Spherical Splines in Tension
continued ...

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1. Introduction

Wessel and Becker (*GJI,* **174**, 21-28, 2008) consider the generalization of my spherical splines by adding a terms that allow tension, increasing the order of the Euler-Lagrange equations by two. The basis functions remain circularly symmetric about the knot points but each assumes the following form:

$$g_p(\theta) = \frac{\pi P_\nu(-\cos\theta)}{\sin\nu\pi} - \ln(1-\cos\theta) \tag{1}$$

where $p > 0$ is an adjustable parameter for the user to select, $\nu = -(1-\sqrt{1-4p^2})/2$, which may be complex, θ is the angle from the knot point, and P_ν is the Legendre function. Our (1) is WB's (22) in a slightly different notation. The goal is to evaluate or approximate g_p in an efficient manner.

In the derivation of this equation WB derived the following expression for the first term on the right of (1)

$$\frac{\pi P_\nu(-\cos\theta)}{\sin\nu\pi} = -\sum_{l=0}^{\infty} \frac{2l+1}{l(l+1)+p^2} P_l(\cos\theta)\,. \tag{2}$$

For our initial stab at evaluation we consider simply summing the series.

1. Summing the Series

If the parameter p is not too large, say $p < 100$ we can consider this approach. We see in (2) that when $l < p$ the rational factor increases proportionally to l, then when $l \gg p$ it decays at l^{-1}. The Legendre polynomial of large degree has this asymptotic behavior (Olver, *Asymptotics and Special Functions,* p 129):

$$P_l(\cos\theta) = \left(\frac{2}{\pi l \sin\theta}\right)^{\frac{1}{2}} \sin(l\theta + \tfrac{1}{2}\theta + \tfrac{1}{4}\pi) + O l^{-3/2}, \;\; \theta \neq 0, \pi\,. \tag{3}$$

So we see that for large l the overall decay of the terms is only as $l^{-3/2}$, not a stellar rate.

The situation is vastly improved if we include the second term in (1) as a series. We note (Backus, Parker and Constable, *Foundations of Geomagnetism*, p 166) that

$$\ln(1-\cos\theta) = \ln 2 - 1 - \sum_{l=1}^{\infty} \frac{2l+1}{l(l+1)} P_l(\cos\theta) \tag{4}$$

Thus we combine (2) and (4) to give

$$g_p = -\ln 2 + \frac{p^2 - 1}{p^2} + \sum_{l=1}^{\infty} \frac{(2l+1)p^2}{l(l+1)\,(l^2+l+p^2)}\, P_l(\cos\theta) \tag{5}$$

The terms in this series, if we disregard the oscillations of P_l for the moment, decrease as $l^{-3/2}$ while $l < p$, then die away as $l^{-7/2}$ once $l > p$. In Figure 1, we plot the quantity

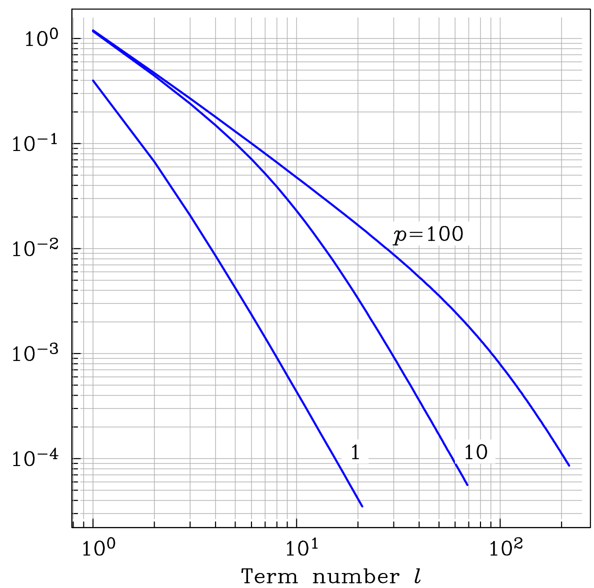
$$\beta_l = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{(2l+1)p^2}{l^{3/2}(l+1)\,(l^2+l+p^2)} \tag{6}$$

which gives an approximate upper bound on the magnitude of the l-th term, from (3) and (5), since the oscillating factor, according to (5), is of unit amplitude. The plot shows that, provided we require only a modest accuracy, and p is not too large, summing the series is a viable technique. To be efficient we evaluate the $P_l(\cos\theta)$ by recursion using the three-term relation (Backus et al., p109):

$$P_{l+1}(\mu) = \frac{2l+1}{l+1}\,\mu\, P_l(\mu) - \frac{l}{l+1}\, P_{l-1}(\mu), \quad l = 1, 2, \cdots L \tag{7}$$

so that (with β_l and other fixed coefficients stored) each term requires only 6 flops. Certainly for $p \le 10$ this method will be competitive with almost any other.

Figure 1: Approximate bound on the term magnitude, β_l, as given by (6).



2. The Tale of the Tail

We have been too cavalier about the accuracy attained when we have summed to L terms: it is certainly not as good as (6) and Figure 1. We need to estimate the remainder; for simplicity we will assume that we have taken $L-1$ terms in (5). We would like to estimate the magnitude of

$$R_L = \sum_{l=L}^{\infty} \frac{(2l+1)p^2}{l(l+1)\,(l^2+l+p^2)}\, P_l(\cos\theta)\,. \tag{8}$$

Assume that $p \ll L$ (perhaps a factor of 3 will do), then by (3) and a bit of algebra

$$R_L = 2p^2\left(\frac{2}{\pi\sin\theta}\right)^{\frac{1}{2}} \sum_{l=L}^{\infty} \frac{\sin(l\theta + \frac{1}{2}\,\theta + \frac{1}{4}\,\pi)}{l^{7/2}} \left(1 - \frac{3}{2l} + \frac{2-p^2}{l^2} + Ol^{-3}\right). \tag{9}$$

A crude bound results from taking the absolute value everywhere :

$$|\,R_L\,| < p^2\left(\frac{8}{\pi\sin\theta}\right)^{\frac{1}{2}} \sum_{l=L}^{\infty} \frac{1}{l^{7/2}} \sim \left(\frac{8}{\pi\sin\theta}\right)^{\frac{1}{2}} \frac{2p^2}{5L^{5/2}}\,. \tag{10}$$

This bound overestimates for two reasons: first the oscillations cancel terms in the tail; second, particularly near $\theta = 0$ or π, the leading factor in the asymptotic expansion is too large. An alternative bound can be found by exploiting the inequality $|\,P_l(\cos\theta)\,| \le 1$ directly in (8):

$$|\,R_L\,| < \sum_{l=L}^{\infty} \frac{(2l+1)p^2}{l(l+1)\,(l^2+l+p^2)} \sim \sum_{L}^{\infty} \frac{2p^2}{l^3} \sim \frac{p^2}{L^2} \tag{11}$$

This bound will be smaller than (10) for small enough angles, and should be used then. The bounds (10) and (11) can be turned around to compute the number of terms needed to achieve a desired accuracy. This is more efficient and reliable than testing the size of each term during summation.

There are some things we can do to improve matters. Just as we integrated (10) to estimate the sum, we can apply the Euler-Maclaurin expansion in (9) to obtain a better estimate. That estimate can then be added to the sum to correct for the missing tail. It would also help if a better asymptotic form could be employed that was not singular at $\theta = 0$; there is a uniform asymptotic expansion with this property (Olver, p 463).

The convergence rate can also be increased by adding and subtracting a function with the Legendre expansion

$$F(\theta) = \sum_{l=1}^{\infty} a_l P_l(\cos\theta) \tag{12}$$

where the coefficients have the asymptotic behavior

$$a_l \sim 2p^2 l^{-3}\,. \tag{13}$$

We add the function and subtract the terms in the series, thus improving the convergence rate by another factor of l^{-1}. Exact expansions like (12) can easily be constructed from known expansions; the dilogarithm is of the correct form, for example. These refinements should be added to improve computational speed for the largest values of p, as well as using Euler-Maclaurin for remainder estimation.

3. More on Tail Estimation

The use of the bounds (10) and (11) will cause excessive caution because the effects of the oscillation of the Legendre factor have been ignored. Near $\theta = 0$ this is less important, but near π it is a significant factor. The E-M series leads to integrals that themselves must be estimated asymptotically. Here I propose a simpler, but less rigorous idea. Concentrating on the leading term in the asymptotic for the rational factor, we write (9) as

$$\tilde{R}_L = C \,\mathrm{Im} \sum_{l=L}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(l\theta+\theta/2+\pi/4)}}{l^{7/2}} \tag{14}$$

$$= C \,\mathrm{Im}\; \mathrm{e}^{\mathrm{i}(L+½)\theta+\mathrm{i}\pi/4} \sum_{n=0}^{\infty} \exp\left(\mathrm{i}n\theta - \tfrac{7}{2}\ln(L+n)\right) \tag{15}$$

Now we expand the log under the exponential, but we can only take the linear term, because any more will lead to a divergent series!

$$\tilde{R}_L \sim \frac{C}{L^{7/2}} \,\mathrm{Im}\; \mathrm{e}^{\mathrm{i}(L+½)\theta+\mathrm{i}\pi/4} \sum_{n=0}^{\infty} \mathrm{e}^{n(\mathrm{i}\theta-7/2L)} \tag{16}$$

$$= \frac{C}{L^{7/2}} \,\mathrm{Im}\; \frac{\mathrm{e}^{\mathrm{i}(L+½)\theta+\mathrm{i}\pi/4}}{1-\mathrm{e}^{-7/2L+\mathrm{i}\theta}} \tag{17}$$

We might use (17) to calculate the tail contribution, or we can find a bound by taking the magnitude, since the imaginary part is never more than the absolute value:

$$|\,\tilde{R}_L\,| < \frac{C}{L^{7/2}} \frac{\mathrm{e}^{7/4L}}{\sqrt{2(\cosh\frac{7}{2L} - \cos\theta)}} \tag{18}$$

$$= \frac{p^2}{L^{7/2}} \frac{2\exp\frac{7}{4L}}{\sqrt{\pi\sin\theta\,(\cosh\frac{7}{2L} - \cos\theta)}} \tag{19}$$

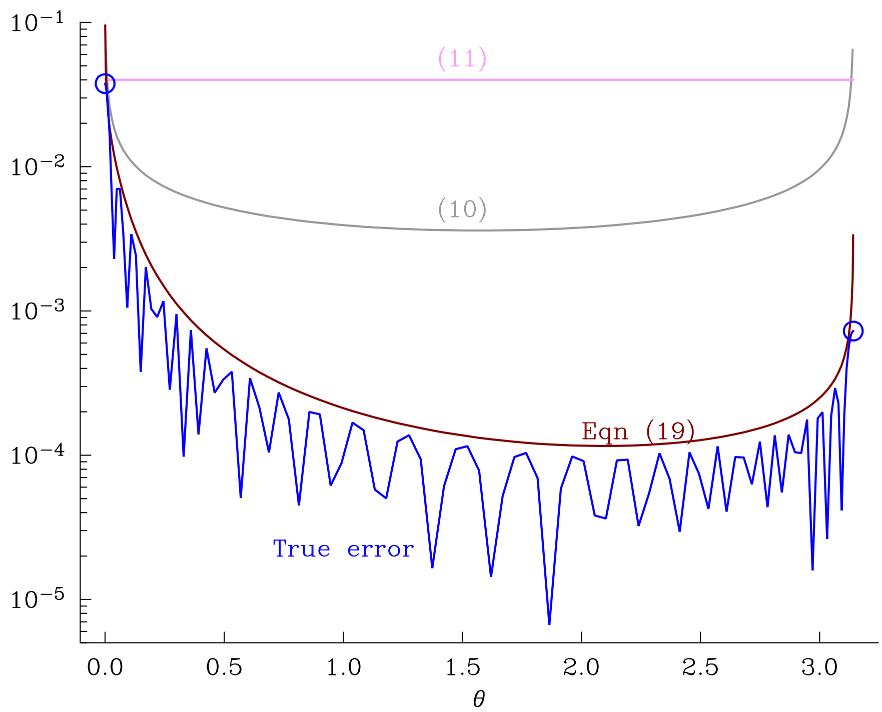
The essentail point to notice is that this bound is a factor of L smaller than the one in (10).

The performance of these various bounds on the remainder is illustrated in Figure 2. Here we consider the case of $p = 10$, and calculate the error and the estimates when $L = 50$. Equation (19) gives amazingly accurate estimates: it captures the correct shape of the error envelope, and the failure due to the singularities at $\theta = 0$ and π affects only a tiny portion of the interval. We see that the bound given in (11) gives almost the exact error at $\theta = 0$ although it is hopeless everywhere else. To make a similarly precise estimate at $\theta = \pi$ we simply note that then $P_l(-1) = (-1)^l$ in (8). It is well known that the remainder of a slowly converging alternating series is roughly equal to one half of the first neglected term, and so

$$R_L(\pi) \sim \frac{p^2}{L^3} \tag{20}$$

which gives 8×10^{-4} in our example; the computed error is 7.26×10^{-4}. Obviously equation (19) should be used to estimate the value of L that will achieve a desired accuracy.

Figure 2: Actual error and bounds after summing 50 terms in (5) with $p = 10$. The true error at $\theta = 0$ and π is indicated by a circle.



4. Ridiculous Pedantry

For a working algorithm we need to invert (19) and solve for L when $R_L = \varepsilon$ is given as a target error. We may assume that L is large and so we can replace the exponential and hyperbolic cosine with low-order Taylor expressions. We cannot approximate cosh by unity because when θ is small it becomes important that this quantity exceeds one. Introducing those approximations, squaring (19) and rearranging, we find

$$L^7\left(1+\tfrac{7}{4L}\right)^{-2}\left(1-\cos\theta+\tfrac{48}{8L^2}\right)=\frac{4p^4}{\pi\varepsilon^2\sin\theta}=\beta \tag{21}$$

Here β will always be a large number. To order L^{-1} we can combine the first two factors into $(L-\tfrac{1}{2})^7$. In a final analysis we can neglect the difference between L and $L-\tfrac{1}{2}$. So, ignoring this small perturbation, and tidying up (21) becomes

$$L^7+\frac{49/16}{\sin^2\tfrac{1}{2}\theta}L^5=\frac{\beta}{2\sin^2\tfrac{1}{2}\theta} \tag{22}$$

which is a degree-7 polynomial equation. We can reduce (22) to a single parameter system by scaling: let

$$\lambda=\tfrac{4}{7}L\sin\tfrac{1}{2}\theta \tag{23}$$

and then (22) becomes

$$\lambda^7+\lambda^5=\gamma \tag{24}$$

where

$$\gamma=\tfrac{1}{2}\left(\tfrac{4}{7}\right)^7\beta\sin^5\tfrac{1}{2}\theta=\frac{p^4}{\pi\varepsilon^2}\left(\frac{4}{7}\right)^7\frac{\sin^4\tfrac{1}{2}\theta}{\cos\tfrac{1}{2}\theta} \tag{25}$$

While β is a large number, γ can easily be less than unity owing to the fifth power on the sine. As a first approximation suppose we split the γ interval at $\gamma=1$ and we make a simple approximation in each subinterval: we find this system

$$\lambda=\begin{cases}\left(\dfrac{\gamma}{1+\gamma^{2/5}}\right)^{1/5}, & \gamma\le 1\\[2ex] \left(\dfrac{\gamma}{1+\gamma^{-2/7}}\right)^{1/7}, & \gamma>1\end{cases} \tag{26}$$

At the discontinuity there is a jump from 0.87055 to 0.90572, and the exact solution is 0.88989; this is an error of about 2 percent in either approximation, which is surely acceptable.