ON THE GAUSS-KUZMIN-WIRSING CONSTANT

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Abstract. We give strong supporting evidence for the fact that the Gauss-Kuzmin-Wirsing constant is

$$|\lambda_2| = 0.30366\,30028\,98732\,65859\,74481\,21901\,5\mathit{5623} \pm 10^{-31}.$$

If x_0 is uniformly distributed in $[0,1]$, then the nth iterate $x_n = T^{(n)}(x_0)$ of the continued fraction transformation

$$T(x) = \{\frac{1}{x}\}$$

(where $\{x\} = x - \lfloor x \rfloor$ denotes the fractional part) has a distribution $F_n(x) = \Pr(x_n < x)$ that converges geometrically to the invariant density $F_\infty(x)$ found by Gauß, namely,

$$F_\infty(x) = \log_2(1+x)\,.$$

The rate of convergence is exponential being of the form $O(\lambda_2^n)$, as established by Wirsing [8] using operator methods (the Perron-Frobenius theory). Babenko [1] and Mayer (see [7] for a survey) later provided a complete spectral decomposition of the form

$$F_n(x) = F_\infty(x) + \sum_{k=2}^{\infty} \lambda_k^n \Psi_k(x),$$

for some eigenvalues λ_k and some analytic eigenfunctions $\Psi_k(x)$.

In the course of a joint work with H. Daudé relative to an average-case analysis of lattice reduction in dimension 2, we came accross a need to compute quantities analogous to the Gauss-Kuzmin-Wirsing constant, $\lambda_2 \approx -0.30366$ (obtained to 20 decimal places by Wirsing and quoted by Knuth in [5], p. 350). Our problem was relative to the average-case analysis of lattice reduction in dimension 2 and it is discussed in the extended abstract [2] with the corresponding computational methods being developed in the full paper [3].

There is renewed interest in these questions (see [4] and "around" for many fascinating pages). The analysis involves an operator introduced by Wirsing whose properties were further elucidated by Babenko and Mayer. The eigenvalues of that operator as originally computed by Babenko are very likely to contain some spurious ones. Knuth [5, p. 350] following Babenko gives $\lambda_4 = -0.0408$ which is almost certainly *not* an eigenvalue. Scepticism has been expressed over the last decade by many people, like Mayer (see the references in [2, 3, 7]), Knuth (personal communication, 1994), MacLeod (see [6], cited in [4]).

The computational approach of [3] yields *highly plausible values* for the dominant eigenvalues, a theoretical possibility to transform numerical computations into certified proofs —for $\lambda_2 \approx -0.30366$ at least—, and finally a global numerical check by means of trace formulæ of Babenko and Mayer.

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1. We want to find the spectrum of the operator which to a function $f(t)$ (of the argument t) associates another function (of the argument x)

$$\mathcal{G}_2[f(t)](x) := \sum_{n=1}^{\infty} \frac{1}{(n+x)^2} f(\frac{1}{n+x}).$$

The idea is simply to look at the effect of this operator on Taylor expansions. For instance, the operator $\mathcal{G}_2$ acting on Taylor expansions at 0 corresponds to an infinite matrix whose entries are simply zeta functions since

$$\mathcal{G}_2[t^r](x) = \zeta(r+2, x+1),$$

and the Taylor expansion of the Hurwitz zeta function $\zeta(s,a)$ just involves the Riemann zeta function. From numerical experiments, there appears that an expansion around $\frac{1}{2}$ even leads to faster convergence; we are then dealing with matrices whose entries involve finite combinations of zeta values at the integers. Of course, we know that such zeta values are "easily" computable, and Maple will kindly do this for us.

2. Next, we hope for the best and expect that *the finite truncations of the infinite matrix have eigenvalues that converge (when truncation order becomes larger) to eigenvalues of the operator $\mathcal{G}_2$.* The idea is easy to try, and we find some values that stabilize fast, others that tend to disappear as the truncation order increases. For instance, using an accuracy of 100 digits and truncation to order $m = 64$, we find the plausible eigenvalues (the vertical bar indicates our estimated limit of accuracy[3]; we claim the last digit before the vertical bar to be correct!):

$$\begin{aligned}
\lambda_1 &= +0.99999999999999999999999999999999|600 \\
\lambda_2 &= -0.30366300289873265859744812190155|493 \\
\lambda_3 &= +0.10088450929310407530563764299 2|35579 \\
\lambda_4 &= -0.03549615902165984540889168113|760384.
\end{aligned}$$

Of course we know that $\lambda_1 = 1$. Now the "plausible" accuracy is obtained by making sure that 100 digits is amply sufficient for $m = 64$, by comparing increasing truncation orders, and by developing empirical estimates on error[4]. Some sort of weird alchemy! (See below for tables.) In Maple, the reference computation ($m = 64$) takes only about 30 minutes on a DEC Alpha station (≈ 100 Mips).

3. We can go much farther if we further relax rigor but, strangely enough, at the same time we even get a better confirmation for the *whole collection* of eigenvalues found. First, we observe as MacLeod did before us that the ratio between eigenvalues is close to -2.6. There are good reasons to believe this unproven fact for the $\mathcal{G}_2$ operator to be true, as discussed in [3]. Roughly, if we approximate $\mathcal{G}_2[f(t)](x)$ by its first term,

$$\frac{1}{(1+x)^2} f(\frac{1}{1+x}),$$

[3]This limit is based on extrapolation of the error pattern observed for smaller values of the truncation order m *and* on a computation with $digits = 110$ and $m = 70$ done in 4400 seconds of CPU time. Both approaches essentially agree and the estimates cited are conservative.

[4]Rougly, for a truncation of order m, we get about $m/2$ digits of accuracy for the first two eigenvalues; then we loose a little less than 1 digit for each successive eigenvalue

then we get an operator whose spectrum can be determined explicitly and the ratio between consecutive eigenvalues is then *exactly*

$$-\phi^2 = -2.61803.$$

(We expect the further terms in the definition of $\mathcal{G}_2$ to act as small perturbations.)

With this process, we can "filter" spurious eigenvalues without a need to go to exorbitant truncation orders. Some more alchemy is needed here to design an automatic filtering routine (eliminate complex values, impose a ratio between consecutive eigenvalues in $[-2.75, -2.45]$ except for the very first ones), but in this way we get an *a priori* plausible set of 42 eigenvalues, the last one obtained being about $0.5\,10^{-17}$.

4. The wild extrapolation of §3 seems rather unjustifiable. However, from Babenko's paper and subsequent work by Mayer, we do have trace formulæ. Actually, the trace of the $\mathcal{G}_2$ operator can be computed to very high accuracy by means of a zeta function expansion, the details being explained in our paper [3]. For the trace,

$$Tr\mathcal{G}_2 = \sum_{j=1}^{\infty} \lambda_j,$$

we find here

$$\begin{aligned} Tr\mathcal{G}_2 &= \frac{1}{2} - \frac{1}{2\sqrt{5}} + \frac{1}{2}\sum_{k=1}^{\infty}(-1)^{k-1}\binom{2k}{k}(\zeta(2k)-1) \\ &= 1 - \frac{1}{2\sqrt{2}} - \frac{1}{2\sqrt{5}} + \frac{1}{2}\sum_{k=1}^{\infty}(-1)^{k-1}\binom{2k}{k}(\zeta(2k) - 1 - \frac{1}{2^{2k}}) \\ &= 0.7711255236555658909317317763277706906373 \pm 10^{-40}, \end{aligned}$$

with *guaranteed* accuracy. (One could get several hundred digits of this trace with limited computational effort.) Similarly, we can compute to great accuracy:

$$Tr\mathcal{G}_2^2 = 1.103839653617613250075195387345 \pm 10^{-30}.$$

Now, we just take our 42 eigenvalues (filtered out of the set of 64), sum them and get a quantity that differs by about $2 \cdot 10^{-17}$ from the exact trace. This is of the same order as the last neglected eigenvalue. In addition, the sum of the squares differs from $7 \cdot 10^{-29}$ from the $Tr\mathcal{G}^2$. So, we can be quite confident that all this makes sense!

Some of the next eigenvalues found in this way are:

$$\begin{aligned} \lambda_5 &= +0.0128437903624402648151602952 9|9518118 \\ \lambda_6 &= -0.004717777511571031073875474 9|84732768 \\ \lambda_7 &= +0.001748675124305511913311709 6|56958713 \\ \lambda_8 &= -0.000652020858320502900330267|646264028 \\ \lambda_9 &= +0.000244131465524515812136 85|1087309327 \\ \lambda_{10} &= -0.00009168908376859330297|7684599961 \end{aligned}$$

5. The empirical computational complexity is somewhere around n^5 or n^6 for n digits. With a full day of Maple computations, one can double the truncation order. (For our $\mathcal{G}_4$, we did more minutious computations and went to truncation orders till 100). By using other lower-level systems like Pari, one could probably get a further speedup of 10. So, over a weekend, it should be possible to go to orders like 200, and get an accurate estimate with somewhere between 50 and 100 significant digits for the Gauss-Kuzmin-Wirsing constant. But getting 1024 digits, which is the goal of Simon Plouffe's tables, see

`http://www.cecm.sfu.ca/people/Simon_Plouffe.html`,

by these methods appears to be completely out of reach.

A last word about proof. For the Gauss-Kuzmin-Wirsing constant at least, it would be possible *in principle* to get *certificates*. The paper [3] gives indications on how to proceed by adapting arguments of [8]. The point is that a suitable variant of the $\mathcal{G}_2$ operator studied by Wirsing is positive (Perron-Frobenius) and admits $-\lambda_2$ as its dominant eigenvalue. Then, the numerical process based on truncation furnishes additionally a good candidate approximation to the corresponding dominant eigenfunction. Any such dominant "near-eigenfunction" can in turn be transformed "mechanically" into proven bounds on the dominant eigenvalue ($-\lambda_2$ here). As we say in [3]: "*We observe that, if required, such numerical computations can be completely validated by purely algebraic manipulations only; it suffices to use truncated Taylor expansions of the Hurwitz zeta function, then rational coefficient approximations, and finally exact computations with algebraic numbers (for determining the maximum and minimum of a rational functions with rational coefficients). We have not deemed this tedious verification necessary since the numerical evidence gathered is overwhelming.*"

6. Here are two tables showing the speed of convergence as a function of the truncation order, m, for the two dominant eigenvalues.

Truncation order (m)	$\lvert\lambda_1^{[m]} - 1\rvert$
2	$3.0 \cdot 10^{-2}$
4	$2.1 \cdot 10^{-3}$
8	$1.5 \cdot 10^{-5}$
16	$1.2 \cdot 10^{-9}$
32	$1.5 \cdot 10^{-17}$
64	$4.0 \cdot 10^{-33}$

Truncation order (m)	$\lvert\lambda_2^{[m]} - \lambda_2\rvert$
2	$2.1 \cdot 10^{-2}$
4	$1.6 \cdot 10^{-3}$
8	$7.1 \cdot 10^{-5}$
16	$1.3 \cdot 10^{-9}$
32	$2.3 \cdot 10^{-18}$
64	$1.2 \cdot 10^{-33}$

The observed ratio between successive eigenvalues is:

i	1	2	3	4	5	6	7	8	9	10	32
λ_i/λ_{i+1}	-3.29	-3.01	-2.84	-2.76	-2.72	-2.69	-2.68	-2.67	-2.66	-2.65	-2.625.

The beginning of the continued fraction expansion of $|\lambda_2|$ (that extends [5, p. 350]) is

$$|\lambda_2| = /3, 3, 2, 2, 3, 13, 1, 174, 1, 1, 1, 2, 2, 2, 1, 1, 1, 2, 2, 1, 5, 6, 1, 1, 73, 1, 4, 2, 3, 8, \ldots/.$$

Finally, the computation with $m = 70$ and $digits = 110$ yields

$$\lambda_2 = -0.30366\,30028\,98732\,65859\,74481\,21901\,55623\,.$$

which is most probably within $\pm 10^{-35}$ of the true value, but further consistency checks on this estimate haven't been performed!

References

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