mathscape — Combining Mathematica and TeX

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Preliminaries

Millions of mathematical formulas are typeset annually. Most of the numbers we see in print are produced by computer. So are the indexes and catalogs issued by database publishers. Charts and diagrams and other products of computer graphics have replaced manually drafted copy. But most of the formulas in mathematics, engineering and science publications are still derived and coded by hand.

The `TeXForm` function in Release 2 of Mathematica [1], and some more extensive resources in Release 3 [2], provide a bridge between symbolic computation and computer composition. The author's mathscape system was designed to strengthen the bridge. Written in Release 2 of Mathematica, it is in ongoing use by the author, and it has produced several hundred typeset pages of heavily mathematical material already. It subsumes work reported previously as `bilo` and `forTeX` [3]. It produces a document from a control file containing:

- statements that Mathematica evaluates for inclusion in the output,
- formatting information and other statements to be executed silently, flagged by the `#` symbol,
- text coded in LaTeX, with each record flagged with an `*`, or in a `text` environment between `# beginText` and `# endText` markers.

Then, within a Mathematica session, the mathscape package is loaded, and the mathscape statement `autorecord[`*controlFileName*`]`:

- makes Mathematica read the control file and convert its contents to the LaTeX coded representation of the document that is being created,
- invokes LaTeX to convert this to a `dvi` file,
- invokes a preview program, and
- prints the typeset product if requested.

In this way, the document can be crafted interactively. Graphics can be incorporated with ease.

The system was started to meet some major needs of research publication. The production of problem sets and worked examples for teaching has been addressed extensively. So has the production of tables of formulas for reference. A tutorial introduction to mathscape and a systematic review are available [4].

The production of the following boxed output illustrates the control file conventions.

$$y^2 - x^2$$

is converted by `Factor` to:

$$(y - x)(y + x)$$

Here, formatting is needed to override the default arrangement $-x^2 + y^2$ and $(-x + y)(x + y)$ imposed by Mathematica. mathscape converts the immediate result v of a Mathematica evaluation to `prep[`v`]`. `prep` is initialized to `Identity` and reassigned dynamically, in the present case to a function that reverses every `Plus`. The portion of the input that produced the contents of the preceding box is:

```
# prep = toEach[Plus][reverse]
s = y^2 - x^2
* is converted by \verb|Factor| to:
s // Factor
```

mathscape supports a large open-ended class of functions, typified by `toEach[Plus]`, that "target" particular portions of an expression. This can be identified by head, e.g., `toEach[Plus]`, `toEach[log]`, as a Mathematica pattern e.g., `toThe[_Integer+_]`, by part name, e.g., `toTheLhs`, `toTheNumerator` or, as in `to[Plus][containing[x], outermost]`, by head and criterion, or by pattern and criterion.

Playing through to TeX

mathscape passes elementary algebraic expressions to the Mathematica `TeXForm` function for conversion to corresponding TeX code. Greek letters, the names of all the special symbols in the TeX vocabulary and some other unparameterized objects, e.g., `strut`, are denoted by the TeX control sequence names without the `\`. The names of binary operators (e.g., `oplus`) are given appropriate mathematical properties, too. Function expressions are used for parameterized objects, e.g., `hat[x]`, `rule[`*rise*`]` `[`*width*, *height*`]`, `overbrace[`*tag*`][`*expr*`]` that map into TeX codes in just a few simple ways.

Other names can be used in the body of a calculation and then changed to the TeX names by replacement rules assigned to `prep`. The statement `newSymbol[`v`]` makes `mathscape` append v to the list of identifiers for unparameterized TeX codes. Symbols can be appended to the lists of other control sequence names by further functions that write the definitions to the output.

The built-in Mathematica names and the lowercase names, e.g., `Cos`, `cos`, for the typographically "cos-like" functions are converted to TeX sequences that provide the conventional omission/inclusion of parentheses and placement of exponent, as in:

`cos[x], cos[x]^2, cos[x+y]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $\cos x\,,\quad \cos^2 x\,,\quad \cos(x+y)$

(We use the $\rhd\!\!\!\Longrightarrow$ and $\overset{resp}{\rhd\!\!\!\Longrightarrow}$ symbols between single or multiple verbatimized input expressions and the typeset products.) In the output, parentheses are put around the arguments of functions that do not have special typographic status. Thus:

`f[x], g[u,v]` $\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $f(x),\ \ g(u,v)$

Special bracketing is illustrated by:

`enbr[x], f[enbr[x]]` $\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $[x],\ \ f[x]$

`enpr[enpr[x]], f[ompr[x]]` $\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $((x)),\ \ fx$

`ensp["|", ">"][x, y]` $\rhd\!\!\!\Longrightarrow$ $|x,\ \ y>$

`sapr[x/y]` $\rhd\!\!\!\Longrightarrow$ $\left(\dfrac{x}{y}\right)$

Further `en` and `sa` functions provide other fixed-size and self-adjusting bracketing symbols. Typically, these are introduced after the body of a symbolic computation by targetting expressions in `prep`.

The infix treatment of binary operators, relationship symbols and arrows in the output, is shown by:

`otimes[x, oplus[u,v,w]]` $\rhd\!\!\!\Longrightarrow$ $x \otimes (u \oplus v \oplus w)$
`ll[a,b,c]` $\rhd\!\!\!\Longrightarrow$ $a \ll b \ll c$
`not[prec][u,v]` $\rhd\!\!\!\Longrightarrow$ $u \not\prec v$
`rightarrow[a,b,c]` $\rhd\!\!\!\Longrightarrow$ $a \to b \to c$
`arrowoo[u,v]` $\rhd\!\!\!\Longrightarrow$ $u \rhd\!\!\!\Longrightarrow v$

The conventions for single and multiple subscripts and superscripts, on the right and/or left of a symbol are illustrated by:

`x@sub@1, x@sup@enpr[m@sub@1], P@subsup[n, m]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $x_1,\ \ x^{(m_1)},\ \ P_n^m$

`x@subscriptSequence[a,b]` $\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $x_{a,b}$

`E@lsub@r, E@lsubsup[r, epsilon]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ ${}_rE,\quad {}_r^{\epsilon}E$

The conventions for decorations, ties, rules and composites are illustrated by:

`hat@x, breve@Psi, widetilde@enpr[tilde@A]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $\hat{x},\ \ \breve{\Psi},\ \ \widetilde{(\tilde{A})}$

`underline[x+underline[y]]` $\rhd\!\!\!\Longrightarrow$ $\underline{x+\underline{y}}$

`f[u] + overbrace["time\ dependent"][`
`g[t,u] + g[t,w]]`

$\rhd\!\!\!\Longrightarrow$ $f(u) + \overbrace{g(t,u) + g(t,w)}^{time\ dependent}$

`rule[5pt][30pt, 1pt]` $\rhd\!\!\!\Longrightarrow$ $\rule[5pt]{30pt}{1pt}$

`atop[a, b], above[1pt][a, b]` $\overset{resp}{\rhd\!\!\!\Longrightarrow}$ ${a \atop b},\ \ \dfrac{a}{b}$

`stackrel[F, "="], ddrel[arrowcc, a, b]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $\stackrel{F}{=},\ \ \overset{a}{\underset{b}{\rhd\!\!\rhd}}$

`overlay[vee, wedge]` $\rhd\!\!\!\Longrightarrow$ $\vee\!\!\!\!\wedge$

The effects of some simple catenation functions are shown by:

`sequence[a, b, c, d]` $\rhd\!\!\!\Longrightarrow$ $a,\ \ b,\ \ c,\ \ d$

`catenation[X, scriptscriptstyle[path], Y]`

$\rhd\!\!\!\Longrightarrow$ $X{\scriptscriptstyle path}Y$

`markedCatenation[cdots][a, b, c]`

$\rhd\!\!\!\Longrightarrow$ $a \cdots b \cdots c$

Fonts styles and sizes are specified by TeX names. Also, `sizedFont[1]`, ... alias `tiny`, ... Thus,

`rm[a b^2], bf[a b^2], sansSerif[a b^2]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $\mathrm{ab}^2,\ \ \mathbf{ab^2},\ \ \mathsf{ab}^2$

`boldmath[a b^2], boldmath[cal[ABCD]]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $\boldsymbol{ab^2},\ \ \boldsymbol{\mathcal{ABCD}}$

`tiny[a b], sizedFont[3][a b]`

$\overset{resp}{\rhd\!\!\!\Longrightarrow}$ $\text{\tiny a b},\ \ ab$

`mathscape` uses TeX primitives in the basic alignment process, too. Every display is built using `hbox`, `vbox`, `hboxTo`, `vboxTo`, `hspace`, `vspace`, `newlength`, `addtowidth`, `newbox`, `phantom`, `setbox`, `copy`, `wd`, `ht`, `dp`, and related constructs that translate directly to TeX or to local macros.

Varying the style

Alternative notations often exist for the same mathematical expression. mathscape lets the user change these freely. Thus, logical expressions are set in $\&|\neg$ notation by default. The assignment `logicStyle=2` changes this to the $\wedge \vee -$ notation. `logicStyle=1` restores the default.

Square roots introduce a more general tactic. Following the action of `prep`, `sqrt[`z`]` is converted to `style[sqrt, defaultSqrtStyle][`z`]`. Initially, the style parameter is 1, giving the radical notation $\sqrt{z}$. Changing it to 2 and 3 give $z^{1/2}$ and $z^{\frac{1}{2}}$ respectively. In general, `useStyle[`n`]` converts f`[`z`]` to `style[`f, n`][`z`]`. It is used to mix styles within a single expression, as in the production of:

$$(1 - \sqrt{\delta})^{1/2}$$

from

```
# prep = to[sqrt][1][useStyle[2]]
sqrt[1 - sqrt[delta]]
```

Fractions are built up, with the numerator and denominator of just the outermost fractions in the `displaystyle` mode, when `defaultFractionStyle` is 1. Style 2 puts all the numerators and denominators in `displaystyle`. Styles 3 and 4 give shilling and reciprocal notations. Styles 1.1, 1.2, …, and 2.1, 2.2, … strengthen the fraction bar and lengthen the shilling slash. For powers, style 2 gives radical notation, e.g., $\sqrt[3]{x}$, when the exponent is a fraction.

Representations

We represent derivatives, integrals, matrices, sums and many other composite mathematical objects in a way that facilitates mechanical operations and allows flexible styling in the typeset output. The handling of partial derivatives, shown next, is typical.

```
D$[x][y], D$[x, 2][y], D$[x,y,z][phi]
```

$$\overset{resp}{\longrightarrow} \quad \frac{\partial y}{\partial x}, \quad \frac{\partial^2 y}{\partial x^2}, \quad \frac{\partial^3 \phi}{\partial x \partial y \partial z}$$

mathscape contains extensive suites of procedures to manipulate expressions represented by "compound heads", such as `D$[x]`, `Dt$[x]` (for a total derivative), `sum[i, j, k]`, `integral[x, 0, infinity]`, and `matrix[m,n,M,N]`. Style is controlled by the `setOptions[D$, placement -> subscript]` statement and its counterparts. These create intermediate `style[...][...]` expressions, that for the current `D$` example, leads to subscript placement of the variables of differentiation, as in $\phi_{x,y,z}$.

Environments

By default, mathscape centers the typeset Mathematica statements in a field that is `widthForMath` wide. The commands `alignLeft`, `alignRight` and `alignCenter` are put in `#` statements to change the alignment. `leftIndent` and `rightIndent` control the indentions. The `displayBoth` command produces verbatimized input and conventionally styled output. `pairHorizontally` makes the output run-on, and `pairVertically` makes it start a new line. The commands `displayInput` and `displayOutput` display just the input and output, respectively. The input can be modified before evaluation and/or before display, by actions that the user specifies.

Within an `alignOnEvalSym` environment, begun and ended by appropriate `begin`… and `end`… statements, all the displays, containing input and output are aligned on the $\triangleright\!\!\!\Rightarrow$ and $\overset{resp}{\longrightarrow}$ symbols. The arrows are placed at the middle of the print region, by default. This is overridden by assigning a value to `inputField`.

Consecutive tags are created in the `tagging` environment. By default, these are parenthesized undivided Arabic numerals, i.e., (1), (2), …. In general, the tag consists of the left marker, `tagPrefix`, `tagSeparator`, `tagNumber`, and the right marker. `tagStyle`, e.g., `letter`, `roman`, `Letter`, determines the style of the sequence number. The markers are combined in `tagMarker`. `tagDown` uses the present prefix, separator and tag number to prefix the subordinate sequence numbers that start again at 1. `tagUp` restores all the tagging parameters in force before tagging down. `tagSide` defaults to `right`, and can be reassigned to `left`.

The `alignOnEqual` environment aligns on the first `=` symbol in the concomitant displays. These may be separated by text. The left and right fields have equal width by default. This is overridden by assignment to `leftWidth`. The environment is an alias for `alignOnRelSym`, which treats all the relationship symbols and `Infix` operators as equivalent.

The `aligningItems` environment is used in:

```
# beginAligningItems; itemWidth = 25pt;
  leftIndent = sequenceGap = 0pt;
  itemsPerLine = 6; itemAlignment = right;
  bar = rule[10pt, 0.2pt]
* Fill in the blanks, in this list:
Table[Prime[Prime[n]], {n, 12}] //
 ReplacePart[#, bar, {{1},{2},{6},{9}}]&
* and in this:
{14, 34, bar, 59, bar, 125}
# endAligningItems;
```

This produced:

Fill in the blanks, in this list:

__	__	11	17	31	__
59	67	__	109	127	157

and in this:

14	34	__	59	__	125

The runOnGroup and tabbedRunOnGroup environments can be used in a variety of ways. The following simple example

$$\sum_i s_i \qquad \sum_{i=j}^{k} s_i \qquad \prod_{i=j}^{k} s_i$$

$$\begin{pmatrix} 1 & 2 \\ 4 & 5 \end{pmatrix} \qquad \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

is produced by

```
# beginRunOnGroup; runOnStyle = compressed;
  continuationSymbol = "";
sum[i][s@sub@i]
sum[i,j,k][s@sub@i]
prod[i,j,k][s@sub@i]
# turnRunOnGroup
matrix[{1,2},{4,5}]
matrix[{1,2,3},{4,5,6}]
# endRunOnGroup;
```

In a runOnGroup, space between items on each line may be compressed or expanded. In runOnGroup and tabbedRunOnGroup, items may be tagged left or right, or untagged. Each group may be tagged left or right, or untagged, independent of item tagging. continuationSymbol defaults to ",". We set it to an arrow when successive items trace a reduction.

The next display shows another tracing tactic. pipe generalizes composition, so as to allow rules.

```
# newBinaryOperator[lplus, "+"];
  continuationSymbol = "rightArrow";
  s = lplus[a, times[b, c]];
  cm = toThe[times][Reverse];
  ca = toThe[lplus][Reverse];
  markWithAction;
  prep = pipe[toEach[_String][
   StringReplace[#,
    {"(cm)" -> "{\\cal C}_m",
    "(ca)" -> "{\\cal C}_a"}]&],
   List -> catenation]
s // pipeList[cm,ca]
```

$\rhd\!\!\!\rightarrow$

$$a + b \times c \xrightarrow{\mathcal{C}_m} a + c \times b \xrightarrow{\mathcal{C}_a} c \times b + a$$

texTab[*lcrString*][{*lineData*}] plays through to the tabular environment. hline and cline symbols and multicolumn heads are wrapped into the data, using prep, to form the *lineData* list.

The boxedPair environment creates TeX files consisting of the codes for verbatimized input and the fully processed output. By default, these are input to frameboxes joined by an $\rhd\!\!\!\rightarrow$. An option defers this to later input statements in the text.

The textExpansion and runOnMath environments embed evaluated results in the run-on text.

Interactive development

autorecord is recursive. A lengthy mathscape document is developed, typically, by writing separate control files for the successive parts, and invoking these from an overall control file. Optional arguments omit the xdvi step, convert to PostScript, invoke ghostview or xpsview, and print. The recursivity is used by boxedPair.

The bypass environment and autobreak function facilitate incremental testing. By conditionalizing the beginBypass and endBypass statements, different versions of a document, e.g., terse and detailed, can be produced from the same file. The silentExecution environment is used to set up variables and operators which are taken for granted in the printed exposition. The evaluation environment, in which work usually is conducted, is exited to allow the output of statements without execution.

The Mathematica graphics shell script psfix has been modified to omit boilerplate. New shell scripts wrap ghostscript and dvips to compensate.

Restructuring

The rearrangement and abbreviation of mathematical expressions is extremely important. reverse, used earlier, belongs to an extensible suite of procedures for these purposes. Several are used to form the next display from an equation that was saved in ordinary Mathematica style from a previous run. They all suspend Orderlessness of Plus and Times and encase the final result in HoldForm.

$$\begin{aligned}&\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}[4\epsilon m A_{l,\,m,\,n-1} L_l(u) L_{m-2}(v) - \\ &\quad 4\epsilon m^2 A_{l,\,m,\,n-1} L_l(u) L_{m-2}(v) + \\ &\quad << 361 terms >> - \\ &\quad 4(n+1)\epsilon m^2 A_{l,\,m,\,n+1} L_l(u) L_{m+2}(v)] \times \\ &\quad L_n(w) = 0\end{aligned}$$

This is produced by

```
# alignLeft; turnIndent = 1pc;
  prep =
   toTheLhs[
    to[Plus][outermost][
     showTerms[{1, 2, -1}]],
    toEach[_Integer + _][
     sortByAbsence[_Integer]],
    allowFurtherSorting,
   to[Times][outermost][
    splitBeforeFactor[2, times]],
   allowFurtherSorting,
   to[Plus][outermost][
    toTerms[containing[v]][
     sortByAbsence[v]],
    splitBeforeTerm[4,, "\\left."],
    splitBeforeTerm[3],
    splitBeforeTerm[2, "\\right."], sabr],
   disallowFurtherSorting,
   A[l_, m_, n_] ->
    A@subscriptSequence[l, m, n],
   L[n_, x_] -> L[sub[n]][x], e -> epsilon]
eqn[4.13]
```

The functions and rules in the arguments list of `toTheLhs` are executed consecutively, just like those of `pipe`. All the targetting functions act this way.

The two procedures `sortByAbsence[`$v_1, v_2, \ldots$`]` and `sortByPresence[`$v_1, v_2, \ldots$`]` meet many needs. These wrap `sortByCriteria` which works by selecting subsequences that satisfy the successive criteria instead of repeated swapping.

`splitBeforeTerm[`n`][`s`]` and the corresponding `After`, `Factor`, `Element` and `Equal` expressions can specify continuity symbols, e.g., $\times$, and codes to balance stretchable brackets.

The procedure `showTerms[{`*indices*`][`s`]` and the similar `Factors`, `Elements`, `Arguments` procedures are used for `Plus`, `sum`, `Times` and `prod` expressions, and lists, matrices and arbitrary functions. Optional arguments control the depiction of of omitted items.

`allowFurtherSorting` removes `Orderless`ness and any `HoldForm`s. `disallowFurtherSorting` imposes `HoldForm` and restores `Orderless`ness.

Numerous situations arise that can be handled by adapting the general principles used in the procedures of this section, e.g., forcing the expressions that Mathematica ordinarily returns as $-u - v$ and z^{1-m} into $-(u + v)$ and $1/z^{m-1}$.

Because ease of understanding is our objective, mathscape contains substantial suites of procedures for convenient cross referencing between statements, and for fine-tuned factoring, distribution and collection. Graphics provides a powerful supplement in many ways. The abstract shows a depiction of a class of sparse matrices, that occur in an electronic energy calculation. Zero and non-zero elements are displayed as spaces and dots, respectively. Symbolic computation, graphics and typesetting come together in the production of diagrams and the synthesis of text throughout scholarly publication.

Past, present, future

The production of readable copy from the numerically represented results of symbolic computation motivated some of the earliest work on electronic typesetting. Formulas, produced by simple array manipulation were converted mechanically to the code of a paper tape driven photo-mechanical typesetter, for work in theoretical chemistry and planetary theory [5].

mathscape, started about six years ago, has gone through a few name changes, but has not undergone any structural change in the last three years. Its application to a variety of material has highlighted the need for the resources it provides. By enabling the mechanical production of readable discourse, this kind of work gives a fresh incentive to the formal study of mathematical derivation.

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Appendix

The main account [5] of mathscape contains numerous examples produced in the `boxedPair` environment. The TEX files for a selection of these were reset separately, converted to PostScript, and `input` to construct this Appendix.

The helium calculation

This page shows a summary of an automated check and extension of Pekeris' classical calculation of the electronic structure of helium like atoms. An `autorun` session produced a detailed narrative of both the conventional mathematical activity and its mechanization. Intermediate results were written out for subsequent computational use. The summary was produced from these.

The calculation involved partial differential equations, changes of variable, infinite series expansion, special functions of mathematical physics, determinants, and multiple integrals. Part of the calculation carried expressions that run to hundreds of terms. At several points, lengthy equations were broken into sets of smaller equations of specified form, for display and manipulation, using further `mathscape` procedures.

Graphics was used to plot numerical results conventionally, and to display the structure of a matrix as mentioned earlier. Also, the published version of a very lengthy formula was scanned, the image dissected, and the pieces imported as pictures between the corresponding pieces of the newly calculated result, for visual comparison. Some are shown in [3, 4].

We begin with the Schrödinger equation for a 2-electron atom with nuclear charge Z.

$$\frac{\partial^2\psi}{\partial r_1^2}+\frac{2}{r_1}\frac{\partial\psi}{\partial r_1}+\frac{\partial^2\psi}{\partial r_2^2}+\frac{2}{r_2}\frac{\partial\psi}{\partial r_2}+2\frac{\partial^2\psi}{\partial r_{12}^2}+\frac{4}{r_{12}}\frac{\partial\psi}{\partial r_{12}}+\frac{r_1^2-r_2^2+r_{12}^2}{r_1 r_{12}}\frac{\partial^2\psi}{\partial r_1\partial r_{12}}+ \frac{r_2^2-r_1^2+r_{12}^2}{r_2 r_{12}}\frac{\partial^2\psi}{\partial r_2\partial r_{12}}+2(E+\frac{Z}{r_1}+\frac{Z}{r_2}-\frac{1}{r_{12}})\psi=0 \qquad (1)$$

This is in standard texts. It is converted to the perimetric coordinates (2) where $\epsilon=\sqrt{-E}$.

$$u=\epsilon(r_2-r_1+r_{12}),\qquad v=\epsilon(r_1-r_2+r_{12}),\qquad w=2\epsilon(r_1+r_2-r_{12}) \qquad (2)$$

We use the equation for $\partial(u,v,w)/\partial(r_1,r_2,r_{12})$ and the consequent equations for the $\partial^2/\partial r_1^2,\ldots$ in terms of the $\partial^2/\partial u^2$. Hence:

$$4\epsilon^2\left\{u(2uv+2v^2+2uw+2vw+w^2)\psi_{uu}+\ll 6 \text{ terms} \gg +2(2u^2+2v^2-w^2)\psi_w\right\}+ \left\{E(u+v)(2u+w)(2v+w)-2\epsilon(2u+w)(2v+w)+8\epsilon Z(u+v)(u+v+w)\right\}\psi=0 \qquad (3)$$

The wave function ψ is written as:

$$\psi=\mathrm{e}^{-(u+v+w)/2}F(u,v,w) \qquad (4)$$

Substitution in (3) gives an equation for F that is, in abbreviated form:

$$\{4Z(u+v)(u+v+w)-(2u+w)(2v+w)\}F+ 2\epsilon\left\{u(2uv+2v^2+2uw+2vw+w^2)F_{uu}+\ll 6 \text{ terms}\gg + (4u^2+4v^2-2u^2w-2v^2w-2w^2-uw^2-vw^2)F_w-2F(u+v)(u+v+w)\right\}=0 \qquad (5)$$

F is expanded as a triple series in Laguerre functions of u, v, w.

$$F=\sum_{\{l,m,n\}\geq 0} A_{l,m,n}L_l(u)L_m(v)L_n(w) \qquad (6)$$

Hence (8). The coefficient of each A contains Laguerre functions and their first two derivatives.

$$\sum_{\{l,m,n\}\geq 0}\left[-4\epsilon(u+v)(u+v+w)L_l(u)L_m(v)L_n(w)+\ll 8 \text{ terms}\gg + 4\epsilon w(2u^2+2v^2+uw+vw)L_l(u)L_m(v)L_n''(w)\right]A_{l,m,n}=0 \qquad (7)$$

Occurrences of $L_l(u)$ and its derivatives times u and u^2 are converted to terms in $L_{l+\lambda}(u), |\lambda|\leq 2$, using simple recurrence formulas. Terms containing v and w are treated correspondingly, giving a summand that contains (u,v,w) only as arguments of undifferentiated Laguerre functions.

$$\sum_{\{l,m,n\}\geq 0}\left[nL_l(u)L_m(v)L_{n-2}(w)+\ll 234 \text{ terms}\gg -4L_n(w)L_{l+1}(u)L_{m+1}(v)+ \ll 127 \text{ terms}\gg -n^2L_l(u)L_m(v)L_{n+2}(w)\right]A_{l,m,n}=0 \qquad (8)$$

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The coefficients of $L_{n+\nu}(w)$ are collected for each $v=-2,\ldots,2$. The summation is split into 5 parts corresponding to the different ν. These are re-indexed and combined, to give:

$$\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\left[4\epsilon mA_{l,m,n-1}L_l(u)L_{m-2}(v)-4\epsilon m^2A_{l,m,n-1}L_l(u)L_{m-2}(v)+ \ll 361 \text{ terms}\gg -4\epsilon m^2(n+1)A_{l,m,n+1}L_l(u)L_{m+2}(v)\right]L_n(w)=0 \qquad (10)$$

The dependences on v and u are treated similarly, to give:

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\left[4\epsilon lA_{l-2,m,n}+\ll 362 \text{ terms}\gg +4l^2ZA_{l+2,m,n}\right]L_l(u)L_m(v)L_n(w)=0 \qquad (11)$$

Orthogonality of the Laguerre functions gives a 33-term recurrence formula for the $A_{l,m,n}$.

$$4(l+1)(l+2)\{-Z+\epsilon(1+m+n)\}A_{l+2,m,n}+\ll 31 \text{ terms}\gg + 2mn\{1-2Z+\epsilon(2l+n+1)\}A_{l,m-1,n-1}=0 \qquad (12)$$

Let (l_j,m_j,n_j) be the j'th triple in the sequencing (12), where $w_j=l_j+m_j+n_j$ and $j<k$.

$$w_j\leq w_k;\qquad n_j\leq n_k \ \text{ if } \ w_j=w_k;\qquad l_j<l_k \ \text{ if } \ w_j=w_k \ \text{ and } \ n_j=n_k \qquad (13)$$

In symmetric states, $A_{l,m,n}=A_{m,l,n}$, so we write $B_k=A_{l_k,m_k,n_k}$, where $\{l_k,m_k,n_k\}$ is the kth triple in the sequence that also satisfies $l_k\leq m_k$. The restriction $l+m+n<=q$ gives the q'th approximation to wave function and energy. $q=1$ takes the first 10 A's in the sequence (12). These map into $B_1,\ldots,B_7$. The equations formed from (11) for these by setting the $B_k=0, k>7$ require the following determinant in $\xi=Z-\epsilon$ to be zero.

$$\begin{vmatrix} 5-16\xi & -4+4\xi & -6+28\xi & 1 & 2-4\xi & -8\xi & 2-4\xi \\ -4+4\xi & 15-48\xi+24Z & 2+8\xi-12Z & -12+16\xi-8Z & -10+60\xi-24Z & -8\xi+8Z & 0 \\ -6+28\xi & 2+8\xi-12Z & 26-144\xi+32Z & -4\xi+4Z & -12+16\xi & -12+104\xi-16Z & -14+72\xi-28Z \\ 1 & -12+16\xi-8Z & -4\xi+4Z & 31-96\xi+64Z & 4+20\xi-28Z & 0 & 0 \\ 2-4\xi & -10+60\xi-24Z & -12+16\xi & 4+20\xi-28Z & 54-336\xi+192Z & 4+32\xi-40Z & 2+4\xi-8Z \\ -8\xi & -8\xi+8Z & -12+104\xi-16Z & 0 & 4+32\xi-40Z & 34-320\xi+96Z & 8-24\xi+8Z \\ 2-4\xi & 0 & -14+72\xi-28Z & 0 & 2+4\xi-8Z & 8-24\xi+8Z & 25-208\xi+104Z \end{vmatrix} \qquad (14)$$

In terms of the normalizing factor $\mathcal{N}$, the first approximation to the wave function is:

$$\psi_1=\frac{\mathrm{e}^{-(u+v+w)/2}}{\mathcal{N}_1}\left[B_1L_0(u)L_0(v)L_0(w)+B_2L_0(u)L_0(v)L_1(w)+ B_3\{L_1(u)L_0(v)L_0(w)+L_0(u)L_1(v)L_0(w)\}+\ll 3 \text{ terms}\gg +B_7L_1(u)L_1(v)L_0(w)\right] \qquad (15)$$

Expansion of the determinant followed by some simple rearrangement leads to:

$$\xi=0.3125+\frac{1}{Z}(0.808039-7.07288\xi+14.0571\xi^2)+\ll 4 \text{ terms}\gg + \frac{1}{Z^6}(0.000735782+\ll 6 \text{ terms}\gg -100.288\xi^7) \qquad (16)$$

For helium, $Z=2$, and numerical solution gives $\xi=0.2961$ for the lowest root, whence ϵ. Given ϵ, the B_j are determined relative to an arbitrary scaling factor. B_1 is set to 1, and the equations that led to 13 are solved numerically. Hence:

$$B_1=1,\quad B_2=0.03859,\quad B_3=-0.04876,\quad B_4=0.002969,\quad \ldots \qquad (17)$$

We replace the Laguerre functions in (14) by explicit polynomials in (u,v,w), and replace these coordinates by $(r_1,r_2,r_{12}$, by reference to (1). Hence the wave function in the form:

$$\psi_1=\frac{\mathrm{e}^{\epsilon(-r_1-r_2)}}{\mathcal{N}_1}\left[d_1+d_2(r_1+r_2)+d_3(r_1^2+r_2^2)+d_4r_1r_2+r_{12}\{d_5+d_6(r_1+r_2)\}+d_7r_{12}^2\right] \qquad (18)$$

where the d_i are linear combinations of the Bs.

$$d_1=B_1+B_2+2B_3+B_4+2B_5+2B_6+B_7,\quad d_2=-2\epsilon(B_2+2B_4+2B_5),\quad \ldots \qquad (19)$$

The normalizing factor is found from the volume integral $\int\psi^2d\tau=1$, using:

$$\int f\ d\tau=\frac{\pi^2}{32\epsilon^6}\int_{u=0}^{\infty}\int_{v=0}^{\infty}\int_{w=0}^{\infty}(u+v)(2u+w)(2v+w)f\ du\ dv\ dw \qquad (20)$$

whence

$$\mathcal{N}_1=\frac{\pi}{2\epsilon^3}(4B_1^2-5B_1B_2+\ll 22 \text{ terms}\gg +52B_6B_7+55B_7^2)^{\frac{1}{2}} \qquad (21)$$

The radial density distribution is found from:

$$\rho(r_1)=8\pi^2\left(\int_{r_2=0}^{r_1}\int_{r_{12}=r_1-r_2}^{r_1+r_2}\psi^2r_1r_2r_{12}\ dr_2\ dr_{12}+\int_{r_2=r_1}^{\infty}\int_{r_{12}=r_2-r_1}^{r_1+r_2}\psi^2r_1r_2r_{12}\ dr_2\ dr_{12}\right) \qquad (22)$$

Some formulas for reference

Table 1. $S_q = \sum_{k=1}^{n} k^q$

q	S_q	q	S_q
1	$(n^2+n)/2$	2	$(2n^3+3n^2+n)/6$
3	$(n^4+2n^3+n^2)/4$	4	$(6n^5+15n^4+10n^3-n)/30$
5	$(2n^6+6n^5+5n^4-n^2)/12$	6	$(6n^7+21n^6+21n^5-7n^3+n)/42$
7	$(3n^8+12n^7+14n^6-7n^4+2n^2)/24$	8	$(10n^9+45n^8+60n^7-42n^5+20n^3-3n)/90$
9	$(2n^{10}+10n^9+15n^8-14n^6+10n^4-3n^2)/20$		
10	$(6n^{11}+33n^{10}+55n^9-66n^7+66n^5-33n^3+5n)/66$		

Problem sets and worked solutions

Fold this worksheet, factor the expressions and check your answers

1. $54n^2+3fn-77f^2$	__________	$(11f+9n)(6n-7f)$
2. $70m^2-83mu+18u^2$	__________	$(10m-9u)(7m-2u)$
3. $30i^2+59ip-56p^2$	__________	$(10i-7p)(3i+8p)$
4. $35p^2+34kp-33k^2$	__________	$(11k+7p)(5p-3k)$
⋮	⋮	⋮

Consider the thermal decomposition of a sample of H_2O_2. The temperature is 22° C. The pressure is 773 torr. The volume of gaseous product is 6.01 liter. Calculate the mass of the sample.

$$\textbf{Answer}: \text{moles of gas} = \frac{\text{pressure} \times \text{volume}}{\text{gas constant} \times \text{temperature Kelvin}} =$$

$$= \frac{(773\ \text{torr}) \times (6.01\ \text{liter})}{(62.36\ \text{liter torr/ deg mol}) \times (295\ \text{deg})} = 0.253\ \text{mol;}$$

$$\text{Hence}: \text{mass of sample} = \frac{\text{molecular mass} \times \text{number of moles of gas}}{\text{mole factor}} =$$

$$= \frac{(34\ \text{gm}) \times (0.253)}{(0.5)} = 17.2\ \text{gm.}$$

0.103 mol of $CaCO_3$ undergoes thermal decomposition. The pressure is 795 torr. The temperature is 24° C. Compute the volume of gaseous product.

$$\textbf{Answer}: \text{moles of gas} = \text{mole factor} \times \text{moles in sample} =$$

$$= (1) \times (0.103\ \text{mol}) = 0.103\ \text{mol;}$$

$$\text{Hence}: \text{volume} = \frac{\text{gas constant} \times \text{moles of gas} \times \text{temperature Kelvin}}{\text{pressure}} =$$

$$= \frac{(62.36\ \text{liter torr/ deg mol}) \times (0.103\ \text{mol}) \times (297\ \text{deg})}{(795\ \text{torr})} = 2.4\ \text{liter.}$$

This ruled table was produced in an experimental reconstruction of portions of the reference work commonly known by the names of the authors Gradshteyn and Ryzhik. The entire first section of indefinite algebraic integrals has been derived anew — many of the citations in the monograph are unhelpful or inaccessible. The process of mechanization provided several useful prototype derivations and new insights of wider application.

The factoring example, like many others in [5] was produced by working back from the solutions. These were formed by random choice of the letters used to name the variables. The coefficients also were random, within a limited range, and rejected if the expanded expression would contain coefficients outside a particular range.

The gas law example is part of a much larger set. The procedure accepted a sequence of n-tuples that specified the property to be found (*e.g.* pressure, number of moles), the compound undergoing decomposition, the units, the values of the given variables, within acceptable ranges, the sentence order, and certain words and phrases. This work is in direct line with an earlier project of the author sponsored by the NSF under their CAUSE initiative some years ago.

The envelope examples

• Example 1: Plot the family of lines $y = m^4 + 2mx$ and its envelope. The canonical and derivative equations are, respectively,

$$y - m^4 - 2mx = 0 \qquad (1.1) \qquad\qquad 2(2m^3 + x) = 0 \qquad (1.2)$$

The parametric form of the discriminant is

$$x = -2m^3 \qquad (1.3) \qquad\qquad y = -3m^4 \qquad (1.4)$$

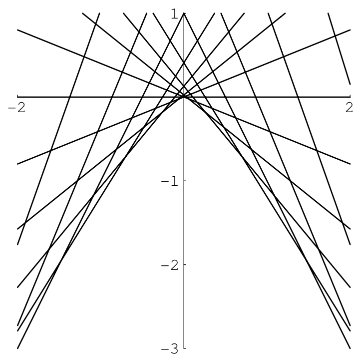


Figure 1a

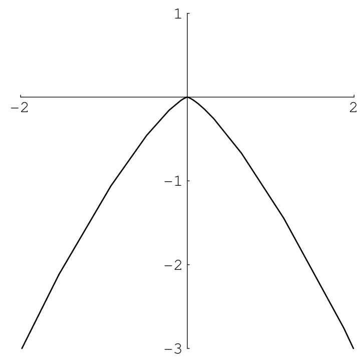


Figure 1b

The existence of an envelope is shown by inspection of

$$F_x = -2m,\ \ F_y = 1,\ \ F_{mx} = -2,\ \ F_{my} = 0 \qquad (1.5)$$

$$F_{mm} = -12m^2,\ \ \begin{vmatrix} F_x & F_y \\ F_{kx} & F_{ky} \end{vmatrix} = \begin{vmatrix} -2m & 1 \\ -2 & 0 \end{vmatrix} = 2 \qquad (1.6)$$

• Example 4: Plot the family of parabolas $y^2 = a(x - a)$ and its envelope. The canonical and derivative equations are, respectively,

$$a(a - x) + y^2 = 0 \qquad (4.1) \qquad\qquad -2a + x = 0 \qquad (4.2)$$

The direct form of the discriminant has the two solutions

$$y = -\frac{x}{2} \qquad (4.3a) \qquad\qquad y = \frac{x}{2} \qquad (4.3b)$$

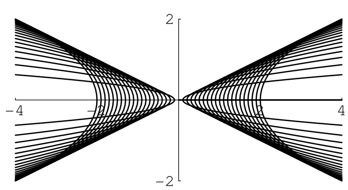


Figure 4a

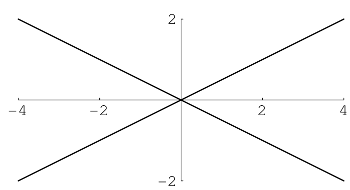


Figure 4b

The existence of an envelope is shown by inspection of

$$F_x = -a,\ \ F_y = 2y,\ \ F_{ax} = -1,\ \ F_{ay} = 0 \qquad (4.4)$$

$$F_{aa} = 2,\ \ \begin{vmatrix} F_x & F_y \\ F_{kx} & F_{ky} \end{vmatrix} = \begin{vmatrix} -a & 2y \\ -1 & 0 \end{vmatrix} = 2y \qquad (4.5)$$

Envelopes have long been of interest in popular mathematics and education. mathscape was used to produce graphically illustrated worked solutions to the exercises on this topic in a problem book that was widely used in the former Soviet Union. Each example begins with the generic equation for a family of curves. The problem is to determine whether the family has an envelope and, if it does, to find the equation and to plot it. The first step finds the "discriminant equation." Sometimes, this is best found in direct form, in other instances parametrically. It may have one or more solutions. Direct, implicit or parametric plotting may be optimal for the envelope.

The process was encapsulated in a single, heavily conditionalized control file. The data for each example consisted of the noun that identified the members of the family (e.g., "line", "curve"), the generic equation, and the choices needed to navigate the alternative paths.

The work was done by Artur v. Solecki, as an undergraduate project in a computer graphics course that the author taught.

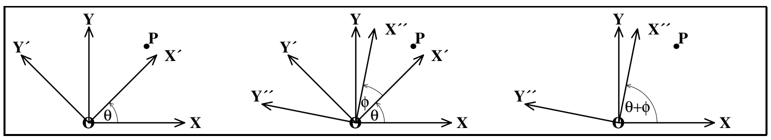
1. $$\begin{pmatrix}1&2\\3&4\end{pmatrix}\cdot\begin{pmatrix}5&6\\7&8\end{pmatrix}=\begin{pmatrix}\boxed{1\times5+2\times7}&\boxed{1\times6+2\times8}\\\boxed{3\times5+4\times7}&\boxed{3\times6+4\times8}\end{pmatrix}=\begin{pmatrix}19&22\\43&50\end{pmatrix}$$

2. $$\begin{pmatrix}3&4\\1&2\end{pmatrix}\cdot\begin{pmatrix}5&6\\7&8\end{pmatrix}=\begin{pmatrix}\boxed{3\times5+4\times7}&\boxed{3\times6+4\times8}\\\boxed{1\times5+2\times7}&\boxed{1\times6+2\times8}\end{pmatrix}=\begin{pmatrix}43&50\\19&22\end{pmatrix}$$

3. $$\begin{pmatrix}1&2\\3&4\end{pmatrix}\cdot\begin{pmatrix}6&5\\8&7\end{pmatrix}=\begin{pmatrix}\boxed{1\times6+2\times8}&\boxed{1\times5+2\times7}\\\boxed{3\times6+4\times8}&\boxed{3\times5+4\times7}\end{pmatrix}=\begin{pmatrix}22&19\\50&43\end{pmatrix}$$

4. $$\begin{pmatrix}5&7\\6&8\end{pmatrix}\cdot\begin{pmatrix}1&3\\2&4\end{pmatrix}=\begin{pmatrix}\boxed{5\times1+7\times2}&\boxed{5\times3+7\times4}\\\boxed{6\times1+8\times2}&\boxed{6\times3+8\times4}\end{pmatrix}=\begin{pmatrix}19&43\\22&50\end{pmatrix}$$

Compare the starting matrices and the results in examples 1 and 2.
Make the corresponding comparisons for examples 1 and 3, and for examples 1 and 4.



Rationalize the denominator in:

$$\frac{\sqrt{x-y}-\sqrt{x+y}}{\sqrt{x-y}+\sqrt{x+y}} \tag{1}$$

Multiply the numerator and the denominator by the numerator, and expand.

$$\frac{(\sqrt{x-y})^2-2\sqrt{x-y}\sqrt{x+y}+(\sqrt{x+y})^2}{(\sqrt{x-y})^2-(\sqrt{x+y})^2} \tag{2}$$

Use $(\sqrt{a})^2 = a$ and $\sqrt{a}\sqrt{b}=\sqrt{ab}$.

$$-\frac{2x-2\sqrt{(x-y)(x+y)}}{2y} \tag{3}$$

Simplify:

$$\frac{\sqrt{x^2-y^2}-x}{y} \tag{4}$$

Consider the geometric series:

$$S(n)=\sum_{i=0}^{n} x^i \tag{1}$$

Multiply throughout by x and restructure the right hand side.

$$xS(n)=\sum_{i=0}^{n} x^{i+1}=\sum_{i=1}^{n+1} x^i=\sum_{i=0}^{n} x^i+x^{n+1}-1 \tag{2}$$

Subtract (2) from (1).

$$S(n)-xS(n)=1-x^{n+1} \tag{3}$$

Solve for $S(n)$.

$$S(n)=\frac{1-x^{n+1}}{1-x} \tag{4}$$

This depiction of a matrix multiplication illustrates the use of fonts to show "where things come from" in a derivation. The entire set of four traced multiplications is parameterized on the eight starting matrix elements, enabling the rapid production of further examples of numerical and symbolic matrix operations. In teaching a course on mathematics for humanists some years ago, the author found it helpful to use worked examples of two-step linear transformations, expressed in terms of verbal matrix elements, e.g., the number of locomotives (coaches) per starter (advanced) train set, and the number of nuts (bolts) per locomotive (coach), and the corresponding product elements.

The axis diagrams are part of an explanation of rotation matrix multiplication, that uses symbolic calculation to generate the associated equations. Diagrams and associated matrix equations are used, too, in the connectivity matrix treatment of n-step path counts in a directed graph.

The next few examples illustrate different styles of discourse. The displays may be expressions or statements (in mathematical, not Mathematica, terminology). They may be joined by text or relationship symbols, such as = or >, or by arrows.

In the rationalization example, the identities embedded in the explanatory sentence are applied mechanically, as an example of the avoidance of possibly inconsistent results and narrative.

In the geometric series example, the referencing between equations also is performed mechanically by mention of the tag. This uses the implied rule formation feature of mathscape.

(1)	Definition : $A \subseteq B$ iff $x \in A$ implies $x \in B$.
(2)	Suppose $A \subseteq B$ and $B \subseteq C$.
(3)	Then $x \in A$ implies $x \in B$ and $x \in B$ implies $x \in C$.
(4)	Hence $x \in A$ implies $x \in C$.
(5)	Consequently $A \subseteq C$.

{1}	(1)	$A \Rightarrow B \vee C$	P
{2}	(2)	$B \Rightarrow -A$	P
{3}	(3)	$D \Rightarrow -C$	P
{4}	(4)	A	P
{1, 4}	(5)	$B \vee C$	*law of detachment*(4, 1)
{2, 4}	(6)	$-B$	*modus tollendo tollens extended*(4, 2)
{1, 2, 4}	(7)	C	*modus tollendo ponens*(6, 5)
{1, 2, 3, 4}	(8)	$-D$	*modus tollendo tollens extended*(7, 3)
{1, 2, 3, 4}	(9)	$A \Rightarrow -D$	*c.p.*(4, 8)

The successive examples of simple algebraic operations in the display below this paragraph were formed by a single assignment to `prep` followed by the pairs `{Expand, (1+x)^2}, ...`.

1. *Expand* : $(1+x)^2$. *Answer* : $1+2x+x^2$.
2. *Factor* : x^2-y^2. *Answer* : $(x-y)(x+y)$.
3. *Cancel* : $\dfrac{x^2+2xy+y^2}{x^2-y^2}$. *Answer* : $\dfrac{x+y}{x-y}$.

The production of the proof of transitivity of the $\subseteq$ operator (above left) involved the conversion of functional expressions to sentence form. Both this example and the logic proof (left) can serve as prototypes for quite large classes of application.

Alignment and tags: some more examples

Items can be labelled collectively and individually. The Legendre functions of degrees 0–3 of the first and second kinds follow.

5.7.1.	(a)	1	(b)	x
	(c)	$\frac{3x^2-1}{2}$	(d)	$\frac{5x^3-3x}{2}$
5.7.2.	(a)	$\frac{1}{2}\log\frac{1+x}{1-x}$	(b)	$-1+\frac{x}{2}\log\frac{1+x}{1-x}$
	(c)	$-\frac{3x}{2}+\frac{3x^2-1}{4}\log\frac{1+x}{1-x}$	(d)	$\frac{-15x^2+4}{6}+\frac{5x^3-3x}{4}\log\frac{1+x}{1-x}$

The outer horizontal lines are `itemWidth` long and the central line is `runOnGap` long.

$1+x$	(1)	$1+2x+x^2$	(2)
$1+3x+3x^2+x^3$	(3)	$1+4x+6x^2+4x^3+x^4$	(4)

The centering allows for the tags and the `runOnGap`.

Items can be labelled collectively:

(5.7.1)	$\int e^x x^2\,dx$	$\rightarrow$	$e^x x^2 - 2\int e^x x\,dx$	$\rightarrow$
	$e^x(-2x+x^2)+2\int e^x\,dx$	$\rightarrow$	$e^x(2-2x+x^2)$	
(5.7.2)	$\int \cos^2 x\ \,dx$	$\rightarrow$	$\frac{2x+\ \sin 2x}{4}$	

The examples on the left show grouped items tagged individually and/or collectively, and variations in the tag style. The examples below show multi-expression bracing, and alignment on single and multiple relationship symbols.

$$\left.\begin{aligned}(1+x)^2 &= 1+2x+x^2\\ (1-x)^2 &= 1-2x+x^2\\ (1-x)(1+x) &= 1-x^2\end{aligned}\right\}\quad (1)$$

$$\begin{aligned}(1+x)^2 &= 1+2x+x^2 && (1)\\ 2x^4 &\geq x^4 && (2)\\ 1 &< 2 && (3)\\ a+b &\hookrightarrow c+d && (4)\end{aligned}$$

For $x > 1$,

$$e^{x^2} \quad > \quad e^x \quad > \quad x \quad > \quad \log x$$

For $0 <= \theta <= \pi/2$,

$$0 \quad \leq \quad \sin^2\theta \quad \leq \quad \sin\theta$$