# Derivatives of Isogeometric Functions on $n$-dimensional Rational Patches in $\mathbb{R}^d$

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**Abstract**

We consider isogeometric functions and their derivatives. Given a geometry mapping, which is defined by an $n$-dimensional NURBS patch in $\mathbb{R}^d$, an isogeometric function is obtained by composing the inverse of the geometry mapping with a NURBS function in the parameter domain. Hence an isogeometric function can be represented by a NURBS parametrization of its graph. We take advantage of the projective representation of the NURBS patch as a B-spline patch in homogeneous coordinates.

We derive a closed form representation of the graph of a partial derivative of an isogeometric function. The derivative can be interpreted as an isogeometric function of higher degree and lower smoothness on the same piecewise rational geometry mapping, hence the space of isogeometric functions is closed under differentiation. We distinguish the two cases $n = d$ and $n < d$, with a focus on $n = d - 1$ in the latter one.

As a first application of the presented formula we derive conditions which guarantee $\mathscr{C}^1$ and $\mathscr{C}^2$ smoothness for isogeometric functions on several singularly parametrized planar and volumetric domains as well as on embedded surfaces. It is interesting to note that the presented conditions not only depend on the general structure of the patch, but on the exact representation of the interior of the given geometry mapping.

*Keywords:* isogeometric analysis, isogeometric function, derivative, NURBS, singular patch, smoothness, embedded manifold

## 1. Introduction

The aim of this work is to contribute to a better understanding of the properties of derivatives of the functions that occur in isogeometric analysis. Our starting point is the

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notion of *isogeometric functions*. It is inspired by the seminal article by Hughes et al. (2005), which introduced the framework of isogeometric analysis (IgA). An isogeometric function is the composition of a NURBS function defined on some parameter domain with the inverse of a NURBS geometry mapping defined on the same parameter domain. Ideally, the geometry mapping is directly obtained from the NURBS representations in an existing CAD model. In this case, the numerical simulations can be performed directly based on the exact geometric representations provided by the CAD framework.

In IgA, the space of isogeometric functions is used to discretize and solve a partial differential equation. The underlying physical domain is defined by the NURBS geometry mapping. The numerical simulation uses the isogeometric functions as test/trial functions for a Galerkin discretization of the variational formulation (see e.g. Hughes et al., 2005; Gomez et al., 2008; Cottrell et al., 2009). Alternatively, these functions can be used as a basis for a collocation approach (see Auricchio et al., 2010; Schillinger et al., 2013). Consequently, it is necessary to find a good representation of the derivatives of the test functions, either for approximation or for point-wise evaluation. In addition, it may be necessary to establish smoothness and regularity properties of the spaces of isogeometric functions, which possibly entail additional constraints, e.g., for singularly parametrized domains.

The properties of derivatives of NURBS patches are well understood. When it comes to derivatives of isogeometric functions defined on these patches, however, many questions are still open. An exact representation is hard to obtain, since the derivatives of piecewise rational functions and their inverse functions are involved.

The approach presented in the paper leads to a closed-form representation of the derivatives of isogeometric functions which can be evaluated in a stable way. Moreover, this representation is quite helpful for analyzing the $C^k$ smoothness or the $H^k$ regularity of an isogeometric function. We consider the most general setting, i.e. domains represented by $n$-dimensional patches in $\mathbb{R}^d$, for both $n = d$ and $n < d$, where we especially focus on $n = d-1$ (such as surface patches in $\mathbb{R}^3$). The present paper is an extension of a conference article by Takacs and Jüttler (2013), which was limited to the case $n = d = 2$.

An isogeometric function on a physical domain, defined by a NURBS patch, can be represented as a NURBS patch parametrizing its graph. If the domain is an $n$-dimensional patch in $\mathbb{R}^d$, then the graph of an isogeometric function is an $n$-dimensional patch in $\mathbb{R}^{d+1}$. Throughout this paper we will use homogeneous coordinates to simplify the notation. Using this approach, we develop a closed form representation of the graphs of the partial derivatives of an isogeometric function. The derivatives can again be interpreted as isogeometric functions of higher degree and lower smoothness defined on the image of the same piecewise rational geometry mapping.

Consequently, the space of isogeometric functions on a given domain patch is closed under differentiation. We derive an exact representation of the derivatives of isogeometric functions. This may be of interest for symbolic manipulations, for other applications where an exact evaluation of derivatives is necessary, and for the formulation of regularization methods for solving inverse problems using the isogeometric approach.

As a first application, we investigate conditions that guarantee smoothness when dealing with patches with singular parametrizations. Related results concerning the smoothness of singular rational Bézier patches were developed e.g. by Bohl and Reif (1997) and Sederberg et al. (2011). We consider a slightly different framework. First, we keep the domain parametrization fixed and consider the space of isogeometric functions defined over this domain parametrization. Second, we investigate not only surfaces, but parameterizations of general $n$-dimensional patches in $\mathbb{R}^d$. Our method provides a systematic approach to derive conditions which characterize smoothness of arbitrary order. We demonstrate the capabilities of the proposed approach to smoothness analysis by presenting results for parametrizations of planar and volumetric domains and for surfaces in $\mathbb{R}^3$.

Regularly mapped, tensor-product NURBS can describe quadrilateral ($n = 2$) or hexahedral ($n = 3$) domains only. When it comes to representing more general domains, a standard approach is to consider singular patches. Consequently, surface patches such as the spherical shell presented in Section 6 are used in many applications (see e.g. Kiendl et al., 2009; Benson et al., 2010). The results concerning the smoothness of isogeometric functions are related to the results by Takacs and Jüttler (2011, 2012) concerning $H^1$ and $H^2$ regularity properties on singular patches.

When using singular patches, certain isogeometric basis functions may not be $C^1$- or $C^2$-smooth, hence some derivatives cannot be evaluated properly. This may affect the stability and convergence properties of the numerical schemes applied. Contributions to the numerical analysis in IgA include consistency, stability and approximation power of the method (Bazilevs et al., 2006; Cottrell et al., 2007; Hughes et al., 2010; Echter and Bischoff, 2010). However, singularly parametrized domains are not covered by these general results and have to be dealt with differently.

The first strategy that comes to mind when dealing with singular patches is to cut out the near-singular part of the patch, i.e. not evaluating functions at points where the Jacobian determinant is close to zero. However, this will lead to a reduced order of convergence in many situations. Another approach to handle singularities is to define some auxiliary basis functions locally at the singularity. We suggest to define new basis functions that lie in the span of the standard basis, i.e. that are smooth linear combinations of the non-smooth basis functions. We derive conditions on the isogeometric functions that guarantee the desired smoothness. These conditions can be used to define new basis functions and thus a smooth function space for discretization. It turns out that the dimension of this smooth function space is very sensitive to changes of the geometry mapping.

The remainder of the paper is organized as follows. In Section 2 we introduce the notation of isogeometric functions on rational patches. We first introduce the homogeneous coordinate representation of rational $n$-dimensional patches in $\mathbb{R}^d$. In the second part we introduce isogeometric functions on such patches. In Section 3 we treat the case of derivatives on patches with $n = d$. We then discuss $\mathscr{C}^1(\bar{\Omega})$ and $\mathscr{C}^2(\bar{\Omega})$ smoothness properties of isogeometric functions on planar domains $\Omega$ in Subsection 4. We denote by $\mathscr{C}^k(\bar{\Omega})$ the space of functions where the $k$-th derivatives are continuous in the interior of the domain $\Omega$ and can be extended continuously to the boundary $\partial\Omega$. In Section 5 we extend the results to $n$-dimensional patches in $\mathbb{R}^d$ with $n < d$. We especially focus on surfaces in $\mathbb{R}^3$ in Section 6, where we consider four examples corresponding to two types of model cases. We conclude the paper with some final remarks in Section 7.

## 2. Isogeometric functions on rational patches

We introduce rational $n$-dimensional patches, which are embedded into the Euclidean space of dimension $d$ and we define *isogeometric functions* on these patches.

### *2.1. Rational n-dimensional patches in* $\mathbb{R}^d$

Throughout this section we deal with piecewise rational parametrizations of patches in $\mathbb{R}^d$. In order to keep the notation simple we will adopt the concept of *homogeneous coordinates*. This is a common approach when dealing with rational functions or NURBS (see e.g. Farin, 1999).

Any Cartesian coordinate vector $\mathbf{r} = [r_1, \ldots, r_d]^T$ in $\mathbb{R}^d$ can be represented in homogeneous coordinates by

$$\tilde{\mathbf{r}} = (\tilde{r}_0, \tilde{r}_1, \ldots, \tilde{r}_d)^T \in \mathbb{R}\backslash\{0\} \times \mathbb{R}^d,$$

where $r_i = \tilde{r}_i/\tilde{r}_0$ for $i \in \{1, \ldots, d\}$. Hence any two points $\mathbf{r}$ and $\mathbf{s}$ are identical if and only if the homogeneous coordinate vectors $\tilde{\mathbf{r}}$ and $\tilde{\mathbf{s}}$ are linearly dependent. More precisely, a point with the Cartesian coordinates $\mathbf{r}$ corresponds to the equivalence class $\tilde{\mathbf{r}}\mathbb{R}$ of points in homogeneous coordinates. In the remainder of this paper, homogeneous coordinates are always denoted with a tilde ($\tilde{\mathbf{r}}$) and Cartesian coordinates without it ($\mathbf{r}$).

A piecewise rational patch in Cartesian coordinates

$$\mathbf{r}(\mathbf{u}) = \left( \frac{\tilde{r}_1(\mathbf{u})}{\tilde{r}_0(\mathbf{u})}, \ldots, \frac{\tilde{r}_d(\mathbf{u})}{\tilde{r}_0(\mathbf{u})} \right)^T \quad \text{for } \mathbf{u} \in \mathbf{B} \subset \mathbb{R}^n$$

can be represented by a piecewise polynomial parametrization in homogeneous coordinates,

$$\tilde{\mathbf{r}}(\mathbf{u}) = (\tilde{r}_0(\mathbf{u}), \tilde{r}_1(\mathbf{u}), \ldots, \tilde{r}_d(\mathbf{u}))^T \quad \text{for } \mathbf{u} \in \mathbf{B}.$$

The parameter domain $\mathbf{B}$ of the patch is the $n$-dimensional open box

$$\mathbf{B} = (0, 1)^n.$$

We assume that $\tilde{r}_0(\mathbf{u}) > 0$ for all $\mathbf{u} \in \bar{\mathbf{B}}$. Here $\bar{\mathbf{B}}$ is the closure of $\mathbf{B}$. The homogeneous coordinates are piecewise polynomial spline functions, $\tilde{r}_0, \tilde{r}_1, \ldots, \tilde{r}_{d+1} \in \mathcal{S}^{\mathbf{p},\mathbf{s}}$. Here $\mathcal{S}^{\mathbf{p},\mathbf{s}}$ is the space of $C^{\mathbf{s}}$-smooth tensor-product spline functions of degree $\mathbf{p} = (p_1, \ldots, p_n)$ with the inner knots $\theta_j^\nu$, $\nu = 1, \ldots, n$, where the vector $\mathbf{s} = (s_1, \ldots, s_n)$ specifies the order of smoothness (differentiability) with respect to the parameters $\mathbf{u} = (u_1, \ldots, u_n)$. Consequently, the knot vectors take the form

$$\boldsymbol{\theta}^\nu = (\underbrace{0, \ldots, 0}_{p_\nu+1 \text{ times}}, \ldots, \underbrace{\theta_j^\nu, \ldots, \theta_j^\nu}_{p_\nu - s_\nu \text{ times}}, \ldots, \underbrace{1, \ldots, 1}_{p_\nu+1 \text{ times}}). \tag{1}$$

We will not consider spline spaces with more general knot vectors in this paper. The bounds for the degree and smoothness of the derivative patches, which will be derived in the later sections, can be generalized to more general spline spaces. For details on NURBS and B-splines and their applications in computer aided geometric design we refer to Farin (1999); Prautzsch et al. (2002); Hoschek and Lasser (1993).

We recall the tensor-product B-spline representation of $\tilde{\mathbf{r}}$ with respect to the tensor-product B-spline basis $\{B_{\mathbf{i}}\}_{\mathbf{i}\in\mathbb{I}}$ of $\mathcal{S}^{\mathbf{p},\mathbf{s}}$,

$$\tilde{\mathbf{r}} : \; \mathbf{u} \mapsto (\tilde{r}_0(\mathbf{u}), \ldots, \tilde{r}_d(\mathbf{u}))^T = \sum_{\mathbf{i}\in\mathbb{I}} \tilde{\mathbf{c}}_{\mathbf{i}} B_{\mathbf{i}}(\mathbf{u}), \tag{2}$$

with homogeneous control points $\tilde{\mathbf{c}}_{\mathbf{i}} \in \mathbb{R}^{d+1}$. When using Cartesian coordinates, this is transformed into

$$\mathbf{r} : \; \mathbf{u} \mapsto (r_1(\mathbf{u}), \ldots, r_d(\mathbf{u}))^T = \sum_{\mathbf{i}\in\mathbb{I}} \mathbf{c}_{\mathbf{i}} R_{\mathbf{i}}(\mathbf{u}), \tag{3}$$

with Cartesian control points $\mathbf{c}_{\mathbf{i}} = (\tilde{c}_{\mathbf{i},1}/\tilde{c}_{\mathbf{i},0}, \ldots, \tilde{c}_{\mathbf{i},d}/\tilde{c}_{\mathbf{i},0})^T \in \mathbb{R}^d$, weights $\tilde{c}_{\mathbf{i},0}$ and piecewise rational (NURBS) basis functions

$$R_{\mathbf{i}}(\mathbf{u}) = \frac{\tilde{c}_{\mathbf{i},0} B_{\mathbf{i}}(\mathbf{u})}{\tilde{r}_0(\mathbf{u})}, \qquad \text{with} \qquad \tilde{r}_0(\mathbf{u}) = \sum_{\mathbf{j}\in\mathbb{I}} \tilde{c}_{\mathbf{j},0} B_{\mathbf{j}}(\mathbf{u}). \tag{4}$$

The (physical) domain $\Omega \subset \mathbb{R}^d$ is given as the image of the geometry mapping $\mathbf{r}$, i.e. $\Omega = \mathbf{r}(\mathbf{B})$, where we assume that the mapping $\mathbf{r} : \mathbf{B} \to \Omega$ is bijective. In the following subsection we define isogeometric functions on the domain $\Omega$.

### 2.2. Isogeometric functions on rational patches

We consider a bijective NURBS patch $\mathbf{r} : \mathbf{B} \to \Omega \subset \mathbb{R}^d$ as in (3) with $\tilde{\mathbf{r}}$ as in (2) such that $\tilde{r}_j \in \mathcal{S}^{\mathbf{p},\mathbf{s}}$, for $0 \leq j \leq d$.

**Definition 1.** Consider an auxiliary spline function $\tilde{r}_{d+1} \in \mathcal{S}^{\mathbf{p},\mathbf{s}}$,

$$\tilde{r}_{d+1}(\mathbf{u}) = \sum_{\mathbf{i} \in \mathbb{I}} \tilde{f}_{\mathbf{i}} B_{\mathbf{i}}(\mathbf{u}).$$

The function $f : \Omega = \mathbf{r}(\mathbf{B}) \to \mathbb{R}$, which is defined via

$$f(\mathbf{r}(\mathbf{u})) = \frac{\tilde{r}_{d+1}(\mathbf{u})}{\tilde{r}_0(\mathbf{u})} = r_{d+1}(\mathbf{u})$$

is called an *isogeometric function* on the physical domain $\Omega$. The symbol $\mathcal{V}^{\mathbf{p},\mathbf{s}}$ denotes the space of all isogeometric functions obtained by considering $\tilde{r}_{d+1} \in \mathcal{S}^{\mathbf{p},\mathbf{s}}$.

Clearly, due to the nestedness of spline spaces, it is possible to use spline spaces of higher degree $\mathbf{p}' \geq \mathbf{p}$ and lower smoothness $\mathbf{s}' \leq \mathbf{s}$ with the same inner knots (with suitably increased knot multiplicities). The space $\mathcal{V}$ of *all* isogeometric functions is obtained by considering piecewise polynomial functions $\tilde{r}_{d+1}$ of any degree over the given knot sequences. Strictly speaking, these functions are defined only in the interior of the boxes defined by the knot sequences, since they need not be continuous.

The *graph* of an isogeometric function $f \in \mathcal{V}^{\mathbf{p},\mathbf{s}}$ can be represented by the *parametric surface*

$$\tilde{\mathbf{f}}(\mathbf{u}) = (\tilde{r}_0(\mathbf{u}), \tilde{r}_1(\mathbf{u}), \ldots, \tilde{r}_d(\mathbf{u}), \tilde{r}_{d+1}(\mathbf{u}))^T, \tag{5}$$

which possesses the B-spline representation

$$\tilde{\mathbf{f}}(\mathbf{u}) = \sum_{\mathbf{i} \in \mathbb{I}} \begin{pmatrix} \tilde{\mathbf{c}}_{\mathbf{i}} \\ \tilde{f}_{\mathbf{i}} \end{pmatrix} B_{\mathbf{i}}(\mathbf{u}),$$

with homogeneous control points $(\tilde{c}_{\mathbf{i},0}, \ldots, \tilde{c}_{\mathbf{i},d}, \tilde{f}_{\mathbf{i}})^T \in \mathbb{R}^{d+2}$ for $\mathbf{i} \in \mathbb{I}$.

If all weights $\tilde{c}_{\mathbf{i},0}$ are non-zero, then an isogeometric function $f \in \mathcal{V}^{\mathbf{p},\mathbf{s}}$ has a representation in the basis $R_{\mathbf{i}} \circ \mathbf{r}^{-1}$ with coefficients $\tilde{f}_{\mathbf{i}}/\tilde{c}_{\mathbf{i},0}$ where the rational basis functions $R_{\mathbf{i}}$ are given as in (4), i.e.

$$f = \left(\frac{\tilde{r}_{d+1}}{\tilde{r}_0}\right) \circ \mathbf{r}^{-1} = \sum_{\mathbf{i} \in \mathbb{I}} \frac{\tilde{f}_{\mathbf{i}}}{\tilde{c}_{\mathbf{i},0}} \left(R_{\mathbf{i}} \circ \mathbf{r}^{-1}\right).$$

We present two simple examples to give a geometric interpretation of isogeometric functions. The left part of Figure 1 depicts a bivariate geometry mapping $\mathbf{r}$ of a planar domain $\Omega$

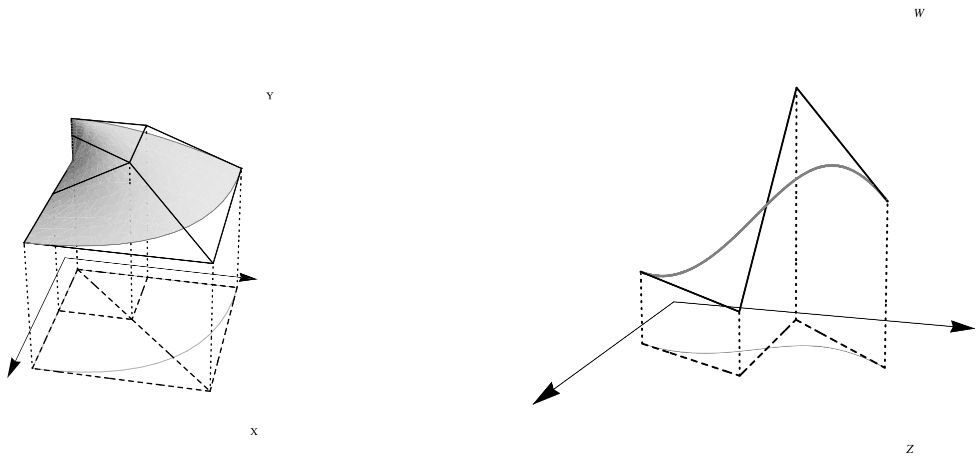


Figure 1: Planar patch $\mathbf{r}$ (left), planar curve $\mathbf{r}$ (right) and corresponding graph surfaces $\mathbf{f}$.

and the graph surface $\mathbf{f}$ of an isogeometric function $f$ defined on $\Omega$. The right part visualizes an isogeometric function $f$ defined over a planar curve given by $\mathbf{r}$.

In the following sections we derive a closed form representation of the derivatives of isogeometric functions $f \in \mathcal{V}^{\mathbf{p},\mathbf{s}}$ and, more generally, $f \in \mathcal{V}$. The main results, which will be presented in Theorem 3 and 5, are valid for NURBS. In the examples in Sections 4 and 6, however, we will restrict ourselves to rational tensor-product Bézier patches. There we consider $\mathcal{S}^{\mathbf{p},\mathbf{s}} = \mathcal{S}^{\mathbf{p},\mathbf{p}} = \Pi^{\mathbf{p}}$, where $\Pi^{\mathbf{p}}$ is the space of polynomials of degree $\mathbf{p}$. The Bernstein polynomials

$$B_{\mathbf{i}}(\mathbf{u}) = \prod_{j=1}^{n} \binom{p_j}{i_j} (1-u_j)^{p_j - i_j} {u_j}^{i_j}$$

for $\mathbf{u} = (u_1, \ldots, u_n)$ and

$$\mathbf{i} \in \mathbb{I} = \{(i_1, \ldots, i_n) : 0 \leq i_j \leq p_j \; \forall \, 1 \leq j \leq n\}$$

form a basis of the space $\Pi^{\mathbf{p}}$. In this context we will omit the index $\mathbf{s} = \mathbf{p}$ for the order of smoothness and write simply $\mathcal{S}^{\mathbf{p}}$, $\mathcal{V}^{\mathbf{p}}$ instead of $\mathcal{S}^{\mathbf{p},\mathbf{p}}$, $\mathcal{V}^{\mathbf{p},\mathbf{p}}$. Clearly, any NURBS parametrization can be transformed into a piecewise Bézier representation via knot insertion.

## 3. Derivatives of isogeometric functions for $n = d$

In this section we assume that the geometry mapping takes the form

$$\mathbf{r} : \mathbf{B} \subset \mathbb{R}^d \to \Omega \subset \mathbb{R}^d.$$

We derive a representation of the partial derivatives of an isogeometric function $f \in \mathcal{V}$ with respect to the coordinates in physical space $x_i$ for $i \in \{1, \ldots, d\}$. More precisely, we define an operator $D_i$, such that $D_i\tilde{\mathbf{r}}$ represents the graph of $\nabla_i f$, similar to the representation (5). Here $\nabla_i f = \frac{\partial f}{\partial x_i}$ is the $i$-th component of the gradient of $f$.

Note that the graph $\mathbf{f}$ of an isogeometric function $f$ is a hypersurface in $\mathbb{R}^{d+1}$. We recall the homogeneous representation of the tangent space to a parametrized hypersurface $\mathbf{f}$ at a point $\mathbf{f}(\mathbf{u})$ (cf. Ovsienko and Tabachnikov, 2005):

**Lemma 2.** *Let $\mathbf{f}$ be a $d$-dimensional patch in $\mathbb{R}^{d+1}$, which is given in the form (5) with $n = d$. We consider the tangent hyperplane $T_{\mathbf{u}}$ to the manifold at the point $\mathbf{f}(\mathbf{u})$, which is assumed to be regular. The points of this hyperplane satisfy the equation*

$$\tilde{\mathbf{g}}(\mathbf{u})^T \tilde{\mathbf{x}} = 0,$$

*where the vector $\tilde{\mathbf{g}}(\mathbf{u})$ has the entries*

$$\tilde{g}_j(\mathbf{u}) = \det(\tilde{\mathbf{e}}_j, \tilde{\mathbf{f}}(\mathbf{u}), \partial_1\tilde{\mathbf{f}}(\mathbf{u}), \ldots, \partial_d\tilde{\mathbf{f}}(\mathbf{u})), \quad j = 0, \ldots, d+1. \tag{6}$$

In these formulas, the vectors $\tilde{\mathbf{e}}_j$ are the unit vectors spanning the coordinate axes in $\mathbb{R}^{d+1}$, i.e. $\tilde{\mathbf{e}}_0 = (1, 0, \ldots, 0)^T$, $\tilde{\mathbf{e}}_1 = (0, 1, 0, \ldots, 0)^T$, etc., and

$$\partial_i\tilde{\mathbf{f}}(\mathbf{u}) = \frac{\partial \tilde{\mathbf{f}}}{\partial u_i}(\mathbf{u})$$

denotes the partial derivative with respect to the $i$-th parameter $u_i$.

The proof of this observation results from the fact that a point $\tilde{\mathbf{x}}$ belongs to the tangent hyperplane if and only if its homogeneous coordinates are linearly dependent on $\tilde{\mathbf{f}}$ and the $d$ partial derivatives of the vector $\tilde{\mathbf{f}}$ of homogeneous coordinates.

We use this well-known result from projective geometry to derive a representation of the derivatives of isogeometric functions as rational hypersurface patches. More precisely, given the graph of an isogeometric function $f$ as a $d$-dimensional patch in $\mathbb{R}^{d+1}$, the following theorem provides a representation of the graph of a partial derivative of $f$, again as a $d$-dimensional patch in $\mathbb{R}^{d+1}$:

**Theorem 3.** *The graph of the partial derivative $\nabla_i f = \frac{\partial f}{\partial x_i}$ of an isogeometric function $f \in \mathcal{V}$, which is given in the form (5) with $n = d$, can be represented by the parametric hypersurface*

$$D_i\tilde{\mathbf{f}} = \left(\tilde{r}_0\tilde{g}_{d+1}, \tilde{r}_1\tilde{g}_{d+1}, \ldots, \tilde{r}_d\tilde{g}_{d+1}, -\tilde{r}_0\tilde{g}_i\right)^T. \tag{7}$$

*Proof.* We consider a fixed parameter value $\mathbf{u}$. According to Lemma 2, the tangent hyperplane of the hypersurface $\tilde{\mathbf{f}}$ at $\mathbf{u}$ is

$$T_{\mathbf{u}} = \left\{ \tilde{\mathbf{x}} \in \mathbb{R}^{d+2} : \ \tilde{\mathbf{g}}(\mathbf{u})^T \tilde{\mathbf{x}} = 0 \right\}.$$

Let $T_1 f(\mathbf{x})$ be the first order Taylor approximation of $f$ at $\mathbf{r}(\mathbf{u})$. Inserting $(1, x_1, \ldots, x_d, T_1 f(\mathbf{x}))^T$ into the equation of the tangent plane gives

$$\tilde{g}_0(\mathbf{u}) + \sum_{j=1}^{d} \tilde{g}_j(\mathbf{u}) x_j + \tilde{g}_{d+1}(\mathbf{u}) T_1 f(\mathbf{x}) = 0,$$

with $\tilde{g}_j$ as in (6). Solving for $T_1 f(\mathbf{x})$ leads to

$$T_1 f(\mathbf{x}) = -\frac{\tilde{g}_0(\mathbf{u})}{\tilde{g}_{d+1}(\mathbf{u})} - \sum_{j=1}^{d} \frac{\tilde{g}_j(\mathbf{u})}{\tilde{g}_{d+1}(\mathbf{u})} x_j$$

hence

$$\frac{\partial T_1 f}{\partial x_i}(\mathbf{x}) = -\frac{\tilde{g}_i(\mathbf{u})}{\tilde{g}_{d+1}(\mathbf{u})}.$$

Since $T_1 f(\mathbf{x})$ is the first order Taylor approximation of $f$ at the point $\mathbf{x} = \mathbf{r}(\mathbf{u})$,

$$\frac{\partial f}{\partial x_i}(\mathbf{r}(\mathbf{u})) = \frac{\partial T_1 f}{\partial x_i}(\mathbf{x}) = -\frac{\tilde{g}_i(\mathbf{u})}{\tilde{g}_{d+1}(\mathbf{u})}.$$

Therefore the graph of the derivative in Cartesian coordinates fulfills

$$\left( \frac{\tilde{r}_1(\mathbf{u})}{\tilde{r}_0(\mathbf{u})}, \ldots, \frac{\tilde{r}_d(\mathbf{u})}{\tilde{r}_0(\mathbf{u})}, \frac{\partial f}{\partial x_i}(\mathbf{r}(\mathbf{u})) \right)^T = \left( \frac{\tilde{r}_1(\mathbf{u})}{\tilde{r}_0(\mathbf{u})}, \ldots, \frac{\tilde{r}_d(\mathbf{u})}{\tilde{r}_0(\mathbf{u})}, -\frac{\tilde{g}_i(\mathbf{u})}{\tilde{g}_{d+1}(\mathbf{u})} \right)^T$$

which directly leads to the representation (7) in homogeneous coordinates. □

Assume that $\mathbf{r}$ is a regular mapping. Then, given an isogeometric function $f \in \mathcal{V}^{\mathbf{p},\mathbf{s}}$ corresponding to the spline space $\mathcal{S}^{\mathbf{p},\mathbf{s}}$, the derivative $\nabla_i f = \frac{\partial f}{\partial x_i}$ is again an isogeometric function. It fulfills $\nabla_i f \in \mathcal{V}^{\hat{\mathbf{p}},\hat{\mathbf{s}}}$, with $\hat{\mathbf{p}} = (d+2)\mathbf{p} - \mathbf{1}$ and $\hat{\mathbf{s}} = \mathbf{s} - \mathbf{1}$. The space $\mathcal{V}^{\hat{\mathbf{p}},\hat{\mathbf{s}}}$ is the space of isogeometric functions corresponding to $\mathcal{S}^{\hat{\mathbf{p}},\hat{\mathbf{s}}}$. Note that $\mathcal{S}^{\mathbf{p},\mathbf{s}} \subseteq \mathcal{S}^{\hat{\mathbf{p}},\hat{\mathbf{s}}} \subset \mathcal{P}$ and $\mathcal{V}^{\mathbf{p},\mathbf{s}} \subseteq \mathcal{V}^{\hat{\mathbf{p}},\hat{\mathbf{s}}} \subset \mathcal{V}$ (see Definition 1). Hence, we can directly conclude that the space $\mathcal{V}$ of all isogeometric functions on $\Omega$ is closed under differentiation.

The bounds on the degree and smoothness are derived from the representation of Theorem 3 and are stated for generic functions on generic geometries. For certain choices of the function $f$ or of the geometry mapping $\mathbf{r}$, the degree of the derivatives may be decreased and/or the smoothness may be increased. In the following we use the representation of the partial derivatives from Theorem 3 to analyze the smoothness properties of isogeometric functions defined on singular patches. Note that the smoothness may decrease when singularities are present.

## 4. Isogeometric functions on singular patches for $n = d$

We use Theorem 3 to analyze the order of smoothness of isogeometric functions defined on patches containing singularities. In the following we assume that a homogeneous representation of a rational patch in Bernstein-Bézier form is given. Since any NURBS patch can be split into a collection of rational patches, we restrict ourselves to rational patches.

We denote with $\mathrm{D}_0 \subset \bar{\mathbf{B}}$ the set of singular points of the geometry mapping $\mathbf{r}$. Recall that $\bar{\mathbf{B}}$ is the closure of $\mathbf{B}$. Let $\det \nabla_{\mathbf{u}} \mathbf{r}(\mathbf{u}) \geq 0$ for all $\mathbf{u} \in \bar{\mathbf{B}}$ and $\det \nabla_{\mathbf{u}} \mathbf{r}(\mathbf{u}) = 0$ if and only if $\mathbf{u} \in \mathrm{D}_0$. Note that the Jacobian determinant $\det \nabla_{\mathbf{u}} \mathbf{r}(\mathbf{u})$ is a rational function of the form

$$\det \nabla_{\mathbf{u}} \mathbf{r}(\mathbf{u}) = (-1)^{d+1} \frac{\tilde{g}_{d+1}(\mathbf{u})}{(\tilde{r}_0(\mathbf{u}))^{d+1}},$$

where the numerator $\tilde{g}_{d+1}(\mathbf{u})$ is the function defined in (6). Recall that $\tilde{r}_0(\mathbf{u}) > 0$ for all $\mathbf{u} \in \bar{\mathbf{B}}$. Consequently, the set $\mathrm{D}_0$ is the zero set of the multivariate polynomial $\tilde{g}_{d+1}(\mathbf{u})$.

We exemplify two types of singular planar patches (types P1 and P2) and three types of singular volumetric patches (types V1, V2 and V3). Patches of type P1, which were already studied by Takacs and Jüttler (2013), possess collapsing control points. Patches of type P2 have singularities caused by parallel tangents at a corner of the parameter domain. The trivariate patches of type V1 represent four-sided pyramids by collapsing the control points of one of the faces. The patches of type V2 describe tetrahedral patches by collapsing two faces to a point and to a curve, respectively. The patch described by type V3 contains a different kind of singularity. In this case the singularity is caused by two edges being collinear in the physical domain. The boundary of the patch consists of five quadrilateral faces and one degenerate triangular face.

We will derive $\mathscr{C}^1(\bar{\Omega})$ and $\mathscr{C}^2(\bar{\Omega})$ smoothness conditions for isogeometric functions defined on these model patches. Note that we consider a non-standard notion of $\mathscr{C}^k(\bar{\Omega})$ smoothness on the closed domain $\bar{\Omega}$ which is defined below. Usually, $\mathscr{C}^k$ smoothness is defined on open domains.

**Definition 4.** Let $\Omega \subset \mathbb{R}^d$ be an open set. We say that $f \in \mathscr{C}^k(\bar{\Omega})$ if and only if $f \in C^k(\Omega)$ and the derivatives of $f$ up to order $k$ can be extended continuously to the boundary $\partial\Omega$ of the domain $\Omega$. We call such a function $f$ a $\mathscr{C}^k$ *smooth function.* Here the space $C^k(\Omega)$ consists of all functions that satisfy the standard definition of $C^k$ smoothness on an open domain $\Omega$.

All presented types of patches are (rational) Bézier patches, which can be seen as restrictions of NURBS patches to one of its elements (knot spans). Since the boundary of the Bézier element may be in the interior of the full NURBS patch, the smoothness of the functions at the boundary of the Bézier element is also of interest, and this is reflected by the definition. In addition, the functions covered by the definition possess certain regularity properties which may be required in isogeometric analysis, e.g., in order to guarantee the existence of the integrals needed to derive the discretization.

The approach to derive the smoothness conditions for isogeometric functions on a singular patch consists of two major steps. First we compute the derivatives up to the desired order, second we derive $C^0$ continuity conditions for the resulting singular patches.

More precisely, given an isogeometric function with arbitrary coefficients $f_{\mathbf{i}}$ (as in Table 1), we compute the derivatives according to Theorem 3. Hence all derivatives are given via a hypersurface representing their graphs. These hypersurfaces are given as homogeneous patches in Bernstein-Bézier form. Each homogeneous control point of such a patch is either a basepoint, a point at infinity, or real point in Euclidean space.

The second task consists in the analysis of the continuity of such patches. First one can identify linear conditions on the coefficients $f_{\mathbf{i}}$ such that no points at infinity occur, resulting in a singular hypersurface consisting of real control points and basepoints only. Depending on the type of the singularity, one may then be able to cancel out basepoints. Again there exist linear conditions on the coefficients $f_{\mathbf{i}}$ that guarantee $C^0$-continuity for the resulting singular hypersurfaces. Here we refer to Warren (1990) which deals with the properties of surfaces containing basepoints. Related results concerning toric patches are presented in Krasauskas (2002).

See Takacs and Jüttler (2013) for further details on deriving smoothness conditions for isogeometric functions on planar patches.

**Type P1: Planar patch with a collapsing edge (triangle).** We exemplify this case by considering an isogeometric function $f^\delta \in \mathcal{V}^{(2,2)}$, which is represented by its graph surface

$$\tilde{\mathbf{f}}^\delta(\mathbf{u}) = \sum_{i_1=0}^{2} \sum_{i_2=0}^{2} \tilde{\mathbf{f}}_{(i_1,i_2)} B_{i_1,i_2}(u_1, u_2) \tag{8}$$

with the control points given in Table 1, where the basis functions $B_{i_1,i_2}$ are the tensor-product Bernstein polynomials of degree $(2, 2)$. The singular points form the set $\mathrm{D}_0 = \{(0, u_2), 0 \leq u_2 \leq 1\}$.

The left part of Figure 2 depicts an example of a patch of type P1. Note that the position of the inner control point with index $(1, 1)$ depends on the value of the perturbation parameter $\delta = (\delta_1, \delta_2)$.

| $i_1 \setminus i_2$ | 0 | 1 | 2 |
|---|---|---|---|
| 0 | $(1,0,0,f_{(0,0)})^T$ | $(1,0,0,f_{(0,1)})^T$ | $(1,0,0,f_{(0,2)})^T$ |
| 1 | $(1,2,0,f_{(1,0)})^T$ | $(1,1{+}\delta_1,1{+}\delta_2,f_{(1,1)})^T$ | $(1,0,2,f_{(1,2)})^T$ |
| 2 | $(1,4,0,f_{(2,0)})^T$ | $(1,2,2,f_{(2,1)})^T$ | $(1,0,4,f_{(2,2)})^T$ |

| $i_1 \setminus i_2$ | 0 | 1 | 2 |
|---|---|---|---|
| 0 | $(1,2,2,f_{(0,0)})^T$ | $(1,3,1,f_{(0,1)})^T$ | $(1,4,0,f_{(0,2)})^T$ |
| 1 | $(1,1,3,f_{(1,0)})^T$ | $(1,\frac{3}{2}{+}\delta_1,\frac{3}{2}{+}\delta_2,f_{(1,1)})^T$ | $(1,2,0,f_{(1,2)})^T$ |
| 2 | $(1,0,4,f_{(2,0)})^T$ | $(1,0,2,f_{(2,1)})^T$ | $(1,0,0,f_{(2,2)})^T$ |

Table 1: Control points of a planar patch of type P1 (top) and P2 (bottom)

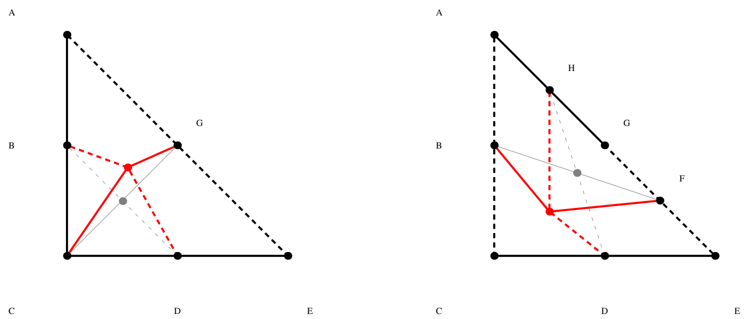


Figure 2: The grid of control points and the corresponding indices of boundary points for type P1 (left) and P2 (right)

Using Theorem 3, we conclude that $f^\delta \in \mathscr{C}^1(\bar{\Omega})$ if and only if

$$f_{(0,0)} = f_{(0,1)} = f_{(0,2)} \tag{9}$$

$$\delta_1(f_{(0,0)} - f_{(1,0)}) + \delta_2(f_{(0,0)} - f_{(1,2)}) + 2f_{(1,1)} - f_{(1,2)} - f_{(1,0)} = 0. \tag{10}$$

This condition admits the (well-known) geometric interpretation that the Cartesian control points $\mathbf{f}_{(0,0)}$, $\mathbf{f}_{(0,1)}$, $\mathbf{f}_{(0,2)}$, $\mathbf{f}_{(1,0)}$, $\mathbf{f}_{(1,1)}$ and $\mathbf{f}_{(1,2)}$ must be coplanar to secure $\mathscr{C}^1(\bar{\Omega})$ smoothness.

Using again Theorem 3 to compute the graph surfaces of the second partial derivatives from the first order ones, we conclude that $f^\delta \in \mathscr{C}^2(\bar{\Omega})$ if and only if equations (9), (10) and

$$\delta_1(f_{(1,0)} - f_{(2,0)}) + \delta_2(f_{(1,0)} - f_{(2,1)}) + 2f_{(1,1)} - f_{(1,2)} - f_{(1,0)} = 0 \tag{11}$$

$$\delta_1(f_{(0,0)} - f_{(1,0)} + f_{(1,2)} - f_{(2,1)}) + \delta_2(f_{(0,0)} - f_{(2,2)}) + 4f_{(1,1)} - 2f_{(1,2)} - 2f_{(1,0)} = 0 \tag{12}$$

are satisfied. Note that the equations (10), (11) and (12) are equivalent if $\delta_1 = \delta_2 = 0$.

The spaces of $\mathscr{C}^1$ and $\mathscr{C}^2$ smooth isogeometric functions obtained from the biquadratic parametrization have generally the dimensions 6 and 4, respectively. If $\delta_1 = \delta_2 = 0$, however, then both spaces possess the dimension 6. In fact, in this case the space consists of all quadratic polynomials on the physical domain.

**Type P2: Planar patch with collinear edges (triangle).** Here we consider an isogeometric function $f^\delta \in \mathcal{V}^{(2,2)}$ represented in the form (8) with the control points given in Table 1. The set $\mathrm{D}_0$ of singularities contains only one point, $\mathrm{D}_0 = \{(0,0)\}$. The right part of Figure 2 depicts a patch of type P2. Again, the inner control point depends on $\delta$. Similar to type P1 we conclude that $f^\delta \in \mathscr{C}^1(\bar{\Omega})$ if and only if

$$\begin{aligned} 2f_{(0,0)} &= f_{(0,1)} + f_{(1,0)} \\ f_{(2,0)} - f_{(0,2)} &= 2f_{(1,0)} - 2f_{(0,1)}. \end{aligned} \tag{13}$$

Moreover, $f^\delta \in \mathscr{C}^2(\bar{\Omega})$ if and only if (13) and

$$4\delta_2 f_{(0,0)} + (4 + 2\delta_1 - 2\delta_2) f_{(0,1)} - 2f_{(0,2)} = 4f_{(1,1)} - (1 - \delta_1 - \delta_2)(f_{(2,1)} + f_{(1,2)}) \tag{14}$$

$$\begin{aligned} (f_{(0,2)} + f_{(2,0)})(\delta_1 - \delta_2) &= (4\delta_1 - 6\delta_2) f_{(0,1)} + 2\delta_1 f_{(1,0)} \\ &+ (\delta_1 + \delta_2)(f_{(1,2)} - f_{(2,1)}) \end{aligned} \tag{15}$$

are satisfied. If $(\delta_1, \delta_2) = (0,0)$ then equation (15) can be omitted since both sides vanish.

The spaces of $\mathscr{C}^1$ and $\mathscr{C}^2$ smooth isogeometric functions obtained from the biquadratic parametrization have generally the dimensions 7 and 5, respectively. If $\delta_1 = \delta_2 = 0$, however, then the latter space has dimension 6.

**Type V1: Volumetric patch with a collapsing face (pyramid).** We consider an isogeometric function $f^\delta \in \mathcal{V}^{(2,2,2)}$ represented by

$$\tilde{\mathbf{f}}^\delta(u_1, u_2, u_3) = \sum_{i_1=0}^{2} \sum_{i_2=0}^{2} \sum_{i_3=0}^{2} \tilde{\mathbf{f}}_{(i_1,i_2,i_3)} B_{i_1,i_2,i_3}(u_1, u_2, u_3) \tag{16}$$

with tensor-product Bernstein polynomials $B_{i_1,i_2,i_3}$ of degree $(2,2,2)$ and control points

$$\begin{aligned} \tilde{\mathbf{f}}_{(i_1,i_2,i_3)} &= (1, i_1, \tfrac{i_1 i_2}{2}, \tfrac{i_1 i_3}{2}, f_{(i_1,i_2,i_3)})^T && \text{for } (i_1,i_2,i_3) \neq (1,1,1), \\ \tilde{\mathbf{f}}_{(1,1,1)} &= (1, 1+\delta_1, \tfrac{1}{2}+\delta_2, \tfrac{1}{2}+\delta_3, f_{(1,1,1)})^T && \text{otherwise,} \end{aligned}$$

as depicted in Figure 3. Note that the inner control point depends on $\delta$. The set of singular points is $\mathrm{D}_0 = \{(0, u_2, u_3), 0 \le u_2, u_3 \le 1\}$.

One can show that $f^\delta \in \mathscr{C}^1(\bar{\Omega})$ if and only if the coefficients of the isogeometric function satisfy

$$f_{(0,i_2,i_3)} = f_{(0,0,0)} \text{ for all } 0 \le i_2, i_3 \le 2 \tag{17}$$

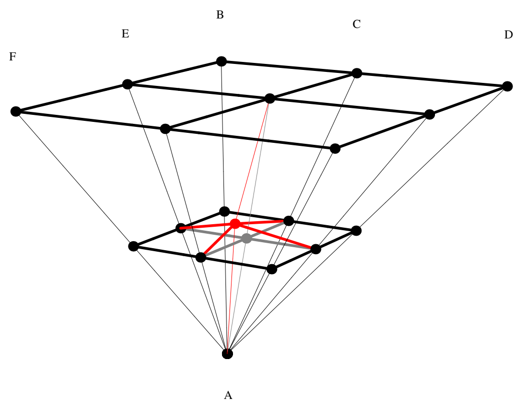


Figure 3: Control point grid for type V1. Only indices of selected control points are shown.

and six additional linearly independent equations. We do not write down the equations explicitly, since this would not give any further insight. Equation (17) leaves one degree of freedom for the coefficients with index $i_1 = 0$. The six additional equations restrict the coefficients with $i_1 = 1$. The remaining coefficients remain unrestricted. Summing up, the dimension of the space of $\mathscr{C}^1$ smooth functions is equal to $1 + 3 + 9 = 13$.

Similarly we can characterize $\mathscr{C}^2(\bar{\Omega})$ smoothness by (17) and 12 further equations. Generally, the space of $\mathscr{C}^2$ smooth functions has dimension 7. If $\delta_1 = \delta_2 = \delta_3 = 0$, the dimension raises to 10. In this case, the space of $\mathscr{C}^2$ smooth isogeometric functions is described by equations (17), as well as

$$
\begin{aligned}
f_{(1,0,1)} &= \tfrac{1}{2}(f_{(1,0,0)} + f_{(1,0,2)}) \qquad & f_{(1,2,1)} &= f_{(1,2,0)} + \tfrac{1}{2}(f_{(1,0,2)} - f_{(1,0,0)}) \\
f_{(1,1,0)} &= \tfrac{1}{2}(f_{(1,0,0)} + f_{(1,2,0)}) \qquad & f_{(1,1,2)} &= f_{(1,0,2)} + \tfrac{1}{2}(f_{(1,2,0)} - f_{(1,0,0)}) \\
f_{(1,1,1)} &= \tfrac{1}{2}(f_{(1,0,2)} + f_{(1,2,0)}) \qquad & f_{(1,2,2)} &= f_{(1,0,2)} + f_{(1,2,0)} - f_{(1,0,0)}
\end{aligned}
$$

and

$$
\begin{aligned}
f_{(2,1,2)} &= f_{(2,0,0)} - 2f_{(2,0,1)} + f_{(2,0,2)} - f_{(2,1,0)} + 2f_{(2,1,1)} \\
f_{(2,2,1)} &= f_{(2,0,0)} - f_{(2,0,1)} - 2f_{(2,1,0)} + 2f_{(2,1,1)} + f_{(2,2,0)} \\
f_{(2,2,2)} &= 3f_{(2,0,0)} - 4f_{(2,0,1)} + f_{(2,0,2)} - 4f_{(2,1,0)} + 4f_{(2,1,1)} + f_{(2,2,0)}.
\end{aligned}
$$

This space is equal to the space of quadratic polynomials on the physical domain. If a perturbation is present, however, this is no longer true and the approximation power is reduced.

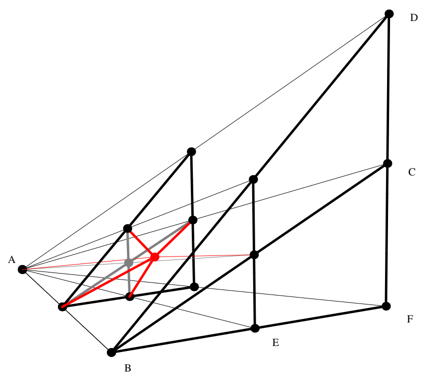


Figure 4: Control point grid for type V2. Only indices of selected control points are shown.

**Type V2: Volumetric patch with two collapsing faces (tetrahedron).** We consider an isogeometric function $f^\delta \in \mathcal{V}^{(2,2,2)}$ represented in the form (16) with control points

$$\begin{aligned}
\tilde{\mathbf{f}}_{(i_1,i_2,i_3)} &= (1, i_1, \tfrac{i_1 i_2}{2}, \tfrac{i_1 i_2 i_3}{4}, f_{(i_1,i_2,i_3)})^T && \text{for } (i_1,i_2,i_3) \neq (1,1,1),\\
\tilde{\mathbf{f}}_{(1,1,1)} &= (1, 1+\delta_1, \tfrac{1}{2}+\delta_2, \tfrac{1}{4}+\delta_3, f_{(1,1,1)})^T && \text{otherwise,}
\end{aligned}$$

as shown in Figure 4. The patch is singular for all points in the set $\mathrm{D}_0 = \{(0,u_2,u_3), 0 \leq u_2, u_3 \leq 1\} \cup \{(u_1,0,u_3), 0 \leq u_1, u_3 \leq 1\}$. Again, the inner control point $\tilde{\mathbf{f}}_{(1,1,1)}$ depends on $\delta = (\delta_1, \delta_2, \delta_3)$.

The conditions for $\mathscr{C}^1(\bar{\Omega})$ smoothness lead to 17 independent equations, leading to a space of dimension 10. If no perturbation is applied, then this space is equal to the space of $\mathscr{C}^2$ smooth functions (which is equal to the space of all quadratic polynomials on the tetrahedron in this case). Generally, however, the space of $\mathscr{C}^2$ smooth functions has dimension 7 only.

**Type V3: Volumetric patch with collinear edges.** This example covers a different class of singularities. The top face of the object is equivalent to the triangular patch P2. All other faces are non-degenerate quadrilaterals. We consider an isogeometric function $f^\delta \in \mathcal{V}^{(2,2,2)}$ represented in the form (16) with control points

$$\begin{aligned}
\tilde{\mathbf{f}}_{(i_1,i_2,0)} &= (1, i_1, i_2, 0, f_{(i_1,i_2,0)})^T && \text{for } 0 \leq i_1, i_2 \leq 2\\
\tilde{\mathbf{f}}_{(i_1,0,i_3)} &= (1, i_1, 0, i_3, f_{(i_1,i_2,0)})^T && \text{for } 0 \leq i_1, i_3 \leq 2\\
\tilde{\mathbf{f}}_{(0,i_2,i_3)} &= (1, 0, i_2, i_3, f_{(0,i_2,i_3)})^T && \text{for } 0 \leq i_2, i_3 \leq 2
\end{aligned}$$

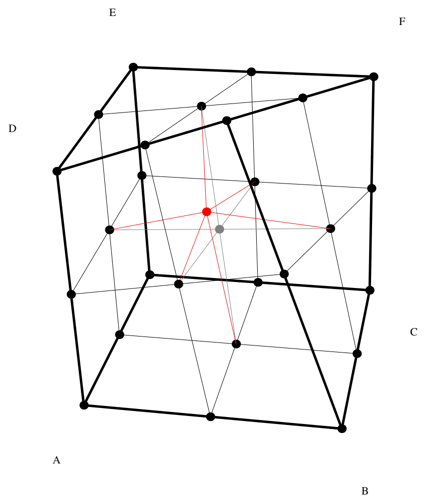


Figure 5: Control point grid for type V3. Only indices of selected control points are shown.

and

$$\begin{aligned}
\tilde{\mathbf{f}}_{(1,1,1)} &= (1, \tfrac{7}{8}+\delta_1, \tfrac{7}{8}+\delta_2, 1+\delta_3, f_{(1,1,1)})^T, & \tilde{\mathbf{f}}_{(1,1,2)} &= (1, \tfrac{3}{4}, \tfrac{3}{4}, 2, f_{(1,1,2)})^T, \\
\tilde{\mathbf{f}}_{(1,2,1)} &= (1, \tfrac{3}{4}, \tfrac{7}{4}, 1, f_{(1,2,1)})^T, & \tilde{\mathbf{f}}_{(1,2,2)} &= (1, \tfrac{1}{2}, \tfrac{3}{2}, 2, f_{(1,2,2)})^T, \\
\tilde{\mathbf{f}}_{(2,1,1)} &= (1, \tfrac{7}{4}, \tfrac{3}{4}, 1, f_{(2,1,1)})^T, & \tilde{\mathbf{f}}_{(2,1,2)} &= (1, \tfrac{3}{2}, \tfrac{1}{2}, 2, f_{(2,1,2)})^T, \\
\tilde{\mathbf{f}}_{(2,2,1)} &= (1, \tfrac{3}{2}, \tfrac{3}{2}, 1, f_{(2,2,1)})^T, & \tilde{\mathbf{f}}_{(2,2,2)} &= (1, 1, 1, 2, f_{(2,2,2)})^T
\end{aligned}$$

as shown in Figure 5. There is exactly one singular point, $\mathrm{D}_0 = \{(1,1,1)\}$, which corresponds to the control point with index $(2,2,2)$. In the unperturbed case, the parametrization of the domain (i.e., the control points without the last coordinate, which corresponds to the isogeometric function) have been constructed by applying degree elevation to a tri-linear patch. The $\mathscr{C}^1(\bar{\Omega})$ smoothness of $f^\delta$ is characterized by four linearly independent equations, leaving a space of dimension 23. The space of $\mathscr{C}^2$ smooth isogeometric functions has dimension 18. The basis functions with indices $(0,0,0)$, $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ are not involved in the nine equations. In this example the dimension of the space of $\mathscr{C}^2$ smooth isogeometric functions is not reduced if the inner control point is perturbed. This, however, is not true when the perturbation is applied to control points different from $\tilde{\mathbf{f}}_{(1,1,1)}$.

In all but the last of the presented examples, the dimension of the $\mathscr{C}^2$ smooth subspace of the isogeometric function space depends on the location of the “free” inner control point. Using perturbations of other control points lead to similar results.

Hence, the smoothness properties are very sensitive with respect to the choice of the parametrization. This should be taken into account when dealing with applications that need very smooth functions, since using $\mathscr{C}^2$ smooth isogeometric functions will often be too restrictive. In the vicinity of the singularity, the space spanned by these functions does not provide a representation of low-degree polynomials in the physical space (see especially types P1, V1, V2). This indicates the reduction of approximation power.

In concrete applications, one should try to find a parameterization that leads to a high-dimensional space. We observed that parameterizations obtained by degree elevation of (bi-/tri-) linear ones are quite useful.

## 5. Intrinsic derivatives of isogeometric functions on patches with $n < d$

We extend the result of Section 3 to functions on $n$-manifolds embedded into $\mathbb{R}^d$, where $n < d$. More precisely, we derive a representation of the intrinsic gradient of an isogeometric function $f \in \mathcal{V}$.

We consider an $n$-dimensional patch $\mathbf{r}(\mathbf{u})$ with homogeneous representation

$$\tilde{\mathbf{r}}(\mathbf{u}) = (\tilde{r}_0(\mathbf{u}), \tilde{r}_1(\mathbf{u}), \ldots, \tilde{r}_d(\mathbf{u}))^T$$

embedded into $\mathbb{R}^d$, with $n < d$, and an isogeometric function $f$ defined on $\mathbf{r}$. Let $\mathbf{x}_0 \in \mathbb{R}^d$ be a point on the patch $\mathbf{r}$. Let $F$ be an extension of $f$ to an open neighborhood $\mathcal{N}_{\mathbf{x}_0} \subset \mathbb{R}^d$ of $\mathbf{x}_0$. The *intrinsic gradient* $\nabla_{\mathbf{r}} f$ of $f$ is

$$\nabla_{\mathbf{r}} f(\mathbf{x}_0) = \Pi_{\mathbf{r}} \left(\nabla_{\mathbf{x}} F(\mathbf{x}_0)\right),$$

where $\nabla_{\mathbf{x}} F$ is the gradient of $F$ with respect to $\mathbf{x}$ in $\mathcal{N}_{\mathbf{x}_0}$ and the operator $\Pi_{\mathbf{r}}$ projects a vector orthogonally into the tangent space of the patch $\mathbf{r}$ at $\mathbf{x}_0$ (see e.g. Šír et al., 2008). When considering a surface in the three-dimensional space (i.e. $n = 2$, $d = 3$), this projection takes the form

$$\Pi_{\mathbf{r}} \left(\nabla_{\mathbf{x}} F\right) = \nabla_{\mathbf{x}} F - \left((\nabla_{\mathbf{x}} F)^T \mathbf{n}\right) \mathbf{n},$$

where $\mathbf{n}$ is the unit normal vector of $\mathbf{r}$ in $\mathbf{x}_0$.

The projection of the gradient onto the tangent space does not depend on the extension $F$ of the function $f$ into the embedding space, but it is fully determined by values of $F$ on the patch (i.e. $\nabla_{\mathbf{r}} f$ only depends on $f$). The intrinsic gradient is therefore well-defined.

We choose a particular extension $F$ of $f$ that allows to obtain the intrinsic gradient without the projection. The $n$-dimensional patch $\tilde{\mathbf{r}}(\mathbf{u})$, with $\mathbf{u} \in \mathbb{R}^n$, is extended to a $d$-dimensional patch in $\mathbb{R}^d$. Consider a basis $\mathbf{n}^{n+1}(\mathbf{u}), \ldots, \mathbf{n}^d(\mathbf{u})$ of the normal space at $\mathbf{u}$, i.e. $(\partial_j \mathbf{r})^T \mathbf{n}^k = 0$ for all $j = 1, \ldots, n$ and $k = n+1, \ldots, d$, where $\mathbf{r}$ is the representation of $\tilde{\mathbf{r}}$ in

Cartesian coordinates. Moreover let $\mathbf{N} = (\mathbf{n}^{n+1}, \ldots, \mathbf{n}^d)$. We denote by

$$\mathbf{F}(\mathbf{u}, \mathbf{u}^+) = \begin{pmatrix} \mathbf{r}(\mathbf{u}) \\ r_{d+1}(\mathbf{u}) \end{pmatrix} + \begin{pmatrix} \mathbf{u}^+\mathbf{N}(\mathbf{u}) \\ 0 \end{pmatrix}$$

the extended graph of $f$, with the row vector $\mathbf{u}^+ = (u_{n+1}, \ldots, u_d)$ and

$$\mathbf{u}^+\mathbf{N}(\mathbf{u}) = \sum_{j=n+1}^{d} u_j\, \mathbf{n}^j(\mathbf{u}).$$

There are several possibilities to obtain a basis of the normal space. In the case $d = 3$ and $n = 2$, the normal space is spanned simply by the normal vector $\partial_1\mathbf{r} \times \partial_2\mathbf{r}$. For other values of $d$ and $n$, however, the choice of the directions of the normal vectors is not unique. We outline an approach to generate the homogeneous representation of the normal space directly.

In order to generate a set $\tilde{\mathbf{N}}$ of normal vectors $\tilde{\mathbf{n}}^k$, $n+1 \le k \le d$, of low degree, we consider the hyperplanes

$$\{\tilde{\mathbf{x}} \ : \ \det(\tilde{\mathbf{r}}, \partial_1\tilde{\mathbf{r}}, \ldots, \partial_n\tilde{\mathbf{r}}, \tilde{\mathbf{q}}_{n+1}, \ldots, \tilde{\mathbf{q}}_{d-1}, \tilde{\mathbf{x}}) = 0 \ \}$$

which are spanned by $\tilde{\mathbf{r}}$, by the $n$ partial derivatives of $\tilde{\mathbf{r}}$ and by $d-n-1$ arbitrarily chosen auxiliary points $\tilde{\mathbf{q}}_{n+1}, \ldots, \tilde{\mathbf{q}}_{d-1}$. The coordinates of their normal vectors are the coefficients of $\tilde{x}_1, \ldots, \tilde{x}_n$ in the expansion of the determinant. These hyperplanes contain the tangent space of the patch $\tilde{\mathbf{r}}$. Hence their normal vectors are possible choices for the vectors $\tilde{\mathbf{n}}^k$, with $n+1 \le k \le d$. Applying this construction for $(d-n)$ sets of auxiliary points in general position leads to a set of $(d-n)$ linearly independent normal vectors of degree $\mathbf{p_n} \le (n+1)\mathbf{p} - \mathbf{1}$.

Rewriting the representation of the graph of the extended function $F$ in homogeneous coordinates gives

$$\tilde{\mathbf{F}}(\mathbf{u}, \mathbf{u}^+) = \begin{pmatrix} \tilde{\mathbf{r}}(\mathbf{u}) \\ \tilde{r}_{d+1}(\mathbf{u}) \end{pmatrix} + \begin{pmatrix} \mathbf{u}^+\tilde{\mathbf{N}}(\mathbf{u}) \\ 0 \end{pmatrix}, \tag{18}$$

where $\tilde{\mathbf{N}} = (\tilde{\mathbf{n}}^{n+1}, \ldots, \tilde{\mathbf{n}}^d)$. The entries $\tilde{n}_j^k$ of the vectors $\tilde{\mathbf{n}}^k$ are chosen as $\tilde{n}_j^k = n_j^k$ and $\tilde{n}_0^k = 0$ for all $n+1 \le k \le d$ and $1 \le j \le d$. The graph of the isogeometric function defined on the patch $\tilde{\mathbf{r}}$ is represented by $\tilde{\mathbf{F}}(\mathbf{u}, \mathbf{0}) = (\tilde{r}_0(\mathbf{u}), \ldots, \tilde{r}_{d+1}(\mathbf{u}))^T = \tilde{\mathbf{f}}(\mathbf{u})$. We denote with $\tilde{\mathbf{e}}_j$ the unit vector that spans the $j$-th coordinate axis in $\mathbb{R}^{d+1}$.

**Theorem 5.** *The graph of the i-th component $\nabla_{\mathbf{r},i} f$ of the intrinsic gradient is represented by the parametric surface*

$$D_i \tilde{\mathbf{f}} = \left(\tilde{r}_0 \tilde{g}_{d+1}, \tilde{r}_1 \tilde{g}_{d+1}, \ldots, \tilde{r}_d \tilde{g}_{d+1}, -\tilde{r}_0 \tilde{g}_i\right)^T,$$

*where*

$$\tilde{g}_j = \det(\tilde{\mathbf{e}}_j, \tilde{\mathbf{f}}, \partial_1 \tilde{\mathbf{f}}, \ldots, \partial_n \tilde{\mathbf{f}}, \tilde{\mathbf{m}}^{n+1}, \ldots, \tilde{\mathbf{m}}^d) \quad \textit{with} \quad \tilde{\mathbf{m}}^k = \begin{pmatrix} \tilde{\mathbf{n}}^k \\ 0 \end{pmatrix}.$$

*Proof.* Applying Theorem 3 to the extended graph $\tilde{\mathbf{F}}$ gives

$$D_i \tilde{\mathbf{F}} = \left(\tilde{F}_0 \tilde{q}_{d+1}, \tilde{F}_1 \tilde{q}_{d+1}, \ldots, \tilde{F}_d \tilde{q}_{d+1}, -\tilde{F}_0 \tilde{q}_i\right)^T,$$

with

$$\tilde{q}_j = \det(\tilde{\mathbf{e}}_j, \tilde{\mathbf{F}}, \partial_1 \tilde{\mathbf{F}}, \ldots, \partial_d \tilde{\mathbf{F}}).$$

The hypersurface $D_i \tilde{\mathbf{F}}$ represents the $i$-th component of the gradient $\nabla_{\mathbf{x}} F$. Restricting the gradient $\nabla_{\mathbf{x}} F$ to the patch $\mathbf{r}$ is equivalent to restricting the parameter value to $(\mathbf{u}, \mathbf{u}^+) = (\mathbf{u}, \mathbf{0})$. Hence,

$$D_i \tilde{\mathbf{F}} \mid_{\{\mathbf{u}^+ = \mathbf{0}\}} = \left(\tilde{r}_0 \tilde{g}_{d+1}, \tilde{r}_1 \tilde{g}_{d+1}, \ldots, \tilde{r}_d \tilde{g}_{d+1}, -\tilde{r}_0 \tilde{g}_i\right)^T,$$

with

$$\tilde{g}_j = \tilde{q}_j \mid_{\{\mathbf{u}^+ = \mathbf{0}\}} = \det(\tilde{\mathbf{e}}_j, \tilde{\mathbf{f}}, \partial_1 \tilde{\mathbf{f}}, \ldots, \partial_n \tilde{\mathbf{f}}, \tilde{\mathbf{m}}^{n+1}, \ldots, \tilde{\mathbf{m}}^d).$$

The gradient $\nabla_{\mathbf{x}} F$ can be decomposed as

$$\nabla_{\mathbf{x}} F = \Pi_{\mathbf{r}} \left(\nabla_{\mathbf{x}} F\right) + \Pi_{\mathbf{n}} \left(\nabla_{\mathbf{x}} F\right),$$

where $\Pi_{\mathbf{r}}$ and $\Pi_{\mathbf{n}}$ are the orthogonal projections into the tangent space and into the normal space, respectively. The extended function $F$ is constant in any normal direction. Hence, the normal component $\Pi_{\mathbf{n}} \left(\nabla_{\mathbf{x}} F\right)$ vanishes and

$$\nabla_{\mathbf{x}} F = \Pi_{\mathbf{r}} \left(\nabla_{\mathbf{x}} F\right) = \nabla_{\mathbf{r}} f,$$

which concludes the proof. □

Consider an isogeometric function $f \in \mathcal{V}^{\mathbf{p},\mathbf{s}}$. If the homogeneous normal vectors $\tilde{\mathbf{n}}^j$ can be represented as polynomials of degree $\mathbf{p_n}$, then the degree of the derivative patches is bounded by $(d-n)\mathbf{p_n} + (n+2)\mathbf{p} - \mathbf{1}$.

Higher order derivatives of $f$ can be computed recursively. The Hessian of $f$, as a tensor in $\mathbb{R}^{d \times d}$ can be computed by applying the gradient operator $\nabla_{\mathbf{r}}$ again to each component of $\nabla_{\mathbf{r}} f$.

| $i_1 \setminus i_2$ | 0 | 1 | 2 |
|---|---|---|---|
| 0 | $(1,0,0,1,f_{(0,0)})^T$ | $\frac{1}{\sqrt{2}}(1,0,0,1,f_{(0,1)})^T$ | $(1,0,0,1,f_{(0,2)})^T$ |
| 1 | $\frac{1}{\sqrt{2}}(1,1,0,1,f_{(1,0)})^T$ | $\frac{1}{2}(1,1,1,1,f_{(1,1)})^T$ | $\frac{1}{\sqrt{2}}(1,0,1,1,f_{(1,2)})^T$ |
| 2 | $(1,1,0,0,f_{(2,0)})^T$ | $\frac{1}{\sqrt{2}}(1,1,1,0,f_{(2,1)})^T$ | $(1,0,1,0,f_{(2,2)})^T$. |

Table 2: Control points of a rational patch of type S1 representing an octant of the sphere

## 6. Isogeometric functions on singular surfaces in $\mathbb{R}^3$

When considering a surface in $\mathbb{R}^3$, the normal space in $\mathbf{u}$ is spanned by the normal vector $\mathbf{n}(\mathbf{u}) = \partial_1\mathbf{r}(\mathbf{u}) \times \partial_2\mathbf{r}(\mathbf{u})$. In homogeneous coordinates this leads to

$$\tilde{\mathbf{m}} = -\begin{pmatrix} 0 \\ \det(\tilde{\mathbf{e}}_1, \tilde{\mathbf{r}}, \partial_1\tilde{\mathbf{r}}, \partial_2\tilde{\mathbf{r}}) \\ \det(\tilde{\mathbf{e}}_2, \tilde{\mathbf{r}}, \partial_1\tilde{\mathbf{r}}, \partial_2\tilde{\mathbf{r}}) \\ \det(\tilde{\mathbf{e}}_3, \tilde{\mathbf{r}}, \partial_1\tilde{\mathbf{r}}, \partial_2\tilde{\mathbf{r}}) \\ 0 \end{pmatrix}.$$

Hence the degree of the normal vector is bounded by $\mathbf{p_n} = 3\mathbf{p} - \mathbf{1}$, leading to $\mathbf{p_n} + 4\mathbf{p} - \mathbf{1} = 7\mathbf{p} - \mathbf{2}$ as a bound on the degree of the gradient patches. We analyze the smoothness of isogeometric functions on several singular surface patches which are embedded in the three-dimensional space $\mathbb{R}^3$.

Patches of type S1 contain a singularity caused by an edge collapsing to a point in physical space (similar to P1). Patches of type S2 possess parallel tangents at the corner points (similar to P2).

The first example from type S1 is an octant of the unit sphere (cf. Piegl and Tiller, 1995), while the second one is a polynomial approximation of the same patch.

**Type S1: Surface patch with collapsing edge.** We consider an isogeometric function $f$ represented by its graph surface as in (8) with the control points given in Table 2. Using Theorem 5, we conclude that $f \in \mathscr{C}^1(\bar{\Omega})$ if and only if

$$\begin{aligned} f_{(0,0)} = f_{(0,1)} &= f_{(0,2)} \\ f_{(1,2)} - f_{(1,1)} + f_{(1,0)} - f_{(0,0)} &= 0. \end{aligned} \tag{19}$$

Similar to the results for type P1, the equation (19) expresses the condition that the points $\mathbf{f}_{(0,0)}$, $\mathbf{f}_{(0,1)}$, $\mathbf{f}_{(0,2)}$, $\mathbf{f}_{(1,0)}$, $\mathbf{f}_{(1,1)}$ and $\mathbf{f}_{(1,2)}$ are contained in a 2-plane in $\mathbb{R}^4$.

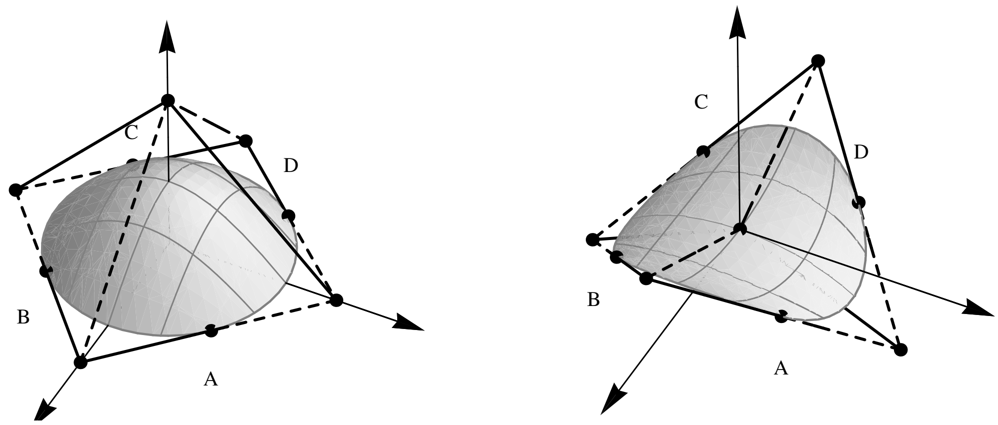


Figure 6: Two surface patches with singularities of type S2

When considering $\mathscr{C}^2(\bar{\Omega})$ smoothness, we obtain a more restrictive result. We apply Theorem 5 to each component of the intrinsic gradient. The isogeometric function satisfies $f \in \mathscr{C}^2(\bar{\Omega})$ if and only if equation (19) and

$$\begin{aligned} f_{(2,1)} - f_{(1,1)} + f_{(2,0)} - f_{(1,0)} &= 0 \\ f_{(2,2)} - f_{(2,0)} + f_{(1,0)} - f_{(1,2)} &= 0. \end{aligned} \tag{20}$$

Consequently, the space of $\mathscr{C}^2$ smooth isogeometric functions of this type has dimension 4.

Now we modify the previous patch by setting the denominator to 1, i.e., we omit the factors in front of the homogeneous coordinate vectors in Table 2. This gives a polynomial approximation to the octant of the sphere. Similar to the previous example, $f \in \mathscr{C}^1(\bar{\Omega})$ if and only if equation (19) is satisfied. The conditions

$$\begin{aligned} f_{(0,0)} = f_{(0,1)} = f_{(0,2)} = f_{(1,0)} = f_{(1,1)} &= f_{(1,2)} \\ f_{(2,0)} + f_{(2,1)} &= 2f_{(0,0)} \\ f_{(2,2)} &= f_{(2,0)} \end{aligned} \tag{21}$$

for $\mathscr{C}^2(\bar{\Omega})$ smoothness, however, are now far more restrictive and leave only 2 degrees of freedom. This is due to the lack of smoothness of the surface itself at the singularity.

**Type S2: Surface patch with collinear edges.** Finally we consider the two surface patches shown in Figure 6 with the control points listed in Table 3. The boundary of the first patch is a circle, and the boundary of the second one is a smooth curve.

The space of $\mathscr{C}^1$ smooth isogeometric functions of the degree $(2, 2)$ has dimension 4 for the first patch, but only 1 for the second one. Both patches admit only constant $\mathscr{C}^2$ smooth isogeometric functions.

| $i_1 \setminus i_2$ | 0 | 1 | 2 |
|---|---|---|---|
| 0 | $(1,-1,-1,0,f_{(0,0)})^T$ | $\frac{1}{\sqrt{2}}(1,0,-2,0,f_{(0,1)})^T$ | $(1,1,-1,0,f_{(0,2)})^T$ |
| 1 | $\frac{1}{\sqrt{2}}(1,-2,0,0,f_{(1,0)})^T$ | $2(1,0,0,2,f_{(1,1)})^T$ | $\frac{1}{\sqrt{2}}(1,2,0,0,f_{(1,2)})^T$ |
| 2 | $(1,-1,1,0,f_{(2,0)})^T$ | $\frac{1}{\sqrt{2}}(1,0,2,0,f_{(2,1)})^T$ | $(1,1,1,0,f_{(2,2)})^T$ |

| $i_1 \setminus i_2$ | 0 | 1 | 2 |
|---|---|---|---|
| 0 | $(1,-1,-1,0,f_{(0,0)})^T$ | $\frac{1}{\sqrt{2}}(1,0,-2,-1,f_{(0,1)})^T$ | $(1,1,-1,0,f_{(0,2)})^T$ |
| 1 | $\frac{1}{\sqrt{2}}(1,-2,0,1,f_{(1,0)})^T$ | $(1,0,0,0,f_{(1,1)})^T$ | $\frac{1}{\sqrt{2}}(1,2,0,1,f_{(1,2)})^T$ |
| 2 | $(1,-1,1,0,f_{(2,0)})^T$ | $\frac{1}{\sqrt{2}}(1,0,2,-1,f_{(2,1)})^T$ | $(1,1,1,0,f_{(2,2)})^T$ |

Table 3: Control points of the two patches shown in Fig. 6

For these examples, perturbations of the control points change the surfaces themselves. In the second example, the conditions do not depend on the position and the weight of the control point with index $(1,1)$. Comparing the two surfaces of type S1 leads to the conclusion that even minor changes of a surface can reduce the dimension of smooth function spaces dramatically. This has to be taken into account when dealing with singular patches in isogeometric analysis, where it is crucial to have sufficient degrees of freedom locally in order to maintain sufficient approximation power.

## 7. Conclusion

We derived a closed form representation of the derivatives of an isogeometric function using homogeneous coordinates. We took advantage of the fact that the graph of an isogeometric function defined on an $n$-dimensional NURBS patch in $\mathbb{R}^d$ can be interpreted as an $n$-dimensional patch in $\mathbb{R}^{d+1}$. The graphs of the partial derivatives of an isogeometric function are again given as NURBS patches, which are defined with respect to the same NURBS geometry mapping. Hence the space of isogeometric functions is closed with respect to differentiation.

We used the representation of the derivatives to obtain smoothness conditions for isogeometric functions on patches containing singularities. The method provides a systematic approach to derive smoothness conditions of arbitrary order. The presented analysis of various models indicates that the smoothness conditions depend heavily on perturbations of the geometry mapping. The results developed here are related to the $H^1$ and $H^2$ regularity results from Takacs and Jüttler (2011, 2012).

Future work will be devoted to isogeometric vector fields. Consider a vector field that is defined on a surface $\mathbf{r}$ in space, i.e. $n = 2$ and $d = 3$, and assume that the vector field is tangential to the surface. Hence the vector field is orthogonal to the surface normal $\mathbf{n_r}$. To represent such a vector field one may define a general vector-valued isogeometric function $\mathbf{V} \in \mathbb{R}^3$ on the surface patch and enforce the orthogonality condition weakly via $\|\mathbf{V}^T \mathbf{n_r}\| \approx 0$. This ansatz can then be used to compute a vector field fulfilling certain properties, such as interpolating given data. In that case a regularization of the vector field may be necessary. Using the approach proposed in this paper, a regularization functional based on the covariant derivatives of the vector field can be constructed. We refer to Kirisits et al. (2013), where a similar approach was employed to approximate the optical flow of an image on a moving surface.

More generally, we plan to use the results presented in this paper to formulate regularization methods based on coefficient norms for the derivatives. Since all norms on finite-dimensional spaces are equivalent, the $H^1$ or $H^2$ semi-norm on an isogeometric function space of given degree can be replaced by suitable coefficient norms obtained from the closed-form representations of the derivatives. These norms should be quite useful for regularization in the context of inverse problems, e.g., for applications in image processing on manifolds (cf. Dong, 2014).


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