The design of efficient algorithms for enumeration

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Abstract

Many algorithms have been developed for enumerating various combinatorial objects in time exponentially less than the number of objects. Two common classes of algorithms are dynamic programming and the transfer matrix method. This paper covers the design and implementation of such algorithms.

A host of general techniques for improving efficiency are described. Three quite different example problems are used for examples: 1324 pattern avoiding permutations, three-dimensional polycubes, and two-dimensional directed animals.

For those new to the field, this paper is designed to be an introduction to many of the tricks for producing efficient enumeration algorithms. For those more experienced, it will hopefully help them understand the interrelationship and implications of a variety of techniques, many or most of which will be familiar. The author certainly found his understanding improved as a result of writing this paper.

1 Introduction

There are many problems in combinatorics where one wants to know the number of some type of object for a given size \( n \) (e.g. the number of polygons of perimeter \( n \) on a given lattice\(^{[1]} \)), but no formula is known. In this case computer enumeration is helpful to get the first few terms of the series, which can then be analysed to estimate their asymptotic behaviour. For many combinatorial problems the series terms grow rapidly - frequently exponentially - and it rapidly becomes computationally intractable to examine each object individually. An algorithm that groups multiple objects together can be more efficient, and can enable enumeration of more terms, which is usually highly desirable. Many such algorithms have been designed for many different problems. Many of them can be described as dynamic programming algorithms or as transfer matrix algorithms. This paper gives ways of thinking about and optimizing such algorithms.

The paper does not intend to be exhaustive - that would be impractical - but rather to describe a coherent group of techniques in a common language.

1.1 Enumeration problems as a set of equations

Ignoring efficiency for the moment, consider how one could count a combinatorial object of size \( n \). Often this involves starting with some base state \( S_b \) (which typically includes \( n \)) and adding
something to it - in the case of a geometrical object, this could be the presence or absence of a bond or a site. This then produces a set of other states \( S_i \) which consist of the base state plus the information about the new site. For each of these states \( S_i \), one adds the next possible item to get a new set of (more complex) states. Continue doing this recursively until one gets to an end state, at which point one increments a counter and then continues with the next substate (or \textit{child state}) in the recursive algorithm. At the end the answer is what is left in the counter.

The set of states and connections to their child states defines a directed acyclic graph, called the \textit{call graph} as it represents the calls in the recursive evaluation of the set of equations. Example call graphs for different formulations of the same problem are given in figures 1, 3 and 4.

This can be written out more formally as a set of equations. Let \( f(S) \) be the number of objects with state \( S \). So what one wants to calculate is \( f(S_b) \). For each state \( S \) define a set of next-possible-states (or \textit{child states}) \( N(S) \) as the states one can get to by doing the next thing to \( S \). This may be empty for an end state. Let \( k(S) \) be a constant (typically 0, or 1 if \( S \) is an end state). Then one can say

\[
f(S) = k(S) + \sum_{s \in N(S)} f(s).
\]

We require that there be no loops in the directed graph implied by \( N(S) \) in order to make the above equation, in principle, straightforward to evaluate without having to solve simultaneous equations. That is, there is no set of \( k > 1 \) states \( s_i \), such that \( s_{i+1} \in N(s_i) \) and \( s_1 = s_k \). This is normally obvious, and one can often define a \textit{hierarchy} function from states to integers (or other well ordered values), \( h(s) \), with the property \( \forall s, \forall t \in N(s), h(t) < h(s) \). Clearly if there exists a hierarchy function, there cannot be any loops. A hierarchy function is called \textit{ideal} if \( \forall s, \forall t \in N(s), h(t) = h(s) - 1 \).

An example is given in figure 4 which builds up all directed animals on a square lattice of size 4. Each rectangle is a state, with arrows pointing to its child states. The hierarchy function of a state in this case is a pair of integers; the number of sites left to add, and the number of grey sites. Ordering on the tuples is primarily by the number of sites to add, and secondarily by the number of grey sites.

Frequently an ideal hierarchy function is obvious — the number of elements to add to the partially constructed object, or the number of sites left to consider when passing over a finite lattice.

Sometimes there are weights associated with the substates - this is particularly common when the value of \( f \) is a partial generating function (typically of integers) rather than an integer. Let \( w(s, S) \) be the (easy to compute) weight associated with state \( s \) coming from state \( S \), giving us a more general formula

\[
f(S) = k(S) + \sum_{s \in N(S)} w(s, S) f(s)
\]

Sometimes the series term number, \( n \), is not explicitly in the state but is implicitly stored and is represented in the structure of \( f \) (e.g. the size of the lattice when enumerating on a finite lattice) and/or in the size of the partial generating function that is the value of \( f \).
Figure 1: Generation of all directed animals of 4 steps. Each box contains, at top, the animal so far. Black sites are occupied; grey sites are potentially occupied, and white sites are unoccupied or not reached yet. At each step, the rightmost grey site in the uppermost row containing a grey site is processed. It is determined to be either unoccupied (left child) or occupied (right child). If it becomes occupied, then the sites accessible from it are set to grey. If the site is the last grey, then it may not be unoccupied as such a child would never be able to grow to the desired size, so there is only one child. If the animal is the desired size, it is finished and has no children. Below the picture of the animal so far is derived information on the border; the grey sites (ignoring surrounding, unreachable sites), and the number of sites left to be occupied to reach the desired size. Above and to the left of each box is the number of directed animals descending from that state; it is one for a leaf box and otherwise equal to the sum of its direct children. The root node’s number, 13, is the number of four site directed animals.
We call a definition of $N$ clean if there is no path from the base state to a state $s$ where $f(s) = 0$. If $N$ is not clean then extra, useless, work will be done. Unfortunately it can be difficult to be clean.

It turns out that a large class of combinatorial enumeration problems fall into this formalism, although the notation may be somewhat different. Sometimes the formalism is slightly different, requiring modifications of the techniques below (e.g. section 3.1).

As an example, consider enumerating the set of well-formed bracket expressions with $n$ open and $n$ closing brackets. Define a state as a pair of integers, $S = (o, c)$, meaning the state where one has $o$ open and $c$ closing brackets left to add. So the stating state would be $S_b = (n, n)$, the ending state would be $(0, 0)$, and adding an open or closing bracket would decrease $o$ or $c$ respectively. Overall one has

$$f(o, c) = \begin{cases} 
1 & \text{if } o = 0 \text{ and } c = 0 \\
0 & \text{if } o > c \\
f(o - 1, c) & \text{if } o = c > 0 \\
 f(o - 1, c) + f(o, c - 1) & \text{otherwise}
\end{cases}$$

Note that this definition is redundant. The second line could be omitted, as such states will never be reached as the definition is clean. Alternatively, the third line could be omitted, but then the system would not be clean and the second line would be used. Also note that there are many other ways of enumerating well formed bracket expressions, with different state definitions.

The straightforward recursive implementation of this function typically takes time proportional to $f(S_b)$ as the only terminal state is 1. In the case of the well-formed bracket expressions (and many others of interest), this grows exponentially with $n$.

### 1.2 Dynamic programming

Recursive functions of this kind often have a simple optimization - whenever one has calculated $f(S)$ for some $S$, one adds $S \rightarrow f(S)$ in some table. Whenever one try to compute $f(s)$, one checks whether $s$ is present in the table already, and if so use the stored value rather than recomputing it. This is generally called dynamic programming (DP), memoization, or caching.

DP takes up memory, but can vastly reduce the running time. Of course it relies on the same state being reachable multiple ways - otherwise the table will never be used.

As an easy to analyze case study, consider the well formed bracket expressions from above, and suppose one is trying to compute $f(10, 10)$. The first step is forced, $f(10, 10) = f(9, 10)$. The next step has two legal choices, $f(9, 10) = f(8, 10) + f(9, 9)$. Now comes the interesting bit. $f(8, 10) = f(7, 10) + f(8, 9)$ and $f(9, 9) = f(8, 9)$. Both use $f(8, 9)$. Using dynamic programming, the second time the program attempts to evaluate $f(8, 9)$ it would just use the value previously computed. The total number of legal signatures needed to compute $f(n, n)$ is the number of pairs of integers $(o, c)$ where $n \geq c \geq o \geq 0$. This is clearly $O(n^2)$ which means the total number of

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1. A well formed bracket (or parenthesis) expression has the same number of open and closing brackets, and there are never more closing brackets than open brackets for any prefix of the expression. So $()$ is OK, as is $(()$, but not $(())$. This is a well known (and solved) problem whose series is the Catalan numbers.
states visited (and thus time and memory use) of the algorithm is $O(n^2)$. This compares with the naive recursive function which is $O(4^n n^{-1.5})$ which is clearly much worse.

In this case dynamic programming reduced the complexity of the algorithm from exponential to polynomial, and this sometimes happens in practice. When it does, the problem becomes computationally easy, a long series is generated, and people don’t bother enumerating it again! Frequently indeed it means that it is plausible to get a closed form solution. In other problems DP only reduces the exponential growth rate, which can significantly extend the number of terms one can get, although it rapidly becomes computationally intractable again. People tend to spend most of their time on such problems, as they are the unsolved ones.

1.3 Transfer matrix

Another approach is to keep a set of states and associated values (or *multiples*), starting off with $S_b$, multiple 1. Then, in each iteration of the algorithm one takes each state $S$ and associated value $v$, and applies the function $f$ to it, adding each of the states $s \in N(S)$ with multiple $m$ (or $m \cdot w(s, S)$ if weights are present) to the new set of states and associated multiples. Also one keeps a counter and whenever applying $f$ to a state $S$ produces a constant, one adds the associated multiple times the constant to the counter. Then one replaces the old set of states and multiples with the new set of states and multiples and iterates until the set of states becomes empty.

So far nothing has been gained; one is effectively doing a breadth first search of the recursive algorithm rather than the obvious depth first search. But crucially, when one ends up putting the same state into the new set of states multiple times, one can merge them together and sum the associated multiples. Now, in a very similar manner to DP, one has bunched together a variety of ways to get to the same state, preventing redundant computation. This technique is often called the transfer matrix technique (TM).

Again going through the well formed brackets example, we have

$$f(10, 10) = f(9, 10)$$
$$= f(8, 10) + f(9, 9)$$
$$= f(7, 10) + 2f(8, 9)$$
$$= f(6, 10) + 3f(7, 9) + 2f(8, 8)$$
$$= \ldots$$

Typically a TM algorithm reduces the total amount of computation to the number of valid signatures reachable from the initial state, the same as DP\footnote{If one can reach the same state via two different routes of different lengths through $f$, then one will end up with the same state in multiple iterations and the amount of computation will be higher - worse than DP. This can usually be avoided. In particular, if one has a hierarchy function $h$ defined on states, then one can, at each pass, process only the states with the highest hierarchy value.}. The memory use is somewhat less than DP, as one is effectively ordering computation so that one has some states that one can discard information about once one knows that one can never revisit them. The memory use is the maximum
number of states one gets in a breadth first search of the structure of $f$. This is bounded above by the number of states from DP, and bounded below by said number of states divided by the number of iterations of $f$ before reaching a final state, which is typically $n$ or at least polynomial in $n$. This means that the memory use is better than DP, but still growing with the same exponent if it is exponential.

1.4 Comparison and interconversion of DP and TM

The computational complexity of DP and TM are generally the same, but TM generally has somewhat lower memory requirements. So why would anyone ever use DP?

One reason is algorithm design complexity. TM is somewhat more complex to think about, implement, and test and debug than DP, while useful tools like Maple sometimes have direct support for DP (Maple calls it memoization). The resources used to implement TM could possibly be better spent making other changes to the algorithm that give a better return on the implementer’s time.

Another reason is lack of awareness of the trick of doing TM on DP problems. The main purpose of this paper is to raise awareness of such tricks, and introduce a way of thinking about the algorithms such that the interconversion is conceptually straightforward.

A third reason is that DP can be used to solve non-linear equations for $f$ - see section 3.1. This can be the real deciding factor.

A TM algorithm can almost always be converted to a DP algorithm, possibly requiring adding some information to the state - undoing the effect of section 4.1. But there is rarely a point in doing so.

1.5 Finite Lattice Method

For enumeration of geometrical objects on a lattice, it is common to split up the problem into enumeration on each possible finite lattice. Then the TM method is used, where each step consists of dealing with one extra element of the lattice (usually site). The ideal hierarchy function is the number of elements left to be added. The desired series is then produced by combining the series from the finite lattices. This is commonly referred to as the Finite Lattice Method.

Typically the sites are added in a systematic way that minimises the size of the boundary between processed and unprocessed sites, and the state then describes that boundary and connectivity information. On a rectangular lattice the boundary would be a cross sectional line through the lattice, possibly with a kink in it if the number of sites processed is not an even multiple of the lattice width. This is shown in figure 2.

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3 Actually roughly twice this value, as one needs to have two sets of states in memory at once; the set being processed and the set being produced

4 A rectangular subset of the square lattice $Z^2$
Doing it on multiple lattices has several advantages

- It makes it easy to deal with uniqueness under translation invariance
- One can commonly require that the object on the finite lattice touches all edges of the lattice. While keeping track of the information required to track this increases the total number of legal states, in practice it often decreases the number of states that will be visited in a clean implementation restricted to a particular size.
- One can use lattice symmetries. Enumerating on the $n \times m$ lattice is usually the same as the $m \times n$ lattice. The orientation is chosen to minimize the length of the boundary, and thus the number of states.

The finite lattice method has been used to great effect on two dimensional lattices, e.g. [2, 3, 4, 5, 6, 7, 8, 9, 10]. When enumerating size $n$ objects, one generally has a maximum boundary length of roughly $n/2$. The number of states usually grows exponentially in the boundary length, although pruning can mean that the peak number of states actually encountered is highest at a smaller portion of $n$.

On $d > 2$ dimensional lattices, the boundary is now a $d - 1$ dimensional surface, typically of size $(n/d)^{d-1}$. The number of states can grow exponentially in this cross section, which can, in a unclean system, easily produce a number of states far greater than the number of objects being enumerated, making it a dreadfully inefficient algorithm. Making a clean system can be difficult, and even if it is clean the performance advantage over direct enumeration is much smaller than in two dimensions.
A technique occasionally used in the finite lattice method (e.g. [5]) is to enumerate subportions of the objects being enumerated and construct the objects being enumerated from the subportions. This enables smaller lattices to be used, producing smaller boundary sizes and vast reductions in the number of states.

This has been used for a long time [11].

1.6 Examples

There are three significantly different examples that will be described in detail. They are used throughout the rest of this paper to provide specific examples of some techniques and trade-offs.

1.6.1 2D directed animals

A directed animal on some directed lattice is a set of sites such that each site apart from a single root site is directly downstream of another site. We will deal here with directed animals on a square lattice $\mathbb{Z}^2$ with the direction constraint being in the positive direction of either the $x$ or $y$ axes (north or east). Often the lattice will be shown rotated clockwise by 135 degree, so that the directed constraint becomes down and left or down and right. This is a well solved problem [12, 13, 14]; it is included as it is a simple example. Similar techniques can be used in many other two dimensional problems and on other lattices. It is solved for the square and triangular lattice but not for the hexagonal or most other lattices. Hereafter we will assume the square lattice.

There is one size one directed animal, the root. There are two size two directed animals, the root and one of the two downstream sites. There are five size three directed animals: four coming from the root, one of the two downstream sites, and also one of the two further downstream sites; the fifth is the root and both of the two downstream sites. There are thirteen size four directed animals; their construction is shown in figure 1.

These can be solved in a straightforward manner using both the dynamic programming and transfer matrix techniques, although the dynamic programming method is more obvious. One starts from the root, and add sites along a line perpendicular to the preferred direction (north east). Connectivity is then not an issue, as everything reached on this line must have come from the root, meaning the presence or absence of the sites on this line, along with the number of sites used, is sufficient information. The line will end up having a kink in it at the site being added, and will be partly the line being processed and partly the subsequent line. In practice one can do even better by using the (kinked) line one beyond the line to which sites have just been added, and record which sites are reachable rather than which sites have been reached. This is because there can be multiple sets of reached sites that can produce the same set of reachable sites. The call graph of such a formulation is given in figure 3 with corresponding equations in table 1. An alternate formulation is given in figure 4 and the transfer matrix algorithm applied to it is presented in table 2.

\[^{5}\text{The generating function } f(x) \text{ for the square lattice satisfies } (3x - 1)f^2 + (3x - 1)f + x = 0, \text{ the triangular similar.}\]
Figure 3: A simplification of figure 1 just showing the border information, which is the only thing that can affect children. This allows coalescing of now identical states together to produce a smaller tree, which will be able to take advantage of dynamic programming. Note there is an arrow skipping the fifth row.
Figure 4: An alternative algorithm for enumeration, like figure 3, except instead of processing one grey site at each step, the algorithm goes through grey sites until one is determined to be occupied. This is a more complex algorithm, but is better suited to the transfer matrix method as there are no row skipping arrows - see section 4.1.

Table 1: The equations corresponding to the graph in figure 3. The first two arguments to the function are binary numbers representing the pattern of grey sites, with a 1 meaning a grey site. Leading zeros are not shown. The third argument is the number of sites remaining to be added. The three arguments together define the state.

| Equation     | Description                                                                 |
|--------------|-----------------------------------------------------------------------------|
| $f(?, ?, 0)$ = 1, otherwise                      |                                                                             |
| $f(1, 0, n) = f(11, 0, n - 1)$                   |                                                                             |
| $f(11, 0, n) = f(1, 0, n) + f(10, 11, n - 1)$     |                                                                             |
| $f(10, 11, n) = f(11, 0, n) + f(111, 0, n - 1)$   |                                                                             |
| $f(111, 0, n) = f(11, 0, n) + f(110, 11, n)$     |                                                                             |

Table 1: The equations corresponding to the graph in figure 3. The first two arguments to the function are binary numbers representing the pattern of grey sites, with a 1 meaning a grey site. Leading zeros are not shown. The third argument is the number of sites remaining to be added. The three arguments together define the state.
\[ f(1, 0, 4) = f(11, 0, 3) \]
\[ = f(10, 11, 2) + f(11, 0, 2) \]
\[ = f(111, 0, 1) + 2f(11, 0, 1) + 2f(10, 11, 1) \]
\[ = f(110, 11, 0) + 5f(11, 0, 0) + 5f(10, 11, 0) + 2f(111, 0, 0) \]
\[ = 1 + 5 + 5 + 2 \]
\[ = 13 \]

Table 2: Transfer matrix style evaluation of the graph in figure 4 with function arguments as described in table 1.

1.6.2 1324 Pattern avoiding permutations

A permutation \( P \) of the integers \( 1 \ldots n \) is said to avoid the pattern \( p \) where \( p \) is itself a permutation of \( 1 \ldots l \) if there does not exist an \( l \) length subsequence (consecutive or not) of \( P \) that has the same relative order of elements as in \( p \). For instance the permutation 15342 contains the pattern 123 through the subsequence 134. The enumeration problem is to compute the number of such permutations for a given \( n \).

Surprisingly, all pattern avoiding permutations grow roughly exponentially, rather than the factorial growth of the permutations. \[15\]

The series are well understood for all 2, 3, and 4 length patterns except for 1324 and its complement 4231. This has been enumerated using a dynamic programming algorithm. Conceptually the permutations are built up one element at a time, and the state consists of the remaining integers and constraints upon their order. This was done in \[16\] enumerating to 31 terms and improved on in \[17\] with a more efficient state definition extending the series to 36 terms. The latter algorithm will be used in this paper.

The state definition consists of a series of numbers separated by brackets like \( 4(5(6)3)5 \). Each number represents a set of consecutive integers yet to be chosen, and the value is the length of this set. The sum of all the numbers is the number of elements left to add. This sum is an ideal hierarchy function. One may not use an element inside a bracketed expression until all numbers after the bracketed expression have been dealt with. That is, in the example, there are 4 low numbers and 5 high numbers that are legal as the next number to be chosen for the permutation being built up. That is, \( N \) of the example will have 9 elements. There may also be a comma at the start of the state indicating that at least one number lower than all remaining numbers has been already taken. See \[17\] for a more precise definition and rules for computing \( N \). The start state is the simple integer \( n \), and the end state is the empty state. The system is clean.

1.6.3 3D polycubes

A polycube is a connected set of unit length cubes in \( Z^3 \). An example is in figure 5. This is the 3D equivalent of a polyomino. The objective is determining the number of polycubes consisting of \( n \) cubes. This is an open problem in two or higher dimensions, with a roughly exponential growth rate.
There is one size 1 polycube - the single cube. There are three size two polycubes - two adjacent blocks, pointing along one of the three axes.

Polycubes are difficult to count efficiently. There has been extensive direct enumeration based on [18]. As the series grows rapidly, the most recent [19] has only got to 18 terms. The techniques in this paper have generally not been used for this or other three dimensional problems, as the number of intermediate states is large, and if one is not sufficiently careful, can be larger than the number of objects being enumerated.

Here is presented a transfer matrix method as a demonstration of the difficulty but not uselessness of TM on three dimensional problems. It is not clean, and will be a dreadful algorithm asymptotically, but may be reasonable for intermediate values. Enumeration will be done on finite lattices, adding one site at a time, with a two dimensional cross section as shown in figure 6. Initial evidence indicates it may be possible to get another couple of terms using this algorithm with comparable computational resources to [19].

The two dimensional equivalent, polyominoes, has been well studied and enumerated using the TM method in [2], significantly improved with pruning in [3], tweaked by Knuth to add a symmetry (public talk), and parallelized in [4].

2 Techniques common to both algorithms

The algorithms are very similar in the sense that the number of states is the primary driver of efficiency and memory use. The efficiency of these techniques comes from the conflation of different states when it can be recognised that they produce the same result. The more that states can be conflated, the more efficient the algorithm.

One can think of starting with a simple algorithm that builds up the objects being enumerated one element at a time, with the state being the entire history (as in figure 1). There is no gain from dynamic programming so far as these states are never reached twice. Then one works out a way of abstracting some reduced information about a state called a signature which is sufficient to

\footnote{Work in progress.}
Figure 6: The boundary of a polycube finite lattice enumeration. This is the bottom of a finite lattice two wide, three deep, and at least three tall. Sites are processed starting with the bottom back left cube. Subsequent cubes are processed left to right. When the right boundary is reached (quickly in this case), the row starts again one step closer to the front. When the whole layer is done, the next layer starts again at the back left. The cubes shown are processed. The six light grey cubes are on the boundary; the nine dark grey cubes are behind the boundary and only matter in so far as they affect connectivity of the boundary cubes and which edge faces have been touched at least once. The next to be processed is the one in the top middle right indentation, adjacent to three light grey cubes labelled P (prior plane), R (prior row) and C (prior column).
identify the state sufficiently precisely to compute downstream computations (as in figure 3). The expectation is that many states map to one signature. One then redefines the signatures to be the states and one has a more efficient algorithm.

So a signature is just a state, although with the connotation of being a summary of many other original states.

2.1 Signature design

Design of a signature is usually the most important part of the algorithm. The more states that map into a signature, the more efficient the algorithm. The specifics depend very much on the problem, but there are a couple of approaches that can be tried.

One approach is to think about different ways of describing the state. This can be exemplified by 1324 PAPs. In [17] the same basic state is used as in the earlier work [16], but a different way of describing it is used. The information is basically what numbers in the permutation are left and what restrictions there are on their use. In [16] these restrictions are, for each available number, an index pointing back at which prior numbers are unlocked after all numbers after this one are dealt with. In [17] it is noticed that this can be represented by a set of nested brackets. Looking at things this way, it becomes clear that consecutive brackets can be simplified, reducing the number of states. It also makes some state factorizations more obvious.

Another approach is to think about storing different information in the state. The following sections give several examples of this.

2.1.1 Signature design on a finite lattice

For the frequent case of enumerating objects on a finite lattice, where each operation consists of considering one extra site to be processed, the state generally consists of the boundary of the processed sites. This is generally one dimension smaller than the lattice being processed. The state then consists of the elements on the boundary, plus any needed connection information. The boundary consists of the set of points in the processed set that have at least one neighbour in the unprocessed set. Connectivity information is necessary in order to prevent counting disconnected or otherwise invalid objects.

In the 3D polycube case, this connectivity information is basically which sites on the boundary are connected to which other sites. This can be practically implemented by assigning an (arbitrary) integer to each site. Sites with the same integer are connected. It is important to canonicalize such information to prevent the same state being referred to in two different ways by different choices of integers. A simple canonicalization in this case is to order the sites, and define the canonical choice of integers to be the one that would come first in lexicographic order if the integers were written out as a series in site order.

For 2D lattices, the connectivity information is simpler as there are frequently restrictions on
crossings. So for the 2D version of polyominoes, the boundary is a line (possibly with a kink in it).
It is impossible to have a series of sites A,B,C,D where A is connected to C, and B is connected to
D, but A is not connected to B. This means that connectivity information can often be defined as
“connected to the next appropriate thing” or “connected to the last appropriate thing” [2]. This
does not intrinsically improve the algorithm, but it does improve implementation as it removes the
need for canonicalization, and means that the state can be stored in a small number of bits, which
is good for speed and memory usage of the big hash map typically used.

For the 2D directed animals case, the connectivity information is trivial... everything on the line
perpendicular to the preferred direction must have come from the root, so is all connected, so no
connectivity information is needed, just the state of the sites on the boundary.

For the enumeration of objects where bonds between sites have a meaning, it is worth considering
the boundary along either sites or bonds - usually one will be significantly more efficient than the
other.

Another common technique is to move the boundary forward one step to be just in front of the
processed sites. That is, the sites that are in the unprocessed set but have a neighbour in the
processed set. Instead of recording what is on the processed sites, one records what could be in
the unprocessed site. Directed animals are an excellent example. Consider the following two states
when recording what is present on the boundary. State A has three consecutive sites occupied -
subsequent growth can come from any of the four sites in the next row (figure [4] left). State B is
the same, except the middle of those three sites is not occupied (figure [7] right). But subsequent
growth for state B is the same as state A, as the same four sites are reachable from state A. So
\( f(A) = f(B) \), and A and B should be considered the same state. This can be done by storing
which sites in the next row could be occupied - the new state replacing A and B would be four
occupiable sites in a row.

A similar technique can be used with 3D polycubes. The kink in the boundary will usually (de-
pending on which site one is currently processing) have a single place where there are three sites
adjacent to the next-to-be-added site. These three sites are in the prior plane \( P \), the prior row \( R \),
and the prior column $C$ (see figure 6). Sites $R$ and $C$ have multiple sites still to be considered that they are adjacent to, but $P$ is only adjacent to the site about to be processed. If $P$ is occupied, and connected to at least one of $R$ or $C$, then the $P$’s presence does not affect anything, as any site added will be connected to the group containing $P$ by dint of $R$ or/and $C$. So the number of states could be reduced slightly by removing $P$ in such a circumstance. This is a minor optimization as it only affects one site.

Instead of storing what is connected to what in the past, one could store the information about what should be connected to what. This is different information with a significantly different set of child states. In [10] this reduced the number of states slightly, but more importantly made the trimming (see later) much faster.

### 2.1.2 Touching boundaries on a finite lattice

Suppose one wants to enumerate polycubes of size 15. This can be done by enumerating all polycubes in a 15 by 15 by 15 finite lattice. Of course smaller polycubes will appear multiple times differing only by translation. This can be accounted for by enumerating polycubes on all subsets of the 15 by 15 by 15 lattice and doing appropriate subtractions.

There are ways of improving this. For many symmetric lattices the result is independent of the order of the dimensions. For instance, the number of 3D polycubes on a 3 by 5 by 7 lattice is the same as on a 7 by 3 by 5 lattice. This clearly reduces the number of lattices that must be enumerated upon, but, more importantly, one can choose the largest dimension to be in the direction perpendicular to the boundary. The size of the border (which is often the main driver of algorithm complexity) is determined by all but that dimension, so choosing it as the longest reduces the maximum size of the border.

This means the biggest border that one will come across to enumerate polycubes of size 15 will be 5 by 6, a much more tractable problem.

Furthermore, if one is counting polycubes on an $A$ by $j$ lattice, where $A$ is the boundary area and $j$ the depth, then instead of enumerating separately for each $j$, one can just work up to the maximum $j$ and one will pass through all lower values in the process, and whenever an object is finished in a layer $l \leq j$, one stores for the $A$ by $l$ lattice. One generally also wants to add the requirement that, after the first layer (of size $A$) is done, the empty boundary is not accepted. This provides uniqueness in the $j$ dimension, avoiding having to explicitly canonicalize, but, more importantly, it reduces the number of states that will be processed, improving efficiency.

Another way to get translational uniqueness is to require each edge of the lattice to be touched. Intuitively, this seems a bad idea, as it makes the state more complex as the state will now contain

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7Define $U_L$ to be the total number of objects on a lattice $L$ (or a generating function of them), and $C_L$ to be a canonicalized version only counting objects that fit into $L$ but not any smaller lattice. Then $C_L$ can be generally computed as $U_L$ minus some multiples of $C_l$ for lattices $l$ smaller than $L$. For the zero size lattice, typically $C_l = 0$. Then by induction given all $U_l$ for $l$ a subset of $L$, one can compute $C_l$. One can then add up all $C_l$ to get the number of objects that fit on lattice $L$ without multiple counting. In practice it is usually simpler than this due to constraints on touching boundaries
flags indicating whether each lattice edge has been touched. This increases the total number of legal states, which is an upper bound on the number of states that will be reached, and a useful heuristic for algorithm complexity. However, in practice adding the boundary requirement often significantly reduces the number of states that will be reached, as it will take too many sites or bonds to get to that state and still be in a position to finish the object (see next section on trimming).

2.2 Signature trimming

Trimming is the process of making sure that the algorithm is clean. That is, it never produces a state \( Z \) such that \( f(Z) = 0 \). The number of states processed, which is the main driver of efficiency, is bounded above for a clean algorithm by the number of objects being enumerated times the maximum length of a chain from the start state to an end state (which is typically linear in the length of the sequence being computed). An unclean algorithm can be much worse. So trimming is of comparable importance to state design.

An example is in two dimensional polyomino enumeration where the TM algorithm with trimming in [3] is much more efficient than the prior algorithm [2], even though the states are more complex, as they involve keeping track of whether the boundaries have been reached. Similarly it has been very effective in 2D polygon enumeration with [8] improving on [1], and in many other problems.

The trimming algorithm is used on each state processed to discard useless next possible states. Sometimes this is obvious, and not even worth mentioning. In other cases it is quite complex [8], which can be problematic if it is time consuming, as it is executed for each state. In [10] trimming is made faster by changing the state definitions from describing the connectivity in the processed space to describing the required connectivity in the unprocessed states.

In the finite lattice case, trimming basically consists of determining the minimum number of sites or bonds needed to complete the object, usually by resolving connectivity issues including to the boundaries. If this minimum number is too high the state can be rejected. Typically “too high” means that the lowest term of the generating function associated with the state plus the minimum completion number is greater than the desired length of the series.

Sometimes it is difficult to come up with a perfect trimming algorithm, in which case an imperfect algorithm may be used which leaves the algorithm still not clean, but better than with no trimming algorithm. An imperfect (or conservative) trimming algorithm generally produces a lower bound on the number of elements needed to finish rather than the number itself. The enumeration algorithm will then still produce the correct answer, but will waste time dealing with states that will go to zero. This is the case for the 3D polycube algorithm presented here as an example of a difficult trim.

\[8\text{Not including the two edges dealt with in the prior paragraph}\]
2.2.1 Polycube trimming

Specific details of the algorithm for trimming polycubes is presented here. It is not provided as an example of a good algorithm; to the contrary, it is a horrible algorithm. It is slow, complex (and therefore error prone), and imperfect. Rather it is presented to show how this is difficult, and the why it is sometimes worth changing the signature design to make trimming easier. Bad as it is, without it the algorithm would be totally impractical. Hopefully a reader will be able to improve it!

The finite lattice method applied to 3D polycubes adds one site at a time. So there are three nested loops, the outermost iterating over layer (z) then row (y) and then column (x). The boundary is a slice through the finite lattice, with a kink - some sites are in the layer currently being processed (z), some are in the prior layer (z - 1, or empty if z = 0). The state consists of the occupied sites on this border, and their connectivity. This is defined as a number for each site. Zero means unoccupied; a positive integer means occupied and connected to all other sites with the same number. For the rest of this section, these numbers will be called colors. Flags are also kept for which of the four sides of the finite lattice are attached (the z = 0 side is connected by construction - no zero states are allowed after the last site of the z = 0 layer is processed, and so the last z layer touched is always the one currently being processed).

The task for the trimmer is to compute what the minimum number of sites is that needs to be added to finish the polycube. This requires adding cubes to:

- connect each distinct color,
- connect to the unconnected sides,
- connect to the minimum value of z that ending is allowed\(^9\).

A fast precise answer is unknown to the author. A reasonably fast, conservative algorithm is presented here.

Ignore for the moment everything other than connecting all the colors. The only sites that need to be considered for this are the ones one layer beyond the boundary, with an extra row above the kink to allow connectivity between above and below the kink. Any minimal connection using other sites could be done equivalently using just this set of sites. Call this set of sites the grid \(G\).

For any color \(c\), we can define \(table(c)\) to be a number for each site in \(G\), being the minimum number of sites needed to get to that cell from any cell of color \(c\) on the boundary. This can be computed in polynomial time using depth first search. Alternatively, define a consistency function \(C(t)\) which takes a table \(t\) and makes it consistent, that is, reduces any value to no more than one more than any of its neighbours. Then \(table(c)\) is \(C\) of the table which is infinite other than neighbours of \(c\) which are 1.

\(^9\)By symmetry, one can always have z be the biggest dimension. So polyominoes can be required to reach to a certain minimum z, being the maximum of the width and height
In the one color case, the color connectivity cost is trivially zero.

In the two color \((a \text{ and } b)\) case, the cost is the minimum in \(table(a) + table(b) - 1\), alternatively the minimum cost in \(table(a)\) of anything adjacent to \(b\). Indeed, the minimum cost of connecting \(a\) and \(b\), going via a given grid element, is \(bitable(a, b) = C(table(a) + table(b))\)

In the three color \((a, b, \text{ and } c)\) case the connectivity cost is the minimum value of \(bitable(a, b) + table(c) - 1\), alternatively the minimum cost in \(bitable(a, b)\) of anything adjacent to \(c\).

Indeed, we can now define \(tritable_c(a, b, c) = C(bitable(a, b) + table(c) - 1)\). Then \(tritable(a, b, c) = \min \{tritable_c(a, b, c), tritable_b(a, c, b), tritable_a(b, c, a)\}\) is now the cost of connecting \(a, b\) and \(c\) going via a particular site.

This lets us now do the four color case \((a,b,c,d)\), in which case the connectivity cost is the minimum value of \(tritable(a, b, c)\) adjacent to \(d\).

For the five or more color case, the cost of continuing this is becoming prohibitive. A conservative lower bound is used, being just the cost to connect four of the colors\(^{10}\).

Now consider the cost to connect to the edges as well. Ignoring connection costs, one could find the sites with minimum and maximum \(x\) and \(y\) values, and take the distance to the edges from them. The connection cost will be that, probably with some extra as one also usually\(^{11}\) need to go up a site in order to build out. If one adds in the color connection cost, frequently the sites used in that will provide the extra height. Working out exactly when extra sites are needed is difficult. The sites in the color connection cost will almost never\(^{12}\) detour outside the minimum and maximum \(x\) and \(y\) values, so the color connection cost can be safely added to this edge connection cost\(^{13}\) to get a lower bound.

Similarly, to get to the maximum \(z\) one has to have sites going from the current layer up to the minimum \(z\) layer. One of these may be counted in the color connection cost if it is non-zero. So this distance can be added, with a 1 discount in the case of a non-zero color connection cost.

This ends up with a somewhat conservative trimming function which produces an algorithm that performs vastly better than with no trimming. Asymptotically it will be a dreadful algorithm as the number of states that end up being zero will become huge, but appears to be reasonable for currently calculable polycube sizes.

\(^{10}\)In practice this was done by computing \(tritable(a, b, c)\) and then finding for each remaining color the minimum value adjacent to it, and taking the maximum of these values

\(^{11}\)The exception is when an edge site is in the kink

\(^{12}\)Exception: sometimes the connection cost can be done in the row below the kink at the same cost as the row above the kink.

\(^{13}\)With a 1 discount for the case of the previous footnote, when one needs to get to the bottom and the kink is up to the last or second last row.
2.3 Binning

A process, sometimes described as binning, can be occasionally used to reduce memory use at the
cost of execution time. One chooses some intermediate set of states, divides them into groups, and,
for each group, one does the enumeration repeatedly, requiring that group to be passed through.
Then one adds up the results. This is rarely useful as the time penalty is usually significantly
greater than the memory advantage.

3 Techniques particular to dynamic programming

Dynamic programming is generally inferior to a transfer matrix algorithm, but is still used exten-
vively as it is conceptually easier, and has some optimizations not available to the transfer matrix
method.

3.1 Factorizations

Sometimes it is possible to factorize a state, that is say \( f(S) = f(S_1)f(S_2) \), for some states \( S_1 \) and
\( S_2 \). Generally \( S_1 \) and \( S_2 \) will be significantly smaller than \( S \), vastly reducing the work needed to
compute them. For instance, in the 1324 PAPs, the state \( S = (S_1)S_2 \) has this property, as the
brackets mean that all things to the right of the bracket must be processed before anything inside
the bracket.

As far as dynamic programming is concerned, multiplication is insignificantly different from addi-
tion. But multiplication of two states does not fit into the transfer matrix paradigm of cumulative
sums at all. This ability is the main advantage of the dynamic programming method over the
transfer matrix method.

It is possible to use a hybrid algorithm, where one basically uses a transfer matrix technique, but
when a factorization is encountered, the simpler state is evaluated using a dynamic programming
algorithm, and then becomes a constant multiplier for the more complex state. A constant multi-
plier is then fine from a transfer matrix perspective, apart from frequently having skipped ahead
some steps in the transfer matrix. This skip makes one have to store it and merge it back in when
other states have caught up. The advance storage of states plus the extra overhead of dynamic
programming storage as well somewhat undoes the smaller memory use advantage of the transfer
matrix method. It turned out to look promising but not actually help significantly for 1324 PAPs
(unpublished work). Such hybrid algorithms are almost twice as complex to implement as either
base algorithm, increasing the likelihood of programming errors.

\[ \text{There is another similar but not quite as effective optimization used... if } S = S_1(S_2)S_3 \text{ then } f(S) = \sum m_i f(s_iS_2) \]
where integers \( m_i \) and prefix states \( s_i \) are functions of \( S_1 \) and \( S_3 \) but not \( S_2 \).
3.2 Probabilistic caching

When memory is a greater issue than speed, it is possible to reduce memory use by only caching results probabilistically. That is, after computing $f(S)$, instead of storing $S \rightarrow f(S)$ in some table, only store it with some probability $p$. If $f(S)$ is never needed again (as often happens), then there is no cost in not storing it. If $f(S)$ is needed frequently, then eventually it will be stored, and there will be no subsequent penalty. A smaller $p$ produces more memory savings, but a greater time penalty, allowing some tuning of the algorithm to just fit in the memory available. A high quality random number generator is not needed; one fast and simple approach is to use a simple accumulator. Each time one wants to see if something should be stored, add $p$ to the accumulator. If the result is at least one, subtract one and store the value.

Superficially, this may sound as if it reduces the memory use to a factor of $p$, and increases the time by a factor of $1/p$, but it is not that simple. The total number of calls made will be increased, and so the amount stored will be $p$ times a larger number. So memory is reduced to a factor between $p$ and 1. Execution time increase is not as bad as may be expected because the number of times each particular state is referenced changes the effect of $p$ on the running time, with large and small numbers both improving matters. It is difficult to theoretically determine this factor, as it depends on the call graph, so empirical results are needed.

Empirical results show that this works surprisingly well and was used in the memory constrained enumeration of 1324 PAPs [17] to get an extra term. Figures 8 and 9 show the empirical effects of $p$ on directed animals and 1324 PAPs. The patterns are surprisingly similar given that the directed animals have a maximum of two children while the 1324 PAPs can have dozens. A $p$ of 0.3 gives roughly a 40 percent reduction in memory and takes roughly twice as long in the two cases shown.

This optimization cannot be used in transfer matrix algorithms as the data store is a cumulative sum, rather than a cache.

3.3 Cache inspection

One is trying to canonicalize states such that two states that can be proven to produce the same result are actually encoded as one state. In the absence of infinite wisdom, a method that can be used to check that nothing obvious has been missed is to inspect the cache after the algorithm has run to see if there are multiple states with the same value. To reduce the chance of coincidences, one can run the algorithm until there are a hundred thousand or so entries in the cache, and look at those entries with associated values over a million. If there are multiple states producing the same large value, an inspection of those states will hopefully inspire a realisation of some equivalence of states, producing a more efficient definition of states.

This has been recently applied by the author to the 1324 PAPs algorithm in [17] to notice that signatures starting with a 1 or a comma allow commutation of some of the ending terms. Proving this then led to other useful realisations leading to a more efficient algorithm (not yet published).

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15 The actual time and memory use for the 1324 PAPs is a little more complex due to factorizations.
Figure 8: Probabilistic caching in 27 step PAPs as a function of the probability of caching a newly computed result. Memory use is roughly proportional to the bottom line; time is roughly proportional to the top line.
Figure 9: Probabilistic caching in 70 site directed animals on the square lattice as a function of the probability of caching a newly computed result. Memory use is roughly proportional to the bottom line; time is roughly proportional to the top line.
This is easy to do for a dynamic programming algorithm; for a TM algorithm a similar technique can be used, but is less directly associated with state equivalence.

4 Techniques particular to transfer matrix

There are also some techniques primarily applicable to the transfer matrix method.

4.1 Part of the signature is the iteration number

For directed animals, the obvious state is the combination of the sites on the boundary eligible for occupancy, and the number of sites left to include. For children there are two main implementation choices:

- One can take a processing step to consider a certain eligible site on the boundary, and have one child if it is occupied, and another if it is not occupied. In the first case the number of sites left to include will have decreased, in the second the number of available sites on the boundary will have reduced. One can define a hierarchy function based primarily upon the number of sites left to include and secondarily on the number of available sites; this hierarchy function will be lower for both child states, so loops are impossible. The call graph for this algorithm is shown in figure 3.

- One can take a processing step to mean the next used site is chosen. There can be many substates in this case (one for each available site in the boundary). The number of sites left to include is decreased by one each time; it makes an ideal hierarchy function; loops are impossible. The call graph for this algorithm is shown in figure 4.

For dynamic programming implementations the two are comparable. The latter is slightly more complex to implement but will be slightly faster and use a little less memory. However for a transfer matrix style implementation they are significantly different. Both algorithms can be implemented with each iteration processing one value of the hierarchy function. For the first algorithm this is somewhat fiddly and has the issue that a child may have a value of the hierarchy function a few steps further on; these need to be tracked. For the second algorithm, each child will go directly into the list to be processed at the next iteration as the hierarchy function is ideal.

In both cases, the number of sites to be included is implicit in the current TM iteration number. Therefore one does not have to store it as part of the signature, saving memory in the states, a large number of which will be stored. This is shown in table 2 where the third argument of each state is determined by the row number in the table, and therefore does not need to be stored with each state.

This implicit storage of part of the state is obvious for the finite lattice methods where each iteration corresponds to moving the boundary out by one site. The shape of the boundary is identical for each element of a particular iteration, and so does not have to be stored with each state.
4.2 Signature Invariants

Sometimes it is possible to divide the states into groups that have the property that there is no state that is a child of a member of two different groups (or bins). For instance, in the 3D polycubes case, define a group by the occupied/unoccupied status of each site other than the one about to be covered. Adding (or not) a new site may affect connectivity, but it won’t change other sites’ occupancy. These are signature invariants.

This division means that instead of processing each signature sequentially, putting all the results in a giant hash map, one can do each group separately, using a small hash map (with better cache locality), and then, when a group is finished, extract the states and associated multiples, store them in some more compact format, and reuse the hash table for the next group. This enables the use of a sparsely filled hash map, improving speed, without the massive memory hit of having a huge sparse hash map. One does have to be very careful with the overhead of small groups and cache clearing.

Processing this way, it is often possible to make the construction of the next set of groups implicit. In the 3D polycube case, it makes sense to assign each group a number whose binary representation contains the occupied status of each site, with the most recent site added as the most significant bit. Then the output from the processing of each group will be in one of two groups, identified by shifting the current groups’ number down one bit and adding a new 0 or 1 as the most significant bit. These can be serialized into two piles based on the most significant bit, and then when all groups are processed, the two piles are concatenated. If the groups started off in order, they will now again be in order, this time for the next set of groups. Since the initial null state is by definition in order, the groups will always be in order.

This can be used to efficiently use disk as storage instead of memory. Current low latency SSDs are too slow to be used as swap space for a giant hash map (2016 unpublished tests), but using them as storage for the serialized group outputs requires many fewer random accesses and is reasonable in some situations.

Of probably greatest importance, this can be very useful on multiprocessor systems, as each group can be assigned to a node, and the node can process that group knowing it will not have to share the hash map with any other node. Examples of such use include 2D self avoiding walks [6, 7], polygons [9] and polyominos [4].

This sort of construction is often possible for geometric entities on finite lattices; it is less clear for other cases like 1324 PAPs which has proven difficult to parallelize.

4.3 Finite lattice techniques

Finite lattice enumerations generally involve enumerating objects on a set of finite lattices individually, and reconstructing the total number of objects from the results on finite lattices.

Finite lattice enumerations are ideal for the TM algorithm as each iteration is well defined (add
one more portion, typically site, of the lattice). The techniques described here can be used for DP algorithms as well, but there is rarely any reason to use DP rather than TM for such algorithms.

4.3.1 Finite lattice symmetries

As mentioned before, when enumerating all the objects on a symmetric lattice of a certain size, the result is often identical to enumerating it on other sizes determined by the lattice symmetry. For instance, enumerating 3D polycubes on a 3*8*2 lattice is the same as a 2*3*8 lattice (and four others). This reduces the number of finite lattices that need to be computed.

This is not always possible - if one of the sides of the lattice is special (e.g. enumeration of paths that are attached to one side of the lattice) or if the dimensions are different (e.g. enumeration of polygons on the square lattice by both horizontal and vertical bonds).

Generally it is better to make the boundary go across the shorter dimension(s), as this makes the states simpler, and probably less numerous, although with good trimming this can be less important than one might expect.

4.3.2 State reflection

When the iteration is such that the kink does not preclude symmetry (e.g. when finishing a row or a plane), frequently the boundary condition is equivalent to its mirror image. At this point a consolidation can be done, declaring one of these arbitrarily to be the canonical one, and merging the two.

This can in principle halve the number of states to process, although this is somewhat misleading as the number of states will continue to grow up to almost the number it would have been anyway during the subsequent iterations where the kink prevents this consolidation. It also breaks many of the invariants (section 4.2).

4.3.3 Reconstruction from fragments

Some of the objects being enumerated can be split up into fragments and then reconstructed by enumerating those fragments. This can reduce the number of items being enumerated. The fragments being enumerated are often called irreducible.

For instance, a bridge on a lattice $L$ is a path on $L$ that has one end at one side of $L$, and the other at the opposite side of $L$. The bridge is irreducible if there is no plane slicing through $L$ parallel to the attached sides of $L$ that intersects only one bond. For many problems one can reconstruct all bridges from just the reducible bridges by chaining them with single bonds connecting the irreducible bridges. That is, if $b(x)$ is the bridge generating function, and $b_i(x)$ is the irreducible
bridge generating function, then

\[ b(x) = b_1(x) + x b_1(x)^2 + x^2 b_1(x)^3 + \cdots = \frac{b_1(x)}{1 - x b_1(x)} \]

Enumerating irreducible objects can potentially be faster than enumerating all objects as there are fewer of them, and therefore there will probably be fewer states reached. Also this can be used to reduce the size of the signature as irreducible objects are more compact and fit onto narrower lattices. This was critical to [5] but later advances in understanding of pruning made this less useful.

## 5 Associated values

The associated values for dynamic programming usually are integers as that fits in well with the paradigm. The state is then the boundary condition and number of elements yet to be included.

With the transfer matrix, one could do the same thing, although it is often more efficient to have the state be the boundary condition, and the associated value is then an array of integers; the polynomial coefficients of a generating function multiple. This is more efficient as the state only needs to be stored once, and trimming calculations only need to be done once for each state. This is difficult to do with a dynamic programming algorithm as one usually does not know in advance how big the generating function will need to be, which is essential information to pass to the child state evaluator.

The number of non-zero entries in a generating function is usually quite small. This is because most of the states are complex, as there are only small numbers of simple states, and complex states typically take a lot of elements to produce, leaving few spare elements for the series. To take advantage of this, avoid storing zero elements. In the majority of cases, the non-zero elements are consecutive, so that means each generating function can be represented by a start index, a length, and an array of coefficients of that length.

Of course if most generating functions are only length 1, then that is a lot of overhead to store one integer, but the total overhead is generally less storing generating functions, especially if the alternative of storing the number of elements left with the state just makes it have similar extra overhead instead. See figure 10 for an example distribution of lengths, and the effect of even imperfect trimming on reducing not just the total number of states, but the size of the associated generating functions as well.

Sometimes only even (or odd) terms can be non-zero, in which case only those terms should be stored. This is particularly common with enumeration by bonds.
Figure 10: Number of generating functions of each length encountered midway through the enumerating of up to 16 element polycubes on and spanning the 3 by 5 by 5 lattice. Computations were done with and without using the (imperfect) trimming.
5.1 Multi variable series and moments

It is straightforward to have more than one variable in the generating function. Suppose instead of counting polycubes just by number of cubes, one also wants to count by surface area (3D perimeter). Let $A_{i,j}$ be the number of polycubes with $i$ cubes and perimeter $j$. Instead of having a 1D array as the generating function associated with each state, one would have a 2D generating function, and update it in the same way. Trimming becomes a little more complex to describe, as does the highest term of the enumeration.

Sometimes however, that can take up too much memory, and having a moment series is useful. The $m$-th moment of surface area series, counting by volume, would then be

$$M_m(x) = \sum_{i,j} A_{i,j} x^i j^m$$

Note that $M_0(x)$ is just the normal enumeration by volume (number of cubes).

In a finite lattice computation, when a state is being processed for a site, the new generating function needs to be modified by adding $c$ cubes and surface area $s$. With a 2D generating function, this is straightforward, one just shifts it $c$ in one dimension and $s$ in another dimension. For $M_0(x)$ it is also straightforward, just shift $c$. For other moments it is not quite as obvious, but it turns out to be straightforward. Let $M^*_m$ be the new desired moment, and $M_m$ be the existing moment. Then

$$M^*_m(x) = \sum_{i,j} A_{i,j} x^{i+c} (j+s)^m = x^c \sum_{i,j} A_{i,j} x^i \sum_{k=0}^m \binom{m}{k} j^{m-k} s^k = x^c \sum_{k=0}^m \binom{m}{k} s^k M_{m-k}$$

which means if one has existing moments from 0 to $m$, one can easily compute the new moments from 0 to $m$.

Given moments, one can compute, say, the mean surface area for size $i$ polycubes by dividing the $i$-th coefficient of $M_1$ by the $i$-th coefficient of $M_0$. Different variables allow different properties of the object to be studied.

This is described in detail in [2] for the 2D polyonimo case. By a similar process one can compute percolation series, where the generating function is of the form $\sum A_{i,j} p^i (1-p)^j$ storing just a single generating function for each state.

6 Implementation issues

Generally, an efficient algorithm is more powerful than an efficient implementation. An efficient algorithm can be many orders of magnitude better than a competitor, whereas an efficient implementation is typically only a couple of orders of magnitude better than a simpler, less efficient implementation. With that said, the implementation does matter.
6.1 Chinese remainder theorem

The numbers being computed often are larger than the native size of an integer. Many languages have libraries for big integers (data structures representing large integers). However these tend to be slow and memory consuming.

One can use the Chinese remainder theorem to deal with this problem. One does the enumeration with small integers by doing everything modulo some number (typically a prime). Do this for several different, coprime, moduli, and this is enough information to be able to simply regenerate the number modulo the product of the original moduli. This is generally faster, and more memory efficient than using a big integer library. It also has the advantage of offering some redundancy; a concern in long running computations can be an error somewhere in the computer (e.g. from gamma ray strikes). Such an error in one of the moduli will usually produce a very large, noticeable, inconsistency in the results.

This is probably the most commonly used trick in implementation.

Knuth\textsuperscript{16} implementing TM algorithms, faced with the inefficiency of repeating the computations multiple times, separated out the state part from the value part. He made two programs, the first of which would carry around all the state information, and would produce as output a long stream of instructions for another program to execute, to actually do the additions and trimming of generating functions. This is more complex and introduces significant disk IO, but has two advantages:

- The first program only needs to be run once, while the second program can be run for each modulus, rather than recomputing the states for each modulus. This is particularly useful if trimming is computationally expensive and therefore a majority of the time.

- The memory consumption can be slightly lower (in principle up to a factor of 2) than doing both at the same time.

6.2 Parallelization

Multi-processor machines are the norm, and to use a big computer effectively, a parallel algorithm is usually needed. This is usually quite difficult, as distributed hash maps take a large amount of inter-processor communication which can be the bottleneck, even on shared memory systems due to the expense of cache synchronization.

Most parallelized success stories with transfer matrices have used signature invariants (see section 4.2). If speed rather than memory is the constraint, then the problem can be partitioned cleanly by different moduli and lattice sizes.

Writing parallelized code is very difficult and error prone. Writing efficient communication code is

\textsuperscript{16}Public talk
even more difficult and requires a deep understanding of the architecture used. One can use distributed libraries, although they generally don’t do exactly what one wants and have an associated overhead. There are no clear general answers.

TM algorithms are usually easier to parallelize than DP algorithms, as the distributed hash map lookup of DP is particularly unfriendly to parallel architectures.

6.3 Hash map

Both TM and DP require a large amount of storage for a map from state to value. For DP this is the cache; it must be a map as the operations are look up value for a state and store calculated value for a state. For TM the operations are iterate over state, value pairs and store value for a state, adding to existing if available. These are most obviously performed by a map, although the map-reduce framework (such as Apache Hadoop) is also possible. Also if invariants are used, a small hash and long list may be used. But most frequently a map (usually a hash map) is used.

This hash map is usually very large. This makes some of its properties affect the performance of the program significantly. The load factor of the hash map is important - higher values mean a slower program using less memory.

Having a good hash function of the state is very important as the state tends to have many similar values, and a poor hash function can lead to a very large number of collisions.

Most languages come with support for hash maps built into a standard library. However this is generally optimized for convenience and flexibility rather than performance, and a less general purpose one can give order of magnitude improvements particularly to memory but also time.

For instance, in Java, the standard hash map is from one object to another object. It is often possible to encode the state as a bit string and therefore as an integer. Similarly the values are often integer. When the generic map is used from integers to integers, then each integer has to be wrapped in an object, causing a large overhead. Similarly, many standard library hash maps handle collisions by storing at each entry a list of values that mapped to that entry. This causes another level of wrapping for each entry. There exist much more memory efficient (and fast) hash maps, such as the GNU Trove library which includes multiple versions for each combination of primitives as key or value.

It is frequently useful to have multiple maps instead of one big one. Some function of the key determines which map to use, and some other function of the key is used in that map. Reasons for doing this include:

- Many hash map libraries have limited size hash maps. Many use 32 bit integers in the indexing (and hash values). On current computers this can be a serious limit to the size of the map.

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17 Integer is used as a generic name for a natively handled data type. It may be called long or something other than integer.
• If one doesn’t set the size of a map in advance, it will typically automatically increase in size when needed. This operation is usually implemented by creating a new data store of larger size and copying values across. During this process both the new and old datastore are in memory, which can exceed available memory. By splitting up the maps, this situation causes less transient memory increase.

• In a multithreaded, shared memory program, it can reduce contention for write locks.

• Some of the key can be implicitly stored in the map selection stage. In [17] the keys for 1324 enumeration were encoded as 128 bit integers. The first 64 bits were used to determine which hash map to use (in a reversible manner). The remaining 64 bits were used as the key in the map. This reduced the memory used for the keys in the maps.

Another way of reducing memory use at the cost of time is by using multiple hash maps with different size values depending upon the actual size of the value. Suppose the values are 64 bit integers. Many of the actual values may fit in a 32 bit integer. This is because a large portion of the states produced will have very restricted paths to endpoints resulting in modest actual values. This means one uses two hash maps, one mapping to 64 bit values and one to 32 bit values. Reads have to check both maps; writes just go to the best fitting map. This is easy for DP; for TM it may require changing which map a value is stored in when another value is added to it. Of course one could get an even greater effect by using 32 bit moduli in the Chinese remainder theorem, but the multiple maps method can achieve much the same effect with a smaller performance hit. Profiling of the bit length in the 1324 PAPs algorithm found it looked useful to have 24 bit, 40 bit, and 64 bit results (see figure 11).

7 Conclusion

The art of efficient enumeration algorithms is, like most skills, enhanced by knowledge of a host of techniques, only a few of which will be appropriate for any specific problem. This paper has described many such techniques with consistent terminology and a discussion of their relative merits and applicability. This will hopefully help the reader to realise when given tricks can be used. The exercise of writing this paper certainly helped me realise how I could have improved various algorithms I came up with in the past.

In particular, the transfer matrix technique is well known and used for two dimensional lattice enumeration problems where it seems natural, but it is rarely used outside of that domain. However, totally unrelated problems with an ideal hierarchy function can often use the transfer matrix technique instead of the dynamic programming that has been typically used. This can provide a reduction in memory usage and significant advantages for parallelization. This paper has emphasised the similarities of the two techniques and the issues in converting from dynamic programming to transfer matrix.

Each enumeration problem will have its own special requirements and peculiarities, but many tricks can be reused.
Figure 11: Bits used in cache for 1324 PAPs, length 20, 25 and 30, as a proportion of the total cache entries. The full answer for length 30 is 78 bits
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References

[1] IG Enting. Generating functions for enumerating self-avoiding rings on the square lattice. *Journal of Physics A: Mathematical and General*, 13(12):3713, 1980.

[2] Andrew Conway. Enumerating 2d percolation series by the finite-lattice method: Theory. *Journal of Physics A: Mathematical and General*, 28(2):335, 1995.

[3] Iwan Jensen. Enumerations of lattice animals and trees. *Journal of Statistical Physics*, 102(3-4):865–881, 2001.

[4] Iwan Jensen. Counting polyominoes: A parallel implementation for cluster computing. In *International Conference on Computational Science*, pages 203–212. Springer, 2003.

[5] Andrew R Conway, Ian G Enting, and Anthony J Guttmann. Algebraic techniques for enumerating self-avoiding walks on the square lattice. *Journal of Physics A: Mathematical and General*, 26(7):1519, 1993.

[6] AR Conway and Anthony J Guttmann. Square lattice self-avoiding walks and corrections to scaling. *Physical Review Letters*, 77(26):5284, 1996.

[7] Iwan Jensen. A new transfer-matrix algorithm for exact enumerations: self-avoiding walks on the square lattice. *arXiv preprint arXiv:1309.6709*, 2013.

[8] Iwan Jensen and Anthony J Guttmann. Self-avoiding polygons on the square lattice. *Journal of Physics A: Mathematical and General*, 32(26):4867, 1999.

[9] Iwan Jensen. A parallel algorithm for the enumeration of self-avoiding polygons on the square lattice. *Journal of Physics A: Mathematical and General*, 36(21):5731, 2003.

[10] Nathan Clisby and Iwan Jensen. A new transfer-matrix algorithm for exact enumerations: self-avoiding polygons on the square lattice. *Journal of Physics A: Mathematical and Theoretical*, 45(11):115202, 2012, 1309.6709.

[11] T De Neef and IG Enting. Series expansions from the finite lattice method. *Journal of Physics A: Mathematical and General*, 10(5):801, 1977.

[12] Deepak Dhar. Equivalence of the two-dimensional directed-site animal problem to baxter’s hard-square lattice-gas model. *Physical Review Letters*, 49(14):959, 1982.

[13] D Gouyou-Beauchamps and Gérard Viennot. Equivalence of the two-dimensional directed animal problem to a one-dimensional path problem. *Advances in Applied Mathematics*, 9(3):334–357, 1988.

[14] J Bétréma and JG Penaud. Animaux et arbres guingois. *Theoretical computer science*, 117(1):67–89, 1993.
[15] Adam Marcus and Gábor Tardos. Excluded permutation matrices and the stanley–wilf conjecture. *Journal of Combinatorial Theory, Series A*, 107(1):153–160, 2004.

[16] Fredrik Johansson and Brian Nakamura. Using functional equations to enumerate 1324-avoiding permutations. *Advances in Applied Mathematics*, 56:20–34, 2014, 1309.7117.

[17] Andrew R Conway and Anthony J Guttmann. On 1324-avoiding permutations. *Advances in Applied Mathematics*, 64:50–69, 2015, 1405.6802.

[18] D Hugh Redelmeier. Counting polyominoes: yet another attack. *Discrete Mathematics*, 36(3):191–203, 1981.

[19] Sebastian Luther and Stephan Mertens. Counting lattice animals in high dimensions. *Journal of Statistical Mechanics: Theory and Experiment*, 2011(09):P09026, 2011, 1106.1078.