A Bernstein-Bézier Sufficient Condition for Invertibility of Polynomial Mapping Functions
(Draft)

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Abstract

We propose a sufficient condition for invertibility of a polynomial mapping function defined on a cube or simplex. This condition is applicable to finite element analysis using curved meshes. The sufficient condition is based on an analysis of the Bernstein-Bézier form of the columns of the derivative.

1 Invertibility of polynomial mapping functions

In finite element analysis, it is common to subdivide the domain into elements that are images of a reference domain under polynomial functions. This approach gives rise to the popular isoparametric elements [6]. The reference domain is the unit square $I^2 = \{(\xi, \eta) : 0 \leq \xi, \eta \leq 1\}$ or triangle $\Delta^2 = \{(\xi, \eta) : 0 \leq \xi, \eta; \xi + \eta \leq 1\}$ in $\mathbb{R}^2$ or the unit cube $I^3 = \{(\xi, \eta, \zeta) : 0 \leq \xi, \eta, \zeta \leq 1\}$ or tetrahedron $\Delta^3 = \{(\xi, \eta, \zeta) : 0 \leq \xi, \eta, \zeta; \xi + \eta + \zeta \leq 1\}$ in $\mathbb{R}^3$.

Polynomials defined on $\Delta^d$ for $d = 2, 3$, generally include monomial terms up to degree $p$ for some $p > 0$. On the other hand, for the unit cube $I^d$, the monomial terms are generally up to degree $p$ individually in each coordinate. Therefore, for the rest of the paper we use $p$ to denote the maximum total

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degree of polynomials on $\Delta^2$ or $\Delta^3$, and the maximum degree in individual coordinates of polynomials defined on $I^2$ or $I^3$.

Let $F : U \rightarrow \mathbb{R}^d$ be a polynomial function, where $U$ is either $I^d$ or $\Delta^d$ and $d$ is 2 or 3. Suppose $F$ is injective on $U$, implying that it has an inverse $G$ defined on $F(U)$ such that $G(F(u)) = u$. If such a $G$ exists and is smooth, then we say that $F$ is invertible. Invertibility is important for correctness of a finite element mesh. This definition of invertibility is sometimes called “global invertibility” in order to distinguish it from “local invertibility.” The function $F$ is locally invertible if its derivative, denoted as $J$, is nonsingular on the entire reference element $U$. Local invertibility is necessary for global invertibility but is not sufficient. A function can be locally but not globally invertible if $F(U)$ “wraps around” (e.g., consider $F(r, \theta) = r(\cos \theta, \sin \theta)$ for $(r, \theta) \in [1, 2] \times [0, 4\pi]$). Additional sufficient conditions for global invertibility in the general setting are considered by Ivanenko [5]. Beyond local invertibility, one would also like an upper bound on the “condition number”

$$\text{cond}(F) = \max_{u \in U} \|J(u)\| \cdot \max_{u \in U} \|J(u)^{-1}\|$$

of $F$. Even more strongly, one would like bounds on the higher derivatives of $F$ in terms of $\text{cond}(F)$ to satisfy the Ciarlet-Raviart [2] conditions on convergence of order-$p$ finite element approximation.

Unfortunately, even the first problem, namely, determining nonsingularity of the Jacobian, is a difficult problem. We know of simple necessary and sufficient conditions only for the following special cases:

1. linear polynomials, that is, $p = 1$, defined on $\Delta^d$ of all dimensions,
2. quadratic polynomials on $\Delta^2$ in the case $d = 2$, in the special case that $F$ is linear on two of the three edges of the reference triangle [6], and
3. bilinear elements (i.e., $p = 1$) defined on $I^2$ [14].

For all other cases, we know of only separate necessary and sufficient conditions, and this paper also proposes only a sufficient condition. To our knowledge, the only necessary condition for the general case proposed in the literature is that $\det(J)$ have the same sign (strictly positive or strictly negative) at some finite list of test points. In engineering applications, it is common to test invertibility at the Gauss points used for quadrature on the
element [13]. This test is known not to be sufficient; see further remarks on this point below.

Sufficient conditions have been proposed for a few settings. For example Ushakova [15] presents a sufficient condition for the case $p = 1$ on domain $I^3$. Her sufficient condition is interpreted as requiring that certain tetrahedra formed by choosing subsets of four of the eight vertices of $F(I^3)$ have positive volume. Sufficient conditions for quadratic triangles and tetrahedra have been proposed by Salem, Canann and Saigal [9, 11, 10, 12].

In this work, we present a sufficient condition to ensure both local and global invertibility of $F$ for any of the four domains $I^d$, $\Delta^d$, $d = 2, 3$ and for any polynomial degree $p$. Our condition appears to be weaker (i.e., not able to certify invertibility in more cases) than existing sufficient tests for specific reference domains and values of $p$ but is considerably more general.

Our condition is based on writing $J$ in Bernstein-Bézier form and then considering the convex hull of the derivatives at the control points. In the next section we describe the new sufficient condition and establish that it is sufficient for local invertibility. In Section 3 we provide an equivalent characterization of the sufficient condition that is amenable to efficient testing. In Section 4 we use the equivalent characterization to prove that the condition also implies global invertibility. Our condition has a desirable property that we term “affinity,” which we define in the last section.

2 Bernstein-Bézier form

Bernstein-Bézier (BB) form is a popular way to write polynomials in computer-aided geometric design [4]. A univariate polynomial of degree $p$ in BB form would be written:

$$F(\xi) = \sum_{i=0}^{p} f_i (1 - \xi)^{p-i} \xi^i \frac{p!}{i!(p-i)!}$$

and has natural parametric domain $\xi \in [0,1]$. A bivariate polynomial with maximum degree $p$ individually in $\xi, \eta$ is written in the form:

$$F(\xi, \eta) = \sum_{i=0}^{p} \sum_{j=0}^{p} f_{i,j} (1 - \xi)^{p-i} \xi^i (1 - \eta)^{p-j} \eta^j \frac{p!p!}{i!(p-i)!j!(p-j)!}$$
and has as its natural parametric domain \((\xi, \eta) \in I^2\). A trivariate polynomial with maximum degree \(p\) individually is written

\[
F(\xi, \eta, \zeta) = \sum_{i=0}^{p} \sum_{j=0}^{p} \sum_{k=0}^{p} f_{i,j,k} (1-\xi)^{p-i}\xi^i(1-\eta)^{p-j}\eta^j(1-\zeta)^{p-k}\zeta^k \frac{p!p!p!}{i!(p-i)!j!(p-j)!k!(p-k)!},
\]

and has as its natural parametric domain \((\xi, \eta, \zeta) \in I^3\).

A bivariate polynomial with total degree at most \(p\) is written in the BB form

\[
F(\xi, \eta) = \sum_{i=0}^{p} \sum_{j=0}^{p-i} f_{i,j} \xi^i\eta^j (1-\xi-\eta)^{p-i-j} \frac{p!}{i!j!(p-i-j)!},
\]

and has natural parametric domain \((\xi, \eta) \in \Delta^2\).

Finally, a trivariate polynomial with total degree at most \(p\) is written in the BB form

\[
F(\xi, \eta, \zeta) = \sum_{i=0}^{p} \sum_{j=0}^{p-i} \sum_{k=0}^{p-i-j} f_{i,j,k} \xi^i\eta^j\zeta^k (1-\xi-\eta-\zeta)^{p-i-j-k} \frac{p!}{i!j!k!(p-i-j-k)!},
\]

and has natural parametric domain \((\xi, \eta, \zeta) \in \Delta^3\).

In all five cases, the vectors \(f_i\) (in 1D), \(f_{i,j} \in \mathbb{R}^2\) (in 2D) or \(f_{i,j,k} \in \mathbb{R}^3\) (in 3D) are called the control points. A fundamental theorem about BB form is:

**Theorem 1** Let \(U\) be the natural parametric domain of BB form for the five cases listed above. Then \(F(U)\) is contained in the convex hull of the control points.

Farin [4] proves this as a consequence of the deCasteljau algorithm for evaluating \(F\), but here is a sketch of a more direct proof. One observes that on the natural parametric domain, all the factors in the summations like \(\xi\), \((1-\xi-\eta)\), etc., are nonnegative. Furthermore, one observes that the value of all the sums, if the control points are excluded, is exactly 1. For example, consider (2) without control points:

\[
\sum_{i=0}^{p} (1-\xi)^{p-i}\xi^i \frac{p!}{i!(p-i)!},
\]

This sum is identically 1, as seen by considering a binomial expansion of \((\xi + (1-\xi))^p\). Similar argument apply to (3)–(6). Thus, in the natural
parametric domains, the above summations may be regarded as weighted averages of the control points, proving the theorem.

The next feature of BB form is that once a function is in BB form, the derivatives can be easily put into BB form. In all cases, the derivative is a BB expansion of one degree lower, multiplied by $p$, and with control points that are finite differences of the control points for $F$ in the direction of the variable being differentiated. Thus, for example, in the case of (5), we have

\[
\frac{\partial F}{\partial \xi} = \sum_{i=0}^{p-1} \sum_{j=0}^{p-1-i} \sum_{i=0}^{p-1} \sum_{j=0}^{p-1-i} p(f_{i+1,j} - f_{i,j})\xi^i \eta^j (1 - \xi - \eta)^{p-i-j-1} \frac{(p-1)!}{i!j!(p-i-j-1)!}
\]

and

\[
\frac{\partial F}{\partial \eta} = \sum_{i=0}^{p-1} \sum_{j=0}^{p-1-i} \sum_{i=0}^{p-1} \sum_{j=0}^{p-1-i} p(f_{i,j+1} - f_{i,j})\xi^i \eta^j (1 - \xi - \eta)^{p-i-j-1} \frac{(p-1)!}{i!j!(p-i-j-1)!}.
\]

In this case, the list of $p(p+1)/2$ vectors of the form $p(f_{i+1,j} - f_{i,j})$ are control points of $\partial F/\partial \xi$, and analogously $p(f_{i,j+1} - f_{i,j})$ are control points for $\partial F/\partial \eta$. Let us denote these two lists of control points $G_\xi$ and $G_\eta$ respectively. Similar expressions hold for the other four BB forms described above. In 3D there is a third list $G_\zeta$. We now state our condition:

**Condition 1** In the case $d = 2$, the matrix $[u, v]$ is invertible for every $u \in \text{hull}(G_\xi)$ and every $v \in \text{hull}(G_\eta)$. In the case $d = 3$, the matrix $[u, v, w]$ is invertible for every $u \in \text{hull}(G_\xi)$, $v \in \text{hull}(G_\eta)$, $w \in \text{hull}(G_\zeta)$.

In this condition, “hull” denotes the convex hull. The main result of this section is as follows.

**Theorem 2** If Condition 1 holds, then the matrix $J$ is invertible on the entire reference element.

The proof of this theorem follows from the arguments in the previous paragraphs: Condition 1 is sufficient since the actual Jacobians that occur on the domain have their first columns chosen from $\text{hull}(G_\xi)$, etc.
3 A computational characterization of the sufficient condition

Condition 1 specifies our sufficient condition in somewhat nonconstructive terms. In this section we provide a computational means to verify the sufficient condition.

Theorem 3 In the case of $\mathbb{R}^2$, Condition 1 is equivalent to the following condition:

- there exists a vector $h \in \mathbb{R}^2$ such that for all $f \in G_\xi \cup G_\eta$, $h^T f > 0$, and
- there exists a vector $\bar{h} \in \mathbb{R}^2$ such that for all $f \in G_\xi$, $\bar{h}^T f > 0$ and for all $f \in G_\eta$, $\bar{h}^T f < 0$.

Proof. Let $u, v$ be arbitrary in hull$(G_\xi)$ and hull$(G_\eta)$ respectively. This is equivalent to saying there exist nonnegative $\alpha_1, \ldots, \alpha_n$ summing to 1 such that $u = \alpha_1 f_1 + \cdots + \alpha_n f_n$, where $f_1, \ldots, f_n$ is an enumeration of $G_\xi$. Similarly, there exist nonnegative $\beta_1, \ldots, \beta_m$ summing to 1 such that $v = \beta_1 g_1 + \cdots + \beta_m g_m$, where $g_1, \ldots, g_m$ is an enumeration of $G_\eta$. The condition that $[u, v]$ is invertible is equivalent to saying that $u, v$ are independent, i.e., that there do not exist $\delta, \gamma$, at least one nonzero such that $\delta u + \gamma v = 0$. Suppose they are dependent, and let $\delta, \gamma$ be the two coefficients of dependence. Without loss of generality, $\delta \geq 0$. There are now two cases: either $\gamma \geq 0$ or $\gamma < 0$. If $\gamma \geq 0$, define $\bar{\alpha}_1, \ldots, \bar{\alpha}_n$ to be $\delta \alpha_1, \ldots, \delta \alpha_n$ and define $\bar{\beta}_1, \ldots, \bar{\beta}_m$ to be $\gamma \beta_1, \ldots, \gamma \beta_n$. Then the condition that the $\alpha$’s are nonnegative and the assumption that $\delta \geq 0$ is equivalent to the hypothesis that $\bar{\alpha}_1, \ldots, \bar{\alpha}_n$ are nonnegative (with no restriction on their sum). Similarly, the condition on the $\bar{\beta}_i$’s is that they are nonnegative.

Thus, in the case that $\gamma \geq 0$, a dependence is equivalent to the existence of nonnegative $\bar{\alpha}_i$’s and $\bar{\beta}_i$’s, not all zeros, such that

$$\sum_{i=1}^n \bar{\alpha}_i f_i + \sum_{i=1}^m \bar{\beta}_i g_i = 0.$$

This problem is solved by linear programming. By Farkas’ lemma [16], there is a nonnegative solution to this problem, with not all the coefficients zero, if
and only if there does not exist a vector \( \mathbf{h} \) such that \( \mathbf{h}^T \mathbf{f}_i > 0 \) and \( \mathbf{h}^T \mathbf{g}_i > 0 \) for all \( \mathbf{f}_i \)'s and \( \mathbf{g}_i \)'s.

Now we turn to the case of dependence when \( \gamma < 0 \). In this case, using the analogous argument, there is no dependence provided that there is a vector \( \mathbf{h} \) such that \( \mathbf{h}^T \mathbf{f}_i > 0 \) for all \( i \) and \( \mathbf{h}^T (-\mathbf{g}_i) > 0 \) for all \( i \).

This shows that in the case of \( \mathbb{R}^2 \), Condition 1 can be tested by solving two linear programming problems over \( \mathbb{R}^2 \) to find \( \mathbf{h} \) and \( \mathbf{h} \). In fact, there is a much simpler algorithm, namely, compute the args of all the points in \( G_\xi \cup G_\eta \). To determine whether \( \mathbf{h} \) exists, one checks whether the max arg differs by less than \( \pi \) from the min arg. (The branch cut for defining the arg function must be chosen outside the min-max range). A similar test can determine whether \( \mathbf{h} \) exists.

In the three-dimensional setting, the algorithm is not so simple but it is still linear time. Following the same approach as in the previous proof, we see that in 3D, Condition 1 is equivalent to the following conditions:

- there exists a vector \( \mathbf{h}_1 \in \mathbb{R}^3 \) such that \( \mathbf{h}_1^T \mathbf{f} > 0 \) for any \( \mathbf{f} \in G_\xi \cup G_\eta \cup G_\zeta \),
- there exists a vector \( \mathbf{h}_2 \in \mathbb{R}^3 \) such that \( \mathbf{h}_2^T \mathbf{f} > 0 \) for any \( \mathbf{f} \in G_\xi \cup G_\eta \cup (-G_\zeta) \), where \( -G_\zeta \) means \( \{ -\mathbf{f} : \mathbf{f} \in G_\zeta \} \),
- there exists a vector \( \mathbf{h}_3 \in \mathbb{R}^3 \) such that \( \mathbf{h}_3^T \mathbf{f} > 0 \) for any \( \mathbf{f} \in G_\xi \cup (-G_\eta) \cup G_\zeta \), and
- there exists a vector \( \mathbf{h}_4 \in \mathbb{R}^3 \) such that \( \mathbf{h}_4^T \mathbf{f} > 0 \) for any \( \mathbf{f} \in G_\xi \cup (-G_\eta) \cup (-G_\zeta) \).

Each of these can be verified with linear programming, which is linear time in three dimensions [8]. Alternatively, they can be verified in \( O(n \log n) \) time using a convex hull algorithm [3].

4 Global invertibility

We are now in a position to prove that Condition 1 in fact implies global invertibility of the mapping function. To demonstrate global invertibility, we will show that \( F \) is injective, i.e., for all \( \mathbf{u}, \mathbf{v} \) in the reference domain, \( \mathbf{u} \neq \mathbf{v} \Rightarrow F(\mathbf{u}) \neq F(\mathbf{v}) \). Injectivity is sufficient for global invertibility: if an injective smooth function has a nonsingular derivative at all points of
its domain, then the global inverse is also smooth by the inverse mapping theorem. The nonsingularity of the derivative is already established.

**Theorem 4** If Condition 1 holds, then $F$ is globally invertible on the reference element.

**Proof.** Let us start with the proof of injectivity in two dimensions. Choose $u, v$ in the reference element such that $u \neq v$. Let $w = v - u$. Then by the definition of directional derivative,

$$F(v) - F(u) = \int_0^1 J(u + tw)w \, dt \tag{7}$$

Assume without loss of generality that $w_1 \geq 0$, where $(w_1, w_2)$ denotes the entries of $w$. (The case $w_1 < 0$ is handled by exchanging the roles of $u, v$.) Now there are two cases: either $w_2 \geq 0$ or $w_2 < 0$. Suppose first that $w_2 \geq 0$. Because we assume Condition 1 and because we have established Theorem 3, we conclude that there exists a vector $h \in \mathbb{R}^2$ such that $h^T f > 0$ for all $f \in G_\xi \cup G_\eta$. By convexity, this implies $h^T f > 0$ for all $f \in \text{hull}(G_\xi \cup G_\eta)$. This implies that $h^T J(\xi, \eta)$ is a vector both of whose entries are positive for any $\xi, \eta$ in the reference domain since both columns of $J$ are taken from $\text{hull}(G_\xi \cup G_\eta)$. Since $w$ has both entries nonnegative, and at least one entry of $w$ is positive (because $u \neq v$), this means $h^T J(\xi, \eta)w > 0$ for all $\xi, \eta$ in the reference domain. Thus, taking the inner product of both sides of (7) with $h$ shows that $h^T (F(v) - F(u)) > 0$, and in particular, $F(v) \neq F(u)$.

The second case is $w_2 < 0$. The argument is analogous, except we use $\bar{h}$ instead of $h$.

Finally, the extension to 3D follows the same lines. We assume $w_1 \geq 0$. Depending on the signs of entries $w_2, w_3$ of $w$, we select one of $h_1, h_2, h_3, h_4$.

5 Discussion

We say that a sufficient condition for invertibility has the “affinity” property provided that it is always satisfied if the mapping function is a nondegenerate affine linear mapping, or a sufficiently small perturbation of a nondegenerate affine linear mapping.
Affinity is a desirable property since the affine linear mapping is obviously the easiest case for invertibility. Furthermore, if a sufficient condition for invertibility has the affinity property, then it can be turned into a necessary and sufficient condition if applied to each subcell of a sufficiently fine subdivision of the original domain. This is because an invertible mapping on a fine subdivision will behave like an affine mapping plus a small perturbation on each subcell, and the small perturbation tends to zero as the subdivision gets finer.

It is fairly easy to see that our test has the affinity property. Recall that the BB control points for a constant function are all identical. Thus, if \( F \) is affine linear, then \( G_\xi, G_\eta \) and \( G_\zeta \) are all singleton sets. Assuming that \( F \) is affine and invertible means that the condition must be satisfied. Furthermore, a sufficiently small perturbation of \( F \) will give \( G_\xi, G_\eta \), and \( G_\zeta \) a positive radius, but the condition of separability by planes will still hold.

Ushakova’s condition also has the affinity property. We suggest that any proposed sufficient condition should possess the affinity property in order to be considered useful.

Ushakova’s sufficient condition for the \( p = 1 \) and \( \mathbf{U} = I^3 \) case is less restrictive (i.e., is able to validate more elements) than the condition proposed here.

We conclude with a few open questions raised by this work.

1. In the case \( p = 1 \) and \( \mathbf{U} = I^3 \), our condition is more restrictive than Ushakova’s. On the other hand, it is not obvious how to generalize her condition to higher degrees or to tetrahedral elements. It would be interesting to combine her techniques with the ones in this paper to come up with less restrictive conditions for higher degrees. Ushakova (private communication) found that experiments with randomly generated elements indicate that for \( p = 1, \mathbf{U} = I^3 \), the conditions stated here overly restrictive in the sense that most of the valid (invertible) elements among a randomly generated test set would not satisfy the sufficient condition proposed here.

2. In practical application of isoparametric mesh generation, one defines the polynomial function only on one face of the boundary of the element (namely, the face adjacent to a curved exterior boundary). The remaining coefficients defining \( F \) can be determined by a formula such as the formula proposed by Lenoir \[7\], which has certain theoretical
guarantees. How does the sufficient condition here specialize if we assume that interior degrees of freedom of $F$ are determined by Lenoir’s formula? Our very preliminary computational tests seem to indicate that using Lenoir’s formula seems to make the element more amenable to our sufficient condition (i.e., it seems to minimize the diameters of the sets $G_\xi, G_\eta, G_\zeta$ compared to other choices for interior degrees of freedom).

3. The test proposed here could be strengthened to obtain an upper bound on $\text{cond}(F)$ defined by (1) in terms of the numerical values of $h^T f_i$ as $f_i$ ranges over the sets $G_\xi, G_\eta, G_\zeta$ and $h$ is the vector defining one of the halfspaces in Theorem 3. This raises the possibility of a sufficient condition not only for invertibility but also for confirming the Ciarlet-Raviart conditions. Recall that the Ciarlet-Raviart conditions require that higher derivatives of $F$ are bounded in terms of $\text{cond}(F)$.

Note that other condition numbers besides $\text{cond}(F)$ may be useful in practice. For example, Branets and Garanzha [1] have developed a distortion measure related to structured grid generation. It would be interesting to get bounds on all of these condition numbers in terms of the numerical values of $h^T f_i$.

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