

On reducing overestimation of ranges of multinomials without splitting boxes

Ramon Moore

March 16, 2006

Consider the problem of computing the **range of values of a multinomial over a box** (interval vector) **of any size**, not necessarily small.

We often need to determine, for instance, whether the range of values over a given box does not contain zero, to lend certainty to order tests; to prove non-existence in connection with deleting sub-boxes; to test for infeasibility, etc. Another important application of multinomial range bounding occurs with Taylor model methods, which produce a multinomial expressions whose ranges contain components of exact solution values, at later times, to systems of nonlinear ODEs with initial values in some given box.

We consider here only **techniques** for reducing overestimation, **that do not involve box splitting**.

As shown more than 40 years ago, we can compute enclosures with arbitrarily small excess width (over-estimation) by subdividing boxes, and taking the union of the subranges. For a small number of variables, this works fine. For a large number of variables, it can be prohibitively slow, depending on how quickly one comes to a result that is of sufficient sharpness for whatever purpose the containment of the range is needed. The cross-over point, between adequately efficient and prohibitively slow, depends on computing power available, of course, but in this paper, we will not consider box splitting at all.

Similarly, the systematic examination of a box for local minima and maxima in the interior and on the faces can be slow for a large number of variables,

again depending, in any particular example, on how quickly one comes to a result that is of sufficient sharpness for whatever purpose the containment of the range is needed. We will consider techniques for improving the efficiency of monotonicity tests, because these can reduce the number of dimensions over which the range must be bounded. The techniques will be illustrated on an example throughout the paper, in order to make the basic ideas as clear as possible, without excessively cumbersome notation for the general case.

Hansen&Walster, Ratschek&Rokne and many others may have considered most, perhaps all, of the techniques discussed here, in one context or another, but here we focus on the single problem of computing intervals containing ranges of multinomials over boxes of arbitrary size. It seems worth reviewing available techniques for this central problem. The goal here is to see what we can do with simple tools to quickly achieve at least *some* reduction in overestimation. We will not consider such algebraic tools as Bernstein polynomials, nor the Buchberger algorithm for finding the Gröbner basis of a system of multinomials, because while these have interesting and important properties, they are not designed for efficiency, but are slow.

Let us consider, first, techniques that can be implemented for general multinomials (for use at compile time?), involving only **computer algebra and special interval functions for exact ranges of commonly occurring sub-expressions** in the given multinomial. Of course, we can make use throughout of the subdistributivity of interval arithmetic, and use nesting whenever it helps.

Consider the multinomial:

$$p(x, y, z) = 4 - x + 2y - 3z + 2x^2 - xy + y^2 + xz - 3yz - 2z^2 + xyz - x^3 + x^2z - yz^2 + y^3 + z^3$$

We want to find intervals containing the range of values, for all $(x, y, z) \in X = ([-1, 2], [0, 2], [-4, -3])$,

and to study simple ways of reducing over-estimation.

Scaling X to the unit cube $U = ([0, 1], [0, 1], [0, 1])$: (we can do this for any number of variables)

We can make a simple change of variables to transform the box $X = ([-1, 2], [0, 2], [-4, -3])$

to the unit cube $U = ([0, 1], [0, 1], [0, 1])$ via

$$x = -1 + u(2 - (-1)) = -1 + 3u$$

$$x = -1 + 3u$$

$$y = 2v$$

$$z = -4 + w$$

so that $(x, y, z) \in X = ([-1, 2], [0, 2], [-4, -3]) \Leftrightarrow (u, v, w) \in U = ([0, 1], [0, 1], [0, 1])$.

In terms of (u, v, w) , $p(x, y, z)$ becomes, after algebraic expansion to the form of a multinomial in u, v, w

$$\begin{aligned} p(x, y, z) = f(u, v, w) = & -76 - 12u + 6v + 61w + 9u^2 - 30vu - 3uw + 8v \\ & w - 14w^2 + 9u^2w - 2vw^2 \\ & + 4v^2 + 8v^3 + 6vuw - 27u^3 + w^3 \end{aligned}$$

Now we can separate the terms with positive coefficients from those with negative coefficients.

$$\begin{aligned} f(u, v, w) = & (6v + 61w + 9u^2 + 8vw + 9u^2w + 4v^2 + 8v^3 + 6vuw + w^3) \\ & - (76 + 12u + 30vu + 3uw + 14w^2 + 2vw^2 + 27u^3) \end{aligned}$$

Now for $(x, y, z) \in X \Leftrightarrow (u, v, w) \in U$, we will can enclose the range of values by simply summing the

positive and negative coefficients, which will be faster than doing the interval evaluation. We find that

$$f(u, v, w) \in [-(76 + 12 + 30 + 3 + 14 + 2 + 27), (6 + 61 + 9 + 8 + 9 + 4 + 8 + 6 + 1) - 76] = [-164, 36].$$

Of course, in floating point, we would use upward rounding on each of the sums of positive numbers, in general, to maintain containment.

We can narrow the interval of containment using special formulas for exact ranges of commonly occurring sub-expressions.

We can rewrite $f(u, v, w)$ in various ways, such as

$$f(u, v, w) = -76 + (-12 + (9 - 27u)u)u + (61 - (14 - w)w - (3 - 9u)u)w + (6 + (8 - 2w)w + 4v + 8v^2 + (6w - 30)u)v$$

With each of the variables ranging over $[0, 1]$, **the ranges of subexpressions involving only positive or only negative coefficients can be found exactly.** For example $4v + 8v^2 = [0, 12]$ for $v \in [0, 1]$.

We can also find exact ranges for certain kinds of subexpressions involving changes of sign in coefficients.

In particular, consider a **quadratic** expression of the form

$$q(u) = au - bu^2 = (a - bu)u, \text{ for positive } a \text{ and } b.$$

We have $q'(u) = 0$ at $u = \frac{a}{2b}$, so q is monotonic increasing from $u = 0$ until $q(u)$ reaches its maximum value

$$q\left(\frac{a}{2b}\right) = \frac{1}{4} \frac{a^2}{b} \text{ at } u = \frac{a}{2b}, \text{ after which it is monotonic decreasing. More precisely,}$$

$q(u) = (a - bu)u$, for positive a and b has the range of values, for all $u \in [0, 1]$ given by (three cases):

$$1) \text{ for } a < b, \text{ we have } (a - bu)u \in [a - b, \frac{1}{4} \frac{a^2}{b}]$$

$$2) \text{ for } b \leq a \leq 2b, \text{ we have } (a - bu)u \in [0, \frac{1}{4} \frac{a^2}{b}]$$

$$3) \text{ for } a > 2b, \text{ we have } (a - bu)u \in [0, a - b].$$

In all three cases, the interval **enclosures** obtained from the formulas above **are narrower** than the direct evaluation of $(a - b[0, 1])[0, 1]$. Here are examples of comparisons in each case:

$$1) \text{ For } a = 2, b = 8 \text{ we have } [a - b, \frac{1}{4} \frac{a^2}{b}] = [-6, 0.125] \text{ vs. } (a - b[0, 1])[0, 1] = [a - b, a] = [-6, 2]$$

$$2) \text{ For } a = 6, b = 4, \text{ we have } [0, \frac{1}{4} \frac{a^2}{b}] = [0, 2.25] \text{ vs. } (a - b[0, 1])[0, 1] = [0, a] = [0, 6]$$

$$3) \text{ For } a = 8, b = 2, \text{ we have } [0, a - b] = [0, 6] \text{ vs. } (a - b[0, 1])[0, 1] = [0, a] = [0, 8]$$

Note that in case 1), $a - b$ is negative, while in case 3) $a - b$ is positive.

Thus, in the above expression for $f(u, v, w)$, we can find ranges of values of the quadratic sub-expressions as follows. For all $(x, y, z) \in X \Leftrightarrow (u, v, w) \in U$, we have

$$(9 - 27u)u \in [-18, 0.75]$$

$$(14 - w)w \in [0, 13]$$

$$(3 - 9u)u \in [-6, 0.25]$$

$$(8 - 2w)w \in [0, 6]$$

and so

$$\begin{aligned} f(u, v, w) = & -76 + (-12 + (9 - 27u)u)u + (61 - (14 - w)w - (3 - 9u)u)w + \\ & + (6 + (8 - 2w)w + 4v + 8v^2 + (6w - 30)u)v \end{aligned}$$

is contained in the interval

$$\begin{aligned} f(u, v, w) \in & -76 + (-12 + [-18, 0.75])[0, 1] + (61 - [0, 13] - [-6, 0.25])[0, 1] \\ & + (6 + [0, 6] + 4[0, 1] + 8[0, 1] + (6[0, 1] - 30)[0, 1])[0, 1] \\ = & -76 + [-30, 0] + [0, 66] + [-24, 24] = [-\mathbf{130}, \mathbf{14}] \end{aligned}$$

This is less than the width of the enclosure $[-\mathbf{164}, \mathbf{36}]$ obtained above using the form

$$\begin{aligned} f(u, v, w) = & (6v + 61w + 9u^2 + 8vw + 9u^2w + 4v^2 + 8v^3 + 6vuw + w^3) \\ & - (76 + 12u + 30vu + 3uw + 14w^2 + 2vw^2 + 27u^3). \end{aligned}$$

Scaling U to the symmetric box $S = ([-0.5, 0.5], [-0.5, 0.5], [-0.5, 0.5])$

Symmetric intervals simplify interval multiplication. For any interval $[a, b]$, we have

$$[a, b][-c, c] = c \max(|a|, |b|)[-1, 1].$$

This can speed up evaluation of multinomials over symmetric boxes.

Let's expand $f(u, v, w)$ about the midpoint $(1/2, 1/2, 1/2)$ of U , and define the symmetric box S by

$$S = ([-0.5, 0.5], [-0.5, 0.5], [-0.5, 0.5]).$$

We have

$$f\left(\frac{1}{2} + u, \frac{1}{2} + v, \frac{1}{2} + w\right) = -\frac{445}{8} - \frac{135}{4}u - 27u^2 - 27u^3 + 53w - \frac{27}{2}w^2 + w^3 + 9uw + 9u^2w + 9wv - 2w^2v + 6v + 16v^2 + 8v^3 - 27uv + 6uvw$$

$$\text{Rename this, for convenience, } g(u, v, w) = f\left(\frac{1}{2} + u, \frac{1}{2} + v, \frac{1}{2} + w\right)$$

We have, after algebraic expansion into the standard form of a multinomial (sums of products of powers of the variables),

$$g(u, v, w) = -\frac{445}{8} - \frac{135}{4}u - 27u^2 - 27u^3 + 53w - \frac{27}{2}w^2 + w^3 + 9uw + 9u^2w + 9wv - 2w^2v + 6v + 16v^2 + 8v^3 - 27uv + 6uvw$$

We now have a third equivalent formulation of the problem of finding the range of values. We have

$$\{p(x, y, z) \in X\} \Leftrightarrow \{f(u, v, w) \in U\} \Leftrightarrow \{g(u, v, w) \in S\}.$$

For the symmetric interval $[-0.5, 0.5] = 0.5[-1, 1]$, we have, of course,

$$[-0.5, 0.5]^k = \begin{cases} (0.5)^k [0, 1] & \text{for } k \text{ even} \\ (0.5)^k [-1, 1] & \text{for } k \text{ odd} \end{cases}$$

since, in general, we define $[a, b]^k = \{t^k : t \in [a, b]\}$.

Of course, the range of a product of two *independent* variables uw is not the same as the square function, so for $u, w \in [-0.5, 0.5]$, we have $uw \in [-0.5, 0.5][0.5, 0.5] = (0.5)^2[-1, 1] = \{uw : u, w \in [-0.5, 0.5]\}$

Thus, we can compute another enclosure by evaluating the above expression with interval arithmetic, substituting the symmetric interval $[-0.5, 0.5]$ for u, v and w .

$$\begin{aligned} g(u, v, w) &= -\frac{445}{8} - \frac{135}{4}u - 27u^2 - 27u^3 + 53w - \frac{27}{2}w^2 + w^3 + 9uw + 9u^2w + 9wv - 2w^2v + 6v + 16v^2 + 8v^3 - 27uv + 6uvw \\ &\in -\frac{445}{8} + \left(\frac{135}{4}(0.5) + 27(0.5)^3 + 53(0.5) + (0.5)^3 + 9(0.5)^2 + 9(0.5)^3 + 9(0.5)^2 \right. \\ &\quad \left. + 2(0.5)^3 + 6(0.5) + 8(0.5)^3 + 27(0.5)^2 + 6(0.5)^3\right)[-1, 1] + (-27)(0.5)^2[0, 1] - \\ &\quad \frac{27}{2}(0.5)^2[0, 1] + 16(0.5)^2[0, 1] \end{aligned}$$

$$= -55.625 + 64.25[-1, 1] + [-27/4 - 27/8, 4] = [-126.625, 12.625]$$

This is slightly narrower than what we had before, $[-126.625, 12.625] \subset [-130, 14]$.

We can find exact ranges for monotonic sub-expressions.

For example, in

$$g(u, v, w) = -\frac{445}{8} - \frac{135}{4}u - 27u^2 - 27u^3 + 53w - \frac{27}{2}w^2 + w^3 + 9uw + 9u^2w + 9wv - 2w^2v + 6v + 16v^2 + 8v^3 - 27uv + 6uvw$$

we may have some monotonic sub-expressions. Thus is easy to check for polynomial subexpressions in a single variable.

First there is

$$h(w) = (53w - \frac{27}{2}w^2 + w^3) \uparrow \text{ for } w \in [-0.5, 0.5],$$

since $h'(w) = 53 - 27w + 3w^2 \in 53 + (3/4 + 27/2)[-1, 1] = [38.75, 67.25] > 0$ for $w \in [-0.5, 0.5]$.

$$\text{So } h(w) \in [h(-0.5), h(0.5)] = [-30.0, 23.25].$$

Then there is

$$k(u) = (-\frac{135}{4}u - 27u^2 - 27u^3) \downarrow \text{ (since } k'(u) = -\frac{135}{4} - 54u - 81u^2 < 0 \text{ for } u \in [-0.5, 0.5],$$

because it has its max at $k''(u) = -54 - 162u = 0$, i.e., at $u = -54/162 = 1/3$ and $k'(1/3) = -\frac{243}{4} < 0$)

$$\text{So } k(u) \in [k(0.5), k(-0.5)] = [-27.0, 13.5].$$

Next is the interesting subexpression

$$m(v) = 6v + 16v^2 + 8v^3 = 2v(2v + 3)(2v + 1)$$

It is not monotonic, but we can find its exact range of values anyway.

$$m'(v) = 6 + 32v + 24v^2 = 0 \text{ at } v = -0.2257.. \in [-0.5, 0.5],$$

where we have $m(-0.2257...) = -0.63113...$

which is the minimum value of $m(v)$ in $[-0.5, 0.5]$.

We have $m(v) \in [-0.631\ 2, m(0.5)] = [-0.631\ 2, 8.0]$.

With these observations, we can compute another interval containing the range of values.

More generally, if we find sub-expressions in a single variable, even as multiplicative factors when grouping terms, we can find, in principle, sharp ranges of their values. In practise, the overestimation for these can be made very small with not much computing. We can have a sub-program (like a macro) defining the range of values of some simple sub-expressions (quadratics, cubics?, etc.) in terms of the coefficients in the sub-expression and the input box.

For $(u, v, w) \in ([-0.5, 0.5], [-0.5, 0.5], [-0.5, 0.5])$, we have, using the above bounds for sub-expressions,

$$\begin{aligned} g(u, v, w) &\in -\frac{445}{8} + [-27.0, 13.5] + [-30.0, 23.25] + [-0.631\ 130\ 31, 8.0] \\ &+ 13.375[-1, 1] = [-\frac{445}{8} - 27 - 30 - 0.63113031 - 13.375, -\frac{445}{8} + 13.5 + 23.25 + \\ &8 + 13.375] \\ &= [-126.631\ 130\ 31, 2.5] \end{aligned}$$

We can intersect this with the previous containing interval to get

$$[-126.625, 12.625] \cap [-126.631\ 130\ 31, 2.5] = [-126.625, 2.5]$$

Let's see if more work can narrow this interval further. It is not hard to differentiate multinomials, so we will look at the gradient of $g(u, v, w) = -\frac{445}{8} - \frac{135}{4}u - 27u^2 - 27u^3 + 53w - \frac{27}{2}w^2 + w^3 + 9uw + 9u^2w + 9wv - 2w^2v + 6v + 16v^2 + 8v^3 - 27uv + 6uvw$

Computer algebra in Scientific Workplace (using Maple tools) finds

$$D_u g(u, v, w) = -\frac{135}{4} - 54u - 81u^2 + 9w + 18uw - 27v + 6wv$$

$$D_v g(u, v, w) = 9w - 2w^2 + 6 + 32v + 24v^2 - 27u + 6uw$$

$$D_w g(u, v, w) = 53 - 27w + 3w^2 + 9u + 9u^2 + 9v - 4wv + 6uv$$

We can verify by direct interval evaluation that

$$D_w g(u, v, w) > 0 \text{ in } S = \{(u, v, w) \in ([-0.5, 0.5], [-0.5, 0.5], [-0.5, 0.5])\}$$

In fact

$$\begin{aligned} D_w g(u, v, w) &\in 53 - 27[-0.5, 0.5] + 3[-0.5, 0.5]^2 + 9[-0.5, 0.5] + 9[-0.5, 0.5]^2 + \\ &9[-0.5, 0.5] \\ &- 4[-0.5, 0.5][-0.5, 0.5] + 6[-0.5, 0.5][-0.5, 0.5] \\ &= 53 + 25[-1, 1] + [0, 3] = [28, 81] > 0. \end{aligned}$$

It follows that the min of g in S is on the face $w = -0.5$ and the max is on $w = 0.5$.

So we have the following two sub-problems

1) Find the maximum value of $g(u, v, w)$ in S by finding the max of

$$g(u, v, 0.5) = -32.375 - 29.25u - 22.5u^2 - 27u^3 + 10.0v + 16v^2 + 8v^3 - 24.0uv$$

for $(u, v) = ([-0.5, 0.5], [-0.5, 0.5])$.

2) Find the min of g in S by finding the min of

$$g(u, v, -0.5) = -85.625 - 38.25u - 31.5u^2 - 27u^3 + 1.0v + 16v^2 + 8v^3 - 30.0uv$$

for $(u, v) = ([-0.5, 0.5], [-0.5, 0.5])$.

For this and other applications involving quadratics, the following interval-valued function may be helpful. We will come back to the example above in more detail, later.

For the general quadratic with real coefficients, $q(x, a, b, c) = ax^2 + bx + c$, $a > 0$, we have

$$D_x q(x, a, b, c) = 2ax + b = 0 \text{ at } x = -\frac{b}{2a}, \text{ where } q\left(-\frac{b}{2a}, a, b, c\right) = -\frac{1}{4a}b^2 + c.$$

We can write down a general formula for the range of values of $q(x, a, b, c) = ax^2 + bx + c$, $a > 0$

for all x in any interval $X = [\underline{X}, \overline{X}]$.

We construct the interval-valued function

$$Q(X, a, b, c) = \{q(x, a, b, c) = ax^2 + bx + c : a > 0 \text{ and } x \in X = [\underline{X}, \overline{X}]\}.$$

It is easy to see that, if we first define $q(x, a, b, c) = ax^2 + bx + c$, then

$$Q(\underline{X}, \overline{X}, a, b, c) = \begin{cases} [q(\underline{X}, a, b, c), q(\overline{X}, a, b, c)] & \text{if } -\frac{b}{2a} \leq \underline{X} \\ [-\frac{1}{4a}b^2 + c, \max(q(\underline{X}, a, b, c), q(\overline{X}, a, b, c))] & \text{if } \underline{X} < -\frac{b}{2a} \leq \overline{X} \\ [q(\overline{X}, a, b, c), q(\underline{X}, a, b, c)] & \text{if } \overline{X} < -\frac{b}{2a} \end{cases}$$

We can construct other such general interval-valued functions for giving ranges of values of other types of factors commonly occurring in multinomial expressions.

We can also directly determine ranges of values of single variable polynomial sub-expressions over interval components of boxes, using standard interval methods for such problems (interval Newton, e.g.).

Let us now go back to the example at hand, let us proceed using some of the approaches just discussed.

Problem 1) Find the maximum value of $g(u, v, w)$ in S by finding the max of

$$g(u, v, 0.5) = -32.375 - 29.25u - 22.5u^2 - 27u^3 + 10.0v + 16v^2 + 8v^3 - 24.0uv$$

Recall that $[-0.5, 0.5]^2 = [0, 0.25]$ whereas $[-0.5, 0.5][0.5, 0.5] = [-0.25, 0.25]$.

By direct interval evaluation of $g(u, v, 0.5)$ we find that

$$\begin{aligned} g(u, v, 0.5) \in & -32.375 - 29.25[-0.5, 0.5] - 22.5[-0.5, 0.5]^2 - 27[-0.5, 0.5]^3 \\ & + 10.0[-0.5, 0.5] + 16[-0.5, 0.5]^2 + 8[-0.5, 0.5]^3 - 24.0[-0.5, 0.5][0.5, 0.5] = \\ & [-68, 1.625] \end{aligned}$$

So the max is no greater than 1.625.

We might be able to find a lower upper bound, if it is not already exact, by sharply bounding the ranges of the single variable subexpressions indicated in parentheses in the following expression

$$g(u, v, 0.5) = -32.375 - (29.25u - 22.5u^2 - 27u^3) + (10.0v + 16v^2 + 8v^3) - 24.0uv$$

We want to find the ranges of $r(u) = 29.25u - 22.5u^2 - 27u^3$ and $s(v) = 10.0v + 16v^2 + 8v^3$.

For $r(u) = 29.25u - 22.5u^2 - 27u^3$, we have $r'(u) = 29.25 - 45.0u - 81.0u^2$ has a root in $[-0.5, 0.5]$,

namely at $u = 0.38424307154516583078\dots$,

where $r(0.38424307154516583078) = 6.3854193599022579948$.

Also we find that $r''(u) = -45.0 - 162.0u < 0$ for $u > -\frac{5}{18} = 0.2777777\dots$

So we have $r(u) \in [\min(r(-\frac{5}{18}), r(0.5)), 6.38542] \cup \{r(u) : u \in [-0.5, \frac{5}{18}]\}$

Now $\min(r(-\frac{5}{18}), r(0.5)) = -9.2824074074074074$, so

$r(u) \in [-9.282408, 6.38542] \cup \{r(u) : u \in [-0.5, -\frac{5}{18}]\}$.

By direct interval evaluation, for $u \in [-0.5, -\frac{5}{18}]$, using the nested form

$r(u) = u(29.25 + u(-22.5 + u(-27)))$, we find that $\{r(u) : u \in [-0.5, -\frac{5}{18}]\} \subset [-18.375, -8.8194]$

so $r(u) \in [-9.282408, 6.38542] \cup [-18.375, -8.8194] = [-18.375, 6.38542]$

Next we find an interval, as narrow as possible with this approach, containing the range of $s(v) = 10.0v + 16v^2 + 8v^3$ for all $v \in [-0.5, 0.5]$.

We find that $s'(v) = 10.0 + 32.0v + 24.0v^2 \geq 0$ for all $v \in [-0.5, 0.5]$,

so $s(v) \in [s(-0.5), s(0.5)] = [-2.0, 10.0]$

Thus we have

$g(u, v, 0.5) \in -32.375 - [-18.375, 6.38542] + [-2.0, 10.0] - 24[-0.5, 0.5][-0.5, 0.5]$

so $g(u, v, 0.5) \in [-33.98958, 2.0]$,

and so the maximum value of $g(u, v, w)$ in S is no greater than 2.0. But this is not an improvement over the the upper bound we already found above, namely 1.625

Problem 2) Find the minimum value of $g(u, v, w)$ in S , by finding the min of $g(u, v, -0.5)$.

Let's bound the ranges of the sub-expressions in parentheses for

$$g(u, v, -0.5) = -85.625 - (38.25u + 31.5u^2 + 27u^3) + (v + 16v^2 + 8v^3) - 30.0uv$$

We want to find the ranges of $(38.25u + 31.5u^2 + 27u^3)$ and $(1.0v + 16v^2 + 8v^3)$ for $u, v \in [-0.5, 0.5]$.

For $r(u) = 38.25u + 31.5u^2 + 27u^3$, we find that $r'(u) = 38.25 + 63.0u + 81.0u^2$

$$r'(u) = 38.25 + 63.0u + 81.0u^2 = 38.25 + 63.0u + 81.0u^2 > 38.25 - \frac{63^2}{4(81)} = 26 > 0$$

so the cubic is monotone increasing and has the range $[r(-0.5), r(0.5)] = [-14.625, 30.375]$

For $s(v) = v + 16v^2 + 8v^3$, we have $s'(v) = 1 + 32v + 24v^2$, and $s''(v) = 32 + 48v$

so for $v \in [-0.5, 0.5]$, we have $s''(v) = 32 + 48v > 0$ and $s(v)$ is convex, with a minimum value at

the root of $s'(v)$ in $[-0.5, 0.5]$, namely at $v = -0.03201890784467430953\dots$

where $s(-0.03201890784467430953) > -1.58782 \times 10^{-2}$.

We find that for $v \in [-0.5, 0.5]$, we have

$$s(v) = v + 16v^2 + 8v^3 \in [-1.58782 \times 10^{-2}, \max(s(-0.5), s(0.5))] = [-0.015879, 5.5]$$

Using these results, we find that

$$g(u, v, -0.5) \in -85.625 - [-14.625, 30.375] + [-0.015879, 5.5] - 30.0[-0.5, 0.5][-0.5, 0.5]$$

so

$$g(u, v, -0.5) \in [-123.515879, -58.0]$$

and the minimum value of $g(u, v, w)$ on S is no smaller than -123.515879 .

Thus, we have found that $g(u, v, w) \in [-123.515879, 1.625]$ for all $(u, v, w) \in S$.

Our previous best, without quite so much calculation, was $g(u, v, w) \in [-126.625, 2.5]$.

The crudest estimate using only direct interval evaluation yielded $g(u, v, w) \in [-164, 112]$.

For the example treated, the various methods produced these results, so far.

| <i>computed</i> | remarks |
|---------------------|--|
| $[-164, 36]$ | easiest, but crudest method |
| $[-126.625, 1.625]$ | more work, much better result |
| $[-123.52, 1.625]$ | still more work, only slight improvement |

Let's try to find a sharper upper bound, for $(u, v) \in ([-0.5, 0.5], [-0.5, 0.5])$, of

$$g(u, v, 0.5) = -32.375 - 29.25u - 22.5u^2 - 27.0u^3 + 10.0v + 16.0v^2 + 8.0v^3 - 24.0uv$$

with still more analysis.

Lets pick out at the sub-expression

$z(u, v) = 16v^2 - 24uv - 22.5u^2$ in two variables. Computer algebra finds

$$D_u z(u, v) = -24.0v - 45.0u$$

$$D_v z(u, v) = 32.0v - 24.0u$$

The zero gradient vector occurs only at $(u, v) = (0, 0)$ where

$\partial^2 z(u, v)/\partial u^2 = -45 < 0$ and $\partial^2 z(u, v)/\partial v^2 = 32 > 0$ so $(0, 0)$ is a saddle point, and $z(u, v)$ has no local minima in the interior of S .

The max must lie on the boundary of $(u, v) \in ([-0.5, 0.5], [-0.5, 0.5])$. There are four edges.

1) $u \in [-0.5, 0.5]$ and $v = -0.5$.

On this edge, $z(u, -0.5) = 4.0 + 12u - 22.5u^2$ and $D_u z(u, -0.5) = 12 - 45u$,
and $\partial^2 z(u, -0.5)/\partial u^2 = -45 < 0$

so $z(u, -0.5)$ has its max at $u = 4/15$ with $z(4/15, -\frac{1}{2}) = 4 + 12(4/15) - (45/2)(4/15)^2 = \frac{28}{5} = 5.6$

2) $u \in [-0.5, 0.5]$ and $v = 0.5$

On this edge, $z(u, 0.5) = 4.0 - 12u - 22.5u^2$ and $D_u z(u, \frac{1}{2}) = -12 - 45u$
and $\partial^2 z(u, 0.5)/\partial u^2 = -45 < 0$

so $z(u, 0.5)$ has its max at $u = -4/15$ and $z(-4/15, \frac{1}{2}) = 5.6$ as before.

3) $u = -0.5$ and $v \in [-0.5, 0.5]$

On this edge, $z(-0.5, v) = 16v^2 + 12.0v - 5.625$ and $D_v z(-0.5, v) = 32.0v + 12.0$

and $\partial^2 z(-0.5, v)/\partial v^2 = 32 > 0$, so $z(-0.5, v)$ has its max at one of the corners.

We have $z(-0.5, -0.5) = -7.625$, and $z(-0.5, 0.5) = 4.375$, so max is 4.375

4) $u = 0.5$ and $v \in [-0.5, 0.5]$

On this edge, $z(0.5, v) = 16v^2 - 12.0v - 5.625$ and $D_v z(0.5, v) = 32.0v - 12.0$
and $\partial^2 z(0.5, v)/\partial v^2 = 32 > 0$, so $z(0.5, v)$ has its max at one of the corners.

We have $z(0.5, -0.5) = 4.375$, and $z(0.5, 0.5) = -7.625$, so max is 4.375.

Thus, we have found the maximum value of the sub-expression $z(u, v) = 16v^2 - 24uv - 22.5u^2$

for all $(u, v) \in ([-0.5, 0.5], [-0.5, 0.5])$.

We could define another interval valued function which finds a tight enclosure of the exact range of a quadratic form in two variables over a two-dimensional box. This could be another useful "macro".

Here we have $\max z(u, v) = 5.6$ at the points $(u, v) = (\frac{4}{15}, -\frac{1}{2})$ and $(-\frac{4}{15}, \frac{1}{2})$.

Using that, let's re-examine

$$g(u, v, 0.5) = -32.375 + (-29.25u - 27.0u^3) + (10.0v + 8.0v^3) + z(u, v)$$

Furthermore, let's find the exact max values of $(-29.25u - 27.0u^3)$ and $(10.0v + 8.0v^3)$

for all $u, v \in S$.

$D_u(-29.25u - 27.0u^3) = -29.25 - 81.0u^2 < 0$ in S , so $(-29.25u - 27.0u^3)$ is monotone decreasing,

and therefore the maximum value is at $u = -0.5$. $\text{Max}(-29.25u - 27.0u^3) = 29.25/2 + 27/8 = 18.0$

$D_v(10.0v + 8.0v^3) = 10.0 + 24.0v^2 > 0$ in S , so $\text{Max}(10.0v + 8.0v^3) = 6$.

Therefore, the maximum value of

$$g(u, v, 0.5) = -32.375 + (-29.25u - 27.0u^3) + (10.0v + 8.0v^3) + z(u, v)$$

in S is $\text{Max} g(u, v, 0.5) = -8.375 + \max z(u, v) = -8.375 + 5.6 = -2.775$.

That is, an improved upper bound on the range of values of $g(u, v, 0.5)$, and hence of

$g(u, v, w)$ in S , is -2.775 . We will not bother further with the lower bound, but instead conclude here with a list of results for the *upperbound*.

| <i>computed</i> | <i>best</i> | <i>excess ></i> | remarks |
|-----------------|-------------|--------------------|---|
| 36 | -2.775 | 38.775 | easiest, but crudest method |
| 1.625 | -2.775 | 4.4 | a bit more work, much better result |
| 1.625 | -2.775 | 4.4 | still more work, no further improvement |
| -2.775 | -2.775 | ? | much more work, |

best found

If we could teach the computer this much algebra and elementary calculus, then it could do the same as we have done with this example and on other

examples of multinomials. It is conceivable that could be done. By "teach the computer", I mean, of course, incorporate the various elementary steps used here, but in more general form. Without subdividing, it is difficult, at best to find sharp bounds on ranges of values of multinomials. Probably the best general approach would be to use the best available global optimization software. Of course, such software would, itself, benefit from efficient evaluation of ranges of values.