ldots, \mathbf{M}_r\} \quad \text{Mathematica}.$$

Example 1. The basic irreps for algebras of rank two and three are, respectively:

$$\text{bi}(2) \to (1,0), (0,1); \quad \text{bi}(3) \to (1,0,0), (0,1,0), (0,0,1).$$

When roots and weights are written in the FWS basis, the Weyl formula (27) for the dimension of the irreducible representation $\Lambda = [l_1, \ldots, l_{r'}]$, $r' = r+1$ for A_r and $r' = r$ for B_r, C_r, and D_r, can be simplified to [5, Ch. 5]:

$$A_r \to \dim(\Lambda) = \prod_{k>i=1}^{r+1} \left(\frac{p_i - p_k}{g_i - g_k}\right), \quad g_i = \frac{r}{2} - i + 1,$$
$$B_r \to \dim(\Lambda) = \prod_{i=1}^{r} \frac{p_i}{g_i} \prod_{k>i=1}^{r} \left(\frac{p_i^2 - p_k^2}{g_i^2 - g_k^2}\right), \quad g_i = r - i + \frac{1}{2},$$
$$C_r \to \dim(\Lambda) = \prod_{i=1}^{r} \frac{p_i}{g_i} \prod_{k>i=1}^{r} \left(\frac{p_i^2 - p_k^2}{g_i^2 - g_k^2}\right), \quad g_i = r - i + 1,$$
$$D_r \to \dim(\Lambda) = \prod_{k>i=1}^{r} \left(\frac{p_i^2 - p_k^2}{g_i^2 - g_k^2}\right), \quad g_i = r - i,$$

where

$$p_i = g_i + l_i. \tag{59}$$

When X is one of the four classical algebras, the procedure **irrdim**(Λ, X) uses the formulae above. For the exceptional Lie algebras, the dimensions are directly calculated from the Weyl formula (27). The input highest weight Λ must be in the DYN basis.

Example 2. The dimension of $\Lambda = (1, 1)$ (adjoint representation) of A_2 is computed as follows:

$$\mathrm{irrdim}(\Lambda, {}''\mathrm{A}'') \to 8.$$

In the same way, the dimension of $\Lambda = (2, 0, 0)$ (adjoint representation) of C_3 is:

$$\mathrm{irrdim}(\Lambda, {}''\mathrm{C}'') \to 21.$$

Example 3. Dimensions can also be calculated in algebraic form. For example, the dimension of the representation $\Lambda = (m)$ of A_1, or *su*(2) (the angular momentum algebra), is:

$$\mathrm{irrdim}(\Lambda, {}''\mathrm{A}'') \to m + 1.$$

The weight system $\Delta(\Lambda)$ of an irreducible representation $\Lambda = (\Lambda_1, \ldots, \Lambda_r)$ can be calculated in the DYN basis using the following algorithm [5, Ch. 5]:

Algorithm 1.

- Calculate the height $\delta(\Lambda)$ of the representation Λ;
- Write down all simple roots $\alpha_i = (A_{1i}, \ldots, A_{ri})$ from the Cartan matrix A;
- Starting with the highest weight Λ, whose layer index is $L_\Lambda(\Lambda) = 0$, repeat each of the following steps for each weight of the same layer index:
  (1) For each component $\Lambda_i > 0$, write down the string of weights $\omega^k = \Lambda - (k-1)\alpha_i$, $1 \leqslant k \leqslant \Lambda_i + 1$;
  (2) Group the new weights ω^k according to their layer index, $L_\Lambda(\omega^k)$;
  (3) Move to the next layer index set of weights and repeat the last two steps, switching the highest weight Λ with each new weight ω^k;
- Continue this process until the lowest weight in the last layer $\delta(\Lambda) + 1$ is reached.

Algorithm 1 is used by the procedure **ws(**Λ, X) to calculate the weight system $\Delta(\Lambda)$ for all classical and exceptional Lie algebras X. The output is a set of sets of weights grouped by their layer indices $L_\Lambda(\lambda)$:

$$\mathrm{ws}(\Lambda, \mathrm{X}) \to \mathrm{table}([0 = [\Lambda], \ldots, L_\Lambda(\lambda) = [\lambda, \ldots]]) \quad \text{Maple V},$$
$$\mathrm{ws}[\Lambda, \mathrm{X}] \to \{\{\Lambda\}, \ldots, \{\lambda, \ldots\}\} \quad \text{Mathematica}.$$

Example 4. The fundamental defining representation $\Lambda = (1, 0)$ of dimension 3 of A_2 (or *su*(3)) has the following weight system $\Upsilon \equiv \Delta(\Lambda)$ in the DYN basis:

$$\mathrm{ws}(\Lambda, {}''\mathrm{A}'') \to \begin{array}{rcl} L_\Lambda(\lambda) & \leftrightarrow & \lambda \\ 0 & = & (1,0) \\ 1 & = & (-1,1) \\ 2 & = & (0,-1) \end{array}$$

Note that the lowest weight is $(0, -1)$ instead of $(-1, 0)$. The fundamental representation $\Lambda = (1, 0, 0)$ of dimension 6 of C_3 (or *sp*(6)) has the following weight system $\Upsilon \equiv \Delta(\Lambda)$ in the DYN basis:

$$
\mathrm{ws}(\Lambda,''\mathrm{C}'') \rightarrow \quad
\begin{aligned}
L_\Lambda(\lambda) &\leftrightarrow \lambda\\
0 &= (1,0,0)\\
1 &= (-1,1,0)\\
2 &= (0,-1,1)\\
3 &= (0,1,-1)\\
4 &= (1,-1,0)\\
5 &= (-1,0,0)
\end{aligned}
$$

All weights in these two examples are multiplicity free.

Example 5. The representation $\Lambda = (1,1,0)$ of dimension 64 of C_3 (or $sp(6)$). Its weight system $\Delta(\Lambda)$ in the DYN basis is:

$$
\mathrm{ws}(\Lambda,''\mathrm{C}'') \rightarrow \quad
\begin{aligned}
L_\Lambda(\lambda) &\leftrightarrow \lambda\\
0 &= (1,1,0)\\
1 &= (2,-1,1),(-1,2,0)\\
2 &= (0,0,1),(2,1,-1)\\
3 &= (3,-1,0),(-2,1,1),(1,-2,2),(0,2,-1)\\
4 &= (-2,3,-1),(1,0,0),(-1,-1,2)\\
5 &= (-1,1,0),(1,2,-2),(2,-2,1)\\
6 &= (-3,2,0),(0,-1,1),(-1,3,-2),(2,0,-1)\\
7 &= (0,1,-1),(3,-2,0),(1,-3,2),(-2,0,1)\\
8 &= (-1,-2,2),(1,-1,0),(-2,2,-1)\\
9 &= (-1,0,0),(1,1,-2),(2,-3,1)\\
10 &= (-1,2,-2),(-3,1,0),(0,-2,1),(2,-1,-1)\\
11 &= (-2,-1,1),(0,0,-1)\\
12 &= (1,-2,0),(-2,1,-1)\\
13 &= (-1,-1,0)
\end{aligned}
$$

Here we count only 38 weights instead of 64. Some weights have a multiplicity greater than one. The procedure **wsm** must be used in order to determine the multiplicities. We can see that the layer of index i has the same number of weights as the layer of index $\delta(\Lambda) - i$ ($\delta(\Lambda) = 13$ for this case). This is a general characteristic of any weight system. Note that the lowest weight is equal to $-\Lambda$.

The (inner) multiplicity η_λ of a weight λ in the weight system $\Delta(\Lambda)$ can be calculated recursively by the Freudenthal formula (25) using the following algorithm [5,40]:

Algorithm 2.

- Compute the weight system;
- Split the weight system in sets of equivalent weights;

- Find the dominant weight (or the weight with the lowest layer index) in each set of equivalent weights;
- Sort the dominant weights in ascending order;
- Compute the multiplicity of each dominant weight.

The procedure **wsm**(Λ, X) was implemented using Algorithm 2. Its output is a list of two elements: the first element is the dimension and the second element is a list of lists of equivalent weights in which the multiplicity η is given in the first positions:

$$\mathrm{wsm}(\Lambda, \mathrm{X}) \rightarrow [\mathrm{dim}, [[\eta_\lambda, [\lambda, \ldots]], \ldots]] \quad \text{Maple V},$$

$$\mathrm{wsm}[\Lambda, \mathrm{X}] \rightarrow \{\mathrm{dim}, \{\{\eta_\lambda, \{\lambda, \ldots\}\}, \ldots\}\} \quad \text{Mathematica}.$$

Example 6. The multiplicities in the weight system $\Delta(\Lambda)$, $\Lambda = (1, 1, 0)$, of C_3 are:

$$\mathrm{wsm}(\Lambda, {''}\mathrm{C}{''}) \rightarrow \begin{array}{rl} \eta_\lambda \rightarrow & \lambda \\ 1 \rightarrow & (-1,3,-2), (2,-3,1), (1,-2,2), (1,-3,2), \\ & (-1,-2,2), (2,1,-1), (-2,3,-1), (-2,1,-1), \\ & (1,1,-2), (2,-1,-1), (1,2,-2), (3,-2,0), \\ & (1,-2,0), (1,1,0), (2,-1,1), (-1,-1,2), \\ & (-1,2,0), (-3,1,0), (-1,2,-2), (-2,1,1), \\ & (-2,-1,1), (3,-1,0), (-1,-1,0), (-3,2,0), \\ 2 \rightarrow & (2,0,-1), (0,0,1), (0,-2,1), (-2,0,1), \\ & (0,0,-1), (0,2,-1), (2,-2,1), (-2,2,-1), \\ 4 \rightarrow & (0,1,-1), (-1,0,0), (1,-1,0), \\ & (0,-1,1), (1,0,0), (-1,1,0) \end{array}$$

When grouped by layers and the multiplicities are included, the number of weights in each layer has the following structure:

$$\begin{array}{rcl} L & \leftrightarrow & \text{number of weights} \\ 0 & = & \bullet \\ 1 & = & \bullet\bullet \\ 2 & = & \bullet\bullet\bullet \\ 3 & = & \bullet\bullet\bullet\bullet \\ 4 & = & \bullet\bullet\bullet\bullet\bullet\bullet \\ 5 & = & \bullet\bullet\bullet\bullet\bullet\bullet \\ 6 & = & \bullet\bullet\bullet\bullet\bullet\bullet\bullet \end{array}$$

It can be seen from the structure shown above that number of weights in a given layer is greater than or equal to the number of weights in the previous layer until the middle of the layer tree. The second part (not shown above) is a mirror image of the first part. This is another feature of any weight system.

The power $\delta(\Lambda)$, given in (24), and the layer index $L_\Lambda(\lambda)$ of a weight λ in an irreducible representation Λ, given in (23), are computed by the procedures **power**(Λ, X) and **layer**(λ, Λ, X), respectively. Their outputs are positive numbers.

Example 7. The power of the highest weight $\Lambda = (1, 1, 0)$ for C_3, whose weight system was calculated in Example 5, is

$$\text{power}(\Lambda, {''}\text{C}{''}) \to 13.$$

The power $\delta(\Lambda) = 13$ means that the irreducible representation Λ has 14 layers. The layer index of the weight $\lambda = (1, 0, 0)$ inside that irreducible representation is

$$\text{layer}(\lambda, \Lambda, {''}\text{C}{''}) \to 4.$$

Roots are the weights of the adjoint representation. In the DYN basis we have the following highest weights Λ for the adjoint representations of classical Lie algebras [28,30]:

$$\begin{aligned}
&A_1 \to \Lambda = (2),\\
&A_r \to \Lambda = (1, 0, 0, \ldots, 0, 1), \quad r > 1,\\
&B_1 \to \Lambda = (2),\\
&B_2 \to \Lambda = (0, 2),\\
&B_r \to \Lambda = (0, 1, 0, \ldots, 0), \quad r > 2,\\
&C_r \to \Lambda = (2, 0, \ldots, 0), \quad r \geqslant 1,\\
&D_3 \to \Lambda = (0, 1, 1),\\
&D_r \to \Lambda = (0, 1, 0, \ldots, 0), \quad r > 3;
\end{aligned}$$

and

$$\begin{aligned}
&E_6 \to \Lambda = (0, 0, 0, 0, 0, 1),\\
&E_7 \to \Lambda = (1, 0, 0, 0, 0, 0, 0),\\
&E_8 \to \Lambda = (0, 0, 0, 0, 0, 0, 1, 0),\\
&F_4 \to \Lambda = (1, 0, 0, 0),\\
&G_2 \to \Lambda = (1, 0)
\end{aligned}$$

for exceptional algebras. The orthogonal algebra D_2 can be written as $D_2 = A_1 \oplus A_1$. The highest weights Λ given above are used in the procedure **rs**(X, r) which calls the procedure **ws**(Λ, X) to compute the corresponding root system $\Sigma(\Lambda)$. The output of rs is the output of ws.

Example 8. The A_2 algebra has eight elements and its root system is:

$$\text{rs}({''}\text{A}{''}, 2) \to \quad \begin{aligned}
L_\Lambda(\lambda) &\leftrightarrow \lambda\\
0 &= (1, 1)\\
1 &= (2, -1), (-1, 2)\\
2 &= (0, 0)\\
3 &= (-2, 1), (1, -2)\\
4 &= (-1, -1)
\end{aligned}$$

From the symmetry of a weight system grouped by layers, the null root $(0, 0)$ must have a degeneracy of degree two. For any simple Lie algebra of rank r, the null root, which has a degeneracy of degree r, is the only degenerated root.

Example 9. The C_3 algebra has 21 elements and its root system is:

$$\mathrm{rs}(''\mathrm{C}'', 3) \to \begin{aligned} L_\Lambda(\lambda) &\leftrightarrow \lambda \\ 0 &= (2, 0, 0) \\ 1 &= (0, 1, 0) \\ 2 &= (-2, 2, 0), (1, -1, 1) \\ 3 &= (-1, 0, 1), (1, 1, -1) \\ 4 &= (0, -2, 2), (-1, 2, -1), (2, -1, 0) \\ 5 &= (0, 0, 0) \\ 6 &= (-2, 1, 0), (0, 2, -2), (1, -2, 1) \\ 7 &= (1, 0, -1), (-1, -1, 1) \\ 8 &= (-1, 1, -1), (2, -2, 0) \\ 9 &= (0, -1, 0) \\ 10 &= (-2, 0, 0) \end{aligned}$$

The simple roots are always alone in the first layer before the middle of the layer tree, and the positive roots are in the first half of the layer tree.

The procedure **sr**(X, r) gives a list of simple roots α_i computed from the Cartam matrices for a Lie algebra X of rank r:

$$\mathrm{sr}(\mathrm{X}, r) \to \Pi = [\alpha_1, \ldots, \alpha_r] \quad \text{Maple V},$$
$$\mathrm{sr}[\mathrm{X}, r] \to \Pi = \{\alpha_1, \ldots, \alpha_r\} \quad \text{Mathematica}.$$

Example 10. In the DYN basis, the simple roots of A_2 and C_3 are, respectively:

$$\mathrm{sr}(''\mathrm{A}'', 2) \to \alpha_1 = (2, -1),\ \alpha_2 = (-1, 2),$$
$$\mathrm{sr}(''\mathrm{C}'', 3) \to \alpha_1 = (2, -1, 0),\ \alpha_2 = (-1, 2, -1),\ \alpha_3 = (0, -2, 2).$$

The procedure **check**(Σ) extracts the positive roots from a root system Σ in the DYN basis. Its output is a list with the Weyl vector $\rho = (1, \ldots, 1)$ (half the sum of the positive roots) and a list with the positive roots Σ^+:

$$\mathrm{check}(\Sigma) \to [\rho, \Sigma^+] \quad \text{Maple V},$$
$$\mathrm{check}[\Sigma] \to \{\rho, \Sigma^+\} \quad \text{Mathematica}.$$

Therefore it can be used to check whether the root system is complete or not.

Example 11. From Examples 8 and 9, the positive roots for A_2 and C_3 are, respectively:

$$\begin{aligned}
&\text{check}(\Sigma_{A_2}) \to \rho = (1,1), \quad \Sigma^+_{A_2} = (1,1), (2,-1), (-1,2)\\
&\text{check}(\Sigma_{C_3}) \to \rho = (1,1,1), \Sigma^+_{C_3} = (2,0,0), (0,1,0), (-2,2,0),\\
&\qquad (1,-1,1), (-1,0,1), (1,1,-1),\\
&\qquad (0,-2,2), (-1,2,-1), (2,-1,0)
\end{aligned}$$

The dimension of a given algebra can be calculated directly from the rank r:

$$\begin{aligned}
&\text{algebra} \to \text{dimension}\\
&A_r \to r(r+2),\\
&B_r \to r(2r+1),\\
&C_r \to r(2r+1),\\
&D_r \to r(2r-1),\\
&E_r \to 30r^2 - 335r + 1008, \quad r = 6, 7, 8,\\
&F_4 \to 52, \quad r = 4,\\
&G_2 \to 14, \quad r = 2.
\end{aligned}$$

The procedure **algdim**(X, r) computes the algebra dimension using the formulae above.

4.1.2. Writing weights in different bases

The Cartan matrix A, given in (8), for an algebra X of rank r, is responsible for the exchange of bases between the DYN and SRS bases as indicated in (15). The Cartan matrices are computed by the procedure **Cm**(X, r) using the following explicit non-null matrix elements A_{ij} [5, Ch. 5]:

$$A_r \to A_{ij} = \begin{cases} +2 & \text{if } i = j,\\ -1 & \text{if } |i-j| = 1; \end{cases}$$

$$D_r \to A_{ij} = \begin{cases} +2 & \text{if } i = j,\\ -1 & \text{if } |i-j| = 1 \text{ and } i, j \leqslant r-1,\\ -1 & \text{if } j = i+2 = r,\\ -2 & \text{if } i = j+2 = r; \end{cases}$$

$$B_r \to A_{ij} = \begin{cases} +2 & \text{if } i = j,\\ -1 & \text{if } |i-j| = 1 \text{ and } i, j \leqslant r-1,\\ -1 & \text{if } j = i+1 = r,\\ -2 & \text{if } i = j+1 = r; \end{cases}$$

$$C_r \to A_{ij} = \begin{cases} +2 & \text{if } i = j,\\ -1 & \text{if } |i-j| = 1 \text{ and } i, j \leqslant r-1,\\ -2 & \text{if } j = i+1 = r,\\ -1 & \text{if } i = j+1 = r. \end{cases}$$

Note that the transpose of the Cartan matrix of B_r is equal the Cartan matrix of C_r. The inverse Cartan matrices [5, Ch. 5] are computed by the same procedure using the optional third argument ″inv″: **Cm**(X, r, ″inv″). For the exceptional algebras, the Cartan matrices are computed from (8). The procedures **dyn2srs**(λ, X) and **srs2dyn**(λ, X) implement the exchange of bases DYN $\leftrightarrow$ SRS:

$$\mathrm{Cm}(\mathrm{X}, r) \to A, \quad \mathrm{Cm}(\mathrm{X}, r, {''}\mathrm{inv}{''}) \to A^{-1},$$
$$\mathrm{srs2dyn}(\lambda_{\mathrm{SRS}}, \mathrm{X}) \to \lambda_{\mathrm{DYN}}, \quad \mathrm{dyn2srs}(\lambda_{\mathrm{DYN}}, \mathrm{X}) \to \lambda_{\mathrm{SRS}}.$$

Example 12. The Cartan matrix and its inverse for A_2 are:

$$\mathrm{Cm}({''}\mathrm{A}{''}, 2) \to A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \qquad \mathrm{Cm}({''}\mathrm{A}{''}, 2, {''}\mathrm{inv}{''}) \to A^{-1} = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

The simple roots of A_2, given in Example 10 in the DYN basis, can be rewritten in the SRS basis by multiplying them by A^{-1}:

$$\mathrm{dyn2srs}(\Pi_{\mathrm{DYN}}, {''}\mathrm{A}{''}) \to \alpha_1 = \{1, 0\}, \ \alpha_2 = \{0, 1\}.$$

The positive roots for A_2, given in Example 10 in DYN basis, when rewritten in the SRS basis are:

$$\mathrm{dyn2srs}(\Sigma^+_{\mathrm{DYN}}, {''}\mathrm{A}{''}) \to \Sigma^+_{\mathrm{SRS}} = \{1, 1\}, \{1, 0\}, \{0, 1\}.$$

Since the simple roots are the basis vectors of the SRS basis, this is exactly what we were expecting.

Example 13. We can analogously rewrite the simple roots of C_3, given in Example 10, and the positive roots, given in Example 11, in the SRS basis:

$$\begin{aligned}
&\mathrm{dyn2srs}(\Pi_{\mathrm{DYN}}, {''}\mathrm{C}{''}) \to \alpha_1 = \{1, 0, 0\}, \ \alpha_2 = \{0, 1, 0\}, \ \alpha_3 = \{0, 0, 1\}, \\
&\mathrm{dyn2srs}(\Sigma^+_{\mathrm{DYN}}, {''}\mathrm{C}{''}) \to \Sigma^+_{\mathrm{SRS}} = \{2, 2, 1\}, \{1, 2, 1\}, \{0, 2, 1\}, \\
&\qquad \{1, 1, 1\}, \{0, 1, 1\}, \{1, 1, 0\}, \\
&\qquad \{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}.
\end{aligned}$$

The Cartan matrix and its inverse for C_3 are:

$$\mathrm{Cm}({''}\mathrm{C}{''}, 3) \to A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -2 \\ 0 & -1 & 2 \end{pmatrix}, \qquad \mathrm{Cm}({''}\mathrm{C}{''}, 3, {''}\mathrm{inv}{''}) \to A^{-1} = \frac{1}{2}\begin{pmatrix} 2 & 2 & 2 \\ 2 & 4 & 4 \\ 1 & 2 & 3 \end{pmatrix}.$$

The Weight matrix W associated with an algebra X of rank r is computed by the procedure **Wm**(X, r) using the following explicit non-null matrix elements W_{ij} [5, Ch. 5]:

$$A_r \to W_{ij} = \begin{cases} +1 & \text{if } i = j, \\ -1 & \text{if } j = i + 1, \ j \leqslant r + 1; \end{cases}$$

$$B_r \to W_{ij} = \begin{cases} +2 & \text{if } i = j = r, \\ +1 & \text{if } i = j \text{ and } i, j \leqslant r - 1, \\ -1 & \text{if } j = i + 1 \text{ and } i \leqslant r - 1; \end{cases}$$

$$C_r \to W_{ij} = \begin{cases} +1 & \text{if } i = j, \\ -1 & \text{if } j = i + 1; \end{cases}$$

$$D_r \to W_{ij} = \begin{cases} -1 & \text{if } i = j = r, \\ +1 & \text{if } i = j + 1 = r, \\ +1 & \text{if } j = i + 1 = r, \\ -1 & \text{if } j = i + 1 = r \text{ and } j \leqslant r - 1, \\ +1 & \text{if } i = j \text{ and } i, j \leqslant r - 1. \end{cases}$$

Note that the Weight matrix of A_r has $r+1$ columns. The inverse matrices [5, Ch. 5] are computed by the same procedure **Wm**(X, r, $''$inv$''$) using the optional third argument $''$inv$''$. These matrices are responsible for the exchange of bases between the DYN and FWS bases (for classical Lie algebras only). The procedures **dyn2fws**(λ, X) and **fws2dyn**(λ, X) implement the exchange of bases DYN $\leftrightarrow$ FWS:

$$\mathrm{Wm}(\mathrm{X}, r) \to W, \quad \mathrm{Wm}(\mathrm{X}, r, ''\mathrm{inv}'') \to W^{-1},$$
$$\mathrm{fws2dyn}(\lambda_{\mathrm{FWS}}, \mathrm{X}) \to \lambda_{\mathrm{DYN}}, \quad \mathrm{dyn2fws}(\lambda_{\mathrm{DYN}}, \mathrm{X}) \to \lambda_{\mathrm{FWS}}.$$

Example 14. The Weight matrix and its “inverse” for A_2 are:

$$\mathrm{Wm}(''\mathrm{A}'', 2) \to W = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix},$$
$$\mathrm{Wm}(''\mathrm{A}'', 2, ''\mathrm{inv}'') \to W^{-1} = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ -1 & 1 \\ -1 & -2 \end{pmatrix}.$$

Note that these matrices are not square matrices, and so they occur only in A_r algebras:

$$WW^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad W^{-1}W = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.$$

The weight system Υ of the fundamental representation of A_2, given in Example 4 in the DYN basis, can be rewritten in the FWS basis by multiplying them by W^{-1}:

$$\mathrm{dyn2fws}(\Upsilon_{\mathrm{DYN}}, ''\mathrm{A}'') \to$$
$$\lambda_1 = \tfrac{1}{3}[2, -1, -1],\ \lambda_2 = \tfrac{1}{3}[-1, 2, -1],\ \lambda_3 = \tfrac{1}{3}[-1, -1, 2].$$

The fractions appearing in the components of the weights given in the above example are easily avoided because in the FWS basis for A_r algebras (and only for A_r algebras) the sum of the components of any weight (or root) is zero, that is, the weights are perpendicular to $p = [1, 1, \ldots, 1]$. This is done by the procedure **fws2fws**(λ, m):

$$\mathrm{fws2fws}(\lambda, m) \to \lambda + m.$$

Example 15. Therefore, we can add a constant $m = 1/3$ to each weight in the weight system Υ given in the previous example:

$$\mathrm{fws2fws}(\Upsilon_{\mathrm{FWS}}, \tfrac{1}{3}) \to \lambda_1 = [1, 0, 0],\ \lambda_2 = [0, 1, 0],\ \lambda_3 = [0, 0, 1].$$

This is exactly what we were expecting if the weights of the defining fundamental representation were all linearly independent since they are the basis vectors of the FWS basis. In fact we have $\lambda_3 = -(\lambda_1 + \lambda_2)$, which means that only λ_1 and λ_2, for example, are linearly independent (they form the modified-FWS basis; see Example 17). This is not the case for the other classical Lie algebras. For example, the positive weights in the weight system Υ of the fundamental representation of C_3, given in Example 4 in the DYN basis, can be rewritten in the FWS basis as:

$$\mathrm{dyn2fws}(\Upsilon_{\mathrm{DYN}}, ''\mathrm{C}'') \to \lambda_1 = [1, 0, 0],\ \lambda_2 = [0, 1, 0],\ \lambda_3 = [0, 0, 1].$$

In this case we have three true linearly independent weights.

Example 16. The positive roots Σ^+ given in Example 11, in the DYN basis, for the algebras A_2 and C_3 can respectively be written in the FWS basis as follows:

$$\begin{aligned}
&\text{dyn2fws}(\Sigma^+_{\text{DYN}}, ''\text{A}'') \to \Sigma^+_{\text{FWS}} = [1,0,-1], [1,-1,0], [0,1,-1],\\
&\text{dyn2fws}(\Sigma^+_{\text{DYN}}, ''\text{C}'') \to \Sigma^+_{\text{FWS}} = [2,0,0], [1,1,0], [0,2,0]\\
&\qquad [1,0,1], [0,1,1], [1,0,-1]\\
&\qquad [1,-1,0], [0,1,-1], [0,0,2].
\end{aligned}$$

For A_2, the simple roots are $\alpha_1 = [1,-1,0]$ and $\alpha_2 = [0,1,-1]$, while for C_3 they are $\alpha_1 = [1,-1,0]$, $\alpha_2 = [0,1,-1]$ and $\alpha_3 = [0,0,2]$.

The exchanges of bases given in (19)–(21) for the A_r algebras are implemented by the procedures:

$$\begin{aligned}
&\text{fws2fwsm}(\lambda) \to \lambda - \lambda_{r+1},\\
&\text{dyn2fwsm}(\lambda_{\text{DYN}}) \to \lambda_{\text{FWS}'}, \quad \text{fwsm2dyn}(\lambda_{\text{FWS}'}) \to \lambda_{\text{DYN}},\\
&\text{srs2fwsm}(\lambda_{\text{SRS}}) \to \lambda_{\text{FWS}'}, \quad \text{fwsm2srs}(\lambda_{\text{FWS}'}) \to \lambda_{\text{SRS}}.
\end{aligned}$$

Example 17. The weights shown in Example 14, in the FWS basis, can be rewritten in the FWS' basis as:

$$\text{fws2fwsm}(\Upsilon_{\text{FWS}}) \to \lambda_1 = [1,0],\ \lambda_2 = [0,1],\ \lambda_3 = [-1,-1].$$

Now it is obvious that there are only two linearly independent weights.

The Root matrices $R_A = (W_A)^t$, $R_B = (W_C)^t$, $R_C = (W_B)^t$ and $R_D = (W_D)^t$ are responsible for the exchange SRS $\to$ FWS for classical algebras [5, Ch. 5]. They are computed by the procedure **Rm**(X, r) and their inverse matrices by **Rm**(X, r, ″inv″). The procedures **fws2srs**(λ, ″X″) and **srs2fws**(λ, ″X″) implement the exchange of bases SRS $\leftrightarrow$ FWS:

$$\begin{aligned}
&\text{Rm}(\text{X}, r) \to R, \quad \text{Rm}(\text{X}, r, ''\text{inv}'') \to R^{-1},\\
&\text{srs2fws}(\lambda_{\text{SRS}}, \text{X}) \to \lambda_{\text{FWS}}, \quad \text{fws2srs}(\lambda_{\text{FWS}}, \text{X}) \to \lambda_{\text{SRS}}.
\end{aligned}$$

4.1.3. Operations in the weight space

In a Kronecker product $\Lambda' \times \Lambda''$ between two irreducible representations Λ' and Λ'', every weight in $\Delta(\Lambda' \times \Lambda'')$ is given by:

$$\Delta(\Lambda' \times \Lambda'') = \Delta(\Lambda') + \Delta(\Lambda''). \tag{60}$$

The Kronecker product representation is reducible:

$$\Lambda' \times \Lambda'' = \sum_{\Lambda} \oplus \eta_\Lambda \Lambda, \tag{61}$$

where η_Λ is the (outer) multiplicity of the irreducible representation Λ. It can be shown [41] that all possible highest weights in $\Delta(\Lambda' \times \Lambda'')$ are in $\Delta(\Lambda') + \Lambda''$ or $\Delta(\Lambda'') + \Lambda'$. The irreducible components in the DYN basis and their degeneracies can be found using the following algorithm [5,41]:

Algorithm 3.

- Compute the weight systems of Λ' and Λ'';
- Compute the weights of the Kronecker product $\Lambda' \times \Lambda''$ and group and sort them by their multiplicities;
- Find all possible highest weights and sort them from the highest to the lowest dimensional weights;
- Remove from the weight system $\Delta(\Lambda') + \Delta(\Lambda'')$ the weight systems corresponding to the previous highest weights. The number of times that each irreducible representation is removed from the Kronecker product weight system is its degeneracy.

The procedure **kronecker**(Λ', Λ'', X) was implemented using Algorithm 3. Its output is a list of lists of highest weights Λ with their multiplicities η_Λ in the first positions:

$$\text{kronecker}(\Lambda', \Lambda'', \text{X}) \to [[\eta_\Lambda, \Lambda], \ldots] \quad \text{Maple V},$$
$$\text{kronecker}[\Lambda', \Lambda'', \text{X}] \to \{\{\eta_\Lambda, \Lambda\}, \ldots\} \quad \text{Mathematica}.$$

Example 18. The fundamental representation, $\mathbf{M}_1 = (1,0,0)$, for C_3 has dimension six. The remaining basic representations, $\mathbf{M}_2 = (0,1,0)$ and $\mathbf{M}_3 = (0,0,1)$, both of dimension 14, can be obtained from the Kronecker products $\mathbf{M}_1 \times \mathbf{M}_1$ and $\mathbf{M}_1 \times \mathbf{M}_1 \times \mathbf{M}_1$, respectively:

$$\text{kronecker}(\mathbf{M}_1, \mathbf{M}_1, ''\text{C}'') \to (2,0,0) \oplus (0,1,0) \oplus (0,0,0),$$
$$\text{kronecker}(\mathbf{M}_1, (2,0,0), ''\text{C}'') \to (3,0,0) \oplus (1,1,0) \oplus (1,0,0),$$
$$\text{kronecker}(\mathbf{M}_1, (0,1,0), ''\text{C}'') \to (1,1,0) \oplus (0,0,1) \oplus (1,0,0),$$
$$\text{kronecker}(\mathbf{M}_1, (0,0,0), ''\text{C}'') \to (1,0,0),$$
$$\therefore \mathbf{M}_1 \times \mathbf{M}_1 \times \mathbf{M}_1 = 2(1,1,0) \oplus (3,0,0) \oplus (0,0,1) \oplus 3(1,0,0).$$

The dimension of $(1,1,0)$ is 64, and the dimension of $(3,0,0)$ is 56. The representations which can (cannot) be obtained from Kronecker powers of the fundamental basic representation are called vector (spinor) representations. In general, for A_r and C_r algebras, the basic representations are vector representations and $\mathbf{M}_1^i \not\supset \mathbf{M}_i$.

Example 19. The basic representations $\mathbf{M}_r$ of B_r, $\mathbf{M}_{r-1}$ and $\mathbf{M}_r$ of D_r, and $\mathbf{M}_2$ of G_2 are examples of spinor representations:

$$\text{kronecker}((1,0), (1,0), ''\text{B}'') \to (2,0) \oplus (0,2) \oplus (0,0),$$
$$\text{kronecker}((1,0), (1,0), ''\text{G}'') \to (2,0) \oplus (0,3) \oplus (0,2) \oplus (1,0) \oplus (0,0),$$
$$\text{kronecker}((1,0,0), (1,0,0), ''\text{D}'') \to (2,0,0) \oplus (0,1,1) \oplus (0,0,0).$$

From the examples above, we can see that $\mathbf{M}_1 \times \mathbf{M}_1 \not\supset \mathbf{M}_2$ for B_2, D_3 and G_2.

The equivalence relation between two weights λ and λ' given by a Weyl reflection σ_i through the simple root α_i for an algebra X is computed by the procedure **weyl**(i, λ, X). Its output is a weight λ' equivalent to λ. The reflection through an arbitrary weight λ'' is given by the same procedure: **weyl**(λ'', λ, X).

Example 20. The equivalent weights to the weight $\lambda = (1,0,0)$ of C_3 (see Example 6) through the simple roots α_1, α_2 and α_3 given in Example 10, are:

$$\text{weyl}(1, \lambda, ''\text{C}'') \to (-1,1,0),$$
$$\text{weyl}(2, \lambda, ''\text{C}'') \to (1,0,0),$$
$$\text{weyl}(3, \lambda, ''\text{C}'') \to (1,0,0).$$

Weights can be ordered in any basis. The procedure **sortwts**(wts) sorts a list of weights wts in descending order. As we can see from the following example, the ordering process based only on the difference of weights, as established in Section 2.1, can change from basis to basis.

Example 21. Let us sort the following set of weights for C_2:

$$\omega_{\text{DYN}} = (1, 2), (3, 4), (0, 3),$$
$$\omega_{\text{SRS}} = \{3, 5/2\}, \{7, 11/2\}, \{3, 3\},$$
$$\omega_{\text{FWS}} = [3, 2], [7, 4], [3, 3].$$

Since all their components are positive, they represent irreducible representations of dimension 40, 420 and 30, respectively. Their respective heights are 11, 25 and 12. We have in the DYN, SRS and FWS bases, respectively:

$$\text{sortwts}(\omega_{\text{DYN}}, ''\text{C}'') \to (3, 4), (1, 2), (0, 3),$$
$$\text{sortwts}(\omega_{\text{SRS}}, ''\text{C}'') \to \{7, 11/2\}, \{3, 3\}, \{3, 5/2\} = (3, 4), (0, 3), (1, 2),$$
$$\text{sortwts}(\omega_{\text{FWS}}, ''\text{C}'') \to [7, 4], [3, 3], [3, 2] = (3, 4), (0, 3), (1, 2).$$

Note that the sorting process only coincides for the SRS and FWS basis.

The procedure **dominant**(hwts, X) sorts a list of highest weights hwts in the DYN basis in descending order by their heights and their dimensions, respectively.

Example 22. For the same set of weights in the previous example, the output of the **dominant** procedure is:

$$\text{dominant}(\omega_{\text{DYN}}, ''\text{C}'') \to (3, 4), (0, 3), (1, 2).$$

The scalar product between the weights λ and λ' in the DYN basis is implemented by the procedure **sprod**(λ, λ', X). This scalar product is calculated by [5, Ch. 5]

$$\lambda \cdot \lambda' = \sum_{i=1}^{r} (\lambda)_i^{\text{DYN}} \{\lambda'\}_i^{\text{SRS}} N_i, \qquad N_i = \frac{|\alpha_i|^2}{2}, \tag{62}$$

where α_i represents the simple roots. The normalizing factor $2N_i$ can be set by the user through the global variable **ShortRoots2**. Its default value is 2, corresponding to the length of the short roots equal to $\sqrt{2}$. The angle in radians between the weights λ and λ' is given by the procedure **angle**(λ, λ', X).

Example 23. Let us now determine the lengths of the weights of the DYN, SRS and FWS bases and their relative angles for the A_2 algebra. The DYN basis is formed by the basic representations $\mathbf{M}_1 = (1, 0) = [2, -1, -1]/3$ and $\mathbf{M}_2 = (0, 1) = [1, 1, -2]/3$:

$$\text{sprod}(\mathbf{M}_1, \mathbf{M}_1, ''\text{A}'') \to |\mathbf{M}_1|^2 = 2/3, \quad \text{sprod}(\mathbf{M}_2, \mathbf{M}_2, ''\text{A}'') \to |\mathbf{M}_2|^2 = 2/3,$$
$$\text{sprod}(\mathbf{M}_1, \mathbf{M}_2, ''\text{A}'') \to \mathbf{M}_1 \cdot \mathbf{M}_2 = 1/3, \quad \text{angle}(\mathbf{M}_1, \mathbf{M}_2, ''\text{A}'') \to \pi/3.$$

The SRS basis is formed by the simple roots $\alpha_1 = (2, -1) = [1, -1, 0]$ and $\alpha_2 = (-1, 2) = [0, 1, -1]$:

$$\text{sprod}(\alpha_1, \alpha_1, ''\text{A}'') \to |\alpha_1|^2 = 2, \quad \text{sprod}(\alpha_2, \alpha_2, ''\text{A}'') \to |\alpha_2|^2 = 2,$$
$$\text{sprod}(\alpha_1, \alpha_2, ''\text{A}'') \to \alpha_1 \cdot \alpha_2 = -1, \quad \text{angle}(\alpha_1, \alpha_2, ''\text{A}'') \to 2\pi/3.$$

The FWS basis is formed by the positive weights of the fundamental representation $\lambda_1 = (1, 0) = [2, -1, -1]/3$, $\lambda_2 = (-1, 1) = [-1, 2, -1]/3$ ($\lambda_3 = -\lambda_1 - \lambda_2$):

$$\text{sprod}(\lambda_i, \lambda_i, ''\text{A}'') \to 2/3, \quad \text{sprod}(\lambda_i, \lambda_j, ''\text{A}'') \to -1/3,$$
$$\text{angle}(\lambda_i, \lambda_j, ''\text{A}'') \to 2\pi/3.$$

It must be observe that, although the weights λ_1, λ_2 and λ_3 are not orthogonal vectors for the A_2 algebra, the scalar products can be calculated using a unity metric in the FWS basis [5, Ch. 5]:

$$\mathbf{u} \cdot \mathbf{v} = \sum_i [u]_i [v]_i. \tag{63}$$

It can be seen from the cases above that the same results for all scalar products can be obtained directly from (63) using the FWS components. For all other algebras, the FWS basis has orthogonal vectors. The same is not true when the fractions are eliminated from the FWS basis (modified-FWS) for A_r algebras. The SRS and DYN bases are not orthogonal, but they are dual to each other, that is, $\alpha_1 \cdot \mathbf{M}_2 = \alpha_2 \cdot \mathbf{M}_1 = 0$.

4.1.4. Comments

Before closing this subsection, it is essential to make some comments about the canonical forms (5) (Cartan–Weyl) and (7) (Chevalley) for the commutation relations of A_r algebras. Let us consider the A_2 algebra as an example. Its simple roots in the FWS basis are $\alpha_1 = [1, -1, 0]$ and $\alpha_2 = [0, 1, -1]$ (see Example 16). The third positive root is $\alpha_3 = \alpha_1 + \alpha_2$. Let E_i^+, E_i^- and H_i, $i \leqslant 3$, be the elements associated with the positive, negative and null roots, respectively. Although there are only two null roots, let us assume for a moment that there are three. In that case, using the simple root components given in the FWS basis, we have from (5) the following defining commutation relations:

$$\begin{array}{lll}
[H_1, H_2] = 0, & [H_1, H_3] = 0, & [H_2, H_3] = 0, \\
[H_1, E_1^+] = E_1^+, & [H_2, E_1^+] = -E_1^+, & [H_3, E_1^+] = 0, \\
[H_1, E_2^+] = 0, & [H_2, E_2^+] = E_2^+, & [H_3, E_2^+] = -E_2^+, \\
[H_1, E_3^+] = E_3^+, & [H_2, E_3^+] = 0, & [H_3, E_3^+] = -E_3^+, \\
[E_1^+, E_1^-] = H_1 - H_2, & [E_2^+, E_2^-] = H_2 - H_3, & [E_3^+, E_3^-] = H_1 - H_3.
\end{array} \tag{64}$$

We can see from this adjoint representation that there are only two linearly independent elements H_i since $H_1 + H_2 + H_3 = 0$. This reflects the fact that the roots are perpendicular to $p = [1, 1, 1]$ in the FWS basis (for A_r algebras only). These commutation relations define the special (traceless) general linear Lie algebra $sl(3)$. It is a subalgebra of the non-semisimple general Lie algebra $gl(3)$ which also contains the non-null trace matrices. In general, $gl(r+1) = I \oplus sl(r+1)$, where I is the unidimensional Abelian algebra formed by multiples of the identity and $sl(r+1)$ is the special linear semisimple Lie algebra associated with A_r. The Chevalley commutation relations are simpler than the Cartan–Weyl commutation relations. Indeed, using the simple roots in the DYN basis, $\alpha_1 = (2, -1)$ and $\alpha_2 = (-1, 2)$ in (7) we have (see Example 11):

$$\begin{array}{ll}
[h_1, h_2] = 0, & \\
[h_1, e_1] = 2e_1, & [h_2, e_1] = -e_1, \\
[h_1, e_2] = -e_2, & [h_2, e_2] = 2e_2, \\
[e_1, f_1] = h_1, & [e_2, f_2] = h_2.
\end{array} \tag{65}$$

Comparing (64) with (65), we have $h_1 = H_1 - H_2$, $h_2 = H_2 - H_3$, $e_i = E_i^+$ and $f_i = E_i^-$.

As an introduction to the next subsection, let us use (14) in order to write the matrices of the fundamental representation given in Example 4 for the A_2 algebra. Let the ordering of the weights be $|1\rangle = \lambda_1 = (1, 0)$, $|2\rangle = \lambda_2 = (-1, 1)$ and $|3\rangle = \lambda_3 = (0, -1)$. The positive roots in the DYN basis are $\alpha_1 = (2, -1)$, $\alpha_2 = (-1, 2)$ and $\alpha_3 = (1, 1)$ (see Example 11). This representation is three-dimensional. Since the weights are the eigenvalues of the elements of the Cartan subalgebra, we have:

$$h_1 = \begin{pmatrix} 1 & & \\ & -1 & \\ & & 0 \end{pmatrix}, \qquad h_2 = \begin{pmatrix} 0 & & \\ & 1 & \\ & & -1 \end{pmatrix}. \tag{66}$$

Since $\lambda_2+\alpha_1=\lambda_1$ $(\lambda_1-\alpha_1=\lambda_2)$, $\lambda_3+\alpha_2=\lambda_2$ $(\lambda_2-\alpha_2=\lambda_3)$ and $\lambda_3+\alpha_3=\lambda_1$ $(\lambda_1-\alpha_3=\lambda_3)$, then it follows from (14) that

$$e_1=\begin{pmatrix}0 & x_1 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\qquad e_2=\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & x_2\\ 0 & 0 & 0\end{pmatrix},\qquad e_3=\begin{pmatrix}0 & 0 & x_3\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\tag{67}$$

and $f_i=(e_i)^{\mathrm{t}}$ (real transposition). From the last relation in (65), we can choose $x_1=x_2=1$. Since $\alpha_3=\alpha_1+\alpha_2$ and $\alpha_1-\alpha_2=(3,-3)$ is not a root, then from (7), with $m=0$, we have

$$e_3=\pm[e_1,e_2],\tag{68}$$

from which we can choose $x_3=1$. The matrices in (66)–(67) satisfy the commutation relations given in (65).

4.2. *The Gelfand–Tsetlin method*

The Gelfand–Tsetlin formulae for the matrix elements are known only for unitary A_r and orthogonal B_r and D_r algebras [22,21,4]. For symplectic algebras, there are only a few particular cases [38,34,39,24].

In the following procedures, X is one of the classical algebras $\{''\mathrm{A}'', ''\mathrm{B}'', ''\mathrm{C}'', ''\mathrm{D}''\}$. All weights must be in FWS basis (FWS with integral components for A_r).

4.2.1. *The Gelfand–Tsetlin patterns*

The complete set of Gelfand–Tsetlin patterns (quantum numbers) for a given irreducible representation Λ (in the FWS basis) is computed in two steps: the procedure **patterns**(X, r) must be used to write a specific procedure **vX**$r(\Lambda)$ which is used to compute all vectors of Λ. The procedure vXr is written on the hard disk in a directory specified by the global variable **WorkDir**. Its default value is the current directory "./". The output of vXr is a list with the Gelfand–Tsetlin patterns, where each pattern is a list in one of the following formats:

A_r: A generic Gelfand–Tsetlin pattern for the irreducible representation $\Lambda=[m_{1n},\dots,m_{nn}]$ is

$$\big[[h_1,\dots,h_n],\ \big[[m_{11}],\ [m_{12},m_{22}],\dots,[m_{1n},\dots,m_{nn}]\big]\big],$$

where the components m_{ij} are given in (34) and $[h_1,\dots,h_n]$, $n=r+1$, is a weight of $\Delta(\Lambda)$;

B_r: A generic Gelfand–Tsetlin pattern for the irreducible representation $\Lambda=[m_{1\,2r},\dots,m_{r\,2r}]$ is

$$\big[[m_{11}],\ [m_{12},m_{22}],\dots,[m_{1\,2r-1},\dots,m_{r\,2r-1}],\ [m_{1\,2r},\dots,m_{r\,2r}]\big],$$

where the components m_{ij} are given in (45);

C_r: A generic Gelfand–Tsetlin pattern for the irreducible representation $\Lambda=[\omega_{1r},\dots,\omega_{rr}]$ is

$$\big[[h_1,\dots,h_r],\ [\sigma_1,\dots,\sigma_r],\ \big[[\omega_{11}],\ [\gamma_{12}],\dots,[\omega_{1r},\dots,\omega_{rr}]\big]\big],$$

where the σ_i, γ_{ij} and ω_{ij} are given in (50) and $[h_1,\dots,h_n]$ is a weight of $\Delta(\Lambda)$;

D_{r+1}: A generic Gelfand–Tsetlin pattern for the irreducible representation $\Lambda=[m_{1\,2r+1},\dots,m_{r+1\,2r+1}]$ is

$$\big[[m_{11}],\ [m_{12},m_{22}],\dots,[m_{1\,2r},\dots,m_{r\,2r}],\ [m_{1\,2r+1},\dots,m_{r+1\,2r+1}]\big],$$

where the components m_{ij} are given in (46).

Example 24. The following command

$$\mathrm{patterns}(''\mathrm{A}'',2)\to \mathrm{vA2}$$

writes the procedure vA2 to compute the vectors of a given irreducible representation of A_2. For example, the Gelfand–Tsetlin vectors of the fundamental representation $\Lambda = [1, 0, 0]$ are:

$$\mathrm{vA2}(\Lambda) \to \begin{array}{l} \left|\begin{array}{ccccc} 1 & & 0 & & 0 \\ & 1 & & 0 & \\ & & 1 & & \end{array}\right| \to \lambda_1 = [1, 0, 0], \\ \left|\begin{array}{ccccc} 1 & & 0 & & 0 \\ & 1 & & 0 & \\ & & 0 & & \end{array}\right| \to \lambda_2 = [0, 1, 0], \\ \left|\begin{array}{ccccc} 1 & & 0 & & 0 \\ & 0 & & 0 & \\ & & 0 & & \end{array}\right| \to \lambda_3 = [0, 0, 1]. \end{array}$$

Note that the fractions were eliminated in the components of all weights (see Example 14), therefore, before going to the DYN and SRS bases they have to be rewritten in the FWS' basis (using the procedure fws2fwsm).

Example 25. The following command

$$\mathrm{patterns}(''\mathrm{D}'', 2) \to \mathrm{vD2}$$

writes the procedure vD2 to compute the vectors of a given irreducible representation of D_2. For example, the Gelfand–Tsetlin vectors of the fundamental representation $\Lambda = [1, 0]$ are:

$$\mathrm{vD2}(\Lambda) \to |1\rangle = \left|\begin{array}{ccc} 1 & & 0 \\ & 1 & \\ & 1 & \end{array}\right|,\ |2\rangle = \left|\begin{array}{ccc} 1 & & 0 \\ & 1 & \\ & 0 & \end{array}\right|,\ |3\rangle = \left|\begin{array}{ccc} 1 & & 0 \\ & 1 & \\ & -1 & \end{array}\right|,\ |4\rangle = \left|\begin{array}{ccc} 1 & & 0 \\ & 0 & \\ & 0 & \end{array}\right|.$$

Example 26. The following command

$$\mathrm{patterns}(''\mathrm{C}'', 2) \to \mathrm{vC2}$$

writes the procedure vC2 to compute the vectors of a given irreducible representation of C_2. For example, the Gelfand–Tsetlin vectors of the fundamental representation $\Lambda = [1, 0]$ are:

$$\mathrm{vC2}(\Lambda) \to \begin{array}{l} |1\rangle = \left|\begin{array}{cccc} 1 & & 0 & \\ & 0 & & 0 \\ & & 0 & \\ & & & -1 \end{array}\right|,\ |2\rangle = \left|\begin{array}{cccc} 1 & & 0 & \\ & 0 & & 0 \\ & & 0 & \\ & & & 1 \end{array}\right|, \\ \sigma_1 = 0,\ \sigma_2 = 1,\ \sigma_1 = 0,\ \sigma_2 = 1 \\ |3\rangle = \left|\begin{array}{cccc} 1 & & 0 & \\ & 1 & & -1 \\ & & 1 & \\ & & & 0 \end{array}\right|,\ |4\rangle = \left|\begin{array}{cccc} 1 & & 0 & \\ & 1 & & 1 \\ & & 1 & \\ & & & 0 \end{array}\right|, \\ \sigma_1 = 1,\ \sigma_2 = 0,\ \sigma_1 = 1,\ \sigma_2 = 0. \end{array}$$

4.2.2. Matrix elements

The matrix elements for unitary (classical and deformed) and orthogonal algebras can be calculated either algebraically or numerically.

Unitary algebras

The matrix elements of the generators A_{ij} of $gl(n, R)$, given in (35) and (36), where $i = j \leqslant n$ for the generators associated with the null roots and $j = i + 1 \leqslant n$ $(i = j + 1 \leqslant n)$ for the positive (negative) simple roots, are calculated by the procedure **Ame**$(i, j, |m\rangle)$, where $|m\rangle$ is an arbitrary Gelfand–Tsetlin vector. Its output is a list of lists which have the matrix element in the first positions and the resulting Gelfand–Tsetlin vector in the second positions.

Example 27. A typical Gelfand–Tsetlin vector of the irreducible representation $\Lambda = [m_{12}, m_{22}]$ of $gl(2,R)$ in the chain $gl(2,R) \subset gl(1,R)$ is

$$|m\rangle = \begin{vmatrix} m_{12} & & m_{22} \\ & m_{11} & \end{vmatrix} \to \big[[m_{11}],\ [m_{12}, m_{22}]\big] \quad \text{(Maple V)}. \tag{69}$$

The action of the $gl(2,R)$ elements $A_{11},\ A_{22},\ A_{12}$ and A_{21} on the generic vector given above is:

$$\begin{aligned}
&\text{Ame}(1,1,|m\rangle) \to \big[m_{11},\ \big[[m_{11}],\ [m_{12}, m_{22}]\big]\big] \\
&\qquad \Rightarrow A_{11}|m\rangle = m_{11}|m\rangle, \\
&\text{Ame}(2,2,|m\rangle) \to \big[m_{12}+m_{22}-m_{11},\ \big[[m_{11}],\ [m_{12}, m_{22}]\big]\big] \\
&\qquad \Rightarrow A_{22}|m\rangle = (m_{12}+m_{22}-m_{11})|m\rangle, \\
&\text{Ame}(1,2,|m\rangle) \to \big[b_1^1(m_{11}),\ \big[[m_{11}+1],\ [m_{12}, m_{22}]\big]\big] \\
&\qquad \Rightarrow A_{12}|m\rangle = b_1^1(m_{11})|m_{11}+1\rangle, \\
&\text{Ame}(2,1,|m\rangle) \to \big[b_1^1(m_{11}-1),\ \big[[m_{11}-1],\ [m_{12}, m_{22}]\big]\big] \\
&\qquad \Rightarrow A_{12}|m\rangle = b_1^1(m_{11}-1)|m_{11}-1\rangle,
\end{aligned}$$

where

$$b_1^1(m_{11}) = \big\{(m_{12}-m_{11})(m_{11}-m_{22}+1)\big\}^{1/2}.$$

We can use the prescriptions given in (31)–(32) to get the matrix elements of $sl(2,R)$. Its diagonal generator is $H_{11} = (A_{11} - A_{22})/2$. Note that $H_{22} = -H_{11}$. The vector (69) must be changed to

$$|m'\rangle = \begin{vmatrix} +j & & -j \\ & l & \end{vmatrix}, \qquad j = \tfrac{1}{2}(m_{12} - m_{22}). \tag{70}$$

Now, using $|m'\rangle$ we have:

$$\begin{aligned}
&\text{Ame}(1,1,|m'\rangle) \to \big[l,\ \big[[l],\ [j,-j]\big]\big] \\
&\qquad \Rightarrow A_{11}|jl\rangle = l\ |jl\rangle, \\
&\text{Ame}(2,2,|m'\rangle) \to \big[-l,\ \big[[l],\ [j,-j]\big]\big] \\
&\qquad \Rightarrow A_{22}|jl\rangle = -l\ |jl\rangle, \\
&\qquad \therefore H_{11}|jl\rangle = l\ |jl\rangle, \\
&\text{Ame}(1,2,|m'\rangle) \to \big[\big\{(j-l)(j+l+1)\big\}^{1/2},\ \big[[l+1],\ [j,-j]\big]\big] \\
&\qquad \Rightarrow A_{12}|jl\rangle = \{(j-l)(j+l+1)\}^{1/2}|j\ l+1\rangle, \\
&\text{Ame}(2,1,|m'\rangle) \to \big[\big\{(j-l+1)(j+l)\big\}^{1/2},\ \big[[l-1],\ [j,-j]\big]\big] \\
&\qquad \Rightarrow A_{12}|jl\rangle = \big\{(j-l+1)(j+l)\big\}^{1/2}|j\ l-1\rangle.
\end{aligned}$$

The procedure **m_jk**($|m\rangle, j, k, p$) can be used to modify the jk entry in the Gelfand–Tsetlin vector $|m\rangle$ by p:

$$\text{m\_jk}(|m\rangle, j, k, p) \to |m_{jk} + p\rangle.$$

For convenience when checking commutation relations, the procedure **commute**(A, B) can be used to compute commutators:

$$\text{commute}(A, B) \to [A, B],$$
$$\text{commute}(A, B, q) \to [A, B]_q \equiv A\,B - q\,A\,B.$$

The explicit construction of the irreducible matrices of a particular representation of $gl(n, R)$ in the canonical chain $gl(n, R) \subset gl(n-1, R) \subset \cdots$ is computed by the procedure **Aim**(i, j, M), where the indices i and j have the same meaning as explained before, and M is an explicit Gelfand–Tsetlin basis. Its output is a matrix representing the generator A_{ij}.

Example 28. The Gelfand–Tsetlin vectors of the fundamental representation $\Lambda = [1, 0, 0]$ of A_2 or $gl(3, R)$ are given in Example 24. The ordering of the vectors is given by the procedure vA2 as shown in Example 24. The irreducible matrices for the diagonal operators in the representation Λ are:

$$\text{Aim}(1, 1, M) \to A_{11} = \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix},$$
$$\text{Aim}(2, 2, M) \to A_{22} = \begin{pmatrix} 0 & & \\ & 1 & \\ & & 0 \end{pmatrix},$$
$$\text{Aim}(3, 3, M) \to A_{33} = \begin{pmatrix} 0 & & \\ & 0 & \\ & & 1 \end{pmatrix},$$

where M is a list containing the Gelfand–Tsetlin vectors computed by the procedure vA2. The non-diagonal operators associated with the simple roots are represented by

$$\text{Aim}(1, 2, M) \to A_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{Aim}(2, 3, M) \to A_{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$
$$\text{Aim}(2, 1, M) \to A_{21} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{Aim}(3, 2, M) \to A_{32} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Note that they are the Weyl matrices given in (28) and identical to the matrices calculated in (66)–(67) with $x_1 = x_2 = x_3 = 1$. The Cartan–Weyl commutation relations (5) can be verified using the procedure commute:

$$\text{commute}(A_{12}, A_{21}) \to A_{11} - A_{22}, \quad \text{commute}(A_{23}, A_{32}) \to A_{22} - A_{33}, \quad \ldots$$

The q-deformed matrix elements given in (41) and the q-deformed irreducible matrices are calculated using the deformation parameter q as an optional fourth argument to **Ame**(i, j, $|m\rangle$, q) and **Aim**(i, j, M, q), respectively. The deformation given in (39) is calculated by the procedure **qdeform**(x, q).

Example 29. Since the Weyl matrices defining the $sl(n, R)$ algebras have only unity elements and the unity is not deformed, the defining representation is never deformed. The q-deformed matrices for the adjoint representation $\Lambda = [2, 0]$ of $sl_q(2)$ are:

$$\text{Aim}(1, 2, M, q) \to {}_qA_{12} = \sqrt{[2]_q} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$
$$\text{Aim}(2, 1, M, q) \to {}_qA_{21} = \sqrt{[2]_q} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

where M, the Gelfand–Tsetlin basis, must be calculated by vA1(Λ) which is written by patterns($''$A$''$,1). The elements of the Cartan subalgebra are not deformed:

$$\text{Aim}(1,1,M,q) \to A_{11} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{Aim}(2,2,M,q) \to A_{22} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

The deformation of

$$H_1 = A_{11} - A_{22} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix},$$

is given by

$$\text{qdeform}(H_1, q) \to [H_1]_q = [2]_q \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The defining commutation relations (37) can be checked:

$$\text{commute}({}_qA_{12}, {}_qA_{21}) \to [H_1]_q, \ldots$$

Orthogonal algebras

The matrix elements of the generators X_{ij} given in (47) and (48) are calculated by the procedure **Ome**(i, j, $|m\rangle$), where $j = i - 1$ and $|m\rangle$ is a generic Gelfand–Tsetlin vector. Its output is a list of lists which have the matrix element in the first positions and the resulting Gelfand–Tsetlin vector in the second positions.

Example 30. A generic Gelfand–Tsetlin vector of an irreducible representation $\Lambda = [m_{13}, m_{23}]$ of $D_2 \sim so(4)$ in the canonical chain $D_2 \subset B_1 \subset D_1$ is

$$|m\rangle = \begin{vmatrix} m_{13} & & m_{23} \\ & m_{12} & \\ & m_{11} & \end{vmatrix} \to \big[[m_{11}],\ [m_{12}],\ [m_{13}, m_{23}]\big] \quad \text{(Maple V)}. \tag{71}$$

The generator X_{21} is always diagonal:

$$\text{Ome}(2,1,|m\rangle) \to \Big[\big[\text{i}m_{11}, \big[[m_{11}], [m_{12}], [m_{13}, m_{23}]\big]\big]\Big]$$
$$\Rightarrow X_{21}|m\rangle = \text{i}m_{11}|m\rangle.$$

The generator X_{32} is a tridiagonal matrix with no diagonal elements:

$$\text{Ome}(3,2,|m\rangle) \to \Big[\big[a_1^1(m_{11}),\ \big[[m_{11}+1], [m_{12}], [m_{13}, m_{23}]\big]\big],$$
$$\big[-a_1^1(m_{11}-1),\ \big[[m_{11}-1], [m_{12}], [m_{13}, m_{23}]\big]\big]\Big]$$
$$\Rightarrow X_{32}|m\rangle = a_1^1(m_{11})|m_{11}+1\rangle - a_1^1(m_{11}-1)|m_{11}-1\rangle,$$

where

$$a_1^1(m_{11}) = \tfrac{1}{2}\big\{(m_{12} - m_{11})(m_{12} + m_{11} + 1)\big\}^{1/2}.$$

The matrix elements of X_{43} are:

$$\begin{aligned}\mathrm{Ome}(4,3,|m\rangle) \to \Big[&\big[b_2^1(m_{12}),\ \big[[m_{11}],[m_{12}+1],[m_{13},m_{23}]\big]\big],\\ &\big[b_2^1(m_{12}-1),\ \big[[m_{11}],[m_{12}-1],[m_{13},m_{23}]\big]\big],\\ &\big[\mathrm{i}c_2,\ \big[[m_{11}],[m_{12}],[m_{13},m_{23}]\big]\big]\Big]\\ &\Rightarrow X_{43}|m\rangle = b_2^1(m_{12})|m_{12}+1\rangle - b_2^1(m_{12}-1)|m_{12}-1\rangle + \mathrm{i}c_2|m\rangle,\end{aligned}$$

where

$$\begin{aligned}b_2^1(m_{12}) &= \left\{\frac{(m_{12}+m_{11}+1)(m_{12}+m_{13}+2)(m_{12}+m_{23}+1)}{(m_{12}+1)^2(2m_{12}+3)(2m_{12}+1)}\right\}^{1/2}\\ &\quad\times\left\{(m_{12}-m_{11}+1)(m_{12}-m_{13})(m_{12}-m_{23}+1)\right\}^{1/2},\\ c_2 &= \frac{m_{11}m_{23}(m_{13}+1)}{m_{12}(m_{12}+1)}.\end{aligned}$$

The action of the remaining elements of D_2 can be calculated from (43):

$$X_{31} = [X_{32}, X_{21}], \quad X_{42} = [X_{43}, X_{32}], \quad X_{41} = [X_{43}, X_{31}] = [X_{42}, X_{21}].$$

The explicit construction of the irreducible matrices of a particular representation of $so(n)$ in the canonical chain $so(n) \subset so(n-1) \subset \cdots$ is computed by the procedure **Oim**(i, j, M), where $i = j + 1$ and M is an explicit Gelfand–Tsetlin basis. Its output is a matrix representing the generator X_{ij}.

Example 31. The Gelfand–Tsetlin vectors of the fundamental representation $\Lambda = [1, 0]$ of D_2 are given in Example 25. The ordering of the vectors is given by the procedure vD2 as shown in Example 25. The irreducible matrices in this representation Λ are:

$$\mathrm{Oim}(2,1,M) \to X_{21} = \mathrm{i}\begin{pmatrix}1&&&\\&0&&\\&&-1&\\&&&0\end{pmatrix} = \mathrm{i}(A_{11} - A_{33}),$$

$$\mathrm{Oim}(3,2,M) \to X_{32} = \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0&0\\-1&0&1&0\\0&-1&0&0\\0&0&0&0\end{pmatrix} = \frac{1}{\sqrt{2}}(A_{21} - A_{12} + A_{32} - A_{23}),$$

$$\mathrm{Oim}(4,3,M) \to X_{43} = \begin{pmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&-1&0&0\end{pmatrix} = (A_{24} - A_{42}),$$

where M is a list containing the Gelfand–Tsetlin vectors computed by the procedure vD2. These matrices are not in the Cartan–Weyl canonical form given in (5).

Symplectic algebras

The Gelfand–Tsetlin matrix elements of the generators of C_1 and C_2 in the chain $C_2 \subset C_1 \oplus C_1$ are given in [24] and they will not be reproduced here. They are calculated using the procedure **Cme**$(i, t, |m\rangle)$. Its output is a list of lists which have the matrix elements in the first positions and the resulting Gelfand–Tsetlin vectors in the second positions. Although this procedure is limited to the C_2 case, the matrix elements of some particular generators can be calculated for the general case A_r: (1) The diagonal operators $i \leqslant r$ and $t = 0$; (2) The C_1 non-diagonal operators $i = r$ and $t = \pm 1$; and (3) The C_2 non-diagonal operators $i = r - 1$ and $t = \pm 1$. In general, $i \leqslant r$ and

$t = 0$ for the elements associated with the null roots, and $t = 1$ ($t = -1$) for the positive (negative) roots. The explicit construction of the irreducible matrices is computed by the procedure **Cim**(i, t, M), where M is a given Gelfand–Tsetlin–Cerkaski basis. Its output is a matrix.

Example 32. A typical Gelfand–Tsetlin–Cerkaski vector of an irreducible representation $\Lambda = [\omega_{12}, \omega_{22}]$ of C_2 in the chain $C_2 \subset C_1 \oplus C_1$ is given by:

$$|\omega\rangle = \left|\begin{array}{ccc} \omega_{12} & & \omega_{22} \\ & \gamma_{12} & \quad h_2 \\ & \omega_{11} & \\ & & \quad h_1 \end{array}\right| \rightarrow \big[[h_1, h_2],\ [\sigma_1, \sigma_2],\ \big[[\omega_{11}], [\gamma_{12}],\ [\omega_{12}, \omega_{22}]\big]\big] \tag{72}$$

where

$$\sigma_1 = \omega_{11}, \quad \sigma_2 = \omega_{12} + \omega_{22} + \omega_{11} - 2\gamma_{12}.$$

The matrix element of the operator E_2^+ associated with the simple root $\alpha_2 = [0, 2]$ of C_2 is

$$\begin{aligned} &\mathrm{Cme}(2, +1, |\omega\rangle) \rightarrow \Big[\big[a,\ \big[[h_1, h_2 + 2], [\sigma_1, \sigma_2], \big[[\omega_{11}], [\gamma_{12}], [\omega_{12}, \omega_{22}]\big]\big]\big]\Big] \\ &\qquad\qquad\qquad \Rightarrow E_2^+|\omega\rangle = a\ |h_2 + 2\rangle, \\ &\quad a = \left\{\tfrac{1}{2}(\sigma_2 - h_2)(\sigma_2 + h_2 + 2)\right\}^{1/2}. \end{aligned}$$

Example 33. The Gelfand–Tsetlin vectors of the fundamental representation $\Lambda = [1, 0]$ of C_2 are given in Example 26. The ordering of the vectors is given by the procedure vC2 as shown in Example 26. The irreducible matrices of the generators in the representation Λ are:

$$\mathrm{Cim}(1, 0, M) \rightarrow H_1 = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}, \qquad \mathrm{Cim}(2, 0, M) \rightarrow H_2 = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 0 & \\ & & & 0 \end{pmatrix},$$

$$\mathrm{Cim}(1, 1, M) \rightarrow E_1^+ = \begin{pmatrix} & & -1 & 0 \\ & & 0 & 0 \\ 0 & 0 & & \\ 0 & 1 & & \end{pmatrix}, \qquad \mathrm{Cim}(1, -1, M) \rightarrow E_1^- = \begin{pmatrix} & & 0 & 0 \\ & & 0 & 1 \\ -1 & 0 & & \\ 0 & 0 & & \end{pmatrix},$$

$$\mathrm{Cim}(2, 1, M) \rightarrow E_2^+ = \sqrt{2}\begin{pmatrix} 0 & 0 & & \\ 1 & 0 & & \\ & & 0 & 0 \\ & & 0 & 0 \end{pmatrix}, \qquad \mathrm{Cim}(2, -1, M) \rightarrow E_2^- = \sqrt{2}\begin{pmatrix} 0 & 1 & & \\ 0 & 0 & & \\ & & 0 & 0 \\ & & 0 & 0 \end{pmatrix},$$

where M is a list containing the Gelfand–Tsetlin vectors computed by the procedure vC2. These matrices are in the Cartan–Weyl canonical form given in (5). For example, the generators $E_i^{\pm}$ are associated with the (simple) roots $\pm\alpha_i$, $i = 1, 2$, where $\alpha_1 = [1, -1] = (2, -1)$ and $\alpha_2 = [0, 2] = (-2, 2)$. Their defining commutation relations are:

$$\mathrm{commute}(E_1^+, E_1^-) \rightarrow H_1 - H_2, \quad \mathrm{commute}(E_2^+, E_2^-) \rightarrow 2H_2.$$

4.2.3. Eigenvalues of invariants

The eigenvalues $C_p(\Lambda)$ of the invariants of order p for classical algebras, given in (56), are calculated by the procedure **spectra**(p, Λ, X). The values of p for the independent invariants are given in Table 1.

Example 34. The $gl(2, R)$ algebra has one invariant of order one and one of order two. Their eigenvalues in an irreducible representation given by $\Lambda = [m_1, m_2]$ are, respectively:

$$\text{spectra}(1, \Lambda, ''\text{A}'') \to C_1(\Lambda) = m_1 + m_2,$$
$$\text{spectra}(2, \Lambda, ''\text{A}'') \to C_2(\Lambda) = m_1(m_1 + 1) + m_2(m_2 - 1).$$

The semisimple A_r algebras do not have a linear invariant, therefore, $m_1 + m_2 = 0$. Following the prescription in (32), we have $\Lambda = [j, -j]$ for $sl(2, R)$ and its second order invariant has the eigenvalue:

$$\text{spectra}(2, \Lambda, ''\text{A}'') \to C_2(\Lambda) = 2\,j(j + 1).$$

Example 35. The D_2 algebra has two second order invariants whose eigenvalues in an irreducible representation given by $\Lambda = [m_1, m_2]$ are:

$$\text{spectra}(2, \Lambda, ''\text{D}'') \to C_2(\Lambda) = 2m_1(m_1 + 2) + 2m_2^2,$$
$$\text{spectra}(4, \Lambda, ''\text{D}'') \to C_2'(\Lambda) = -8m_2(m_1 + 1).$$

Note that $p = 2r$ must be used in the procedure spectra for the eigenvalue of C_r'. The eigenvalues C_p calculated with p being odd are not linearly independent:

$$\text{spectra}(1, \Lambda, ''\text{D}'') \to C_1(\Lambda) = 0,$$
$$\text{spectra}(3, \Lambda, ''\text{D}'') \to C_3(\Lambda) = C_2'(\Lambda).$$

It is interesting to calculate the eigenvalue of the Casimir operator (second order invariant) using the procedure casimir. Before doing that, the highest weight Λ must be rewritten in the DYN basis: $\Lambda = [m_1, m_2] = (m_1 + m_2, m_1 - m_2)$. Therefore,

$$\text{casimir}(\Lambda, ''\text{D}'') \to m_1(m_1 + 2) + m_2^2 = \tfrac{1}{2}C_2(\Lambda).$$

5. Installation

The KILLING package was written using the Maple V (Release 5) and Mathematica (Release 3) algebraic programming softwares. Therefore, it can be used in any operational system which has Maple V or Mathematica installed. The source codes come in the following directory structure:

```
$Root/killing/maple/src
$Root/killing/maple/lib
$Root/killing/maple/help
$Root/killing/math/src
$Root/killing/math/Files
$Root/killing/math/Files/Addons/Applications/Killing
$Root/killing/math/Files/Addons/Applications/Killing/Kernel
$Root/killing/math/Files/English/Addons/Applications/Killing
```

where $Root represents the absolute path where the KILLING files are installed.

5.1. Installation under Maple V

The following steps are necessary for a manual installation of the KILLING package under Maple V (Release 5):

(1) Execute the Maple V worksheet

$Root/killing/maple/make.mws

in order to compile all procedures in the KILLING package. The output is written in the binary file

$Root/killing/maple/lib/killing.m

The output is controlled by the ASCII file

$Root/killing/maple/killing

(2) Execute the Maple V worksheet

$Root/killing/maple/help/make.mws

in order to generate the online help files. The output is written in the binary file

$Root/killing/maple/lib/maple.hdb

(3) The following line

libname := ‘$Root/killing/maple/lib’, libname;

must be added to the Maple V initialization file in order to have the KILLING package loaded in a Maple V session by

with(Killing);

It is important here that the absolute path indicating where the files `killing.m` and `maple.hdb` are located, comes before the Maple V library path given by `libname`;

(4) One alternative to the previous step is to redefine the Maple V library search path given by `libname`, as in step (3) above, for each Maple V session.

The Maple V initialization file under Microsoft Windows is named `maple.ini` and should be placed in one of the Maple V subdirectories, either `lib` or `update`. For case in which there is a Maple V subdirectory `update`, then the initialization file `maple.ini` must be created (or modified) there.

5.2. Installation under Mathematica

The KILLING package can be loaded in two ways: (1) using the ASCII file

$Root/killing/math/src/killing

to load all functions inside a Mathematica session (`«killing`); or (2) using the files under

$Root/killing/math/Files

to install it as an Add-On application. This is accomplished by the following steps:

(1) Copy the subdirectory

$Root/killing/math/Files/Addons/Applications/Killing

and its contents to

$RootMath/Files/Addons/Applications/Killing where `$RootMath` is the root of the Mathematica directory tree in single user systems or a user relative path for the Add-On subdirectories in multiple user systems. The KILLING functions must first be declared as stub functions by typing "`«Killing‘`", the full package is loaded when one of the functions is used for the first time;

(2) Copy the subdirectory

$Root/killing/math/Files/English/Addons/Applications/Killing

and its contents to

$RootMath/Files/Documentation/English/Addons/Applications/Killing

This installs the online help files. In order to add an entry to the Add On radio button to the Help Browser, the ASCII file `BrowserCategories.m`

$RootMath/Files/Documentation/English/Addons/

must be modified to include the path for the KILLING help files. There is a commented sample in

$Root/killing/math/Files/English/Addons/

(3) Rebuild the Mathematica help index using the Help menu `Rebuild Help Index` button.

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