Best polynomial approximation: multidimensional case

D. Yost (Federation University)
N. Sukhorukova (Swinburne University of Technology) and
J. Ugon (Federation University)

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Multivariate uniform approximation

- The theory of Chebyshev (uniform) approximation for univariate functions is very elegant.
- The optimality conditions are based on the notion of alternance (maximal deviation points with alternating deviation sign).
- It is not very straightforward, however, how to extend the notion of alternance to the case of multivariate function.
- In this study, we derive optimality conditions (Chebyshev approximation) for multivariate functions.

Let us first formulate the objective function. Suppose that a continuous function $f(\mathbf{x})$ is to be approximated by a functions

$$L(A,\mathbf{x}) = a_0 + \sum_{i=1}^{n} a_i g_i(\mathbf{x}), \tag{1}$$

where $g_i(\mathbf{x})$ are the basis functions and the multipliers $a_i,\ i = 0, \dots, n$ are the corresponding coefficients. Then the approximation problem can be formulated as follows:

$$\text{minimise } \Psi(A), \text{ subject to } A = (a_0, a_1, \dots, a_n)^T \in \mathbb{R}^{n+1}, \tag{2}$$

where

$$\Psi(A) = \sup_{\mathbf{x}\in Q} \max\{f(\mathbf{x}) - a_0 - \sum_{i=1}^{n} a_i g_i(\mathbf{x}), a_0 + \sum_{i=1}^{n} a_i g_i(\mathbf{x}) - f(\mathbf{x})\},$$

$\mathbf{x} \in \mathbb{R}^l$, Q is a hyperbox, such that $c_i \le x_i \le d_i,\ i = 1, \dots, l.$

Convexity

Note that $\Psi(A),\ A \in \mathbb{R}^{n+1}$ is a supremum of affine functions and therefore $\Psi(A)$ is a convex function. Then the following condition is a necessary and sufficient optimality condition for the optimisation problem (2) at A^*:

$$\mathbf{0}_{n+1} \in \underline{\partial}\Psi(A^*), \tag{3}$$

where $\underline{\partial}\Psi(A^*)$ is a subdifferential of $\Psi(A)$ at A^*.

Basing on the calculus rules, a necessary and sufficient optimality condition (3) for (2) at A^* can be written as follows:

$$\mathbf{0}_{n+1} \in \mathrm{co}\left\{ \mathrm{sign}(\Psi(A^*)) \begin{pmatrix} 1 \\ g_1(\mathbf{x}_j) \\ g_2(\mathbf{x}_j) \\ \vdots \\ g_n(\mathbf{x}_j) \end{pmatrix} \right\}, \tag{4}$$

where $\mathbf{x}_j \in \mathcal{E}$ are maximal absolute deviation points (due to Caratheodori's theorem, $\mathbf{0}_{n+1}$ can be constructed a convex combination of no more than $n+2$ points).

The optimality condition (4) can be rewritten as follows: there exists a scalar γ, such that $0 \leq \gamma \leq 1$ and two sets of nonnegative coefficients

$$\alpha_{i+}, \text{ and } \alpha_{i-},\ i+,\ i- = 1, \dots, n+2,\ \sum_{i+=1}^{n+2} \alpha_{i+} = \sum_{i=1}^{n+2} \alpha_{i-} = 1,$$

such that

$$\mathbf{0}_{n+1} = \gamma \sum_{i=1}^{n+2} \alpha_{i+} \begin{pmatrix} 1 \\ g_1(\mathbf{x}_{i+}) \\ \vdots \\ g_n(\mathbf{x}_{i+}) \end{pmatrix} - (1-\gamma) \sum_{i=1}^{n+2} \alpha_{i-} \begin{pmatrix} 1 \\ g_1(\mathbf{x}_{i-}) \\ \vdots \\ g_n(\mathbf{x}_{i-}) \end{pmatrix}, \quad (5)$$

where $\mathbf{x}_{i+}$ are maximal absolute deviation points with positive deviation and $\mathbf{x}_{i-}$ are maximal absolute deviation points with negative deviation (it is possible to construct such convex combination, using at most $n+2$ maximal absolute deviation points, due to Caratheodori's theorem).

Necessary and sufficient optimality conditions, cont.

Therefore, a necessary and sufficient optimality condition for a Chebyshev approximation (2) can be formulated in the following theorem.

Theorem 1 *The convex hulls of the vectors* $(1, g_1(\mathbf{x}), \dots, g_n(\mathbf{x}))^T$, *built over positive and negative maximal deviation points intersect.*

An equivalent theorem is as follows (since the first coordinate is the same for all the vectors).

Theorem 2 *The convex hulls of the vectors* $(g_1(\mathbf{x}), \dots, g_n(\mathbf{x}))^T$, *built over positive and negative maximal deviation points intersect.*

In the case of linear functions (multidimensional case) $n = l$ and the functions $g_i = x_i,\ i = 1, \dots, l$. Then (5) holds and theorem 2 can be formulates as follows.

Theorem 3 *The convex hull of the maximal deviation points with positive deviation and convex hull of the maximal deviation points with negative deviation have common points.*

Note that in general $l \leq n$

Definition 1 *An exponent vector*

$$e = (e_1, \dots, e_l) \in \mathbb{R}^l,\ e_i \in \mathbb{N},\ i = 1, \dots, n$$

for $\mathbf{x} \in \mathbb{R}^l$ *defines a* **monomial** $\mathbf{x}^e = x_1^{e_1} x_2^{e_2} \dots x_l^{e_l}$.

Definition 2 *A product* $c\mathbf{x}^e$, *where* $c \neq 0$ *is called the term, then a multivariate polynomial is a sum of a finite number of terms.*

Definition 3 *The degree of a monomial* $\mathbf{x}^e$ *is the sum of the components of* e*:*

$$\deg(\mathbf{x}^e) = \sum_{i=1}^{l} e_i.$$

Definition 4 *The degree of a polynomial is the largest degree of the composing it monomials*

Theorem 4 *A polynomial of degree m is optimal if and only if there exists a pair of sets of non-negative coefficients*

$$\alpha_{i+},\ \alpha_{i-},\ \sum_{i+=1}^{n+2} \alpha_i = \sum_{i-=1}^{n+2} \alpha_i = 1,$$

such that for any monomial M_j the following equality holds

$$\sum_{i+=1}^{n+2} \alpha_{i+} M_j(\mathbf{x}^{i+}) = \sum_{i-=1}^{n+2} \alpha_{i-} M_j(\mathbf{x}^{i-}),\ j = 1, \dots, n, \qquad (6)$$

where $\mathbf{x}^{i+}$ and $\mathbf{x}^{i-}$ are maximal deviation points with positive and negative deviation signs respectively (we need at most $n+2$ points, due to Carathodori's theorem).

Proof: The proof is obvious, since this is a reformulation of theorem 2 for the case of polynomials.

Lemma 0.1 *Consider two sets of non-negative coefficients*

- $\alpha_i \geq, \ i = 1, \dots, n$ *such that* $\sum_{i=1}^{n} \alpha_i = 1$;
- $\beta_i \geq, \ i = 1, \dots, n$ *such that* $\sum_{i=1}^{n} \beta_i = 1$.

If

$$\sum_{i=1}^{n} \alpha_i a_i x_i = \sum_{i=1}^{n} \beta_i b_i y_i \tag{7}$$

$$\sum_{i=1}^{n} \alpha_i a_i = \sum_{i=1}^{n} \beta_i b_i \tag{8}$$

then for any scalar δ *the following equality holds*

$$\sum_{i=1}^{n} \alpha_i a_i (x_i - \delta) = \sum_{i=1}^{n} \beta_i b_i (y_i - \delta). \tag{9}$$

Proof:

$$\sum_{i=1}^{n} \alpha_i a_i (x_i - \delta) = \sum_{i=1}^{n} \alpha_i a_i x_i - \delta \sum_{i=1}^{n} \alpha_i a_i$$
$$= \sum_{i=1}^{n} \beta_i b_i - \delta \sum_{i=1}^{n} \beta_i b_i y_i$$
$$= \sum_{i=1}^{n} \beta_i b_i (y_i - \delta).$$

$\triangle$

Algorithm

The following algorithm can be used to verify necessary optimality conditions.

- Step 1 Identify maximal deviation points that correspond to positive and negative deviations:

$$\mathcal{P} = \{\mathbf{x}^{i+},\ i = 1, \dots, N^+\};\ \mathcal{N} = \{\mathbf{x}^{i-},\ i = 1, \dots, N^-\};$$

$$N = N^+ + N^-.$$

- Step 2 For each dimension $k : k = 1, \ldots, l$ identify

$$\delta_k = \min\{\min_{i=1,\ldots,N^+} x_k^{i+}, \min_{j=1,\ldots,N^-} x_k^{j-}\},$$

where x_k^{i+} and x_k^{i-} are the $k-$th coordinates of $\mathbf{x}^{i+}$ and $\mathbf{x}^{i-}$ respectively; and

$$\sigma_k = \max\{\max_{i=1,\ldots,N^+} x_k^{i+}, \max_{j=1,\ldots,N^-} x_k^{j-}\},$$

where x_k^{i+} and x_k^{i-} are the $k-$th coordinates of $\mathbf{x}^{i+}$ and $\mathbf{x}^{i-}$ respectively.

- Step 3 Apply the following coordinate transformation (to transform the coordinates of the maximal deviation points to nonnegative numbers):

$$\tilde{x}_k^{i+} = x_k^{i+} - \delta_k;$$

$$\tilde{x}_k^{i-} = x_k^{i-} - \delta_k;$$

and

$$\tilde{\tilde{x}}_k^{i+} = x_k^{i+} - \sigma_k;$$

$$\tilde{\tilde{x}}_k^{i-} = x_k^{i-} - \sigma_k.$$

- Step 4 Reduction
  - Step 4.1 Exclude all the points whose coordinates in the highest degree monomial coincide with δ and check if the intersection of the convex hulls of the remaining points from $\mathcal{N}$ and $\mathcal{P}$ are nonempty.
  - Step 4.2 Exclude all the points whose coordinates in the highest degree monomial coincide with σ and check if the intersection of the convex hulls of the remaining points from $\mathcal{N}$ and $\mathcal{P}$ are nonempty.

- Step 5 If both pairs have common points then the original polynomials may be optimal, otherwise it is not optimal.

Note that theorem 2 can also be used to verify optimality (necessary and sufficient condition). In this case one needs to check if two convex sets are intersecting in $\mathbb{R}^{n+1}$, while the above algorithm requires to check if two convex sets are intersecting in $\mathbb{R}^{l+1}$.
Therefore, there are two main advantages of this algorithm.

1. It demonstrates how the concept of alternance can be generalised to the case of multivariate functions.
2. It is based on the verification whether two convex sets are intersecting or not, but since $l \leq n$ it is much easier to verify it after applying the algorithm.

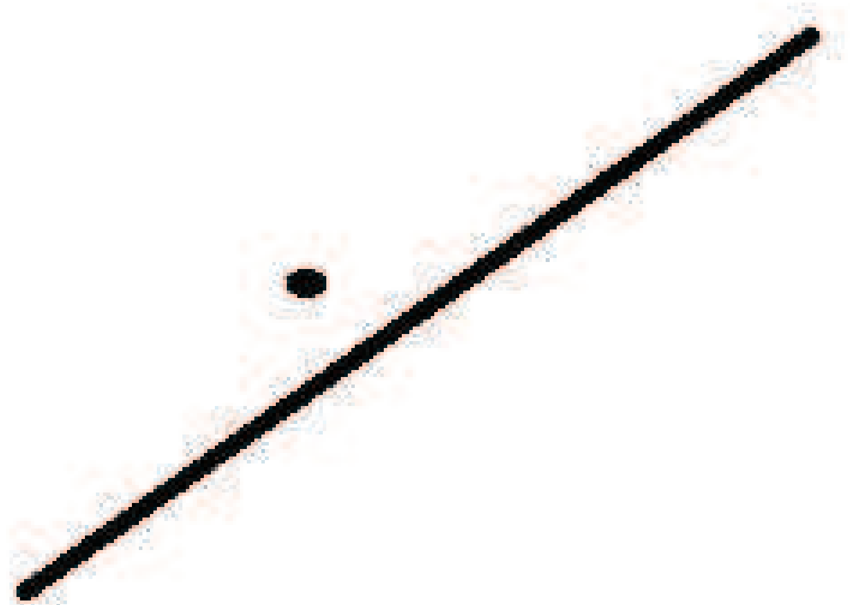
However!!!!!!!!!!! This condition is only necessary, but not sufficient. There are counterexamples.

Optimality for constant (degree zero)

There exists at least one maximal deviation point (positive deviation sing) and one maximal deviation point (negative deviation sign).
In this case, the system contains only one equation

$$\sum_{i=1+}^{N^+} \alpha_{i+} = \sum_{i-=1}^{N^-} \alpha_{i-}.$$

Counter example 1



Another necessary condition

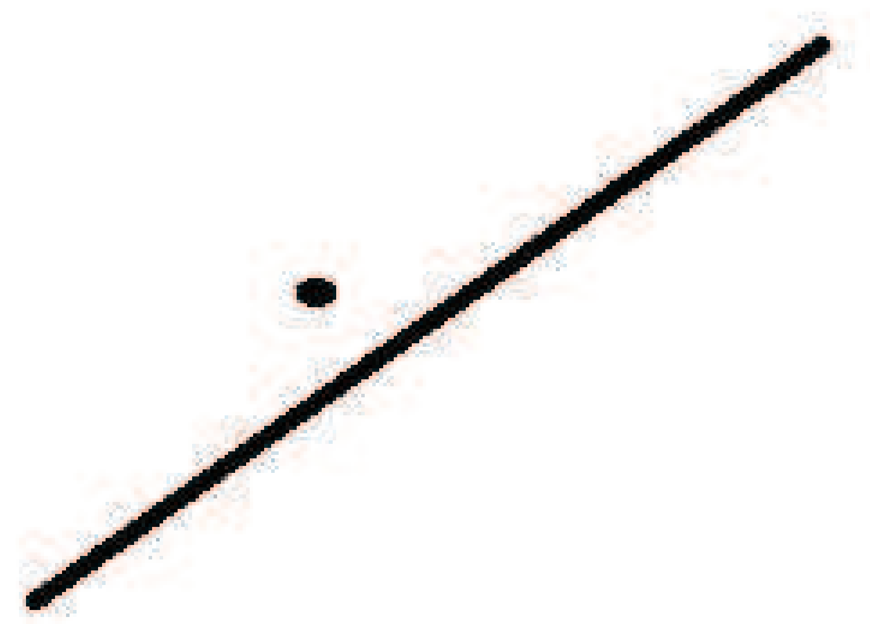
Projections: fix all the coordinates, except one. The alternance condition should satisfy.

Counterexample: Two negative maximal deviation points $A = (x_1, y_1)$ and $B = (x_2, y_2)$; and one positive maximal deviation point $C = (x_3, y_3)$, such that

$$x_1 < x_3 < x_2 \text{ and } y_1 < y_3 < y_2$$

and $C = (x_3, y_3)$ does not belong to the segment AB. In this case, the alternance conditions are satisfied for both dimensions. However, the necessary and sufficient optimality conditions are not satisfied (since C does not belong AB).

Counter example 2



Another formulation of necessary and sufficient optimality conditions

Assume that our maximal deviation points are located in such a way that necessary and sufficient optimality conditions for degree $m-1$ are satisfied.
Therefore, there exists a non-negative solution (at least one of the components is non-zero) to the system

$$A_{m-1}\Lambda = \mathbf{0}.$$

Any solution can be presented as $\Lambda = B\Gamma$ (if non-empty, represents a cone: intersection of a linear space and positive orthant). We can split A_m as

$$\begin{bmatrix} A_{m-1} \\ A_m^d \end{bmatrix}.$$

Necessary and sufficient condition

We need to find non-negative vectors Γ_1 and Γ_2 (at least one coordinate is positive for one of these vectors), such that

$$X_i B\Gamma_1 = B\Gamma_2,\ i = 1,\dots,n,$$

where $X_i = \mathrm{diag}(x_i^1,\dots,x_i^N),\ i = 1,\dots,l$. Finally, we need to find a non-negative vector Γ (at least one coordinate is positive), such that

$$[XB, -\tilde{B}]\Gamma = \mathbf{0},$$

where

$$X = \begin{bmatrix} X_1 \\ \vdots \\ X_l \end{bmatrix},\quad \tilde{B} = \begin{bmatrix} B \\ \vdots \\ B \end{bmatrix},\quad \Gamma = \begin{bmatrix} \Gamma_1 \\ \Gamma_2 \end{bmatrix}.$$

In his paper (1963) J. Rice studies a number of properties of multivariate best approximations. Also, he gives his necessary and sufficient optimality conditions.

Theorem 5 *(Rice) $L(A^*, \mathbf{x})$ is a best approximation to $f(\mathbf{x})$ if and only if the set of extremal points of $L(A^*, \mathbf{x}) - f(\mathbf{x})$ (maximal deviation points) contains a critical point set.*

Definition 5 *A subset of extremal points is called a critical point set if its positive and negative parts $\mathcal{P}$ and $\mathcal{N}$ are not isolable, but if any point is deleted then $\mathcal{P}$ and $\mathcal{N}$ are isolable.*

Definition 6 *The point sets $\mathcal{P}$ and $\mathcal{N}$ are said to be isolable if there is an A, such that*

$$L(A, \mathbf{x}) > 0 \, \mathbf{x} \in \mathcal{P}, \quad L(A, \mathbf{x}) < 0 \, \mathbf{x} \in \mathcal{N}.$$

Connection with John Rice's paper 1963, cont.

- Note that $L(A, \mathbf{x})$ is linear with respect to A. Then the set of points, where $L(A, \mathbf{x}) = 0$ is a linear function (hyperplane). If two convex sets (convex hulls of positive and negative points) are not intersecting, then there is a separating hyperplane, such that these two convex sets lie on opposite sides of this hyperplane.
- Note that in our necessary and sufficient optimality conditions we only consider finite subsets of $\mathcal{P}$ and $\mathcal{N}$, namely, we only consider the set of at most $n + 2$ points from the corresponding sundifferential that are used to form zero on their convex hull. Generally, there are several ways to form zero, but if we choose the one with the minimal number of maximal deviation points, then, indeed, the removal of any of the extremal points will lead to a situation where zero can not be formed anymore and the corresponding subsets of positive and negative points are isolable (their convex hulls do not intersect).

Therefore, our necessary and sufficient optimality conditions are equivalent to Rice's conditions.
The main advantages of our formulations are as follows.

- First of all, our condition is much simpler, easier to understand and connect with the classical theory of univariate chebyshev approximation.
- Second, it is much easier to verify our optimality conditions, which is especially important for the construction of of a Remez-like algorithm, where necessary and sufficient optimality conditions need to be verified at each iteration.

Connection with classical results, obtained by Chebyshev (univariate approximation)

- In the case of univariate linear approximation there exist three maximal deviation points (alternating deviation signs). This means that there are two points with the same deviation sign and one (between them) with the opposite deviation sign. Therefore, the convex hull of the two points (same deviation sign) contain the maximal deviation point (opposite sign). This means that the convex hulls of positive and negative maximal deviation points intersect.
- If we apply our algorithm (optimality verification for higher degree polynomials) to univariate polynomial approximation, then at each step we have to reduce the degree by one (from m to $m-1$). This would be achieved (in the algorithm) by canceling the first maximal deviation point and indeed the remaining maximal deviation points correspond to necessary and sufficient optimality conditions in the case of polynomials of degree $m-1$.

Further directions

For the future we are planning to proceed in the following directions.

1. Extend these results to the case of variable polynomial degrees for each dimension.
2. Develop similar optimality conditions for multivariate trigonometric polynomials and polynomial spline Chebyshev approximations.
3. Develop an approximation algorithm to construct best multivariate approximations (similar to the famous Remez algorithm, developed for univariate polynomials and extended to polynomial splines)