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Micah D Gale, Paul Wilson, Patrick Shriwise

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Idaho National Laboratory
Idaho Falls, Idaho 83415

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Working with Bézier Curves as Nonorthogonal Bases for Functional Expansion Tallies

Micah D. Gale 1,*, Patrick Shriwise2, Paul Wilson3

1Idaho National Laboratory, Idaho Falls, ID; 2Argonne National Laboratory, Argonne, IL;
3University of Wisconsin—Madison, Madison, WI

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ABSTRACT

Functional expansion tallies (FETs) are powerful tools for getting more information per history from Monte Carlo simulations, but in the past they have been constrained to orthogonal bases. Bézier curves are used widely in computer aided design (CAD) geometry kernels and could be well-suited for FETs due to their ability to assume many arbitrary shapes, but they use nonorthogonal bases. Recent developments in 2021 have made nonorthogonal FETs possible. The convergence of Bézier curve FETs in both polynomial order and number of samples is explored in this work. It is shown that these bases are well-suited for representing normal distributions and this opens the door to the possibility of other CAD-derived FET bases.

Keywords: functional expansion tallies, nonorthogonal, Bernstein polynomials, B-splines, NURBS

1. INTRODUCTION

In Monte Carlo particle transport simulations, tallies are the primary means of retrieving information from the simulation. Individual particle events each generate a score, and statistical moments are estimated from the set of scores generated over a large set of events. Although tallies are most commonly evaluated as piecewise constant functions over some domain, there are a number tallies using functional expansions to reconstruct continuous representations of scores [1, 2]. Past implementations of functional expansion tallies (FETs) are dominated by orthogonal FET bases, such as: Legendre polynomials, spherical harmonics, and Zernike polynomials. All of these bases are specialized to specific classes of problems. One commonality of these basis is global support, meaning that their basis functions are non-zero for almost the entirety of the domain, so all scoring events affect all regions in the domain. As a result, these bases cannot represent discontinuities in the function, or its derivatives, so the tally domain must be carefully selected to avoid possible discontinuities. Therefore, these FETs are only appropriate for their specific geometries, and require expertise in FET by the modeler. This work seeks to expand on this by exploring a specific class of nonorthogonal bases for FETs.

A generalized class of FETs is desirable as they would require less domain knowledge by Monte Carlo transport users, leading to the broader use of FETs.

Additionally, an FETs basis with local support (where basis functions are non-zero for only part of the domain) may be able to support general geometry domains and/or geometry interfaces.

*micah.gale@inl.gov

Basis-splines (B-Splines) form a basis with local support, and are widely used in computer-aided design (CAD), meaning they are well developed and implemented [3]. However, B-Splines form a nonorthogonal basis, which makes their use as a FET basis more difficult. The Bézier curve is a subset of B-Splines, and are very simple to work with, though they use a basis with global support. The Bézier curve was used in this work as a demonstration of non orthogonal functional expansion tally (NOFET) for application to more generalized B-Splines. This work explores the behavior of the Bézier curve, one such class of CAD geometry primitive, as an FET basis. This work introduces the theory of using NOFETs, introduces the Bézier curve as a specific nonorthogonal basis class, explores the convergence of this NOFET basis in both polynomial order and number of samples, and test its suitability for NOFETs in Monte Carlo radiation transport by comparing its convergence behavior in polynomial order, and sampling with the Legendre basis set.

2. BACKGROUND

2.1. Orthogonal Functional Expansion Tallies

Fundamental to the use of FETs is the assumption that the function being tallied is a member of the function space defined by the function basis, or that there exists a function in this space such that it approaches the function being expanded as the order of the function approaches infinity [1].

One example of a common functional expansion is the Fourier Series. The functional basis is the set of all sines and cosines with periods that are rational multiples of the function's period. As most engineers may remember, almost all well-behaved periodic functions have a function in the Fourier space that approaches the expanded function. Another way to phrase this is to say that the function is, or can be approached by, a linear combination of the functional basis. This can be written as:

$$f = \sum_{i=1}^{N} a_i \psi_i \tag{1}$$

Where:

- f is the function being expanded
- a_i are the coefficients of the expansion, and
- ψ_i are the basis functions.

For this work, we were constrained to some finite spatial domain, Γ. This is reasonable as almost all Monte Carlo tallies are constrained to some finite domain. We also used an inner product extensively, which will be defined for the arbitrary functions, f and g, as [1]:

$$\langle f(x), g(x) \rangle := \int_\Gamma f(x) g(x) dx \tag{2}$$

The issue now is that Equation 1 defines what the functional expansion is, but the values of $\vec{a}$ are needed. Following the derivation of Han et al. [2], the first step to find these coefficients is to take the inner product of f with all bases, ψ_i, and to substitute in the assumed relationship from Equation 1:

$$\begin{aligned} \langle f, \psi_i \rangle &= \int_\Gamma a_1\psi_1\psi_i + \cdots + a_i\psi_i\psi_i + \cdots + a_n\psi_n\psi_i dx \\ \langle f, \psi_i \rangle &= a_1\langle \psi_1, \psi_i \rangle + \cdots + a_i\langle \psi_i, \psi_i \rangle + \cdots + a_n\langle \psi_n, \psi_i \rangle \end{aligned} \tag{3}$$

We can also define the square of the L_2 norm of a function as the inner product of a function with itself (i.e., $\langle f, f\rangle =: ||f||^2$). Now that this inner product has been expanded into a sum of inner products, we can then simplify the expression if an orthogonal basis is used. Orthogonality for two functions is defined as having a zero inner product between said functions—i.e., $\langle f, g\rangle = 0$. For an orthogonal basis, Equation 3 simplifies significantly to:

$$\langle f, \psi_i\rangle = a_i ||\psi_i||^2 \tag{4}$$

Solving Equation 4 for a_i we then arrive at Griesheimer's form:

$$a_i = \frac{\langle f, \psi_i\rangle}{||\psi_i||^2} \tag{5}$$

Since these functional expansions are used in a Monte Carlo problem, the true inner product isn't known, but rather it must be estimated. Equation 6 then becomes:

$$\widehat{a_i} = \frac{\widehat{\langle f, \psi_i\rangle}}{||\psi_i||^2} \tag{6}$$

The inner product can then be estimated for N events occurring at location $\vec{x_n}$, which are individual realizations of the probability distribution function, f:

$$\widehat{\langle f, \psi_i\rangle} = \frac{1}{N}\sum_{n=1}^{N} \psi_i(\vec{x_n}) f(\vec{x_n}) \tag{7}$$

$$\widehat{a_i} = \frac{1}{N||\psi_i||^2}\sum_{n=1}^{N} \psi_i(\vec{x_n}) f(\vec{x_n}) \tag{8}$$

2.2. Nonorthogonal FET Bases

Traditionally FETs have been constrained to orthogonal bases [1]. However, it has been shown recently that this restriction is not necessary for using FETs by Han et al. [2]. To derive this relation it is necessary to revisit Equation 3. If the assumption of an orthonormal basis is removed, this Equation can then be rewritten as:

$$\langle f, \psi_i\rangle = \sum_{k=0}^{I} a_k \langle \psi_k, \psi_i\rangle \tag{9}$$

Then if the variable t_i is defined as the inner product of the expanded function with a basis function (i.e., $t_i := \langle f, \psi_i\rangle$), this equation can be clearly changed to a matrix form:

$$\vec{t} = \boldsymbol{G}\vec{a} \tag{10}$$

Given that:

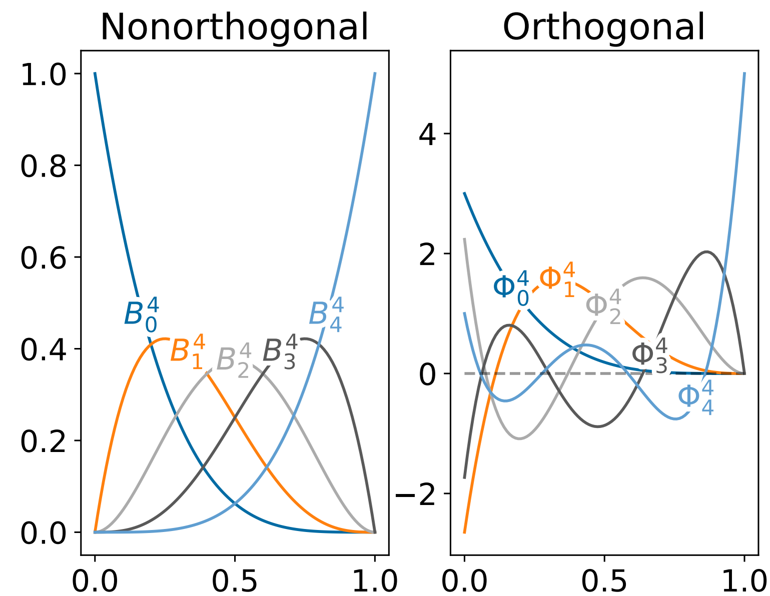

Figure 1. The order-4 Bernstein bases.

$$G_{i,j} := \langle \psi_i, \psi_j \rangle \tag{11}$$

Once we estimate $\vec{t}$ via a Monte Carlo simulation, we can solve for $\vec{a}$ using linear algebra methods, provided that $\boldsymbol{G}$, the Gramian matrix, is invertible, which is true for all linearly independent bases [2]. Notice that the Gramian matrix depends only on the functional basis, and therefore the matrix inversion needs to be only performed once for a given functional basis, and can be completed at any point in the simulation process.

2.3. Bézier Curves

Bézier curves are a class of computer-aided design (CAD) geometry primitives that are used for many arbitrary curves. They are defined by their coefficients, or control points. The curves use the Bernstein polynomials, named after the Ukrainian mathematician Sergei Natanovich Bernstein, as their basis. There are $n + 1$ base polynomials for a basis of order n. They are only defined in the parametric range $[0, 1]$. To apply the curve to the desired tally domain, an affine transformation can be used [3]. The Bernstein polynomials are not orthogonal, but an orthogonalized form exists [4]. Both orthogonal and nonorthogonal Bernstein polynomials were used in this work. The Bernstein polynomials of order n are a set of $n + 1$ polynomials defined as:

$$B_{n,i}(x) := \binom{n}{i} x^i (1-x)^{n-i} \tag{12}$$

The specific polynomial in a set is identified by its index, i, which is in the range $[0, n]$. An example of the order-4 Bernstein basis is shown in Figure 1.

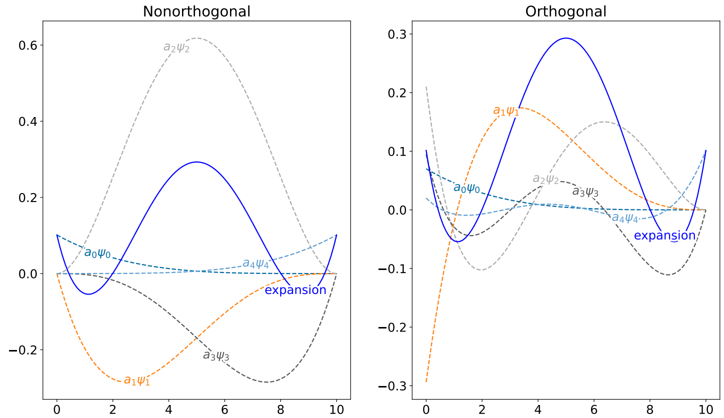

Figure 2. Example functional expansion of a normal distribution using order-4 Bernstein polynomials, showing the contribution from each basis function.

2.3.1. Orthogonal Bernstein Polynomials

The Bernstein polynomials were orthogonalized by Bellucci using the Gram-Schmidt process [4]. These orthogonalized Bernstein polynomials are defined as:

$$\phi_{n,i}(x) = \sqrt{2(n-i)+1} \sum_{k=0}^{i} (-1)^k \frac{\binom{2n+1-k}{i-k}}{\binom{n-k}{i-k}} B_{n-k,i-k}(x) \tag{13}$$

where the $\phi_{n,i}$ functions form the orthogonal Bernstein basis of order n. This basis set was used as the "orthogonal Bernstein" basis. The order-4 basis is also shown in Figure 1.

A demonstration of what a functional expansion in Bernstein polynomials looks like is given in Figure 2. In this demonstration a normal distribution was expanded using order-4 Bernstein bases. The contribution from each basis is shown as the basis function times it expansion coefficient.

3. MEASURING GOODNESS OF FIT

To determine if the Bernstein polynomials form a good basis for NOFETs, metrics are needed to evaluate how well these functional expansions represent the original function. There are generally two processes that could lead to a FET being a poor representation of the function. The first is the truncation error. This is the discrepancy in the functional expansion introduced because the target function is not a member of the basis's function space. In this case the functional expansion is depending on the target function being approached by a member of the function space as the basis order approaches infinity. The discrepancy is then introduced by truncating this infinite basis to be finite. Secondly, there is the statistical error present from using a statistical estimator from a stochastic process.

3.1. Quantifying Truncation Error

Bézier curves of degree n are able to represent all polynomials in their domain, with order $\leq n$, with a unique decomposition onto the basis [3]. It is necessary to quantify the approximation error introduced by using this basis for approximating a continuous function, which is not a member of this polynomial class.

A single scalar (or multiple scalars over smaller subdomains) metric is desirable, and over-and-under fitting should be penalized the same, so the root-mean-square error (RMSE) is a well-suited metric. Though the L-2 norm of the truncation error can be used as well [1]. For this metric to be meaningful, the true function and the basis functions should all be finite and continuous over the domain, Γ, and Γ must be finite.

The definition of the RMSE can be explicitly defined for quantifying the truncation error for a functional expansion:

$$b_n(f) = \sqrt{\frac{1}{\Gamma}\int_\Gamma \left[f(x) - \sum_{i=0}^{I} a_i \psi_i(x)\right]^2 dx} \tag{14}$$

b_n is the RMSE for the given functional expansion of order n.

The L-2 norm of the truncation error is defined as [1]:

$$||E_n|| = \sqrt{\int_\Gamma \left[f(x) - \sum_{i=0}^{I} a_i \psi_i(x)\right]^2 dx} \tag{15}$$

3.2. Measuring Stochastic Uncertainty

As with any tally, FETs experience stochastic noise. It is essential to quantify the uncertainty in the estimator of the tally. Since the quantities estimated by these tallies are the coefficients of the functional expansion $\hat{a}_i$, the uncertainty in these coefficients must be found.

For orthogonal FETs, Griesheimer has derived an estimator [1]. However, this derivation assumes orthogonal bases in order to eliminate the coefficient covariances. Currently, there does not appear to be a simple way to quantify the variance for these coefficient estimators for nonorthogonal bases, and further research is needed [1, 2].

4. RESULTS

In all the analysis presented below a normal distribution with mean of 5 and standard devation of 1 was used as the target function being estimated. The domain was defined as $[0, 10]$, or $\pm 5\sigma$, and includes a large domain where the normal distribution departs significantly from polynomial behavior. For clarity, these are shown in Equation 16.

$$\begin{aligned} f = \mathcal{N}(5,1) &= \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-5)^2}{2}} \\ \Gamma &= [0, 10] \end{aligned} \tag{16}$$

All Monte Carlo FET work was done in 1D, and all samples were in the domain, Γ. The FET methods were all implemented in a simple Python script.

4.1. Truncation Error for the Normal Distribution

To quantify the truncation error of polynomials of a given order for the base function, a functional expansion was completed numerically. The truncation error was evaluated using Equation 3. For this $\langle f, \psi_i \rangle$ was numerically calculated directly instead of using Monte Carlo sampling. These inner products were then used to solve Equations 8 and 10. The truncation errors were then calculated as the RMSE using Equation 14. For this analysis the orthogonal and nonorthogonal Bernstein polynomials, and the Legendre polynomials were used as the functional bases. Histogram, or bin, based tallies were also included in the comparison. This was done by treating each histogram bin as a basis function that was piecewise continuous. These results are given in Figure 3.

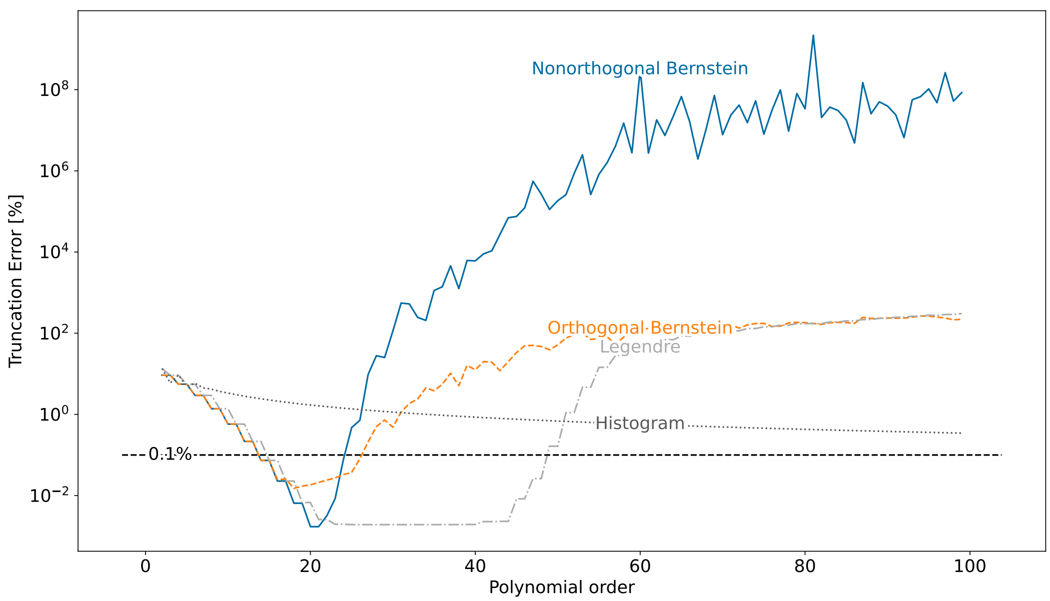

Figure 3. Numerical truncation error of Bernstein polynomials for a given order. The Legendre polynomials are provided for comparison as well.

As expected, the truncation error decreases rapidly with increasing polynomial order. The truncation error is also clearly dominated by odd-even behavior for all bases. This is likely because the normal distribution is symmetric and is best represented by even functions. None of these bases calculated the exact same truncation error, meaning that it cannot be definitively stated that these are the theoretical minimum possible truncation errors possible with a polynomial of a given order, especially given that numerical integration was used. In general, the nonorthogonal, or "traditional," Bernstein basis converges the best for polynomial orders under 20.

As expected as well all polynomials outperformed histogram based representations, in both truncation error magnitude as well as in convergence rate. This of course is exactly what FETs meant to do.

For the Bernstein and for expanding this normal distribution an order 14 polynomial is needed to achieve $< 0.1\%$ error. This order was used going forward for most expansions. The Bernstein functional expansion bases begin to diverge above order 20. This is likely due to numerical precision round-off errors in the evaluation of these higher order polynomials, as well as discrepancies from using numerical integration. If finer precision floating-point arithmetic was used this point of divergence should be higher. However, the Legendre bases do not suffer from this divergence, until numerical integration discrepancies dominate. This is due to their orthogonality, and the fact they span all lower order polynomials. This means that the lower orders of the functional expansions do not change as the polynomial order is increased, and only small changes are made to the higher order coefficients. As a result, the very high order coefficients have minimal round off effects and essentially no effect on the resulting functional expansions in the Legendre bases. The trends in Figure 3 indicate that Bernstein polynomials converge at the same rate as Legendre polynomials with regards to order when used as an FET basis in this case.

4.2. Convergence of 1D Direct Monte Carlo Sampling

Next, Monte Carlo sampling was performed using the normal distribution defined in Equation 16. FETs were deployed with the same stochastic samples for both types of Bernstein bases, the Legendre basis, and the histogram basis. This was performed for a different number of samples in order to observe the convergence behavior. The functional expansion was not restarted for each data point. For example, if only 10 and 100 samples were collected the FET would be paused at 10 samples, and the FET would be evaluated, then another 90 samples would be tallied, and so forth. All FET bases were of order 14. This was repeated for 100 independent trials. These bases are not expected to converge to 0 RMSE due to the truncation error inherent to the finite bases chosen. The truncation error limit for the Bernstein bases is 0.077%. These results are shown in Figure 4.

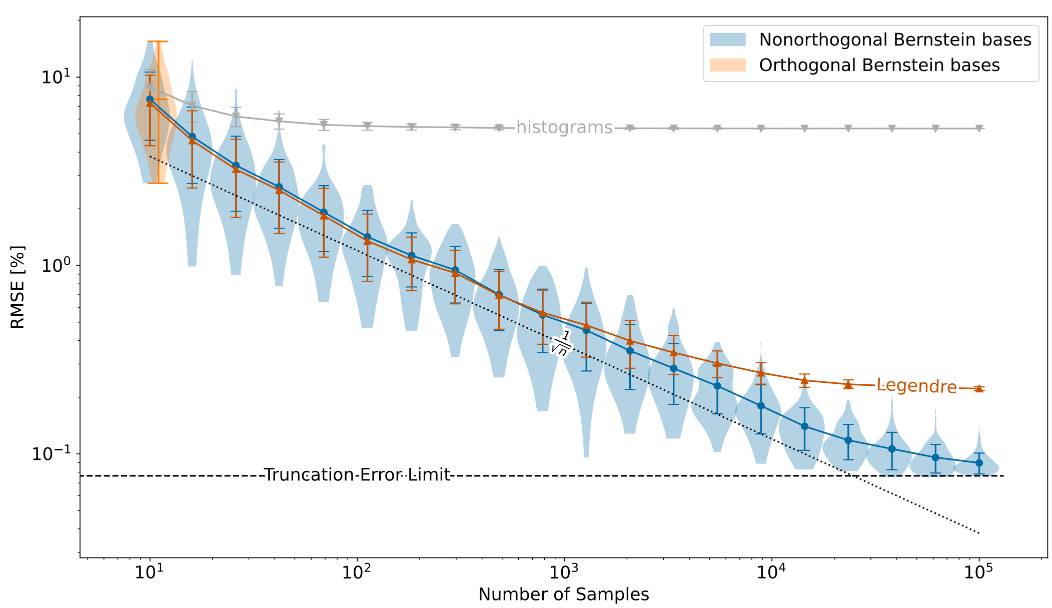

Figure 4. The RMSE of different FET bases for direct Monte Carlo sampling compared to the numerical RMSE achievable for these bases of order 14. 100 trials were performed.

The nonorthogonal and the orthogonal Bernstein bases performed almost identically, and their distributions among the 100 trials were also nearly the same. For this reason only the first set of data for the orthogonal Bernstein bases RMSEs were included for clarity.

The Legendre FET basis performed very similarly to the Bernstein polynomial bases at less than 1,000 samples. This makes sense as both bases are using order-14 polynomials. Above 1,000 samples they begin to diverge as in this implementation the Legendre basis has a truncation error higher than the Bernstein basis for this order, so the Legendre basis begins to approach this limit at around 1,000 samples. Both Legendre and Bernstein bases outperformed the histogram system. This is because 14 histogram bins is far too course in this case, and the truncation limit for this problem is quickly reached for the histogram bases.

The Bernstein data were fit with a linear regression in “log-log” space. The RMSEs for the Bernstein bases converge with $O\left(n^{-0.477}\right)$, based on this regression with $R^2 = 0.98$. This is very close to the theoretical rate of convergence that we would expect: $O\left(\frac{1}{\sqrt{n}}\right)$. The deviation from $n^{-0.5}$ might be due to a few effects. First the far left groups of samples are likely to have very high discrepancies since there are 15 degrees of freedom in these functional expansions, and so anything with less than 30 samples will have very poor statistics. On the right side the distributions are hitting the truncation error limit, and are noticeably asymmetric due to this. The regression was also performed for only the middle 10 groups of samples. This found a convergence rate of: $O\left(n^{-0.488}\right)$ with $R^2 = 0.999$. Based on these results, Bernstein polynomial based FET are well-behaved statistical estimators, that converge at the same rate as Legendre Polynomials with regard to sample size, and had nearly identical RMSEs to the Legendre polynomials for this target function.

4.3. Analysis of Subdomain Error

All previous data analyses were performed on the global RMSEs. However, the goal with this FET basis is for it to be well converged in the low-sampled tails of the normal distribution as well. To investigate the convergence of these tails, a Monte Carlo FET was performed on the normal distribution using order 14 Bernstein bases with 1,000 samples in 100 trials. A numerical functional expansion was performed as well. The square of the L-2 norm of the Error, $||E_{14}||^2$, was then calculated for 10 equally sized subdomains. The error over the entire domain was used to compute the fractional error contribution from each of the 10 subdomains. The results are shown in Figure 5.

From these results, it can be seen that for the numerical case the fractional contributions to the truncation error are nearly uniformly distributed with no extreme outliers. For the Monte Carlo FET, a similar conclusion can be drawn. The tails actually have a lower fractional contribution to the discrepancy than would be expected based on the numerical truncation error alone. This is true for almost all of the trials, showing this is not an anomaly. Likely this is due to the error shifting towards to middle of the distribution. This region has a larger magnitude in the true function, and so the same relative discrepancy will lead to a large fraction contribution to the error. Further research is needed to understand this phenomenon.

5. CONCLUSIONS

The Bézier curves and the underlying Bernstein polynomials are a class of functions well-suited for computer aided design (CAD). The Bernstein polynomials are nonorthogonal and therefore have not widely been considered for use as a basis for Monte Carlo FET. Recent developments have enabled the use of NOFET. Here we have shown that the Bernstein polynomials are well-suited for FET on the normal distribution. They have comparable convergence behavior to Legendre based FET in both order and sample size. In general, the nonorthogonal Bernstein polynomials perform the same as the orthogonal Bernstein polynomials, are simpler to implement, and there exists a wide range of toolkits for them. However, it is not clear yet if it is possible to estimate the statistical moments of NOFETs, and so NOFET should not be used yet in production.

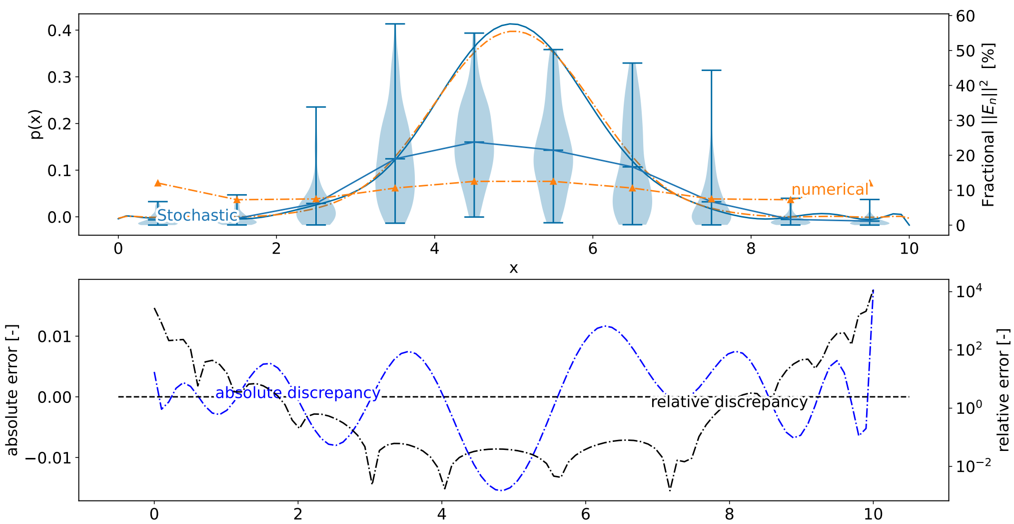

Figure 5. FET of the normal distribution using an order-14 Bernstein basis with 100 trials of 1,000 samples. The fraction contribution from 10 subdomains to the square of the L-2 norm of the error was found for each trial.

We have demonstrated an effective way to evaluate the truncation error of an FET basis deterministically, if the true form of the solution is known a priori, by using a numerical functional expansion. This work with Bernstein polynomials was meant to be a simplified basis to work with before working with general B-Splines. Next, this work should be extended to general B-Splines. In addition, the statistical properties—specifically around convergence—of these NOFET estimators need to be explored further. Specifically the variance of the coefficients of NOFETs, as well as the variance of the NOFET evaluated at an arbitrary point should be derived or approximated.

ACKNOWLEDGMENTS

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