Generalized Catalan Sequences Originating from the Analysis of Special Data Structures

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Abstract

Reinterpreting known results on Carlitz’s $q$-Catalan numbers $c_n(q)$ we find a connection between the number of acyclic DJ graphs and these $q$-analogs. A similar recurrence relation is setup for the number of reducible DJ graphs, a well-known data structure in computer science, this time leading to a different $q$-analog $C_n(q)$ of Catalan numbers. Using arguments from enumerative combinatorics we establish a complete asymptotic expansion of the numbers $C_n(q)$.

1. Introduction

In [10] Fürlinger and Hofbauer have studied several kinds of $q$-analogs of Catalan numbers. In particular, they derive an asymptotic formula for

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Carlitz’s $q$-Catalan numbers $c_n(q)$ ([9, 5]) defined by

\begin{equation}
    z = \sum_{n=1}^{\infty} c_{n-1}(q)(1-z)(1-qz) \cdots (1-q^{n-1}z).
\end{equation}

For $|q| < 1$

\[ c_n(q) \rightarrow \prod_{i=1}^{\infty} (1-q^i)^{-1} \quad \text{as } n \rightarrow \infty, \]

i.e., the $q$-Catalan numbers $c_n(q)$ converge to the partition function.

Eq. (1) can be used to derive a simple recurrence relation for $c_n(q)$ [10]

\begin{equation}
    c_n(q) = \sum_{k=0}^{n-1} c_k(q)c_{n-1-k}(q)q^{(k+1)(n-1-k)}, \quad c_0(q) = 1.
\end{equation}

Writing

\[ \overline{c}_n(q) = q^{\binom{n}{2}}c_n(q^{-1}) \]

the simplest possible $q$-analog of Catalan numbers can be obtained

\begin{equation}
    \overline{c}_n(q) = \sum_{k=0}^{n-1} q^k \overline{c}_k(q)\overline{c}_{n-1-k}(q).
\end{equation}

If we set $q = 2$ in Eq. (3) and let $a_n = \overline{c}_n(2)$, we obtain

\begin{equation}
    a_n = \sum_{k=0}^{n-1} 2^k a_k a_{n-1-k}, \quad a_0 = 1.
\end{equation}

Interestingly, $a_n$ can be interpreted as the number of acyclic DJ graphs, a data structure well-known in computer science.

In the next section we will define DJ graphs and show that the above interpretation is correct. In Section 3 we study a $q$-analog of the Catalan numbers resulting from the enumeration of reducible DJ graphs.

2. DJ Graphs

Flow graphs are directed graphs that model the control flow of computer programs or are used to solve flow problems. A more formal definition is given below.

**Definition 1.** [3] A *flow graph* is a triple $G = (V, E, s)$, where $(V, E)$ is a directed graph, $s \in V$ is a distinguished node, and there is a path from $s$ to every other node.
It is useful to distinguish between ordered and non-ordered flow graphs in the same way as ordered trees are distinguished from other trees, i.e., the order of the successors of a node is significant. We study ordered flow graphs in this paper. In the following the term flow graph always means ordered flow graph.

Let $u$ and $v$ be nodes of a flow graph. If all paths from $s$ to $v$ contain node $u$, we say that node $u$ dominates node $v$. Node $u$ immediately dominates node $v$ if $u$ dominates $v$, and there is no intervening node $w$ such that $u$ dominates $w$ and $w$ dominates $v$. Each node has a unique immediate dominator. The dominator tree is a data structure depicting the dominator relationships. There is an edge from node $u$ to node $v$ if $u$ is an immediate dominator of $v$.

Hecht and Ullman [14] give three equivalent definitions for a reducible flow graph $G = (V, E, s)$:

1. Any depth first search (cf. [21]) on $G$ starting at $s$ determines the same set $B$ of back edges.
2. $G$ does not contain the forbidden flow graph $SP(s,x,y,z)$, shown in Figure 1.
3. For every back edge $(v, w) \in B$, $w$ dominates $v$ (cf. [1]).

Figure 1 shows that the major difference between reducible and irreducible flow graphs is the presence of multiple-entry loops.

Generally speaking, reducible flow graphs allow more efficient algorithms to solve problems based on flow graphs. For example it is easy to implement a linear algorithm to determine the dominator tree of reducible flow graphs while a linear algorithm for general flow graphs is hard to implement (cf. [4, 11]). Even certain concepts are easier to define for reducible flow graphs.
For example, *loops* are easy to define in reducible flow graphs by their back edges. For general flow graphs this is not so easy and cannot be done unambiguously (cf. [16]).

In [19, 20] DJ graphs are introduced as the union of a flow graph and its dominator tree. The name DJ graph reflects that an edge in the graph either originates solely from the dominator tree or not. In the first case it is called d-edge, in the latter case it is called join edge. DJ graphs are an efficient vehicle to solve dataflow equations [17, 19, 20].

In [22, 23] Vernet and Markenzon study maximal reducible flow graphs (MRFs). They prove a decomposition theorem for MRFs which has been generalized to reducible flow graphs in [18]. The corresponding composition operator is denoted by $\oplus$.

A similar decomposition theorem can be proved for reducible DJ graphs. It is best visualized by the symbolic equation (cf. [24]) shown in Fig. 2. The only allowed edges are *forward edges* from nodes in $G_1$ to $r_2$ and *back edges* from nodes in $G_2$ to $r_1$. Note that the edge from $r_1$ to $r_2$, if not present in the underlying flow graph, is contained in its dominator tree.

Now, assume that $G_1$ has $k + 1$ nodes and $G_2$ has $n - k$ nodes. Then $G = G_1 \oplus G_2$ has $n + 1$ nodes and there are $k + (n - k)$ possible edges. Hence a recurrence relation for $r_n$, the number of reducible DJ graphs with $n + 1$ nodes follows immediately

\[
\begin{align*}
    r_0 &= 1 \\
    r_n &= 2^n \sum_{k=0}^{n-1} r_k r_{n-k-1}.
\end{align*}
\]

(5)

If we assume that the underlying flow graph does not contain loops, no back edges exist. Thus Fig. 2 allows to quickly find a recurrence relation for $a_n$, the number of acyclic (reducible) flow graphs with $n + 1$ nodes. Clearly $a_n$ fulfills the recurrence relation in Eq. (4).

The next section will be devoted to the studying of the number of reducible DJ graphs given by (5). However, recurrence relation (5) can neither be brought into a form studied in [10] nor into one that is comparable to those discussed in [5]. Thus (5) needs different treatment. We shall develop from (5) a kind of $q$-Catalan numbers for which we will derive a full asymptotic expansion.
**Figure 2.** $G = G_1 \oplus G_2$: A Symbolic Equation for Enumerating Reducible Flow Graphs

<table>
<thead>
<tr>
<th>$n$</th>
<th>$r_n = \overline{r}_{n+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>16</td>
</tr>
<tr>
<td>3</td>
<td>288</td>
</tr>
<tr>
<td>4</td>
<td>10240</td>
</tr>
<tr>
<td>5</td>
<td>700416</td>
</tr>
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<td>6</td>
<td>92864512</td>
</tr>
<tr>
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<td>24184487936</td>
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<tr>
<td>8</td>
<td>12484798840832</td>
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<tr>
<td>9</td>
<td>12835745584644096</td>
</tr>
<tr>
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</tr>
<tr>
<td>18</td>
<td>56127644484656663221666495855250671194867830902552354881536</td>
</tr>
</tbody>
</table>

**Table 1.** The first few values of $r_n$. 

**back edges**

**G**

**1**

**r**

**1**

**G**

**2**

**forward edges**

**r**

**2**

$G_1$

$G_2$
3. Enumerating Reducible DJ Graphs, and a q-analog of Catalan Numbers

In order to obtain an asymptotic expansion of \( r_n \), the first few values of which are displayed in Table 1, we let \( r_n = 2^{\frac{n^2+3n}{2}} p_n \) and find for \( n \geq 1 \)

\[
p_n = \frac{1}{2} \sum_{k=0}^{n-1} \frac{p_k p_{n-k-1}}{2^k(n-k-1)}
\]

\( p_0 = 1. \)

In addition, we let \( C_n = 2^n \cdot p_n \) and get

\[
C_n = \sum_{k=0}^{n-1} \frac{C_k C_{n-k-1}}{2^k(n-k-1)}
\]

\( C_0 = 1. \)

Generalizing we define now q-Catalan numbers \( C_n(q) \) by

\[
C_n(q) = \sum_{k=0}^{n-1} C_k(q) C_{n-k-1}(q) q^{k(n-k-1)}
\]

\( C_0(q) = 1. \)

and an auxiliary sequence \( p_n(q) \) by

\[
p_n(q) = \frac{1}{2} \sum_{k=0}^{n-1} p_k(q) p_{n-k-1}(q) q^{k(n-k-1)}
\]

\( = p_{n-1}(q) + \frac{1}{2} \sum_{k=1}^{n-2} p_k(q) p_{n-k-1}(q) q^{k(n-k-1)} \)

\( p_0(q) = 1, \)

so that \( C_n(q) = 2^n p_n(q). \)

Observe that \( C_n(1) = c_n \), the classical Catalan numbers, \( C_n(\frac{1}{2}) = C_n \), and observe the difference between recurrences (2) and (8).

Using arguments from enumerative combinatorics we will show in the next proposition that for all \( n \) and for \( 0 \leq q < 1 \), \( p_n(q) \) is bounded from above by some \( C(q) \).

**Proposition 1.** For \( n \geq 1 \) and for \( 0 \leq q < 1 \) we have

\[
C_n(q) = 2^n p_n(q) \leq 2^n \prod_{k \geq 1} \left( 1 + \frac{q^k}{2(1 - q^k)} \right).
\]
Figure 3. Lattice path visualizing the recurrence relation for $C_n(q)$.

Figure 4. Ferrers graph of partition $56 = 1 + 1 + 1 + 3 + 3 + 3 + 3 + 7 + 8 + 8 + 8 + 10$ if lattice path is viewed from the NW side. Note that if the light gray squares are removed, no valid partition is left.
Proof. We start by observing that similar to [10] recurrence relation (8) can be interpreted by considering a certain part of the area “above” a lattice path in Figure 3. Note however that our situation differs from the one occurring in [10] for standard $q$-Catalan numbers in that the area of the light gray squares is not counted, the reason being the presence of the term $(n - k - 1)$ in (8) instead of $(n - k)$ in (2).

If we proceed recursively we may arrive at a graph shown in Figure 4, and the contribution of this lattice path to $C_n(q)$ is given by $q^m$, where $m$ is the area of all middle and dark gray squares in Figure 4. Unfortunately in our situation, viewed from the NW side, this graph cannot be interpreted as a Ferrers graph of a certain partition. In general, as the example in Figure 4 shows, this makes our situation more complicated than the one in [10]. Note that the light gray squares do not appear in our sum, but the two darker gray ones do.

Nevertheless our interpretation of $C_n(q)$ as the counting function of the area in middle and dark gray “above” the corresponding lattice paths is still helpful to derive an upper estimate. In order to find an upper bound for $C_n(q)$ we may eliminate additional squares from the ones colored in middle or dark gray. The reason is that the resulting function $U_n(q)$ will then contain terms with smaller exponents of $q$. When evaluating $U_n(q)$ for some fixed $0 \leq q < 1$ we will then obtain $U_n(q) \geq C_n(q)$.

In particular, we eliminate all squares of the first appearance of a summand in the partitions corresponding to all gray squares. In our example in Figure 4 the eliminated squares are those of the first summand 3 and the summands 7, 8, and 10. The corresponding squares are shown in middle gray.

A short consideration shows that the generating function of these partitions is given by the infinite product

$$(2 + q + q^2 + \ldots) \cdot (2 + q^2 + q^4 + \ldots) \cdot (2 + q^3 + q^6 + \ldots) \cdot \ldots$$

The number “2” comes from the fact that either the corresponding summand was not present from the beginning (light gray squares) or it has been eliminated (middle gray squares).

Since none of the summands both in the original and in the partition after the elimination process can be greater than $n$, we have

$$C_n(q) \leq \prod_{k=1}^{n} \left( 2 + \frac{q^k}{1 - q^k} \right),$$

*Why we have three different gray colors, will soon be clear.
Figure 5. Plot of $\beta(q) = \lim_{n \to \infty} C_n(q) \cdot 2^{-n}$

resp.

$$p_n(q) \leq \prod_{k=1}^{n} \left(1 + \frac{q^k}{2(1-q^k)}\right).$$

Since $\sum_{k \geq 1} \frac{q^k}{2(1-q^k)} = \frac{1}{2} \sum_{k,j \geq 1} q^{kj}$ converges absolutely, the infinite product converges for $0 \leq q < 1$. Thus the proposition is proved.

From (9) it is easy to see that for fixed $0 \leq q < 1$ $p_n(q)$ is monotonically increasing.

Hence we conclude from Proposition 1 that for some fixed $0 \leq q < 1$ $p_n(q)$ converges to a limit $\beta(q)$. A plot of $\beta(q)$ is shown in Figure 5.

Thus we have proved that

$$r_n \sim 2^{n^2 + 3n \frac{2}{2}} \cdot \beta(1/2) \quad \text{as } n \to \infty.$$

By numerical computations we find that

$$\beta(1/2) = 0.715337433614869740944075474484711589980951273610256 \ldots.$$

In the following we derive the complete asymptotic expansion of $C_n(q)$ for $n \to \infty$. First we give a representation of $p_n(q)$ in terms of a double
series

\[ p_n(q) = p_1(q) + \sum_{j=2}^{n} (p_j(q) - p_{j-1}(q)) \]

\[ = \frac{1}{2} + \frac{1}{2} \sum_{j=2}^{n} p_j(q) \cdot p_{j-1-k}(q) \cdot q^{k(j-1-k)} \]

\[ = \frac{1}{2} + \frac{1}{2} \sum_{k=1}^{n-2} p_k(q) \sum_{j=2}^{n-2} p_{j-1-k}(q) \cdot q^{k(j-1-k)}. \]

By a change of variable \( m = j - 1 - k \) we obtain for \( n \geq 2 \)

\[ p_n(q) = \frac{1}{2} + \frac{1}{2} \sum_{k=1}^{n-2} p_k(q) \sum_{m=1}^{n-1-k} p_m(q) \cdot q^{km}. \]

By extending the domain of summation to \( \infty \) we find

\[ p_n(q) = \frac{1}{2} + \frac{1}{2} \sum_{k,m=1}^{\infty} p_k(q) \cdot p_m(q) \cdot q^{km} \]

where \( B_n^{(1)} \) is a suitably defined set of pairs of integers. A diagram of \( B_n^{(s)} \), a generalized form of \( B_n^{(1)} \), can be found in Figure 6.

As the \( p_n(q) \) are bounded, the series is absolutely convergent.

In the next step we are going to estimate the last term of (10). We have

\[ \frac{1}{2} \sum_{(k,m) \in B_n^{(1)}} p_k(q) \cdot p_m(q) \cdot q^{km} \leq \frac{\beta(q)^2}{2} \sum_{(k,m) \in B_n^{(1)}} q^{km} \]

\[ \leq \frac{\beta(q)^2}{2} \sum_{j=n-1}^{\infty} j \cdot q^j \left\{ (k,m) \in B_n^{(1)} \mid km = j \right\} \leq \frac{\beta(q)^2}{2} \sum_{j=n-1}^{\infty} j \cdot q^j. \]

Because of \( \sum_{j=n-1}^{\infty} j \cdot q^j = \frac{q^{n-1}(n(1-q) + 2q - 1)}{(1-q)^2} \) we get

\[ \frac{1}{2} \sum_{(k,m) \in B_n^{(1)}} p_k(q) \cdot p_m(q) \cdot q^{km} \leq \frac{\beta(q)^2}{2} \frac{q^{n-1}(n(1-q) + 2q - 1)}{(1-q)^2} \]

Hence we have proved for \( n \to \infty \)

\[ p_n(q) = \frac{1}{2} + \frac{1}{2} \sum_{k,m=1}^{\infty} p_k(q) \cdot p_m(q) \cdot q^{km} + O(n \cdot q^n). \]
In particular, we have

\begin{align*}
\beta(q) &= \lim_{n \to \infty} p_n(q) = \frac{1}{2} + \frac{1}{2} \sum_{k,m=1}^{\infty} p_k(q) p_m(q) q^{km} \\
&= \frac{1}{2} + \frac{1}{2} \sum_{j=1}^{\infty} q^j \sum_{d|j} p_d(q) \cdot p_{j/d}(q)
\end{align*}

and

\begin{align*}
p_n(q) &= \beta(q) \cdot (1 + O(n q^n)), n \to \infty.
\end{align*}

Therefore

\begin{align*}
C_n(q) &= \beta(q) \cdot 2^n \cdot (1 + O(n q^n)), n \to \infty.
\end{align*}

The following theorem provides a complete asymptotic expansion of $C_n(q)$ as $n \to \infty$.

**Theorem 1.** Let $0 \leq q < 1$ and the sequence $(\alpha_j(q))$ be defined by

\[ \alpha_0(q) = 1, \]
\[ \alpha_j(q) = -\frac{1}{q-j-1} \sum_{i=1}^{j} q^{-j(i+1)} p_i(q) \alpha_{j-i}(q) \]

for $j \geq 1$.

Then we have for each $s \geq 0$

\begin{align*}
C_n(q) &= \beta(q) \cdot 2^n \cdot \left( \sum_{r=0}^{s} \alpha_r(q) q^{rn} + O_{s+1} \left( n q^{(s+1)n} \right) \right), n \to \infty.
\end{align*}

**Proof.** The proof is by induction.

For $s = 0$ we get (13). Thus the induction basis is settled.

Now, assume that (14) is already proved for $1, \ldots, s-1$. For $s$ we obtain

\begin{align*}
p_n(q) &= \beta(q) - \frac{1}{2} \sum_{(k,m) \in B_n^{(s)}} p_k(q) p_m(q) q^{km} \\
&= \beta(q) - \sum_{k=1}^{s} p_k(q) \sum_{m=n-k}^{\infty} p_m(q) q^{km} - \frac{1}{2} \sum_{(k,m) \in B_n^{(s)}} p_k(q) p_m(q) q^{km}
\end{align*}

Figure 6 shows the domains $D_n^{(s)}$ and $B_n^{(s)}$ valid for the second and third term, respectively.

Similar to (11) the third term can be estimated by $O\left( n q^{(s+1)n} \right)$.
Using the induction hypothesis the second term can be written

$$\beta(q) \sum_{k=1}^{s} p_k(q) \sum_{m=n-k}^{\infty} q^{km} \left( \sum_{j=0}^{s-k} \alpha_j(q) q^{jm} + O_{s-k+1} \left( m q^{(s-k+1)m} \right) \right).$$
Temporarily ignoring the O-terms, we obtain \((r = j + k)\)

\[
\beta(q) \sum_{r=1}^{s} \sum_{k=1}^{r} p_k(q) \alpha_{r-k}(q) \sum_{m=n-k}^{\infty} q^{rm} = \beta(q) \sum_{r=1}^{s} \sum_{k=1}^{r} p_k(q) \alpha_{r-k}(q)q^{-r(k+1)} \sum_{m+k+1 \geq n+1}^{\infty} q^{r(m+k+1)} \]

\[
= \beta(q) \sum_{r=1}^{s} \sum_{k=1}^{r} p_k(q) \alpha_{r-k}(q)q^{-r(k+1)} \cdot \frac{q^{r(n+1)}}{1 - q^r} \]

\[
= \beta(q) \sum_{r=1}^{s} q^{rn} (-\alpha_r(q))
\]

by the recurrence relation for \(\alpha_j\).

The O-terms can be estimated by

\[
\beta(q) \sum_{k=1}^{s} p_k(q) \sum_{m=n-k}^{\infty} O_{s-k+1} \left( m q^{(s+1)m} \right) = \sum_{k=1}^{s} p_k(q)O_{s-k+1} \left( n q^{(s+1)n} \right) = O_{s+1} \left( n q^{(s+1)n} \right).
\]

Hence the theorem is proved. \(\Box\)

Summing up, we have proved the complete asymptotic expansion for the number of reducible DJ graphs.

**Proposition 2.** The number of reducible DJ graphs with \(n\) nodes fulfills for each \(s\)

\[
\tau_n = r_{n-1} = \beta(1/2) \cdot 2^{\frac{n^2 + n - 2}{2}} \cdot \left( \sum_{r=0}^{s} \frac{\alpha_r(1/2)}{2^{rn}} + O_{s+1} \left( \frac{n}{2(s+1)n} \right) \right), \quad (n \to \infty)
\]

where

\[
\beta(1/2) = 0.715337433614869740944075474484711589980951273610256 \ldots
\]

and the \(\alpha_r(q)\) are defined in Theorem 1. \(\Box\)

### 4. Related Work

Until now enumerating flow graphs was not in the center of interest of scientific research. On the other hand flow graphs themselves are and have always been very useful for designing and analyzing software. Flowcharts are part of the UML ([8]) and flow graphs are prominently used in compilers
for code optimization. They are of fundamental importance for dataflow analysis (cf. e.g. [13, 17]) and for solving flow problems in general ([2]).

Vernet and Markenzon have studied maximal reducible flow graphs in [22, 23] which is the starting point for our analysis in Section 2. Independently Joshi et al. [15] have derived similar results for MRFs, but they did not find Vernet and Markenzon’s decomposition of MRFs. The decomposition theorem has been generalized to reducible flow graphs in [18].

Bender and Butler derived enumeration results for structured flowcharts in [6]. Their results cannot be directly related to ours because they study non-ordered, so-called BJ_m-charts. These are flow graphs consisting of if-then-else and do-while statements with m exits from the loops.

In [12] Gessel uses a decomposition process to setup relations for generating functions of rooted non-ordered digraphs. These graphs constitute non-ordered flow graphs in our terms.

In [7] the average case of an algorithm based on DJ graphs is studied. Only a subset of DJ graphs is considered in [7]. This subset consists of all DJ graphs which are built from goto-free programs (exits from loops are allowed, though). This subset can be derived by a graph grammar and the number of these graphs are calculated by studying this grammar.

5. Conclusions

Reinterpreting known results on q-Catalan numbers we found a connection between the number of acyclic DJ graphs and q-Catalan numbers \(C_n(q)\). A similar recurrence relation has been setup for the number of reducible DJ graphs, a well-known data structure in computer science. We have derived a full asymptotic expansion for a q-analog of the number of these graphs.

The recurrence relations we have studied in this paper show that there are hitherto unexplored q-analogs of Catalan numbers. Besides being interesting for their own, they are worth studying because they are useful in the analysis of data structures.

References


