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Estimating Coefficients of Frobenius Series by Legendre Transform and WKB Approximation

Amna Noreen and Kåre Olaussen

***Abstract*—The Frobenius method can be used to represent solutions of ordinary differential equations by (generalized) power series. It is useful to have prior knowledge of the coefficients of this series. In this contribution we demonstrate that the magnitude of the coefficients can be predicted to surprisingly high accuracy by a Legendre transformation of WKB approximated solutions to the differential equations.**

***Index Terms*—Second order ODEs, Regular singular points, Frobenius method, Legendre transformation, WKB approximation.**

I. Introduction

RECENTLY we have developed and used code for solving ordinary Frobenius type differential equations to very high precision [1], [2], [3], like finding the lowest eigenvalue of

$$-\psi''(x) + x^4\psi(x) = \varepsilon\psi(x) \tag{1}$$

to one million decimals. The general class of equations treated in [3] is of the type

$$-\left(\frac{d^2}{dz^2} + \frac{1-\nu_+-\nu_-}{z}\frac{d}{dz} + \frac{\nu_+\nu_-}{z^2}\right)\psi(z) + \frac{1}{z}\sum_{n=0}^{N} \mathrm{v}_n\, z^n\, \psi(z) = 0. \tag{2}$$

Following the Frobenius method our solution is represented by a convergent series

$$\psi(z) = \sum_{m=0}^{\infty} a_m\, z^{m+\nu}, \tag{3}$$

where the coefficients a_m is generated recursively in parallel with a brute force summation of the series. The individual terms in (3) may grow very big, leading to huge cancellations and large roundoff errors. It is therefore useful to have some prior knowledge of the magnitude of the a_m's before a high-precision evaluation — to set the computational precision required for a desired accuracy of the final result, and to estimate the time required to complete the computation.

We have found that $|a_m|$ can be estimated surprisingly accurate from a WKB approximation of the solution, followed by a Legendre transform. For the general class of equations (2) the WKB integrals and the Legendre transform must be done by (ordinary precision) numerical methods.

In the remainder of this paper we first derive a Legendre transform relation between the magnitudes $|a_m|$ and $|\psi(z)|$, slightly generalized to take into account a logarithmic correction, and next use the WKB approximation to estimate $\psi(z)$.

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A. Noreen is with the Department of Physics, NTNU, N-7048 Trondheim, Norway. e-mail: Amna.Noreen@ntnu.no.
K. Olaussen is with the Department of Physics, NTNU, N-7048 Trondheim, Norway. e-mail: Kare.Olaussen@ntnu.no.

II. Legendre transform method of solution

Our method of solution is based on the hypothesis that the sum (3) for large $|z|$ receives its main contribution from a relatively small range of m-values. Introduce quantities u and $s(m)$ so that

$$x = \mathrm{e}^u, \quad |a_m| = \mathrm{e}^{s(m)}.$$

Our assumption is that

$$\mathrm{e}^{S(u)} \equiv \max_{\varphi} \psi(\mathrm{e}^{u+i\varphi}) \approx \sum_m \mathrm{e}^{s(m)+(\nu+m)u}, \tag{4}$$

with the main contribution to the sum coming from a small range of m-values around a maximum value $\bar{m}$. The latter is defined so that $s'(\bar{m}) + u = 0$, $s''(\bar{m}) < 0$. Now write $m = \bar{m} + \Delta m$, and approximate the sum (4) over Δm by a gaussian integral. This gives

$$\mathrm{e}^{S(u)} \approx \sqrt{-2\pi/s''(\bar{m})}\, \mathrm{e}^{s(\bar{m})+(\nu+\bar{m})u}.$$

In summary, we have found the relations

$$u = -s'(m), \tag{5}$$

$$S(u) = s(m) - (\nu+m)s'(m) + \frac{1}{2}\log\left(\frac{2\pi}{-s''(m)}\right)$$
$$\equiv S_0(u) + \frac{1}{2}\log\left(\frac{2\pi}{-s''(m)}\right). \tag{6}$$

This is essentially a Legendre transformation between $s(m)$ and $S(u)$. Consider a small change $u \to u + \delta u$. To maintain the maximum condition we must also make a small change $m \to m + \delta m$, with $\delta m = -\delta u/s''(m)$. I.e. $s''(m) = -u'(m)$. This is consistent with the result of taking the m-derivative of equation (5). One further finds that $S_0(u)$ becomes

$$S_0(u+\delta u) = S_0(u) + S_0'(u)\,\delta u + \frac{1}{2}S_0''(u)\,\delta u^2 + \cdots$$
$$= s(m) + (\nu+m)u + (m+\nu)\,\delta u - \frac{1}{2s''(m)}\,\delta u^2 + \cdots,$$

giving the relations

$$(m+\nu) = S_0'(u), \tag{7}$$

$$s(m) = S_0(u) - uS_0'(u), \tag{8}$$

$$s''(m) = -S_0''(u)^{-1}. \tag{9}$$

Equation (9) just says that $(dm/du) = (du/dm)^{-1}$. We are only able to compute $S(u)$ directly, not $S_0(u)$. However, they only differ by a logarithmic term, hence we will approximate $\log(-s''(m)) = -\log S_0''(u) \approx -\log S''(u)$. This gives

$$S_0(u) \approx S(u) - \frac{1}{2}\log\left(2\pi\, S''(u)\right), \tag{10}$$

which can be used in equations (7–9) when we have computed $S(u)$.

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III. WKB APPROXIMATION

It remains to find $S(u)$. Here we will use the leading order WKB approximation to find a sufficiently accurate estimate. When $z = 0$ is an ordinary point, i.e. when $\nu_- = 0$, $\nu_+ = 1$, the leading order WKB solution to (2) is

$$\psi(z) \approx \sqrt{Q_0/Q(z)} \exp\left(\frac{1}{s}\int_0^z Q(t)\mathrm{d}t\right), \qquad (11)$$

where $Q^2(z) = \sum_{n=1}^{N} \mathrm{v}_n z^{n-1}$, and $Q_0 = Q(0)$. This represents a superposition of the solutions $\psi_\pm(z)$. The difference between the ν_+ and ν_- solutions is at worst comparable to accuracy of our approximation; hence we will not distinguish between them.

When $z = 0$ is a regular singular point we use the Langer corrected WKB approximation to obtain leading order solutions in the form

$$\psi_\pm(z) \approx z^{\nu_\pm}\sqrt{Q_0/Q(z)} \times \exp\left(\pm\frac{1}{s}\int_0^z \frac{\mathrm{d}t}{t}\left[\sqrt{Q^2(t)} - Q_0\right]\right). \qquad (12)$$

Here $Q^2(z) = \frac{1}{4}s^2(\nu_+ - \nu_-)^2 + \sum_{n=0}^{N} \mathrm{v}_n z^{n+1}$, and $Q_0 = Q(0)$. In equation (12) we distinguish between the ν_+- and ν_--solutions, because the difference $\nu_+ - \nu_-$ may in principle be large.

The WKB integrals must in general be done numerically, sometimes along curves in the complex plane. This requires careful attention to branch cuts. Here we will only give some examples where most of the calculations can be done analytically.

A. *Example 1: Anharmonic oscillators*

Consider the equation

$$-\frac{\partial^2}{\partial y^2}\Psi(y) + \left(y^2 + c^2\right)^2 \Psi(y) = 0, \qquad (13)$$

for real c so that $c^2 \geq 0$. For large y the typical solution behaves like

$$\Psi(y) \sim \mathrm{e}^{\frac{1}{3}y^3 + c^2 y}, \qquad (14)$$

neglecting the slowly varying prefactor. For a given value of $|y|$ this is maximum along the positive real axis. Hence, with $x = y^2 = \mathrm{e}^u$, we find as a leading approximation

$$S(u) = \tfrac{1}{3}\left(\mathrm{e}^{\frac{3}{2}u} + 3c^2\mathrm{e}^{\frac{1}{2}u}\right).$$

In this case the Frobenius series can be written

$$\Psi(y) = \sum_{m=0}^{\infty} a_m\, y^{2m+\nu} \equiv \sum_{m=0}^{\infty} A_m(y), \qquad (15)$$

with $\nu = 0,\ 1$. Ignoring the $\log(S''(u))$-term in (7, 8, 10) we find

$$m = \tfrac{1}{2}\left(\mathrm{e}^{\frac{3}{2}u} + c^2\,\mathrm{e}^{\frac{1}{2}u}\right), \qquad (16)$$

$$\log\left(|a_m|\right) = \left(\tfrac{1}{3} - \tfrac{1}{2}u\right)\mathrm{e}^{\frac{3}{2}u} + c^2\left(1 - \tfrac{1}{2}u\right)\mathrm{e}^{\frac{1}{2}u}. \qquad (17)$$

For $c = 0$ an explicit representation is

$$\log|a_m| = \frac{2}{3}m\left(1 - \log 2m\right). \qquad (18)$$

This is plotted as the lower curve in figure 1. It fits satisfactory with the high-precision coefficients generated numerically, but there remains a correction which depends logarithmically on m. For nonzero c the parametric representation provides equally good results, as shown by the upper curve in figure 1.

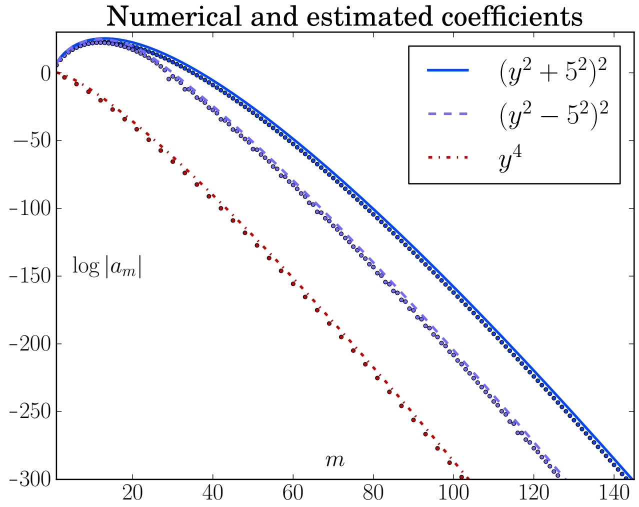

Fig. 1. Comparison of numerical coefficients a_m (points) with estimates (full-drawn lines) based on (16, 17) and (28, 29). The estimates of $\log|a_m|$ are accurate up to corrections which depend logarithmically on m.

The conclusion of this example is that for a fixed (large) x we expect the largest term of the power series to be

$$\max_m |A_m(x)| \sim \mathrm{e}^{\frac{1}{3}(x^{3/2} + 3c^2 x^{1/2})}, \qquad (19)$$

neglecting a slowly varying prefactor. Further, the maximum should occur at

$$m \approx \tfrac{1}{2}\left(x^{3/2} + c^2 x^{1/2}\right). \qquad (20)$$

Finally, estimates like equation (18) for the coefficients a_m may be used to predict how many terms $\mathcal{M}$ we must sum to evaluate $\psi(x)$ to a given precision P, based on the stopping criterium

$$|a_{\mathcal{M}}|\, x^{\mathcal{M}} \leq 10^{-P}. \qquad (21)$$

As can be seen in figure 2 the agreement with the actual number of terms used by our evaluation routine is good, in particular for high precision P. But keep in mind that a logarithmic scale makes it easier for a comparison to look good.

Next consider the logarithmic corrections. Including the prefactor of equation (14) changes $S(u)$ by an amount

$$\Delta S(u) = -\frac{1}{2}\log\left(\mathrm{e}^u + c^2\right). \qquad (22)$$

Including the $\log(S''(u))$-term in the relation between $S(u)$ and $S_0(u)$ changes S_0 by an additional amount

$$\Delta S_0(u) = -\frac{1}{2}\log\left(\frac{3}{4}\mathrm{e}^{\frac{3}{2}u} + \frac{1}{4}c^2\,\mathrm{e}^{\frac{1}{2}u}\right). \qquad (23)$$

For $c^2 = 0$ this changes the relation (18) to

$$\log|a_m| = \frac{1}{3}\left(2m + 5/2\right)\left(1 - \log\left(2m + 5/2\right)\right). \qquad (24)$$

For $|a_m|$ this essentially corresponds to a factor $m^{-5/6}$.

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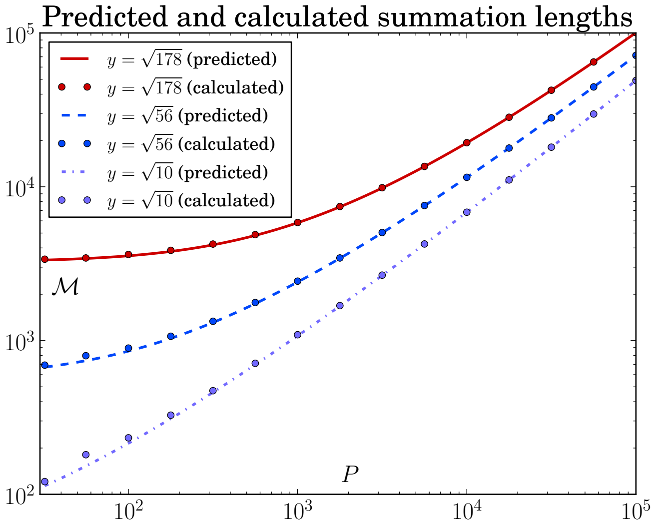

Fig. 2. This figure compares the *a priori* prediction, based on equation (18), of the number of terms $\mathcal{M}$ which must be summed in order to evaluate $\Psi(y)$ for $c = 0$ to a desired precision P with the actual number of terms computed by.

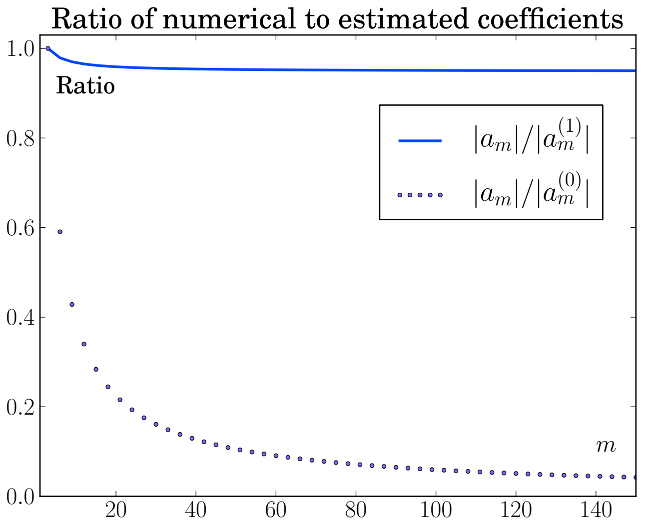

Fig. 3. This figure shows the ratio between the computed coefficients a_m and the crude prediction (18) (labelled $|a_m^{(0)}|$) and the logarithmically corrected prediction (24) (labelled $|a_m^{(1)}|$). For easy comparison we have in both cases adjusted an overall constant such that the ratio is unity for $m = 3$.

B. Example 2: Double well oscillators

The same procedure also work for the equation

$$-\frac{\partial^2}{\partial y^2}\Psi(y) + \left(y^2 - c^2\right)^2 \Psi(y) = 0, \tag{25}$$

which however is a little more challenging since the maximum value of $|\Psi(y e^{i\varphi}|$ sometimes occur for $\varphi \neq 0$, i.e. for complex arguments.

For large y the typical solution behaves like

$$\Psi(y) \sim e^{\frac{1}{3}y^3 - c^2 y}, \tag{26}$$

neglecting the slowly varying prefactor. Equation (25) can be transformed to the form (2) by introducing $x = y^2$, $\Psi(y) = \psi(x)$. Hence, with $x = y^2 = e^u$

$$S(u) = \max_{\varphi} \tfrac{1}{3}\mathrm{Re}\left(e^{\frac{3}{2}(u+i\varphi)} - 3c^2 e^{\frac{1}{2}(u+i)\varphi}\right).$$

The maximum occurs for $\cos\frac{1}{2}\varphi = -\frac{1}{2}\left(1 + c^2 e^{-u}\right)^{1/2}$ when $e^u \geq \frac{1}{3}c^2$, and for $\cos\frac{1}{2}\varphi = -1$ otherwise. This gives

$$S(u) = \begin{cases} c^2 e^{u/2} - \frac{1}{3}e^{3u/2} & \text{for } e^u \leq \frac{1}{3}c^2, \\ \frac{1}{3}(e^u + c^2)^{3/2} & \text{for } e^u \geq \frac{1}{3}c^2. \end{cases} \tag{27}$$

This implies that

$$\bar{m} = \begin{cases} \frac{1}{2}e^{u/2}\left(c^2 - e^u\right) & \text{for } e^u \leq \frac{1}{3}c^2, \\ \frac{1}{2}e^u\,\left(e^u + c^2\right)^{1/2} & \text{for } e^u \geq \frac{1}{3}c^2, \end{cases} \tag{28}$$

$$\log\left(|a_{\bar{m}}|\right) = \begin{cases} \left(1 - \frac{1}{2}u\right)c^2 e^{u/2} - \left(\frac{1}{3} - \frac{1}{2}u\right)e^{3u/2} & \text{for } e^u \leq \frac{1}{3}c^2, \\ \left[\left(\frac{1}{3} - \frac{1}{2}u\right)e^u + \frac{1}{3}c^2\right]\left(e^u + c^2\right)^{1/2} & \text{for } e^u \geq \frac{1}{3}c^2. \end{cases} \tag{29}$$

This representation compares fairly well with the numerically generated coefficients, as shown by the middle curve in figure 1. However, in this case the coefficients a_m have a local oscillating behaviour. The representation (28, 29) should be interpreted as the local amplitude of this oscillation.

The conclusion of this example is that we expect the largest term of the power series to be term of the series to be

$$\max_m |A_m(x)| \sim e^{\frac{1}{3}(x+c^2)^{3/2}}, \tag{30}$$

neglecting the slowly varying prefactor. Further, the maximum should occur at

$$m \approx \tfrac{1}{2}x\left(x + c^2\right)^{1/2} \approx \tfrac{1}{2}x^{3/2} + \tfrac{1}{4}c^2 x^{1/2}. \tag{31}$$

IV. Conclusion

As illustrated in this contribution the coefficients of Frobenius series can be predicted to surprisingly high accuracy by use of Legendre transformations and lowest order WKB approximations. We have also tested the validity of the method on many other cases.

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