The Smoothing Effect of the ANOVA Decomposition

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Abstract

We show that the lower-order terms in the ANOVA decomposition of a function $f(\boldsymbol{x}) := \max(\phi(\boldsymbol{x}), 0)$ for $\boldsymbol{x} \in [0,1]^d$, with ϕ a smooth function, may be smoother than f itself. Specifically, f in general belongs only to $\mathcal{W}^1_{d,\infty}$, i.e., f has one essentially bounded derivative with respect to any component of $\boldsymbol{x}$, whereas, for each $\mathbf{u} \subseteq \{1,\ldots,d\}$, the ANOVA term $f_{\mathbf{u}}$ (which depends only on the variables x_j with $j \in \mathbf{u}$) belongs to $\mathcal{W}^{1+\tau}_{d,\infty}$, where τ is the number of indices $k \in \{1,\ldots,d\} \setminus \mathbf{u}$ for which $\partial\phi/\partial x_k$ is never zero.

As an application, we consider the integrand arising from pricing an arithmetic Asian option on a single stock with d time intervals. After transformation of the integral to the unit cube and employing also a boundary truncation strategy, we show that for both the standard and the Brownian bridge constructions of the paths, the ANOVA terms that depend on $(d+1)/2$ or fewer variables all have essentially bounded mixed first derivatives; similar but slightly weaker results hold for the principal components construction. This may explain why quasi-Monte Carlo and sparse grid approximations of option pricing integrals often exhibit nearly first order convergence, in spite of lacking the smoothness required by the conventional theories.

Key words: ANOVA decomposition, smoothing, option pricing

1. Introduction

The *analysis of variance* (ANOVA) decomposition [5, 17] of a multivariate function has in the last decade become an important tool in the understanding of high-dimensional functions, allowing us to explain why quadrature algorithms such as *quasi-Monte Carlo* (QMC) methods [15, 19] and *sparse grid* (SG) techniques [3, 9] are successful for many practical high dimensional integration problems. The ANOVA representation of a d-dimensional function decomposes the function into 2^d terms (or "effects"), one for each subset of the d coordinates, with the *order* of each term being the cardinality of the corresponding subset. Because the ANOVA terms are mutually orthogonal in the L_2 sense, the variance is the sum of the variances of the separate terms. Caflisch, Morokoff and Owen [5] suggested that the reason for the observed success of QMC methods for many problems of finance is that most of the variance is explained either by the terms arising from just a small number of the leading variables (in which case the "truncation dimension" is small), or is mostly accounted for by the terms that involve just two or three variables at a time (in which case the "superposition dimension" is small). This suggestion has by now achieved wide acceptance, because it fits with a recognition that QMC methods of all kinds are almost invariably of better quality for the leading variables, or for projections that involve only a small number of variables.

While arguments in [5] based on *low effective dimensionality* are plausible for the problem of valuing mortgage backed securities [18], they encounter a difficulty for other problems of mathematical finance such as option pricing [8]. The difficulty is that in a typical option pricing problem the "payoff" has a factor of the form

$$\phi(\boldsymbol{x})_+ := \max(\phi(\boldsymbol{x}), 0), \tag{1}$$

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where ϕ is smooth. The integrand therefore has a "kink", and thus does not in general lie in any of the typical mixed-derivative function spaces used for the theoretical analysis of QMC methods and SG techniques [3, 9, 13]. Note that even the 2-variable function $f(x, y) = (x - y)_+$ does not have a mixed derivative $\partial^2 f/(\partial x \partial y)$, except in a distributional sense.

In this paper we address the problem posed by kinks such as (1) by showing that the lower-order ANOVA terms for functions with a kink are typically smooth, and under appropriate precise conditions *do* lie in function spaces with mixed first or higher derivatives. In this way we give mathematical substance to the observation by Liu and Owen (see the remark in [17] and the explanatory example in [16]) who appear to have been the first to notice the phenomenon. The point of the observation is that if the effective dimension is small and the lower-order ANOVA terms of f are smooth, then the theoretical error bounds can be applied to the smooth terms, while the small non-smooth terms can be neglected, or approximated in some other way. No such error analysis is carried out in the present paper, but we are laying a foundation for such an analysis in the future, by giving precise results on the function spaces to which various ANOVA components belong.

This paper is organized as follows. In Section 2 we give necessary background information on the ANOVA decomposition and on different Sobolev spaces, and state simple properties for functions with bounded mixed derivatives. In Section 3 we consider a family of functions with a kink typical of option pricing problems, and derive the smoothness properties of the ANOVA terms; the main result is stated in Theorem 7. In Section 4 we deal with the more extreme case of a function with a jump. In Section 5 we consider some option pricing problems as examples. In Section 6 we present numerical results. We finally give some concluding remarks in Section 7.

Option pricing problems, if mapped to the unit cube in a conventional way, give rise to integrands that have singularities at the boundaries, and that therefore have a second reason for failing to belong to the usual mixed-derivative function spaces. In Section 5 we therefore employ a novel "truncation-near-the-boundary" strategy when mapping the option pricing problem to the unit cube, so that the lower-order ANOVA terms in the ANOVA decomposition of the resulting integrand really do have the claimed smoothness properties. The truncation strategy introduces an error, by omitting a portion of the original integrand near the boundary. To help make this a practical strategy, our analysis in Section 5 includes an estimate of the error from neglecting the contribution from the boundary.

A striking observation from the option pricing discussion in Section 5 is that, with the truncation step included, the ANOVA terms for pricing the arithmetic average Asian call options of a single stock have square integrable mixed first derivatives, for all ANOVA terms with order up to at least $d/2$ (that is, half of the 2^d ANOVA terms), for both the standard and Brownian bridge constructions of the Brownian paths. For the principal components construction the smoothing effect may be reduced, but substantial smoothing is still expected. Even more remarkably, a similar result holds for the binary arithmetic average Asian call option in which the integrand itself is discontinuous.

2. ANOVA decomposition and Sobolev spaces

In this paper the analysis will be carried out for functions defined on the d-dimensional unit cube. Thus for standard option pricing problems (see Section 5) we shall assume that the problem has already been mapped to the d-dimensional unit cube, and that the common problem of singularities at the boundaries has been avoided in some way. (One such way is discussed in Section 5.) For f a continuous function defined on the unit cube $[0, 1]^d$, we write

$$I_d f \;=\; \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

Throughout this paper we assume that the dimension d is fixed, and we write

$$\mathfrak{D} \;=\; \{1, 2, \ldots, d\}.$$

2.1. ANOVA decomposition

For $j \in \mathfrak{D}$, let P_j be the projection defined by

$$(P_j f)(\boldsymbol{x}) \;=\; \int_0^1 f(x_1, .., x_{j-1}, t, x_{j+1}, \ldots, x_d)\,\mathrm{d}t \qquad \text{for} \quad \boldsymbol{x} = (x_1, \ldots, x_d) \in [0, 1]^d.$$

Thus $P_j f$ is the function obtained by integrating out the jth component of $\boldsymbol{x}$, and so is a function that is constant with respect to x_j. For convenience we often say that $P_j f$ does not depend on this component x_j, and we write interchangeably

$$(P_j f)(\boldsymbol{x}) \;=\; (P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}),$$

where $\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}$ denotes the $d-1$ components of $\boldsymbol{x}$ apart from x_j. For $\mathbf{u} \subseteq \mathfrak{D}$ we write

$$P_{\mathbf{u}} \;=\; \prod_{j\in\mathbf{u}} P_j.$$

Here the ordering within the product is not important because, by the Fubini theorem, $P_j P_k = P_k P_j$ for all $j,k \in \mathfrak{D}$. Thus $P_{\mathbf{u}} f$ is the function obtained by integrating out all the components of $\boldsymbol{x}$ with indices in $\mathbf{u}$. Note that $P_{\mathbf{u}}^2 = P_{\mathbf{u}}$ and $P_{\mathfrak{D}} = I_d$.

The ANOVA decomposition of f (see, e.g., [5, 17]) is

$$f \;=\; \sum_{\mathbf{u}\subseteq\mathfrak{D}} f_{\mathbf{u}}, \tag{2}$$

with $f_{\mathbf{u}}$ depending only on the variables x_j with indices $j \in \mathbf{u}$, and with $f_{\mathbf{u}}$ satisfying $P_j f_{\mathbf{u}} = 0$ for all $j \in \mathbf{u}$. The functions $f_{\mathbf{u}}$ satisfy the recurrence relation

$$f_{\emptyset} \;=\; I_d f \qquad \text{and} \qquad f_{\mathbf{u}} \;=\; P_{\mathfrak{D}\setminus\mathbf{u}} f - \sum_{\mathbf{v}\subsetneq\mathbf{u}} f_{\mathbf{v}}.$$

Often this recurrence relation is used as the defining property of the ANOVA terms $f_{\mathbf{u}}$. It is known from the recent paper [14] that the ANOVA terms $f_{\mathbf{u}}$ are given explicitly by

$$f_{\mathbf{u}} \;=\; \sum_{\mathbf{v}\subseteq\mathbf{u}} (-1)^{|\mathbf{u}|-|\mathbf{v}|} P_{\mathfrak{D}\setminus\mathbf{v}} f \;=\; P_{\mathfrak{D}\setminus\mathbf{u}} f \;+\; \sum_{\mathbf{v}\subsetneq\mathbf{u}} (-1)^{|\mathbf{u}|-|\mathbf{v}|} P_{\mathbf{u}\setminus\mathbf{v}} (P_{\mathfrak{D}\setminus\mathbf{u}} f). \tag{3}$$

In the latter form it becomes plausible that *the smoothness of* $f_{\mathbf{u}}$ *is determined by* $P_{\mathfrak{D}\setminus\mathbf{u}} f$, since we do not expect the further integrations $P_{\mathbf{u}\setminus\mathbf{v}}$ in the terms of the second sum to reduce the smoothness of $P_{\mathfrak{D}\setminus\mathbf{u}} f$; this expectation is proved in Theorem 4 below.

2.2. Sobolev spaces and weak derivatives

For $j \in \mathfrak{D}$, let D_j denote the partial derivative operator

$$(D_j f)(\boldsymbol{x}) \;=\; \frac{\partial f}{\partial x_j}(\boldsymbol{x}).$$

For a multi-index $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$, with each α_j a nonnegative integer, let

$$D^{\boldsymbol{\alpha}} \;=\; \prod_{j=1}^{d} D_j^{\alpha_j} \;=\; \prod_{j=1}^{d} \left(\frac{\partial}{\partial x_j}\right)^{\alpha_j} \;=\; \frac{\partial^{|\boldsymbol{\alpha}|}}{\prod_{j=1}^{d} \partial x_j^{\alpha_j}},$$

where $|\boldsymbol{\alpha}| = \alpha_1 + \cdots + \alpha_d$.

In this paper we consider two kinds of Sobolev space: the *isotropic Sobolev space* with smoothness parameter $r \geq 1$,

$$\mathcal{W}_{d,p}^{r} \;=\; \left\{ f \,:\, D^{\boldsymbol{\alpha}} f \in \mathcal{L}_p[0,1]^d \quad \text{for all} \quad |\boldsymbol{\alpha}| \leq r \right\},$$

and the *mixed Sobolev space* with smoothness multi-index $\boldsymbol{r} = (r_1, \ldots, r_d)$,

$$\mathcal{W}_{d,p,\mathrm{mix}}^{\boldsymbol{r}} \;=\; \left\{ f \,:\, D^{\boldsymbol{\alpha}} f \in \mathcal{L}_p[0,1]^d \quad \text{for all} \quad \boldsymbol{\alpha} \leq \boldsymbol{r} \right\},$$

where $\boldsymbol{\alpha} \leq \boldsymbol{r}$ is to be understood componentwise, and $p \in [1,\infty]$. For convenience we also write $\mathcal{W}_{d,p}^{0} = \mathcal{L}_p[0,1]^d$.

The derivatives in the above definitions of Sobolev spaces are *weak* derivatives, i.e., $D^{\boldsymbol{\alpha}} f$ is a function which satisfies

$$\int_{[0,1]^d} (D^{\boldsymbol{\alpha}} f)(\boldsymbol{x})\, v(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} \;=\; (-1)^{|\boldsymbol{\alpha}|} \int_{[0,1]^d} f(\boldsymbol{x})\, (D^{\boldsymbol{\alpha}} v)(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} \quad \text{for all } v \in \mathcal{C}_0^\infty[0,1]^d, \tag{4}$$

where $\mathcal{C}_0^\infty[0,1]^d$ denotes the space of infinitely differentiable functions with support in the open unit cube $(0,1)^d$, and the derivatives on the right-hand side of (4) are classical partial derivatives. See e.g., [1, 2] for detailed discussions of Sobolev spaces and weak derivatives.

The norms corresponding to the two kinds of Sobolev space are

$$\|f\|_{\mathcal{W}^r_{d,p,q}} \;=\; \left\| \left(\|D^{\boldsymbol{\alpha}} f\|_{\mathcal{L}_p} \right)_{|\boldsymbol{\alpha}| \le r} \right\|_{\ell_q}, \tag{5}$$

$$\|f\|_{\mathcal{W}^{\boldsymbol{r}}_{d,p,q,\mathrm{mix}}} \;=\; \left\| \left(\|D^{\boldsymbol{\alpha}} f\|_{\mathcal{L}_p} \right)_{\boldsymbol{\alpha} \le \boldsymbol{r}} \right\|_{\ell_q}, \tag{6}$$

where $\|\cdot\|_{\mathcal{L}_p}$ denotes the $\mathcal{L}_p[0,1]^d$ norm of a function, that is

$$\|g\|_{\mathcal{L}_p} \;=\; \begin{cases} \left(\int_{[0,1]^d} |g(\boldsymbol{x})|^p \, \mathrm{d}\boldsymbol{x} \right)^{1/p} & \text{if } 1 \le p < \infty, \\ \operatorname{ess\,sup}_{\boldsymbol{x} \in [0,1]^d} |g(\boldsymbol{x})| & \text{if } p = \infty, \end{cases}$$

and $\|\cdot\|_{\ell_q}$ denotes the ℓ_q norm of a k-dimensional vector, $k < \infty$,

$$\|\boldsymbol{v}\|_{\ell_q} \;=\; \begin{cases} \left(\sum_{j=1}^k |v_j|^q \right)^{1/q} & \text{if } 1 \le q < \infty, \\ \max_{1 \le j \le k} |v_j| & \text{if } q = \infty. \end{cases}$$

Typically, the norms of Sobolev spaces are defined with $p = q$ in (5) and (6), although some people argue the merits of taking p and q to be Hölder conjugates, i.e., $1/p + 1/q = 1$ (see, e.g., [10, 11]). For fixed p, the value of q only affects the size of the norm and does not change the function space. This is why we often suppress the dependence on q in our notation, i.e., we write $\|f\|_{\mathcal{W}^r_{d,p}}$ and $\|f\|_{\mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}}}$ instead of $\|f\|_{\mathcal{W}^r_{d,p,q}}$ and $\|f\|_{\mathcal{W}^{\boldsymbol{r}}_{d,p,q,\mathrm{mix}}}$, respectively. On the other hand, we have

$$\mathcal{W}^r_{d,p'} \subseteq \mathcal{W}^r_{d,p} \qquad \text{and} \qquad \mathcal{W}^{\boldsymbol{r}}_{d,p',\mathrm{mix}} \subseteq \mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}} \qquad \text{for} \qquad 1 \le p \le p' \le \infty, \tag{7}$$

which follows from $\mathcal{L}_{p'}[0,1]^d \subseteq \mathcal{L}_p[0,1]^d$ for $1 \le p \le p' \le \infty$.

It is easily seen that the isotropic and the mixed Sobolev spaces are related by

$$\mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}} \subseteq \mathcal{W}^r_{d,p} \quad \text{iff} \quad \min_{j \in \mathfrak{D}} r_j \ge r \qquad \text{and} \qquad \mathcal{W}^r_{d,p} \subseteq \mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}} \quad \text{iff} \quad r \ge |\boldsymbol{r}|. \tag{8}$$

In particular, we have

$$\mathcal{W}^{(s,..,s)}_{d,p,\mathrm{mix}} \subseteq \mathcal{W}^r_{d,p} \quad \text{iff} \quad s \ge r \qquad \text{and} \qquad \mathcal{W}^r_{d,p} \subseteq \mathcal{W}^{(s,..,s)}_{d,p,\mathrm{mix}} \quad \text{iff} \quad r \ge s\, d. \tag{9}$$

For the special case of $p = q = 2$, we have the commonly used Hilbert spaces $\mathcal{H}^r_d = \mathcal{W}^r_{d,2}$ and $\mathcal{H}^{\boldsymbol{r}}_{d,\mathrm{mix}} = \mathcal{W}^{\boldsymbol{r}}_{d,2,\mathrm{mix}}$. Another interesting special case is when $p = \infty$ and $q = 1$, which leads to the Sobolev spaces $\mathcal{W}^r_{d,\infty}$ and $\mathcal{W}^{\boldsymbol{r}}_{d,\infty,\mathrm{mix}}$, with norms

$$\|f\|_{\mathcal{W}^r_{d,\infty,1}} = \sum_{|\boldsymbol{\alpha}| \le r} \left(\operatorname*{ess\,sup}_{\boldsymbol{x} \in [0,1]^d} |(D^{\boldsymbol{\alpha}} f)(\boldsymbol{x})| \right) \text{ and } \|f\|_{\mathcal{W}^{\boldsymbol{r}}_{d,\infty,1,\mathrm{mix}}} = \sum_{\boldsymbol{\alpha} \le \boldsymbol{r}} \left(\operatorname*{ess\,sup}_{\boldsymbol{x} \in [0,1]^d} |(D^{\boldsymbol{\alpha}} f)(\boldsymbol{x})| \right).$$

We finish this subsection on Sobolev spaces with an instructive example which is pertinent to the present paper.

Example 1 Setting $d = 2$, we define a simple function with a kink,

$$f(x_1, x_2) := (x_1 - x_2 + \tfrac{1}{2})_+, \qquad (x_1, x_2) \in [0,1]^2,$$

where, as in (1), we use the common notation $a_+ := \max(a, 0)$ for $a \in \mathbb{R}$.

To which of our Sobolev spaces does f belong? From the definition (4) of the weak derivative it is easily verified that

$$(D^{(1,0)} f)(x_1, x_2) = \begin{cases} 0 & \text{for } x_1 < x_2 - \frac{1}{2}, \\ 1 & \text{for } x_1 > x_2 - \frac{1}{2}, \end{cases} \quad \text{and} \quad (D^{(0,1)} f)(x_1, x_2) = \begin{cases} 0 & \text{for } x_1 < x_2 - \frac{1}{2}, \\ -1 & \text{for } x_1 > x_2 - \frac{1}{2}. \end{cases}$$

Since both of these first derivatives of f are essentially bounded functions on $[0,1]^2$, we have

$$f \in \mathcal{W}^1_{2,\infty} \subseteq \mathcal{W}^1_{2,p} \qquad \text{for all} \quad p \in [1, \infty].$$

On the other hand, $D^{(1,1)} f$ exists only as a distribution (a "delta function"), and does not exist as a member of any $\mathcal{L}_p$ space, thus

$$f \notin \mathcal{W}^{(1,1)}_{2,p,\mathrm{mix}} \qquad \text{for all} \quad p \in [1, \infty].$$

In the subsequent sections we shall be concerned with functions in $\mathcal{W}^1_{d,\infty}$, the space of measurable functions f whose first derivatives $D_j f$ for $j \in \mathfrak{D}$ are essentially bounded. From the Sobolev imbedding theorem (see, e.g., [1]) we have

$$\mathcal{W}^1_{d,\infty} \subseteq \mathcal{C}[0,1]^d, \tag{10}$$

that is, the functions $f \in \mathcal{W}^1_{d,\infty}$ are continuous. Indeed, since the first derivatives of $f \in \mathcal{W}^1_{d,\infty}$ are almost everywhere bounded by $\|f\|_{\mathcal{W}^1_{d,\infty,\infty}}$, the functions in $\mathcal{W}^1_{d,\infty}$ are Lipschitz continuous.

2.3. Notations

We now introduce a number of notations used throughout the paper.

For a given index $j \in \mathfrak{D}$, we sometimes need to separate out the jth component of a given vector $\boldsymbol{x} \in [0,1]^d$, and we achieve this by writing

$$\boldsymbol{x} = (x_j, \boldsymbol{x}_{\mathfrak{D} \setminus \{j\}}),$$

where as noted previously $\boldsymbol{x}_{\mathfrak{D} \setminus \{j\}}$ denotes the $d - 1$ components of $\boldsymbol{x}$ apart from x_j. More generally, for a given set $\mathbf{u} \subseteq \mathfrak{D}$ we write

$$\boldsymbol{x}_{\mathbf{u}} = (x_j)_{j \in \mathbf{u}}$$

to denote the set of components x_j of $\boldsymbol{x}$ for which $j \in \mathbf{u}$. The cardinality of a set $\mathbf{u}$ is denoted by $|\mathbf{u}|$.

For $\mathbf{u} \subseteq \mathfrak{D}$ and $\boldsymbol{r}_{\mathbf{u}} = (r_j)_{j \in \mathbf{u}}$, we define

$$\mathcal{W}^r_{\mathbf{u},p} \qquad \text{and} \qquad \mathcal{W}^{\boldsymbol{r}_{\mathbf{u}}}_{\mathbf{u},p,\mathrm{mix}}$$

to be the *subspaces* of $\mathcal{W}^r_{d,p}$ and $\mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}}$, respectively, which contain those functions that are constant with respect to the components whose indices are outside of $\mathbf{u}$ (that is, functions that depend only on the variables $\boldsymbol{x}_{\mathbf{u}}$). To help to identify the relevant variables, we write the domain of the functions as

$$[0,1]^{\mathbf{u}}.$$

The norm of a function from $\mathcal{W}^r_{\mathbf{u},p}$ (or $\mathcal{W}^{\boldsymbol{r}_{\mathbf{u}}}_{\mathbf{u},p,\mathrm{mix}}$) is the same as its norm in $\mathcal{W}^r_{d,p}$ (or $\mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}}$). With this new notation, we have $\mathcal{W}^r_{\mathfrak{D},p} = \mathcal{W}^r_{d,p}$ and $\mathcal{W}^{\boldsymbol{r}}_{\mathfrak{D},p,\mathrm{mix}} = \mathcal{W}^{\boldsymbol{r}}_{d,p,\mathrm{mix}}$.

2.4. Weak derivatives and classical derivatives

Although in principle the derivatives we consider are weak derivatives, for functions in $\mathcal{W}^1_{d,\infty}$ there is a close relation between weak derivatives and classical derivatives. We state this connection in the following theorem. In effect it states, via the fundamental theorem of calculus, that whenever the classical derivative of f with respect to x_j exists, it equals the weak derivative $D_j f$.

Theorem 2 *Let $f \in \mathcal{W}^1_{d,\infty}$. For arbitrary $j \in \mathfrak{D}$ and $x_j \in [0,1]$ we have*

$$f(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) - f(0, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = \int_0^{x_j} (D_j f)(t_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \, \mathrm{d}t_j,$$

where the equality is to be understood in the weak sense, i.e., it holds after multiplying both sides by arbitrary $v \in \mathcal{C}_0^\infty[0,1]^{\mathfrak{D}\setminus\{j\}}$ and integrating over $[0,1]^{\mathfrak{D}\setminus\{j\}}$. It follows that for almost all $\boldsymbol{x} \in [0,1]^d$ the pointwise partial derivative of f with respect to x_j exists and is equal to $(D_j f)(\boldsymbol{x})$.

The proof follows in a standard way by multiplying the right-hand side by $v \in \mathcal{C}_0^\infty[0,1]^{\mathfrak{D}\setminus\{j\}}$ and integrating, then using the definition of weak derivative (that is, using partial integration) to transfer the derivative onto v, and then making a clever choice of $v \in \mathcal{C}_0^\infty[0,1]^{\mathfrak{D}\setminus\{j\}}$.

2.5. Extending the Leibniz theorem

The classical Leibniz theorem says that

$$\frac{\mathrm{d}}{\mathrm{d}y} \int_0^1 f(x,y) \, \mathrm{d}x = \int_0^1 \frac{\partial f}{\partial y}(x,y) \, \mathrm{d}x$$

under the condition that f and $\partial f / \partial y$ are continuous functions for $x, y \in [0,1]$. In our notation this may be stated as

$$D_k P_j f = P_j D_k f \qquad \text{for all} \quad j,k \in \mathfrak{D} \quad \text{with} \quad j \neq k.$$

Thus the Leibniz theorem allows us to swap the order of differentiation and integration.

In this section we assume at least $f \in \mathcal{W}^1_{d,\infty}$, thus f is a continuous function (see (10)), and therefore $(P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})$ exists and belongs to $\mathcal{C}[0,1]^{\mathfrak{D}\setminus\{j\}}$. We are especially interested in the case in which f is a kink function as in (1). But in this case the classical Leibniz theorem does not apply because the kink function (1) does *not* have a continuous derivative. We therefore need a more general form of the Leibniz theorem as given below.

Theorem 3 (The Extended Leibniz Theorem) *For $r \geq 1$ and $f \in \mathcal{W}^r_{d,\infty}$ we have*

$$D_k P_j f = P_j D_k f \qquad \textit{for all} \quad j,k \in \mathfrak{D} \quad \textit{with} \quad j \neq k.$$

Proof. For $r \geq 2$, we have $D_k f \in \mathcal{W}^{r-1}_{d,\infty} \subseteq \mathcal{C}[0,1]^d$ for all $k \in \mathfrak{D}$, and the result follows immediately from the classical Leibniz theorem. Therefore it suffices to prove the result for $r = 1$.

Let $f \in \mathcal{W}^1_{d,\infty}$ and $j,k \in \mathfrak{D}$ with $j \neq k$. We consider the weak derivative D_k of $P_j f$, see (4). For arbitrary $v \in \mathcal{C}_0^\infty[0,1]^d$ we have

$$\begin{aligned}
-\int_{[0,1]^d} (P_j f)(\boldsymbol{x})(D_k v)(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} &= -\int_{[0,1]^d} \left(\int_0^1 f(t_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \, \mathrm{d}t_j \right) (D_k v)(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \\
&= \int_0^1 \left(-\int_{[0,1]^d} f(t_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \, (D_k v)(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \right) \mathrm{d}t_j,
\end{aligned}$$

where in the last step we used Fubini's theorem [4, Section 5.4] to interchange the order of integration. Now we use again the definition of weak derivative (4), this time in the inner integral, followed again by Fubini's theorem, to obtain from the last expression

$$\begin{aligned}
\int_0^1 \left(\int_{[0,1]^d} (D_k f)(t_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \, v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \right) \mathrm{d}t_j &= \int_{[0,1]^d} \left(\int_0^1 (D_k f)(t_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \, \mathrm{d}t_j \right) v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \\
&= \int_{[0,1]^d} (P_j D_k f)(\boldsymbol{x}) \, v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}.
\end{aligned}$$

With (4) this shows for $j \neq k$ that $D_k P_j f$ exists, and is equal to $P_j D_k f$. This completes the proof. $\square$

Later we shall refer to Theorem 3 as the Leibniz theorem.

The next theorem is an application of the Leibniz theorem which establishes that $P_j f$ inherits the smoothness of f.

Theorem 4 (The Inheritance Theorem) *For $r \geq 1$ and $f \in \mathcal{W}^r_{d,\infty}$ we have*

$$P_j f \;\in\; \mathcal{W}^r_{\mathfrak{D}\setminus\{j\},\infty} \qquad \textit{for all} \quad j \in \mathfrak{D}.$$

Proof. The case $r = 1$ follows immediately from the Leibniz theorem (Theorem 3) with $r = 1$. Here we give a proof for general $r \geq 1$.

Let $f \in \mathcal{W}^r_{d,\infty}$ and $j \in \mathfrak{D}$. To show that $P_j f \in \mathcal{W}^r_{\mathfrak{D}\setminus\{j\},\infty}$ we need to show that

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_j f \;\in\; \mathcal{L}_\infty \qquad \text{for all } a \leq r \text{ and all possible combinations of } k_i \in \mathfrak{D} \setminus \{j\},$$

with repetitions allowed in k_i. We write successively

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_j f \;=\; \left(\prod_{i=2}^{a} D_{k_i}\right) P_j D_{k_1} f \;=\; \cdots \;=\; D_{k_a} P_j \left(\prod_{i=1}^{a-1} D_{k_i}\right) f \;=\; P_j \left(\prod_{i=1}^{a} D_{k_i}\right) f,$$

where each step involves a single differentiation under the integral sign, and is justified by the Leibniz theorem (Theorem 3) because $(\prod_{i=1}^{\ell} D_{k_i}) f \in \mathcal{W}^{r-\ell}_{d,\infty} \subseteq \mathcal{W}^1_{d,\infty}$ for all $\ell = 0, 1, \ldots, a-1$ with $a \leq r$. Since $P_j(\prod_{i=1}^{a} D_{k_i}) f \in \mathcal{L}_\infty$, this completes the proof. $\square$

2.6. Implicit function theorem

In this paper we shall make repeated use of the implicit function theorem. In the following, $\overline{S}$ denotes the closure of the set S. By a $\mathcal{C}^\infty(\overline{U})$ function, we mean that all the partial derivatives of the function exist on an open set U and have continuous extensions to $\overline{U}$.

Theorem 5 *Let $j \in \mathfrak{D}$. Suppose $\phi \in \mathcal{C}^\infty[0,1]^d$ satisfies*

$$(D_j \phi)(\boldsymbol{x}) \;\neq\; 0 \qquad \textit{for all} \quad \boldsymbol{x} \in [0,1]^d. \tag{11}$$

Let

$$U \;=\; U_j \;:=\; \left\{ \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in (0,1)^{\mathfrak{D}\setminus\{j\}} \;:\; \phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = 0 \textit{ for some (unique) } x_j \in (0,1) \right\}.$$

If U is not empty then there exists a unique function $\psi \in \mathcal{C}^\infty(\overline{U})$ such that

$$\phi(\,\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; 0 \qquad \textit{for all} \quad \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in \overline{U},$$

and for all $k \neq j$ we have

$$(D_k \psi)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; -\frac{(D_k \phi)(\boldsymbol{x})}{(D_j \phi)(\boldsymbol{x})}\bigg|_{x_j = \psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})} \qquad \textit{for all} \quad \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in U. \tag{12}$$

Proof. If $\boldsymbol{x} = (x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \in (0,1)^d$ satisfies $\phi(\boldsymbol{x}) = 0$ and $(D_j\phi)(\boldsymbol{x}) \neq 0$, then [12, Theorem 3.2.1] asserts the existence of an open set $A_{\boldsymbol{x}} \subseteq [0,1]^{\mathfrak{D}\setminus\{j\}}$, depending on j and $\boldsymbol{x}$, such that $\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in A_{\boldsymbol{x}}$, and the existence of a unique continuously differentiable function $\psi_{\boldsymbol{x}} : A_{\boldsymbol{x}} \to \mathbb{R}$ such that $x_j = \psi_{\boldsymbol{x}}(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})$ and

$$\phi(\,\psi_{\boldsymbol{x}}(\boldsymbol{x}'_{\mathfrak{D}\setminus\{j\}}),\, \boldsymbol{x}'_{\mathfrak{D}\setminus\{j\}}\,) \;=\; 0 \qquad \text{for all} \quad \boldsymbol{x}'_{\mathfrak{D}\setminus\{j\}} \in A_{\boldsymbol{x}}.$$

If we take two points $\boldsymbol{x}$ and $\boldsymbol{y}$ such that the corresponding sets $A_{\boldsymbol{x}}$ and $A_{\boldsymbol{y}}$ overlap, then in the overlap region the functions $\psi_{\boldsymbol{x}}$ and $\psi_{\boldsymbol{y}}$ for each of these two domains must give the same values, by uniqueness. Given that (11) holds for all $\boldsymbol{x} \in [0,1]^d$, we therefore have a globally defined, single unique continuously differentiable function $\psi : U \to \mathbb{R}$ such that for $\boldsymbol{x} \in (0,1)^d$

$$\phi(\boldsymbol{x}) \;=\; 0 \qquad \text{if and only if} \qquad x_j \;=\; \psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}).$$

Implicit differentiation of

$$\phi(\,\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}),\,\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}\,)\;=\;0,\qquad \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}\in U,$$

then yields (12), and repeated differentiation shows that ψ and all its derivatives can be extended continuously to the boundary of U. $\square$

We stress that the set U need not be connected: the claim in the theorem is only that ψ is $\mathcal{C}^\infty$ on the closure of each connected subset.

3. Smoothing for functions with kinks

3.1. A special function with a kink

In this subsection we consider a function of the form

$$f(\boldsymbol{x})\;=\;\phi(\boldsymbol{x})_+,\qquad \boldsymbol{x}\in[0,1]^d. \tag{13}$$

We assume for simplicity that $\phi:[0,1]^d\to\mathbb{R}$ is a $\mathcal{C}^\infty$ function. It will become clear that $\mathcal{C}^\infty$ can be replaced by $\mathcal{C}^k$ for a suitably large value of k. We shall always assume that the equation $\phi(\boldsymbol{x})=0$ defines a smooth, but not necessarily connected, $(d-1)$-dimensional manifold. From the implicit function theorem (Theorem 5) this is the case if, for example, there exists at least one $j\in\mathfrak{D}$ such that $(D_j\phi)(\boldsymbol{x})\neq 0$ for $\boldsymbol{x}\in[0,1]^d$.

The function f is continuous but has a kink along the $(d-1)$-dimensional manifold $\phi(\boldsymbol{x})=0$. Clearly f can be differentiated pointwise once with respect to any one of the d variables except on the manifold $\phi(\boldsymbol{x})=0$. Indeed for $k\in\mathfrak{D}$ we have

$$(D_kf)(\boldsymbol{x})\;=\;\begin{cases}(D_k\phi)(\boldsymbol{x}) & \text{if } \phi(\boldsymbol{x})>0,\\ 0 & \text{if } \phi(\boldsymbol{x})<0.\end{cases}$$

It can be easily verified that this is the weak derivative of f by checking the condition (4). Since D_kf is measurable and essentially bounded on $[0,1]^d$, we conclude that

$$f\;\in\;\mathcal{W}^1_{d,\infty}. \tag{14}$$

It then follows from the inheritance theorem (Theorem 4) with $r=1$ that

$$P_jf\;\in\;\mathcal{W}^1_{\mathfrak{D}\setminus\{j\},\infty}\qquad\text{for all}\quad j\in\mathfrak{D}.$$

In other words, integration with respect to x_j leaves the smoothness of the function f unchanged.

More remarkably, we shall see in Theorem 7 below (and this is the core result of the paper) that integration with respect to x_j can have a smoothing effect: indeed, for f given by (13) we shall as a first illustration prove

$$\text{if}\quad (D_j\phi)(\boldsymbol{x})\neq 0\quad\text{for all}\quad \boldsymbol{x}\in[0,1]^d\quad\text{then}\quad P_jf\;\in\;\mathcal{W}^2_{\mathfrak{D}\setminus\{j\},\infty}, \tag{15}$$

where the special feature is that the smoothness parameter of the space is 2 instead of 1. Thus the claim is that P_jf is in this situation one order smoother than f with respect to the variables other than x_j (while x_j itself has, of course, been integrated out). We now formulate (15) as a lemma and provide a proof.

Lemma 6 *Let $f(\boldsymbol{x})=\phi(\boldsymbol{x})_+$, where $\phi\in\mathcal{C}^\infty[0,1]^d$. Let $j\in\mathfrak{D}$ and suppose that $(D_j\phi)(\boldsymbol{x})\neq 0$ for all $\boldsymbol{x}\in[0,1]^d$. Then for any $k\in\mathfrak{D}\setminus\{j\}$ we have $D_kP_jf\in\mathcal{W}^1_{\mathfrak{D}\setminus\{j\},\infty}$, and in turn $P_jf\in\mathcal{W}^2_{\mathfrak{D}\setminus\{j\},\infty}$.*

Proof. For the function $f(\boldsymbol{x})=\phi(x_j,\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})_+$ we can write P_jf as

$$(P_jf)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})\;=\;\int_{x_j\in[0,1]\,:\,\phi(x_j,\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})\geq 0}\phi(x_j,\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})\,\mathrm{d}x_j. \tag{16}$$

Note that the condition $(D_j\phi)(\boldsymbol{x}) \neq 0$, when combined with the continuity of $D_j\phi$, means that $D_j\phi$ is either everywhere positive or everywhere negative. For definiteness we assume that

$$(D_j\phi)(\boldsymbol{x}) \;>\; 0 \quad \text{for all} \quad \boldsymbol{x} \in [0,1]^d;$$

the other case is similar. It follows that, for fixed $\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}$, $\phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})$ is a strictly increasing function of x_j. Using this, we now determine the limits of integration in (16). If $\phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \geq 0$ for all x_j (this is equivalent to $\phi(0, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \geq 0$), then we integrate x_j from 0 to 1. On the other hand, if $\phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \leq 0$ for all x_j (this is equivalent to $\phi(1, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \leq 0$), then the integral is 0 and can be interpreted as integrating x_j from 1 to 1. The remaining scenario is that $\phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})$ changes sign once as x_j goes from 0 to 1. Then there exists a unique $x_j^* \in (0,1)$ for which $\phi(x_j^*, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = 0$; in this case we integrate x_j from x_j^* to 1. Hence we can write (16) as

$$(P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; \int_{\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})}^{1} \phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \,\mathrm{d}x_j, \tag{17}$$

where, for $\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in [0,1]^{\mathfrak{D}\setminus\{j\}}$,

$$\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;:=\; \begin{cases} 0 & \text{if} \;\; \phi(0, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \geq 0, \\ x_j^* & \text{if} \;\; \phi(x_j^*, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = 0 \;\text{ with }\; x_j^* \in (0,1), \\ 1 & \text{if} \;\; \phi(1, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \leq 0. \end{cases} \tag{18}$$

Moreover, if we define

$$U \;:=\; \Big\{ \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in (0,1)^{\mathfrak{D}\setminus\{j\}} \;:\; \phi(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = 0 \text{ for some } x_j \in (0,1) \Big\}, \tag{19}$$

then (18) and the implicit function theorem (Theorem 5) lead us to conclude that

$$\psi \in \mathcal{C}[0,1]^{\mathfrak{D}\setminus\{j\}} \qquad \text{and} \qquad \psi|_{\overline{U}} \in \mathcal{C}^\infty(\overline{U}).$$

Now we differentiate (17) with respect to x_k for any $k \neq j$ and obtain

$$(D_k P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; \int_{\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})}^{1} (D_k\phi)(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \,\mathrm{d}x_j \;-\; \phi(\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \times (D_k\psi)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}).$$

Observe that the second term above is zero, since it follows from (18) that $\phi(\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = 0$ for $\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in U$ and $(D_k\psi)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) = 0$ for $\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \notin U$. Writing

$$g(t, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;:=\; \int_t^1 (D_k\phi)(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \,\mathrm{d}x_j, \qquad t \in [0,1], \tag{20}$$

we conclude that

$$(D_k P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; g(\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}). \tag{21}$$

It is easily seen that (21) can be differentiated again with respect to any variable other than x_j, since for $\ell \neq j$ we have

$$\begin{aligned} &(D_\ell D_k P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \\ &\quad = \int_{\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})}^{1} (D_\ell D_k\phi)(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \,\mathrm{d}x_j \;-\; (D_k\phi)(\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \times (D_\ell\psi)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \end{aligned}$$

which is essentially bounded. Thus $D_k P_j f \in \mathcal{W}^1_{\mathfrak{D}\setminus\{j\},\infty}$, and in turn $P_j f \in \mathcal{W}^2_{\mathfrak{D}\setminus\{j\},\infty}$. $\square$

Example 1 continued. For this example we have $\phi(x_1,x_2) = x_1 - x_2 + 1/2$, thus $(D_1\phi)(x_1,x_2) > 0$ for all $(x_1,x_2) \in [0,1]^2$. Explicit integration gives

$$
\begin{aligned}
(P_1 f)(x_2) \;&=\; \begin{cases} \displaystyle\int_0^1 (x_1 - x_2 + \tfrac{1}{2})\,\mathrm{d}x_1 \;=\; 1 - x_2 & \text{for } x_2 \le \tfrac{1}{2}, \\ \displaystyle\int_{x_2-1/2}^1 (x_1 - x_2 + \tfrac{1}{2})\,\mathrm{d}x_1 \;=\; 1 - x_2 + \tfrac{1}{2}(x_2 - \tfrac{1}{2})^2 & \text{for } x_2 \ge \tfrac{1}{2}, \end{cases} \\
&=\; 1 - x_2 + \tfrac{1}{2}(x_2 - \tfrac{1}{2})_+^2,
\end{aligned} \tag{22}
$$

which is clearly twice differentiable. Indeed

$$(D_2 P_1 f)(x_2) \;=\; -1 + (x_2 - \tfrac{1}{2})_+,$$

and hence $(D_2 D_2 P_1 f)(x_2)$ is the characteristic function of $x_2 - 1/2$. This is consistent with the proof of Lemma 6: indeed, for $j = 1$ and $k = 2$ we have $(D_2 P_1 f)(x_2) = g(\psi(x_2), x_2)$, with $\psi(x_2) = (x_2 - 1/2)_+$ and $g(t,x_2) = \int_t^1 (-1)\,\mathrm{d}x_1 = -1 + t$.

We are now ready to present the core result of this paper. In the following theorem the property $D_j\phi \ne 0$ is assumed to hold for all j in a subset $\mathbf{z} \subseteq \mathfrak{D}$. Here and later, the notation $\mathbf{z} \setminus \mathbf{u} := \{j : j \in \mathbf{z} \text{ and } j \notin \mathbf{u}\} = \mathbf{z} \setminus (\mathbf{u} \cap \mathbf{z})$ denotes set difference.

Theorem 7 *Let $\mathbf{z}$ be a non-empty subset of $\mathfrak{D}$, i.e., $\emptyset \ne \mathbf{z} \subseteq \mathfrak{D}$, and let*

$$f(\boldsymbol{x}) \;=\; \phi(\boldsymbol{x})_+, \quad \textit{with} \quad \begin{cases} \phi \in \mathcal{C}^\infty[0,1]^d, \\ (D_j\phi)(\boldsymbol{x}) \ne 0 \quad \forall\, j \in \mathbf{z} \quad \forall\, \boldsymbol{x} \in [0,1]^d. \end{cases} \tag{23}$$

Then

$$f \;\in\; \mathcal{W}^1_{d,\infty} \qquad \textit{and} \qquad P_{\mathbf{u}} f \;\in\; \mathcal{W}^{1+|\mathbf{z}\cap\mathbf{u}|}_{\mathfrak{D}\setminus\mathbf{u},\infty} \quad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

Moreover, the ANOVA terms of f satisfy

$$f_{\mathbf{u}} \;\in\; \mathcal{W}^{1+|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u},\infty} \qquad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

We will give the proof in the next subsection. Note that the conclusions in the theorem also hold with ∞ replaced by any $p \in (1,\infty)$ because of the imbedding property (7).

The heart of the matter is that if $D_j\phi$ is never zero (thus never changes sign), then we can show that P_j has a "once-smoothing" effect in all variables, in the sense illustrated in (15) and proved in Lemma 6. We have assumed in the theorem that $D_j\phi \ne 0$ holds for indices j in some set $\mathbf{z} \subseteq \mathfrak{D}$, and so we can gain up to $|\mathbf{z}|$ additional degrees of smoothness by successive applications of projections P_j, with the maximum value $|\mathbf{z}|$ achieved when we have $P_{\mathbf{u}}$ with $\mathbf{u} = \mathbf{z}$.

To gain more insight into the theorem, suppose now that we have the best case $\mathbf{z} = \mathfrak{D}$, that is, suppose $(D_j\phi)(\boldsymbol{x}) \ne 0$ for all $j \in \mathfrak{D}$ and all $\boldsymbol{x} \in [0,1]^d$. Then we have the following corollary.

Corollary 8 *Take $\mathbf{z} = \mathfrak{D}$ in Theorem 7. Then for f given by (23) we have*

$$f \;\in\; \mathcal{W}^1_{d,\infty} \qquad \textit{and} \qquad f_{\mathbf{u}} \;\in\; \mathcal{W}^{1+d-|\mathbf{u}|}_{\mathbf{u},\infty} \quad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}. \tag{24}$$

Consequently, for $s \ge 1$ and $\boldsymbol{r} \ge (1,\ldots,1)$ we have

(i) $f_{\mathbf{u}} \in \mathcal{W}^{(s,\ldots,s)}_{\mathbf{u},\infty,\mathrm{mix}}$ *for all* $\mathbf{u} \subseteq \mathfrak{D}$ *satisfying* $|\mathbf{u}| \le \dfrac{d+1}{s+1}$,
and in particular,
$f_{\mathbf{u}} \in \mathcal{W}^{(1,\ldots,1)}_{\mathbf{u},\infty,\mathrm{mix}}$ *for all* $\mathbf{u} \subseteq \mathfrak{D}$ *satisfying* $|\mathbf{u}| \le \dfrac{d+1}{2}$,

(ii) $f_{\mathbf{u}} \in \mathcal{W}^{\boldsymbol{r}_{\mathbf{u}}}_{\mathbf{u},\infty,\mathrm{mix}}$ *for all* $\mathbf{u} \subseteq \mathfrak{D}$ *satisfying* $|\mathbf{u}| \le d + 1 - \sum_{j\in\mathbf{u}} r_j$.

Proof. Part (i) follows from (24) and the second part of the imbedding property (9) with d replaced by $|\mathbf{u}|$. It can also be easily explained as follows. Since $f_{\mathbf{u}} \in \mathcal{W}^{1+d-|\mathbf{u}|}_{\mathbf{u},\infty}$, we can differentiate $f_{\mathbf{u}}$ up to $1+d-|\mathbf{u}|$ times in total. On the other hand, to have $f_{\mathbf{u}} \in \mathcal{W}^{(s,\ldots,s)}_{\mathbf{u},\infty,\mathrm{mix}}$ we need to be able to differentiate $f_{\mathbf{u}}$ exactly s times with respect to each variable in $\mathbf{u}$. Thus we need

$$s\,|\mathbf{u}| \,\le 1 + d - |\mathbf{u}|,$$

which yields the upper bound on $|\mathbf{u}|$ in (i). Part (ii) can be deduced in a similar way from (24) and the second part of the imbedding property (8). □

The special case of part (i) with $s = 1$ indicates that approximately half of all the ANOVA terms of f belong to the space of functions with essentially bounded mixed first derivatives.

Example 1 continued again. For this example we found already $(P_1 f)(x_2)$, see (22), and in a similar way we find

$$(P_2 f)(x_1) \;=\; x_1 + \tfrac{1}{2}(\tfrac{1}{2} - x_1)_+^2.$$

Thus from the ANOVA formula (3) we have

$$f_\emptyset \;=\; P_1P_2 f \;=\; \frac{25}{48}, \quad f_{\{1\}}(x_1) \;=\; (P_2 f)(x_1) - \frac{25}{48}, \quad f_{\{2\}}(x_2) \;=\; (P_1 f)(x_2) - \frac{25}{48},$$

and

$$f_{\{1,2\}}(x_1,x_2) \;=\; f - (P_1 f)(x_2) - (P_2 f)(x_1) + \frac{25}{48}.$$

As expected from (24), $f_{\{1\}}$ belongs to $\mathcal{W}^{1+2-1}_{\{1\},\infty} = \mathcal{W}^2_{\{1\},\infty}$, and similarly $f_{\{2\}}$ belongs to $\mathcal{W}^2_{\{2\},\infty}$.

3.2. Proof of the main theorem – Theorem 7

The proof of Lemma 6 provides the base step for an inductive argument to prove Theorem 7. We shall begin with a discussion which will lead us to the induction step, that is, Lemma 9 below, and then prove the theorem at the end.

The inductive step will act on functions of the form $g(\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})$, see (21), where g is a smooth function and ψ is what we call a "cutoff nice function" – ψ is essentially a smooth function, but since it refers to coordinates in the unit cube its range must be limited to the interval $[0,1]$.

More precisely, a "cutoff nice function" ψ, see (18) for example, is a continuous function consisting of three pieces: the middle piece is a monotone $\mathcal{C}^\infty(\overline{U})$ function, where U is an open subset of $(0,1)$ and $\psi(U) \subseteq (0,1)$, while the two end pieces take the constant values of 0 and 1, respectively. In degenerate cases we may have only one or two of the three pieces.

In the proof of Lemma 6, the middle piece of the function ψ given by (18) arises from applying the implicit function theorem to the smooth function ϕ. The set U, see (19), defines the domain of the middle piece of ψ. We considered in that proof the case $D_j\phi > 0$. If, in addition, we have $D_k\phi \neq 0$ for $k \neq j$, then we see from (12) that $D_k\psi$ is also nonzero on U and takes the opposite sign to $D_k\phi$. In other words, ψ is strictly increasing (or decreasing) on U with respect to x_k if ϕ is strictly decreasing (or increasing, respectively) in x_k.

Instead of the definition (19), we can also refer to the domain of the middle piece of ψ by

$$U \;:=\; \Big\{\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in (0,1)^{\mathfrak{D}\setminus\{j\}} \;:\; \psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \in (0,1)\Big\}.$$

To integrate some expression involving ψ, we shall need to determine the "end points" of U with respect to the variable of integration, say x_k, and split the integral into three pieces. The "end points" of U determine the limits of integration and they can be defined by

$$\begin{aligned} y(\boldsymbol{x}_{\mathfrak{D}\setminus\{j,k\}}) \;&:=\; \inf\big\{x_k \in (0,1) \;:\; \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in U\big\} \\ z(\boldsymbol{x}_{\mathfrak{D}\setminus\{j,k\}}) \;&:=\; \sup\big\{x_k \in (0,1) \;:\; \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}} \in U\big\}. \end{aligned}$$

As we shall explain in the proof of Lemma 9 below, the functions y and z are also "cutoff nice functions". The middle pieces of y and z arise from applying the implicit function theorem to the middle piece of

ψ (for $\psi = 0$ and $\psi = 1$, respectively). This requires a slightly modified version of the implicit function theorem, Theorem 5, in which $(0,1)^{\mathfrak{D}\setminus\{j\}}$ and $[0,1]^{\mathfrak{D}\setminus\{j\}}$ are replaced by a connected open set and its closure.

We are now ready to prove the induction step of the argument.

Lemma 9 *Let $\mathbf{z}$ and f be as in Theorem 7. For $1 \le a \le |\mathbf{z}|$, let $j_1, \ldots, j_a$ be distinct elements of $\mathbf{z}$, $\mathbf{u} := \mathfrak{D} \setminus \{j_1, \ldots, j_a\}$, and let $k_1, \ldots, k_a$ be elements of $\mathbf{u}$. Then it is possible to write*

$$\left(\left(\prod_{i=1}^{a} D_{k_i} P_{j_i} \right) f \right) (\boldsymbol{x}_{\mathbf{u}}) \;=\; \sum_{p=1}^{M_a} h_{a,p}(\boldsymbol{x}_{\mathbf{u}}), \tag{25}$$

for some integer $M_a \ge 1$, where each term in the finite sum on the right can be expressed in the form

$$h_{a,p}(\boldsymbol{x}_{\mathbf{u}}) \;=\; g_{a,p}(\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}), \boldsymbol{x}_{\mathbf{u}}), \tag{26}$$

with

$$\begin{cases} g_{a,p} \in \mathcal{C}^\infty([0,1] \times [0,1]^{\mathbf{u}}), \\ \psi_{a,p} \in \mathcal{C}[0,1]^{\mathbf{u}}, \\ \psi_{a,p} : [0,1]^{\mathbf{u}} \to [0,1] \textit{ is non-decreasing (or non-increasing) in } x_k \textit{ for all } k \in \mathbf{u} \cap \mathbf{z}, \\ \psi_{a,p}|_{\overline{U_{a,p}}} \in \mathcal{C}^\infty(\overline{U_{a,p}}), \\ \psi_{a,p}|_{\overline{U_{a,p}}} \textit{ is strictly increasing (or decreasing, respectively) in } x_k \textit{ for all } k \in \mathbf{u} \cap \mathbf{z}, \end{cases}$$

where

$$U_{a,p} \;:=\; \{\boldsymbol{x}_{\mathbf{u}} \in (0,1)^{\mathbf{u}} \;:\; \psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}) \in (0,1)\}\,. \tag{27}$$

We have $h_{a,p} \in \mathcal{W}^1_{\mathbf{u},\infty}$ for all a and p, and hence $(\prod_{i=1}^{a} D_{k_i} P_{j_i}) f \in \mathcal{W}^1_{\mathbf{u},\infty}$.

Proof. The proof is again by induction. The case $a = 1$ has already been proved in Lemma 6, see (21). For this case we have $M_a = 1$. That $\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})$ is non-increasing or non-decreasing in x_k for $k \in \mathbf{z}$ and $k \neq j$ follows from (12), and has been explained in the discussion before this lemma.

Now we assume that the lemma holds for some $a < |\mathbf{z}|$, and we seek to prove the result with a replaced by $a+1$. Then with $j_{a+1} \in \mathbf{u} \cap \mathbf{z}$ (that is, j_{a+1} belongs to the set $\boldsymbol{z}$ but is different from $j_1, \ldots, j_a$), we have from (25) that

$$\begin{aligned} \left(\left(\prod_{i=1}^{a+1} D_{k_i} P_{j_i} \right) f \right) (\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) \;&=\; \left((D_{k_{a+1}} P_{j_{a+1}}) \left(\prod_{i=1}^{a} D_{k_i} P_{j_i} \right) f \right) (\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) \\ &=\; \sum_{p=1}^{M_a} (D_{k_{a+1}} P_{j_{a+1}} h_{a,p})(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}), \end{aligned}$$

and it follows from (26) that

$$(P_{j_{a+1}} h_{a,p})(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) \;=\; \int_0^1 g_{a,p}(\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}), \boldsymbol{x}_{\mathbf{u}})\, \mathrm{d}x_{j_{a+1}}.$$

Suppose for definiteness that $\psi_{a,p}$ is a non-decreasing (rather than non-increasing) function of each variable x_k with $k \in \mathbf{u} \cap \mathbf{z}$; the other case is similar. Then from the assumed properties of $\psi_{a,p}$ we can write

$$\begin{aligned} (P_{j_{a+1}} h_{a,p})(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) \;=\; &\int_0^{y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})} g_{a,p}(0, \boldsymbol{x}_{\mathbf{u}})\, \mathrm{d}x_{j_{a+1}} + \int_{y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})}^{z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})} g_{a,p}(\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}), \boldsymbol{x}_{\mathbf{u}})\, \mathrm{d}x_{j_{a+1}} \\ &+ \int_{z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})}^1 g_{a,p}(1, \boldsymbol{x}_{\mathbf{u}})\, \mathrm{d}x_{j_{a+1}}, \end{aligned} \tag{28}$$

where we define, for given $\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}} \in [0,1]^{\mathbf{u}\setminus\{j_{a+1}\}}$,

$$y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) := \inf\left\{x_{j_{a+1}} \in (0,1) \,:\, \boldsymbol{x}_{\mathbf{u}} \in U_{a,p}\right\}$$
$$z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) := \sup\left\{x_{j_{a+1}} \in (0,1) \,:\, \boldsymbol{x}_{\mathbf{u}} \in U_{a,p}\right\},$$

with $U_{a,p}$ given by (27).

Since by assumption $\psi_{a,p}$ is a strictly increasing function of $x_{j_{a+1}}$ on $U_{a,p}$, which we recall is the set of values of $\boldsymbol{x}_{\mathbf{u}} \in (0,1)^{\mathbf{u}}$ for which $\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}) \in (0,1)$, it follows that there are only three possibilities for $y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})$: either $y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 1$ (in which case $z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 1$ also); or $y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 0$; or $y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = x^*_{j_{a+1}} \in (0,1)$ is such that $\psi_{a,p}(x^*_{j_{a+1}}, \boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 0$. In the latter case it follows from the implicit function theorem that y is a $\mathcal{C}^\infty$ function on $\overline{Y}$, where

$$Y := \left\{\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}} \in (0,1)^{\mathbf{u}\setminus\{j_{a+1}\}} \,:\, y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) \in (0,1)\right\},$$

and it is strictly decreasing on $\overline{Y}$ for each x_k with $k \in (\mathbf{u}\cap\mathbf{z}) \setminus \{j_{a+1}\}$; the latter property can be deduced using (12). This shows that y is a "cutoff nice function" as described at the beginning of this subsection.

In a similar way, there are only three possibilities for $z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})$: either $z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 0$ (in which case $y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 0$); or $z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 1$; or $z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = x^{**}_{j_{a+1}} \in (0,1)$ is such that $\psi_{a,p}(x^{**}_{j_{a+1}}, \boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) = 1$. In the latter case the implicit function theorem (applied to $\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}) - 1 = 0$) gives that z is a $\mathcal{C}^\infty$ function on $\overline{Z}$, where

$$Z := \left\{\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}} \in (0,1)^{\mathbf{u}\setminus\{j_{a+1}\}} \,:\, z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) \in (0,1)\right\},$$

and it is again strictly decreasing on $\overline{Z}$ for each x_k with $k \in (\mathbf{u}\cap\mathbf{z}) \setminus \{j_{a+1}\}$. This shows that z is also a "cutoff nice function".

Now we can differentiate (28) to obtain (noting that the contribution from differentiating the limits of integration cancel)

$$\begin{aligned}
(D_{k_{a+1}} P_{j_{a+1}} h_{a,p})(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}}) &= \int_0^{y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})} (D_{k_{a+1}} g_{a,p})(0, \boldsymbol{x}_{\mathbf{u}})\,\mathrm{d}x_{j_{a+1}} \\
&+ \int_{y(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})}^{z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})} \left[(D_{k_{a+1}} g_{a,p})(\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}), \boldsymbol{x}_{\mathbf{u}}) + (D_0 g_{a,p})(\psi_{a,p}(\boldsymbol{x}_{\mathbf{u}}), \boldsymbol{x}_{\mathbf{u}}) \times (D_{k_{a+1}} \psi_{a,p})(\boldsymbol{x}_{\mathbf{u}})\right] \mathrm{d}x_{j_{a+1}} \\
&+ \int_{z(\boldsymbol{x}_{\mathbf{u}\setminus\{j_{a+1}\}})}^{1} (D_{k_{a+1}} g_{a,p})(1, \boldsymbol{x}_{\mathbf{u}})\,\mathrm{d}x_{j_{a+1}},
\end{aligned}$$

where D_0 is the derivative with respect to the first variable in $g_{a,p}$. Rewriting the integrals using definitions similar to (20), we see that this is a sum of terms of exactly the form required. In particular, the roles of the function $\psi_{a,p}$ and the set $U_{a,p}$ are now taken by the function y together with the set Y, and the function z together with the set Z. Thus the proof by induction is complete.

To show the last point of the lemma, we observe that $D_k h_{a,p} \in \mathcal{L}_\infty$ for all $k \in \mathbf{u}$ and hence $h_{a,p} \in \mathcal{W}^1_{\mathbf{u},\infty}$, concluding the proof of this lemma. □

Finally we prove our main theorem.

Proof of Theorem 7. We have from (14) that $f \in \mathcal{W}^1_{d,\infty}$, and we wish to show that

$$P_{\mathbf{u}} f \in \mathcal{W}^{1+|\mathbf{z}\cap\mathbf{u}|}_{\mathfrak{D}\setminus\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D}. \tag{29}$$

Since $P_{\mathbf{u}} f = P_{\mathbf{u}\setminus\mathbf{z}}(P_{\mathbf{z}\cap\mathbf{u}} f)$, it is enough to prove that

$$P_{\mathbf{z}\cap\mathbf{u}} f \in \mathcal{W}^{1+|\mathbf{z}\cap\mathbf{u}|}_{\mathfrak{D}\setminus(\mathbf{z}\cap\mathbf{u}),\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D},$$

and then to use the inheritance theorem (Theorem 4) to conclude that $P_{\mathbf{u}} f$ has the desired smoothness property (29). It then follows that it is sufficient to prove

$$P_{\mathbf{u}} f \in \mathcal{W}^{1+|\mathbf{u}|}_{\mathfrak{D}\setminus\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathbf{z}.$$

Equivalently, we have to prove that

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_{\mathbf{u}} f \,\in\, \mathcal{W}^1_{\mathfrak{D}\setminus\mathbf{u},\infty} \quad \text{for all } a \le |\mathbf{u}| \text{ and all possible combinations of } k_i \in \mathfrak{D}\setminus\mathbf{u}.$$

Note there is no requirement that the numbers k_i be distinct. Thus we allow for repeated differentiations with respect to the same variable, so long as the total number of differentiations does not exceed $|\mathbf{u}|$.

Labeling the distinct projections in $P_{\mathbf{u}}$ as $P_{j_1}, \ldots, P_{j_{|\mathbf{u}|}}$, we now write

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_{\mathbf{u}} f \,=\, \left(\prod_{i=1}^{a} D_{k_i}\right)\left(\prod_{\ell=1}^{|\mathbf{u}|} P_{j_\ell}\right) f \,=\, \left(\prod_{i=2}^{a} D_{k_i}\right)\left(\prod_{\ell=2}^{|\mathbf{u}|} P_{j_\ell}\right)(D_{k_1} P_{j_1} f),$$

where we moved the differential operator D_{k_1} past $P_{j_2}, \ldots, P_{j_{|\mathbf{u}|}}$ by repeated use of the Leibniz theorem (Theorem 3). Each step is justified since $P_{\mathbf{w}} f \in \mathcal{W}^1_{\mathfrak{D}\setminus\mathbf{w},\infty}$ for all $\mathbf{w} \subseteq \mathfrak{D}$ by the inheritance theorem (Theorem 4).

Next we use the last point of Lemma 9 to claim that $D_{k_1} P_{j_1} f$ belongs to $\mathcal{W}^1_{\mathfrak{D}\setminus\{j_1\},\infty}$. We may now again use the Leibniz theorem (Theorem 3), this time to move D_{k_2} to the right until we achieve

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_{\mathbf{u}} f \,=\, \left(\prod_{i=3}^{a} D_{k_i}\right)\left(\prod_{\ell=3}^{|\mathbf{u}|} P_{j_\ell}\right)(D_{k_2} P_{j_2})(D_{k_1} P_{j_1} f).$$

Each step is justified since $P_{\mathbf{w}}(D_{k_1} P_{j_1} f) \in \mathcal{W}^1_{\mathfrak{D}\setminus(\mathbf{w}\cup\{j_1\}),\infty}$ for all $\mathbf{w} \subseteq \mathfrak{D}$ by the inheritance theorem (Theorem 4).

Then we use Lemma 9 to claim that $(D_{k_2} P_{j_2})(D_{k_1} P_{j_1} f)$ belongs to $\mathcal{W}^1_{\mathfrak{D}\setminus\{j_1,j_2\},\infty}$. The Leibniz theorem (Theorem 3) can now be used to move D_{k_3} to the right. We continue this way, using repeatedly the Leibniz theorem (Theorem 3) and Lemma 9 until we obtain finally

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_{\mathbf{u}} f \,=\, \left(\prod_{\ell=a+1}^{|\mathbf{u}|} P_{j_\ell}\right)(D_{k_a} P_{j_a}) \cdots (D_{k_2} P_{j_2})(D_{k_1} P_{j_1} f) \,\in\, \mathcal{W}^1_{\mathfrak{D}\setminus\mathbf{u},\infty}.$$

This proves that $P_{\mathbf{u}} f \in \mathcal{W}^{1+|\mathbf{u}|}_{\mathfrak{D}\setminus\mathbf{u},\infty}$ for all $\mathbf{u} \subseteq \mathbf{z}$, which completes the proof of (29).

Substituting $\mathbf{u}$ by $\mathfrak{D}\setminus\mathbf{u}$ in (29), we obtain

$$P_{\mathfrak{D}\setminus\mathbf{u}} f \,\in\, \mathcal{W}^{1+|\mathbf{z}\cap(\mathfrak{D}\setminus\mathbf{u})|}_{\mathbf{u},\infty} \,=\, \mathcal{W}^{1+|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

Then the inheritance theorem (Theorem 4) gives

$$P_{\mathbf{u}\setminus\mathbf{v}}(P_{\mathfrak{D}\setminus\mathbf{u}} f) \,\in\, \mathcal{W}^{1+|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{v} \subseteq \mathbf{u} \subseteq \mathfrak{D}.$$

The identity (3) now allows us to conclude that

$$f_{\mathbf{u}} \,\in\, \mathcal{W}^{1+|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

This completes the proof of Theorem 7. □

3.3. More general functions with kinks

Theorem 7 extends in a trivial way to the absolute value function, because of the identity

$$|\phi(\boldsymbol{x})| \,=\, \phi(\boldsymbol{x})_+ \,+\, (-\phi(\boldsymbol{x}))_+.$$

Similarly, it extends to any linear combination of functions of the form (23), provided that the required derivative property holds with the same set $\mathbf{z}$ for every function in this linear combination. We can also generalize Theorem 7 by considering functions f of a more complicated form. For example, we can allow the kink to depend only on the variables $\boldsymbol{x}_{\mathbf{w}}$ for some subset $\mathbf{w} \subseteq \mathfrak{D}$, so that the functions f are smooth with respect to $\boldsymbol{x}_{\mathfrak{D}\setminus\mathbf{w}}$. In the following, $\mathcal{W}^1_{\mathbf{w},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus\mathbf{w},\infty}$ denotes the space of functions which are once differentiable with respect to the variables $\boldsymbol{x}_{\mathbf{w}}$ and infinitely differentiable with respect to the remaining variables.

Theorem 10 *Let* $\mathbf{z}$ *be a non-empty subset of* $\mathbf{w}$*, which is a non-empty subset of* $\mathfrak{D}$*, i.e.,* $\emptyset \neq \mathbf{z} \subseteq \mathbf{w} \subseteq \mathfrak{D}$*, and let*

$$f(\boldsymbol{x}) \;=\; g(\phi(\boldsymbol{x}_{\mathbf{w}})_+, \boldsymbol{x}), \quad \textit{with} \quad \begin{cases} g \in \mathcal{C}^\infty([0,1]\times[0,1]^d), \\ \phi \in \mathcal{C}^\infty[0,1]^{\mathbf{w}}, \\ (D_j\phi)(\boldsymbol{x}_{\mathbf{w}}) \neq 0 \quad \forall\, j \in \mathbf{z} \quad \forall\, \boldsymbol{x}_{\mathbf{w}} \in [0,1]^{\mathbf{w}}. \end{cases}$$

Then

$$f \;\in\; \mathcal{W}^1_{\mathbf{w},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus\mathbf{w},\infty} \qquad \textit{and} \qquad P_{\mathbf{u}} f \;\in\; \mathcal{W}^{1+|\mathbf{z}\cap\mathbf{u}|}_{\mathbf{w}\setminus\mathbf{u},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus(\mathbf{w}\cup\mathbf{u}),\infty} \quad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

Moreover, the ANOVA terms of f *satisfy*

$$f_{\mathbf{u}} \;\in\; \mathcal{W}^{1+|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u}\cap\mathbf{w},\infty} \otimes \mathcal{W}^\infty_{\mathbf{u}\setminus\mathbf{w},\infty} \qquad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

Proof. Since g is a $\mathcal{C}^\infty$ function, we see immediately that f can be differentiated infinitely many times with respect to the variables $\boldsymbol{x}_{\mathfrak{D}\setminus\mathbf{w}}$. On the other hand, due to the term $\phi(\boldsymbol{x}_{\mathbf{w}})_+$ we can only differentiate f once with respect to one of the variables in $\boldsymbol{x}_{\mathbf{w}}$. Hence clearly we have $f \in \mathcal{W}^1_{\mathbf{w},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus\mathbf{w},\infty}$. It then follows from the inheritance theorem (Theorem 4) that $P_{\mathbf{u}} f \in \mathcal{W}^1_{\mathbf{w}\setminus\mathbf{u},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus(\mathbf{w}\cup\mathbf{u}),\infty}$ for all $\mathbf{u} \subseteq \mathfrak{D}$. Under the condition that $D_j\phi$ is never zero for all $j \in \mathbf{z}$, we now prove that $P_{\mathbf{u}} f$ is of order $|\mathbf{z}\cap\mathbf{u}|$ smoother with respect to $\boldsymbol{x}_{\mathbf{w}\setminus\mathbf{u}}$ than we have shown so far.

Since $P_{\mathbf{u}} f = P_{\mathbf{u}\setminus\mathbf{z}}(P_{\mathbf{z}\cap\mathbf{u}} f)$, to prove the desired smoothness property of $P_{\mathbf{u}} f$ it suffices to show that

$$P_{\mathbf{z}\cap\mathbf{u}} f \;\in\; \mathcal{W}^{1+|\mathbf{z}\cap\mathbf{u}|}_{\mathbf{w}\setminus(\mathbf{z}\cap\mathbf{u}),\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus\mathbf{w},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D},$$

and then to use the inheritance theorem (Theorem 4). It is sufficient to establish that

$$P_{\mathbf{u}} f \;\in\; \mathcal{W}^{1+|\mathbf{u}|}_{\mathbf{w}\setminus\mathbf{u},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus\mathbf{w},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathbf{z},$$

which is equivalent to proving, for all $\mathbf{u} \subseteq \mathbf{z}$,

$$\left(\prod_{i=1}^{a} D_{k_i}\right) P_{\mathbf{u}} f \;\in\; \mathcal{W}^1_{\mathbf{w}\setminus\mathbf{u},\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus\mathbf{w},\infty} \quad \text{for all } a \le |\mathbf{u}| \text{ and all possible } k_i \in \mathbf{w}\setminus\mathbf{u}.$$

Lemma 9 needs obvious modification for the new function f. Omitting the details, we simply say here that the above property can be obtained by using a suitably modified version of Lemma 9 and arguing as in the proof of Theorem 7.

Finally, since the smoothness of the ANOVA term $f_{\mathbf{u}}$ is determined by $P_{\mathfrak{D}\setminus\mathbf{u}} f$, we obtain

$$f_{\mathbf{u}} \in \mathcal{W}^{1+|\mathbf{z}\cap(\mathfrak{D}\setminus\mathbf{u})|}_{\mathbf{w}\setminus(\mathfrak{D}\setminus\mathbf{u}),\infty} \otimes \mathcal{W}^\infty_{\mathfrak{D}\setminus(\mathbf{w}\cup(\mathfrak{D}\setminus\mathbf{u})),\infty} \;=\; \mathcal{W}^{1+|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u}\cap\mathbf{w},\infty} \otimes \mathcal{W}^\infty_{\mathbf{u}\setminus\mathbf{w},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

This completes the proof. $\square$

The above theorem demonstrates that the smoothing effect of the ANOVA decomposition can be established for more general functions.

4. Functions with jumps

Now we consider functions with a jump along a manifold $\phi(\boldsymbol{x}) = 0$. For convenience, we introduce a new notation for the Heaviside step function:

$$a_{\#} \;:=\; \begin{cases} 1 & \text{if } a \ge 0, \\ 0 & \text{if } a < 0. \end{cases}$$

We have the following result.

Theorem 11 *Let $\mathbf{z}$ be a non-empty subset of $\mathfrak{D}$, i.e., $\emptyset \neq \mathbf{z} \subseteq \mathfrak{D}$, and let*

$$f(\boldsymbol{x}) \;=\; \eta(\boldsymbol{x})\,\phi(\boldsymbol{x})_{\#}, \quad \textit{with} \quad \begin{cases} \eta \in \mathcal{C}^{\infty}[0,1]^d, \\ \phi \in \mathcal{C}^{\infty}[0,1]^d, \quad \phi \neq \eta, \\ (D_j\phi)(\boldsymbol{x}) \neq 0 \quad \forall\, j \in \mathbf{z} \quad \forall\, \boldsymbol{x} \in [0,1]^d. \end{cases}$$

Then

$$f \,\in\, \mathcal{W}^{0}_{d,\infty} \qquad \textit{and} \qquad P_{\mathbf{u}} f \,\in\, \mathcal{W}^{|\mathbf{z}\cap\mathbf{u}|}_{\mathfrak{D}\setminus\mathbf{u},\infty} \quad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

Moreover, the ANOVA terms of f satisfy

$$f_{\mathbf{u}} \,\in\, \mathcal{W}^{|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u},\infty} \quad \textit{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

Proof. We have

$$f(\boldsymbol{x}) \;=\; \begin{cases} \eta(\boldsymbol{x}) & \text{if } \phi(\boldsymbol{x}) \geq 0, \\ 0 & \text{if } \phi(\boldsymbol{x}) < 0. \end{cases}$$

Thus clearly $f \in \mathcal{W}^{0}_{d,\infty}$. For any $j \in \mathbf{z}$ we have

$$(P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; \int_{x_j \in [0,1]\,:\,\phi(x_j,\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \geq 0} \eta(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})\,\mathrm{d}x_j.$$

For definiteness we may assume as in the proof of Lemma 6 that $(D_j\phi)(\boldsymbol{x}) > 0$ for all $\boldsymbol{x} \in [0,1]^d$ (the other case is similar), and we can write

$$(P_j f)(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) \;=\; \int_{\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})}^{1} \eta(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})\,\mathrm{d}x_j \;=\; g(\psi(\boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}), \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}),$$

where ψ is given by (18) and $g(t, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}}) := \int_t^1 \eta(x_j, \boldsymbol{x}_{\mathfrak{D}\setminus\{j\}})\,\mathrm{d}x_j$. This proves that $P_j f$ is of the form (26) with $\mathbf{u} = \mathfrak{D} \setminus \{j\}$.

Hence we can argue as in the proof of Theorem 7, provided that we begin with $P_j f$ for some $j \in \mathbf{z}$. This indicates that we lose one order of smoothness here compared to Theorem 7. The remainder of this proof is omitted. □

5. Option pricing examples

As examples of our theory, we now consider some standard option pricing problems. We deal with the case of a single asset undergoing geometric Brownian motion. We first define the problem as a multivariate expected value on $\mathbb{R}^d$, then transform it to a bounded region by using the cumulative normal distribution. In one respect, however, the following discussion is non-standard: namely, that we additionally truncate the Gaussian integrals at some sufficiently large distance away from the boundary of the finite domain. We do this to avoid the well known problem caused by the unboundedness of the inverse cumulative normal distribution near the boundary.

5.1. Option pricing

As usual, a risky asset with value S_t at time t is assumed to follow (under risk neutral measure) the geometric Brownian motion

$$\mathrm{d}S_t \;=\; rS_t\,\mathrm{d}t + \sigma S_t\,\mathrm{d}W_t, \quad t \geq 0, \tag{30}$$

where r is the risk-free interest rate, σ is the volatility, and W_t is standard Brownian motion, i.e., the increments $W_t - W_s$ for $t > s$ are independent zero-mean Gaussian random variables with variance $t - s$. The solution of (30) is

$$S_t \;=\; S_0\,\exp\left(\left(r - \frac{\sigma^2}{2}\right)t + \sigma W_t\right), \quad t \geq 0.$$

The pay-off $G(\boldsymbol{S})$, with $\boldsymbol{S} = (S_1, \ldots, S_d)^{\mathrm{T}}$, is assumed to depend on the asset prices $S_j = S_{t_j}$ at equally spaced times $t_j = j\Delta t$ for $j = 1, \ldots, d$, where $\Delta t = T/d$ with T denoting the final time. Later we will focus on three standard option pricing problems:

- Arithmetic average Asian call option with strike price K,

$$G(\boldsymbol{S}) \;=\; \left(\frac{1}{d}\sum_{j=1}^{d} S_j - K\right)_+ . \tag{31}$$

- Geometric average Asian call option with strike price K,

$$G(\boldsymbol{S}) \;=\; \left(\left(\prod_{j=1}^{d} S_j\right)^{1/d} - K\right)_+ . \tag{32}$$

- Binary arithmetic average Asian call option with strike price K,

$$G(\boldsymbol{S}) \;=\; \left(\frac{1}{d}\sum_{j=1}^{d} S_j\right)\left(\frac{1}{d}\sum_{j=1}^{d} S_j - K\right)_\# . \tag{33}$$

The first two are examples with a kink, while the third one is an example with a jump. We included the geometric average Asian option for benchmarking purposes only, since a closed form solution is known.

Continuing our discussion for a general general pay-off $G(\boldsymbol{S})$, the discounted expected value of the option at the final time T is

$$V \;=\; \frac{e^{-rT}}{(2\pi)^{d/2}\sqrt{\det(C)}}\int_{\mathbb{R}^d} G(\boldsymbol{S}(\boldsymbol{W}))\, e^{-\frac{1}{2}\boldsymbol{W}^{\mathsf{T}}C^{-1}\boldsymbol{W}}\,\mathrm{d}\boldsymbol{W},$$

where $\boldsymbol{W} = (W_1,\ldots,W_d)^{\mathsf{T}}$ with $W_j = W_{t_j}$ for $j = 1,\ldots,d$, $\boldsymbol{S}(\boldsymbol{W}) = (S_1(\boldsymbol{W}),\ldots,S_d(\boldsymbol{W}))^{\mathsf{T}}$, and C is a $d\times d$ covariance matrix with entries given by $C_{ij} = \min(t_i,t_j) = \Delta t\,\min(i,j)$. Let $C = AA^{\mathsf{T}}$ be a factorization of C with A a $d\times d$ matrix. Then the change of variables $\boldsymbol{W} = A\boldsymbol{z}$ with $\boldsymbol{z} = (z_1,\ldots,z_d)^{\mathsf{T}}$ transforms the expected value into an integral with a standard Gaussian probability distribution, i.e.,

$$V \;=\; \frac{e^{-rT}}{(2\pi)^{d/2}}\int_{\mathbb{R}^d} G(\boldsymbol{S}(A\boldsymbol{z}))\, e^{-\frac{1}{2}\boldsymbol{z}^{\mathsf{T}}\boldsymbol{z}}\,\mathrm{d}\boldsymbol{z}. \tag{34}$$

It is well known [8] that the factorization of C can be carried out in several ways. Here we will consider three methods:

- In the *standard construction*, the Brownian motions are generated sequentially in time:

  $$W_0 = 0,\; W_{t_j} = W_{t_{j-1}} + \sqrt{\Delta t}\, z_j, \qquad j = 1,\ldots,d.$$

  The corresponding matrix A has entries

  $$A_{j\ell} \;=\; \begin{cases} \sqrt{\Delta t} & \text{if } j \ge \ell,\\ 0 & \text{otherwise,}\end{cases} \tag{35}$$

  which is just the Cholesky factor of C.

- In the *Brownian bridge construction*, assuming that $d = 2^m$, the Brownian motions are generated in the order of $T, T/2, T/4, 3T/4, \ldots$ as follows:

  $$\begin{aligned} W_0 &= 0,\\ W_T &= \sqrt{T}\, z_1,\\ W_{T/2} &= (W_0 + W_T)/2 + \sqrt{T/4}\, z_2,\\ W_{T/4} &= (W_0 + W_{T/2})/2 + \sqrt{T/8}\, z_3,\\ W_{3T/4} &= (W_{T/2} + W_T)/2 + \sqrt{T/8}\, z_4,\\ &\;\;\vdots\\ W_{(d-1)T/d} &= (W_{(d-2)T/d} + W_T)/2 + \sqrt{T/(2d)}\, z_d. \end{aligned} \tag{36}$$

This leads to a matrix A different to that obtained from the Cholesky factorization. Note that the approach can be generalized to include unequal length intervals, allowing d to be not a power of 2.

- In the *principal components construction*, the matrix A is

$$A = [\sqrt{\lambda_1}\boldsymbol{\eta}_1, \sqrt{\lambda_2}\boldsymbol{\eta}_2, \ldots, \sqrt{\lambda_d}\boldsymbol{\eta}_d],$$

where $\lambda_1, \ldots, \lambda_d$ are the eigenvalues of C in non-increasing order and $\boldsymbol{\eta}_1, \ldots, \boldsymbol{\eta}_d$ are the corresponding eigenvectors normalized by $\boldsymbol{\eta}_\ell^{\mathrm{T}}\boldsymbol{\eta}_{\ell'} = \delta_{\ell\ell'}$ for $1 \le \ell, \ell' \le d$. Furthermore, we know the precise formulas for the eigenpairs (see, e.g., [8])

$$\lambda_\ell = \frac{T}{4d\,\sin^2(h_\ell)}, \qquad h_\ell = \frac{(2\ell-1)\pi}{2(2d+1)},$$

$$\boldsymbol{\eta}_\ell = \frac{2}{\sqrt{2d+1}}\left(\sin(2h_\ell), \sin(4h_\ell), \ldots, \sin(2dh_\ell)\right)^{\mathrm{T}}.$$

Thus

$$A_{j\ell} = \sqrt{\frac{T}{d(2d+1)\,\sin^2(h_\ell)}}\,\sin(2jh_\ell), \qquad h_\ell = \frac{(2\ell-1)\pi}{2(2d+1)}. \tag{37}$$

The final step in setting up the problem is to map the integral to the unit cube. The standard way of doing this is to introduce the cumulative normal integral $\Phi(\boldsymbol{z})$ as a new variable,

$$\boldsymbol{x} = \Phi(\boldsymbol{z}) := (\Phi(z_1), \ldots, \Phi(z_d))^{\mathrm{T}}, \quad \Phi(z) = \frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{z} e^{-\frac{1}{2}s^2}\,\mathrm{d}s.$$

(Note our slight abuse of notation here: Φ denotes both a function on $\mathbb{R}^d$ and a function on $\mathbb{R}$.) Under this transformation the integral (34) becomes

$$V = e^{-rT}\int_{[0,1]^d} G(\boldsymbol{S}(A\Phi^{-1}(\boldsymbol{x})))\,\mathrm{d}\boldsymbol{x}, \tag{38}$$

where $\Phi^{-1}(\boldsymbol{x}) := (\Phi^{-1}(x_1), \ldots, \Phi^{-1}(x_d))^{\mathrm{T}}$, with $\Phi^{-1} : [0,1] \to \mathbb{R}$ denoting the inverse function of $\Phi : \mathbb{R} \to [0,1]$.

5.2. Eliminating the unboundedness by truncation

As explained at the beginning of this section, we do not make the above-mentioned mapping to the unit cube here, since if we did so then none of our integrands would lie in $\mathcal{W}^1_{d,\infty}$, or even in $\mathcal{W}^0_{d,\infty}$. Instead we choose to split V by truncating the infinite integral of (34), writing

$$V = V_0 + R \tag{39}$$

where

$$V_0 = \frac{e^{-rT}}{(2\pi)^{d/2}}\int_{B_{\boldsymbol{q},d}} G(\boldsymbol{S}(A\boldsymbol{z}))\,e^{-\frac{1}{2}\boldsymbol{z}^{\mathrm{T}}\boldsymbol{z}}\,\mathrm{d}\boldsymbol{z},$$

with $B_{\boldsymbol{q},d} := \prod_{i=1}^d[-q_i, q_i]$ being a box of edge length $2q_i$ for $i = 1, \ldots, d$, centered at the origin, and $\boldsymbol{q} = (q_1, \ldots, q_d)$. Thus $V_0 = V_0(\boldsymbol{q})$ is the contribution to the integral from the box $B_{\boldsymbol{q},d}$ and $R = R(\boldsymbol{q})$ is the remainder.

Then with the transformation $\boldsymbol{y} = \Phi(\boldsymbol{z})$, we obtain, instead of (38),

$$V_0 = e^{-rT}\int_{b_{\boldsymbol{q},d}} G(\boldsymbol{S}(A\Phi^{-1}(\boldsymbol{y})))\,\mathrm{d}\boldsymbol{y}, \tag{40}$$

where $b_{\boldsymbol{q},d} = \prod_{i=1}^d[1-\Phi(q_i), \Phi(q_i)]$. On rescaling to the unit cube, that is, substituting $x_i - 1/2 = (y_i - 1/2)/(2\Phi(q_i) - 1)$ for each $i = 1, \ldots, d$, this can be written as

$$V_0 = e^{-rT}\int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

where

$$f(\boldsymbol{x}) \;:=\; f_{\boldsymbol{q}}(\boldsymbol{x}) \;=\; \left(\prod_{i=1}^{d}(2\Phi(q_i)-1)\right) G(\boldsymbol{S}(A\Theta_{\boldsymbol{q}}(\boldsymbol{x}))), \tag{41}$$

with

$$\Theta_{\boldsymbol{q}}(\boldsymbol{x}) \;:=\; (\Theta_{q_1}(x_1),\ldots,\Theta_{q_d}(x_d))^{\mathrm{T}}, \qquad \Theta_q(x) \;:=\; \Phi^{-1}((2\Phi(q)-1)x+1-\Phi(q)).$$

We note for future use that

$$\Theta_q'(x) \;=\; (2\Phi(q)-1)\,\sqrt{2\pi}\exp\left(\frac{1}{2}(\Theta_q(x))^2\right) \;>\; 0.$$

Thus $\Theta_q(x)$ is a monotone increasing function, with the values $-q$ at $x=0$ and q at $x=1$. The graph is simply a rescaled portion of the graph of Φ^{-1} that excludes the boundary singularities. Thus Θ_q is a $\mathcal{C}^\infty$ function on $[0,1]$.

We stress that the standard construction, the Brownian bridge construction, and the principal components construction discussed in Subsection 5.1 give different matrices A in the factorization of the covariance matrix $C = AA^{\mathrm{T}}$. Therefore the integrands (41) corresponding to the three construction methods are different, so a given variable x_i has a different role with different constructions. We now consider the different pay-offs mentioned in Subsection 5.1, and discuss the smoothness properties of the integrands and their ANOVA terms under different construction methods.

Example 12 (Arithmetic average Asian call option) For the case of (31), the integrand (41) can be written as

$$f(\boldsymbol{x}) \;=\; \phi(\boldsymbol{x})_+,$$

where

$$\phi(\boldsymbol{x}) \;=\; \left(\prod_{i=1}^{d}(2\Phi(q_i)-1)\right)\left(\frac{S_0}{d}\sum_{j=1}^{d}\exp\left(\left(r-\frac{\sigma^2}{2}\right)j\Delta t+\sigma\sum_{i=1}^{d}A_{ji}\Theta_{q_i}(x_i)\right)-K\right), \tag{42}$$

which is a $\mathcal{C}^\infty$ function on $[0,1]^d$. Its first partial derivatives are given by

$$(D_\ell\,\phi)(\boldsymbol{x}) \;=\; \left(\prod_{i=1}^{d}(2\Phi(q_i)-1)\right)\frac{\sigma S_0}{d}\,\beta_\ell(\boldsymbol{x})\,\Theta_{q_\ell}'(x_\ell), \quad \ell=1,\ldots,d,$$

with

$$\beta_\ell(\boldsymbol{x}) \;:=\; \sum_{j=1}^{d}\exp\left(\left(r-\frac{\sigma^2}{2}\right)\frac{j\,T}{d}+\sigma\sum_{i=1}^{d}A_{ji}\Theta_{q_i}(x_i)\right)A_{j\ell}.$$

Since $\Theta_q'(x)>0$ for all $x\in[0,1]$, the sign of $(D_\ell\,\phi)(\boldsymbol{x})$ depends on the sign of $\beta_\ell(\boldsymbol{x})$.

For the standard construction and the Brownian bridge construction, the elements $A_{j\ell}$ of the matrix A are always nonnegative. Thus $\beta_\ell(\boldsymbol{x})>0$ and so $(D_\ell\,\phi)(\boldsymbol{x})>0$ for all $\ell=1,\ldots,d$ and all $\boldsymbol{x}\in[0,1]^d$. Hence Theorem 7 applies with $\mathbf{z}=\mathfrak{D}$, that is, we have $f\in\mathcal{W}_{d,\infty}^{1}$ and

$$f_{\mathbf{u}} \;\in\; \mathcal{W}_{\mathbf{u},\infty}^{1+d-|\mathbf{u}|} \qquad \text{for all} \quad \mathbf{u}\subseteq\mathfrak{D}.$$

For the principal components construction of the matrix A the elements A_{j1} are positive, so that $\beta_1(\boldsymbol{x})>0$, but for $\ell\ge 2$ the elements $A_{j\ell}$ take both positive and negative signs. Thus negative values of $\beta_\ell(\boldsymbol{x})$, and hence of $(D_\ell\,\phi)(\boldsymbol{x})$, are possible. It may be that in some cases $\beta_\ell(\boldsymbol{x})$, and hence $(D_\ell\,\phi)(\boldsymbol{x})$, will change sign in the domain $[0,1]^d$. Nevertheless, Theorem 7 applies and we have

$$f_{\mathbf{u}} \;\in\; \mathcal{W}_{\mathbf{u},\infty}^{1+|\mathbf{z}\setminus\mathbf{u}|} \qquad \text{for all} \quad \mathbf{u}\subseteq\mathfrak{D},$$

with $\mathbf{z}$ denoting the set of the indices ℓ such that $D_\ell\,\phi$ is never zero.

Example 13 (Binary Arithmetic average Asian call option) For the case of (33), the integrand (41) can be written as

$$f(\boldsymbol{x}) \;=\; \eta(\boldsymbol{x})\,\phi(\boldsymbol{x})_{\#},$$

with ϕ given as in (42) and $\eta(\boldsymbol{x}) = \phi(\boldsymbol{x})/(\prod_{i=1}^{d}(2\Phi(q_i)-1))+K$. Thus Theorem 11 applies and $f \in \mathcal{W}^{0}_{d,\infty}$. For the standard and the Brownian bridge constructions, we have

$$f_{\mathbf{u}} \;\in\; \mathcal{W}^{d-|\mathbf{u}|}_{\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D}.$$

For the principal components construction, we have

$$f_{\mathbf{u}} \;\in\; \mathcal{W}^{|\mathbf{z}\setminus\mathbf{u}|}_{\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D},$$

with $\mathbf{z}$ denoting the set of the indices ℓ such that $D_\ell\,\phi$ is never zero.

Example 14 (Geometric average Asian call option) For the case of (32), the integrand (41) can be written as

$$f(\boldsymbol{x}) \;=\; \phi(\boldsymbol{x})_{+},$$

where

$$\begin{aligned}
\phi(\boldsymbol{x}) \;&=\; \left(\prod_{i=1}^{d}(2\Phi(q_i)-1)\right)\left(\prod_{j=1}^{d}\left[S_0\exp\left(\left(r-\frac{\sigma^2}{2}\right)j\Delta t+\sigma\sum_{i=1}^{d}A_{ji}\Theta_{q_i}(x_i)\right)\right]^{1/d}-K\right)\\
&=\; \left(\prod_{i=1}^{d}(2\Phi(q_i)-1)\right)\left(S_0\exp\left(\left(r-\frac{\sigma^2}{2}\right)\frac{(d+1)\,\Delta t}{2}+\frac{\sigma}{d}\sum_{i=1}^{d}\left(\sum_{j=1}^{d}A_{ji}\right)\Theta_{q_i}(x_i)\right)-K\right),
\end{aligned}$$

which is a $\mathcal{C}^\infty$ function on $[0,1]^d$. Its first partial derivatives are given by

$$\begin{aligned}
(D_\ell\,\phi)(\boldsymbol{x}) \;&=\; \left(\prod_{i=1}^{d}(2\Phi(q_i)-1)\right)\frac{\sigma S_0}{d}\left(\sum_{j=1}^{d}A_{j\ell}\right)\Theta'_{q_\ell}(x_\ell)\\
&\qquad\times\exp\left(\left(r-\frac{\sigma^2}{2}\right)\frac{(d+1)\,\Delta t}{2}+\frac{\sigma}{d}\sum_{i=1}^{d}\left(\sum_{j=1}^{d}A_{ji}\right)\Theta_{q_i}(x_i)\right).
\end{aligned}$$

Thus the sign of $(D_\ell\,\phi)(\boldsymbol{x})$ depends on the sign of $\sum_{j=1}^{d}A_{j\ell}$, which is the sum of the ℓth column of the matrix A, and is independent of $\boldsymbol{x}$. We conclude that there can be no change of sign in $(D_\ell\,\phi)(\boldsymbol{x})$. Clearly this sum is positive for the standard and the Brownian bridge constructions, since all elements of the matrix A are nonnegative. For the principal components construction, we have from (37)

$$\sum_{j=1}^{d}A_{j\ell} \;=\; \sqrt{\frac{T}{d(2d+1)\,\sin^2(h_\ell)}}\;\sum_{j=1}^{d}\sin(2jh_\ell).$$

Now with $u := 2h_\ell = (2\ell-1)\pi/(2d+1)$ and $\mathrm{i}=\sqrt{-1}$, we have

$$\begin{aligned}
\sum_{j=1}^{d}\sin(j\,u) \;&=\; \sum_{j=1}^{d}\frac{e^{\mathrm{i}ju}-e^{-\mathrm{i}ju}}{2\,\mathrm{i}} \;=\; \frac{1}{2\,\mathrm{i}}\left(\frac{1-e^{\mathrm{i}u(d+1)}}{1-e^{\mathrm{i}u}}-\frac{1-e^{-\mathrm{i}u(d+1)}}{1-e^{-\mathrm{i}u}}\right)\\
&=\; \frac{1}{2\,\mathrm{i}}\left(\frac{e^{-\mathrm{i}u/2}-e^{\mathrm{i}u(d+1/2)}}{e^{-\mathrm{i}u/2}-e^{\mathrm{i}u/2}}-\frac{e^{\mathrm{i}u/2}-e^{-\mathrm{i}u(d+1/2)}}{e^{\mathrm{i}u/2}-e^{-\mathrm{i}u/2}}\right)\\
&=\; \frac{1}{2\,\mathrm{i}}\,\frac{\left(e^{\mathrm{i}u(d+1)/2}-e^{-\mathrm{i}u(d+1)/2}\right)\left(e^{\mathrm{i}ud/2}-e^{-\mathrm{i}ud/2}\right)}{e^{\mathrm{i}u/2}-e^{-\mathrm{i}u/2}}\\
&=\; \frac{\sin\left(u\frac{d+1}{2}\right)\,\sin\left(u\frac{d}{2}\right)}{\sin\left(\frac{u}{2}\right)}\\
&=\; \frac{\sin\left((2\ell-1)\frac{d+1}{2d+1}\frac{\pi}{2}\right)\,\sin\left((2\ell-1)\frac{d}{2d+1}\frac{\pi}{2}\right)}{\sin\left(\frac{2\ell+1}{2d+1}\frac{\pi}{2}\right)},
\end{aligned}$$

which is not zero for all $\ell = 1,\dots,d$ because both d and $d+1$ are relatively prime to $2d+1$, and as a result in the arguments of the sine function in the numerator we never have an integer multiple of π. Hence Theorem 7 applies with $\mathbf{z} = \mathfrak{D}$, the best case. That is, we have $f \in \mathcal{W}^1_{d,\infty}$ and

$$f_{\mathbf{u}} \in \mathcal{W}^{1+d-|\mathbf{u}|}_{\mathbf{u},\infty} \qquad \text{for all} \quad \mathbf{u} \subseteq \mathfrak{D}$$

for all three construction methods. This is in contrast to the arithmetic Asian option for which we were unable to show $\mathbf{z} = \mathfrak{D}$ for the principal components construction.

5.3. Estimating the remainder

Here we obtain an upper bound on the option price remainder R given by (38), (39) and (40), that is

$$R = e^{-rT} \int_{[0,1]^d \setminus b_{\boldsymbol{q},d}} G(\boldsymbol{S}(A\Phi^{-1}(\boldsymbol{x})))\,\mathrm{d}\boldsymbol{x} = \frac{e^{-rT}}{(2\pi)^{d/2}} \int_{\mathbb{R}^d \setminus B_{\boldsymbol{q},d}} G(\boldsymbol{S}(A\boldsymbol{z}))\, e^{-\frac{1}{2}\boldsymbol{z}^{\mathrm{T}}\boldsymbol{z}}\,\mathrm{d}\boldsymbol{z}.$$

Throughout this subsection, we will assume that we have a general pay-off which satisfies

$$G(\boldsymbol{S}) \le \frac{1}{d}\sum_{j=1}^d S_j. \tag{43}$$

This is clearly true for the binary arithmetic average Asian call option (33). For the arithmetic average Asian call option (31), we have

$$G(\boldsymbol{S}) = \left(\frac{1}{d}\sum_{j=1}^d S_j - K\right)_+ \le \left(\frac{1}{d}\sum_{j=1}^d S_j\right)_+ = \frac{1}{d}\sum_{j=1}^d S_j.$$

The bound also holds for the geometric average Asian call option (32), since the geometric average is always less than or equal to the arithmetic average.

From (43) we have

$$G(\boldsymbol{S}(A\boldsymbol{z})) \le \frac{1}{d}\sum_{j=1}^d S_0 \exp\left(\left(r - \frac{\sigma^2}{2}\right) j\Delta t + \sigma \sum_{i=1}^d A_{ji} z_i\right),$$

giving

$$R \le \frac{S_0}{d}\sum_{j=1}^d \exp\left(-r(T - j\Delta t) - \frac{\sigma^2}{2} j\Delta t\right) \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d \setminus B_{\boldsymbol{q},d}} \exp\left(\sum_{i=1}^d \left(\sigma A_{ji} z_i - \frac{z_i^2}{2}\right)\right) \mathrm{d}\boldsymbol{z}.$$

Now we complete the square in the exponent inside the integral, giving

$$\sum_{i=1}^d \left(\sigma A_{ji} z_i - \frac{z_i^2}{2}\right) = -\frac{1}{2}\sum_{i=1}^d (z_i - \sigma A_{ji})^2 + \frac{\sigma^2}{2}\sum_{i=1}^d A_{ji}^2,$$

where we have, since $AA^{\mathrm{T}} = C$,

$$\sum_{i=1}^d A_{ji}^2 = (AA^{\mathrm{T}})_{jj} = C_{jj} = t_j = j\Delta t.$$

Hence

$$\begin{aligned} R &\le \frac{S_0}{d}\sum_{j=1}^d e^{-r(T-j\Delta t)} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d \setminus B_{\boldsymbol{q},d}} \exp\left(-\frac{1}{2}\sum_{i=1}^d (z_i - \sigma A_{ji})^2\right) \mathrm{d}\boldsymbol{z} \\ &\le S_0 \left(1 - \frac{1}{d}\sum_{j=1}^d \prod_{i=1}^d \frac{1}{\sqrt{2\pi}} \int_{-q_i}^{q_i} \exp\left(-\frac{1}{2}(z_i - \sigma A_{ji})^2\right) \mathrm{d}z_i\right), \end{aligned}$$

where we used the estimate $e^{-r(T-j\Delta t)} \le 1$. This leads to the following result.

Theorem 15 *Let R denote the remainder due to the truncation of the domain for an option pricing problem where the pay-off satisfies* (43). *Then we have the estimate*

$$R \leq S_0 \left(1 - \frac{1}{d} \sum_{j=1}^{d} \prod_{i=1}^{d} \left(\Phi(q_i - \sigma A_{ji}) - \Phi(-q_i - \sigma A_{ji}) \right) \right).$$

Given $\boldsymbol{q}$ and the matrix A, it is easy to compute this upper bound. However, from a practical point of view, we would like to use this upper bound to help in choosing the numbers q_i so that a certain accuracy is guaranteed, e.g., for a given $\varepsilon > 0$ we want

$$R \leq \varepsilon S_0.$$

Consider the function $w(u) := \Phi(q-u) - \Phi(-q-u)$. We can easily verify that for all $u \in \mathbb{R}$, $w(u) > 0$ as long as $q > 0$, $w(-u) = w(u)$, and $w'(u) < 0$ for $u \neq 0$. This indicates that $w(u)$ is minimized when $|u|$ is as large as possible. Thus the upper bound in Theorem 15 can be overestimated by

$$R \leq S_0 \left(1 - \prod_{i=1}^{d} \left(\Phi(q_i - \sigma M_i) - \Phi(-q_i - \sigma M_i) \right) \right), \quad \text{with} \quad M_i \geq \max_{1 \leq j \leq d} |A_{ji}|, \tag{44}$$

that is, M_i is an upper bound to the largest value in magnitude in the ith column of the matrix A.

For the standard construction, clearly we see from (35) that we may take

$$M_i = \sqrt{\Delta t} = \sqrt{\frac{T}{d}}.$$

For the Brownian bridge construction, we may take

$$M_1 = \sqrt{T}, \quad M_2 = \sqrt{\frac{T}{4}}, \quad M_3 = \sqrt{\frac{T}{8}}, \quad M_4 = \sqrt{\frac{T}{8}}, \quad \ldots \quad M_d = \sqrt{\frac{T}{2d}}.$$

The reasoning is that, although the variable z_i occurs both explicitly and implicitly in (36), the largest matrix coefficient occurs at the first (explicit) entry of the variable. It is this largest coefficient of z_i that we need to take as M_i. For the principal components construction, we see from (37) that we may take

$$M_i = \sqrt{\frac{T}{d(2d+1)\,\sin^2(h_i)}}, \qquad h_i = \frac{(2i-1)\pi}{2(2d+1)}.$$

Then $R \leq \varepsilon S_0$ can be achieved by choosing the numbers q_i so that each factor in the product in (44) satisfies

$$\Phi(q_i - \sigma M_i) - \Phi(-q_i - \sigma M_i) \geq (1-\varepsilon)^{1/d} \qquad \text{for all} \quad i = 1, \ldots, d.$$

Since $\Phi(q-u) - \Phi(-q-u) = \Phi(q-u) + \Phi(q+u) - 1 \geq 2\,\Phi(q-u) - 1$, it is sufficient that we take the numbers q_i such that

$$2\,\Phi(q_i - \sigma M_i) - 1 \geq (1-\varepsilon)^{1/d} \qquad \text{for all} \quad i = 1, \ldots, d.$$

This leads to the following theorem.

Theorem 16 *Consider an option pricing problem where the pay-off satisfies* (43). *For a given $\varepsilon > 0$ and a chosen method for factorizing the covariance matrix $C = AA^{\mathrm{T}}$, the choice $\boldsymbol{q} = (q_1, \ldots, q_d)$, with*

$$q_i \geq \Phi^{-1}\left(\frac{(1-\varepsilon)^{1/d} + 1}{2} \right) + \sigma M_i \qquad \textit{for all} \quad i = 1, \ldots, d,$$

and $M_i \geq \max_{1 \leq j \leq d} |A_{ji}|$, ensures that the remainder $R = R(\boldsymbol{q})$ due to the truncation of the domain $\mathbb{R}^d$ to the box $B_{\boldsymbol{q},d}$ satisfies $R \leq \varepsilon S_0$.

Table 1: $\Phi^{-1}(\frac{(1-\varepsilon)^{1/d}+1}{2})$ for a few choices of ε and d

$\varepsilon \setminus d$	1	2	3	4	5	10	50	100	200
0.1	1.64	1.95	2.11	2.23	2.31	2.56	3.08	3.28	3.47
0.01	2.58	2.81	2.93	3.02	3.09	3.29	3.72	3.89	4.05
0.001	3.29	3.48	3.59	3.66	3.72	3.89	4.26	4.42	4.56
0.0001	3.89	4.06	4.15	4.21	4.26	4.42	4.75	4.89	5.02

Table 2: Cutoff values q_i (rounded *up* to 2 decimal places) corresponding to $\varepsilon = 0.01$

q_i	$d=2$		$d=4$			
Standard	2.95	2.95	3.13	3.13	3.13	3.13
Brownian bridge	3.01	2.91	3.23	3.13	3.10	3.10
Principal components	3.02	2.89	3.22	3.09	3.07	3.06

Table 1 contains some values of $\Phi^{-1}(\frac{(1-\varepsilon)^{1/d}+1}{2})$. We shall make use of entries in this table in our numerical experiments.

We remark that the result of this subsection can be easily generalized by replacing the assumption (43) with

$$G(\boldsymbol{S}) \,\le\, \frac{C_d}{d}\sum_{j=1}^{d} S_j,$$

where C_d is some constant which may depend on d, S_0, K, r, σ, but it does *not* depend on the stock prices $S_1,\ldots,S_d$. Then we should replace $(1-\varepsilon)^{1/d}$ in Theorem 16 by $(1-\varepsilon/C_d)^{1/d}$. This allows us to deal with a larger class of options: for example, for the pay-off $G(\boldsymbol{S}) = (\max_{1\le j\le d} S_j - K)_+$ we can take $C_d = d$.

6. Numerical results

We consider the arithmetic average Asian call option (Example 12) and the binary arithmetic average Asian call option (Example 13), combined with the standard construction (35), the Brownian bridge construction (36), and the principal components construction (37). We use the parameters

$$S_0 = 100, \quad \sigma = 0.2, \quad r = 0.1, \quad T = 1, \quad \text{and} \quad K = 100.$$

Since our purpose is to illustrate the smoothing process rather than to price options, we restrict ourselves to $d = 2$ and $d = 4$.

Taking $\varepsilon = 0.01$ in Theorem 16 (and thus ensuring that the truncation error is no more than 1% of the initial price), we present in Table 2 the values q_i for the three construction methods.

Figure 1. In the top row of Figure 1 we plot the integrand f, see (41), for the arithmetic average Asian call option with $d = 2$ and the three construction methods, using the cutoff values q_i given in Table 2. The kink in the integrand is clearly visible. We observe that the kink appears to straighten out when we switch from the standard construction over the Brownian bridge construction to the principal components construction. Furthermore, we note that the kink for the principal components construction is almost a straight line and nearly parallel to an axis. For the principal components construction, $(D_2\phi)(\boldsymbol{x})$ changes sign in the domain $[0,1]^2$ and thus Theorem 7 applies with $\mathbf{z} = \{1\}$. For the standard and Brownian bridge constructions, Theorem 7 applies with $\mathbf{z} = \{1,2\}$.

We show in the next three rows the two-dimensional ANOVA term $f_{\{1,2\}}$ and the one-dimensional ANOVA terms $f_{\{1\}}$ and $f_{\{2\}}$ for the three construction methods. We see that, while $f_{\{1,2\}}$ still has a kink, the lower-order ANOVA terms $f_{\{1\}}$ and $f_{\{2\}}$ appear smooth, with the exception of $f_{\{1\}}$ having an apparent kink point under the principal components construction, which is consistent with Theorem 7. Observe also that the use of a specific construction method influences the size of the ANOVA term $f_{\{2\}}$: there is a decay in magnitude from approximately 24 over 14 to 4 for the different constructions.

In the bottom two rows we plot the first derivative of the one-dimensional ANOVA terms $f_{\{1\}}$ and $f_{\{2\}}$. Clearly, the derivatives appear to be smooth functions, with the exception of $f'_{\{1\}}$ under the principal components construction.

Figure 2. Next we consider the case of the arithmetic average Asian call option with $d = 4$. In Figure 2 we display the (x_1, x_2)-projection of the integrand f at $x_3 = x_4 = 0.5$ and the four one-dimensional ANOVA terms $f_{\{1\}}$, $f_{\{2\}}$, $f_{\{3\}}$ and $f_{\{4\}}$ for the three construction methods. We observe again that the one-dimensional ANOVA terms appear smooth, with the exception of $f_{\{1\}}$ under the principal components construction. This is consistent with Theorem 7, since for the principal components construction $(D_2\phi)(\boldsymbol{x})$, $(D_3\phi)(\boldsymbol{x})$, and $(D_4\phi)(\boldsymbol{x})$ all change sign in the domain $[0,1]^4$. We also observe for $f_{\{2\}}$, $f_{\{3\}}$ and $f_{\{4\}}$ a similar decay in scale to that in the case $d = 2$ when switching from the standard construction to the Brownian bridge construction and then to the principal components construction.

Figure 3. Finally we consider the binary arithmetic average Asian call option with $d = 2$. We produce in Figure 3 plots similar to those in Figure 1. The location of the kink is exactly as in Figure 1, but the nature of the singularity in f is different: now it is a jump discontinuity (see the top row). It follows from Theorem 11 that $f_{\{1,2\}}$ should inherit the jump from f, while $f_{\{1\}}$ and $f_{\{2\}}$ should be smooth, with the exception of $f_{\{1\}}$ under the principal components construction.

In all our figures, the integrals in the ANOVA terms were approximated using $50,000$ Sobol′ points. (An increase to $100,000$ points makes no noticeable difference, and thus we are confident that the quadrature error is sufficiently small.) The derivatives were approximated via a standard central difference formula using 100 points in each direction. Since the graphics package interpolates linearly over the data points, the kink or the jump may not always be visible in the plots.

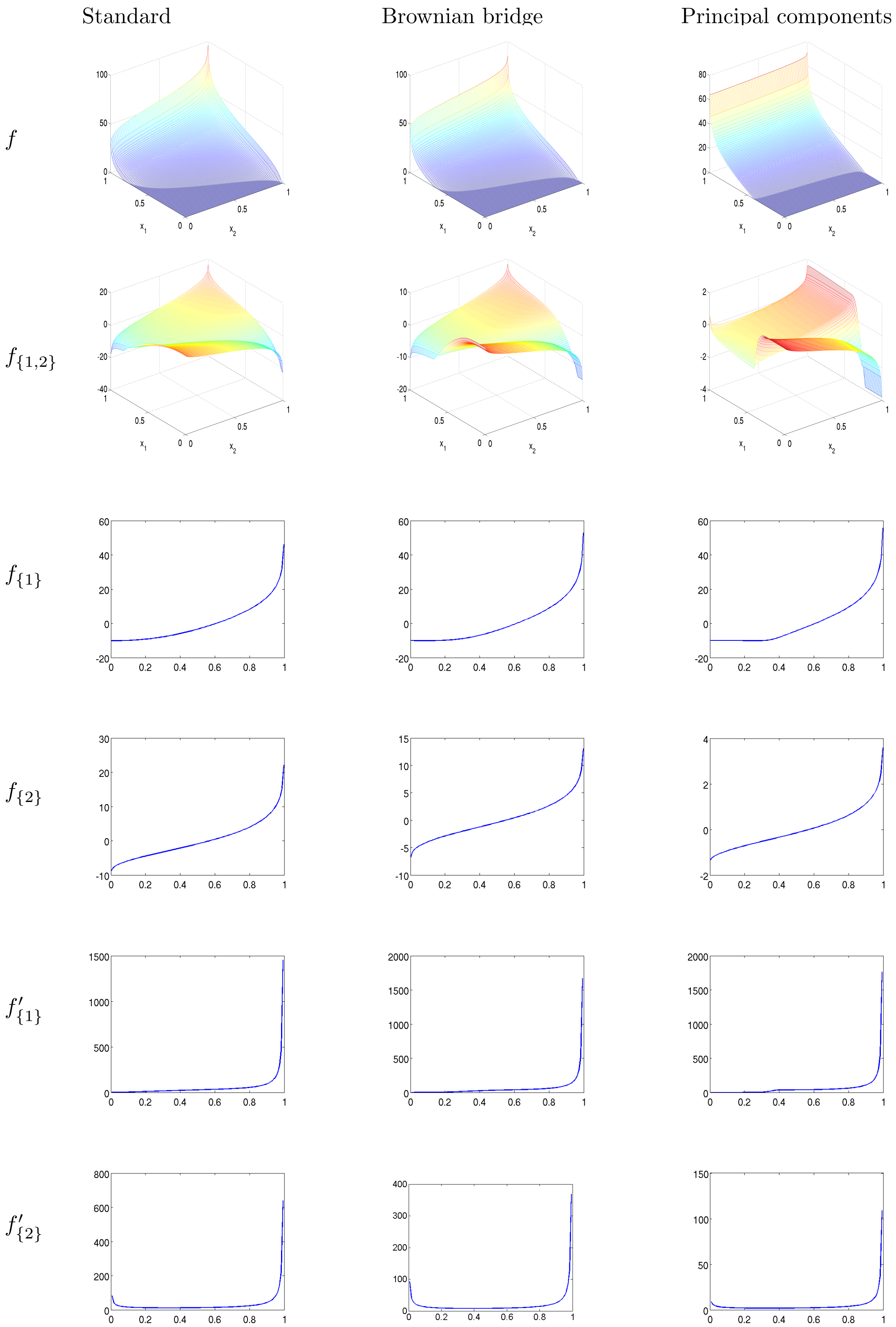

Figure 1: The integrand, its ANOVA terms, and their derivatives for the arithmetic average Asian call option with $d = 2$ and the three construction methods.

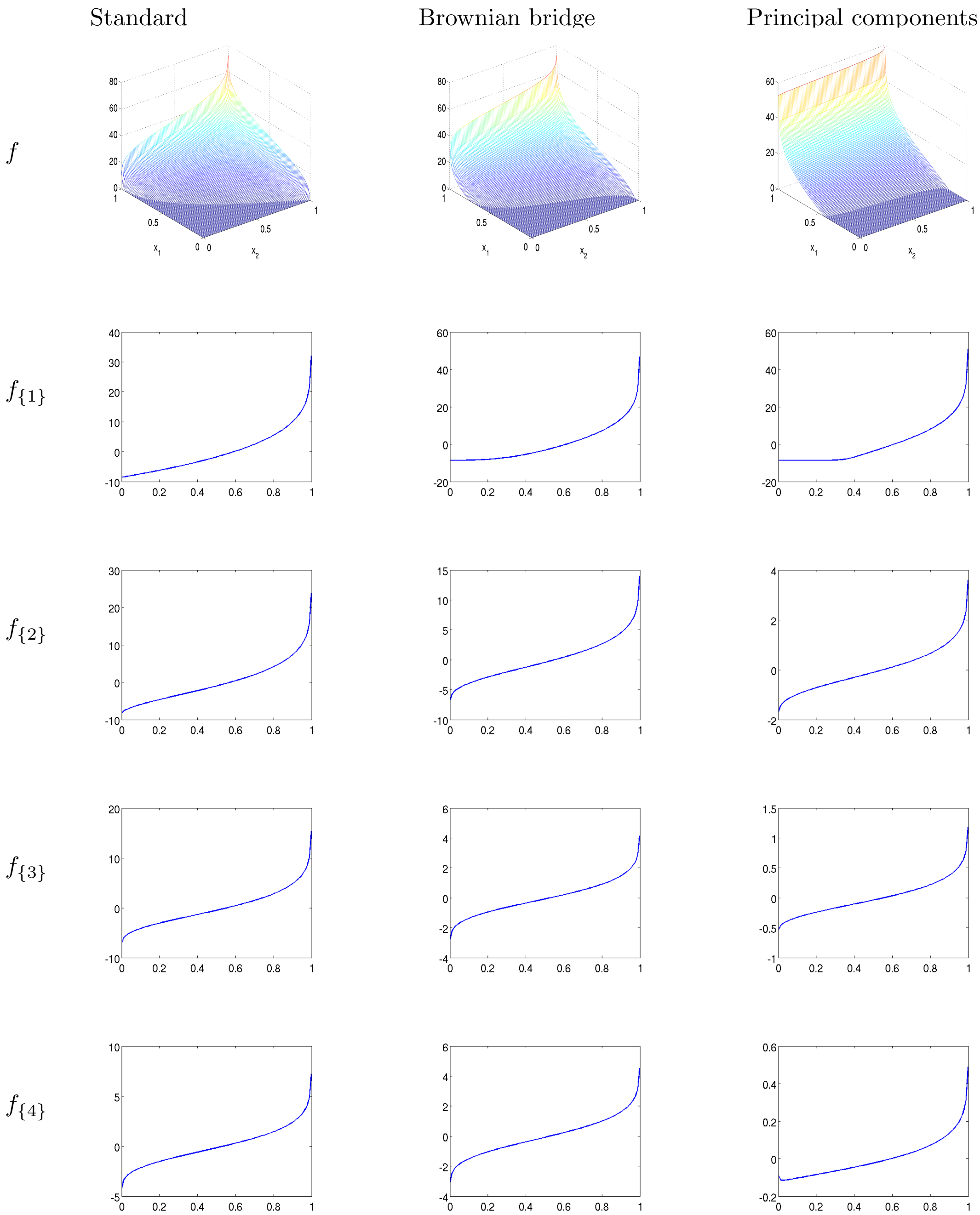

Figure 2: (x_1, x_2)-projection of the integrand at $x_3 = x_4 = 0.5$ and some ANOVA terms for the arithmetic average Asian call option with $d = 4$ and the three construction methods.

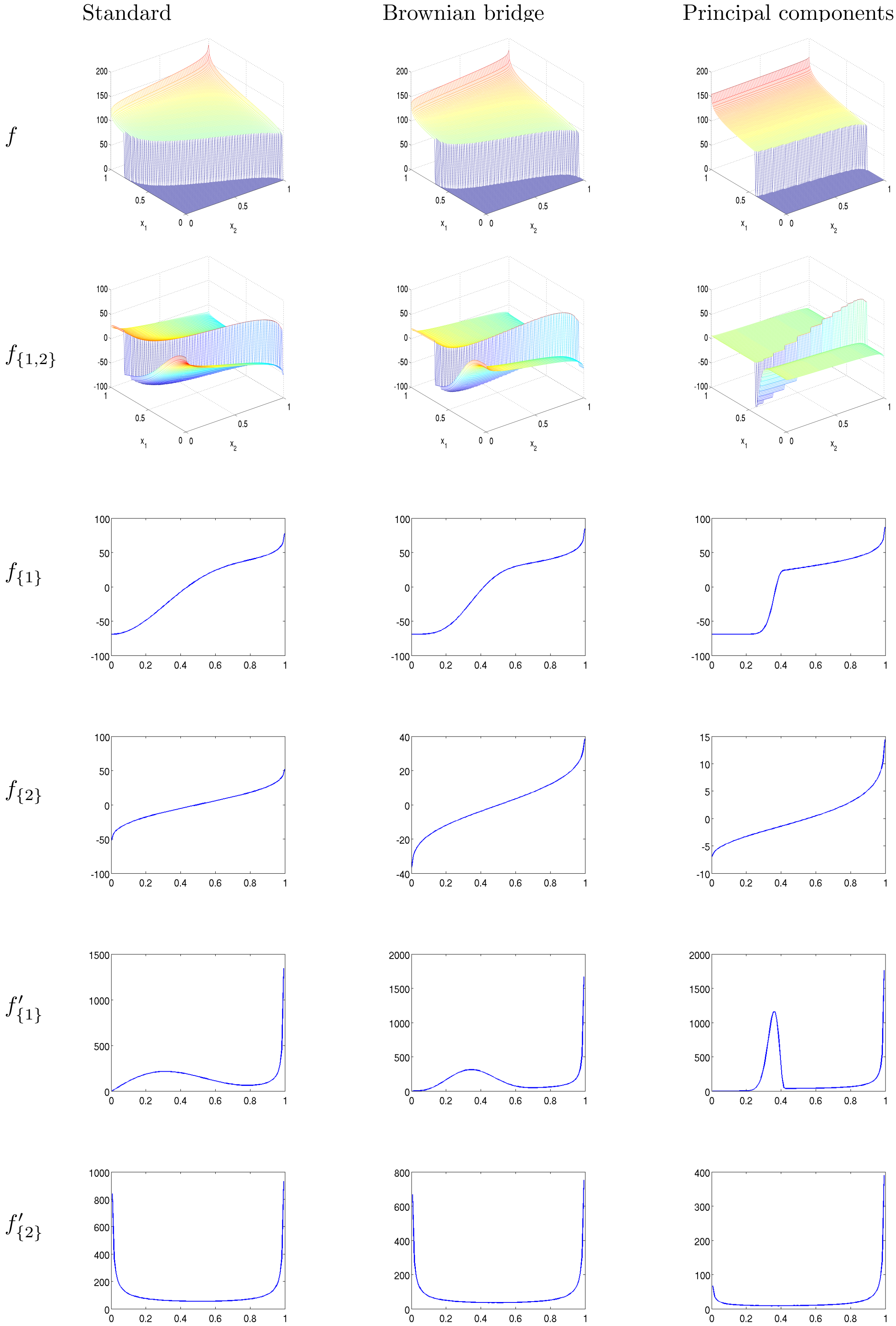

Figure 3: The integrand, its ANOVA terms, and their derivatives for the *binary* arithmetic average Asian call option with $d = 2$ and the three construction methods.

7. Concluding remarks

In this paper we gave precise results on the smoothness properties of the ANOVA terms for integrands characterized by single kinks or jumps as they typically arise in option pricing problems. The ANOVA decomposition indeed results in smooth lower-order terms as long as the kink- or jump-manifold is not parallel to an axis. This may explain, at least in part, why quadrature rules like quasi-Monte Carlo (QMC) methods and sparse grid (SG) techniques are successful for option pricing problems. Indeed, for an integration problem

$$I_d f \;=\; \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

and quadrature rules of the form

$$Q_{n,d} f \;=\; \sum_{i=1}^{n} \alpha_i f(\boldsymbol{x}_i)$$

with weights α_i and evaluation points $\boldsymbol{x}_i$, the quadrature error can be written with the help of the ANOVA decomposition (2) of f as

$$(I_d - Q_{n,d})f \;=\; (I_d - Q_{n,d})\bigg(\sum_{\mathbf{u}\subseteq\mathfrak{D}} f_{\mathbf{u}}(\boldsymbol{x}_{\mathbf{u}})\bigg) \;=\; \sum_{\mathbf{u}\subseteq\mathfrak{D}} (I_d f_{\mathbf{u}} - Q_{n,d} f_{\mathbf{u}}) \;=:\; \sum_{\mathbf{u}\subseteq\mathfrak{D}} e_{\mathbf{u}},$$

i.e., we have a sum of error contributions $e_{\mathbf{u}}$ where the d-dimensional integral and the d-dimensional quadrature rule, projected onto a $|\mathbf{u}|$-dimensional cube, are applied to the different ANOVA terms $f_{\mathbf{u}}$ of f. The larger smoothness of the lower-order terms is exploited implicitly by the QMC methods and SG techniques, while the contribution from the non-smooth higher-order terms might be small enough to be neglected, if the superposition dimension of the option pricing problem is small, as suggested by [5].

More precisely, we showed that the lower-order half of the ANOVA terms of the integrand arising from pricing the arithmetic Asian option under both the standard and Brownian bridge constructions belong to $\mathcal{W}^{(1,\ldots,1)}_{d,\infty,\mathrm{mix}}$ (see Corollary 8(ii)), which is contained in the Sobolev space $\mathcal{W}^{(1,\ldots,1)}_{d,2,\mathrm{mix}}$ that is typically considered in the theoretical analysis of QMC methods. Thus the existing theory on QMC error bounds can be applied to these lower-order ANOVA terms. In a similar way, the lower-order one-third of the ANOVA terms belong to $\mathcal{W}^{(2,\ldots,2)}_{d,\infty,\mathrm{mix}}$, and so on. It might be possible to exploit this higher smoothness using higher-order SG techniques and the recent higher-order QMC methods [6, 7]. Further work is needed in this direction.

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