

GMBE Derivation

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1 Definitions

Let:

- \mathbb{S} be a set of finite cardinality
- s be an element of \mathbb{S} .
- $\mathbb{F}^{(m)}$ be a (ordered) family of sets over \mathbb{S} with cardinality m .
- f_i be the i -th element of $\mathbb{F}^{(m)}$.
- $\mathcal{P}(\mathbb{X})$ be the powerset of the set \mathbb{X} .
- f be a function which takes a set \mathbb{X} and maps it to a scalar, $f(\mathbb{X})$.

2 Problem Descriptions

Ultimately we would like to compute $f(\mathcal{P}(\mathbb{S}))$; however, the computational cost of computing $f(\mathcal{P}(\mathbb{S}))$ scales exponentially with N . Instead we propose a series of systematic approximations to $f(\mathcal{P}(\mathbb{S}))$.

In the first order approximation we divide \mathbb{S} into m subsets such that:

$$\mathcal{P}(\mathbb{S}) \approx \bigcup_{f_i \in \mathbb{F}^{(m)}} \mathcal{P}(f_i). \quad (1)$$

Of note we do not assume that the various f_i are disjoint. Using the inclusion-exclusion principle (IEP), we can approximate $f(\mathcal{P}(\mathbb{S}))$ via:

$$\begin{aligned} f(\mathcal{P}(\mathbb{S})) \approx & \sum_{i=1}^m f(\mathcal{P}(f_i)) - \sum_{i=1}^{m-1} \sum_{j=i+1}^m f(\mathcal{P}(f_i \cap f_j)) + \cdots \\ & + (-1)^{m-1} f(\mathcal{P}(f_1 \cap f_2 \cap \cdots \cap f_m)), \end{aligned} \quad (2)$$

where $f_i \cap f_j$ is the intersection of sets f_i and f_j . For brevity, and because there is a one-to-one mapping between a set \mathbb{X} and its powerset, we define a new function g such that:

$$g(\mathbb{X}) \equiv f(\mathcal{P}(\mathbb{X})). \quad (3)$$

In terms of g , our first order approximation, $g^{(1,m)}(\mathbb{S})$, becomes:

$$g^{(1,m)}(\mathbb{S}) = \sum_{i=1}^m g(f_i) - \sum_{i=1}^{m-1} \sum_{j=i+1}^m g(f_i \cap f_j) + \dots \\ + (-1)^{m-1} g(f_1 \cap f_2 \cap \dots \cap f_m). \quad (4)$$

As a second order approximation to $\mathcal{P}(\mathbb{S})$ we take all pairwise unions of the initial m subsets:

$$\mathcal{P}(\mathbb{S}) \approx \bigcup_{i=1}^{m-1} \bigcup_{j=i+1}^m \mathcal{P}(f_i \cup f_j). \quad (5)$$

Like f_i and f_j individually, each of the various $f_i \cup f_j$ are subsets of \mathbb{S} as well. Thus the various $f_i \cup f_j$ also form a family of sets over \mathbb{S} ; we define the ordered family of sets generated from pairs of elements of $\mathbb{F}^{(m)}$ to be $\mathbb{F}^{(2,m)}$, and we define $f_i^{(2,m)}$ to be the i -th element of $\mathbb{F}^{(2,m)}$. With these definitions the second order approximation to $\mathcal{P}(\mathbb{S})$ can be written more compactly as:

$$\mathcal{P}(\mathbb{S}) \approx \bigcup_{f_i^{(2,m)} \in \mathbb{F}^{(2,m)}} \mathcal{P}(f_i^{(2,m)}). \quad (6)$$

Using the IEP the second order approximation to $g(\mathbb{S})$, $g^{(2,m)}(\mathbb{S})$, is:

$$g^{(2,m)}(\mathbb{S}) = \sum_{f_i^{(2,m)} \in \mathbb{F}^{(2,m)}} g(f_i^{(2,m)}) - \sum_{f_i^{(2,m)} \in \mathbb{F}^{(2,m)}} \sum_{f_j^{(2,m)} \in \mathbb{F}^{(2,m)} \setminus f_i^{(2,m)}} g(f_i^{(2,m)} \cap f_j^{(2,m)}) + \dots \\ + (-1)^{|\mathbb{F}^{(2,m)}|-1} g\left(f_1^{(2,m)} \cap f_2^{(2,m)} \cap \dots \cap f_{|\mathbb{F}^{(2,m)}|}^{(2,m)}\right), \quad (7)$$

where $|\mathbb{F}^{(2,m)}|$ is the cardinality of $\mathbb{F}^{(2,m)}$ (which because the sets are possibly non-disjoint may be less than m choose 2) and $\mathbb{F}^{(2,m)} \setminus f_i^{(2,m)}$ is $\mathbb{F}^{(2,m)}$ without $f_i^{(2,m)}$. In order to write this more compactly we realize that the various intersections are also subsets of \mathbb{S} . The intersections involving combinations of j elements of $\mathbb{F}^{(2,m)}$ form a family of sets over \mathbb{S} which we define as $\mathcal{I}^{(2,m,j)}$. We define $f_i^{(2,m,j)}$ as the i -th member of $\mathcal{I}^{(2,m,j)}$. With these definitions $g^{(2,m)}(\mathbb{S})$ becomes:

$$g^{(2,m)}(\mathbb{S}) = \sum_{j=1}^{|\mathbb{F}^{(2)}|} \sum_{f_i^{(2,m,j)} \in \mathcal{I}^{(2,m,j)}} (-1)^{j-1} g(f_i^{(2,m,j)}) \quad (8)$$

The above readily generalizes to an ℓ -order approximation to $\mathcal{P}(\mathbb{S})$:

$$\mathcal{P}(\mathbb{S}) \approx \bigcup_{f_i^{(\ell,m)} \in \mathbb{F}^{(\ell,m)}} \mathcal{P}(f_i^{(\ell,m)}). \quad (9)$$

and using the IEP we may write the ℓ -order approximation to $g(\mathbb{S})$, $g^{(\ell,m)}(\mathbb{S})$, as:

$$g^{(\ell,m)}(\mathbb{S}) = \sum_{j=1}^{|\mathbb{F}^{(\ell)}|} \sum_{f_i^{(\ell,m,j)} \in \mathcal{I}^{(\ell,m,j)}} (-1)^{j-1} g(f_i^{(\ell,m,j)}). \quad (10)$$

As written this equation express the ℓ -order approximation in terms of subsets of $\mathcal{I}^{(\ell,m,j)}$. The subsets in $\mathcal{I}^{(\ell,m,j)}$ are intersections formed from elements of sets $\mathbb{F}^{(\ell,m)}$. The elements of $\mathbb{F}^{(\ell,m)}$ are themselves unions of elements from the family of sets $\mathbb{F}^{(1,m)}$. Hence if we flatten the nested families of sets we end up with subsets of \mathbb{S} where each subset can be written as intersections of unions of the elements from $\mathbb{F}^{(1,m)}$. Since intersection distributes over union it should be possible to rewrite $g^{(\ell,m)}(\mathbb{S})$ in terms of unions of intersections of elements from $\mathbb{F}^{(1,m)}$. Inverting this relationship is the first problem.

In practice we actually prefer to write $g^{(\ell,m)}(\mathbb{S})$ as:

$$g^{(\ell,m)}(\mathbb{S}) = g^{(1,m)}(\mathbb{S}) + \left(g^{(2,m)}(\mathbb{S}) - g^{(1,m)}(\mathbb{S}) \right) + \dots + \left(g^{(\ell,m)}(\mathbb{S}) - g^{(\ell-1,m)}(\mathbb{S}) \right), \quad (11)$$

which projects $g^{(\ell,m)}(\mathbb{S})$ into:

- the first order approximation,
- corrections stemming from the second order approximation,
- corrections from the third-order through $(\ell - 1)$ -order approximations (the ellided terms), and
- the corrections that come from the ℓ order approximation.

In this form, $g^{(\ell,m)}(\mathbb{S})$ is written in terms of subsets from not only $\mathcal{I}^{(\ell,m,j)}$, but also using subsets from all of the families of sets $\mathcal{I}^{(k,m,j)}$ with k in the range $[1, \ell]$. Writing $g^{(\ell,m)}(\mathbb{S})$ in this form, but using the inverted relationships from solving problem one, is the second problem.

3 Problem One

Our overall strategy is deduce the general form of $g^{(\ell,m)}(\mathbb{S})$, by first determining the general form for select ℓ values. Writing the order-one approximation in terms of the elements of $\mathbb{F}^{(1,m)}$ is trivial (it is just Eq. 4). The first non-trivial order is $\ell = 2$.

3.1 $\ell = 2$

To deduce the general form for $\ell = 2$ we systematically consider increasing values of m . For $m = 1$, there is no $\ell = 2$ term, and $m = 2$ has a trivial $\ell = 2$ term:

$$g^{(2,2)}(\mathbb{S}) = g(f_1 \cup f_2). \quad (12)$$

Hence the first non-trivial m is $m = 3$.

For $m = 3$ we have:

$$g^{(2,3)}(\mathbb{S}) = g(f_{12}) + g(f_{13}) + g(f_{23}) - g(f_{12} \cap f_{13}) - g(f_{12} \cap f_{23}) - g(f_{13} \cap f_{23}) + g(f_{12} \cap f_{13} \cap f_{23}), \quad (13)$$

where we have further simplified the notation by defining:

$$f_{ijk\dots} \equiv f_i \cup f_j \cup f_k \cup \dots \quad (14)$$

Noting that:

$$(a \cup b) \cap (a \cup c) = a \cup (b \cap c) \quad (15)$$

and that:

$$\begin{aligned}
(a \cup b) \cap (a \cup c) \cap (b \cup c) &= (a \cup (b \cap c)) \cap (b \cup c) \\
&= (a \cap (b \cup c)) \cup ((b \cap c) \cap (b \cup c)) \\
&= (a \cap b) \cup (a \cap c) \cup (b \cap c),
\end{aligned} \tag{16}$$

we can rewrite Eq. (13) as:

$$\begin{aligned}
g^{(2,3)}(\mathbb{S}) &= g^{(2,2)}(\mathbb{S}) + g(f_{13}) + g(f_{23}) - g(f_3 \cup s_{12}) - g(f_2 \cup s_{13}) - \\
&\quad g(f_2 \cup s_{23}) + g(s_{12} \cup s_{13} \cup s_{23})
\end{aligned} \tag{17}$$

where we have defined:

$$s_{ijk\dots} \equiv f_i \cap f_j \cap f_k \cap \dots \tag{18}$$

and identified the $m = 2$ approximation.

For $m = 4$ there are 63 terms. Stemming from the $\mathcal{I}^{(2,4,1)}$ family of sets are 6 trivial terms:

$$\begin{aligned}
\sum_{f_i^{(2,4,1)} \in \mathcal{I}^{(2,4,1)}} g\left(f_i^{(2,4,1)}\right) &= g(f_{12}) + g(f_{13}) + g(f_{23}) + g(f_{14}) + g(f_{24}) + g(f_{34}) \\
&= \sum_{f_i^{(2,3)} \in \mathbb{F}^{(2,3)}} g\left(f_i^{(2,3)}\right) + \sum_{f_i^{(2,4)} \in \mathbb{F}^{(2,4)} \setminus \mathbb{F}^{(2,3)}} g\left(f_i^{(2,4)}\right),
\end{aligned} \tag{19}$$

where in the second line we separated the six terms into the three that are common to the $\mathbb{F}^{(2,3)}$ family of sets and the three which are unique to the $\mathbb{F}^{(2,4)}$ family of sets.

Stemming from $\mathcal{I}^{(2,4,2)}$ are 15 terms:

$$\begin{aligned}
\sum_{f_i^{(2,4,2)} \in \mathcal{I}^{(2,4,2)}} g\left(f_i^{(2,4,2)}\right) &= g(f_{12} \cap f_{13}) + g(f_{12} \cap f_{23}) + g(f_{12} \cap f_{14}) + g(f_{12} \cap f_{24}) + \\
&\quad g(f_{12} \cap f_{34}) + g(f_{13} \cap f_{23}) + g(f_{13} \cap f_{14}) + g(f_{13} \cap f_{24}) + \\
&\quad g(f_{13} \cap f_{34}) + g(f_{23} \cap f_{14}) + g(f_{23} \cap f_{24}) + g(f_{23} \cap f_{34}) + \\
&\quad g(f_{14} \cap f_{24}) + g(f_{14} \cap f_{34}) + g(f_{24} \cap f_{34}),
\end{aligned} \tag{20}$$

which respectively simplify to:

$$\begin{aligned}
\sum_{f_i^{(2,4,2)} \in \mathcal{I}^{(2,4,2)}} g\left(f_i^{(2,4,2)}\right) &= g(f_1 \cup s_{23}) + g(f_2 \cup s_{13}) + g(f_1 \cup s_{24}) + g(f_2 \cup s_{14}) + \\
&\quad g(s_{13} \cup s_{23} \cup s_{14} \cup s_{24}) + g(f_3 \cup s_{12}) + g(f_1 \cup s_{34}) + \\
&\quad g(s_{12} \cup s_{23} \cup s_{14} \cup s_{34}) + g(f_3 \cup s_{14}) + g(s_{12} \cup s_{13} \cup s_{24} \cup s_{34}) + \\
&\quad g(f_2 \cup s_{34}) + g(f_3 \cup s_{24}) + g(f_4 \cup s_{12}) + g(f_4 \cup s_{13}) + g(f_4 \cup s_{23}),
\end{aligned} \tag{21}$$

where we have used:

$$\begin{aligned}
(a \cup b) \cap (c \cup d) &= (a \cap (c \cup d)) \cup (b \cap (c \cup d)) \\
&= (a \cap c) \cup (a \cap d) \cup (b \cap c) \cup (b \cap d)
\end{aligned} \tag{22}$$

Identifying the terms which were present for $\mathcal{I}^{(2,3,2)}$:

$$\begin{aligned} \sum_{f_i^{(2,4,2)} \in \mathcal{I}^{(2,4,2)}} g\left(f_i^{(2,4,2)}\right) &= \sum_{f_i^{(2,3,2)} \in \mathcal{I}^{(2,3,2)}} g\left(f_i^{(2,3,2)}\right) + g(f_1 \cup s_{24}) + g(f_2 \cup s_{14}) + \\ &g(s_{13} \cup s_{23} \cup s_{14} \cup s_{24}) + g(f_1 \cup s_{34}) + \\ &g(s_{12} \cup s_{23} \cup s_{14} \cup s_{34}) + g(f_3 \cup s_{14}) + g(s_{12} \cup s_{13} \cup s_{24} \cup s_{34}) + \\ &g(f_2 \cup s_{34}) + g(f_3 \cup s_{24}) + g(f_4 \cup s_{12}) + g(f_4 \cup s_{13}) + g(f_4 \cup s_{23}), \end{aligned} \quad (23)$$

Stemming from $\mathcal{I}^{(2,4,3)}$ are 20 terms:

$$\begin{aligned} \sum_{f_i^{(2,4,3)} \in \mathcal{I}^{(2,4,3)}} g\left(f_i^{(2,4,3)}\right) &= g(f_{12} \cap f_{13} \cap f_{23}) + g(f_{12} \cap f_{13} \cap f_{14}) + g(f_{12} \cap f_{13} \cap f_{24}) + \\ &g(f_{12} \cap f_{13} \cap f_{34}) + g(f_{12} \cap f_{23} \cap f_{14}) + g(f_{12} \cap f_{23} \cap f_{24}) + \\ &g(f_{12} \cap f_{23} \cap f_{34}) + g(f_{12} \cap f_{14} \cap f_{24}) + g(f_{12} \cap f_{14} \cap f_{34}) + \\ &g(f_{12} \cap f_{24} \cap f_{34}) + g(f_{13} \cap f_{23} \cap f_{14}) + g(f_{13} \cap f_{23} \cap f_{24}) + \\ &g(f_{13} \cap f_{23} \cap f_{34}) + g(f_{13} \cap f_{14} \cap f_{24}) + g(f_{13} \cap f_{14} \cap f_{34}) + \\ &g(f_{13} \cap f_{24} \cap f_{34}) + g(f_{23} \cap f_{14} \cap f_{24}) + g(f_{23} \cap f_{14} \cap f_{34}) + \\ &g(f_{23} \cap f_{24} \cap f_{34}) + g(f_{14} \cap f_{24} \cap f_{34}), \end{aligned} \quad (24)$$

which respectively simplify to:

$$\begin{aligned} \sum_{f_i^{(2,4,3)} \in \mathcal{I}^{(2,4,3)}} g\left(f_i^{(2,4,3)}\right) &= g(s_{12} \cup s_{13} \cup s_{23}) + g(f_1 \cup s_{234}) + g(s_{12} \cup s_{14} \cup s_{23}) + \\ &g(s_{13} \cup s_{14} \cup s_{23}) + g(s_{12} \cup s_{13} \cup s_{24}) + g(f_2 \cup s_{134}) + \\ &g(s_{13} \cup s_{23} \cup s_{24}) + g(s_{12} \cup s_{14} \cup s_{24}) + g(s_{13} \cup s_{14} \cup s_{24}) + \\ &g(s_{14} \cup s_{23} \cup s_{24}) + g(s_{12} \cup s_{13} \cup s_{34}) + g(s_{12} \cup s_{23} \cup s_{34}) + \\ &g(f_3 \cup s_{124}) + g(s_{12} \cup s_{14} \cup s_{34}) + g(s_{13} \cup s_{14} \cup s_{34}) + \\ &g(s_{14} \cup s_{23} \cup s_{34}) + g(s_{12} \cup s_{24} \cup s_{34}) + g(s_{13} \cup s_{24} \cup s_{34}) + \\ &g(s_{23} \cup s_{24} \cup s_{34}) + g(f_4 \cup s_{123}). \end{aligned} \quad (25)$$

Identifying the terms which stem from $\mathcal{I}^{(2,3,3)}$:

$$\begin{aligned} \sum_{f_i^{(2,4,3)} \in \mathcal{I}^{(2,4,3)}} g\left(f_i^{(2,4,3)}\right) &= \sum_{f_i^{(2,3,3)} \in \mathcal{I}^{(2,3,3)}} g\left(f_i^{(2,3,3)}\right) + g(f_1 \cup s_{234}) + g(s_{12} \cup s_{14} \cup s_{23}) + \\ &g(s_{13} \cup s_{14} \cup s_{23}) + g(s_{12} \cup s_{13} \cup s_{24}) + g(f_2 \cup s_{134}) + \\ &g(s_{13} \cup s_{23} \cup s_{24}) + g(s_{12} \cup s_{14} \cup s_{24}) + g(s_{13} \cup s_{14} \cup s_{24}) + \\ &g(s_{14} \cup s_{23} \cup s_{24}) + g(s_{12} \cup s_{13} \cup s_{34}) + g(s_{12} \cup s_{23} \cup s_{34}) + \\ &g(f_3 \cup s_{124}) + g(s_{12} \cup s_{14} \cup s_{34}) + g(s_{13} \cup s_{14} \cup s_{34}) + \\ &g(s_{14} \cup s_{23} \cup s_{34}) + g(s_{12} \cup s_{24} \cup s_{34}) + g(s_{13} \cup s_{24} \cup s_{34}) + \\ &g(s_{23} \cup s_{24} \cup s_{34}) + g(f_4 \cup s_{123}). \end{aligned} \quad (26)$$

At this point we have identified all terms which are also present in $g^{(2,3)}(\mathbb{S})$ and remaining terms are unique to $g^{(2,4)}(\mathbb{S})$.

Stemming from $\mathcal{I}^{(2,4,4)}$ are 15 terms:

$$\begin{aligned} \sum_{f_i^{(2,4,4)} \in \mathcal{I}^{(2,4,4)}} g\left(f_i^{(2,4,4)}\right) = & g(f_{12} \cap f_{13} \cap f_{23} \cap f_{14}) + g(f_{12} \cap f_{13} \cap f_{23} \cap f_{24}) + \\ & g(f_{12} \cap f_{13} \cap f_{23} \cap f_{34}) + g(f_{12} \cap f_{13} \cap f_{14} \cap f_{24}) + \\ & g(f_{12} \cap f_{13} \cap f_{14} \cap f_{34}) + g(f_{12} \cap f_{13} \cap f_{24} \cap f_{34}) + \\ & g(f_{12} \cap f_{23} \cap f_{14} \cap f_{24}) + g(f_{12} \cap f_{23} \cap f_{14} \cap f_{34}) + \\ & g(f_{12} \cap f_{23} \cap f_{24} \cap f_{34}) + g(f_{12} \cap f_{14} \cap f_{24} \cap f_{34}) + \\ & g(f_{13} \cap f_{23} \cap f_{14} \cap f_{24}) + g(f_{13} \cap f_{23} \cap f_{14} \cap f_{34}) + \\ & g(f_{13} \cap f_{23} \cap f_{24} \cap f_{34}) + g(f_{13} \cap f_{14} \cap f_{24} \cap f_{34}) + \\ & g(f_{23} \cap f_{14} \cap f_{24} \cap f_{34}), \end{aligned} \quad (27)$$

which respectively simplify to:

$$\begin{aligned} \sum_{f_i^{(2,4,4)} \in \mathcal{I}^{(2,4,4)}} g\left(f_i^{(2,4,4)}\right) = & g(s_{12} \cup s_{13} \cup s_{234}) + g(s_{12} \cup s_{23} \cup s_{134}) + g(s_{13} \cup s_{23} \cup s_{124}) + \\ & g(s_{12} \cup s_{14} \cup s_{234}) + g(s_{13} \cup s_{14} \cup s_{234}) + g(s_{14} \cup s_{23}) + \\ & g(s_{12} \cup s_{24} \cup s_{134}) + g(s_{13} \cup s_{24}) + g(s_{23} \cup s_{24} \cup s_{134}) + \\ & g(s_{14} \cup s_{24} \cup s_{123}) + g(s_{12} \cup s_{34}) + g(s_{13} \cup s_{34} \cup s_{124}) + \\ & g(s_{23} \cup s_{34} \cup s_{124}) + g(s_{14} \cup s_{34} \cup s_{123}) + g(s_{24} \cup s_{34} \cup s_{123}), \end{aligned} \quad (28)$$

Stemming from $\mathcal{I}^{(2,4,5)}$ are 6 terms:

$$\begin{aligned} \sum_{f_i^{(2,4,5)} \in \mathcal{I}^{(2,4,5)}} g\left(f_i^{(2,4,5)}\right) = & g(f_{12} \cap f_{13} \cap f_{23} \cap f_{14} \cap f_{24}) + g(f_{12} \cap f_{13} \cap f_{23} \cap f_{14} \cap f_{34}) + \\ & g(f_{12} \cap f_{13} \cap f_{23} \cap f_{24} \cap f_{34}) + g(f_{12} \cap f_{13} \cap f_{14} \cap f_{24} \cap f_{34}) + \\ & g(f_{12} \cap f_{23} \cap f_{14} \cap f_{24} \cap f_{34}) + g(f_{13} \cap f_{23} \cap f_{14} \cap f_{24} \cap f_{34}), \end{aligned} \quad (29)$$

which respectively simplify to:

$$\begin{aligned} \sum_{f_i^{(2,4,5)} \in \mathcal{I}^{(2,4,5)}} g\left(f_i^{(2,4,5)}\right) = & g(s_{12} \cup s_{134} \cup s_{234}) + g(s_{13} \cup s_{124} \cup s_{234}) + g(s_{23} \cup s_{124} \cup s_{134}) + \\ & g(s_{14} \cup s_{123} \cup s_{234}) + g(s_{24} \cup s_{123} \cup s_{134}) + g(s_{34} \cup s_{123} \cup s_{124}), \end{aligned} \quad (30)$$

Finally there is one term stemming from $\mathcal{I}^{(2,4,6)}$:

$$\sum_{f_i^{(2,4,6)} \in \mathcal{I}^{(2,4,6)}} g\left(f_i^{(2,4,6)}\right) = g(f_{12} \cap f_{13} \cap f_{23} \cap f_{14} \cap f_{24} \cap f_{34}) = g(s_{123} \cup s_{124} \cup s_{134} \cup s_{234}) \quad (31)$$

At this point we make a number of observations:

- There are $2^{\binom{m}{2}} - 1$ terms. So $m = 5$ and 6 respectively contain 1023, and 32,768 terms. Meaning explicitly writing out higher-orders is impractical.

- The expressions involve unions of elements from $\mathcal{I}^{(1,m)}$ (where $\mathcal{I}^{(1,m)}$ is the set $\{\mathcal{I}^{(1,m,i)} \mid i \in [1, \binom{m}{2}]\}$) instead of intersections of elements from $\mathcal{I}^{(2,m)}$.
- Algorithmically this allows us to reuse information from the dramatically smaller $\mathcal{I}^{(1,m)}$ family of sets (namely which elements of $\mathcal{I}^{(1,m)}$ are empty) to decrease the number of terms we must consider.