(The difficulties of) Computing $\left\langle \sin(x), x^k \right\rangle$

MATHEMAGICA
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March 2, 2014

We are asked to find the polynomial $P_n(x)$ of degree n that minimizes

$$\min_{P_n \in \Pi_n} \|P_n - \sin\|^2 = \min_{P_n \in \Pi_n} \int_{-1}^{1} (P_n(x) - \sin(\pi x)) dx$$

it turns out that by a famous theorem, suppose we have an orthonormal basis $U_n = \{u_0, u_1, \cdots, u_n\}$ of polynomial functions (wrt to the $\|\cdot\|$ defined above) where u_k is a degree k polynomial, then $P_n \in U_n$ and furthermore, let

$$P_n = \sum_k c_k u_k$$

then by orthonormality,

$$c_k = \langle u_k(x), \sin(\pi x) \rangle$$

Now, irregardless of which set U_n you choose, at some point, you're going to need to be able to evaluate $\left\langle x^k, \sin(\pi x) \right\rangle$. I thought this was going to be easily done with a quadrature, but it turns out that $x^k \sin(\pi x)$ becomes extremely stiff and all of the conventional quadratures I've tried have been unable to evaluate this integral satisfactorily for large values of n. Most immediately holds on to the solution of a nearby function (by slightly perturbing n) and attempts to go to zero. I'm going to now discuss the various unforseen issues of computing $\int_{-\pi}^{\pi} \left(\frac{x}{\pi}\right)^n \sin(x) dx$.

A first attempt

I thought that I was rather clever when I poured through my high school AP calculus text book and rediscovered integration by parts. I constructed two objects:

$$S_k = \int_{-\pi}^{\pi} \left(\frac{x}{\pi}\right)^n \sin(x) dx, \text{and} \quad C_k = \int_{-\pi}^{\pi} \left(\frac{x}{\pi}\right)^n \cos(x) dx.$$

Now, consider S_k, we know that

$$\int u dv = uv - \int v du,$$

so if we let $u = \left(\frac{x}{\pi}\right)^k, du = k\left(\frac{x}{\pi}\right)^{k-1}dx$ and $dv = \sin(x)dx, v = -\cos(x)$, then we'll find that

$$\begin{aligned}
S_n &= \int_{-\pi}^{\pi}\left(\frac{x}{\pi}\right)^n \sin(x)dx \\
&= -\left(\frac{x}{\pi}\right)^n \cos(x)\Big|_{-\pi}^{\pi} + n\int_{-\pi}^{\pi}\left(\frac{x}{\pi}\right)^{n-1}\cos(x)dx \\
&= 2[\text{n is odd}] + \frac{n}{\pi}C_{n-1} \\
C_n &= 0 - \frac{n}{\pi}S_{n-1}
\end{aligned}$$

which means that

$$S_n = \begin{cases} 0 & \text{if } n \text{ is even} \\ 2 & \text{if } n = 1 \\ 2 - \frac{n(n-1)}{\pi^2}S_{n-2} & \text{if } n \text{ is odd} \end{cases}$$

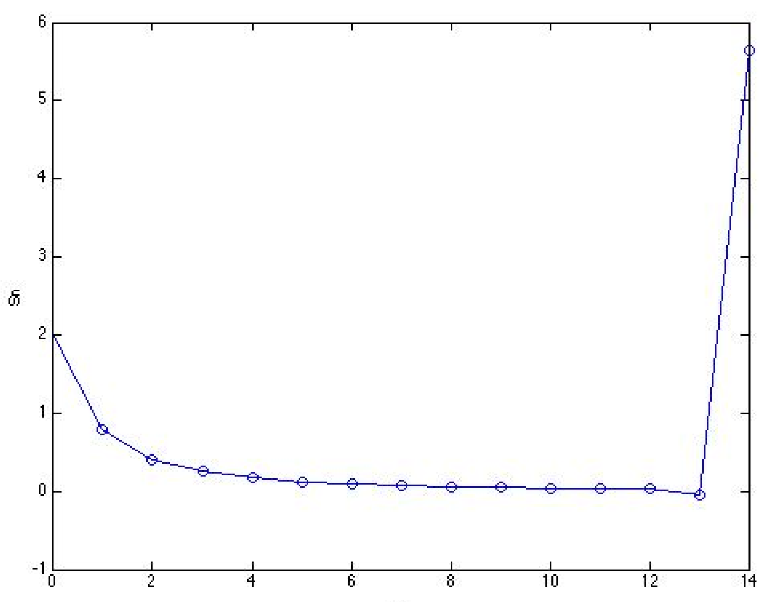
Notice here that if we let

$$\hat{S}_n = 1 - \frac{(2n+1)2n}{\pi^2}\hat{S}_{n-1}, \quad \hat{S}_0 = 1$$

then $2\hat{S}_n = S_{2n+1}$! This is great because we only need to compute the odd S_ns anyways:

```
function [ Sn ] = Snk( n )
    Sn = 2;
    for k = 1:n
        Sn = [Sn; 2 - (2*k+1)*(2*k)/(pi*pi)*Sn(k)];
    end
```

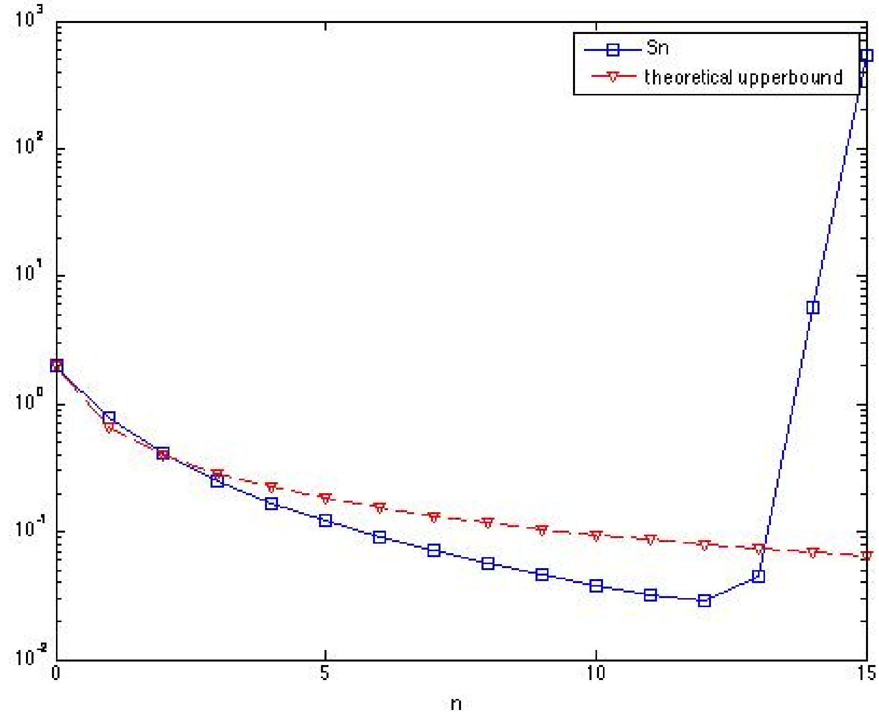
Figure 1: Uhoh...



Hmmm, that looks a little suspicious. Recall that S_k is only defined for odd k, so we know that $\left(\frac{x}{\pi}\right)^n \sin(x) = \left(\frac{-x}{\pi}\right)^n \sin(-x)$. Furthermore, since $\left(\frac{x}{\pi}\right)^n \sin(x) < \left(\frac{x}{\pi}\right)^n$ between $-\pi, \pi$, we can bound this integral by

$$0 \leq 2\hat{S}_k \leq \frac{2}{2k+1}$$

Figure 2: $2\hat{S}_n$ violates the theoretic upper bound!



What's going on here? To analyze the error, suppose that there was just some error in the computation of $\hat{S}_1$ so that we instead got $\hat{S}_1 + \frac{3!}{\pi^2}\epsilon$, then let's look at how this error propagates:

$$\begin{aligned}
\hat{S}_2' &= 1 - \frac{5 \cdot 4}{\pi^2}\left(\hat{S}_1 + \frac{3!}{\pi^2}\epsilon\right) = \hat{S}_2 - \frac{5!}{\pi^4}\epsilon \\
\hat{S}_3' &= 1 - \frac{7 \cdot 6}{\pi^2}\left(\hat{S}_2 + \frac{5!}{\pi^4}\epsilon\right) = \hat{S}_3 + \frac{7!}{\pi^6}\epsilon \\
\hat{S}_4' &= \hat{S}_4 - 9!\pi^{-8}\epsilon \\
&\vdots \\
\hat{S}_k' &= \hat{S}_k \pm (2k+1)!\pi^{-2k}\epsilon
\end{aligned}$$

By stirling's approximation, our error is growing at the rate of $O\left(\left(\frac{2k+1}{\pi e}\right)^{2k+1}\right)$! This is clearly unacceptable. We resorted to various techniques to overcome this difficulty: pre-computing a table of $\hat{S}_n$ values using big-number packages, quadratures, but these methods all seem to fall short.

A second attempt

At this point, it dawned on us that we can transform this into a linear recurrence, which may give us a more stable method to compute this integral by. Suppose we define

$$X_n = \prod_k^n -\frac{(2k+1)2k}{\pi^2} = (-1)^n \frac{(2k+1)!}{\pi^{2k}}$$

then

$$\begin{aligned}\frac{\hat{S}_n}{X_n} &= \frac{1}{X_n} - \frac{\frac{(2n+1)2n}{\pi^2}}{\prod_k^n -\frac{(2k+1)2k}{\pi^2}} \hat{S}_{n-1} \\ &= (-1)^n \frac{\pi^{2n}}{(2n+1)!} + \frac{\hat{S}_{n-1}}{X_{n-1}}\end{aligned}$$

so if we let $T_n = \frac{\hat{S}_n}{X_n}$, then

$$\begin{aligned}T_0 &= 1 \\ T_n &= (-1)^n \frac{\pi^{2n}}{(2n+1)!} + T_{n-1} \\ &= \sum_{k=0}^n (-1)^k \frac{\pi^{2k}}{(2k+1)!} \\ \hat{S}_n &= \sum_{k=0}^n (-1)^k \frac{(2n-2k)!\binom{2n+1}{2(n-k)}}{\pi^{2(n-k)}}\end{aligned}$$

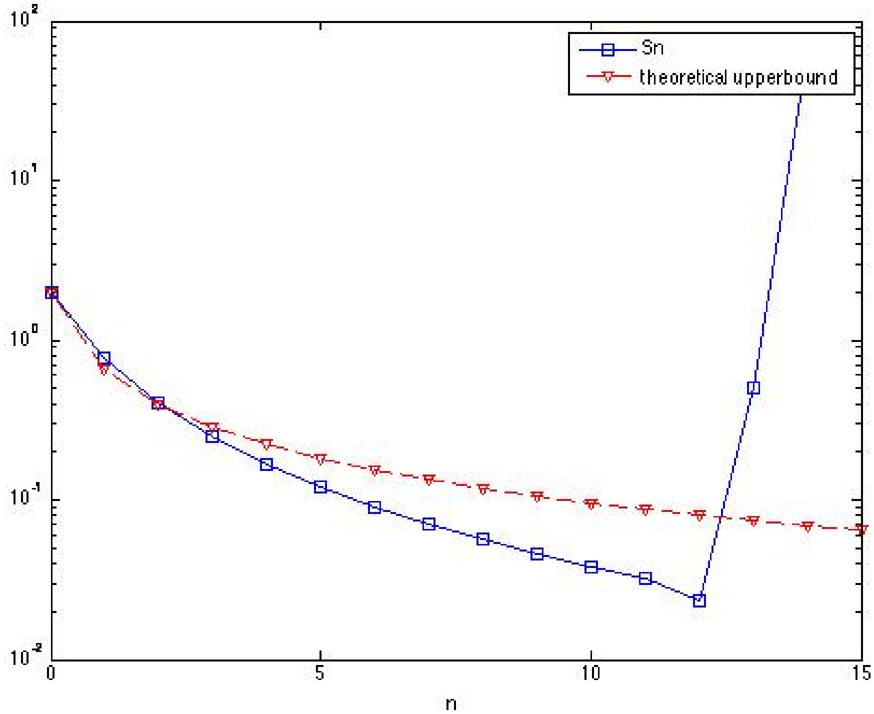
Which lends to the code

```
function [ r ] = Snk( nn )
    r = [1];
    for n = 1:nn
        a = 0;
        for k = n:-1:0
            a = a + (-1).^k .* factorial(2*n+1) ./ (pi.^(2*(n-k)).*factorial(2*k+1));
        end
        r = [r;abs(a)];
    end
    r = 2*r;
end
```

Unfortunately, if we plot out the error again using

```
semilogy(0:n,abs(Sn(n)), '-s' ,0:n,2./(2*(0:n)+1),'--vr')
xlabel('n')
legend('Sn','theoretical upperbound')
```

We find once again that this new series is still unstable!



This makes sense since we're essentially adding up really large parts in the hope that it will converge to something really small. Small amounts of relative error is guaranteed to doom our endeavors as the error gets amplified. At this point, it seems like we're doomed to failure :(Most of us gave up at this point, but a sudden surge of brilliance ended up giving us the nudge that saved the day.

Third time's the charm

While playing on Wolfram | Alpha, one of our members realized that the partial series

$$\pi T_n = \sum_{k=0}^{n} (-1)^k \frac{\pi^{2k+1}}{(2k+1)!}$$

is just the truncated taylor expansion of $\sin(x)$ evaluated at π using just the first $n+1$ terms! This means that

$$\lim \pi T_n = \sin(\pi) = 0$$

This may look not very important or obvious right now, but it opens up a whole new approach to this problem. If we consider T_n as the truncated expansion of function $x^{-1} \cdot \sin(x)$ at π, then we can view it in two ways:

1. as a forward series: basically what we've been looking at it as this entire time

2. as the residual: in other words, because T_n is the prefix sum of the first n terms of this series, it is also the entire infinite sum minus the sum of the $n+1$ term onwards.

using the second interpretation, we can say that

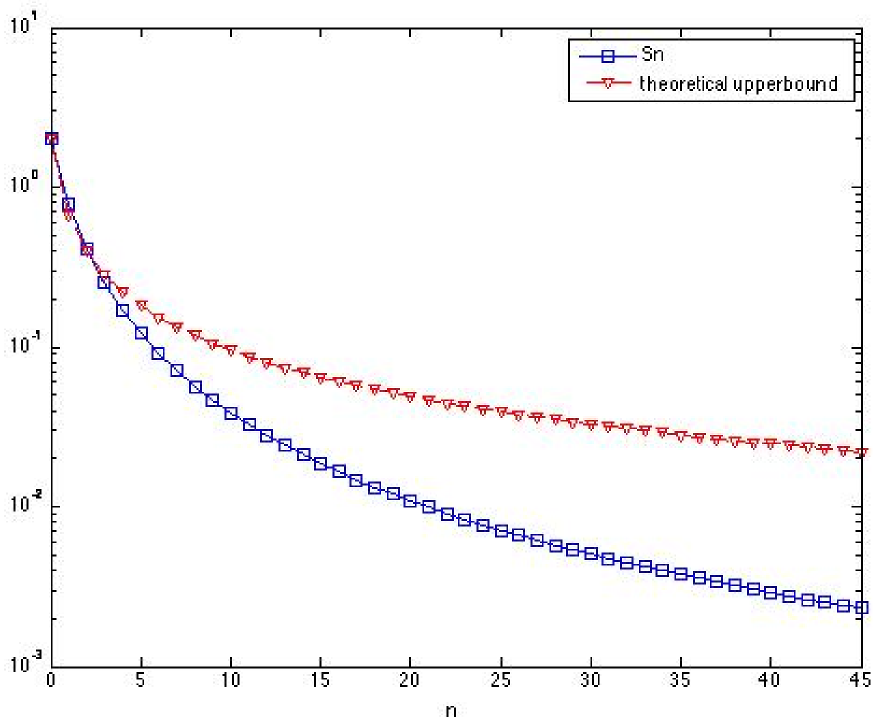
$$\begin{aligned}
T_n &= \frac{\sin(\pi)}{\pi} - \sum_{k=n+1}^{\infty} (-1)^k \frac{\pi^{2k+1}}{(2k+1)!} \\
&= -\sum_{k=n+1}^{\infty} (-1)^k \frac{\pi^{2k+1}}{(2k+1)!} \\
\hat{S}_n &= X_n T_n
\end{aligned}$$

let $\left[{n \atop k} \right] = k!\binom{n}{k}$ be a short hand for k-permutations of a set of n items

$$\begin{aligned}
&= -\sum_{k=n+1}^{\infty} (-1)^{n+k} \frac{\pi^{2(k-n)}}{\left[{2k+1 \atop 2(k-n)} \right]} \\
&= \left| \sum_{\Delta=1}^{\infty} (-1)^{\Delta} \frac{\pi^{2\Delta}}{\left[{2(n+\Delta)+1 \atop 2\Delta} \right]} \right|
\end{aligned}$$

what's remarkable about this series is that unlike the finitary summation version of S_n, this infinite sum is guaranteed to have monotonically decreasing terms in the series, therefore the series doesn't diverge as long as we don't use a stupidly many set of terms. In fact, it seems extremely stable.

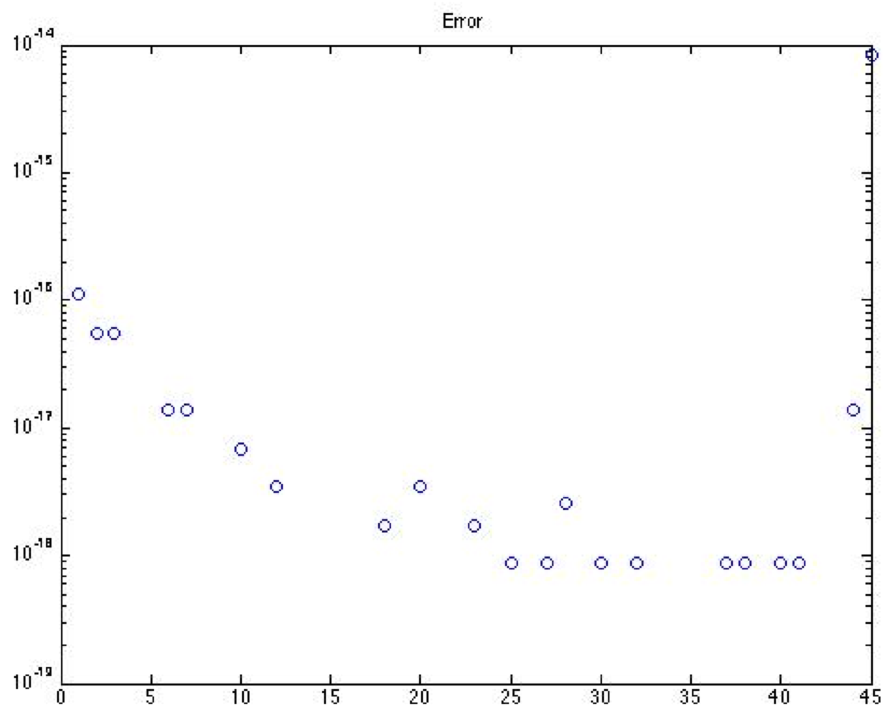
Figure 3: Stable computation of $\hat{S}n$.



```
function [ r ] = Sn( nn,k )
    r = [1];
    for n = 1:nn
        d = k:-1:1;
        r = [r;abs(sum((-1).^d .* pi.^(2*d)./ ( factorial(2*(n+d)+1)./factorial(2*n+1)
            ) ))];
    end
    r = 2*r;
end
```

After using an arbitrary precision solver in MATHEMATICA, I plotted out the error using our method.

Figure 4: Error of $\hat{S}n$.



this seems pretty nifty. Furthermore, we get the extra comfort in knowing also that

$$\hat{S}_n = \frac{4\pi^2}{\binom{2n+3}{2}} - O\left(\pi^4 n^{-4}\right)$$