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ORTHOGONAL POLYNOMIALS AND REGRESSION-BASED SYMMETRIC DERIVATIVES

Abstract

We demonstrate how certain types of symmetric derivatives originate from a simple least-squares regression problem involving discrete Chebyshev polynomials. As the number of data points used in this regression tends to infinity, the resulting integrals, which involve Legendre polynomials, lead to Lanczos derivatives, a result that demonstrates how this latter entity is merely a continuous version of the symmetric derivative.

1 Introduction.

A well-known fact is that the symmetric derivative

$$f'_s(x) = \lim_{h\to 0} \frac{f(x+h) - f(x-h)}{2h}, \tag{1}$$

is a proper extension of the usual derivative f'.

A variety of means exist for constructing second-order symmetric derivatives. Two examples are given by

$$\lim_{h\to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \tag{2}$$

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and

$$\lim_{h\to 0}\frac{4}{7}\cdot\frac{2f(x+h)-f\left(x+\frac{h}{2}\right)-2f(x)-f\left(x-\frac{h}{2}\right)+2f(x-h)}{h^2}. \tag{3}$$

That each of these limits yields a proper extension of the usual second-order derivative can be seen by considering the function $f(x)=x|x|$ at the origin.

A typical method for constructing such difference quotients involves algebraically manipulating Taylor polynomial approximations of f based at x. The purpose of this note is to view this situation from a statistical perspective. We demonstrate how each difference quotient also arises from a polynomial regression problem in which the number of data points determines the number of terms in the difference quotient. The polynomial of best fit is written as a discrete Chebyshev polynomial expansion, one of whose coefficients leads to a symmetric difference quotient. As the number of data points tends to infinity, these symmetric difference quotients give rise to integral-based derivative extensions involving Legendre polynomials. The process by which this is carried out utilizes a number of important properties of orthogonal polynomials.

2 Preliminaries.

Let $\alpha(x)$ be a nondecreasing function defined on some finite interval I. To this function, we may associate the distribution $d\alpha(x)$, an inner product

$$\langle f,g\rangle=\int_I f(x)g(x)\,d\alpha(x),$$

and the normed inner product space L^2_α. The family of orthogonal polynomials corresponding to α is then constructed using the Gram-Schmidt process. For an elaboration of this process, we refer the reader to Szegö's text ([9], Sections 1.4, 2.1, 2.2, 2.8).

The discrete Chebyshev polynomials and Legendre polynomials are the two relevant polynomial families for purposes of this discussion. The former arises by letting $\alpha(x)$ denote a step function with jumps of one unit at the points $x=0,1,\ldots,N-1$, where N is any fixed positive integer. In this case,

$$\langle f,g\rangle=\sum_{j=0}^{N-1}f(j)g(j). \tag{4}$$

The Legendre polynomials are the continuous analog of the Chebyshev family and arise when $\alpha(x)$ is constant and equal to one on the interval $[-1,1]$. Typical notation for either family involves scaling by a conventional factor. The table below gives this scaling factor and summarizes other useful properties to be used in later discussions. A summary of these identities may be found in the texts of Abramowiz and Stegun ([1], 22.2) and Nikiforov, et al. ([6], Table 2.2).

Family	Norm squared	Leading coefficient
Discrete Chebyshev, T_m, $m = 0, 1, \ldots, N-1$	$\dfrac{(N+m)!}{(2m+1)(N-m-1)!}$	$\dfrac{(2m)!}{(m!)^2}$
Legendre, P_m, $m = 0, 1, 2, \ldots$	$\dfrac{2m+1}{2}$	$\dfrac{(2m)!}{2^m(m!)^2}$

Table 1: Summary of discrete Chebyshev and Legendre polynomial properties

Explicit formulas for Legendre polynomials can be found in a variety of sources. For the discrete Chebyshev polynomials, we will use Rodrigues' formula:

$$T_m(x) = \Delta^m \phi_m(x),\ m = 0, 1, 2, \ldots, N-1, \tag{5}$$

where

$$\phi_m(x) = \frac{(x-m+1)_m(x-N-m+1)_m}{m!}, \tag{6}$$

$(x)_m$ denotes the pochhammer symbol $x(x+1)\cdots(x+m-1)$, and Δ denotes the forward difference operator ([3], 10.23).

3 Regression and Chebyshev Polynomials.

Let m denote an arbitrary integer satisfying $m \geq 1$, and let n be any other integer such that $m \leq 2n$. We use the discrete Chebyshev polynomials and regression to construct a symmetric difference quotient whose limit yields a proper extension of the usual m^{th}-order derivative $f^{(m)}$. This difference quotient involves $2n$ terms when m is odd and $2n+1$ terms when m is even.

Fix x and assume f is defined in some open interval about x. For h sufficiently small, $f(x+ht)$, considered as a function of t, is defined at the data points $t_j = \dfrac{j}{n}$, where $-n \leq j \leq n$.

Set $N = 2n+1$ in (4). Then as j increases from $-n$ to n, the points $n(t_j+1)$ vary between 0 and $2n$. Hence, the functions

$$T_{n,k}(t) = T_k\left(n(t+1)\right) \tag{7}$$

form an orthogonal family with respect to the distribution $d\tilde{\alpha}(t)$, where $\tilde{\alpha}(t)$ is a step function having unit jumps at each of the $2n+1$ points t_j.

The m^{th} degree least-squares polynomial of best fit using the data points t_j, where $-n \leq j \leq n$, is the polynomial Q_m that minimizes the sum of squares

$$\sum_{j=-n}^{n} \left(f(x+ht_j) - Q_m(t_j)\right)^2 . \tag{8}$$

Properties of orthogonal polynomials associated with the distribution $d\tilde{\alpha}(t)$ then dictate that Q_m can be expressed as a discrete Chebyshev polynomial expansion as follows:

$$Q_m(t) = \sum_{k=0}^{m} \frac{\langle f(x+ht), T_{n,k}(t)\rangle}{\|T_{n,k}\|^2} T_{n,k}(t). \tag{9}$$

The focus of the ensuing discussion will be on the leading coefficient of (9), which we denote by $a_m(n,h)$, and which, by the second and third columns of Table 1, simplifies to

$$\begin{aligned} a_m(n,h) &= \frac{\langle f(x+ht), T_{n,m}(t)\rangle}{\|T_{n,m}\|^2} \frac{(2m)!}{(m!)^2} n^m \\ &= \frac{(2m+1)!(2n-m)!}{(2n+m+1)!} \frac{n^m}{(m!)^2} \sum_{j=-n}^{n} f(x+ht_j) T_{n,m}(t_j). \end{aligned} \tag{10}$$

4 Symmetric Difference Quotients.

The expression $a_m(n,h)$ leads to a symmetric difference quotient that extends the usual m^{th} order derivative $f^{(m)}$. The motivation for this construction is as follows.

If f possesses an m^{th}-degree Taylor polynomial about x in the variable t, then the coefficient of t^m is $\dfrac{f^{(m)}(x)h^m}{m!}$. At the same time, the corresponding coefficient of the approximating polynomial Q_m is given by $a_m(n,h)$. Given that both Q_m and the Taylor polynomial approximate f near x when this latter polynomial does in fact exist, we are motivated to consider the limit

$$\begin{aligned} f_{s,n}^{(m)}(x) &\stackrel{\text{def}}{=} \lim_{h\to 0} \frac{m!}{h^m} a_m(n,h) \\ &= \lim_{h\to 0} \frac{(2m+1)!(2n-m)!}{(2n+m+1)!} \frac{n^m}{m! h^m} \sum_{j=-n}^{n} f(x+ht_j) T_{n,m}(t_j). \end{aligned} \tag{11}$$

Before establishing that $f_{s,n}^{(m)}$ is a proper extension of the usual m^{th} order derivative, we demonstrate, through simple examples, how (11) reduces to a symmetric difference quotient.

Consider the case when $m = n = 1$. Then calculations establish that $T_m(t) = 2t - 2$, in which case (11) yields the usual symmetric first derivative (1). In a similar manner, if $m = 2$, then $T_m(t) = 6t^2 - 24t + 12$. The combination $m = 2$ and $n = 1$ yields (2) and that of $m = n = 2$ leads to (3). We also observe that for each fixed value of m, there exist infinitely many difference quotients as n varies. Finally, the example $f(x) = \operatorname{sgn}(x)\sqrt{|x|}$ with $m = 2$ and $x = 0$ illustrates how $f_{s,n}^{(m)}(x)$ can exist even if $f_{s,n}^{(m-1)}(x)$ does not.

We now state our main result.

Theorem 4.1. *Fix m, and let n be such that $2n \geq m$. Suppose that f is $(m-1)$-times continuously differentiable in some neighborhood of x and that $f^{(m)}$ exists and is continuous in a neighborhood of x, except possibly at x itself, where the limits of both the left and right m^{th} derivatives, $f_-^{(m)}(x) = \lim_{h\to 0^+} f^{(m)}(x-h)$ and $f_+^{(m)}(x) = \lim_{h\to 0^+} f^{(m)}(x+h)$ exist. Then $f_{s,n}^{(m)}(x)$ exists and*

$$f_{s,n}^{(m)}(x) = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{2}.$$

PROOF. Begin by considering the expression from (11). Summation by parts m times, Rodrigues' formula (5), and the behavior of ϕ at the boundary terms of summation yield the following, where we've set $\beta_{n,m,h} = \frac{(2m+1)!(2n-m)!}{(2n+m+1)!}$.

$$\begin{aligned}
&\beta_{n,m,h}\frac{n^m}{m!h^m}\sum_{j=-n}^{n} f(x+ht_j)T_{n,m}(t_j)\\
=&\beta_{n,m,h}\frac{n^m}{m!h^m}\sum_{j=-n}^{n} f\left(x+h\frac{j}{n}\right)T_m(j+n)\\
=&\beta_{n,m,h}\frac{n^m(-1)^m}{m!h^m}\sum_{j=-n}^{n} \Delta^m f\left(x+h\frac{j}{n}\right)\phi(j+m+n).
\end{aligned}$$

The above sum is written in terms of a forward difference operator. We now carefully manipulate it to introduce symmetric differences. The polynomial ϕ has $2m$ roots at $x = 0, 1, \ldots, m-1$ and at $x = 2n+1, N+1, \ldots, N+m-1 = 2n+m$. To exploit the symmetry of the roots about $x = n + \frac{m}{2}$, we make the change of index $j' = j + \frac{m}{2}$ in the above sum. The upper limit may be written as $j' = n - \dfrac{m}{2}$ due to the fact $n - \dfrac{m}{2} < j' \leq n + \dfrac{m}{2}$ implies $2n+1 \leq j+m+n \leq 2n+m$; i.e., $j+m+n$ is a root of ϕ. Performing this change of index and relabelling j' as j, we may rewrite (11) as

$$f_{s,n}^{(m)}(x) = \lim_{h\to 0} \beta_{n,m,h} \frac{n^m(-1)^m}{m!h^m} \sum_{j=-n+m/2}^{n-m/2} \Delta^m f\left(x + h\left(\frac{j-m/2}{n}\right)\right)\phi(j+m/2+n).$$

Note that if m is odd, we interpret this sum to start at the fraction $j = -n+m/2$ and increase by 1 through $j = n - m/2$.

The function $\phi(j+m/2+n)$ is an even function of j, implying that

$$\begin{aligned} f_{s,n}^{(m)}(x) =& \beta_{n,m,h} \frac{n^m(-1)^m}{m!} \times \\ & \lim_{h\to 0}\left[\frac{1}{h^m} \sum_{j=j_0}^{n-m/2} \Delta^m f\left(x + h\Big(\frac{j-m/2}{n}\Big)\right)\phi(j+m/2+n)\right. \\ & + \frac{1}{h^m} \sum_{j=j_0}^{n-m/2} \Delta^m f\left(x + h\Big(\frac{-j-m/2}{n}\Big)\right)\phi(j+m/2+n) \\ & \left. + \frac{1}{h^m}\Delta^m f\left(x + h\Big(\frac{j-m/2}{n}\Big)\right)\Big|_{j=0} \phi(m/2+n)\right], \end{aligned} \tag{12}$$

where $j_0 = \dfrac{m}{2} \pmod 2$. We now proceed with the proof under the assumption that m is even. The case when m is odd is slightly simpler owing to the fact that (12) has no central term corresponding to $j = 0$.

The m^{th} order forward difference operator is given by

$$\Delta^m f\left(x + h\left(\frac{j-m/2}{n}\right)\right) = \sum_{i=0}^{m} f\left(x + h\left(\frac{j+i-m/2}{n}\right)\right)(-1)^{m-i}\binom{m}{i}.$$

From this, it follows that

$$\Delta^m f\left(x + h\left(\frac{-j-m/2}{n}\right)\right) = (-1)^m \Delta^m f\left(x - h\left(\frac{j-m/2}{n}\right)\right),$$

so that (12) simplifies to

$$f_{s,n}^{(m)}(x) = \beta_{n,m,h} \frac{n^m(-1)^m}{m!} \times \lim_{h\to 0} \left[\frac{1}{h^m} \sum_{j=1}^{n-m/2} \left[\Delta^m f \left(x + h\Big(\frac{j-m/2}{n} \Big) \right) \right.\right.$$
$$\left. + (-1)^m \Delta^m f \left(x - h\Big(\frac{j-m/2}{n} Big) \right) \right] \phi(j+m/2+n) \tag{13}$$
$$\left. + \frac{1}{h^m} \Delta^m f \left(x + h\Big(\frac{j-m/2}{n} \Big) \right) \Big|_{j=0} \phi(m/2+n) \right].$$

A second useful forward difference operator identity is given by

$$\begin{aligned} \Delta^m \left(\left(\frac{j-m/2}{n} \right)^k \right) &= \sum_{i=0}^{m} \left(\frac{j-m/2}{n} \right)^k (-1)^{m-i} \binom{m}{i} \\ &= \begin{cases} 0, & \text{if } k < m; \\ \frac{m!}{n^m}, & \text{if } k = m. \end{cases} \end{aligned} \tag{14}$$

This second case follows from the fact $\left(\frac{j-m/2}{n} \right)^m$ is an m^{th} degree polynomial in j having leading coefficient $\frac{1}{n^m}$ [7].

We now consider what results as h tends to zero in (13). By L'Hospital's rule, the chain rule, the continuity of the first $m-1$ derivatives of f at x, and (14), we obtain

$$\begin{aligned} &\lim_{h\to 0} \frac{1}{h^m} \left[\Delta^m f \left(x + h\Big(\frac{j-m/2}{n} \Big) \right) + (-1)^m \Delta^m f \left(x - h\Big(\frac{j-m/2}{n} \Big) \right) \right] \\ &= \lim_{h\to 0} \frac{1}{m!h} \left[\Delta^m f^{(m-1)} \left(x + h\Big(\frac{j-m/2}{n} \Big) \right) \Big(\frac{j-m/2}{n} \Big)^{m-1} \right. \\ &\quad \left. + (-1)^m \Delta^m f^{(m-1)} \left(x - h\Big(\frac{j-m/2}{n} \Big) \Big(\frac{j-m/2}{n} \Big)^{m-1} \right) (-1)^{m-1} \right] \\ &= \lim_{h\to 0} \frac{1}{m!h} \Delta^m \left[\left[f^{(m-1)} \left(x + h\Big(\frac{j-m/2}{n} \Big) \right) \right.\right. \\ &\quad \left.\left. - f^{(m-1)} \left(x - h\Big(\frac{j-m/2}{n} \Big) \right) \right] \Big(\frac{j-m/2}{n} \Big)^{m-1} \right]. \end{aligned}$$

Since the symmetric first derivative is the average of the left- and right-first derivatives, the limiting value of this final difference quotient introduces

$f_-^{(m)}(x) + f_+^{(m)}(x)$ and one additional factor of $\left(\dfrac{j+i-m/2}{n}\right)$ so that the preceding simplifies further to become

$$\begin{aligned} \lim_{h\to 0} \frac{1}{m!h}\Delta^m \Bigg[\Bigg[f^{(m-1)} \left(x + h\Big(\frac{j-m/2}{n}\Big)\right) & \\ - f^{(m-1)} \left(x - h\Big(\frac{j-m/2}{n}\Big)\right) \Bigg] \Big(\frac{j-m/2}{n} Big)^{m-1} \Bigg] & \qquad (15) \\ = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{m!}\Delta^m \left(\frac{j-m/2}{n}\right)^m = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{n^m}. & \end{aligned}$$

For the second limit in (13), we have

$$\begin{aligned} \Delta^m f\left(x + h\left(\frac{j-m/2}{n}\right)\right)\Bigg|_{j=0} &= \sum_{i=0}^{m} f\left(x + h\left(\frac{i-m/2}{n}\right)\right)(-1)^{m-i}\binom{m}{i} \\ = -f(x)(-1)^{m/2}\binom{m}{m/2} &+ \sum_{i=0}^{m/2-1}\left(f\left(x + h\left(\frac{i-m/2}{n}\right)\right)\right. \\ &\left. + f\left(x - h\left(\frac{i-m/2}{n}\right)\right)\right)(-1)^{m-i}\binom{m}{i}. \end{aligned}$$

Using this identity and proceeding in a manner very similar to before, our limit becomes

$$\begin{aligned} \lim_{h\to 0} \frac{1}{h^m}\Delta^m f\left(x + h\left(\frac{j-m/2}{n}\right)\right)\Bigg|_{j=0} & \\ = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{m!} \sum_{i=0}^{m/2-1}\left(\frac{i-m/2}{n}\right)^m (-1)^{m-i}\binom{m}{i} & \\ = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{2m!} \cdot 2\sum_{i=0}^{m/2-1}\left(\frac{i-m/2}{n}\right)^m (-1)^{m-i}\binom{m}{i} & \\ = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{2m!} \sum_{i=0}^{m}\left(\frac{i-m/2}{n}\right)^m (-1)^{m-i}\binom{m}{i} & \\ = \frac{f_-^{(m)}(x) + f_+^{(m)}(x)}{2n^m}. & \qquad (16) \end{aligned}$$

We now are ready to substitute the results of (15) and (16) into (13). Again utilizing the fact that $\phi(j + m/2 + n)$ is even, we obtain

$$
\begin{aligned}
&f_{s,n}^{(m)}(x) = \beta_{n,m,h}\frac{n^m(-1)^m}{m!}\times\\
&\Big[\frac{f_-^{(m)}(x)+f_+^{(m)}(x)}{2n^m}\phi(m/2+n)+\sum_{j=1}^{n-m/2}\frac{f_-^{(m)}(x)+f_+^{(m)}(x)}{n^m}\phi(j+m/2+n)\Big]\\
&= \quad \frac{f_-^{(m)}(x)+f_+^{(m)}(x)}{2}\cdot\frac{(-1)^m\beta_{n,m,h}}{m!}\cdot\Big[\phi(m/2+n)+2\sum_{j=1}^{n-m/2}\phi(j+m/2+n)\Big]\\
&\qquad = \frac{f_-^{(m)}(x)+f_+^{(m)}(x)}{2}\cdot\beta_{n,m,h}\frac{(-1)^m}{m!}\sum_{k=0}^{2n-m}\phi(k+m). \qquad (17)
\end{aligned}
$$

To evaluate this last sum, we utilize the Chu-Vandermonde Sum Identity [2]. It yields

$$\sum_{k=0}^{2n-m}\phi(k+m) = \phi(m)\frac{(-2n-m-1)_{2n-m}}{(-2n)_{2n-m}} = (-2n)_m\frac{(-2n-m-1)_{2n-m}}{(-2n)_{2n-m}}.$$

Substituting this result into (17) and carefully simplifying the factorials, we ultimately arrive at our desired result:

$$f_{s,n}^{(m)}(x) = \frac{f_-^{(m)}(x)+f_+^{(m)}(x)}{2}. \qquad \square$$

5 From Symmetric Derivatives to Lanczos Derivatives.

The symmetric difference quotient whose limit yields $f_{s,n}^m$ is defined for all n satisfying $m \le 2n$. As n increases, it is natural to ask what happens to the values of these difference quotients. Because our convention has been to space inputs $\frac{h}{n}$ units apart, we should not be surprised that a definite integral results from this process.

Recall that Legendre polynomials are the continuous analog of the discrete Chebyshev polynomials. One means of expressing this fact is through the asymptotic relation that exists between the two families. Namely, that for m fixed and for t in $[-1,1]$,

$$(2n)^{-m}T_{n,m}(t) = P_m(t) + \mathrm{O}\left(\frac{1}{n}\right) \text{ as } n\to\infty \qquad (18)$$

([6], p. 42). Using this formula, we can formally establish that, for m and h fixed, (10) converges to a definite integral as $n \to \infty$, an integral that can be viewed as the leading coefficient in a Legendre series expansion.

If we assume that f is square integrable in a sufficiently small neighborhood of x, then the calculations establishing that (10) converges to an integral are fairly straightforward and are as follows:

$$\begin{aligned} a_m(n,h) &= \beta_{n,m,h} \frac{n^m}{(m!)^2} \sum_{j=-n}^{n} f(x+ht_j) T_{n,m}(t_j) \\ &= \beta_{n,m,h} \frac{2^m n^{2m+1}}{(m!)^2} \sum_{j=-n}^{n} f(x+ht_j) \left(P_m(t_j) + \mathrm{O}\left(\frac{1}{n}\right)\right) \frac{1}{n} \\ &= \beta_{n,m,h} \frac{2^m n^{2m+1}}{(m!)^2} \sum_{j=-n}^{n} f(x+ht_j) P_m(t_j) \frac{1}{n} + \frac{(2n-m)! n^{2m+1}}{(2n+m+1)!} \mathrm{O}\left(\frac{1}{n}\right) \end{aligned}$$

Since $\displaystyle\lim_{n\to\infty} \frac{(2n-m)!}{(2n+m+1)!} n^{2m+1} = \frac{1}{2^{2m+1}}$, we arrive at

$$a_m(h) \stackrel{\text{def}}{=} \lim_{n\to\infty} a_m(n,h) = \frac{(2m+1)!}{2^{m+1}(m!)^2} \int_{t=-1}^{t=1} f(x+ht) P_m(t)\, dt.$$

This same integral would arise had we instead sought to determine the polynomial Q_m that minimizes the mean-square error

$$\int_{t=-1}^{t=1} \left(f(x+ht) - Q_m(t)\right)^2 \, dt,$$

which is analogous to the sum of squares in (8). Indeed, properties of Legendre polynomials dictate that this integral is minimized when

$$Q_m(t) = \sum_{k=0}^{m} \frac{1}{\|P_k\|^2} \left(\int_{t=-1}^{t=t} f(x+ht) P_k(t)\, dt \right) P_k(t).$$

Referring to properties given in Table 1, we deduce that the leading coefficient of Q_m is precisely $a_m(h)$. Thus, $a_m(h)$ is a Legendre coefficient scaled by the leading term of the corresponding Legendre polynomial.

The transition in the preceding paragraphs has all taken place with m and h fixed. If we proceed in the spirit of our earlier approach of comparing coefficients of orthogonal polynomial expansions to like coefficients in Taylor expansions in order to obtain an extension of the usual m^{th} order derivative, it makes sense to consider the limit

$$\begin{aligned} f_L^{(m)}(x) &\stackrel{\text{def}}{=} \lim_{h\to 0} \frac{m!}{h^m} a_m(h) \\ &= \lim_{h\to 0} \frac{(2m+1)!}{2^{m+1}h^m m!} \int_{t=-1}^{t=1} f(x+ht)P_m(t)\,dt. \end{aligned} \tag{19}$$

The quantity $f_L^{(m)}$ in (19) has been the recent focus of investigation by the authors and is referred to as the m^{th} order Lanczos derivative, named in honor of Cornelius Lanczos. A general discussion of the Lanczos derivative may be found in [5], [8], and [4]. In particular, the authors prove in [4] that Theorem 1 remains valid if $f_{s,n}^{(m)}(x)$ is replaced by $f_L^{(m)}(x)$. What is new about the results contained in this note is that they spell out in detail how the the Lanczos derivative is a continuous analog of certain symmetric derivatives and how it is derived from them via a limiting process.

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