Sequential barycentric interpolation

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Abstract Polynomial interpolators may exhibit oscillating behavior which often makes them inadequate for modeling functions. A well known correction to this problem is to use Chebyshev design points. However, in a sequential strategy it is not very clear how to add points, while still improving polynomial interpolation.
We present a sequential design alternative by allocating an extra observation where the difference between consecutive interpolators is largest. Our proposal is independent of the response and does not require distributional assumptions. In simulated examples, we show the good interpolation performance of our proposal and its asymptotical convergence to the Chebyshev distribution.

1 Introduction

In classical optimal design theory, a connection can be established between a certain optimality criterion, a linear polynomial model and a design constructed with zeros of Chebyshev polynomials, i.e. Chebyshev points. This connection was first noted by Studden (1968). Subsequent research led to various articles and books which also exhibited designs whose points are zeros of Jacobi, Laguerre, or Hermite polynomials, among others. Among some of the better known examples of the connection between polynomial models and Chebyshev points, we may cite, classified by optimality criteria, Pukelsheim and Torsney (1991) for *A*-optimal designs, Fedorov (1972, pp.85), Pázman (1986, pp.178), Pukelsheim (1993, pp.214–216) and Kar-

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lin and Studden (1966) for D-optimality, Dette (1993) for D_s-optimality; and Dette (1993) and Heiligers (1998) for E-optimality.

In the analysis of computer experiments, usually there is no random error associated with the response and models interpolate the observed response values. A variety of models are available for the analysis of such experiments. Spline models can be used, but also models based on radial bases and kriging are have become widely used, see Müller (2001), O'Hagan (2006) and Fedorov and Müller (2007).

We are concerned with sequential polynomial interpolation. Polynomials are simple and potentially effective models, often with a straightforward interpretation. However, they have a tendency to oscillate between design points. Those oscillations are called the *Runge phenomenon*, which in some cases can only get worse as the number of data points increases. It is a well-known classical result that the oscillation caused by Runge's phenomenon can be minimized by interpolating at the Chebyshev nodes. In Epperson (1987), additional conditions for mitigating the phenomenon are studied. In the literature of approximation theory there are several proposals which use Chebyshev points and may be used to interpolate. In Boyd and Ong (2009) and Boyd and Xu (2009) the authors use a subsample of the uniform distribution to generate "mock Chebyshev" (i.e. approximate Chebyshev) points, while in Platte and Driscoll (2005), interpolation points are selected using more general polynomial approximation techniques. The methods produce good interpolation results, although the strategies are non-sequential.

The aim of the present paper is to introduce a sequential design strategy for univariate polynomial interpolation. Our proposal is based on an equivalent form of the Lagrange interpolator called barycentric interpolator. In Section 2 we review the Lagrange and barycentric interpolators. In Section 3 we present our sequential problem, introduce a design algorithm and prove that it does not depend on response values. Section 4 presents simulated examples to evaluate the performance of our algorithm. Conclusions, future work and a conjecture are presented in Section 5.

2 Barycentric Lagrange interpolation

Let $D_n = \{d_1, \dots, d_n\}$ be a design of n distinct univariate points. The values $f_1, \dots, f_n$ are observations, one for every design point. Those values are assumed to be evaluations of a deterministic (but unknown) function which is to be interpolated. A classic solution is the Lagrange interpolator $g_n(x) = \sum_{j=1}^n f_j \prod_{i=1, i\neq j}^n \frac{x-d_i}{d_j-d_i}$. Lagrange interpolation exhibits numerical and computational drawbacks and an alternative form of it is available, known as the barycentric interpolator:

$$g_n(x) = m_n(x) \sum_{j=1}^n \frac{w_{n,j} f_j}{x - d_j}, \tag{1}$$

with barycentric weights defined by $w_{n,j} = \left(\prod_{i=1, i\neq j}^{n}(d_j - d_i)\right)^{-1}$ and $m_n(x) = \prod_{i=1}^{n}(x - d_i)$. The first subindex in $w_{n,j}$ denotes number of design points used for computing it, while the second subindex relates the weight to a design point.

3 Sequential interpolation

Barycentric formulæ allow sequential interpolation of data, that is, adding an extra observation to an existing data set and updating the barycentric interpolator. Sequential updating can be made part of an adaptive procedure, in which using information from the interpolation process helps in selecting a new design point.

3.1 Response based update

Consider two interpolators, one of which is considered to be more accurate than the other, as it is built with one extra observation. We postulate that the difference between them can be used as a guide to future experimentation. In other words, the more accurate interpolator may be used to validate the less accurate fit and to insert another design point where this difference is largest over an arbitrary design region. We set the design region to $[0,1]$ but it can be adapted to other design region $[a,b]$.

The starting point is $g_n(x)$, the barycentric interpolator as defined in Equation (1). Consider an extra design point d^*_{n+1} and its corresponding observation. We term d^*_{n+1} a *dummy point* and only require it to be different from existing design points. Denote by $G_{n+1}(x)$ the interpolator constructed with the temporary design consisting of the original design plus the dummy point, $D_n \cup d^*_{n+1}$. A new design point is selected according to

$$d_{n+1} = \arg\max_{x\in[0,1]} |G_{n+1}(x) - g_n(x)|. \tag{2}$$

After the search, the dummy point d^*_{n+1} is discarded and the original design D_n is augmented to $D_{n+1} = D_n \cup d_{n+1}$. The search problem is well posed, i.e. maximisation of a bounded function over a closed compact set.

Example 1. Consider the function $f(x) = 1/(1+25(2x-1)^2)$, which is to be interpolated using the design $D_{10} = \{0, \frac{1}{9}, \ldots, 1\}$. Let $g_{10}(x)$ be the interpolator function constructed with observations of $f(x)$ at D_{10}. The dummy point $d^*_{11} = \frac{1}{2}$ is added to build an updated interpolator $G_{11}(x)$. The next point is selected where the absolute difference between the interpolators $G_{11}(x)$ and $g_{10}(x)$ is largest over $[0,1]$; this occurs at the points 0.0325 and 0.9675. Any of these two points can be added to D_{10} and d^*_{11} is discarded.

3.2 Sequential design algorithm

The sequential design procedure described above simplifies to a response-independent alternate maximization and update of $m_n(x)$. We now describe the algorithm.

Input An initial design D_n of n distinct points $d_1,\dots,d_n \subset [0,1]$; a number k of extra design points required.
Output A set of additional runs $d_{n+1},\dots,d_{n+k} \subset [0,1]$.
Initialization Set $m_n(x) := \prod_{i=1}^n (x-d_i)$; set $j := 0$.
Step 1 Maximize $|m_{n+j}(x)|$ with respect to x, in the interval $[0,1]$, i.e. let $d_{n+j+1} := \arg\max_{x\in[0,1]} |m_{n+j}(x)|$.
Step 2 Update $m_{n+j+1}(x) := m_{n+j}(x)(x-d_{n+j+1})$ and $j := j+1$. If $j<k$, repeat from Step 1.

The algorithm does not depend on actual response values observed, but only on the design points. Additionally, it does not depend on the actual location of the dummy point. These two characteristics are implied by Theorem 1, which is proven in the Appendix.

Theorem 1. *For $n>0$, let $g_n(x)$ and $G_{n+1}(x)$ for $n>0$, be two barycentric interpolators, where $g_n(x)$ is defined as in Equation (1); and $G_{n+1}(x)$ is constructed with an additional dummy design point d^*_{n+1}. Then*

$$G_{n+1}(x) - g_n(x) = m_n(x) \sum_{j=1}^{n+1} w_{n+1,j} f_j. \tag{3}$$

The right hand side of Equation (3) is the product of $m_n(x)$, which depends on x and on D_n (but not on the dummy d^*_{n+1}), and a second quantity $\sum_{j=1}^{n+1} w_{n+1,j} f_j$ that depends on design points and responses (including dummy data), but not on x and thus it can be ignored when searching for the new design point. Theorem 1 makes the search for a new design point independent of the response, indeed it makes Equation (2) equivalent to $d_{n+1} = \arg\max_{x\in[0,1]} |m_n(x)|$.

Example 2. Consider again the design of Example 1. The sequential algorithm is applied for $k=10$ extra runs and points d_{11} to d_{20} are sequentially obtained: 0.0325, 0.9684, 0.9335, 0.0662, 0.8306, 0.1677, 0.4999, 0.0099, 0.9902 and 0.2813.

A special condition arises from Equation (3), when $\sum_{j=1}^{n+1} w_{n+1,j} f_j = 0$ holds. This implies that $G_{n+1}(x) - g_n(x) \equiv 0$, in other words, that the dummy point d^*_{n+1} does not update the interpolator and consequently, this step does not yield information for the next design point d_{n+1}. This condition appears, for instance, when all f_j values are equal. This could occur when sampling a constant function or a periodic function at the same point in every period. A different instance appears when response data truly comes from a polynomial of degree at most $n-1$. In any of the above situations, any point in the interval $[0,1]$ could be selected as new design point. However, in all the examples we tried, none of them occurred and we suggest that they should not be cause of concern.

4 Performance and large sample properties

In this section we first evaluate the performance of our sequential design strategy to interpolate. We then study the large sample properties of our sequential designs.

4.1 Interpolating performance

The accuracy of polynomial interpolators with our sequential design algorithm was assessed in a simulation study. The following four functions with domain $[0,1]$ were used as test functions: $s_1(x)$ is the function of Example 1; $s_2(x) = \frac{1}{20}\exp(u^{1/3})\sin(u/2)\phi(u)$ with $\phi(u)$ the Heaviside unit step function and $u = 60x-30$; $s_3(x) = \sin(10x)$ and $s_4(x) = 2\frac{1-cos(v)}{v^2}$ with $v = 35x-15$. The functions were selected to exhibit features which are not easy for modeling with polynomials, such as flat regions followed by regions with sharp change, or periodic behavior.

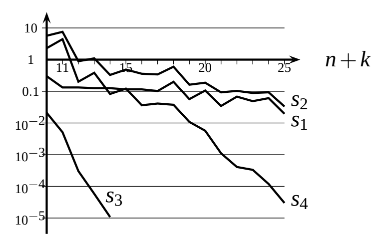

Fig. 1 Maximum distance between simulators and barycentric interpolators, plotted against number of extra points k added.

From a uniform design of size ten, fifteen points were sequentially added, totalling 25 points. At every step, barycentric interpolators were fitted independently for each function. The maximum distance between the true function $s_1(x),\ldots,s_4(x)$ and its barycentric interpolator, over the design region, was recorded. Decreasing values of this distance show good approximation, while or increasing values point to the presence of Runge phenomenon.

The results are plotted in Figure 1, where a decreasing trend is evident, thus showing good approximation to simulators for all cases. Convergence to the true function s_3 was faster than the other cases, while convergence was slower for s_2.

4.2 Large sample properties of points

The points generated with our algorithm cluster in the borders of the design region. We studied whether the points converge asymptotically to a known distribution.

To study large sample behavior, points were sequentially added to each of the following eight initial designs of size n: uniform designs $0, \frac{1}{n-1}, \ldots, 1$ (termed UI) and $\frac{1}{n+1}, \ldots, \frac{n}{n+1}$ (termed UII); first n points of Sobol's space filling sequence (termed S), see Bratley and Fox (1988); Chebyshev type I and II points (CI and CII, respectively), see Berrut and Trefethen (2004); the designs labelled TI and TII were generated by transforming UI and UII to the symmetric triangular distribution with mode in $\frac{1}{2}$; and a design with random points (termed R). We used initial design sizes $n = 5, 10, 35, 50, 100, 150$, in each case sequentially adding points with our algorithm up to one thousand. Two statistics were computed: a) Quantile-Quantile (QQ) plot and b) goodness of fit Kolmogorov-Smirnoff (KS) statistic. The Beta distribution $\beta(\frac{1}{2}, \frac{1}{2})$ (also known as the Chebyshev or arcsine distribution) was used in computations. This choice was suggested by literature on polynomial interpolation convergence Berrut and Trefethen (2004).

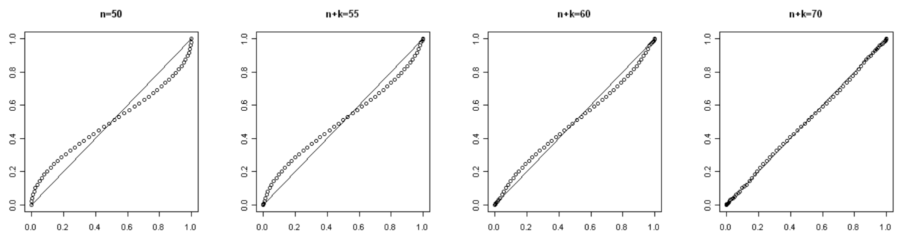

Fig. 2 QQ plot for design UI.

We show results for $n = 50$, which are representative of the results for other initial sizes. Figure 2 shows QQ plot for UI, which converges to Chebyshev distribution with 20 extra points. QQ plots for other initial designs exhibit similar pattern.

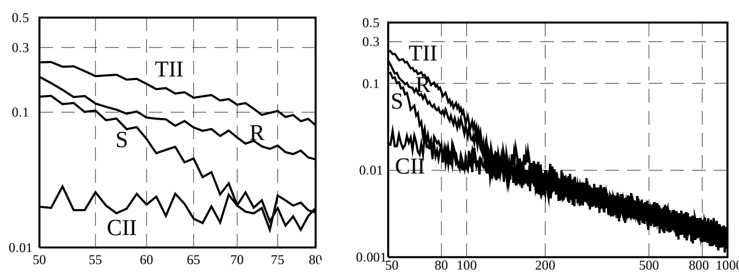

Fig. 3 KS statistic vs. design size.The left-hand panel is a close up view of the right-hand panel.

The KS statistic "grouped" designs according to their initial performance, with best (i.e. low) values obtained by Chebyshev points (CI, CII). In second place were uniform designs (UI, UII, S), followed by random design R. The worst values were observed for designs with points clustered in the centre of the design region (TI, TII). Figure 3 shows the evolution of KS statistic for one design for each of the observed "groups": CII, R, S and TII. After adding about two times as many points as the initial design size, designs behave similarly, showing non-monotonous decreasing linear trend (in the log-log scale) for the KS statistic. Simulation results suggest a value for the slope of the linear trend between -0.8 and -1, see also Figure 3.

5 Discussion and future work

We introduced a univariate sequential adaptive design algorithm. In the examples we tried, the algorithm produced good points for polynomial interpolation, which converged rapidly to the Chebyshev distribution and lead to the following claim.

Conjecture 1. For any initial design in $[0,1]$, as the number of extra points k tends to infinity, the algorithm of Section 3.2 produces samples from the distribution $\beta(\frac{1}{2},\frac{1}{2})$; and the KS statistic is of order $O(k^{\alpha})$, with α a suitable constant.

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Appendix A: Proof of Theorem 1

The barycentric interpolator $G_{n+1}(x)$ is

$$G_{n+1}(x) = m_n(x)(x-d^*_{n+1})\left(\sum_{j=1}^{n}\frac{w_{n+1,j}f_j}{x-d_j}+\frac{w_{n+1,n+1}f_{n+1}}{x-d^*_{n+1}}\right),$$

where barycentric weights $w_{n+1,j}$ are computed using design and dummy point. We have that $G_{n+1}(x)-g_n(x)=m_n(x)A$, where

$$A = (x-d^*_{n+1})\left(\sum_{j=1}^{n}\frac{w_{n+1,j}f_j}{x-d_j}+\frac{w_{n+1,n+1}f_{n+1}}{x-d^*_{n+1}}\right)-\sum_{j=1}^{n}\frac{w_{n,j}f_j}{x-d_j}.$$

We now show that A does not depend on x. After simplifying and using the updating formula of barycentric weights $w_{n+1,j}=w_{n,j}(d_j-d^*_{n+1})^{-1}$, we have

$$\begin{aligned} A &= \sum_{j=1}^{n}\frac{f_j}{x-d_j}\left((x-d^*_{n+1})\frac{w_{n,j}}{(d_j-d^*_{n+1})}-w_{n,j}\right)+w_{n+1,n+1}f_{n+1} \\ &= \sum_{j=1}^{n}\frac{w_{n,j}f_j}{(d_j-d^*_{n+1})}+w_{n+1,n+1}f_{n+1}=\sum_{j=1}^{n+1}w_{n+1,j}f_j. \end{aligned}$$

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