Combinatorial Enumeration: Theory and Practice

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For many applications we wish to only consider subsets of a fixed size — the \( k \)-subsets of an \( n \)-set.

There are two common orderings used to list \( k \)-subsets, shown here for 2-subsets of a 5-set.

- **Lexicographic**

  12, 13, 14, 15, 23, 24, 25, 34, 35, 45

- **Co-lexicographic**

  12, 13, 23, 14, 24, 34, 15, 25, 35, 45

Note: Here we are using 12 as shorthand for \( \{1, 2\} \).
The number of $k$-subsets of an $n$-set is given by the binomial coefficient
\[
\binom{n}{k} = \frac{n!}{k!(n-k)!}.
\]

**Proof.**

The number of *sequences* of $k$ distinct elements from an $n$-set is
\[n(n-1)(n-2)\cdots(n-k+1).\]

Every $k$-subset will occur in $k!$ different orders in this list of sequences, and so the total number of $k$-subsets is
\[\frac{n(n-1)(n-2)\cdots(n-k+1)}{k!}.\]
Binomial Identities

A significant area of “classical” combinatorics is the discovery and proof of the many binomial identities relating appropriate binomial coefficients.

For example,

\[
\binom{n}{k-1} + \binom{n}{k} = \binom{n+1}{k}
\]

Many of these identities can be proved in two ways - an algebraic proof or a combinatorial proof.
Algebraic Proofs

Algebraic proofs simply involve manipulation of the formulas to get the stated identity.

\[
\binom{n}{k-1} + \binom{n}{k} = \frac{n!}{(n-(k-1))!(k-1)!} + \frac{n!}{(n-k)!k!} = \frac{kn! + (n+1-k)n!}{(n+1-k)!k!} = \binom{n+1}{k}
\]
Combinatorial Proofs

A combinatorial proof aims to *explain* the identity, rather than simply verify it.

Suppose there are $n + 1$ objects, one of which is “distinguished” from the others. Any $k$-subset of this set either

- contains the distinguished object, or
- doesn’t contain the distinguished object.

There are $\binom{n}{k-1}$ sets in the first category and $\binom{n}{k}$ in the second category and so the stated identity holds.

A combinatorial proof is usually viewed as conveying more information than an algebraic proof, but there are many situations where only an algebraic proof is known.
Exercise

Find a combinatorial proof of the following identity:

\[ \sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n} \]

Hint: Consider the $2n$ objects as consisting of two groups of $n$ objects.
The odometer principle

Lexicographic order is related to the “odometer” principle used in a car odometer: increase the least significant digit if possible, and otherwise roll that digit over to 0 and increase the next least significant digit.

\[
\begin{array}{ccccc}
1 & 4 & 3 & 2 & 2 \\
1 & 4 & 3 & 2 & 3 \\
2 & 3 & 7 & 9 & 9 \\
2 & 3 & 8 & 0 & 0
\end{array}
\]
Representing a $k$-set

We will represent a $k$-set $T$ by a sequence (or array) listing its elements in increasing order

$$t_1 < t_2 < \ldots < t_k,$$

which we can view as a sort of $k$-digit odometer

$$
\begin{array}{cccc}
t_1 & t_2 & \cdots & t_k \\
\end{array}
$$

with strange properties.
Example: 3-subsets of a 7-set

This “odometer” starts at the smallest possible value

```
1 2 3
```

because no digits can be repeated.

Using the odometer principle is easy for the first few successors:

```
1 2 4
1 2 5
1 2 6
1 2 7
```
Successor of \{1, 2, 7\}

We cannot increase the last position any more, so we

- propagate the increase one position to the left, and
- put the lowest possible value in the last position.

\[
\begin{array}{ccc}
1 & 2 & 7 \\
1 & 3 & 4 \\
\end{array}
\]

If the next position over is already in its highest possible position, then the increase must be propagated further to the left:

\[
\begin{array}{ccc}
1 & 6 & 7 \\
2 & 3 & 4 \\
\end{array}
\]
In GAP

nextLex := function(T,n,k) local S,pos,i;
    pos := k;
    while (pos > 0) and (T[pos] = n+pos-k) do
        pos := pos-1;
    od;
    if (pos = 0) then
        S := [1..k];
    else
        S := T;
        S[pos] := S[pos]+1;
        for i in [pos+1..k] do
            S[i] := S[i-1]+1;
        od;
    fi;
    return S;
end;
A ranking function is much less pleasant to calculate for this ordering — for example, consider finding the rank of \{2, 5, 7\} in the ordering of 3-subsets of a 7-set. This equivalent to finding the number of sets that occur before \{2, 5, 7\} in the ordering, which are the sets of the form:

\[
\begin{array}{ccc}
1 & ? & ? \\
2 & 3 & ? \\
2 & 4 & ? \\
2 & 5 & 6
\end{array}
\]

The key to counting these is to observe that the number of each type is just a binomial coefficient, and in fact we have

\[
\binom{6}{2} + \binom{4}{1} + \binom{3}{1} + 1 = 23.
\]
The number of subsets before 

\[ t_1 \ t_2 \ \cdots \ t_k \]

is the sum of the numbers of subsets that

- Start with \( u_1 \), where \( u_1 < t_1 \), or
- Start with \( t_1 u_2 \) where \( u_2 < t_2 \), or
- Start with \( t_1 t_2 u_3 \) where \( u_3 < t_3 \), or
- \( \ldots \)
- Start with \( t_1 t_2 \cdots t_{k-1} u_k \) where \( u_k < t_k \).
The number of subsets whose \( i \) lowest values are \( t_1 \ t_2 \ldots t_i \) is

\[
\binom{n - t_i}{k - i}
\]

because the remaining positions determine a \( k - i \) subset chosen from a set of size \( n - t_i \).
So, the number of subsets that start with $u_1$, where $u_1 < t_1$ is

$$
\sum_{j=1}^{t_1-1} \binom{n-j}{k-1}
$$

with the index $j$ running over all the feasible values for $u_1$. Similarly the number of subsets that start with $t_1 u_2$ is

$$
\sum_{j=t_1+1}^{t_2-1} \binom{n-j}{k-2}
$$

again with the index $j$ running over all possible values for $u_2$ (notice that the lowest possible value for $u_2$ is $t_1 + 1$).
The final expression

The rank of the subset \( \{t_1, t_2, \ldots, t_k\} \) is

\[
\sum_{i=1}^{k} \left( \sum_{j=t_{i-1}+1}^{t_i-1} \binom{n-j}{k-i} \right)
\]

where \( t_0 = 0 \).

(This is the kind of equation that you derive once, then program in a reusable manner and hope you never have to derive again!)
Colexicographic order

The other ordering on $k$-sets that is common is called \textit{colexicographic} order. To determine this order, we represent a $k$-set by a sequence $t_1, t_2, \ldots, t_k$ with the property that

$$t_1 > t_2 > \cdots > t_k.$$
Colexicographic order (cont)

Colexicographic (colex) order is then defined by listing these representatives in normal lexicographic order:

\[321, 421, 431, 432, 521, 531, 532, 541, 542, 543\]

One of the important properties of colex order is that the ordering does not depend on \(n\). More precisely, the colex ordering for the \(k\)-subsets of an \(n\)-set is the leading portion of the colex ordering for the \(k\)-subsets of an \((n + 1)\)-set.
Colex successors

It is quite easy to find a successor function for colex order.

To find the successor of

\[ T = \{t_1, t_2, \ldots, t_k\} \]

do the following steps:

- Find the largest index \( i \) such that \( t_{i-1} \neq t_i + 1 \).
- Increase \( t_i \) by 1.
- Replace \( t_{i+1}, \ldots, t_k \) by \( k - i, \ldots, 2, 1 \)
Example successor

To find the successor of \([8, 5, 4, 3, 2]\) in colex order.

- The specified index is \(i = 2\)

\[
[8, 5, 4, 3, 2]
\]

- Increase \(t_i\) by 1

\[
[8, 6, 4, 3, 2]
\]

- Replace \(t_3 \ldots t_5\) with \(3, 2, 1\)

\[
[8, 6, 3, 2, 1]
\]
Colex rank

How many $k$-sets occur before $T = \{t_1, t_2, \ldots, t_k\}$ in the colex order? Once again we can divide them into $k$ groups:

- Those starting $u_1$ where $u_1 < t_1$, or
- Those starting $t_1 u_2$ where $u_2 < t_2$, or
- Those starting $t_1 t_2 u_3$ where $u_3 < t_3$, or
- \ldots
- Those starting $t_1 t_2 \cdots t_{k-1} u_k$ where $u_k < t_k$.

This sum is much easier to calculate than the corresponding sum for lexicographic order.
**Colex rank (cont.)**

The number of subsets whose largest element is less than $t_1$ is simply the number of $k$ subsets of the set $\{1, 2, \ldots, t_1 - 1\}$, which is

$$\binom{t_1 - 1}{k}.$$

Similarly, those starting with $t_1$ but then having no other element larger than $t_2$ is

$$\binom{t_2 - 1}{k - 1}.$$

Continuing in this fashion we get

$$r(\{t_1, t_1, \ldots, t_k\}) = \sum_{i=1}^{k} \binom{t_i - 1}{k - (i - 1)}.$$
In GAP

colLexRank := function(T,k) local rk,i;

    rk := 0;
    for i in [1..k] do
        rk := rk + Binomial(T[i]-1,k-(i-1));
    od;

    return rk;
end;
Permutations

A permutation is defined to be a one-to-one mapping

\[ \pi : \{1, \ldots, n\} \to \{1, \ldots, n\}. \]

We can express a permutation by listing the images of each element of the domain under this mapping:

\[
\begin{pmatrix}
1 & 2 & \cdots & n \\
\pi(1) & \pi(2) & \cdots & \pi(n)
\end{pmatrix}
\]

It should be clear that the number of permutations of degree \( n \) is

\[ n(n - 1)(n - 2) \cdots 1 = n!. \]
Permutations of degree 4

\[
\begin{align*}
(1 & 2 & 3 & 4) & (1 & 2 & 3 & 4) & (1 & 2 & 3 & 4) & (1 & 2 & 3 & 4) \\
1 & 2 & 3 & 4 & 1 & 2 & 4 & 3 & 1 & 3 & 2 & 4 & 1 & 3 & 4 & 2 \\
1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\
1 & 4 & 2 & 3 & 1 & 4 & 3 & 2 & 1 & 4 & 3 & 2 & 1 & 4 & 3 & 2 \\
1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\
2 & 3 & 1 & 4 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 \\
1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\
3 & 1 & 2 & 4 & 3 & 1 & 4 & 2 & 3 & 1 & 4 & 2 & 3 & 1 & 4 & 2 \\
1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\
3 & 4 & 1 & 2 & 3 & 4 & 2 & 1 & 4 & 3 & 2 & 1 & 4 & 3 & 2 & 1 \\
1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\
4 & 2 & 1 & 3 & 4 & 2 & 3 & 1 & 4 & 3 & 2 & 1 & 4 & 3 & 2 & 1 \\
\end{align*}
\]
Image notation

This notation can be condensed a bit by dropping the top line, and simply giving the list of images in order:

$$\left[\pi(1), \pi(2), \ldots, \pi(n)\right].$$

So the 24 permutations of degree 4 are:

- [1, 2, 3, 4] [1, 2, 4, 3] [1, 3, 2, 4] [1, 3, 4, 2] [1, 4, 2, 3] [1, 4, 3, 2]
- [2, 1, 3, 4] [2, 1, 4, 3] [2, 3, 1, 4] [2, 3, 4, 1] [2, 4, 1, 3] [2, 4, 3, 1]
- [3, 1, 2, 4] [3, 1, 4, 2] [3, 2, 1, 4] [3, 2, 4, 1] [3, 4, 1, 2] [3, 4, 2, 1]
- [4, 1, 2, 3] [4, 1, 3, 2] [4, 2, 1, 3] [4, 2, 3, 1] [4, 3, 1, 2] [4, 3, 2, 1]
Cycle Notation

Another notation that is frequently used is *cycle notation*. Given a permutation $\pi$ consider the sequence of values

$$1, \pi(1), \pi^2(1) = \pi(\pi(1)), \pi^3(1), \ldots$$

obtained by repeatedly applying the mapping $\pi$.

This sequence must eventually return to 1 and the sequence of values obtained is called a *cycle* of the permutation.

For example, if $\pi_1 = [4, 3, 1, 2]$ then we get

$$1 \rightarrow 4 \rightarrow 2 \rightarrow 3 \rightarrow 1$$

which is expressed more succinctly as

$$(1, 4, 2, 3).$$
Cycle Notation (cont.)

The cycle that starts with 1 may not include all the elements of \( \{1, 2, 3, 4\} \), but by starting with an unused element we can obtain another cycle. For example, if \( \pi_2 = [2, 1, 4, 3] \), then both \((1, 2)\) and \((3, 4)\) are cycles of \( \pi_2 \).

We can represent a permutation completely by listing all its cycles:

\[
\pi_1 = (1, 4, 2, 3) \quad \pi_2 = (1, 2)(3, 4).
\]

This representation is not unique, because we could equally well say that

\[
\pi_1 = (4, 2, 3, 1)
\]

but by convention we express each cycle by putting its smallest element first.
### Permutations of degree 4

In cycle notation, the 24 permutations of degree 4 are:

<table>
<thead>
<tr>
<th>Cycle 1</th>
<th>Cycle 2</th>
<th>Cycle 3</th>
<th>Cycle 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>(2)</td>
<td>(3)</td>
<td>(4)</td>
</tr>
<tr>
<td>(1) (2, 4, 3)</td>
<td>(1) (2, 4) (3)</td>
<td>(1, 2) (3) (4)</td>
<td>(1, 2) (3, 4)</td>
</tr>
<tr>
<td>(1, 3, 2) (4)</td>
<td>(1, 3, 4, 2)</td>
<td>(1, 3) (2) (4)</td>
<td>(1, 3, 4) (2)</td>
</tr>
<tr>
<td>(1) (3, 2, 4)</td>
<td>(1, 3, 2, 4)</td>
<td>(1, 4, 3, 2)</td>
<td>(1, 4, 2) (3)</td>
</tr>
<tr>
<td>(1) (4, 3) (2)</td>
<td>(1, 4) (2) (3)</td>
<td>(1, 4, 2, 3)</td>
<td>(1, 4) (2, 3)</td>
</tr>
</tbody>
</table>
Fixed points

Cycles of length 1 are called \textit{fixed points} and are usually omitted from the cycle notation.

\begin{align*}
(2, 4, 3) & \quad (3, 4) & \quad (2, 3) & \quad (2, 3, 4) \\
(2, 4) & \quad (1, 2) & \quad (1, 2)(3, 4) \\
(1, 2, 3) & \quad (1, 2, 3, 4) & \quad (1, 2, 4, 3) & \quad (1, 2, 4) \\
(1, 3, 2) & \quad (1, 3, 4, 2) & \quad (1, 3) & \quad (1, 3, 4) \\
(1, 3)(2, 4) & \quad (1, 3, 2, 4) & \quad (1, 4, 3, 2) & \quad (1, 4, 2) \\
(1, 4, 3) & \quad (1, 4) & \quad (1, 4, 2, 3) & \quad (1, 4)(2, 3)
\end{align*}

It is not very convenient having a blank symbol for the identity mapping, so we usually use either () or a symbol such as $e$ or $\text{id}$. 
Lexicographic Order

The order used above for the permutations was, once again, lexicographic order on the permutations expressed in image notation.

It is possible to define a successor function for permutations in lexicographic order, but the details are surprisingly complicated, so instead we will just specify a pair of ranking/unranking functions.

These hinge on the observation that the permutations with a fixed value of \( \pi(1) \), say \( \pi(1) = a \), all have the form

\[
[a, \pi(2), \pi(3), \ldots, \pi(n)]
\]

where \([\pi(2), \pi(3), \ldots, \pi(n)]\) is a permutation of \( \{1, 2, \ldots, n\} \setminus \{a\} \).
Therefore the rank of $\pi$ is equal to the sum of the following two numbers

- $(a - 1)(n - 1)!$ for the permutations that have $\pi(1) < a$, and
- The rank of $[\pi(2), \pi(3), \ldots, \pi(n)]$ within the list of permutations of $\{1, 2, \ldots, n\}\setminus\{a\}$.

If we form $\pi'$ from $[\pi(2), \pi(3), \ldots, \pi(n)]$ by subtracting 1 from every value greater than $a$, then $\pi'$ is a permutation of $\{1, 2, \ldots, n - 1\}$ and its (normal) rank is the second value above.
Example

The rank of the permutation \([3, 4, 1, 2, 5]\) is equal to

- \(4! \times 2\) for the permutations with \(\pi(1) = 1, 2\), plus
- The rank of \([4, 1, 2, 5]\) within the permutations of \(\{1, 2, 4, 5\}\) which is equal to the rank of \([4 - 1, 1, 2, 5 - 1] = [3, 1, 2, 4]\).

Proceeding recursively we see that:

\[
\begin{align*}
r([3, 4, 1, 2, 5]) & = 48 + r([3, 1, 2, 4]) \\
& = 48 + 12 + r([1, 2, 3]) \\
& = 60.
\end{align*}
\]
Factorial Notation

Unranking a permutation depends on an interesting representation of a number known as the *factorial representation*. A normal decimal number, such as 5476 is a compressed positional notation for

\[
\begin{array}{cccc}
1000s & 100s & 10s & 1s \\
5 & 4 & 7 & 6 \\
\end{array}
\]

Rather than using the values \(10^0, 10^1, 10^2\) and so on as the values associated with each position, we use \(1!, 2!, 3!\), \ldots

\[
\begin{array}{cccccccc}
7! & 6! & 5! & 4! & 3! & 2! & 1! \\
1 & 0 & 3 & 3 & 0 & 2 & 0 \\
\end{array}
\]
Uniqueness

If each “digit” $d_i$ in a factorial representation

$$\cdots d_3d_2d_1$$

satisfies the condition that $d_i \leq i$, then every natural number has a unique factorial representation!

This is a relatively straightforward but interesting proof, in that it requires us to show

- Every natural number has *some* factorial representation, and
- No natural number has *more than one* factorial representation.

Exercise: Prove this.
Unranking

In order to unrank the integer $r$, we first find its factorial representation. For example

$$60 = 0 \times 5! + 2 \times 4! + 2 \times 3! + 0 \times 2! + 0 \times 1! = 2200.$$  

The first digit $d_4 = 2$ tells us that $\pi(1) = 3$, and that the permutation $[\pi(2), \pi(3), \pi(4), \pi(5)]$ has rank $60 - 48 = 12$ among the permutations of $\{1, 2, 4, 5\}$.

We can (recursively) calculate the permutation with rank 12 among the permutations of $\{1, 2, 3, 4\}$ and then transform it to a permutation of $\{1, 2, 4, 5\}$ by incrementing each value that is greater than or equal to 3.
Fixed Points

A classic result in combinatorics is the enumeration of derangements — permutations with no fixed points.

For \( n = 4 \) there are

- 9 derangements
- 8 permutations with 1 fixed point
- 6 permutations with 2 fixed points
- 1 permutation with 4 fixed points
Inclusion/Exclusion

Calculating the number of derangements uses an important counting technique called the *principle of inclusion/exclusion*, which we illustrate with a simple example:

> In a high-school class of 25 children, there are 10 who play cricket, 14 who play football and 6 who play both. How many children play neither sport?

![Venn diagram showing the overlap of children playing different sports](image)
We can calculate the number by calculating separately the number of cricket-but-not-football players \((10 - 6)\), football-but-not-cricket players \((14 - 6)\) and both-cricket-and-football players \((6)\) and subtracting these from the total.

\[
7 = 25 - (10 - 6) - (14 - 6) - 6 = 25 - (10 + 14) + 6
\]

The re-arranged version on the second line shows that we could have obtained the same result by starting with the total number of students, subtracting the football players and the cricket players, and then adding back the number who play both.
Inclusion/Exclusion for two or three sets

If $A$ and $B$ are subsets of $X$, then the number of elements that are not in either $A$ or $B$ is

$$|X| - (|A| + |B|) + (|A \cap B|).$$

If $A$, $B$ and $C$ are subsets of $X$, then the number of elements of $X$ that are not in any of $A$, $B$ or $C$ is

$$|X| - (|A| + |B| + |C|) + (|A \cap B| + |A \cap C| + |B \cap C|) - (|A \cap B \cap C|).$$
Principle of Inclusion/Exclusion

If \( A_1, A_2, \ldots, A_n \) are all subsets of a set \( X \) then for any index set \( I \subseteq X \), define

\[ A_I = \bigcap_{i \in I} A_i \]

(where we take \( A_\emptyset = X \)).

Principle of Inclusion/Exclusion

The number of elements of \( X \) that do not belong to any of the sets \( A_1, A_2, \ldots, A_n \) is given by

\[
\sum_{I \subseteq \{1,2,\ldots,n\}} (-1)^{|I|} |A_I|.
\]
Derangements of degree 4

To count the derangements of degree 4, let $X$ be the set of all permutations of degree 4, and for $1 \leq i \leq 4$, let $A_i$ be the set of permutations that fix $i$. Then the number of permutations that fix no points is equal to:

$$24 - (6 + 6 + 6 + 6) + (2 + 2 + 2 + 2 + 2 + 2) - (1 + 1 + 1 + 1) + 1$$

because

$$|A_i| = 6$$
$$|A_i \cap A_j| = 2$$
$$|A_i \cap A_j \cap A_k| = 1$$

for any choices of distinct $i, j$ and $k$. 
Derangements

It is immediate that the number of derangements of degree $n$ is

$$\sum_{i=0}^{i=n} (-1)^i \binom{n}{i} (n - i)!$$

Expanding the binomial coefficient, this reduces to

$$\sum_{i=0}^{i=n} (-1)^i \frac{n!}{i!} = n! \sum_{i=0}^{i=n} \frac{(-1)^i}{i!}.$$

Is this a good answer?
An infinite series

As $n!$ is the total number of permutations we see that the *fraction* of them that are derangements is found by summing the $n + 1$ leading terms of the series

$$\frac{1}{0!} - \frac{1}{1} + \frac{1}{2} - \frac{1}{6} + \frac{1}{24} - \frac{1}{120} + \frac{1}{720} + \cdots$$

This series converges quickly:

<table>
<thead>
<tr>
<th>$n$</th>
<th>Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.5000</td>
</tr>
<tr>
<td>3</td>
<td>0.3333</td>
</tr>
<tr>
<td>4</td>
<td>0.3750</td>
</tr>
<tr>
<td>5</td>
<td>0.3667</td>
</tr>
<tr>
<td>6</td>
<td>0.3681</td>
</tr>
<tr>
<td>7</td>
<td>0.3679</td>
</tr>
<tr>
<td>8</td>
<td>0.3679</td>
</tr>
</tbody>
</table>
A good answer

Recall that the Taylor series of a suitably differentiable function is

\[ f(x) \approx f(0) + xf'(0) + \frac{x^2}{2!} f''(0) + \frac{x^3}{3!} f'''(0) + \cdots + \frac{x^n}{n!} f^{(n)}(0). \]

If we take \( f(x) = e^{-x} \) then the derivatives of this function are \(-e^{-x}, e^{-x}, -e^{-x}, \) etc, so by putting \( x = 1, \) we get

\[ e^{-1} = 1 - 1 + \frac{1}{2!} - \frac{1}{3!} + \frac{1}{4!} - \cdots \]

With a little bit more work we get the final result:

**Theorem**
The number of derangements of degree \( n \) is given by the closest integer to \( n!/e. \)

The corresponding sequence is given by OEIS A000166