

Roots $x_k(y)$ of a formal power series

$$f(x, y) = \sum_{n=0}^{\infty} a_n(y) x^n$$

with applications to graph enumeration
and q -series

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LECTURE #2

Applications of
the explicit implicit function formula
and the exponential formula

The basic set-up

Consider a formal power series

$$f(x, y) = \sum_{n=0}^{\infty} \alpha_n x^n y^{n(n-1)/2}$$

normalized to $\alpha_0 = \alpha_1 = 1$, or more generally

$$f(x, y) = \sum_{n=0}^{\infty} a_n(y) x^n$$

where

- (a) $a_0(0) = a_1(0) = 1$;
- (b) $a_n(0) = 0$ for $n \geq 2$; and
- (c) $a_n(y) = O(y^{\nu_n})$ with $\lim_{n \rightarrow \infty} \nu_n = \infty$.

Examples:

- The “partial theta function”

$$\Theta_0(x, y) = \sum_{n=0}^{\infty} x^n y^{n(n-1)/2}$$

- The “deformed exponential function” studied in Lecture #1:

$$F(x, y) = \sum_{n=0}^{\infty} \frac{x^n}{n!} y^{n(n-1)/2}$$

- More generally, consider

$$\tilde{R}(x, y, q) = \sum_{n=0}^{\infty} \frac{x^n y^{n(n-1)/2}}{(1+q)(1+q+q^2) \cdots (1+q+\dots+q^{n-1})}$$

which reduces to Θ_0 when $q = 0$, and to F when $q = 1$.

The leading root $x_0(y)$

- Start from a formal power series

$$f(x, y) = \sum_{n=0}^{\infty} a_n(y) x^n$$

where

- (a) $a_0(0) = a_1(0) = 1$
- (b) $a_n(0) = 0$ for $n \geq 2$
- (c) $a_n(y) = O(y^{\nu_n})$ with $\lim_{n \rightarrow \infty} \nu_n = \infty$

and coefficients lie in a commutative ring-with-identity-element R .

- By (c), each power of y is multiplied by only *finitely many* powers of x .
- That is, f is a formal power series in y whose coefficients are *polynomials* in x , i.e. $f \in R[x][[y]]$.
- Hence, for *any* formal power series $X(y)$ with coefficients in R [not necessarily with zero constant term], the composition $f(X(y), y)$ makes sense as a formal power series in y .
- Not hard to see (by the implicit function theorem for formal power series or by a direct inductive argument) that there exists a unique formal power series $x_0(y) \in R[[y]]$ satisfying $f_0(x_0(y), y) = 0$.
- We call $x_0(y)$ the **leading root** of f .
- Since $x_0(y)$ has constant term -1 , we will write $x_0(y) = -\xi_0(y)$ where $\xi_0(y) = 1 + O(y)$.

How to compute $\xi_0(y)$?

1. **Elementary method:** Insert $\xi_0(y) = 1 + \sum_{n=1}^{\infty} b_n y^n$ into $f(-\xi_0(y), y) = 0$ and solve term-by-term.
 2. Method based on the explicit implicit function formula.
 3. Method based on the exponential formula and expansion of $\log f(x, y)$.
- Methods #2 and #3 are computationally very efficient.
 - Can they also be used to give *proofs*?

Tools I: The explicit implicit function formula

- See A.D.S., arXiv:0902.0069 or Stanley, vol. 2, Exercise 5.59
- (Almost trivial) generalization of Lagrange inversion formula
- Comes in analytic-function and formal-power-series versions
- Recall Lagrange inversion: If $f(x) = \sum_{n=1}^{\infty} a_n x^n$ with $a_1 \neq 0$ (as either analytic function or formal power series), then

$$f^{-1}(y) = \sum_{m=1}^{\infty} \frac{y^m}{m} [\zeta^{m-1}] \left(\frac{\zeta}{f(\zeta)} \right)^m$$

where $[\zeta^n]g(\zeta)$ denotes the coefficient of ζ^n in the power series $g(\zeta)$.
More generally, if $h(x) = \sum_{n=0}^{\infty} b_n x^n$, we have

$$h(f^{-1}(y)) = h(0) + \sum_{m=1}^{\infty} \frac{y^m}{m} [\zeta^{m-1}] h'(\zeta) \left(\frac{\zeta}{f(\zeta)} \right)^m$$

- Rewrite this in terms of $g(x) = x/f(x)$: then $f(x) = y$ becomes $x = g(x)y$, and its solution $x = \varphi(y) = f^{-1}(y)$ is given by the power series

$$\varphi(y) = \sum_{m=1}^{\infty} \frac{y^m}{m} [\zeta^{m-1}] g(\zeta)^m$$

and

$$h(\varphi(y)) = h(0) + \sum_{m=1}^{\infty} \frac{y^m}{m} [\zeta^{m-1}] h'(\zeta) g(\zeta)^m$$

- There is also an alternate form

$$h(\varphi(y)) = h(0) + \sum_{m=1}^{\infty} y^m [\zeta^m] h(\zeta) [g(\zeta)^m - \zeta g'(\zeta) g(\zeta)^{m-1}]$$

The explicit implicit function formula, continued

- Generalize $x = g(x)y$ to $x = G(x, y)$, where
 - $G(0, 0) = 0$ and $|(\partial G/\partial x)(0, 0)| < 1$ (analytic-function version)
 - $G(0, 0) = 0$ and $(\partial G/\partial x)(0, 0) = 0$ (formal-power-series version)
- Then there is a unique $\varphi(y)$ with zero constant term satisfying $\varphi(y) = G(\varphi(y), y)$, and it is given by

$$\begin{aligned}\varphi(y) &= \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] G(\zeta, y)^m \\ &= \sum_{m=1}^{\infty} [\zeta^{m-1}] \left[G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1} \right]\end{aligned}$$

More generally, for any $H(x, y)$ we have

$$\begin{aligned}H(\varphi(y), y) &= H(0, y) + \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] \frac{\partial H(\zeta, y)}{\partial \zeta} G(\zeta, y)^m \\ &= H(0, y) + \sum_{m=1}^{\infty} [\zeta^m] H(\zeta, y) \left[G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1} \right]\end{aligned}$$

- First versions are slightly more convenient but require R to contain the rationals as a subring.
- Proof imitates standard proof of the Lagrange inversion formula: the variables y simply “go for the ride”.
- Alternate interpretation: Solving fixed-point problem for the family of maps $x \mapsto G(x, y)$ parametrized by y . Variables y again “go for the ride”.

A possible extension [open problem]

- Conditions on G and φ in the explicit implicit function formula seem natural:
 - If $G(x, y)$ is a formal power series, it ordinarily makes sense to substitute $x = \varphi(y)$ only when $\varphi(y)$ is a formal power series *with zero constant term*.
 - Then a solution to the fixed-point equation $\varphi(y) = G(\varphi(y), y)$ with $\varphi(y)$ having zero constant term can exist only if $G(0, 0) = 0$.
- But there is one important case where these conditions can be weakened: namely, if $G(x, y)$ belongs to $R[x][[y]]$, i.e. if the coefficient of each power of y is a *polynomial* in x .
 - In this case it makes sense to substitute for x an *arbitrary* formal power series $\varphi(y)$, *not necessarily with zero constant term*.
 - The result $G(\varphi(y), y)$ is a well-defined formal power series in y .
 - What can be said about existence and uniqueness of solutions to $\varphi(y) = G(\varphi(y), y)$?
 - And is there an explicit “Lagrange-like” formula for $\varphi(y)$?
 - I suspect that the answer is yes, but I haven’t worked out the details.
 - And it looks like this may be useful in our application.

Application to leading root of $f(x, y)$

- Start from a formal power series $f(x, y) = \sum_{n=0}^{\infty} a_n(y) x^n$ satisfying properties (a)–(c) above.
- Write out $f(-\xi_0(y), y) = 0$ and add $\xi_0(y)$ to both sides:

$$\xi_0(y) = a_0(y) - [a_1(y) - 1]\xi_0(y) + \sum_{n=2}^{\infty} a_n(y) (-\xi_0(y))^n$$

- Insert $\xi_0(y) = 1 + \varphi(y)$ where $\varphi(y)$ has zero constant term. Then $\varphi(y) = G(\varphi(y), y)$ where

$$G(z, y) = \sum_{n=0}^{\infty} (-1)^n \hat{a}_n(y) (1 + z)^n$$

and

$$\hat{a}_n(y) = \begin{cases} a_n(y) - 1 & \text{for } n = 0, 1 \\ a_n(y) & \text{for } n \geq 2 \end{cases}$$

And $\varphi(y)$ is the *unique* formal power series with zero constant term satisfying this fixed-point equation.

- Since this G satisfies $G(0, 0) = 0$ and $(\partial G / \partial z)(0, 0) = 0$ [indeed it satisfies the stronger condition $G(z, 0) = 0$], we can apply the explicit implicit function formula to obtain an explicit formula for $\xi_0(y)$:

$$\xi_0(y) = 1 + \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] \left(\sum_{n=0}^{\infty} (-1)^n \hat{a}_n(y) (1 + \zeta)^n \right)^m$$

More generally, for any formal power series $H(z, y)$, we have

$$\begin{aligned} & H(\xi_0(y) - 1, y) \\ &= H(0, y) + \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] \frac{\partial H(\zeta, y)}{\partial \zeta} \left(\sum_{n=0}^{\infty} (-1)^n \hat{a}_n(y) (1 + \zeta)^n \right)^m \end{aligned}$$

Application to leading root of $f(x, y)$, continued

- In particular, by taking $H(z, y) = (1 + z)^\beta$ we can obtain an explicit formula for an arbitrary power of $\xi_0(y)$:

$$\xi_0(y)^\beta = 1 + \sum_{m=1}^{\infty} \frac{\beta}{m} \sum_{n_1, \dots, n_m \geq 0} \binom{\beta - 1 + \sum n_i}{m - 1} \prod_{i=1}^m (-1)^{n_i} \widehat{a}_{n_i}(y)$$

- Important special case: $a_0(y) = a_1(y) = 1$ and $a_n(y) = \alpha_n y^{\lambda_n}$ ($n \geq 2$) where $\lambda_n \geq 1$ and $\lim_{n \rightarrow \infty} \lambda_n = \infty$. Then

$$[y^N] \frac{\xi_0(y)^\beta - 1}{\beta} = \sum_{m=1}^{\infty} \frac{1}{m} \sum_{\substack{n_1, \dots, n_m \geq 2 \\ \sum_{i=1}^m \lambda_{n_i} = N}} (-1)^{\sum n_i} \binom{\beta - 1 + \sum n_i}{m - 1} \prod_{i=1}^m \alpha_{n_i}$$

- Can this formula be used for proofs of nonnegativity???
- *Empirically* I know that the RHS is ≥ 0 when $\lambda_n = n(n-1)/2$:
 - For $\beta \geq -2$ with $\alpha_n = 1$ (partial theta function)
 - For $\beta \geq -1$ with $\alpha_n = 1/n!$ (deformed exponential function)
 - For $\beta \geq -1$ with $\alpha_n = (1 - q)^n / (q; q)_n$ and $q > -1$
- And I can *prove* this (by a *different* method!) for the partial theta function with $\beta \geq -1$
- **How can we see these facts from this formula???**
[open combinatorial problem]

Tools II: Variants of the exponential formula

- Let R be a commutative ring containing the rationals.
- Let $A(x) = \sum_{n=0}^{\infty} a_n x^n$ be a formal power series (with coefficients in R) satisfying $a_0 = 1$.
- Now consider $C(x) = \log A(x) = \sum_{n=1}^{\infty} c_n x^n$.
- It is well known (and easy to prove) that

$$a_n = \sum_{k=1}^n \frac{k}{n} c_k a_{n-k} \quad \text{for } n \geq 1$$

This allows $\{a_n\}$ to be calculated given $\{c_n\}$, or vice versa.

- Sometimes useful to introduce $\tilde{c}_n = n c_n$, which are the coefficients in

$$\frac{x A'(x)}{A(x)} = \sum_{n=1}^{\infty} \tilde{c}_n x^n$$

- See Scott–Sokal, arXiv:0803.1477 for generalizations to $A(x)^\lambda$ and applications to the multivariate Tutte polynomial
- Now specialize to $R = R_0[[y]]$ and $A(x, y) = \sum_{n=0}^{\infty} a_n(y) x^n$ where $a_0(y) = 1$
- Assume further that $a_1(0) = 1$ and $a_n(0) = 0$ for $n \geq 2$ [conditions (a) and (b) for our $f(x, y)$]
- Then

$$\frac{x A'(x, y)}{A(x, y)} = \sum_{n=1}^{\infty} \tilde{c}_n(y) x^n$$

where $'$ denotes $\partial/\partial x$ and $\tilde{c}_n(y)$ has constant term $(-1)^{n-1}$.

Application to leading root of $f(x, y)$

- Start from a formal power series $f(x, y) = 1 + x + \sum_{n=2}^{\infty} a_n(y) x^n$ satisfying

$$a_n(y) = O(y^{\alpha(n-1)}) \quad \text{for } n \geq 2$$

for some real $\alpha > 0$. [This is a bit stronger than (a)–(c).]

- Define $\{\tilde{c}_n(y)\}_{n=1}^{\infty}$ by

$$\frac{x f'(x, y)}{f(x, y)} = \sum_{n=1}^{\infty} \tilde{c}_n(y) x^n$$

where $'$ denotes $\partial/\partial x$.

- **Theorem:** We have

$$\tilde{c}_n(y) = (-1)^{n-1} \xi_0(y)^{-n} + O(y^{\alpha n})$$

or equivalently

$$\xi_0(y) = [(-1)^{n-1} \tilde{c}_n(y)]^{-1/n} + O(y^{\alpha n})$$

- This theorem provides an extraordinarily efficient method for computing the series $\xi_0(y)$:

– Compute the $\tilde{c}_n(y)$ inductively using the recursion

$$\tilde{c}_n = n a_n - \sum_{k=1}^{n-1} \tilde{c}_k a_{n-k}$$

– Take the power $-1/n$ to extract $\xi_0(y)$ through order $y^{\lceil \alpha n \rceil - 1}$

- This abstracts the recursive method shown in Lecture #1 for the special case $F(x, y) = \sum_{n=0}^{\infty} \frac{x^n}{n!} y^{n(n-1)/2}$.

Proof of Theorem (via complex analysis)

- Use complex-analysis argument to prove Theorem when $R = \mathbb{C}$ and f is a polynomial.
- Infer general validity by some abstract nonsense.

Lemma. Fix a real number $\alpha > 0$, and let $P(x, y) = 1 + x + \sum_{n=2}^N a_n(y)x^n$ where the $\{a_n(y)\}_{n=2}^N$ are polynomials with complex coefficients satisfying $a_n(y) = O(y^{\alpha(n-1)})$. Then there exist numbers $\rho > 0$ and $\gamma > 0$ such that $P(\cdot, y)$ has precisely one root in the disc $|x| < \gamma|y|^{-\alpha}$ whenever $|y| \leq \rho$.

Idea of proof: Apply Rouché's theorem to $f(x) = x$ and $g(x) = 1 + \sum_{n=2}^N a_n(y)x^n$ on the circle $|x| = \gamma|y|^{-\alpha}$.

Proof of Theorem when $R = \mathbb{C}$ and f is a polynomial:
Write

$$P(x, y) = \prod_{i=1}^{k(y)} \left(1 - \frac{x}{X_i(y)}\right)$$

with $k(y) \leq N$. Therefore

$$\frac{x P'(x, y)}{P(x, y)} = \sum_{i=1}^{k(y)} \frac{-x/X_i(y)}{1 - x/X_i(y)}$$

and hence

$$\tilde{c}_n(y) = - \sum_{i=1}^{k(y)} X_i(y)^{-n}.$$

Now, for small enough $|y|$, one of the roots is given by the *convergent* series $-\xi_0(y)$ and is smaller than $\gamma|y|^{-\alpha}$ in magnitude, while the

other roots have magnitude $\geq \gamma|y|^{-\alpha}$ by the Lemma. We therefore have

$$|\tilde{c}_n(y) - (-1)^{n-1}\xi_0(y)^{-n}| \leq (N-1)\gamma^{-n}|y|^{\alpha n}$$

for small enough $|y|$, as claimed. \square

Proof of Theorem in general case: Write

$$a_n(y) = \sum_{m=\lceil \alpha(n-1) \rceil}^{\infty} a_{nm} y^m$$

Work in the ring $R = \mathbb{Z}[\mathbf{a}]$ where $\mathbf{a} = \{a_{nm}\}_{n \geq 2, m \geq \lceil \alpha(n-1) \rceil}$ are treated as indeterminates. Then the claim of the Theorem amounts to a series of identities between polynomials in \mathbf{a} with integer coefficients. We have verified these identities when evaluated on collections \mathbf{a} of complex numbers of which only finitely many are nonzero; and this is enough to prove them as identities in $\mathbb{Z}[\mathbf{a}]$. \square

There is also a direct formal-power-series proof (due to Ira Gessel) at least in the case $\alpha = 1$. I don't know whether it extends to arbitrary real $\alpha > 0$.

Computational use of Theorem

- Can compute $\xi_0(y)$ through order y^{N-1} by computing $\tilde{c}_N(y)$
- Do this by computing $\tilde{c}_n(y)$ for $1 \leq n \leq N$ using recursion
- Observe that all $\tilde{c}_n(y)$ can be truncated to order y^{N-1}
[no need to keep the full polynomial of degree $n(n-1)/2$]
- For F , have done $N = 900$
[$N = 400$ takes a minute, $N = 900$ takes less than 6 hours;
but $N = 900$ needs 24 GB memory!]
- For Θ_0 , have done $N = 7000$
[$N = 500$ takes a minute, $N = 1500$ takes less than an hour;
 $N = 7000$ took 11 days and 21 GB memory]
- For \tilde{R} , have done $N = 350$
[$N = 50$ takes a minute, $N = 100$ takes less than an hour;
 $N = 350$ took a month and 10 GB memory]

Some positivity properties of formal power series

- Consider formal power series with real coefficients

$$f(y) = 1 + \sum_{m=1}^{\infty} a_m y^m$$

- For $\alpha \in \mathbb{R}$, define the class \mathcal{S}_α to consist of those f for which

$$\frac{f(y)^\alpha - 1}{\alpha} = \sum_{m=1}^{\infty} b_m(\alpha) y^m$$

has all nonnegative coefficients (with a suitable limit when $\alpha = 0$).

- In other words:
 - For $\alpha > 0$ (resp. $\alpha = 0$), the class \mathcal{S}_α consists of those f for which f^α (resp. $\log f$) has all nonnegative coefficients.
 - For $\alpha < 0$, the class \mathcal{S}_α consists of those f for which f^α has all *nonpositive* coefficients after the constant term 1.
- Containment relations among the classes \mathcal{S}_α are given by the following fairly easy result:

Proposition (Scott–A.D.S., unpublished):

Let $\alpha, \beta \in \mathbb{R}$. Then $\mathcal{S}_\alpha \subseteq \mathcal{S}_\beta$ if and only if either

- (a) $\alpha \leq 0$ and $\beta \geq \alpha$, or
- (b) $\alpha > 0$ and $\beta \in \{\alpha, 2\alpha, 3\alpha, \dots\}$.

Moreover, the containment is strict whenever $\alpha \neq \beta$.

Application to deformed exponential function F

As shown last week, it seems that $\xi_0(y) \in \mathcal{S}_1$:

$$\begin{aligned}\xi_0(y) = & 1 + \frac{1}{2}y + \frac{1}{2}y^2 + \frac{11}{24}y^3 + \frac{11}{24}y^4 + \frac{7}{16}y^5 + \frac{7}{16}y^6 \\ & + \frac{493}{1152}y^7 + \frac{163}{384}y^8 + \frac{323}{768}y^9 + \frac{1603}{3840}y^{10} + \frac{57283}{138240}y^{11} \\ & + \frac{170921}{414720}y^{12} + \frac{340171}{829440}y^{13} + \frac{22565}{55296}y^{14} \\ & + \dots + \text{terms through order } y^{899}\end{aligned}$$

and indeed that $\xi_0(y) \in \mathcal{S}_{-1}$:

$$\begin{aligned}\xi_0(y)^{-1} = & 1 - \frac{1}{2}y - \frac{1}{4}y^2 - \frac{1}{12}y^3 - \frac{1}{16}y^4 - \frac{1}{48}y^5 - \frac{7}{288}y^6 \\ & - \frac{1}{96}y^7 - \frac{7}{768}y^8 - \frac{49}{6912}y^9 - \frac{113}{23040}y^{10} - \frac{17}{4608}y^{11} \\ & - \frac{293}{92160}y^{12} - \frac{737}{276480}y^{13} - \frac{3107}{1658880}y^{14} \\ & - \dots - \text{terms through order } y^{899}\end{aligned}$$

But I have no proof of either of these conjectures!!!

- Note that $\xi_0(y)$ is analytic on $0 \leq y < 1$ and diverges as $y \uparrow 1$ like $1/[e(1-y)]$.
- It follows that $\xi_0(y) \notin \mathcal{S}_\alpha$ for $\alpha < -1$.

Application to partial theta function Θ_0

It seems that $\xi_0(y) \in \mathcal{S}_1$:

$$\begin{aligned}\xi_0(y) = & 1 + y + 2y^2 + 4y^3 + 9y^4 + 21y^5 + 52y^6 + 133y^7 + 351y^8 \\ & + 948y^9 + 2610y^{10} + \dots + \text{terms through order } y^{6999}\end{aligned}$$

and indeed that $\xi_0(y) \in \mathcal{S}_{-1}$:

$$\begin{aligned}\xi_0(y)^{-1} = & 1 - y - y^2 - y^3 - 2y^4 - 4y^5 - 10y^6 - 25y^7 - 66y^8 \\ & - 178y^9 - 490y^{10} - \dots - \text{terms through order } y^{6999}\end{aligned}$$

and indeed that $\xi_0(y) \in \mathcal{S}_{-2}$:

$$\begin{aligned}\xi_0(y)^{-2} = & 1 - 2y - y^2 - y^4 - 2y^5 - 7y^6 - 18y^7 - 50y^8 \\ & - 138y^9 - 386y^{10} - \dots - \text{terms through order } y^{6999}\end{aligned}$$

Here I *do* have a proof of the first two properties (but not the third).

Coming next week!

- Note that

$$\frac{\xi_0(y)^\alpha - 1}{\alpha} = y + \frac{\alpha + 3}{2}y^2 + \frac{(\alpha + 2)(\alpha + 7)}{6}y^3 + O(y^4)$$

- So $\xi_0(y) \notin \mathcal{S}_\alpha$ for $\alpha < -2$.

Application to $\tilde{R}(x, y, q) = \sum_{n=0}^{\infty} \frac{x^n y^{n(n-1)/2}}{(1+q) \cdots (1+q+\dots+q^{n-1})}$

- Can use explicit implicit function formula to prove that

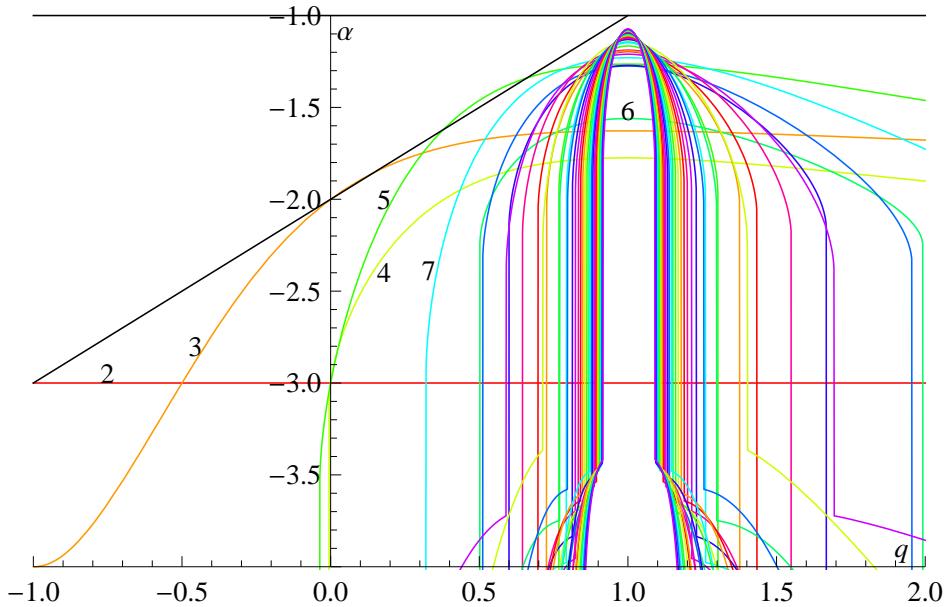
$$\xi_0(y; q) = 1 + \sum_{n=1}^{\infty} \frac{P_n(q)}{Q_n(q)} y^n$$

where

$$Q_n(q) = \prod_{k=2}^{\infty} (1+q+\dots+q^{k-1})^{\lfloor n/\binom{k}{2} \rfloor}$$

and $P_n(q)$ is a self-inversive polynomial in q with integer coefficients.

- *Empirically* $P_n(q)$ has *two* interesting positivity properties:
 - (a) $P_n(q)$ has all nonnegative coefficients. Indeed, all the coefficients are strictly positive except $[q^1] P_5(q) = 0$.
 - (b) $P_n(q) > 0$ for $q > -1$.
- *Empirically* $\xi_0(y; q) \in \mathcal{S}_{-1}$ for all $q > -1$:



Can any of this be proven???

- It seems that $\tilde{R}(x, y, q)$ is the right unification of Θ_0 and F .
- But thus far my proofs are only for $q = 0$ (i.e. Θ_0).

Coming next week!

- Can anything be generalized to $q \neq 0$???
- **Open problem:** For $q = 0$, prove $\xi_0(y) \in \mathcal{S}_1$ or \mathcal{S}_{-1} (or even \mathcal{S}_{-2}) *directly from the explicit implicit function formula.*
- If this works, it might be generalizable to $q \neq 0$.