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CHALLENGING THE BOUNDARIES OF SYMBOLIC COMPUTATION

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editors

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CHALLENGING THE BOUNDARIES OF SYMBOLIC COMPUTATION
Proceedings of the 5th International *Mathematica* Symposium

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Host's Preface

The International *Mathematica* Symposium began, I guess, as a twinkle in the eye of people like Peter Mitic, Gautam Dasgupta and Veikko Keränen, who collectively had the idea at a Wolfram Developer's Conference in Champaign-Urbana, Illinois, back (if I remember rightly) in 1994. How would it be, they wondered, if the worldwide community of *Mathematica* users—in research, in education, in industry and commerce—got together on a regular basis to plot, and scheme, and exchange ideas? How would it be if a Program Committee and a proper peer review process were set up? That way, academic users in particular could gain recognition for their work with *Mathematica*. That way, too, *Mathematica*'s role in research, which orthodox journals and conferences used to treat as something of a shameful secret, (and which some of them, to be honest, still do), could come to the forefront.

Where these flights of imagination led to was Southampton, U.K., in the summer of 1995 and the first IMS of all, which Peter Mitic hosted. Where *that* led was where we are now: back in England again, after travelling via Rovaniemi, Linz and Tokyo. We find ourselves in a computational environment that has changed utterly in those eight years, yet *Mathematica* and IMS are both stronger than ever. In 1995, *Mathematica* development meant writing packages. In 1995, *Mathematica* in Education meant building courses around the Notebook's Front End. Some great truths never change: if you leaf through the papers in this volume, you'll find plenty of packages and plenty of examples of students using Notebooks, but you'll also find *Mathematica* acting in new and exciting ways: powering specialist research, educational and fieldwork tools written by the Symposium's authors, and often available over the Internet, (itself changed in ways we couldn't have imagined as recently as eight years ago).

The word "interdisciplinary" usually strikes dread into me. Too often, it signals either woolly generalities, or specialists talking past one another. But IMS has always been about the best kind of "interdisciplinary". Widely divergent as our fields and backgrounds are, we speak a shared language, and we find ourselves able to strike sparks across disciplinary boundaries. That's the main reason why IMS has become my favourite regular conference of all, and why I'm delighted to see the Symposium in London and even more pleased to welcome IMS to Imperial College.

Phil Ramsden, Imperial College London

Editor's Preface

This year we are fortunate to welcome many new authors to IMS, as well as old friends. Their papers cover, as usual, a wide range of topics, although there seemed to be some concentration on physics and applied maths. Many authors, particularly in education, have webified their applications and made solid advances as a result. There are some unusual papers, too, and they're worth reading just to see what can be done. One of the original aims of IMS was to encourage students and new users to contribute, and I ask you to encourage your students to do just that. IMS is an ideal medium for short precursors to more substantial research or practice.

Before the job of producing final papers started, we spent a lot of time discussing how to present the proceedings. There were two main issues. The first was what format to use, and we settled on the *Mathematica* notebook. That must seem odd, since *Mathematica* is designed for development and to produce technical documents, yet this is the first IMS where we have asked authors to submit notebooks. The results have been positive and uniformity in submissions has eased the task of editing. This issue was originally prompted by the second main issue, which was whether or not to produce the proceedings as a book or on a CD. I was very much in favour of the CD because it has clear advantages, particularly for work in *Mathematica*. Notebooks on CD need not be limited in length, need not suffer from formatting problems, and can be what they should be: live documents that you can use as well as read. It's quite clear that these proceedings are intended almost entirely for the printed page. However, we have found significant problems with the acceptability of proceedings on CD on the part of some academics. They like paper! They are also the ones who control the budgets. Arguing that material on a CD is refereed to the same standard as that in a book, can have an ISBN and a NLC number and can even be printed does not work. I have not yet heard a rational argument against CDs. So, my message is: persuade your senior academics, (yourself if you are one), to agree that a CD is as acceptable as print, if not more so.

Finally, I would like to thank two people. Larry Adelston of Wolfram Research did an excellent job in producing the IMS 2003 stylesheet. He must have been awake all night at times: I often received e-mails when it must have been dark in Champaign IL. My co-editor, Janet Carne, did a meticulous job in editing many papers in these proceedings. You can be sure that if you see extra commas, (she likes those...), or different wording in your text, it has been done for a purpose and is worth emulating.

Peter Mitic, Positive Corporation Ltd.

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- The "CODATA recommended values of the fundamental physical constants:1998" are badly conditioned, i.e. some non-degenerate sub-matrices of the CODATA correlation matrix published on the Web are not positive definite, presumably because of the unjustified independent rounding of the numerical values of the correlation coefficients;
- It will help if the notion of "Hermitian matrix" will appear in *Mathematica,* with the assurance of conservation of the main features of Hermitian matrices in all numerical transformations, especially for Hermitian matrices close to degenerate.

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Boole-Bell-type inequalities in Mathematica

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1 Abstract

The violation of Bell-type inequalities by quantum probabilities represents an important aspect of quantum mechanics which is linked to the mind-boggling quantum features of nonlocality, complementarity and contextuality. Formally, such bounds on the classical probabilities from consistency arguments have already been investigated by Boole in the middle of the nineteenth century. Boole called them "conditions of possible experience." We introduce CddIF, a *Mathematica* package to compute all the Boole-Bell-type inequalities associated with an arbitrary physical setup. We have also computed with *Mathematica* the tractable special cases of two particles with up to three possible detection angles per particle, and the three-particle/two directions (Greenberger-Horne-Zeilinger) case.

2 Boole-Bell Type Inequalities

Would you believe someone telling you that the chances of rain in Vienna and Budapest are 0.1 in each one of the cities alone, and the joint probability of rainfall in both cities is 0.99? I believe you would not. It just does not make any intuitive sense to claim that it rains almost never in one of the cities but almost always in both of them. The nagging question appears, though: which numbers would you believe in? Of course one could argue that the joint probability should not exceed any single probability. This certainly appears to be a necessary condition, but is it a sufficient one? In the middle of the 19th century George Boole, in response to such queries, formulated a theory of "conditions of possible experience" [1,2,3,4,5]. These conditions on the (joint) probabilities of logically connected events are expressed by certain equations or inequalities relating those probabilities. More recently, similar inequalities for a particular setup which are relevant in the quantum mechanical context have been discussed by Clauser and Horne and others [6,7,8]. Pitowsky has given a geometrical interpretation in terms of correlation polytopes [9, 4, 10, 5].

2.1 *Geometrical interpretation [4,5,9,10]*

Consider the truth table (Table 1) of the above example, where a_1 and b_1 represent the statements that *"it rains in Vienna"* and *"it rains in Budapest"*, and $a_1 b_1$ represents the proposition *"it rains in Vienna and in Budapest ,"* respectively; i.e.,

```
In[1]:= TruthTable[2, 1]
```

```
Out[1]//MatrixForm=
```

$$\begin{pmatrix} a_1 & b_1 & a_1 b_1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

Table 1

In the weather example, there are two places with one observable each; hence the arguments 2,1. The third "component bit" of the vector is a function of the first components. Since we are dealing with the classical logical "and" operation here, this function is a multiplication. This amounts to interpreting the rows of the truth table as extremal points; the entries of the rows being the components. The vectors have the following meaning: {0,0,0} stands for the case of neither rain in Vienna nor in Budapest, {1,0,0} stands for the case of rain in Vienna but not in Budapest, and so on. Any probability distribution characterized by the three numbers {a1, b1, a1b1} should be a weighted linear average over all these (weather) conditions.

Interpret the set of all numbers {a1, b1, a1b1} as a set of points in a three-dimensional real space. As pointed out by Pitowsky [4], this set is the polytope formed by a weighted linear average over all extremal points of Table 1 representing the possible (weather) conditions. More precisely, the surface of the convex polytope with vertices {0,0,0}, {1,0,0}, {0,1,0} and {1,1,1} (cf. Figure 1) represents all conceivable classical probability distributions. The faces of the polytope represent the conditions by which

classical probabilities are bound; and these "inside-outside" conditions are expressed as inequalities. These inequalities are called Boole-Bell inequalities.

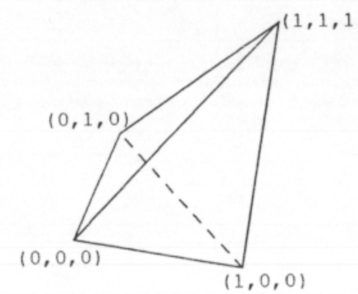

Figure 1

2.2 *Minkowski-Weyl representation theorem*

Generally, according to the Minkoswki-Weyl representation theorem (eg.,[10,p.29]), every convex polytope in an Euclidean space has a dual description: either as the convex hull of its extreme points (vertices), or as the intersection of a finite number of half-spaces, each one given by a linear inequality. The problem to obtain all inequalities from the vertices of a convex polytope is known as the hull problem. For the Boole-Bell type problems at hand, the Minkowski-Weyl representation theorem represents a direct, provable method to obtain a complete set of optimal inequalities for classical probability distributions characterizing any physical setup or arrangement.

3 Calculating Inequalities using CddIF

This package acts as an interface to the cdd-program by Komei Fukuda [11] for a transformation from a vertex to a half-space representation and vice versa, making use of the Minkowski-Weyl representation theorem by means of the Double Description Method [12], which we shall use but not review here. A complete description can be found in [13] and the package can be downloaded from *http://tph.tuwien.ac.at/~svozil/cdd/*. Available *Mathematica* functions are for example **TruthTable[x,y]** to build the corresponding truth table for the configuration *x-particles/y-measurements*, **ConvToHRep** to construct the half-spaces representation or **PlotInequalities** to plot the calculated inequalities.

3.1 *Computation of inequalities corresponding to {{0,0,0}, {1,0,0}, {0,1,0} and {1,1,1}}*

The appropriate inequalities for the probabilities of rain in Vienna (a1), rain in Budapest (b1) and rain in Vienna and in Budapest (a1b1) from the example above can easily be calculated with the use of *CddIF:*

```
In[3]:= InequToRead[GetInequFromHRep[
          ConvToHRep[2, 1]]]
```

```
Out[3]//MatrixForm=
  a1 - a1b1 + b1 ≤ 1
  -a1 + a1b1 ≤ 0
  a1b1 - b1 ≤ 0
  -a1b1 ≤ 0
```

Here **ConvToHRep[2,1]** calculates the half-space representation for this particular configuration. Again, as in the weather example discussed above, there are two places with one observable each; hence the arguments 2, 1. The functions **InequToRead[GetInequFromHRep[...]]** display the inequalities in a human-readable form.

3.2 *Quantum mechanical context*

In the quantum mechanical case elementary events and their probabilities refer to clicks in particle detectors. Quantum probabilities have to be calculated using the formalism of quantum mechanics based on Hilbert space entities (i.e., Gleason's theorem) rather than on Boolean algebras. There exist complementary observables which cannot be measured simultaneously. And unlike classical Boolean algebras, Quantum Hilbert lattices are non-boolean (non-distributive). It is by no means trivial that quantum probabilities should satisfy the consistency conditions for classical probabilities; and indeed Bell has discovered physical configurations where Boole's "conditions of possible experience" are violated by quantum probabilities.

As an example, consider a source that produces pairs of spin-1/2 particles in a singlet-state, meaning that, no matter in what direction the spins of the two particles are measured, they will always be opposed to each other. The particles fly apart along the *z* axis, and after the particles have separated, measurements on spin components along one out of two directions are made. If, for simplicity, the measurements are made in the

x-y plane perpendicular to the trajectory of the particles, the direction of the measurement can be given by angles measured from the vertical x axis (α_1 and α_2 on one side, β_1 and β_2 on the other side). On each side the measurement angle is chosen randomly for each pair of incoming particles and each measurement can yield two results - in $\hbar/2$ units: "+1" for spin up and "-1" for spin down (cf. Figure 2).

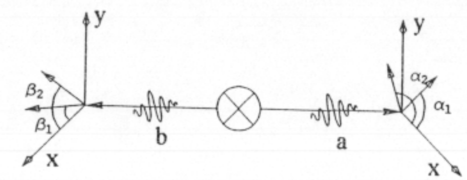

Figure 2

Deploying this configuration we get probabilities to find a particle measured along the axis specified by the angles α_1, α_2, β_1 and β_2 either in spin up or in spin down state denoted as a1, a2, b1, b2 - and we also take the joint event of finding a particle on one side at the angle α_1 (α_2) in a specific spin state and the other particle on the other side along the vector β_1 (β_2) in a specific spin state, denoted by a1b1, a2b1, a1b2 and a2b2.

```
In[4]:= GetInequFromHRep[ConvToHRep[2, 2]] // InequToRead
```

```
Out[4]//MatrixForm=
  [...]
  a1 - a1b1 - a1b2 + a2b1 - a2b2 + b2 ≤ 1
  a1b1 - a1b2 + a2 - a2b1 - a2b2 + b2 ≤ 1
  -a1b1 + a1b2 + a2 - a2b1 - a2b2 + b1 ≤ 1
  a1 - a1b1 - a1b2 - a2b1 + a2b2 + b1 ≤ 1
  [...]
  -a1 + a1b1 + a1b2 - a2b1 + a2b2 - b2 ≤ 0
  -a1b1 + a1b2 - a2 + a2b1 + a2b2 - b2 ≤ 0
  [...]
  -a1b1 ≤ 0
  -a2 + a2b2 ≤ 0
  [...]
  a1 - a1b1 + b1 ≤ 1
```

The first inequalities correspond to the well known CHSH inequalities, which are thereby obtained in a very natural way.

3.3 *Two particles - three measurement directions*

In the case of two particles (a and b) with three properties (whereas the properties are three different angles of the detectors for each particle) denoted by $a_1, a_2, a_3, b_1, b_2, b_3$ 15 different events can be found: $\{a_1, a_2, \ldots, b_3, a_1 \wedge b_1, a_1 \wedge b_2, \ldots, a_3 \wedge b_3\}$. Using

```
In[5]:= TruthTable[2, 3]
```

all vertices of the corresponding correlation polytope can be found - we get a dimension of 15 and 64 vertices as result.
A representation in terms of inequalities of the polytope described by the truth table above can be created by

```
In[6]:= h = ConvToHRep[2, 3]
```

This results in 684 hyper-planes or 684 inequalities, respectively, from the 64 vertices limiting the polytope. All inequalities can be displayed by

```
In[7]:= GetInequFromHRep[h] // InequToRead
```

```
Out[7]//MatrixForm=
               [...]
a1b1 - a1b3 + a2 - a2b1 - a2b3 + b3 ≤ 1
               [...]
             -a2b3 ≤ 0
          a2 - a2b1 + b1 ≤ 1
          a1 - a1b1 + b1 ≤ 1
```

To show all inequalities that are violated at the specific measurement directions $a_1 = b_1 = 0$, $a_2 = b_2 = 2\pi/3$, $a_3 = b_3 = 4\pi/3$ with the functions **P[{x_}]:=1/2** and **P[{x_,y_}]:=1/2 Sin^2[(x-y)/2]** yielding the quantum probabilities to find two spin-1/2 particles (in a singlet state) both either in spin up or both in spin down, we execute


```
In[8]:= P[{x_}] := 1 / 2;
        P[{x_, y_}] := Sin[(x - y) / 2]^2 / 2;
        GetViolInequalities[h,
          {{0, 2π/3, 4π/3}, {0, 2π/3, 4π/3}},
          P, All] // TableForm
```

```
Out[10]//TableForm=
                                   [...]
-a1 + a1b2 + a1b3 + a3b2 - a3b3 - b2 ≤ 0      0.125
a2b1 - a2b2 - a3 + a3b1 + a3b2 - b1 ≤ 0       0.125
-a2 + a2b1 + a2b3 + a3b1 - a3b3 - b1 ≤ 0      0.125
```

A two-dimensional graphical representation of all inequalities (cf. Figure 3) can be generated for example by

```
In[11]:= PlotInequalities[h, {x, 0, π},
           {{0, x, 4π/3}, {0, x, 4π/3}}, P];
```

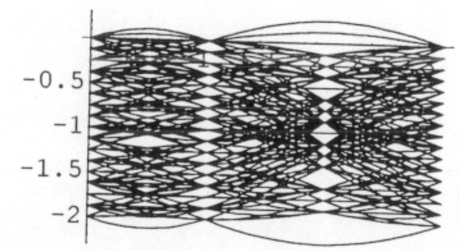

Figure 3

A very similar procedure involving `TruthTable[3,2]` yields all Boole-Bell inequalities for the three-particle and two measurement directions (Greenberger-Horne-Zeilinger) case.

4 Summary

In summary we have implemented a systematic method to compute all optimal Boole-Bell type inequalities satisfied by classical probabilities, given a physical setup. By optimal we mean that there is no condition such as equality or inequality which is satisfied by classical probabilities and which is a less stringent bound thereof. We have used this method to compute well known as well as new types of bounds on probabilities in configurations relevant to quantum physics. We believe that this represents a powerful new tool for the investigation of the nonclassical features of quantum mechanics.

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Reversible Computation and a Toolkit for Quantum Turing Machine Simulation

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1 Abstract

This talk begins with some background information on reversible computation from a Thermodynamics and Quantum Theory point of view, and then introduces a Mathematica® Package *Quantum Turing Machine Simulator* (QTS) that can serve as an educational tool to explore the principles of a reversible computational process within the context of Quantum Mechanics.

2 Reversible Computation

The computational process has long been an interesting and challenging subject of basic research in Mathematics, Physics and Computer Sciences, see [2]. One of the fundamental insights is that Information is indeed *physical* [1,4] and therefore subject to the basic laws of Physics. Well known milestones of that research are Landauer's [3] entropy counting argument that erasure of information decreases the entropy of a system by $k \log 2$ per bit and Bennett's [5] proof, that every computational irreversible process can be re-designed as a reversible one. Turning to Quantum Mechanics, we recognize that the physical laws are reversible in time [7]. Following Deutsch's [6] architecture of a Quantum Turing Machine (QTM) , the machine state advances in time according to $\psi(t) = U(t)\, \psi(0)$, U(t) being the unitary operator acting on the Hilbert space of the machine. Typically, U(t) is given as $U(t) = e^{-iHt}$ with H being the Hamiltonian of the system. For our purposes we are interested in the properties of H as they relate to the computational process. A computational process can be described as a sequence q0,q1,... of steps , and to each such process a linear, bounded operator T ("step operator") can be associated. In general, the step operator T is not associated with a finite time interval; instead T is linked to an infinitesimal time step. According to Feynman [8] one can construct a time-independent Hamiltonian H(T) from the step operator T by H(T) := K(2-T-T*). (Here, T* is the adjoint of T.) H(T) is a generator of a unitary time evolution $U(t) = e^{-iH(T)t}$. Benoff [9] proved, that iff T is *distinct path generating* (dpg) [9],

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