CHARGE DENSITY ESTIMATIONS WITH ORTHOGONAL POLYNOMIALS *

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Abstract

A beam's charge density, treated as a smooth and continuous function can be approximated using an orthogonal series, allowing a solution of Poisson's equation to be found. Getting the most accurate solution to the electric potential requires the best approximated charge density. Several beam distributions are approximated using Jacobi polynomials generated by the recursion relation and the moment method. Varing both the particle number and order of the approximation gives a chance to not only compare the performance of the different polynomials, but allows to determine if a particular combination of order and particle number works better for a particular function. Although all three orthogonal polynomials used give similar results, the approximation coefficients should be allowed to converge and taken to high orders for best results. This is clearly seen on the single Gaussian approximation, where after five million particles, the difference between the distributions remains constant and the highest tested order gives best results.

INTRODUCTION

Solving the single particle equations of motion requires the space-charge fields in addition to those external. These fields can be solved by using Poisson's equation for a given beam distribution [1]. With a vanishing potential at infinity, the solution to (1) only relies on the integral of a charge distribution function, as shown in (2). The charge distribution can then be treated as a smooth function and approximated to a truncated order with a sum of polynomials and their coefficients using Weierstrass theorem [2]; see (3). Minimizing an error function in the approximated charge distribution will result in the best solution for the potential.

$$\nabla^2\Phi(\vec{r}) = -\frac{\rho(\vec{r})}{\epsilon_0} \qquad \Phi(\infty) = 0 \tag{1}$$

$$\Phi(\vec{r'}) = \frac{1}{4\pi}\int \frac{\rho(\vec{r'})}{\left\|\vec{r} - \vec{r'}\right\|} d\vec{r'} \tag{2}$$

$$\rho(\vec{r}) = \sum_{i=0}^{n} a_i P_i(\vec{r}) \tag{3}$$

With Weierstrass theorem, any type of polynomials can be used to approximate the charge distribution. Orthogonal polynomials in particular have very nice properties that simplify mathematical calculations. Because beams are contained in a finite space that can be rescaled to suit, any interval of orthogonality $[a, b]$ can be chosen to define the orthogonal polynomials. Defining it as $[-1, 1]$ results in the orthogonality interval that defines Jacobi polynomials, [3]. More specifically, we choose the cases of Jacobi polynomials where $\alpha = \beta$, i.e. Legendre and Chebyshev I. In addition to the orthogonality properties, these polynomials are also known for minimizing certain errors.

A distribution function, which describes the distribution of the particles inside the beam, usually takes a bell-shaped curve. According to the Central Limit Theorem, many small effects on the beam will eventually transform the distribution into a Gaussian if enough time is allowed [1, 4]. A set of classic beam distributions represent the extremes of a beam distribution, starting with the K-V distribution and moving to the WaterBag, Parabolic and the Gaussian at the other end. Because the beam is not always allowed to fully evolve into a Gaussian, other distributions like these are used to model the charge distributions. All four distributions are defined over phase space. If any of these distributions is integrated over the velocities, the result is the 2D projection of the distribution. In the case of the K-V distribution, the two dimensional representation is known as the Uniform distribution.

CHARGE DENSITY APPROXIMATIONS WITH ORTHOGONAL POLNOMIALS

Although beams are composed of N discrete particles, represented by a sum of delta functions, the charge distribution can be sampled from a smooth function and approximated with orthogonal polynomials. This approximation, written in (4), needs to be truncated to a particular order m in order to be computationally feasible.

$$F(x) = \sum_{j}^{N} \delta(x - x_j)$$
$$\hat{=} \sum_{i}^{\infty} a_i P_i(x) \approx \sum_{i}^{m} a_i P_i(x) \tag{4}$$

Once a polynomial is chosen for the approximation, it is necessary to calculate the coefficients that correspond to the polynomials. By multiplying both sides of (4) by $P_n(x)W(x)$ and integrating on the interval $[a, b]$ with respect to x, the equation is now in form that can be simplified by applying orthogonality conditions and using a delta function property. This equation can then be solved for the

* This work was supported by the Department of Energy under Contract No. DE-FG02-08ER41532 with Northern Illinois University.

ISBN 978-3-95450-115-1

approximated polynomial coefficients a_n in terms of an orthogonal polynomial and its weight function.

$$\sum_j^N \int_a^b \delta(x - x_j) P_n(x) W(x) dx$$
$$= \sum_i^m \int_a^b a_i P_i(x) P_n(x) W(x) dx \quad (5)$$

$$\sum_j^N P_n(x_j) W(x_j) = a_n \int_a^b {P_n}^2(x) W(x) dx \quad (6)$$

$$a_n = \frac{\sum_j^N P_n(x_j) W(x_j)}{\int_a^b {P_n}^2(x) W(x) dx} \quad (7)$$

For the case where instead of a delta function, the distribution function is continuous and defined by $g(x)$, (7) is written in terms of the integral of $g(x)$. These coefficients b_n will serve as a comparison point for the approximated coefficients and help determine whether the coefficients a_n have reached convergence.

$$b_n = \frac{\int_a^b g(x) P_n(x) W(x)}{\int_a^b {P_n}^2(x) W(x) dx} \quad (8)$$

Changing the particle number N and the polynomial used on the calculation will allow determining if a particular combination is best for a distribution. To compare the different combinations, the error between the approximated charge distribution and the distribution based on $g(x)$ is calculated using (9).

$$\epsilon = \int |\rho(\vec{r}) - \rho_a(\vec{r})| \, d\vec{r} \quad (9)$$

RESULTS

Single One Dimensional Gaussian Distribution

The first distribution approximated was a 1D single Gaussian with mean $\mu = 0$ and variance $\sigma^2 = \frac{1}{36}$ with a randomly generated particle set of $1.5{\cdot}10^7$. Using (7) the coefficients up to order $n = 20$ for Legendre and Chevyshev polynomials were approximated for every 10^4 points up to 10^6 million and for every million after that. Figures 1 and 2 shows a sample of the progression of the approximations for the polynomials.

Although all the figures with $n = 20$ show a very good approximation, by looking at the figures with just the naked eye, it is impossible to tell if there is a difference as we move from left to right in the figures, which increases the particle number. On the other hand, by moving from top to bottom which increases the order, there is a clear difference in the approximation. Using (9), we calculated the difference the difference between the plots in order to compare the polynomials to each other. From table 1, we see that for $n = 20$ the approximation has an error of around 0.1% for all polynomials used. Looking across the entire

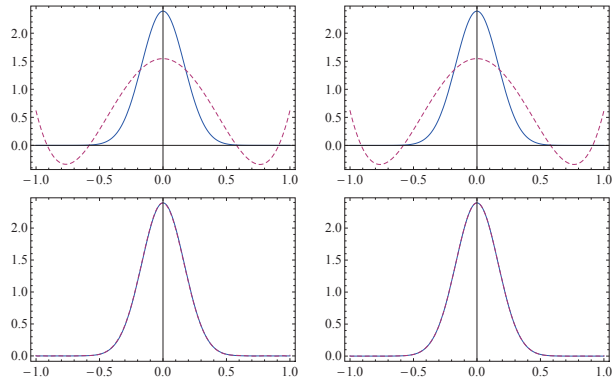

Figure 1: At the top, the Legendre polynomial approximations of the charge density for $n = 4$ with 10^5 and 10^7 points and for $n = 20$ with 10^5 and 10^7 points below.

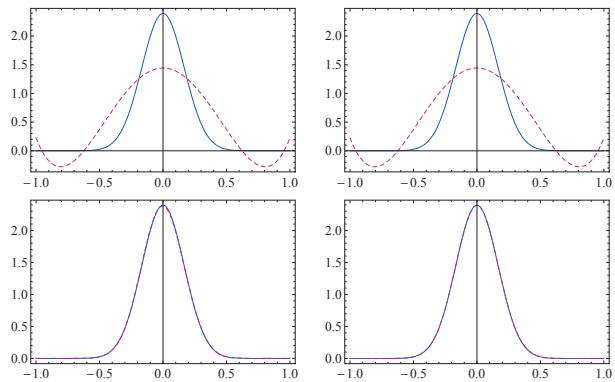

Figure 2: At the top, the Chebyshev I polynomial approximations of the charge density for $n = 4$ with 10^5 and 10^7 points and for $n = 20$ with 10^5 and 10^7 points below.

table that Chebyshev I starts out with a lower error than the other two. This later changes to Legendre giving the best approximated distribution overall. It is also important to point out that after a few million particles, the numbers stop changing drastically and just vary slightly. This is because the coefficients have reached a convergence point after a certain number of particles.

Uniform Distribution

In addition to a single Gaussian, we also approximated a Uniform distribution centered at zero also in the boundary $[-1, 1]$. Similarly to the Gaussian, the number of particles and approximation order reached a maximum of $1.5{\cdot}10^7$ particles and order $n = 20$. The interval for the approximations was also kept constant. Contrary to the Gaussian distribution, the Uniform approximation is not as good. Because of the hard edges on the distribution, it is impossible for polynomials to approximate it exactly. Even at $n = 20$ there is plenty of oscillations around the sharp edges and it is far from an almost perfect approximation. This is supported by the numbers in table 2. For the maximum order and number of particles, the error is around 12% to 16%.

ISBN 978-3-95450-115-1

Table 1: Error between the Gaussian distribution and polynomial approximations for select orders and particle numbers.

N	10^4		10^5		10^6		$5 \cdot 10^6$		10^7		$1.5 \cdot 10^7$	
	L	CI	L	CI	L	CI	L	CI	L	CI	L	CI
4	0.6733	0.6703	0.6732	0.6706	0.6733	0.6706	0.6734	0.6706	0.6734	0.6706	0.6733	0.6707
8	0.2460	0.2500	0.2458	0.2505	0.2458	0.2505	0.2459	0.2506	0.2460	0.2506	0.2459	0.2506
12	0.0637	0.0647	0.0625	0.0648	0.0622	0.0646	0.0622	0.0646	0.0623	0.0646	0.0622	0.0647
16	0.0228	0.0155	0.0141	0.0143	0.0112	0.0121	0.0113	0.0119	0.0113	0.0119	0.0112	0.0119
20	0.0236	0.0113	0.0086	0.0097	0.0020	0.0031	0.0016	0.0018	0.0015	0.0017	0.0016	0.0017

Table 2: Error between the Uniform distribution and polynomial approximations for select orders and particle numbers.

N	10^4		10^5		10^6		$5 \cdot 10^6$		10^7		$1.5 \cdot 10^7$	
	L	CI	L	CI	L	CI	L	CI	L	CI	L	CI
4	0.3145	0.3152	0.3150	0.3152	0.3144	0.3155	0.3144	0.3153	0.3144	0.3153	0.3144	0.3153
8	0.2259	0.2286	0.2265	0.2287	0.2254	0.2305	0.2254	0.2293	0.2253	0.2295	0.2254	0.2296
12	0.2014	0.2026	0.2001	0.1988	0.2008	0.1985	0.2009	0.1987	0.2007	0.1988	0.2010	0.1987
16	0.1441	0.1452	0.1468	0.1511	0.1478	0.1478	0.1484	0.1486	0.1487	0.1486	0.1484	0.1486
20	0.1306	0.1337	0.1270	0.1276	0.1267	0.1235	0.1271	0.1242	0.1273	0.1242	0.1484	0.1243

2D Single Gaussian

In 2D, we expanded a similar normal distribution. In order to perform this approximation, the coefficients necessary increased significantly from 20 to 441 for order 20. Because of this, the number of particles was kept low as to not further increase the computation time. It was found that all polynomials work well in 2D in approximating the distribution, with an error below 3%. At 10^5 particles, the coefficients have not reached convergence.

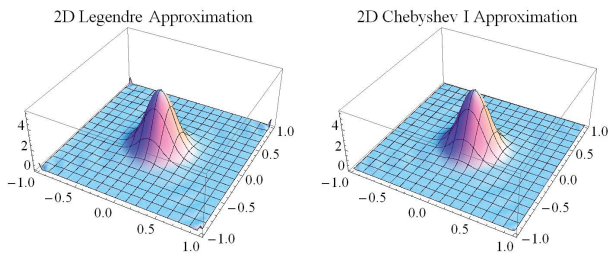

Figure 3: The 2D Gaussian distribution and their polynomial approximations with $n = 20$ and 10^5 particles.

CONCLUSION

To approximate the charge distribution of a beam, we explored one- and two-dimensional distributions. In 1D, we looked at smooth distributions such as the single Gaussian. At the other end of the spectrum of typically used distributions we considered the Uniform. In 2D we restricted ourselves to Multinormal distributions. We obtained fairly good results for the Gaussians, especially using Legendre polynomials. More work done using Legendre polynomials can be seen in [5]. Generally speaking, whether or not one of the polynomials performs better than another might be most likely specific to the function being approximated. However, the differences are expected to be small among the types of polynomials utilized. The best combination seems to be a high number of particles and order number. For example, the 1D single Gaussian returned errors below 0.16% at the highest order with $n = 20$ and 10^7 to $1.5 \cdot 10^7$ particles. For the 2D Gaussians, this approximation method also gives the expansion and approximation straightforwardly. In fact, it works very nicely with an error below 3% for 10^5 particles and $n = 20$, but the major increase of the number of coefficients needed for the approximation lengthens the time of calculation considerably. Non-smooth functions with sharper edges, like the Uniform distribution, require even higher numbers and may still not be as good as those of the smoother functions. If the number of particles must be kept low, increasing the order number will still improve the approximation. Ideally, for best results it is necessary to have a few million particles and a truncation order of at least $n = 16$. This constitutes a reasonable practical advice for production runs that combines good efficiency with acceptable accuracy.

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ISBN 978-3-95450-115-1