On efficient weighted integration via a change of variables

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Abstract

In this paper, we study the approximation of d-dimensional ϱ-weighted integrals over unbounded domains $\mathbb{R}_+^d$ or $\mathbb{R}^d$ using a special change of variables, so that quasi-Monte Carlo (QMC) or sparse grid rules can be applied to the transformed integrands over the unit cube. We consider a class of integrands with bounded L_p norm of mixed partial derivatives of first order, where $p \in [1, +\infty]$.

The main results give sufficient conditions on the change of variables ν which guarantee that the transformed integrand belongs to the standard Sobolev space of functions over the unit cube with mixed smoothness of order one. These conditions depend on ϱ and p.

The proposed change of variables is in general different than the standard change based on the inverse of the cumulative distribution function. We stress that the standard change of variables leads to integrands over a cube; however, those integrands have singularities which make the application of QMC and sparse grids ineffective. Our conclusions are supported by numerical experiments.

1 Introduction

We consider in this paper the approximation of d-variate ϱ_d-weighted integrals of the form

$$I_{d,\varrho}(f) = \int_{D^d} f(\boldsymbol{x})\, \varrho_d(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}, \quad \text{where} \quad \varrho_d(\boldsymbol{x}) = \prod_{j=1}^{d} \varrho(x_j), \tag{1}$$

over an unbounded domain D^d, where

$$D = \mathbb{R}_+ \quad \text{or} \quad D = \mathbb{R}$$

and for a given probability density function

$$\varrho : D \to \mathbb{R}_+.$$

Such integrals in the univariate case are often approximated by Gaussian quadratures that enjoy exponential rate of convergence, see, e.g., [1]. There are also generalized Gaussian rules, see, e.g., [4] and the papers cited there, that achieve exponential rate for integrands with

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singularities at infinity. We stress that those results are about the asymptotic behavior of the integration error and require analytic integrands. In the current paper, we consider integrands of regularity one only, and we analyze the worst case error with respect to a class of integrands.

Indeed, we follow the *Information-Based Complexity* approach (see, e.g., [10]) providing worst case results for all integrands f from the Sobolev space $F_{d,p}(D^d)$ of functions defined on D^d with mixed partial derivatives of first order bounded in the standard $L_p(D^d)$ space, where $p \in [1, +\infty]$. As will be clear later, our results may also be applied to γ-weighted spaces of ∞-variate functions (i.e., $d = +\infty$) as well as for ϱ_d being a product of different probability densities (i.e., $\varrho(\boldsymbol{x}) = \prod_{j=1}^{d} \varrho_j(x_j)$).

The spaces $F_{d,p}(D^d)$ have been considered in a number of papers, and they are naturally related to the Sobolev spaces $W_{d,p}(B^d)$ of functions on a unit cube B^d with mixed partial first order derivatives in $L_p(B^d)$. Indeed, a quite common approach is to use the change of variables $x := \Phi_{\varrho}^{-1}(t)$, where Φ_{ϱ} is the *cumulative distribution function (CDF)* for the probability density ϱ, to reduce the ϱ-weighted integrals over D^d to the standard Lebesgue integration over a unit cube B^d, and next apply algorithms that are efficient for spaces $W_{d,p}(B^d)$. However, as we will show, such an approach is well founded for only $p = 1$, since for $p > 1$ the change of variables based on the inverse of the CDF produces integrands with boundary singularities, and so they **do not** belong to the spaces $W_{d,p}(B^d)$.

To simplify the notation, we will denote $W_{d,p}(B^d)$ and $F_{d,p}(D^d)$, respectively, by

$$W_{d,p} \quad \text{and} \quad F_{d,p}.$$

We investigate changes of variables that transform the weighted integrals $I_{d,\varrho}(f)$ over unbounded D^d into standard Lebesgue integrals over a bounded cube B^d:

$$I_d(g_{f,\nu}) \;=\; \int_{B^d} g_{f,\nu}(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t} \quad \text{with} \quad g_{f,\nu}(\boldsymbol{t}) \;=\; f(\nu(t_1),\ldots,\nu(t_d)) \prod_{j=1}^{d} \left(\varrho(\nu(t_j))\,\nu'(t_j)\right).$$

We are searching for *change of variables functions* $\nu : B \to D$ such that the obtained integrands satisfy

$$g_{f,\nu} \;\in\; W_{d,p} \quad \text{for all } f \;\in\; F_{d,p}. \tag{2}$$

We now explain the significance of the requirement (2). If the integrands $g_{f,\nu}$ satisfy (2), then their integrals can be approximated by cubatures that are known to have small worst case errors with respect to the spaces $W_{d,p}$, including *quasi-Monte Carlo (QMC)* and *sparse grid* methods. This in turn provides efficient cubatures for the original ϱ_d-weighted integration over unbounded D^d. More precisely, let

$$\mathrm{error}(Q_{d,n}; W_{d,p}) \;=\; \sup_{g \in W_{d,p}} \frac{\left|\int_{B^d} g(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t} - Q_{d,n}(g)\right|}{\|g\|_{W_{d,p}}}$$

be the worst case error of a cubature $Q_{d,n}$. Then the cubature $Q_{d,\varrho,n}$ for the weighted integrals $I_{d,\varrho}$ over unbounded domains D^d, given by

$$Q_{d,\varrho,n}(f) \;:=\; Q_{d,n}(g_{f,\nu}), \tag{3}$$

has the worst case error

$$\mathrm{error}(Q_{d,\varrho,n}; F_{d,p}) \;=\; \sup_{f \in F_{d,p}} \frac{|I_{d,\varrho}(f) - Q_{d,\varrho,n}(f)|}{\|f\|_{F_{d,p}}},$$

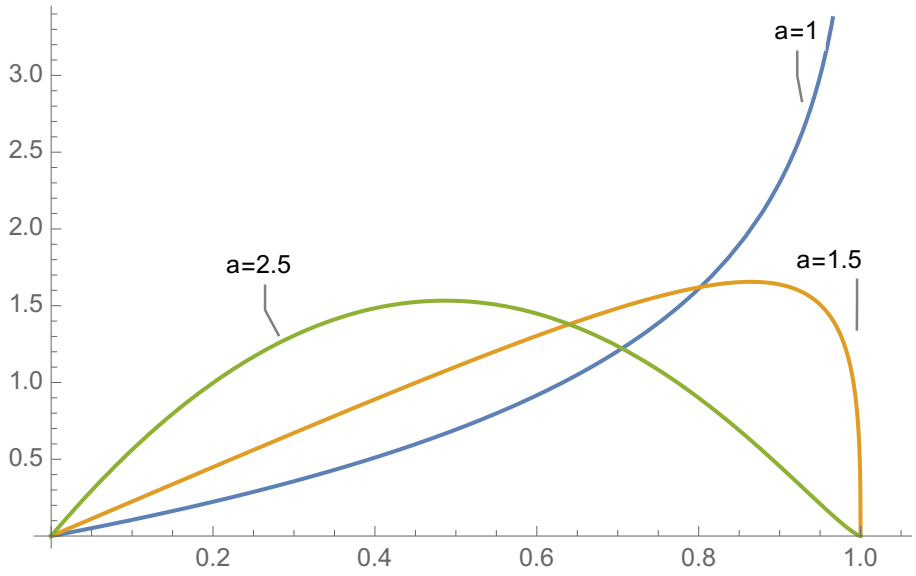

Figure 1: Plot of $g_{f,\nu_a}(t) = -a^2(\ln(1-t))(1-t)^{a-1}$ for $a \in \{1, 1.5, 2.5\}$.

bounded by

$$\text{error}(Q_{d,\varrho,n}; F_{d,p}) \;\le\; \text{error}(Q_{d,n}; W_{d,p}) \;\cdot\; C_{d,p}(\nu), \tag{4}$$

where

$$C_{d,p}(\nu) \;:=\; \sup_{f \in F_{d,p}} \frac{\|g_{f,\nu}\|_{W_{d,p}}}{\|f\|_{F_{d,p}}}.$$

This is why, in our search, we are looking for functions ν with finite and possibly small $C_{d,p}(\nu)$.

As already mentioned, the most common change of variables that uses the inverse of the CDF,

$$\nu(t) \;:=\; \Phi_\varrho^{-1}(t) \quad \text{for} \quad \Phi_\varrho(x) \;=\; \int_{y \le x} \varrho(y)\,\mathrm{d}y, \tag{5}$$

gives $C_{d,p}(\nu) = +\infty$, for all $p > 1$ and *non-trivial* densities ϱ, see Proposition 4. Moreover, it produces functions $g_{f,\nu}$ that have singularities (poles) on the boundary of the cube B^d, even for exceptionally smooth f. We illustrate this by the following example. Let $D = \mathbb{R}_+$, $\varrho(x) = \exp(-x)$, $p = +\infty$, and $f(x) = x$. Then $\|f\|_{F_{1,\infty}} = 1$, yet for ν as in (5) the change of variables produces

$$g_{f,\nu}(t) \;=\; -\ln(1-t),$$

which has a singularity at $t = 1$. Using instead

$$\nu_a(x) \;=\; a\,\Phi_\varrho^{-1}(x) \quad \text{with} \quad a > 1$$

results in

$$g_{f,\nu_a}(t) \;=\; -a^2\,(\ln(1-t))\,(1-t)^{a-1},$$

which even belongs to $W_{1,\infty}$ for $a > 2$ (compare with Fig.1).

Moreover, the midpoint rule with 10^5 samples applied to g_{f,ν_a} with $a \in \{1, 1.5, 2.5\}$ produces, correspondingly, approximations with absolute errors

$$3.47 \times 10^{-6}, \qquad 5.02 \times 10^{-8}, \qquad 2.65 \times 10^{-11},$$

see Numerical Test 10 for more details.

In Theorems 5 and 7, we provide conditions on the change of variables function ν, that guarantee finite $C_{d,p}(\nu)$. It turns out that for a number of specific probability density functions, including $\varrho(x) = \lambda^{-1} \exp(-x/\lambda)$ with $D = \mathbb{R}_+$ and $\varrho(x) = (2\pi\sigma^2)^{-1/2} \exp(-x^2/(2\,\sigma^2))$ with $D = \mathbb{R}$, these conditions are satisfied by $\nu_a = a\,\Phi_\varrho^{-1}$ for a specially chosen $a \geq 1$. However, with the exception of $p = 1$, we still have $C_{1,p}(\nu_1) = +\infty$ for $a = 1$. Moreover, as shown in Example 6, $\nu_a = a\,\Phi_\varrho^{-1}$ need not yield finite $C_{d,p}(\nu_a)$ for any a (unless $p = 1$) for a special probability density function ϱ. In this case, we provide another change of variable function ν with finite $C_{d,p}(\nu)$.

Finally, we add that the results of this paper can be used to produce an efficient implementation of the *Multivariate Decomposition Method (MDM)* for approximation of weighted integrals of functions that belong to γ-weighted spaces $\mathcal{F}_{d,p,\gamma}$ for any d including $d = +\infty$. Due to a number of specific details, we delay the discussion of MDM's to Section 5.

2 Multivariate Integration

In the multivariate integration problem (1), we assume that the integrands f belong to the Sobolev space $F_{d,p}$ of functions anchored at zero and whose mixed first order partial derivatives (in the weak sense) are in the L_p space. By anchored we mean that

$$f(\boldsymbol{x}) \,=\, 0 \quad \text{if} \quad x_j \,=\, 0 \quad \text{for some } j \in \{1, \ldots, d\}.$$

This assumption is not restrictive, as will be explained in Section 5.

Such spaces were introduced for $d = 1$ in [13] and have been later considered in a number of papers. Specifically, see, e.g. [3], a function f is in $F_{d,p}$ iff it is of the form

$$f(\boldsymbol{x}) \,=\, \int_{D^d} h_f(\boldsymbol{z}) \prod_{j=1}^{d} \kappa(x_j, z_j)\, \mathrm{d}\boldsymbol{z}, \tag{6}$$

where

$$\kappa(x, z) \,=\, \begin{cases} 1 & \text{if } x > z \geq 0, \\ -1 & \text{if } x < z < 0, \\ 0 & \text{otherwise.} \end{cases}$$

The mixed first order partial derivative

$$\prod_{j=1}^{d} \frac{\partial}{\partial x_j} f \,:=\, \frac{\partial^d}{\partial x_1 \partial x_2 \cdots \partial x_d} f$$

is then equal to h_f and is assumed to be in the $L_p = L_p(D^d)$ space, $p \in [1, +\infty]$, which is endowed with the norm

$$\|h_f\|_{L_p(D^d)} \,:=\, \left(\int_{D^d} |h_f(\boldsymbol{x})|^p \, \mathrm{d}\boldsymbol{x} \right)^{1/p} \quad \text{for } \; 1 \leq p < +\infty,$$

and

$$\|h_f\|_{L_\infty(D^d)} \,:=\, \operatorname*{ess\,sup}_{\boldsymbol{x} \in D^d} |h_f(\boldsymbol{x})| \quad \text{for } p = +\infty.$$

Then the norm in $F_{d,p}$ is given by

$$\|f\|_{F_{d,p}} \;=\; \|h_f\|_{L_p(D^d)} \;=\; \left\| \prod_{j=1}^{d} \frac{\partial}{\partial x_j}\, f \right\|_{L_p(D^d)},$$

which is well defined since the functions $f \in F_{d,p}$ are anchored at zero.

Throughout the paper, p^* denotes the conjugate of p, i.e.,

$$\frac{1}{p} + \frac{1}{p^*} \;=\; 1.$$

Due to (6) and Hölder's inequality, for $1 < p \le +\infty$ we have

$$\begin{aligned}
\left| \int_{D^d} f(\boldsymbol{x})\, \varrho_d(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} \right| \;&=\; \left| \int_{D^d} h_f(\boldsymbol{z}) \int_{D^d} \prod_{j=1}^{d} \left(\kappa(x_j, z_j)\, \varrho(x_j)\right)\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{z} \right| \\
&\le\; \|f\|_{F_{d,p}} \left(\int_{D^d} \left| \int_{D^d} \prod_{j=1}^{d} (\kappa(x_j, z_j)\, \varrho(x_j))\, \mathrm{d}\boldsymbol{x} \right|^{p^*} \mathrm{d}\boldsymbol{z} \right)^{1/p^*}.
\end{aligned}$$

Since Hölder's inequality is sharp, we conclude that if the integration functional $I_{d,\varrho}$ is bounded, then its operator norm is given by

$$\|I_{d,\varrho}\| \;=\; \left(\int_{D^d} \left| \int_{D^d} \prod_{j=1}^{d} (\kappa(x_j, z_j)\, \varrho(x_j))\, \mathrm{d}\boldsymbol{x} \right|^{p^*} \mathrm{d}\boldsymbol{z} \right)^{1/p^*} \;=\; \|I_{1,\varrho}\|^d$$

with

$$\|I_{1,\varrho}\| \;=\; \left(\int_{D} \left| \int_{D} \kappa(x, z)\, \varrho(x)\, \mathrm{d}x \right|^{p^*} \mathrm{d}z \right)^{1/p^*}.$$

Similarly, for $p = 1$ the equality $\|I_{d,\varrho}\| = \|I_{1,\varrho}\|^d$ holds with

$$\|I_{1,\varrho}\| \;=\; \operatorname*{ess\,sup}_{z \in D} \left| \int_{D} \kappa(x, z)\, \varrho(x)\, \mathrm{d}x \right|.$$

We propose using a change of variables that transforms the original weighted integral over the unbounded domain D^d to the standard Lebesgue integral over the unit cube B^d with the new integrand belonging to the standard Sobolev space $W_{d,p}$, as required in (2), and then use, e.g., QMC or sparse grid methods, which are well suited and quite efficient for such kinds of integrands. Also here we assume, without any loss of generality, that functions $g \in W_{d,p}$ are anchored at zero.

Specifically, we apply (componentwise) a change of variables

$$x_j \;=\; \nu(t_j) \quad \text{for} \quad 1 \le j \le d,$$

where the function $\nu : B \to D$ is monotonically increasing and onto D, and

$$B \;=\; \begin{cases} [0, 1) & \text{if } D = \mathbb{R}_+, \\ (-1/2, 1/2) & \text{if } D = \mathbb{R}. \end{cases}$$

Then, assuming that the derivative ν' exists and is measurable, we obtain

$$I_{d,\varrho}(f) \;=\; \int_{B^d} g(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t} \qquad \text{with} \qquad g(\boldsymbol{t}) \;:=\; f(\nu(t_1),\ldots,\nu(t_d)) \prod_{j=1}^{d} \varrho(\nu(t_j))\,\nu'(t_j). \tag{7}$$

To stress the dependence of g on the functions f and ν, we will often write

$$g_{f,\nu} \text{ or } g_f \text{ instead of } g.$$

We are interested in functions ν such that the corresponding integrands $g = g_{f,\nu}$ are in $W_{d,p}$ and are anchored at zero. That is,

$$\|g\|_{W_{d,p}} \;=\; \left[\int_{B^d} \left|\prod_{j=1}^{d} \frac{\partial}{\partial x_j} g(\boldsymbol{x})\right|^p \mathrm{d}\boldsymbol{x}\right]^{1/p} \;<\; +\infty \quad \text{and } g(\boldsymbol{x}) = 0 \text{ if } x_j = 0 \text{ for some } j$$

(with the obvious modification for $p = +\infty$). Moreover, we would like the ratio

$$C_{d,p}(\nu) \;:=\; \sup_{f\in F_{d,p}} \frac{\|g_f\|_{W_{d,p}}}{\|f\|_{F_{d,p}}} \tag{8}$$

to be not only finite, but also small, as explained in the introduction, see (4). Due to the tensor product form (6), one can show (in a similar way to the derivation of the norm of $I_{d,\varrho}$) that the following holds.

Proposition 1 *The ratio $C_{d,p}(\nu)$ is fully determined by the univariate case, i.e.,*

$$C_{d,p}(\nu) \;=\; \left(C_{1,p}(\nu)\right)^d, \qquad \textit{where} \qquad C_{1,p}(\nu) \;=\; \sup_{f\in F_{1,p}} \frac{\|g_f\|_{W_{1,p}}}{\|f\|_{F_{1,p}}}.$$

This is why, in the analysis of the factor $C_{d,p}(\nu)$, we can restrict our considerations to the univariate case.

Remark 2 Denote by J_d the standard Lebesgue integral over the unit cube B^d, i.e.,

$$J_d(g) \;=\; \int_{B^d} g(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t}.$$

Then its operator norm equals $\|J_d\| = \|J_1\|^d$, where

$$\|J_1\| = \begin{cases} (1+p^*)^{-1/p^*} & \text{if } 1 < p \le +\infty, \\ 1 & \text{if } p = 1, \end{cases}$$

for $B = [0,1)$, and is twice smaller for $B = (-1/2, 1/2)$. Furthermore,

$$|I_{d,\varrho}(f)| = \left|\int_{B^d} g_f(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t}\right| \le \|J_d\|\|g_f\|_{W_{d,p}} \le \|J_d\| C_{d,p}(\nu)\|f\|_{F_{d,p}} = \big(\|J_1\| C_{1,p}(\nu)\big)^d \|f\|_{F_{d,p}}.$$

Hence, if $C_{1,p}(\nu) < +\infty$ for some ν, then the operator $I_{d,\varrho}$ is bounded in $F_{d,\varrho}$, and its norm satisfies

$$\|I_{d,\varrho}\| \;\le\; \Big(\|J_1\|\, C_{1,p}(\nu)\Big)^d.$$

Remark 3 When ϱ_d is a product of different weights depending on j, then also ν being a product of different ν_j should be considered. That is, if $\varrho_d(\boldsymbol{x}) = \prod_{j=1}^d \varrho_{1,j}(x_j)$, then one could consider $\nu(\boldsymbol{t}) = \prod_{j=1}^d \nu_j(t_j)$. Then $C_{d,p}(\nu) = \prod_{j=1}^d C_{1,p}(\nu_j)$.

Before we propose our ways of changing variables, let us see what happens when we apply the standard change that has been commonly used in practice.

Standard Change of Variables. Let $\Phi_\varrho : \mathbb{R}_+ \to [0,1)$ or $\Phi_\varrho : \mathbb{R} \to (0,1)$ be the CDF corresponding to the probability density ϱ, defined by

$$\Phi_\varrho(x) \;=\; \int_D 1_{\{x \geq t\}}\, \varrho(t)\, \mathrm{d}t, \tag{9}$$

where 1_A denotes the indicator function of a given set A. Then the standard change of variables uses $\nu = \Phi_\varrho^{-1}$, i.e.,

$$\int_{D^d} f(\boldsymbol{x})\, \varrho(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} \;=\; \int_{[0,1]^d} g_{f,\Phi_\varrho^{-1}}(\boldsymbol{t})\, \mathrm{d}\boldsymbol{t}, \quad \text{where} \quad g_{f,\Phi_\varrho^{-1}}(\boldsymbol{t}) \;=\; f\left(\Phi_\varrho^{-1}(t_1), \ldots, \Phi_\varrho^{-1}(t_d)\right). \tag{10}$$

We have the following simple yet important proposition.

Proposition 4 *For any $f \in F_{d,p}$, let $g_{f,\Phi_\varrho^{-1}}$ be the function given by* (10)*.*

(i) For $p = 1$, we have

$$\|f\|_{F_{d,1}} \;=\; \|g_{f,\Phi_\varrho^{-1}}\|_{W_{d,1}} \quad \textit{for all } f \in F_{d,1}.$$

(ii) For $p > 1$, we have

$$\|g_{f,\Phi_\varrho^{-1}}\|_{W_{d,p}} \;=\; \left[\int_{D^d} \left| \left(\prod_{j=1}^d \frac{\partial}{\partial x_j} f(\boldsymbol{x})\right) \left(\prod_{j=1}^d \frac{1}{\varrho^{1/p^*}(x_j)}\right)\right|^p \mathrm{d}\boldsymbol{x}\right]^{1/p}. \tag{11}$$

Hence $g_{f,\Phi_\varrho^{-1}} \in W_{d,p}$ if and only if the right-hand side of (11) *is finite.*

Proof. Due to the tensor product structure of the spaces, it is enough to prove the proposition for $d = 1$. We clearly have

$$g'_{f,\Phi_\varrho}(t) \;=\; f'(\Phi_\varrho^{-1}(t))\, \frac{\mathrm{d}}{\mathrm{d}t}\Phi_\varrho^{-1}(t) \;=\; f'(\Phi_\varrho^{-1}(t))\, \frac{1}{\varrho(\Phi_\varrho^{-1}(t))}.$$

Hence for $1 \leq p < +\infty$ we have

$$\begin{aligned} \|g_{f,\Phi_\varrho^{-1}}\|_{W_{1,p}}^p \;&=\; \int_0^1 |g'_{f,\Phi_\varrho^{-1}}(t)|^p\, \mathrm{d}t \;=\; \int_0^1 \left| f'(\Phi_\varrho^{-1}(t))\, \frac{1}{\varrho(\Phi_\varrho^{-1}(t))}\right|^p \mathrm{d}t \\ &=\; \int_D \left| f'(x)\, \frac{1}{\varrho(x)}\right|^p \varrho(x)\, \mathrm{d}x \;=\; \int_D \left| f'(x)\, \frac{1}{\varrho^{1/p^*}(x)}\right|^p \mathrm{d}x, \end{aligned}$$

(with $1/p^* = 0$ for $p = 1$), and for $p = +\infty$ we have

$$\|g_{f,\Phi_\varrho^{-1}}\|_{W_{1,\infty}} = \operatorname*{ess\,sup}_{t\in[0,1]} |g'_{f,\Phi_\varrho^{-1}}(t)| = \operatorname*{ess\,sup}_{t\in[0,1]} \left| \frac{f'(\Phi_\varrho^{-1}(t))}{\varrho(\Phi_\varrho^{-1}(t))}\right| = \operatorname*{ess\,sup}_{x\in D} \left| \frac{f'(x)}{\varrho(x)}\right|,$$

as claimed. □

Proposition 4 states that the change of variables (10) transforms all functions from $F_{d,p}$ to $W_{d,p}$ only for $p = 1$. For $p > 1$, the situation is quite different. Then $1/p^* > 0$ and, therefore, only those functions whose mixed first order partial derivatives converge to zero sufficiently fast have the corresponding functions $g_{f,\Phi_\varrho^{-1}}$ in the space $W_{d,p}$. Indeed, since the weight $\varrho(x)$ has to

converge to zero as $|x| \to \infty$, $\varrho^{-1/p^*}(x)$ has to converge to infinity, resulting in a very restrictive class of integrands f. In particular, if $p^* = 1$ then we need to have

$$\operatorname*{ess\,sup}_{\boldsymbol{x} \in D^d} \left| \frac{\prod_{j=1}^d \frac{\partial}{\partial x_j} f(\boldsymbol{x})}{\prod_{j=1}^d \varrho(x_j)} \right| < +\infty.$$

For instance, for $D = \mathbb{R}$ and Gaussian weight

$$\varrho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

we would need

$$\int_{\mathbb{R}^d} \exp\left(\frac{1}{2\sigma^2 p^*} \sum_{j=1}^d x_j^2\right) \left| \prod_{j=1}^d \frac{\partial}{\partial x_j} f(\boldsymbol{x}) \right|^p \mathrm{d}\boldsymbol{x} < +\infty \qquad \text{for } p < +\infty,$$

and

$$\operatorname*{ess\,sup}_{\boldsymbol{x} \in \mathbb{R}^d} \exp\left(\frac{1}{2\sigma^2} \sum_{j=1}^d x_j^2\right) \left| \prod_{j=1}^d \frac{\partial}{\partial x_j} f(\boldsymbol{x}) \right| < +\infty \qquad \text{for } p = +\infty,$$

which may hold only if the derivative of f decreases to zero faster than exponentially. This is why in the rest of the paper we concentrate on the case of $p > 1$.

We now switch to the univariate case, but will return to the multivariate case in Section 5 with some additional comments.

3 Univariate Functions

Recall that for the univariate case the space $F_{1,p}$ consists of functions anchored at zero and whose weak derivatives are in the $L_p(D)$ space. For $f \in F_{1,p}$ we want to know when the corresponding functions

$$g_f(t) = g_{f,\nu}(t) = f(\nu(t))\, \varrho(\nu(t))\, \nu'(t) \tag{12}$$

belong to the standard Sobolev space $W_{1,p}$ of functions anchored at zero with $g' \in L_p(B)$.

The following functions will play an important role:

$$h_{0,p^*}(t) := \varrho(\nu(t))\, \nu'(t)\, |\nu(t)|^{1/p^*}, \tag{13}$$
$$h_{1,p^*}(t) := \varrho(\nu(t))\, (\nu'(t))^{1+1/p^*}, \tag{14}$$
$$h_{2,p^*}(t) := (\varrho(\nu(t))\, \nu'(t))'\, |\nu(t)|^{1/p^*}. \tag{15}$$

For this to make sense we obviously assume that the corresponding functions ϱ and ν are sufficiently regular.

3.1 Case of $D = \mathbb{R}_+$

Let $\nu : [0, 1) \to \mathbb{R}_+$ be an increasing and twice differentiable function such that

$$\nu(0) = 0 \quad \text{and} \quad \lim_{t \to 1} \nu(t) = +\infty.$$

Theorem 5 *For every $f \in F_{1,p}$, the corresponding function g_f given by* (12) *satisfies:*

(i) $\|g_f\|_{L_\infty(0,1)} < +\infty \quad$ *if* $\quad \|h_{0,p^*}\|_{L_\infty(0,1)} < +\infty$,

(ii) $g_f \in W_{1,p}$ *if* $\|h_{1,p^*}\|_{L_\infty(0,1)} < +\infty$ *and* $\|h_{2,p^*}\|_{L_p(0,1)} < +\infty$. *If so, then*

$$C_{1,p}(\nu) \;\le\; \|h_{1,p^*}\|_{L_\infty(0,1)} + \|h_{2,p^*}\|_{L_p(0,1)}.$$

In particular, for $p = +\infty$,

$$C_{1,\infty}(\nu) \;\le\; \left\|\varrho(\nu(\cdot))\,(\nu'(\cdot))^2\right\|_{L_\infty(0,1)} + \left\|\left(\varrho(\nu(\cdot))\,\nu'(\cdot)\right)'\,\nu(\cdot)\right\|_{L_\infty(0,1)}.$$

Proof. To show *(i)*, observe that, by Hölder's inequality,

$$\begin{aligned} |g_f(t)| &= \varrho(\nu(t))\,\nu'(t)\left|\int_0^{\nu(t)} f'(z)\,\mathrm{d}z\right| \le \varrho(\nu(t))\,\nu'(t)\left(\int_0^{\nu(t)}\mathrm{d}z\right)^{1/p^*}\|f'\|_{L_p(\mathbb{R}_+)} \\ &= h_{0,p^*}(t)\,\|f'\|_{L_p(\mathbb{R}_+)}. \end{aligned}$$

We next prove *(ii)*. Obviously $g_f(0) = 0$ since $\nu(0) = 0$. We will prove the upper bound on $C_{1,p}(\nu)$ only for $1 < p < +\infty$ since the case of $p = +\infty$ is even easier. We have

$$\begin{aligned} g_f'(t) &= f'(\nu(t))\,\varrho(\nu(t))\,(\nu'(t))^2 + f(\nu(t))\,\left(\varrho(\nu(t))\,\nu'(t)\right)' \\ &= f'(\nu(t))\,(\nu'(t))^{1/p}\,\varrho(\nu(t))\,(\nu'(t))^{1+1/p^*} + \left(\varrho(\nu(t))\,\nu'(t)\right)'\int_0^{\nu(t)} f'(z)\,\mathrm{d}z. \end{aligned}$$

Therefore

$$\begin{aligned} \|g_f'\|_{L_p([0,1))} \;\le\; & \left(\int_0^1 |f'(\nu(t))|^p\,\nu'(t)\,\left(\varrho(\nu(t))\,(\nu'(t))^{1+1/p^*}\right)^p\,\mathrm{d}t\right)^{1/p} \\ & + \left(\int_0^1 |(\varrho(\nu(t))\,\nu'(t))'|^p\left|\int_0^{\nu(t)} f'(z)\,\mathrm{d}z\right|^p\,\mathrm{d}t\right)^{1/p}. \end{aligned}$$

Clearly

$$\int_0^1 |f'(\nu(t))|^p\,\nu'(t)\,\mathrm{d}t = \int_0^\infty |f'(x)|^p\,\mathrm{d}x = \|f'\|^p_{L_p(\mathbb{R}_+)}$$

and, again by Hölder's inequality,

$$\left|\int_0^{\nu(t)} f'(z)\,\mathrm{d}z\right| = \left|\int_0^\infty f'(z)\,1_{\{\nu(t)\ge z\}}\,\mathrm{d}z\right| \le \|f'\|_{L_p(\mathbb{R}_+)}\,(\nu(t))^{1/p^*}.$$

Hence indeed,

$$\begin{aligned} \|g'\|_{L_p(0,1)} \;\le\; & \left(\int_0^1 |f'(\nu(t))|^p\,\nu'(t)\,\mathrm{d}t\right)^{1/p}\operatorname*{ess\,sup}_{t\in[0,1)}\varrho(\nu(t))\,(\nu'(t))^{1+1/p^*} \\ & + \left(\int_0^1 |\left(\varrho(\nu(t))\,\nu'(t)\right)'|^p\,\|f'\|^p_{L_p(\mathbb{R}_+)}\,(\nu(t))^{p/p^*}\,\mathrm{d}t\right)^{1/p} \\ \le\; & \|f'\|_{L_p(\mathbb{R}_+)}\,\|\varrho(\nu(\cdot))\,(\nu'(\cdot))^{1+1/p^*}\|_{L_\infty(0,1)} \\ & + \|f'\|_{L_p(\mathbb{R}_+)}\,\left\|\left(\varrho(\nu(\cdot))\,\nu'(\cdot)\right)'\,(\nu(\cdot))^{1/p^*}\right\|_{L_p(0,1)} \\ =\; & \|f'\|_{L_p(\mathbb{R}_+)}\,\left(\|h_{1,p^*}\|_{L_\infty(0,1)} + \|h_{2,p^*}\|_{L_p(0,1)}\right). \end{aligned}$$

This completes the proof. □

We give an example for an application of Theorem 5.

Example 6 Let $D = \mathbb{R}_+$ and $\varrho(x) = (c-1)(1+x)^{-c}$ for sufficiently large c. We use Theorem 5 for

$$\nu_b(t) \;=\; \frac{1}{(1-t)^b} - 1 \quad \text{for } b \;>\; 0.$$

Then

$$\nu_b'(t) \;=\; \frac{b}{(1-t)^{b+1}} \quad \text{and} \quad \varrho(\nu_b(t)) \;=\; (c-1)\,(1-t)^{b\,c}.$$

Therefore, for $p = +\infty$ we have

$$h_{1,1}(t) \;=\; b^2\,(c-1)\,(1-t)^{b\,(c-2)-2} \quad \text{and} \quad \|h_{1,1}\|_{L_\infty(0,1)} \;=\; b^2\,(c-1)$$

for

$$b \;\geq\; \frac{2}{c-2}.$$

Otherwise, $h_{1,1}$ is unbounded. As for $h_{2,1}$, we have

$$\left(\varrho(\nu_b(t))\,\nu_b'(t)\right)' \;=\; b\,(c-1)\,(b\,(c-1)-1)\,(1-t)^{b(c-1)-2}$$

and

$$\begin{aligned} h_{2,1}(t) \;&=\; b\,(c-1)\,(b\,(c-1)-1)(1-t)^{b\,(c-1)-2}\,\left(\frac{1}{(1-t)^b} - 1\right) \\ &=\; b\,(c-1)\,(b\,(c-1)-1)\left((1-t)^{b\,(c-2)-2} - (1-t)^{b\,(c-1)-2}\right). \end{aligned}$$

Hence,

$$\begin{aligned} \|h_{2,1}\|_{L_\infty(0,1)} \;&=\; \operatorname*{ess\,sup}_{x\in(0,1)} b\,(c-1)\,(b\,(c-1)-1)\left(x^{b\,(c-2)-2} - x^{b\,(c-1)-2}\right) \\ &=\; h_{2,1}\left(1 - \left(\frac{b(c-2)-2}{b(c-1)-2}\right)^{1/b}\right) \\ &=\; \frac{b^2(c-1)(b(c-1)-1)}{b(c-1)-2}\left(\frac{b(c-2)-2}{b(c-1)-2}\right)^{c-2-\frac{2}{b}}, \end{aligned}$$

and for $b > 2/(c-2)$ we have

$$C_{1,\infty}(\nu_b) \leq b^2(c-1)\left(1 + \frac{b(c-1)-1}{b(c-1)-2}\left(\frac{b(c-2)-2}{b(c-1)-2}\right)^{c-2-\frac{2}{b}}\right).$$

In view of what follows we mention that here for the change of variables $\nu(t) = b\,\Phi_\varrho^{-1}(t)$, we have $\|h_{0,p^*}\|_{L_\infty(B)} = \|h_{1,p^*}\|_{L_\infty(B)} = \|h_{2,p^*}\|_{L_p(B)} = +\infty$ for any $p > 1$.

3.2 Case of $D = \mathbb{R}$

In this case, we consider $\nu : (-1/2, 1/2) \to \mathbb{R}$ that is increasing, twice differentiable, and for which

$$\nu(0) \;=\; 0 \quad \text{and} \quad \lim_{t \to \pm 1/2} \nu(t) \;=\; \pm\infty.$$

To simplify the presentation, we also assume that the function ϱ is even and ν is odd, i.e.,

$$\varrho(-x) \;=\; \varrho(x) \quad \text{and} \quad \nu(-t) \;=\; -\nu(t), \tag{16}$$

since then it is sufficient to consider only positive values of t. However, if this assumption is not satisfied then one can treat the problem as two subproblems: one with the domain $D = [0, +\infty)$ and the other with $D = (-\infty, 0]$.

The following result is a version of Theorem 5 adapted to the case $D = \mathbb{R}$. Due to (16), the proposition follows easily from the proof of Theorem 5, and hence its proof is omitted.

Theorem 7 *If $\|h_{1,p^*}\|_{L_\infty(-1/2,1/2)} < +\infty$ and $\|h_{2,p^*}\|_{L_p(-1/2,1/2)} < +\infty$, then, for every $f \in F_{1,p}$, the corresponding function g_f belongs to $W_{1,p}$ and*

$$C_{1,p}(\nu) \;\le\; \|h_{1,p^*}\|_{L_\infty(-1/2,1/2)} + \|h_{2,p^*}\|_{L_p(-1/2,1/2)}$$

with h_{1,p^*} and h_{2,p^*} defined by (14) and (15), respectively.

3.3 Special Change of Variables

We propose to use the following change of variables. If $D = \mathbb{R}_+$, define $\nu = \nu_a : [0, 1) \to \mathbb{R}$ by

$$\nu(t) \;=\; \nu_a(t) \;=\; a\, \Phi_\varrho^{-1}(t). \tag{17}$$

If $D = \mathbb{R}$, define $\nu = \nu_a : (-1/2, 1/2) \to \mathbb{R}$ by

$$\nu(t) \;=\; \nu_a(t) \;=\; a\, \Phi_\varrho^{-1}\left(t + \frac{1}{2}\right), \tag{18}$$

where in both cases $a \ge 1$ and, as before, Φ_ϱ^{-1} is the inverse of the CDF for ϱ.

Proposition 8 *Let ν_a be given by (17) or (18), respectively. Then*

$$\begin{aligned}
\|h_{0,p^*}\|_{L_\infty(B)} &= a^{1+1/p^*} \operatorname*{ess\,sup}_{y \in D} \frac{\varrho(a\,y)}{\varrho(y)}\, |y|^{1/p^*}, \\
\|h_{1,p^*}\|_{L_\infty(B)} &= a^{1+1/p^*} \operatorname*{ess\,sup}_{y \in D} \frac{\varrho(a\,y)}{(\varrho(y))^{1+1/p^*}}, \quad \textit{and} \\
\|h_{2,p^*}\|_{L_p(B)} &= a^{1+1/p^*} \left(\int_D \left| \left(\frac{\varrho(a\,y)}{\varrho(y)} \right)' \frac{y^{1/p^*}}{\varrho(y)} \right|^p \varrho(y)\, \mathrm{d}y \right)^{1/p},
\end{aligned}$$

where, as before, $B = [0, 1)$ if $D = \mathbb{R}_+$ and $B = (-1/2, 1/2)$ if $D = \mathbb{R}$.

Proof. The result follows from a change of variables. If $D = \mathbb{R}_+$, then replace t by $\Phi_\varrho(y)$ and use the fact that

$$\nu_a'(t) \;=\; \frac{a}{\varrho(\Phi_\varrho^{-1}(t))} \;=\; \frac{a}{\varrho(y)} \quad \text{and} \quad \mathrm{d}t \;=\; \varrho(y)\,\mathrm{d}y.$$

If $D = \mathbb{R}$, then replace t by $\Phi_\varrho(y) - \frac{1}{2}$ and use the fact that

$$\nu_a'(t) \;=\; \frac{a}{\varrho(\Phi_\varrho^{-1}(t+1/2))} = \frac{a}{\varrho(y)} \quad \text{and} \quad \mathrm{d}t \;=\; \varrho(y)\,\mathrm{d}y.$$

This completes the proof. □

Remark 9 Note that for $p = 1$, the exponent $1/p^* = \infty$. Hence, for $a = 1$, we have

$$\|h_{0,\infty}\|_{L_\infty(B)} \;=\; \|h_{1,\infty}\|_{L_\infty(B)} \;=\; 1 \quad \text{and} \quad \|h_{2,\infty}\|_{L_1(B)} \;=\; 0.$$

This coincides with Part *(i)* of Proposition 4.

4 Particular Weights

We illustrate Proposition 8 for exponential and Gaussian densities ϱ.

4.1 Exponential ϱ

We consider $D = \mathbb{R}_+$ and

$$\varrho(x) \;=\; \frac{1}{\lambda}\,\exp\left(-\frac{x}{\lambda}\right) \quad \text{for} \quad \lambda \;>\; 0.$$

Clearly

$$\|I_{1,\varrho}\| \;=\; \left(\frac{\lambda}{p^*}\right)^{1/p^*}.$$

We use the change of variables

$$\nu_a(t) \;=\; a\,\Phi_\varrho^{-1}(t) \;=\; -\lambda\,a\,\ln(1-t). \tag{19}$$

It is easy to see that the norm of h_{0,p^*} is infinite for $a \leq 1$. Assume that $a > 1$. Then

$$\|h_{0,p^*}\|_{L_\infty(0,1)} \;=\; a^{1+1/p^*}\,\left(\frac{\lambda}{\mathrm{e}\,p^*\,(a-1)}\right)^{1/p^*}.$$

We also have

$$\|h_{1,p^*}\|_{L_\infty(0,1)} \;=\; a^{1+1/p^*}\lambda^{1/p^*}\,\sup_{y\in\mathbb{R}_+}\exp\left(-y\,\frac{a-(1+1/p^*)}{\lambda}\right),$$

and hence

$$\|h_{1,p^*}\|_{L_\infty(0,1)} \;=\; \begin{cases} a^{1+1/p^*}\lambda^{1/p^*} & \text{if } a \;\geq\; 1+\frac{1}{p^*}, \\ +\infty & \text{otherwise,} \end{cases}$$

for any $p \in (1, +\infty]$.

In order to analyze h_{2,p^*}, we consider first $p = +\infty$. It is easy to see that then

$$\|h_{2,1}\|_{L_\infty(0,1)} \;=\; \frac{a^2(a-1)\lambda}{(a-2)\mathrm{e}} \quad \text{for } a > 2$$

and

$$C_{1,\infty}(\nu_a) \le a^2\lambda\left(1 + \frac{a-1}{(a-2)\mathrm{e}}\right) \quad \text{for } a > 2.$$

The upper bound on $C_{1,\infty}(\nu_a)$ is minimal for

$$a^* \;=\; 2 + \frac{4}{\sqrt{17+16\,\mathrm{e}}+1} \;=\; 2.4557\ldots \quad \text{and then} \quad C_{1,\infty}(\nu_{a^*}) \;\le\; \lambda \times 13.1172\ldots. \tag{20}$$

Consider now finite $p > 1$. Observe that

$$\left(\frac{\varrho(a\,y)}{\varrho(y)}\right)' \;=\; -\frac{a-1}{\lambda}\,\exp\left(-y\,\frac{a-1}{\lambda}\right)$$

which results in

$$\|h_{2,p^*}\|_{L_p(0,1)} \;=\; \frac{a^{1+1/p^*}\,(a-1)}{\lambda^{1/p}}\left(\int_0^\infty y^{p-1}\,\exp\left(-y\,\frac{p\,(a-2)+1}{\lambda}\right)\,\mathrm{d}y\right)^{1/p},$$

where we used the fact that $p/p^* = p-1$.

Suppose for the rest of this section that p is an integer. Using integration by parts $p-1$ times, one can show that for any $c > 0$,

$$\int_0^\infty y^{p-1}\,\exp(-y\,c)\,\mathrm{d}y \;=\; \frac{(p-1)!}{c^p},$$

and conclude that

$$\|h_{2,p^*}\|_{L_p(0,1)} \;=\; \frac{(a-1)\,a^{1+1/p^*}}{p\,(a-2)+1}\,\lambda^{1/p^*}\,((p-1)!)^{1/p},$$

whenever $a > 1 + 1/p^*$. Finally,

$$C_{1,p}(\nu_a) \;\le\; a^{1+1/p^*}\,\lambda^{1/p^*}\left(1 + \frac{(a-1)\,((p-1)!)^{1/p}}{p\,(a-2)+1}\right) \;<\; +\infty \tag{21}$$

for $a > 1 + 1/p^*$.

The upper bound on $C_{1,p}(\nu_a)$ is minimal for

$$\begin{aligned} a^* \;=\;& 2p(2p-1)^2 + (7p^2-6p+1)((p-1)!)^{1/p} \\ &+ \frac{\sqrt{p-1}((p-1)!)^{1/(2p)}\sqrt{4p^2(2p-1)^2 + (17p^3-19p^2+7p-1)((p-1)!)^{1/p}}}{2p(2p-1)(p+((p-1)!)^{1/p})}. \end{aligned}$$

For example, for $p = p^* = 2$,

$$a^* \;=\; \frac{53+\sqrt{217}}{36} \;=\; 1.8814\ldots$$

which results in the upper bound

$$C_{1,2}(\nu_{a^*}) \;\le\; \frac{(5+\sqrt{217})\,(53+\sqrt{217})^{3/2}}{144\,(\sqrt{217}-1)}\,\sqrt{\lambda} \;=\; \sqrt{\lambda} \times 5.5624\ldots.$$

Numerical Test 10 Consider $f(x) = x$ and $\varrho(x) = \exp(-x)$. Clearly, f is in our space for $p = +\infty$ and $\|f\|_{F_{1,\infty}} = 1$. The value of the integral is 1, and we use the change of variables ν_a as outlined above. Then the corresponding integrand is equal to

$$g_{f,\nu_a}(t) \;=\; -a^2\,(\ln(1-t))\,(1-t)^{a-1}.$$

Note that for $a = 1$ the function $g_{f,\nu_a}(t) = -\ln(1-t)$ has a singularity at $t = 1$, for $1 < a \le 2$ its derivative has a singularity at $t = 1$, and for $a > 2$ the singularity of g'_{f,ν_a} is removed and $g_{f,\nu_a} \in W_{1,\infty}$.

In the following table, we compare the integration errors of the midpoint rule with n samples applied to g_{f,ν_a} with $a = a^*$ as in (20), $a = 1.5$, and $a = 1$.

n	$a = a^* = 2.4557\ldots$	$a = 1.5$	$a = 1$
10	$4.353949E-03$	$1.118346E-02$	$3.424093E-02$
10^2	$3.471053E-05$	$6.488305E-04$	$3.461569E-03$
10^3	$2.958141E-07$	$3.029058E-05$	$3.465319E-04$
10^4	$2.707151E-09$	$1.271297E-06$	$3.465694E-05$
10^5	$2.596101E-11$	$5.015712E-08$	$3.465732E-06$

4.2 Gaussian ϱ

Consider $D = \mathbb{R}$ and

$$\varrho(x) \;=\; \frac{1}{\sigma\,\sqrt{2\,\pi}}\,\exp\left(-\frac{x^2}{2\,\sigma^2}\right) \quad \text{for } \sigma \;>\; 0.$$

Then

$$\|I_{1,\varrho}\| \;=\; \left(2^{1-p^*}\,\int_0^\infty \left(1-\operatorname{erf}\left(\frac{z}{\sqrt{2}\,\sigma}\right)\right)^{p^*}\,\mathrm{d}z\right)^{1/p^*} \qquad \text{for } p > 1,$$

where erf is the *Gauss error function* defined as $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \mathrm{e}^{-t^2}\,\mathrm{d}t$, and

$$\|I_{1,\varrho}\| \;=\; 1 \quad \text{for } p = 1.$$

Note that $1-\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \mathrm{e}^{-t^2}\,\mathrm{d}t \le \mathrm{e}^{-x^2}$ for $x > 0$ and hence $\|I_{1,\varrho}\| < +\infty$ for all $p \ge 1$.

By Proposition 8, for

$$\nu(t) \;=\; \nu_a(t) \;=\; a\,\Phi_\varrho^{-1}(t+1/2) \quad \text{for } t \;\in\; (-1/2, 1/2),$$

we get

$$\|h_{0,p^*}\|_{L_\infty(-1/2,1/2)} \;=\; a\,\left(\frac{a\,\sigma}{\sqrt{\mathrm{e}\,p^*\,(a^2-1)}}\right)^{1/p^*}.$$

Moreover

$$\|h_{1,p^*}\|_{L_\infty(-1/2,1/2)} \;=\; a^{1+1/p^*}\,(\sigma\sqrt{2\pi})^{1/p^*}\,\operatorname*{ess\,sup}_{y\in\mathbb{R}} \exp\left(-\frac{y^2}{2\sigma^2}\left(a^2-\left(1+\frac{1}{p^*}\right)\right)\right).$$

Hence

$$\|h_{1,p^*}\|_{L_\infty(-1/2,1/2)} \;=\; \begin{cases} \infty & \text{if } a^2 \;<\; 1+\frac{1}{p^*}, \\ c_1(a) & \text{if } a^2 \;\ge\; 1+\frac{1}{p^*}, \end{cases}$$

where

$$c_1(a) \,=\, a^{1+1/p^*}\,(\sigma\,\sqrt{2\,\pi})^{1/p^*}.$$

Again, by Proposition 8 we get

$$\begin{aligned}
\|h_{2,p^*}\|_{L_p(-1/2,1/2)} &= a^{1+1/p^*}\left(\int_{-\infty}^{\infty}\left|\left(\frac{\varrho(ay)}{\varrho(y)}\right)'\right|^p(\varrho(y))^{1-p}\,|y|^{p/p^*}\;\mathrm{d}y\right)^{1/p}\\
&= \frac{a^{1+1/p^*}}{(\sigma\sqrt{2\pi})^{1/p-1}}\\
&\quad\times\left(\int_{-\infty}^{\infty}\left[\exp\left(-\frac{y^2}{2\sigma^2}(a^2-1)\right)\left|\frac{y}{\sigma^2}(a^2-1)\right|\right]^p\exp\left(-\frac{y^2(1-p)}{2\sigma^2}\right)|y|^{p/p^*}\;\mathrm{d}y\right)^{1/p}\\
&= \frac{a^{1+1/p^*}}{(\sigma\sqrt{2\pi})^{1/p-1}}\frac{a^2-1}{\sigma^2}\left(\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{2\sigma^2}(a^2-1)p\right)\exp\left(-\frac{y^2(1-p)}{2\sigma^2}\right)|y|^{p+p/p^*}\;\mathrm{d}y\right)^{1/p}\\
&= \frac{a^{1+1/p^*}(a^2-1)}{(\sqrt{2\pi})^{1/p-1}\sigma^{1/p+1}}\left(\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{2\sigma^2}((a^2-2)p+1)\right)|y|^{p+p/p^*}\;\mathrm{d}y\right)^{1/p}. \qquad (22)
\end{aligned}$$

For p tending to $+\infty$ (and p^* tending to 1) we see that

$$\frac{a^{1+1/p^*}(a^2-1)}{(\sqrt{2\pi})^{1/p-1}\sigma^{1/p+1}} \to c_2(a) \,:=\, \frac{\sqrt{2\pi}\,a^2\,(a^2-1)}{\sigma}.$$

Furthermore, we write

$$\begin{aligned}
&\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{2\sigma^2}((a^2-2)p+1)\right)|y|^{p+p/p^*}\;\mathrm{d}y\\
&=\int_{-\infty}^{\infty}\left[\exp\left(-\frac{y^2}{2\sigma^2}\left((a^2-2)+1-\frac{1}{p^*}\right)\right)|y|^{1+1/p^*}\right]^p\;\mathrm{d}y.
\end{aligned}$$

From this we conclude that

$$\|h_{2,1}\|_{L_\infty(-1/2,1/2)} \,=\, c_2(a)\,\max_{z\in\mathbb{R}} z^2\,\exp\left(-\frac{z^2}{2\,\sigma^2}\,(a^2-2)\right) \,=\, c_2(a)\,\mathrm{e}^{-1}\,\frac{2\,\sigma^2}{a^2-2}$$

for $a^2>2$. Hence

$$C_{1,\infty}(\nu_a) \,\le\, \sqrt{2\,\pi}\sigma\,a^2\,\left(1+\frac{2}{\mathrm{e}}\,\frac{a^2-1}{a^2-2}\right).$$

It is easy to check that the upper bound on $C_{1,\infty}(\nu_a)$, as a function of a, attains its minimum at

$$a^* \,=\sqrt{2+\frac{2}{\sqrt{2+\mathrm{e}}}} \,=\, 1.70902\ldots \quad\text{and then}\quad C_{1,\infty}(a^*) \,=\, \sigma\,\times\,18.5582\ldots \quad\text{for } p=+\infty. \qquad (23)$$

Returning to (22), and using $p(1+1/p^*)=2p-1$, we have for $p<+\infty$,

$$\begin{aligned}
\|h_{2,p^*}\|_{L_p(-1/2,1/2)} &= \frac{a^{1+1/p^*}(a^2-1)}{(\sqrt{2\pi})^{1/p-1}\sigma^{1/p+1}}\left(\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{2\sigma^2}((a^2-2)p+1)\right)|x|^{p+p/p^*}\;\mathrm{d}x\right)^{1/p}\\
&= c_2(a)\,\left(\frac{1}{\sqrt{2\,\pi}\,\sigma\,a}\int_{-\infty}^{\infty}|x|^{2\,p-1}\,\exp\left(-\frac{x^2}{2\,\sigma^2}\,(p\,(a^2-2)+1)\right)\,\mathrm{d}x\right)^{1/p}.
\end{aligned}$$

This means that $\|h_{2,p^*}\|_{L_p(-1/2,1/2)} < +\infty$ if and only if $p(a^2-2)+1 > 0$, i.e.,

$$a^2 \;>\; 1 + \frac{1}{p^*}.$$

By the change $y = \frac{x}{\sigma}\sqrt{p(a^2-2)+1}$ we get that

$$\|h_{2,p^*}\|_{L_p(-1/2,1/2)} \;=\; c_3(a)\,\left(\frac{1}{\sqrt{2\,\pi}}\,\int_{-\infty}^{\infty} |y|^{2\,p-1}\,\exp\left(-\frac{y^2}{2}\right)\,\mathrm{d}y\right)^{1/p},$$

where

$$c_3(a) \;=\; c_2(a)\,\frac{\sigma^{2-1/p}}{(p\,(a^2-2)+1)\,a^{1/p}} \;=\; \frac{\sqrt{2\pi}\,a^{1+1/p^*}\,(a^2-1)\,\sigma^{1/p^*}}{(p\,(a^2-2)+1)}.$$

It is well known that for natural numbers p,

$$\frac{1}{\sqrt{2\,\pi}}\,\int_{-\infty}^{\infty} |y|^{2\,p-1}\,\exp\left(-\frac{y^2}{2}\right)\,\mathrm{d}y \;=\; \frac{1}{\sqrt{2\,\pi}}\,2^p\,(p-1)!\,.$$

Hence, for natural numbers p,

$$\|h_{2,p^*}\|_{L_p(-1/2,1/2)} \;=\; c_3(a)\,\frac{2\,((p-1)!)^{1/p}}{(2\,\pi)^{1/(2p)}},$$

and, for $a^2 > 1 + \frac{1}{p^*}$,

$$\begin{aligned} C_{1,p}(\nu_a) \;&\leq\; c_1(a) + c_3(a)\,\frac{2\,((p-1)!)^{1/p}}{(2\,\pi)^{1/(2p)}} \\ &=\; a^{1+1/p^*}\,(\sigma\,\sqrt{2\,\pi})^{1/p^*} + \frac{\sqrt{2\pi}\,a^{1+1/p^*}\,(a^2-1)\,\sigma^{1/p^*}}{p\,(a^2-2)+1}\,\frac{2\,((p-1)!)^{1/p}}{(2\,\pi)^{1/(2p)}} \\ &=\; a^{1+1/p^*}\,(\sigma\,\sqrt{2\,\pi})^{1/p^*}\,\left(1 + \frac{2\,(a^2-1)\,((p-1)!)^{1/p}}{p\,(a^2-2)+1}\right) < +\infty. \end{aligned}$$

For example, if $p = p^* = 2$, then

$$C_{1,2}(\nu_a) \;\leq\; a^{3/2}\sqrt{\sigma\sqrt{2\pi}}\,\left(2 + \frac{1}{2a^2-3}\right).$$

As a function of a, the upper bound on $C_{1,2}(\nu_a)$ attains its minimum at $a^* = 3/2$ and then

$$C_{1,2}(\nu_{a^*}) \;\leq\; 2\sqrt{6\sqrt{2\pi}}\,\sqrt{\sigma} = \sqrt{\sigma} \times 7.7562\ldots.$$

If p is not a natural number, we can estimate

$$\begin{aligned} \frac{1}{\sqrt{2\,\pi}}\,\int_{-\infty}^{\infty} |y|^{2\,p-1}\,\exp\left(-\frac{y^2}{2}\right)\,\mathrm{d}y \;&\leq\; C \,+\, \frac{1}{\sqrt{2\,\pi}}\,\int_{-\infty}^{\infty} |y|^{2\,\lceil p\rceil-1}\,\exp\left(-\frac{y^2}{2}\right)\,\mathrm{d}y \\ &=\; C \,+\, \frac{1}{\sqrt{2\,\pi}}\,2^{\lceil p\rceil}\,(\lceil p\rceil-1)! \end{aligned}$$

for some absolute constant $C > 0$. Then, $\|h_{2,p^*}\|_{L_p(-1/2,1/2)}$ and $C_{1,p}(\nu_a)$ can be estimated accordingly.

Numerical Test 11 Consider integration of the function $f(x) = |x|$, similar to Numerical Test 10. Then the integral to be computed is

$$\int_{-\infty}^{\infty} \frac{|x|}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \mathrm{d}x = \sqrt{\frac{2}{\pi}}.$$

In this case, our change of variables is defined as $x = \nu_a(t) := a\sqrt{2}\,\mathrm{erfinv}(2t)$, where $a \geq 1$, and erfinv is the inverse of the erf function. This results in the integral

$$\int_{-1/2}^{1/2} g_{f,\nu_a}(t)\,\mathrm{d}t \qquad \text{with} \qquad g_{f,\nu_a}(t) = a\,|\nu(t)| \exp\left(-\frac{\nu^2(t)}{2}\left(1 - \frac{1}{a^2}\right)\right).$$

Note that $g_{f,\nu_a} \in W_{1,\infty}$ for $a > \sqrt{2}$.

In the following table, we compare the absolute integration errors of the midpoint rule with n samples applied to g_{f,ν_a} with $a = a^*$ as in (23), $a = \sqrt{2}$, and $a = 1$.

n	$a = a^* = 1.70902\ldots$	$a = \sqrt{2}$	$a = 1$
10	$6.044012E-03$	$8.241433E-03$	$2.734692E-02$
10^2	$1.096395E-04$	$1.157302E-03$	$2.106636E-03$
10^3	$1.200953E-06$	$6.968052E-05$	$1.770735E-04$
10^4	$1.217389E-08$	$3.509887E-06$	$1.559486E-05$
10^5	$1.219963E-10$	$1.642630E-07$	$1.409149E-06$

5 γ-Weighted Spaces and MDM

We show in this section how the algorithms derived via the change of variables can be used in efficient implementation of the *Multivariate Decomposition Method* (*MDM* for short) that was introduced in [6] (see also [5]). Our presentation follows [11, 12], where more details can be found.

Consider the following γ-weighted space $\mathcal{F}_\gamma = \mathcal{F}_{\gamma,d,p,q}$ of functions $f : D \to \mathbb{R}$ with mixed first order partial derivatives bounded in $L_p(D^d)$ (as before) and for which the following norm of $\mathcal{F}_\gamma$ is finite,

$$\|f\|_{\mathcal{F}_\gamma} := \left[\sum_{\mathfrak{u}} \gamma_{\mathfrak{u}}^{-q}\, \|f^{(\mathfrak{u})}(\cdot_{\mathfrak{u}}; \mathbf{0})\|_{L_p(D^{\mathfrak{u}})}^q\right]^{1/q} < \infty.$$

Here, $q \in [1, \infty]$, the summation above is with respect to all subsets

$$\mathfrak{u} \subseteq \{1, 2, \ldots, d\},$$

$f^{(\mathfrak{u})}$ denotes $\prod_{j\in\mathfrak{u}} \frac{\partial}{\partial x_j} f$, the vector $(\boldsymbol{x}_{\mathfrak{u}}; \mathbf{0})$ is the d-dimensional vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)$ with the j-th component x_j set to zero whenever $j \notin \mathfrak{u}$, and $\gamma_{\mathfrak{u}}$ are given positive numbers quantifying importance of the subsets $\mathfrak{u}$. For $\mathfrak{u} = \emptyset$, we set $f^{(\emptyset)} \equiv f(0)$ and $\gamma_\emptyset = 1$. For simplicity, we consider only so-called *product weights*, introduced in [9], of the form

$$\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j,$$

where $\{\gamma_j\}_{j\geq 1}$ is a given non-increasing sequence of positive numbers.

Remark 12 The results can easily be extended to functions with infinitely many ($d = +\infty$) variables. Then the summation is with respect to all finite subsets $\mathfrak{u}$ of $\mathbb{N}$.

It is well known that any $f \in \mathcal{F}_\gamma$ has a unique *anchored decomposition* of the form

$$f(\boldsymbol{x}) \;=\; \sum_{\mathfrak{u}} f_{\mathfrak{u}}(\boldsymbol{x}),$$

where, for $\mathfrak{u} \neq \emptyset$, $f_{\mathfrak{u}}$ depends only on x_j with $j \in \mathfrak{u}$ and is anchored at zero, i.e.,

$$f_{\mathfrak{u}}(\boldsymbol{x}) = 0 \text{ if there is } j \in \mathfrak{u} \text{ such that } x_j = 0.$$

Moreover,

$$f_{\mathfrak{u}}^{(\mathfrak{u})} \;=\; f^{(\mathfrak{u})}(\cdot_{\mathfrak{u}}; \mathbf{0}), \quad \text{which implies that} \quad \|f\|_{\mathcal{F}_\gamma} \;=\; \left[\sum_{\mathfrak{u}} \gamma_{\mathfrak{u}}^{-q}\, \|f_{\mathfrak{u}}\|_{F_{\mathfrak{u},p}}^q\right]^{1/q} \quad \text{and} \quad f_{\mathfrak{u}} \in F_{\mathfrak{u},p},$$

where the spaces $F_{\mathfrak{u},p}$ are equivalent to $F_{d,p}$ for $d = |\mathfrak{u}|$ with the only difference that the functions in $F_{\mathfrak{u},p}$ depend on the variables x_j with $j \in \mathfrak{u}$. In particular, $F_{d,p} = F_{\{1,2,\ldots,d\},p}$. Therefore

$$I_{d,\varrho}(f) \;=\; \sum_{\mathfrak{u}} I_{|\mathfrak{u}|,\varrho}(f_{\mathfrak{u}}).$$

Suppose now that

$$\left[\sum_{j=1}^{\infty} \gamma_j^{q^*}\right]^{1/q^*} \;<\; \infty. \tag{24}$$

Following [7], one can show that for $\varepsilon > 0$ there is a set $\mathrm{Act}(\varepsilon)$ containing some $\mathfrak{u}$'s with cardinality $|\mathrm{Act}(\varepsilon)| = O(\varepsilon^{-1})$ such that

$$\sum_{\mathfrak{u} \notin \mathrm{Act}(\varepsilon)} |I_{|\mathfrak{u}|,\varrho}(f_{\mathfrak{u}})| \;\le\; \frac{\varepsilon}{2^{1/q^*}} \left\| \sum_{\mathfrak{u} \notin \mathrm{Act}(\varepsilon)} f_{\mathfrak{u}} \right\|_{\mathcal{F}_\gamma} \quad \text{and} \quad d(\varepsilon) \;:=\; \max_{\mathfrak{u} \in \mathrm{Act}(\varepsilon)} |\mathfrak{u}| \;=\; O\left(\frac{\ln(1/\varepsilon)}{\ln(\ln(1/\varepsilon))}\right).$$

As shown recently in [2], the absolute constants in the big-O notations above are very small, see also Example 13. Hence it is enough to aproximate the integrands $I_{|\mathfrak{u}|,\varrho}(f_{\mathfrak{u}})$ for $\mathfrak{u} \in \mathrm{Act}(\varepsilon)$ with the total error bounded by

$$\frac{\varepsilon}{2^{1/q^*}} \left\| \sum_{\mathfrak{u} \in \mathrm{Act}(\varepsilon)} f_{\mathfrak{u}} \right\|_{\mathcal{F}_\gamma}.$$

This can be achieved by using cubatures $Q_{|\mathfrak{u}|,\varrho,n_{\mathfrak{u}}}$ (see (3)) with appropriately chosen natural numbers $n_{\mathfrak{u}}$ such that

$$\left[\sum_{\mathfrak{u} \in \mathrm{Act}(\varepsilon)} \Big(\gamma_{\mathfrak{u}}\, C_{|\mathfrak{u}|,p}(\nu)\, \mathrm{error}(Q_{|\mathfrak{u}|;n_{\mathfrak{u}}}\,;\, W_{|\mathfrak{u}|,p})\Big)^{q^*}\right]^{1/q^*} \;\le\; \frac{\varepsilon}{2^{1/q^*}},$$

which follows from (4). Note that

$$\gamma_{\mathfrak{u}}\, C_{|\mathfrak{u}|,p}(\nu) \;=\; \prod_{j \in \mathfrak{u}} (\gamma_j\, C_{1,p}(\nu)),$$

due to Proposition 1. Hence, as shown in, e.g. [11], the sum of all $n_{\mathfrak{u}}$ is small,

$$\sum_{\mathfrak{u}\in \mathrm{Act}(\varepsilon)} n_{\mathfrak{u}} \;=\; O(\varepsilon^{-1}).$$

This means that the corresponding MDM uses altogether $O(1/\varepsilon)$ function values to approximate $O(1/\varepsilon)$ integrals, each with at most $d(\varepsilon) = O(\ln(1/\varepsilon)/\ln(\ln(1/\varepsilon)))$ variables.

We now illustrate this by the following special case.

Example 13 Let $D = \mathbb{R}_+$, $\varrho(x) = \exp(-x/\lambda)/\lambda$, $\gamma_j = 1/j^\beta$ with some positive β, and $q = 1$. Recall that then $\|I_{1,\varrho}\| = (\lambda/p^*)^{1/p^*}$ and, hence, we can take

$$\mathrm{Act}(\varepsilon) \;=\; \left\{\mathfrak{u} \,:\, \|I_{1,\varrho}\|^{|\mathfrak{u}|}\,\gamma_{\mathfrak{u}} \,>\, \varepsilon\right\} \;=\; \left\{\mathfrak{u} \,:\, \frac{(\lambda/p^*)^{|\mathfrak{u}|/p^*}}{\prod_{j\in\mathfrak{u}} j^\beta} \,>\, \varepsilon\right\},$$

for which

$$d(\varepsilon) \;=\; \max\left\{k \,:\, \frac{(\lambda/p^*)^{k/p^*}}{(k!)^\beta} \,>\, \varepsilon\right\}.$$

For instance for $p = p^* = 2$, $\lambda = 2$, and $\varepsilon = 10^{-4}$ we have:

β	2	3	4	5
$d(\varepsilon)$	4	3	3	3

Numerical Test 14 Let, similarly to Test 10, $D = \mathbb{R}_+$, $\varrho(x) = \exp(-x)$, and define, for $d \geq 1$, $f_d(\boldsymbol{x}) = \prod_{j=1}^d x_j$ for $\boldsymbol{x} = (x_1, \ldots, x_d) \in \mathbb{R}_+^d$. The value of the integral is then 1 and we have $\|f\|_{\infty,d} = 1$. Using the change of variables ν_a from (19), the corresponding integrand is

$$g_{d,a}(\boldsymbol{t}) \;=\; \prod_{j=1}^{d} \left(-a^2\,(\ln(1-t_j))\,(1-t_j)^{a-1}\right).$$

As integration rules, we use lattice rules[1] (cf. [8]) with $n = 2^k$, $k = 10, 11, 12, \ldots, 15$, points in $[0,1)^d$.

We compare the absolute integration errors for $a = a^*$ as in (20), $a = 1.5$, and $a = 1$, and $d = 3$ and $d = 4$. In view of Example 13, it is justified to concentrate on d in this range. The results below indicate that the approach taken in this paper yields effective improvements over the standard change of variables.

$d = 3$

n	$a = a^* = 2.4557\ldots$	$a = 1.5$	$a = 1$
2^{10}	$1.088922E-04$	$9.822891E-04$	$3.702216E-03$
2^{11}	$3.972304E-05$	$3.220787E-04$	$1.725302E-02$
2^{12}	$1.160874E-05$	$1.342448E-04$	$4.356446E-03$
2^{13}	$3.077676E-06$	$1.812985E-04$	$7.678733E-03$
2^{14}	$7.859542E-07$	$1.831772E-05$	$2.343056E-03$
2^{15}	$2.052312E-07$	$2.369181E-06$	$3.260093E-03$

[1]We use lattice rules with generating vectors taken from the website of Frances Y. Kuo. The generating vectors used in this example were generated for equal product weights $\gamma_j = 1$, referred to as "lattice-28001" at `http://web.maths.unsw.edu.au/~fkuo/lattice/index.html` .

$d = 4$			
n	$a = a^* = 2.4557\ldots$	$a = 1.5$	$a = 1$
2^{10}	$2.125335E-05$	$1.461441E-03$	$1.316315E-02$
2^{11}	$1.092869E-05$	$7.043893E-04$	$3.040979E-02$
2^{12}	$5.426712E-06$	$8.995698E-06$	$1.980920E-02$
2^{13}	$6.603896E-06$	$2.797430E-04$	$1.999552E-02$
2^{14}	$8.905416E-06$	$9.166504E-05$	$5.214687E-03$
2^{15}	$2.602460E-06$	$6.881108E-05$	$3.043182E-04$

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