# The problem of simplification of algebraic expressions with indices in computer algebra*

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  - Where and how indexed expression accur in science
- The problem
  - What does it means “simplification”
  - Example: Riemann tensor
- Possible solutions
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- Definitions
- Colored graphs.
- Conclusions

# Introduction

- Areas where calculations are used
  - Theoretical physics
  - Solid state physics
  - Mechanics
  - Mathematics
- Types of calculations
  - Component calculation
  - Indexed expressions with abstract indices
  - Abstract calculations
  - More details see for example:
    - Korol'kova A.V., Kulyabov D.S., Sevast'yanov L.A. Tensor computations in computer algebra systems // Programming and Computer Software. - 39 (2013), No3, pp. 135-142

# Introduction

- We will consider indexed expression T(i,j,k,l) as an object with abstract indices
  - We are not interested in a specific coordinate basis (like for tensor)
    - So, we will not calculate components of the expressions.
- Advantages:
  - We can use properties of expressions: symmetry with respect to permutation of the indices, renaming summation indices, etc.
  - Good method for calculation of invariants.
- Disadvantages:
  - Often at the end we need to calculate the components of the expressions in a particular basis.

# Simplification of indexed expressions

- Expression can have the following properties:
  - Symmetry with respect to permutations of the indices
  - Summation indices
  - Linear relations (multi-term identities)
- There are two main questions:
  - Are the two polynomials equal: P1 == P2?
  - Is the polynomial equal to zero: P1 == 0?
    - The first question can be reduced to the second one: P1-P2 == 0
- One of the solutions is finding of canonical presentation of indexed expression:
  - two expression are equal each other if and only if they have identical canonical form.

# Example: Riemann tensor

- Symmetries in relation to index permutations

  R(i,j,k,l)=-R(j,i,k,l), т.е. 1<-->2
  R(i,j,k,l)=R(k,l,i,j), i.e. {1,2}<-->{3,4}

- Summation indixes
  - Ricci tensor:

    R(j,l)=R(i,j,i,l): $R(j,l)==\sum_i R(i,j,i,l)$
  - Scalar curvature:

    R=R(m,m)=R(i,m,i,m)
- Liniar identities
  - Bianchi identity

    R(i,j,k,l)+R(i,l,j,k)+R(i,k,l,j)=0

# Algorithms

- Double coset
  - Rodionov, A.Y. and Taranov, A.Y., Combinatorial aspects of simplification of algebraic expressions, In Proc. Int. Conf. EUROCAL'89, Lecture Notes in Computer Science, vol.378(1989), pp.192-201
- Group algebra
  - Ilyin, V.A. and Kryukov, A.R., ATENSOR - REDUCE program for tensor simplification, Computer Physics Communications, vol.96(1996), pp.36-52
- Graph isomorphism
  - G. Shpiz and A. Kryukov, Canonical Representation of Polynomial Expressions with Indices // Programming and Computer Software, v.45, no.2, pp.81-87.
- Of course, it is incomplete list of publications.
- *Here we consider the further development of the graph isomorphism methods in the case of several classes of indexes.*

# Problem

- Usually the task is to develop an algorithm that effectively works on large expressions.
- Unfortunately, most available algorithms in the worst case, require complete search.
- We set the task of optimizing calculations for expressions typical of calculations in theoretical physics. These are, as a rule, expressions containing the product of a dozen factors, each of which has several indices.
- The main task is to reduce the number of options studied by working with equivalence classes of color graphs instead of concrete representatives of monomials.
  - In the case of finite number of indexes our approach allows to avoid the complete search.

# Note

- Further consideration is based on the article

G. Shpiz and A. Kryukov, Canonical Representation of Polynomial Expressions with Indices // Programming and Computer Software,  v.45 (2019), no.2, pp.81-87.

# Monomials: basic definition

**Let's**

- ***T*** is a set of symbol types.
- ***I*** is a set of indexes
- ***C*** is a set of index colors

**Definition.** An elementary colored symbol or simply a symbol is an expression of the form $t\,(i_1, \dots, i_n; c_1, \dots c_n)$, where $t \in T$, and $i_1, \dots, i_n \in I$ and $c_1, \dots c_n \in C$. The product of symbols will be called a monomial if no index occurs in it more than twice. Repeated indices will be called summation indices, the others - simple indices.

- We assume that the set of all types of symbols and their indices is linearly ordered, and the following conditions are satisfied:

1) any type less than any index,
2) any summation index is greater than any simple index,
3) summation indices and only they are natural numbers.
4) the color corresponds to the index number in the index sequence, and not its name. That is, when rearranging indices or when renaming them, the sequence of colors does not change.

# Monomials: signature

- We introduce a linear order in the set of all symbols ***$s=t(i_1, \ldots, c_1, \ldots)$*** assuming that ***$t(i_1, \ldots) < t'(i'_1, \ldots)$*** if ***$(t, i_1, \ldots) < (t', i'_1, \ldots)$*** in the sense of a lexicographic order. The set of all monomials will also be considered lexicographically ordered.

**Definition.** A signature of k-th index is a pair ***$sig_k=(c_k,i_k)$***

***Definition.*** By the signature of the symbol ***$s=t(i_1, \ldots i_n)$*** we mean the sequence ***$(t, sig_1, \ldots sig_n)$***, where ***$(sig_1, \ldots sig_n)$*** is an ascending sequence of index signatures ***$sig_1, \ldots sig_n$*** ordered by increasing these signatures.

- The signature of the symbol ***$s=t(i_1, \ldots, c_1, \ldots)$*** will always be identified with the symbol obtained from ***s*** by ordering the indices in increasing order, and the signature of the monomial ***m*** - with the product of the signatures of the factors of the monomial ***m*** ordered by increasing these signatures.

# Monomials: signature

- Index coloring can be used to distinguish the spaces with which these indices are associated. For example, subscripts can be associated with some (arithmetic) vector space, and the superscripts with its conjugate. In particular, indices in various types of characters can be associated with different spaces.

  An example of coloring indexes is the top or bottom position of the index.

  Another example. Indices in the symbols of partial derivatives are associated with the space of linear differential operators with constant coefficients, and indices in the symbols of functions with the space of arguments.

# Monomials

- By the signature of a monomial we will call a class of monomials that differ from each other only by a permutation of the factors between themselves or a permutation of indices within the factors.

**Definition.** A contracted expression or monomial is a product of symbols in which no index occurs more than 2 times. Indices occurring once in a monomial will be called free indexes, occurring 2 times – contracted indexes.

- We assume that any set of characters with pairwise different signatures is linearly independent, and characters with the same signatures can be connected by linear relationships. The set of all such relations will be denoted by ***R*** and we will assume that any renaming of the indices takes a linear relation from ***R*** to ***R*** (that is, the set of relations is invariant under the renaming of the indices).
- Signature of the contracted expression ***m*** is a sequence of the signature of the factors of ***m*** in increasing order.

# Week equivalence

- Linear combinations of convolutional expressions with the same signature are weakly equivalent if they are obtained from each other by replacing factors with equivalent symbols or sums of symbols, expanding parentheses, and rearranging factors in terms.
- The weak equivalence class of a contracted expression with signature ***s*** is called a quasi-monomial with signature ***s***.

# Monomials: quasi-monomial

- Symbols with the same signature can be connected by linear relations. We assume that the following conditions are satisfied.
- C1. Any renaming of indices translates the relation into relation.
- C2. Any set of symbols with pairwise different signatures is linearly independent.

**Definition.** A quasi-monomial is a linear combination of monomials with the same signature. This signature will be called the quasi-monomial signature. The signature of the quasi-monomial ***m*** will be denoted by ***sig(m).***

- Note that the signature of any quasi-monomial is always a monomial.

**Definition**. Quasi-monoms are said to be weakly equivalent if they have the same signature ***sig*** and their difference lies in ***R(sig)***. Quasi-monoms are called equivalent if, after some renaming of the summation indices, they become weakly equivalent. The equivalence class (not weak equivalence) of the monomial ***m*** is denoted by ***[m]***.

# Monomials

**Proposition.**

Any set of nonzero quasi-monomials with pairwise different signatures is linearly independent.

- Quasi-monomials with a fixed signature ***sig*** form a vector space, which will be denoted by ***V(sig)***. In this space, a subspace of relations ***R(sig)*** is defined, which is generated by permutations of factors and linear relations, which are obtained by replacing any factor with an equivalent linear combination of symbols.

# Monomials:

**Definition.** A monomial will be called minimal if it can not be up to weak equivalence represented as a linear combination of smaller monomials (with the same signature).

**Proposition.**

1) Let $\boldsymbol{sig_0}$ – minimal signature. Monomial is minimal if and only if it has signature $\boldsymbol{sig_0}$, any of its factors is minimal as symbols and the factors are ordered in ascending order.

2) The set of all minimal monomials with signature ***sig*** forms a basis in the quotient space ***V(sig)/R(sig)***. The decomposition of the class of a quasi-monomials in this basis will be called the quasi-canonical representation of a monomial.

# Canonical representation of monomials (1)

- For an arbitrary monomial $m = v_1 * \ldots * v_n$, we denote **D*(m)***, the set of all its summation indices.
- Let a set of indices be given ***I***. Any one-to-one mapping ***f: D(I) → D(I)*** defines a one-to-one mapping of the set of all monomials into itself, in which, in a given monomial, any index ***i*** present in it is replaced by ***f(i)***. Such transformations will be called renames of indices from the set **D(*I*)**.

**Definition.** For an arbitrary signature ***sig***, we denote by ***G(sig)*** the group of all renames of its summation indices that take ***sig*** into itself.

- Arbitrary renaming of ***f*** from ***G(sig)*** takes the set of monomials with signature ***sig*** to the set of monomials with signature ***s*** itself and defines an automorphism of the space ***V(sig)***, which takes the subspace of relations into itself. The group ***G(sig)*** will be called the automorphism group of the signature ***sig*** and be considered as the group of linear transformations of the space ***V(sig)***.
- For an arbitrary quasi-monomial we set ***G(m) = G(sig(m))***.

# Canonical representation of monomials (2)

**Definition.** Quasi-monomials will be called equivalent if they become weakly equivalent if the summation indices are appropriately renamed to their terms.

- The equivalence class of a monomial ***m*** will be denoted by ***[m]***, and the set of all signatures of elements from ***[m]*** will be denoted by ***sig[m]***. The minimal element in the set ***sig[m]*** will be denoted by $sig_0(m)$.

- Obviously, by suitable renaming of the indices of summation by any monomial ***m*** can be transferred to the space $V(sig_0(m))$. Thus, for any monomial ***m*** one can find an equivalent monomial with minimal signature.

# Canonical representation of monomials (3)

Let ***m*** be an arbitrary monomial, and $m_0$ be any equivalent quasi-monomial with minimal signature (that is, $m_0 \in V(sig_0(m))$).

**Theorem.**

The quasi-canonical representation $\hat{m}$ of the average of all monomials of the form $g(m_0)$, $g \in G(m_0)$ which does not change signature does not depend on the choice of $m_0$. Thus, $\hat{m}$ is uniquely determined by the class ***[m]*** and in turn defines this class.

- The quasi-monomial $\hat{m}$ will be called the canonical representation of the monomial ***m***.

# Canonical representation of monomials (4)

- It is clear from the definition that the computation of the canonical representation of the monomial ***m*** is reduced to two problems.
  - T1. Calculate the minimum signature ***s*** **=** $\boldsymbol{sig_0(m)}$.
  - T2. Calculation of the automorphism group of the signature ***s***.
    - We reduce monomials to quasi-canonical form during avaraging.
    - Calculating the quasi-canonical representation of symbols.

# Structural monomial graph

Let us $m=v_1*v_2*...v_n$

Consider a graph whose vertices coincide with the symbols in ***v*** and the vertices are counted by an edge if and only if they contain at least one common index.

- The color ***col(α)*** of the index ***α*** common to the vertices ***v_i*** and ***v_j*** for ***i <= j*** is a pair ***(s1, s2)*** of signatures of this index in ***v_i*** and ***v_j***, respectively.
- The color of a vertex will be called its signature.
- The color of the edge connecting the vertices $v_i$ and $v_j$; moreover, $i \leq j$ is the sequence $(i,sig(v_i),j,sig(v_j),c)$ where ***c*** is the sequence of colors of common indices for ***v_i*** and ***v_j***, sorted in ascending order.

# Structural monomial graph

**Definition.** The colored graph described above is called the graph of the contracted expression ***v*** and is denoted by ***Gr(v)***.

- Note that the coloring of the graph ***Gr(v)*** depends on the order of the factors and on the renaming of the summation indices.

**Definition.** The ascending order of the color sequence of all edges of the graph ***Gr(v)*** is called the color of the graph.

- Obviously, the graph is uniquely determined by its color, and the lexicographic order of the colors of the graphs determines the linear order on the set of graphs of the form ***Gr(v)*** for $v \in [v]$.

**Definition.** The minimal element of this set is called the structural graph of the monomial ***[v]*** and is denoted by $Gr_0([v])$ or $Gr_0(v)$.

# Structural monomial graph

- Contracted expressions corresponding to the structural graph are obtained from each other by automorphisms of the structural graph (naturally preserving the coloring of vertices and edges) and permutations of the "multiple" summation indices with the same signatures.

# Structural monomial graph

**Definition.** The numbering of the colored graph, we will call the numbering of its vertices, that is, the embedding of the set of vertices in the initial segment of the natural series.

**Theorem.**

The numbering of the structural graph has the same color if and only if they are obtained from each other by the substitution of the automorphism of the structural graph.

**Theorem.**

Replacing the summation indices of the monomial ***m*** by their numbers with respect to a certain numbering gives a monomial with a minimal signature if and only if this numbering corresponds to a certain optimal numbering of the structural graph of the monomial ***m***.

# Structural monomial graph

- Thus, the tasks of finding the minimal signature and its automorphism group are reduced to finding the list of optimal numberings of the structural graph.
- The numbering of the indices corresponds to the order of the corresponding edges, except for the case of multiple indices, where all permutations of indices with the same signature must be considered.
- Reduction to the canonical form of the contracted expression reduces to reduction to the canonical form of the graph associated with it and calculation of the group of automorphisms of this graph. This lead to calculating a list of optimal vertex numberings, which is obtained by a tree-like process of sequentially “increasing" numbering.

# Conclusion

- We considered the problem of reducing multiplicative expressions with contractions to canonical form.
- The approach  permit to consider different type of index sets which is acting in different spaces.
- The concept of signature and defining a canonical form for monomials from indexed values, taking into account summation indices and linear relations between them, was introduced. The definitions of a structural colored monomial graph and canonical numbering of its edges were introduced too.
- The tasks of finding the minimal signature and its automorphism group was reduced to finding the list of optimal numbering of the structural graph.
- The algorithm of finding the optimal numbering is based on calculating the set of canonical numerations of edges of a structural graph of a monomial, whose computational complexity does not depend on the number of summation indices, but on the number of automorphisms of the structural graph, which is not great for real expressions.

# References (incomplete)


1. G. Shpiz and A. Kryukov, Canonical Representation of Polynomial Expressions with Indices // Programming and Computer Software, v.45(2019), no.2, pp.81-87
2. Королькова А.В., Кулябов Д.С., Севастьянов Л.А. Тензорные расчеты в системах компьютерной алгебры // Программирование, №3(2013), с.47–57
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# THANK YOU!

# QUESTIONS?