Optimization for TCAD Purposes Using Bernstein Polynomials

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Abstract

The optimization of computationally expensive objective functions requires approximations that preserve the global properties of the function under investigation. The RSM approach of using multivariate polynomials of degree two can only preserve the local properties of a given function and is therefore not well-suited for global optimization tasks. In this paper we discuss generalized Bernstein polynomials that provide faithful approximations by converging uniformly to the given function. Apart from being useful for optimization tasks, they can also be used for solving design for manufacturability problems.

1 Introduction

Automated TCAD optimization is difficult since the evaluation of the objective function is usually very computationally expensive. There are two main approaches: the first is to optimize the given objective function, and the second is to optimize an approximation of the objective function. Both approaches are implemented in the SIESTA (Simulation Environment for Semiconductor Technology Analysis) framework [1, 2]. The second approach relies on how good an approximation was chosen, and that it can be evaluated much faster than the original objective function so that conventional optimization algorithms requiring many more evaluations can be applied.

In the RSM (response surface methodology) [3] almost exclusively polynomials of degree two (or less) are used. This method, however, suffers from the fact that there is no reason why such an approximation should preserve the global properties of the given function: the set of of all polynomials of degree two or less is not dense in $C(X)$, $X \subset \mathbb{R}^p$ compact. Moreover, evaluating the objective function at more and more points does generally not improve the RSM approximation – these evaluations are wasted. A simple example for this fact are the functions $e_\lambda : x \mapsto \mathrm{e}^{\lambda x}$ which are ubiquitous in TCAD applications. Other examples are functions containing transitions from exponential to linear behavior.

Although the RSM approach can be improved by transforming the variables before fitting the polynomials, it has to be known a priori which transformations are useful and should be considered. If this knowledge is available, it can of course be applied to other optimization approaches as well.

To overcome the shortcoming of the RSM approach, we propose using generalized Bernstein polynomials for approximating objective functions.

We also note that a good approximation resembling the global properties of the objective function can be used for solving design for manufacturability problems. Furthermore, this method of computing approximations evidently gives rise to a recursive optimization algorithm. After a first approximation either further approximations of interesting areas are computed, or – if needed – the first approximation is refined using additional points.

2 Properties of Bernstein Polynomials

In this section we discuss some important properties of (generalized) Bernstein polynomials. In order to keep the formulas simple we will concern ourselves with functions defined on the (multidimensional) intervals $[0,1] \times \cdots \times [0,1]$. Using affine transformations it is straightforward to apply the results to arbitrary intervals.

The following theorem is due to Sergei N. Bernstein.

2.1 Theorem *Let $f : [0,1] \to \mathbb{R}$ be a continuous function. Then the Bernstein polynomials*

$$B_{f,n}(x) := \sum_{k=0}^{n} f\left(\frac{k}{n}\right) \binom{n}{k} x^k (1-x)^{n-k}$$

converge uniformly to f for $n \to \infty$.

A proof can be found in [4, p. 339]. If f even satisfies a Lipschitz condition, a stronger result can be shown giving an error bound.

2.2 Theorem *If f additionally satisfies a Lipschitz condition $|f(x) - f(y)| < L|x-y|$, then the inequality*

$$|B_{f,n}(x) - f(x)| < \frac{L}{2\sqrt{n}}$$

holds.

Additional to uniform convergence, also the derivatives of the approximation converge to those of the given function.

2.3 Theorem *If f has a continuous i-th order derivative $f^{(i)}(x)$ on $(0,1)$, then $B_{f,n}^{(i)}(x)$ converges uniformly to $f^{(i)}(x)$ on $(0,1)$.*

The proof for this theorem is still elementary but requires more careful analysis.

The generalization for a function of two variables is obtained by first approximating one variable and then the second. But using this straightforward method we can only prove pointwise convergence.

2.4 Theorem *Let $f : [0,1] \times [0,1] \to \mathbb{R}$ be a continuous function. Then the two-dimensional Bernstein polynomials*

$$B_{f,n}(x,y) := \sum_{k=0}^{n} \sum_{\ell=0}^{n} f\left(\frac{k}{n}, \frac{\ell}{n}\right) \binom{n}{k} \binom{n}{\ell} x^k (1-x)^{n-k} y^\ell (1-y)^{n-\ell}$$

converge pointwise to f for $n \to \infty$.

This method can of course be applied recursively.

2.5 Theorem *Let $f : [0,1] \times \cdots \times [0,1] \to \mathbb{R}$ be a continuous function of m variables $x_1, \ldots, x_m$. Then the multi-dimensional Bernstein polynomials*

$$B_{f,n}(x_1,\ldots,x_n) := \sum_{k_1,\ldots,k_m=0}^{n} f\left(\frac{k_1}{n},\ldots,\frac{k_m}{n}\right) \prod_{j=1}^{m} \left(\binom{n}{k_j} x_j^{k_j} (1-x_j)^{n-k_j} \right)$$

converge pointwise to f for $n \to \infty$.

3 Examples

In this section we discuss two examples illustrating the properties of Bernstein polynomials, namely an analytical function and a two-dimensional inverse modeling example.

The example of the function $f : [0,1] \times [0,1] \to \mathbb{R}$,

$$f(x,y) := (1/2)\mathrm{e}^{-10((x-1/2)^2+(y-1/2)^2)} + \mathrm{e}^{-50((x-1)^2+(y-1)^2)}$$

shows that approximation using generalized Bernstein polynomials resembles the global properties of a given function better than using multivariate polynomials of degree 2 or less, even when using a small number of lattice points. The two approaches are compared in Fig. 1. In the left hand figure, f is plotted at the $11 \cdot 11$ lattice points that were used for calculating the two-dimensional Bernstein polynomial $B_{f,10}(x,y)$ and the least squares fit $rsm(x,y)$ of degree 2. f and $B_{f,10}$ have two local maxima on $[0,1] \times [0,1]$, whereas rsm has only one. Their respective values are (up to six digits): $f(0.5, 0.5) = 0.5$, $f(0.999661, 0.999661) = 1.00338$; $B_{f,10}(0.500674, 0.500674) = 0.331634$, $B_{f,10}(1,1) = 1.00337$; $rsm(0.696706, 0.696706) = 0.283076$.

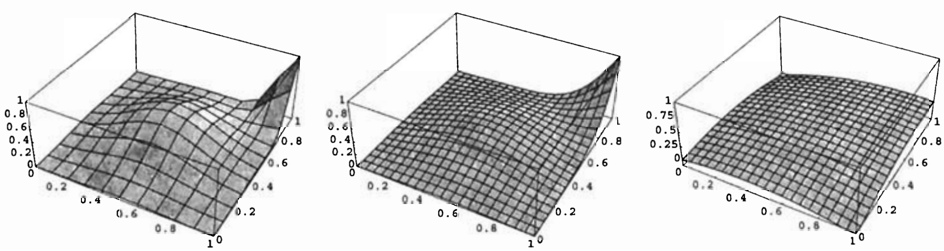

Fig. 1: Comparison of $11 \cdot 11$ lattice points of f (left), the Bernstein approximation $B_{f,10}$ (middle, the variables have been scaled to the interval $[0,1]$), and the RSM approximation rsm (right) as found by MATHEMATICA's `Fit` function.

The second, real world example stems from minimizing the leakage current of a novel SRAM storage cell [5]. First, we extracted seven parameters from the drain currents of the select transistor of the storage cell and tried to fit two transfer characteristics (two bulk voltages, two times 27 points). The seven variables were `ew`, the work function of the gate material, `sr`, the source resistance, `f`, a parameter controlling the doping, and four variables pertaining to the Shockley–Read–Hall model [6, page 71]. In the second step the extracted values were used when minimizing the leakage current.

In the course of the inverse modeling task it was found that two variables, namely the parameter of the gate material (`ew`) and the parameter controlling the doping (`f`), have a major influence on the result. For further investigations, these remaining variables were

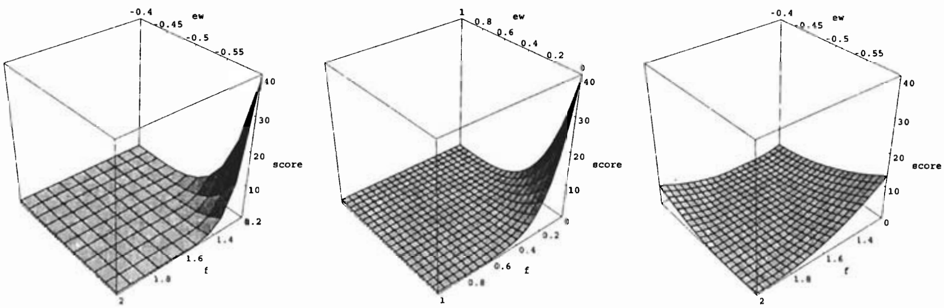

Fig. 2: Comparison of the computed lattice points (left), the Bernstein approximation (middle), and the RSM approximation (right) as found by MATHEMATICA's `Fit` function.

then fixed at the values of the minimum found, and the objective function was evaluated at $11 \cdot 11$ lattice points with these two most sensitive parameters (cf. Fig. 2, left). Using these points, two approximations were calculated: the two-dimensional Bernstein polynomial (where the variables were scaled to the interval $[0, 1]$), and the least squares approximation from the set of all polynomials of degree two or less (cf. Fig. 2). Again the RSM approximation is misleading.

4 Conclusion

For optimization tasks involving computationally expensive functions, we propose using multivariate Bernstein polynomials for approximating objective functions instead of the conventional RSM approach of using polynomials of degree two or less. We show that this approach is mathematically sound and present two examples illustrating its advantages.

Acknowledgment

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