Constructive Representation of Functions in N-Dimensional Sobolev Space*

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Abstract

We propose a new representation of functions in Sobolev spaces on an N-dimensional hyper-rectangle, expressing such functions in terms of their admissible derivatives, evaluated along lower-boundaries of the domain. These boundary values are either finite-dimensional or exist in the space L_2 of square-integrable functions – free of the continuity constraints inherent to Sobolev space. Moreover, we show that the map from this space of boundary values to the Sobolev space is given by an integral operator with polynomial kernel, and we prove that this map is invertible. Using this result, we propose a method for polynomial approximation of functions in Sobolev space, reconstructing such an approximation from polynomial projections of the boundary values. We prove that this approximation is optimal with respect to a discrete-continuous Sobolev norm, and show through numerical examples that it exhibits better convergence behavior than direct projection of the function. Finally, we show that this approach may also be adapted to use a basis of step functions, to construct accurate piecewise polynomial approximations that do not suffer from e.g. Gibbs phenomenon.

1. Introduction

We consider the basic question of the relation between a function and its highest-order partial derivative. In particular, given a differentiable function u, can we uniquely represent u by its highest-order derivative and a set of

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independent boundary values? Conversely, given these boundary values, can we reconstruct the associated function u from its highest-order derivative?

To illustrate, for a first-order differentiable function in a single variable, an answer to both of these questions is given by the fundamental theorem of calculus. This results proves that a differentiable function $u : [a, b] \to \mathbb{R}$ can be represented by its partial derivative $\partial_s u$ and the value of u at a single point in its domain, i.e. $u(s) = u(a) + \int_a^s \partial_s u(\theta) d\theta$. Moreover, given any $v_0 \in \mathbb{R}$ and $v_1 \in L_2[a, b]$ such that $u(s) = v_0 + \int_a^s v_1(\theta) d\theta$, we have $u(a) = v_0$ and $\partial_s u = v_1$. If the function is Nth-order differentiable, this result may be generalized using Cauchy's formula for repeated integration, uniquely expressing u in terms of its Nth-order derivative $\partial_s^N u$ and suitable boundary values. More generally, the theory of Green's functions tells us that for a wide variety of differential operators D, a function u in multiple variables can be expressed in terms of Du using an integral operator with a suitable kernel [1]. Unfortunately, establishing this kernel for a given operator D can be challenging in practice.

In this paper, we provide an explicit relation between a differentiable function $u : \Omega \to \mathbb{R}$ on a hyperrectangle $\Omega := \prod_{i=1}^N [a_i, b_i]$, and each of its derivatives. In particular, let $W_2^\delta[\Omega]$ denote the Sobolev space of δ-differentiable, square-integrable functions, so that $D^\alpha u = \frac{\partial^{\alpha_1}}{\partial s_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_N}}{\partial s_N^{\alpha_N}} u \in L_2[\Omega]$ for every $\alpha \in \mathbb{N}$ with $\alpha_i \leq \delta_i$ for all i. Then, any function $u \in W_2^\delta[\Omega]$ can be expressed in terms of its derivatives $D^\alpha u$, evaluated along lower boundaries of the hyperrectangle, as we show in the following theorem.

Theorem 1. *Suppose* $\mathbf{u} \in W_2^\delta[\Omega]$ *for* $\delta \in \mathbb{N}^N$ *and* $\Omega := \prod_{i=1}^N [a_i, b_i] \subseteq \mathbb{R}^N$. *Then*

$$\mathbf{u}(s) = \sum_{0 \leq \alpha \leq \delta} \big(\mathcal{G}_\alpha^\delta B^{\alpha - \delta} D^\alpha \mathbf{u}\big)(s), \qquad s \in \Omega,$$

where $B^\beta := \prod_{i=1}^N b_i^{\beta_i}$ *and* $\mathcal{G}_\alpha^\delta := \prod_{i=1}^N g_{i,\alpha_i}^{\delta_i}$, *with*

$$(b_i^{\beta_i}\mathbf{u})(s) = \begin{cases} \mathbf{u}(s_1, \ldots, a_i, \ldots, s_N), & \beta_i < 0, \\ \mathbf{u}(s_1, \ldots, s_i, \ldots, s_N), & \beta_i = 0, \end{cases}$$

$$(g_{i,\alpha_i}^{\delta_i}\mathbf{u})(s) = \begin{cases} \mathbf{p}_{\alpha_i}(s_i - a_i)\mathbf{u}(s), & \alpha_i < \delta_i, \\ \int_{a_i}^{s_i} \mathbf{p}_{\alpha_i - 1}(s_i - \theta)\mathbf{u}(s)|_{s_i = \theta} d\theta & \alpha_i = \delta_i, \end{cases}$$

where $\mathbf{p}_k(z) := \frac{z^k}{k!}$.

Moreover, for any $\{\mathbf{v}^\alpha \subseteq L_2[\Gamma^\alpha] \mid 0 \leq \alpha \leq \delta\}$ *on suitable* $\Gamma^\alpha \subseteq \Omega$, *if*

$$\mathbf{u}(s) = \sum_{0 \leq \alpha \leq \delta} \left(\mathcal{G}_\alpha^\delta \mathbf{v}^\alpha\right)(s), \qquad s \in \Omega,$$

then, $\mathbf{v}^\alpha = B^{\alpha-\delta} D^\alpha \mathbf{u}$ *for all* $0 \leq \alpha \leq \delta$.

Thm. 1 shows that any function $\mathbf{u} \in W_2^\delta[\Omega]$ can be represented uniquely by its partial derivatives $D^\alpha \mathbf{u}$ for $0 \leq \alpha \leq \delta$, evaluated at suitable (lower) boundaries of the domain. For example, consider a second-order differentiable function $u \in W_2^{(2,1)}[[a,b] \times [c,d]]$ in two variables. Then, the associated boundary values in Thm. 1 are given by

$$\begin{aligned}
B^{-(2,1)} D^{(0,0)} u &= u(a,c), & (B^{-(2,0)} D^{(0,1)} u)(y) &= \partial_y u(a,y), \\
B^{-(1,1)} D^{(1,0)} u &= \partial_x u(a,c), & (B^{-(1,0)} D^{(1,1)} u)(y) &= \partial_x \partial_y u(a,y), \\
(B^{-(0,1)} D^{(2,0)} u)(x) &= \partial_x^2 u(x,c), & (B^{(0,0)} D^{(2,1)} u)(x,y) &= \partial_x^2 \partial_y u(x,y),
\end{aligned}$$

and Thm. 1 implies

$$\begin{aligned}
u(x,y) &= u(a,c) + (x-a)\partial_x u(a,c) + \int_a^x (x-\theta)\partial_x^2 u(\theta,c) d\theta \\
&+ \int_c^y \partial_y u(a,\eta) d\eta + \int_c^y (x-a)\partial_x \partial_y u(a,\eta) d\eta + \int_a^x \int_c^y (x-\theta)\partial_x^2 \partial_y u(\theta,\eta) d\eta d\theta.
\end{aligned}$$

We prove Thm. 1 in Section 3. In the subsequent section, we then show how this result may be applied to perform optimal polynomial approximation of functions $\mathbf{u} \in W^\delta[\Omega]$, reconstructing such an approximation from a projection of the derivatives $B^{\alpha-\delta} D^\alpha \mathbf{u}$ onto a polynomial subspace. This approach has the advantage that, unlike a direct projection of $\mathbf{u}$ (using the L_2 inner product), it accurately captures each of the derivatives $D^\alpha \mathbf{u}$, thus converging in the Sobolev norm. Moreover, this approach can be adapted to perform projection using a basis of step functions, avoiding undesired oscillatory behavior inherent to smooth basis functions, whilst still capturing each of the derivatives of the function.

2. Notation

We denote the set of integers as $\mathbb{Z}$, and that of natural numbers as $\mathbb{N}$, writing $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. For $N \in \mathbb{N}$ and $\alpha, \beta \in \mathbb{Z}^N$, we write $\alpha \leq \beta$ if $\alpha_i \leq \beta_i$

for all $i \in \{1, \dots, N\}$, and we write $\alpha < \beta$ if $\alpha \leq \beta$ and $\alpha \neq \beta$. We write 0^N and 1^N for the vectors of all zeros and ones in $\mathbb{N}_0^N$, respectively.

Our focus in this paper will be on Sobolev spaces on a hyper-rectangle $\Omega := \Omega_1 \times \dots \Omega_N$, where $\Omega_i = [a_i, b_i] \subseteq \mathbb{R}$ for $i \in \{1, \dots, N\}$. To distinguish the boundaries and interior of this domain, we introduce the notation

$$\Omega^\beta := \Omega_1^{\beta_1} \times \dots \times \Omega_N^{\beta_N}, \qquad \Omega_i^{\beta_i} := \begin{cases} \{a_i\}, & \beta_i < 0, \\ (a_i, b_i), & \beta_i = 0, \\ \{b_i\}, & \beta_i > 0, \end{cases}$$

for all $\beta \in \mathbb{Z}^N$, so that $\Omega = \bigcup_{\beta \in \{-1,0,1\}^N} \Omega^\beta$. We will write $L_2[\Omega^\beta]$ for the Hilbert space of square-integrable functions on Ω^β. If Ω^β corresponds to a boundary of the domain, i.e. $\Omega_i^{\beta_i} = \{a_i\}$ or $\Omega_i^{\beta_i} = \{b_i\}$ for some i, we identify $L_2[\Omega^\beta]$ with the space of square-integrable functions along this boundary, so that e.g. $L_2[[a, b] \times \{c\}] \cong L_2[[a, b]]$ and $L_2[\{b\} \times [c, d]] \cong L_2[[c, d]]$. If Ω^β corresponds to a vertex of the hyper-rectangle, we let $L_2[\Omega^\beta] = \mathbb{R}$, so that e.g. $L_2[\{a\} \times \{d\}] \cong \mathbb{R}$.

For a suitably differentiable function $\mathbf{u} \in L_2[\Omega]$, we define the partial differential operator D^α as

$$D^\alpha \mathbf{u} = \partial_{s_1}^{\alpha_1} \cdots \partial_{s_N}^{\alpha_N} \mathbf{u}, \qquad \text{where} \qquad \partial_{s_i}^{\alpha_i} \mathbf{u} = \frac{\partial^{\alpha_i}}{\partial s_i^{\alpha_i}} \mathbf{u}.$$

For $\delta \in \mathbb{N}_0^N$, we define the Sobolev subspaces of δ-order differentiable functions on Ω as

$$W_2^\delta[\Omega] := \big\{ \mathbf{u} \in L_2[\Omega] \mid D^\alpha \mathbf{u} \in L_2[\Omega],\ \forall \alpha \in \mathbb{N}_0^N : \alpha \leq \delta \}, \tag{1}$$

with the associated Sobolev norm $\|\mathbf{u}\|_{W_2^\delta} := \sum_{0^N \leq \alpha \leq \delta} \|\mathbf{u}\|_{L_2}$. Note that the Sobolev space as defined here differs from that more commonly used in the literature, wherein functions $\mathbf{u}$ in the Sobolev space are required to be differentiable only up to some order $k := \|\delta\|_1$, so that $D^\alpha \mathbf{u} \in L_2$ for all $\alpha \in \mathbb{N}_0^N$ for which $\|\alpha\|_1 \leq k$. However, defining a Sobolev space as in (1), we ensure that the derivative $D^\alpha \mathbf{u}$ of any $\mathbf{u} \in W^\delta[\Omega]$ is classically defined at the boundaries $s_i = a_i$ and $s_i = b_i$ whenever $\alpha_i < \delta_i$, whereas such boundary values may be only weakly defined if e.g. $\|\alpha\|_1 < \|\delta\|_1$. Then, for a function $\mathbf{u} \in W^\delta[\Omega]$ with suitable $\delta > 0^N$, we can define a boundary operator $B^\beta : \mathbf{u} \mapsto \mathbf{u}|_{\Omega^\beta}$ as the restriction of this function to the subdomain Ω^β.

3. Proof of Main Result

In this section, we rephrase and prove the main theorem.

Theorem 1. *Suppose* $\mathbf{u} \in W_2^\delta[\Omega]$ *for* $\delta \in \mathbb{N}_0^N$ *and* $\Omega := \prod_{i=1}^N [a_i, b_i] \subseteq \mathbb{R}^N$. *Then*

$$\mathbf{u}(s) = \sum_{0^N \leq \alpha \leq \delta} \big(\mathcal{G}_\alpha^\delta B^{\alpha-\delta} D^\alpha \mathbf{u}\big)(s), \qquad s \in \Omega, \tag{2}$$

where $\mathcal{G}_\alpha^\delta := \prod_{i=1}^N g_{i,\alpha_i}^{\delta_i}$ *where for all* $i \in \{1, \ldots, N\}$,

$$(g_{i,\alpha_i}^{\delta_i}\mathbf{u})(s) = \begin{cases} \mathbf{u}(s), & 0 = \alpha_i = \delta_i, \\ \mathbf{p}_{\alpha_i}(s_i - a_i)\mathbf{u}(s), & 0 \leq \alpha_i < \delta_i, \\ \int_{a_i}^{s_i} \mathbf{p}_{\alpha_i - 1}(s_i - \theta)\mathbf{u}(s)|_{s_i=\theta} d\theta & 0 < \alpha_i = \delta_i. \end{cases}$$

Moreover, for any $\{\mathbf{v}^\alpha \in L_2[\Omega^{\alpha-\delta}] \mid 0^N \leq \alpha \leq \delta\}$, *if*

$$\mathbf{u}(s) = \sum_{0 \leq \alpha \leq \delta} \big(\mathcal{G}_\alpha \mathbf{v}^\alpha\big)(s), \qquad s \in \Omega, \tag{3}$$

then, $\mathbf{v}^\alpha = B^{\alpha-\delta} D^\alpha \mathbf{u}$ *for all* $0^N \leq \alpha \leq \delta$.

The theorem shows that any function $\mathbf{u} \in W^\delta[\Omega]$ can be expressed in terms of each of its partial derivatives $D^\alpha \mathbf{u}$, evaluated along a suitable lower boundary $\Omega^{\alpha-\delta}$ of the domain. To prove this result, we first show that we can express such a function $\mathbf{u}$ in terms of its derivatives $\partial_{s_i}^{\alpha_i}\mathbf{u}$ with respect to just a single variable s_i, evaluated at the boundary $s_i = a_i$. To illustrate, consider a function $u \in W^{(2,1)}[[a, b] \times [c, d]]$ in just two variables. Applying the fundamental theorem of calculus twice, we can expand this function along $x \in [a, b]$ as

$$\begin{aligned} u(x, y) &= u(a, y) + \int_a^x \partial_x u(\theta, y) d\theta \\ &= u(a, y) + [x - a]\partial_x u(a, y) + \int_a^x \int_a^\theta \partial_x^2 u(\eta, y) d\eta d\theta. \end{aligned}$$

Using Cauchy's formula for repeated integration, the double integral in this expansion can be expressed as a single integral, and we obtain a representation of u as

$$u(x, y) = u(a, y) + [x - a]\partial_x u(a, y) + \int_a^x [x - \theta]\partial_x^2 u(\theta, y) d\theta.$$

The following lemma generalizes this result to functions in N variables, differentiable up to arbitrary order $\delta_i \in \mathbb{N}_0$ with respect to variable $s_i \in [a_i, b_i]$, for any $i \in \{1, \ldots, N\}$. In this lemma, we will write $\mathrm{e}_i \in \mathbb{R}^N$ for the ith standard Euclidean basis vector in $\mathbb{R}^N$.

Lemma 2. *Suppose* $\mathbf{u} \in W_2^{\delta}[\Omega]$ *for* $\delta \in \mathbb{N}_0^N$ *and* $\Omega := \prod_{i=1}^N [a_i, b_i] \subseteq \mathbb{R}^N$. *Then, for any* $i \in \{1, \ldots, N\}$,

$$\mathbf{u}(s) = \sum_{k=0}^{\delta_i} \big(g_{i,k}^{\delta_i} b_i^{k-\delta_i} \partial_{s_i}^k \mathbf{u}\big)(s), \qquad s \in \Omega, \tag{4}$$

where $g_{i,k}^{\delta_i}$ *is as in Thm. 1 and* $b^{\delta_i - k} = B^{(\delta_i - k)e_i}$, *so that*

$$(b_i^{\beta_i}\mathbf{u})(s) = \begin{cases} \mathbf{u}(s_1, \ldots, a_i, \ldots, s_N), & \beta_i < 0, \\ \mathbf{u}(s_1, \ldots, s_i, \ldots, s_N), & \beta_i = 0. \end{cases}$$

Moreover, for any $\{\mathbf{v}^k \in L_2[\Omega^{(k-\delta_i)e_i}] \mid 0 \le k \le \delta_i\}$, *if*

$$\mathbf{u}(s) = \sum_{k=0}^{\delta_i} \big(g_{i,k}^{\delta_i} \mathbf{v}^k\big)(s), \qquad s \in \Omega, \tag{5}$$

then, $\mathbf{v}^k = b_i^{k-\delta_i} \partial_{s_i}^k \mathbf{u}$ *for all* $0 \le k \le \delta_i$.

Proof. Without loss of generality, fix $i = 1$, re-ordering the variables s_i if necessary. Let $\delta \in \mathbb{N}_0^N$. We prove the result through induction on the order of differentiability $\delta_1 \in \mathbb{N}_0$.

Base case $\boldsymbol{\delta_1 = 0}$: For the case $\delta_1 = 0$, the result holds trivially, since $g_{1,0}^0 \mathrm{b}_1^0 \partial_{s_1}^0 = I$ is an identity operator.

Induction step $\boldsymbol{\delta_1 > 0}$: To show that the result holds for all $\delta_1 \in \mathbb{N}_0$,

fix arbitrary $\tilde{\delta}_1 \in \mathbb{N}_0$. Then, for every $\{\mathbf{v}^k \in L_2[\Omega^{(k-\tilde{\delta}_1)\mathrm{e}_1}] \mid 0 \le k \le \tilde{\delta}_1\}$,

$$\begin{aligned}
&\int_{a_1}^{s_1} \left(\sum_{k=0}^{\tilde{\delta}_1} \big(g_{1,k}^{\tilde{\delta}_1} \mathbf{v}^k\big)(\eta) \right) d\eta \\
&\qquad = \sum_{k=0}^{\tilde{\delta}_1 - 1} \int_{a_1}^{s_1} \mathbf{p}_k(\eta - a_1)\mathbf{v}^k \, d\eta + \int_{a_1}^{s_1} \int_{a_1}^{\eta} \mathbf{p}_{\tilde{\delta}_1 - 1}(\eta - \theta)\mathbf{v}^{\tilde{\delta}_1}(\theta) \, d\theta d\eta \\
&\qquad = \sum_{k=0}^{\tilde{\delta}_1 - 1} \int_{a_1}^{s_1} \mathbf{p}_k(\eta - a_1) d\eta \, \mathbf{v}^k + \int_{a_1}^{s_1} \int_{\theta}^{s_1} \mathbf{p}_{\tilde{\delta}_1 - 1}(\eta - \theta) d\eta \, \mathbf{v}^{\tilde{\delta}_1}(\theta) d\theta \\
&\qquad = \sum_{k=0}^{\tilde{\delta}_1 - 1} \mathbf{p}_{k+1}(s_1 - a_1)\mathbf{v}^k + \int_{a_1}^{s_1} \mathbf{p}_{\tilde{\delta}_1}(s_1 - \theta)\mathbf{v}^{\tilde{\delta}_1}(\theta) d\theta \\
&\qquad\qquad = \sum_{k=0}^{\tilde{\delta}_1} \big(g_{1,k+1}^{\tilde{\delta}_1 + 1} \mathbf{v}^k\big)(s_1), \qquad (6)
\end{aligned}$$

where we note that $\int_a^x \mathbf{p}_k(\eta - a) d\eta = \mathbf{p}_{k+1}(x - a)$ by definition of the polynomials $\mathbf{p}_k$. Now, assume for induction that the lemma holds for $\tilde{\delta} \in \mathbb{N}_0^N$, and let $\delta = \tilde{\delta} + \mathrm{e}_1$ so that $\delta_1 = \tilde{\delta}_1 + 1$. Fix arbitrary $\mathbf{u} \in W_2^{\delta}[\Omega]$. To prove that (4) holds for $\mathbf{u}$, note that $\partial_{s_1}\mathbf{u} \in W_2^{\delta - \mathrm{e}_1}[\Omega] = W_2^{\tilde{\delta}}[\Omega]$. Applying the fundamental theorem of calculus, invoking the induction hypothesis, and finally using the relation in (6), it follows that

$$\begin{aligned}
\mathbf{u}(s_1) &= \mathbf{u}(a_1) + \int_{a_1}^{s_1} \partial_{s_1}\mathbf{u}(\eta) d\eta \\
&= \mathbf{u}(a_1) + \int_{a_1}^{s_1} \left(\sum_{k=0}^{\tilde{\delta}_1} g_{1,k}^{\tilde{\delta}_1} \mathrm{b}_1^{k - \tilde{\delta}_1} \partial_{s_1}^k \big(\partial_{s_1}\mathbf{u}\big) \right)(\eta) d\eta \\
&= g_{1,0}^{\delta_1} \mathrm{b}_1^{-\delta_1} \partial_{s_1}^0 \mathbf{u} + \sum_{k=0}^{\tilde{\delta}_1} \Big(g_{1,k+1}^{\tilde{\delta}_1 + 1} \mathrm{b}_1^{k - \tilde{\delta}_1} \partial_{s_1}^k \big(\partial_{s_1}\mathbf{u}\big) \Big)(s_1) \\
&= g_{1,0}^{\delta_1} \mathrm{b}_1^{-\delta_1} \partial_{s_1}^0 \mathbf{u} + \sum_{k=0}^{\delta_1 - 1} \Big(g_{1,k+1}^{\delta_1} \mathrm{b}_1^{k+1-\delta_1} \partial_{s_1}^{k+1} \mathbf{u} \Big)(s_1) = \sum_{k=0}^{\delta_1} \Big(g_{1,k}^{\delta_1} \mathrm{b}_1^{k-\delta_1} \partial_{s_1}^k \mathbf{u} \Big)(s_1).
\end{aligned}$$

Thus (4) holds. To see that also the implication for (5) holds, suppose that for some $\{\mathbf{v}^k \in L_2[\Omega^{(k-\delta_i)\mathrm{e}_i}] \mid 0 \le k \le \delta_1\}$, we have $\mathbf{u}(s_1) = \sum_{k=0}^{\delta_1} \big(g_{1,k}^{\delta_1} \mathbf{v}^k\big)(s_1)$.

Then, using Eqn. (6),

$$\mathbf{u}(s_1) = \mathbf{v}^0 + \sum_{k=0}^{\delta_1-1} \big(g_{1,k+1}^{\delta_1} \mathbf{v}^{k+1}\big)(s_1) = \mathbf{v}^0 + \int_{a_1}^{s_1} \sum_{k=0}^{\delta_1-1} \big(g_{1,k}^{\delta_1-1} \mathbf{v}^{k+1}\big)(\theta) d\theta.$$

It follows that

$$\mathrm{b}^{-\delta_1} \partial_{s_1}^0 \mathbf{u} = \mathbf{u}(a_1) = \mathbf{v}^0, \qquad \text{and} \qquad \partial_{s_1} \mathbf{u} = \sum_{k=0}^{\delta_1-1} \big(g_{1,k}^{\delta_1-1} \mathbf{v}^{k+1}\big).$$

By the induction hypothesis, then, for all $0 \le k \le \tilde{\delta}_1 = \delta_1 - 1$,

$$\mathbf{v}^{k+1} = \mathrm{b}_1^{k-(\delta_1-1)} \partial_{s_1}^k (\partial_{s_1} \mathbf{u}) = \mathrm{b}_1^{(k+1)-\delta_1} \partial_{s_1}^{k+1} \mathbf{u},$$

whence $\mathbf{v}^k = \mathrm{b}_1^{k-\delta_1} \partial_{s_1}^k \mathbf{u}$ for every $0 \le k \le \delta_1$. Thus, for $\delta_1 = \tilde{\delta}_1 + 1 \in \mathbb{N}_0$, both implications of the lemma hold. By induction, the lemma holds for all $\delta_1 \in \mathbb{N}_0$, and hence all $\delta \in \mathbb{N}_0^N$.

Lemma 2 shows that a function $\mathbf{u} \in W_2^\delta[\Omega]$ can be expressed in terms of its partial derivatives $\partial_{s_i}^{\alpha_i} \mathbf{u}$ with respect to a single variable s_i, using a suitable integral operator along $\Omega_i = [a_i, b_i]$. For example, a function $u \in W^{(2,1)}[[a,b] \times [c,d]]$ in two variables can be expressed in terms of its partial derivatives $\partial_x^k u$ for $0 \le k \le 2$ as

$$u(x,y) = u(a,y) + [x-a]\partial_x u(a,y) + \int_a^x [x-\theta] \partial_x^2 u(\theta, y) d\theta,$$

or in terms of its derivatives $\partial_y^k u$ for $0 \le k \le 1$ as

$$u(x,y) = u(x,c) + \int_c^y \partial_y u(x,\theta) d\theta.$$

Combining these expansions, it follows that we can express the function u in terms of all of its partial derivatives $D^{(i,j)} u = \partial_x^i \partial_y^j u$ for $(0,0) \le (i,j) \le (2,1)$ as

$$\begin{aligned} u(x,y) = u(a,c) + [x-a]\partial_x u(a,c) + \int_a^x [x-\theta] \partial_x^2 u(\theta, c) d\theta \\ + \int_c^y \partial_y u(a,\eta) d\eta + \int_c^y [x-a] \partial_x \partial_y u(a,\eta) d\eta + \int_a^x \int_c^y [x-\theta] \partial_x^2 \partial_y u(\theta,\eta) d\eta d\theta. \end{aligned} \tag{7}$$

Thm. 1 generalizes this result to functions $\mathbf{u} \in W_2^\delta[\Omega]$ in N variables, differentiable up to arbitrary order with respect to each variable. The proof of the result follows by applying Lemma 2 along each variable of the function.

Proof of Theorem 1. To prove that the theorem holds for arbitrary $\delta \in \mathbb{N}_0^N$, let $J \in \{0, \ldots, N\}$, and suppose that $\delta_i = 0$ for all $i \in \{J+1, \ldots, N\}$. Then, it suffices to show that the theorem holds for $J = N$, which we will prove through induction on the value of J.

Base case $J = 0$: For $J = 0$, we have $\delta = 0^N$, so that $G_\alpha^\delta B^{\alpha-\delta} D^\alpha = I$ for all $0^N \leq \alpha \leq \delta = 0^N$. In this case, the result holds trivially.

Induction step $J > 1$: Suppose for induction that the theorem holds for some $\tilde{J} \in \{0, \ldots, N-1\}$, and let $J = \tilde{J} + 1$. Let $\delta \in \mathbb{N}_0^N$ be such that $\delta_i = 0$ for $i > J$, and let $\tilde{\delta} = \delta - \delta_J \mathrm{e}_J \in \mathbb{N}_0^N$, so that $\tilde{\delta}_i = \delta_i$ for $i \leq J-1$, and $\tilde{\delta}_i = 0$ for $i > J-1$. Then, for every $0^N \leq \tilde{\alpha} \leq \tilde{\delta}$ we have

$$\mathcal{G}_{\tilde{\alpha}}^{\tilde{\delta}} = \prod_{i=1}^{J-1} g_{i,\tilde{\alpha}_i}^{\delta_i}, \qquad B^{\tilde{\alpha}-\tilde{\delta}} = \prod_{i=1}^{J-1} \mathrm{b}_i^{\tilde{\alpha}_i - \delta_i}, \qquad D^{\tilde{\alpha}} = \prod_{i=1}^{J-1} \partial_{s_i}^{\tilde{\alpha}_i}.$$

Now, fix arbitrary $\mathbf{u} \in W_2^\delta[\Omega] \subseteq W_2^{\tilde{\delta}}[\Omega]$. Invoking the induction hypothesis, and applying Lem. 2, it follows that

$$\begin{aligned}
\mathbf{u} &= \sum_{0^N \leq \tilde{\alpha} \leq \tilde{\delta}} \left(\mathcal{G}_{\tilde{\alpha}}^{\tilde{\delta}} B^{\tilde{\alpha}-\tilde{\delta}} D^{\tilde{\alpha}} \mathbf{u}\right) \\
&= \sum_{0^N \leq \tilde{\alpha} \leq \tilde{\delta}} \left(\mathcal{G}_{\tilde{\alpha}}^{\tilde{\delta}} B^{\tilde{\alpha}-\tilde{\delta}} D^{\tilde{\alpha}} \left(\sum_{\alpha_J=0}^{\delta_J} \left(g_{J,\alpha_J}^{\delta_J} \mathrm{b}_J^{\alpha_J - \delta_J} \partial_{s_J}^{\alpha_J} \mathbf{u} \right) \right) \right) \\
&= \sum_{0^N \leq \alpha \leq \delta} \left(\prod_{i=1}^{J} g_{i,\alpha_i}^{\delta_i} \right) \left(\prod_{i=1}^{J} \mathrm{b}_i^{\alpha_i - \delta_i} \right) \left(\prod_{i=1}^{J} \partial_{s_i}^{\alpha_i} \right) \mathbf{u} \qquad = \sum_{0^N \leq \alpha \leq \delta} \left(\mathcal{G}_\alpha^\delta B^{\alpha-\delta} D^\alpha \mathbf{u} \right).
\end{aligned}$$

Hence $\mathbf{u}$ satisfies (2). To see that the implication given by (3) also holds, let $\{\mathbf{v}^\alpha \in L_2[\Omega^{\alpha-\delta}] \mid 0^N \leq \alpha \leq \delta\}$ be such that

$$\mathbf{u} = \sum_{0^N \leq \alpha \leq \delta} \left(\mathcal{G}_\alpha^\delta \mathbf{v}^\alpha \right) = \sum_{0^N \leq \tilde{\alpha} \leq \tilde{\delta}} \left(\mathcal{G}_{\tilde{\alpha}}^{\tilde{\delta}} \left(\sum_{\alpha_J=0}^{\delta_J} g_{J,\alpha_J}^{\delta_J} \mathbf{v}^\alpha \right) \right),$$

where $\alpha = \tilde{\alpha} + \alpha_J \mathrm{e}_J$. Then, by the induction hypothesis,

$$\sum_{\alpha_J=0}^{\delta_J} g_{J,\alpha_J}^{\delta_J} \mathbf{v}^\alpha = B^{\tilde{\alpha}-\tilde{\delta}} D^{\tilde{\alpha}} \mathbf{u}, \qquad 0^N \leq \tilde{\alpha} \leq \tilde{\delta}.$$

By Lemma 2, it follows that for all $0^N \leq \alpha \leq \delta$,

$$\mathbf{v}^\alpha = \mathrm{b}_J^{\alpha_J - \delta_J} \partial_{s_J}^{\alpha_J} \left(B^{\tilde{\alpha}-\tilde{\delta}} D^{\tilde{\alpha}} \mathbf{u} \right) = B^{\alpha-\delta} D^\alpha \mathbf{u}.$$

Thus, for the given $J = \tilde{J}+1 \in \{0, \dots, N\}$, both implications of the theorem hold. By induction, we conclude that the theorem holds for $J = N$, and thus for all $\delta \in \mathbb{N}_0^N$.

Thm. 1 shows that a differentiable function $\mathbf{u}$ is uniquely defined by its derivatives $D^\alpha \mathbf{u}$ for $0^N \leq \alpha \leq \delta$, evaluated at the lower boundaries $\Omega^{\alpha-\delta}$ of the domain. However, it is clear that a similar expansion of $\mathbf{u}$ may be given in terms of the derivatives $D^\alpha \mathbf{u}$ along upper boundaries $\Omega^{\delta-\alpha}$. For example, just as $u \in W_2^{(2,1)}[[a,b] \times [c,d]]$ can be expressed in terms of its derivatives at $x = a$ and $y = c$ as in (7), so too can it be expressed in terms of its derivatives at $x = b$ and $y = d$ as

$$u(x,y) = u(b,d) - [b-x]\partial_x u(b,d) - \int_x^b [x-\theta]\partial_x^2 u(\theta,d)d\theta$$
$$- \int_y^d \partial_y u(b,\eta)d\eta + \int_y^d [b-x]\partial_x\partial_y u(b,\eta)d\eta + \int_x^b \int_y^d [x-\theta]\partial_x^2\partial_y u(\theta,\eta)d\eta d\theta.$$

Such different expansions of $\mathbf{u}$ in terms of different boundary values are of particular interest when considering functions constrained by boundary conditions, in which case the value of certain terms $B^\beta D^\alpha \mathbf{u}$ is known. Given sufficient and suitable boundary conditions, then, Thm. 1 proves that there exists a unique map between $\mathbf{u}$ and its highest-order derivative $D^\delta \mathbf{u}$. We leave a full derivation of such a relation for future works.

4. Polynomial Approximation of Functions in Sobolev Space

Thm. 1 offers an alternative representation of functions $\mathbf{u} \in W_2^\delta[\Omega]$ on the hyperrectangle $\Omega = \prod_{i=1}^N [a_i, b_i]$ in terms of their derivatives $D^\alpha \mathbf{u}$ along lower boundaries $\Omega^{\alpha-\delta}$ of the domain. The benefit of this representation is that the boundary values $B^{\alpha-\delta} D^\alpha \mathbf{u} \in L_2[\Omega^{\alpha-\delta}]$ in the expansion are elements of L_2 rather than W_2^δ, and therefore not required to be differentiable or even continuous. Specifically, defining an aggregate space of square-integrable functions

$$\mathbf{L}_2^\delta[\Omega] = \prod_{0^N \leq \alpha \leq \delta} L_2[\Omega^{\alpha-\delta}],$$

Thm. 1 shows that there exists a bijective map $\mathcal{G} : \mathbf{L}_2^\delta[\Omega] \to W_2^\delta[\Omega]$ from this space to the Sobolev space, where $\mathcal{G}$ is an integral operator with polynomial kernel. Using this bijection, analysis, approximation, and simulation of functions in $W_2^\delta[\Omega]$ may be performed in the less restrictive space $\mathbf{L}_2^\delta[\Omega]$.

In this section, we illustrate one application of Thm. 1, concerning polynomial approximation of functions in Sobolev space. In particular, rather than constructing a polynomial approximation for $\mathbf{u} \in W_2^\delta$ directly, we propose to approximate each of the derivatives $B^{\alpha-\delta}D^\alpha \mathbf{u}$, and reconstruct an approximation of $\mathbf{u}$ using Thm. 1. We show how this may be achieved using a basis of Legendre polynomials in the following subsection, as well as using step functions in Subsection 4.2. In each case, we assume the domain $\Omega = \prod_{i=1}^N [-1, 1]$ to a be a hypercube for ease of notation.

4.1. Approximation using Legendre Polynomials

As a first method for approximation of functions $\mathbf{u} \in W_2^\delta[\Omega]$, we consider projection using Legendre polynomials. These functions may be recursively defined for $x \in [-1, 1]$ as

$$\begin{aligned} \phi^0(x) &= 1, & \phi^1(x) &= x, \\ \phi^{k+1}(x) &= \frac{2k+1}{k+1}\phi^k(x) - \frac{k}{k+1}\phi^{k-1}(x), & k &\geq 1, \end{aligned}$$

and are orthogonal with respect to the standard L_2 inner product, satisfying

$$\int_{-1}^{1} \phi^m(x)\phi^n(x)dx = \begin{cases} \frac{1}{m+\frac{1}{2}}, & m = n, \\ 0, & \text{else.} \end{cases}$$

Letting $\boldsymbol{\phi}^d(s) := \prod_{i=1}^N \sqrt{d_i + \frac{1}{2}}\, \phi^{d_i}(s_i)$ for $d \in \mathbb{N}_0^N$, we can thus project a function $\mathbf{u} \in W_2^\delta[\Omega]$ onto the space $\mathbb{R}^d[\Omega]$ of polynomials of degree at most $d_i \in \mathbb{N}$ in variables $s_i \in \Omega_i$ as

$$P_d\mathbf{u} = \sum_{0^N \leq \alpha \leq d} c_\alpha \boldsymbol{\phi}^\alpha, \qquad \text{where} \qquad c_\alpha := \int_\Omega \mathbf{u}(s)\boldsymbol{\phi}^\alpha(s)ds. \tag{8}$$

This projection $P_d\mathbf{u}$ offers an L_2-optimal polynomial approximation of $\mathbf{u}$, in the sense that

$$\|\mathbf{u} - P_d\mathbf{u}\|_{L_2} = \min_{\mathbf{v} \in \mathbb{R}^d[\Omega]} \|\mathbf{u} - \mathbf{v}\|_{L_2}. \tag{9}$$

Moreover, in the case that $\delta = \delta_0 \cdot 1^N$ and $d = d_0 \cdot 1^N$, the error in the projection of $\mathbf{u} \in W_2^\delta[\Omega]$ is bounded as [2]

$$\|\mathbf{u} - P_d\mathbf{u}\|_{L_2} \leq C_0 d_0^{-\delta_0} \|\mathbf{u}\|_{W_2^\delta},$$

for some constant C_0, so that the error decays as $\mathcal{O}(d_0^{-\delta_0})$. Unfortunately, such decay is not guaranteed for the Sobolev norm of the error, which is bounded only as [3, 4]

$$\|\mathbf{u} - P_d\mathbf{u}\|_{W_2^\gamma} \leq C_\gamma d_0^{2\gamma_0-\delta_0-\frac{1}{2}}\|\mathbf{u}\|_{W_2^\delta}, \qquad 0 \leq \gamma_0 \leq \delta_0 \in \mathbb{N},$$

for $\gamma = \gamma_0 \cdot 1^N$. This bound does not guarantee convergence of the error in terms of the Sobolev norm, and indeed, the Sobolev norm of the error may actually increase with the degree of the polynomials. Instead, accurate approximation in terms of the Sobolev norm requires projecting not just the function $\mathbf{u}$, but also its derivatives $D^\alpha\mathbf{u}$. Although this can be achieved using a Sobolev inner product with suitable polynomial basis [5, 6, 7, 8], we propose to instead use Thm. 1, to reconstruct an approximation of $\mathbf{u}$ from L_2 projections of its derivatives $\mathbf{v}^\alpha = B^{\alpha-\delta}D^\alpha\mathbf{u}$. In particular, if $\mathbf{u} = \sum_{0^N \leq \alpha \leq \delta} \mathcal{G}_\alpha^\delta \mathbf{v}^\alpha$, we can project each $\mathbf{v}^\alpha \in L_2[\Omega^{\alpha-\delta}]$ onto $\mathbb{R}^d[\Omega^{\alpha-\delta}]$ as

$$P_{\kappa_d^\beta}\mathbf{v}^{\beta+\delta} = \sum_{0^N \leq \gamma \leq \kappa_d^\beta} c_\gamma \boldsymbol{\phi}^\gamma, \qquad \text{where} \qquad c_\gamma := \int_{\Omega^\beta} \mathbf{u}(s)\boldsymbol{\phi}^\gamma(s)ds,$$

where we define $\kappa_d^\beta \in \mathbb{N}_0^N$ by $(\kappa_d^\beta)_i := \begin{cases} d_i, & \beta_i = 0, \\ 0, & \text{else}, \end{cases}$ for $-\delta \leq \beta \leq 0^N$, so that e.g. $P_{\kappa_d^\beta}\mathbf{v}^{\beta+\delta} = c_{0^N}\boldsymbol{\phi}^{0^N} = \mathbf{v}^{\beta+\delta}$ when $\mathbf{v}^{\beta+\delta} \in \mathbb{R}$ is finite-dimensional. Then, for any $0^N \leq \gamma \leq \delta$ and $d \in \mathbb{N}_0^N$, we can construct an *order-γ Sobolev projection* of $\mathbf{u}$ onto $\mathbb{R}^{d+\gamma}[\Omega]$ as

$$P_d^\gamma \mathbf{u} := \sum_{0^N \leq \alpha \leq \gamma} \mathcal{G}_\alpha^\gamma \left(P_{\kappa_d^{\alpha-\gamma}}\left[B^{\alpha-\gamma}D^\alpha\mathbf{u}\right]\right). \tag{10}$$

Approximating $\mathbf{u} \in W_2^\delta[\Omega]$ in this manner is equivalent to projecting the function onto a polynomial subspace using a discrete-continuous Sobolev inner product [9]. In particular, defining a discrete-continuous norm on $W_2^\delta[\Omega]$ as

$$\|\mathbf{u}\|_{\tilde{W}_2^\delta} := \sum_{0^N \leq \alpha \leq \delta} \left\|B^{\alpha-\delta}D^\alpha\mathbf{u}\right\|_{L_2}, \qquad \mathbf{u} \in W_2^\delta[\Omega], \tag{11}$$

the following proposition shows that the approximation $P_d^\delta\mathbf{u}$ is optimal with respect to this norm.

Proposition 3. *Let $\mathbf{u} \in W_2^\delta[\Omega]$ for some $\delta \in \mathbb{N}_0^N$, and define the polynomial approximation $P_d^\gamma \mathbf{u}$ for $0^N \leq \gamma \leq \delta$ as in* (10)*. Then, for every $d \in \mathbb{N}_0^N$,*

$$\|\mathbf{u} - P_d^\gamma \mathbf{u}\|_{\tilde{W}_2^\gamma} = \min_{\mathbf{v} \in \mathbb{R}^{d+\gamma}[\Omega]} \|\mathbf{u} - \mathbf{v}\|_{\tilde{W}_2^\gamma}$$

where the norm $\|.\|_{\tilde{W}_2^\gamma}$ is as defined in (11)*.*

Proof. Fix arbitrary $\mathbf{u} \in W_2^\delta[\Omega]$ and $\mathbf{v} \in \mathbb{R}^{d+\gamma}[\Omega]$. Then $B^{\alpha-\gamma} D^\alpha \mathbf{u} \in W_2^{\delta-\alpha}[\Omega^{\alpha-\gamma}]$ and $B^{\alpha-\gamma} D^\alpha \mathbf{v} \in \mathbb{R}^{d+\gamma-\alpha}[\Omega^{\alpha-\gamma}]$ for every $0^N \leq \alpha \leq \gamma$. By optimality of the projection P_d in $L_2[\Omega]$ (Eqn. (9)), it follows that

$$\begin{aligned}
\|\mathbf{u} - \mathbf{v}\|_{\tilde{W}_2^\gamma} &= \sum_{0^N \leq \alpha \leq \gamma} \left\| B^{\alpha-\gamma} D^\alpha \mathbf{u} - B^{\alpha-\gamma} D^\alpha \mathbf{v} \right\|_{L_2} \\
&\geq \sum_{0^N \leq \alpha \leq \gamma} \left\| B^{\alpha-\gamma} D^\alpha \mathbf{u} - P_{\kappa_d^{\alpha-\gamma}} [B^{\alpha-\gamma} D^\alpha \mathbf{u}] \right\|_{L_2} \\
&= \sum_{0^N \leq \alpha \leq \gamma} \left\| B^{\alpha-\gamma} D^\alpha \big(\mathbf{u} - P_d^\gamma \mathbf{u}\big) \right\|_{L_2} \qquad = \|\mathbf{u} - P_d^\gamma \mathbf{u}\|_{\tilde{W}_2^\gamma} .
\end{aligned}$$

where we remark that $B^{\alpha-\gamma} D^\alpha (P_d^\gamma \mathbf{u}) = P_{\kappa_d^{\alpha-\gamma}} [B^{\alpha-\gamma} D^\alpha \mathbf{u}]$ by Thm. 1 and Eqn. (10).

Numerical Example

To illustrate the proposed polynomial approximation method, we apply it to a univariate function $u \in W_2^5[-1, 1]$ defined by

$$u(s) = \frac{s^4}{36} + \frac{17 s^3}{210} - \frac{3 s^2}{55} + \frac{29 s}{90} - \frac{413}{1140} + \operatorname{sign}(s) \frac{512 |s|^{\frac{19}{4}}}{65835}, \tag{12}$$

so that $\partial_s^5 u(s) = \frac{1}{2|s|^{1/4}}$ is square-integrable. Figure 1 shows the error in the projection $P_d^\gamma u$ for increasing polynomial degrees $d \in \mathbb{N}$, and for $\gamma = 0, 1, 3, 5$. Note that $P_d^0 u = P_d u$ corresponds to the standard Legendre projection using the L_2 inner product. The error $\|u - P_d^\gamma u\|$ is computed both in the L_2 norm and the standard Sobolev norm on W_2^5.

Figure 1 shows that the L_2 norm of the error decreases at a linear rate on log-log scale, independent of the order γ of the Sobolev projection. The slope of each graph is roughly -5, matching the expected rate of decay $\|u - P_N u\|_{L_2} = \mathcal{O}(d^{-\delta}) = \mathcal{O}(d^{-5})$ for the standard L_2 projection. On the other hand, the error in the Sobolev norm decreases only for $\gamma = 5$, displaying a decay $\|u - P_d^{(5)} u\| = \mathcal{O}(d^{-0.25})$.

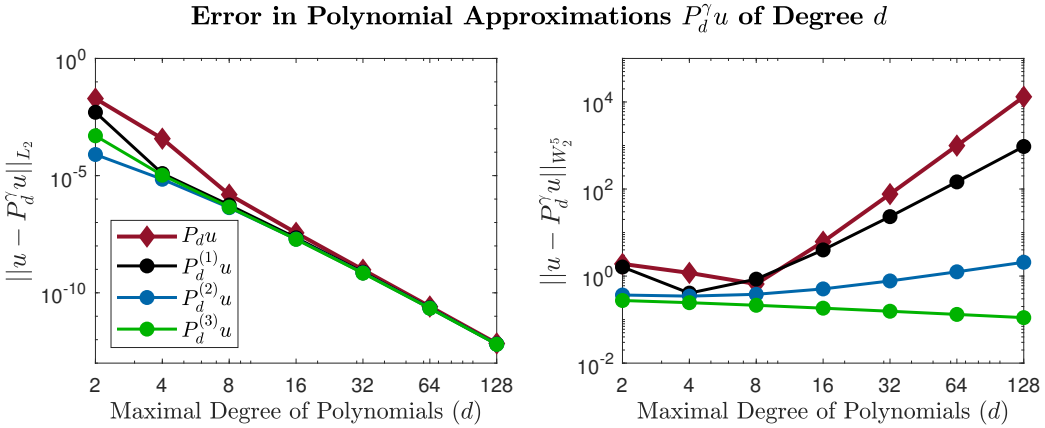

Figure 1: L_2 (left) and Sobolev (right) norms of error in polynomial approximations $P_d^\gamma u$ of function $u \in W_2^5[-1,1]$ defined in (12). The plot $P_d u$ corresponds to a standard Legendre projection of u using the L_2 inner product, as defined in (8). The plots $P_d^\gamma u$ correspond to reconstructing an approximation of u from a projection of $\partial_s^\gamma u$ as in (10), using Thm. 1. Projecting the highest-order derivative $\partial_s^5 u$ of $u \in W_2^5$, both the L_2 and Sobolev norms of the error in the associated approximation $P_d^{(5)} u$ decrease with the degree d, with the L_2 norm decaying at the same rate as observed for the standard projection $P_d u = P_d^{(0)} u$.

Numerical Example in 2D

For a second example, consider the function $w \in W_2^{(3,3)}[[-1,1]^2]$ defined by $w(s_1, s_2) = v(s_1)v(s_2)$, where for $x \in [-1,1]$,

$$v(x) = \begin{cases} \frac{1}{6}x^3 - \frac{1}{2}x^2 + \frac{5}{6}x - \frac{1}{6}, & x < -\frac{1}{2}, \\ -\frac{1}{6}x^3 + \frac{7}{12}x - \frac{5}{24}, & |x| \le \frac{1}{2}, \\ \frac{1}{6}x^3 - \frac{1}{2}x^2 + \frac{5}{6}x - \frac{1}{4}, & x > \frac{1}{2}, \end{cases} \tag{13}$$

so that $\partial_x^3 v = \begin{cases} 1, & |x| > \frac{1}{2} \\ -1, & \text{else} \end{cases}$ is piecewise constant. Figure 2 shows the error in the projection $P_d^\gamma w$ of this function for increasing polynomial degrees (d, d), and for $\gamma = (\gamma_0, \gamma_0)$ with $\gamma_0 = 0, 1, 2, 3$. The figure shows that, again, the L_2 norm of the error decreases as roughly $\mathcal{O}(d^{-\delta_0}) = \mathcal{O}(d^{-3})$, independent of the order γ of the Sobolev projection $P_d^\gamma u$. However, decay of the error in the Sobolev norm is observed only for $\gamma = (2,2)$ and $\gamma = (3,3)$, i.e. when projecting a suitably high-order derivative of the function.

4.2. Expansion using Step Functions Basis

In the previous subsection, we showed how Thm. 1 can be used to construct a polynomial approximation of a differentiable function $\mathbf{u} \in W_2^\delta[\Omega]$,

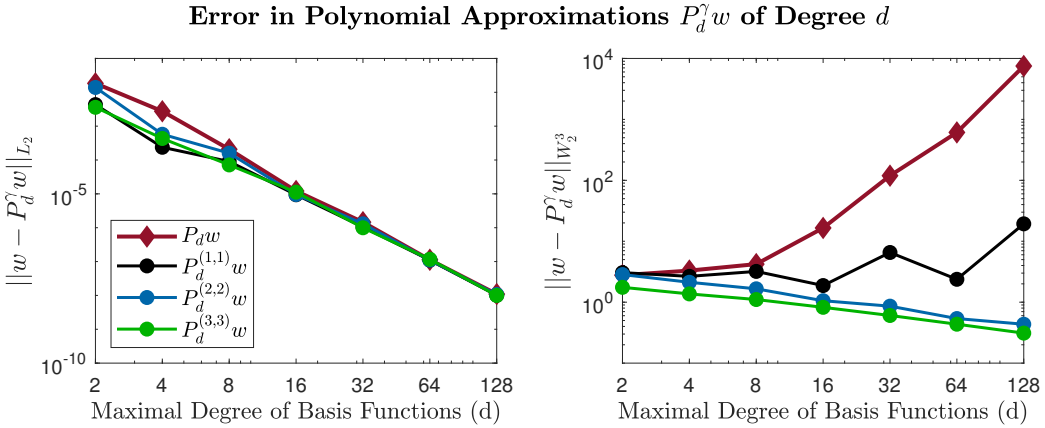

Figure 2: L_2 (left) and Sobolev (right) norms of error in polynomial approximations $P_d^\gamma w$ of $w \in W_2^{(3,3)}[[-1,1]^2]$ defined in (13). Each approximation $P_d^\gamma w$ is computed by projecting the derivative $D^\gamma w$ onto the space of polynomials of degree at most d in each variable, and reconstructing an approximation of w as in (10). The error in the direct projection $P_d w = P_d^{(0,0)} w$ is also plotted. Convergence of the approximation in the Sobolev norm is observed only for $P_d^{(2,2)} w$ and $P_d^{(3,3)} w$, i.e. when projecting $D^{(2,2)} w$ and $D^{(3,3)} w$.

using polynomial projections of the boundary values $\mathbf{v}^\alpha = B^{\alpha-\delta} D^\alpha \mathbf{u}$. However, computing these projections requires integrating the product $\mathbf{v}^\alpha \boldsymbol{\phi}^\gamma$ for each polynomial $\boldsymbol{\phi}^\gamma$ up to degree $\gamma = d$, which becomes numerically challenging for large degrees d. Moreover, since the boundary values $\mathbf{v}^\alpha \in L_2[\Omega^{\alpha-\delta}]$ – and in particular the highest-order derivative $\mathbf{v}^\delta = D^\delta \mathbf{u} \in L_2[\Omega]$ – need not be continuous, a polynomial projection of these functions may not be well-behaved, exhibiting e.g. Gibbs phenomenon.

As an alternative to the polynomial projection method presented in the previous section, we now propose to perform projection using a basis of step functions. In particular, for $K \in \mathbb{N}^N$, we decompose the hypercube $\Omega = [-1,1]^N$ into $\prod_{i=1}^N K_i$ disjoint hypercubes $\Gamma_K^\lambda \subseteq \Omega$ for $1^N \leq \lambda \leq K$ of equal dimensions, each with volume $\Delta_K = \prod_{i=1}^N \frac{2}{K_i}$, so that $\Omega = \bigcup_{1^N \leq \gamma \leq K} \Gamma_K^\lambda$. Then, we define a piecewise constant approximation $S_K \mathbf{v}$ of $\mathbf{v} \in L_2[\Omega]$ as the projection of $\mathbf{v}$ onto a basis of step functions on these cells, as

$$S_K \mathbf{v}\big|_{\Gamma_K^\lambda} = \frac{1}{\Delta_K} \int_{\Gamma_K^\lambda} \mathbf{v}(s) ds, \qquad 1^N \leq \lambda \leq K.$$

Projecting each derivative $\mathbf{v}^\alpha = B^{\alpha-\gamma} D^\alpha \mathbf{u} \in L_2[\Omega^{\alpha-\gamma}]$ in this manner, we

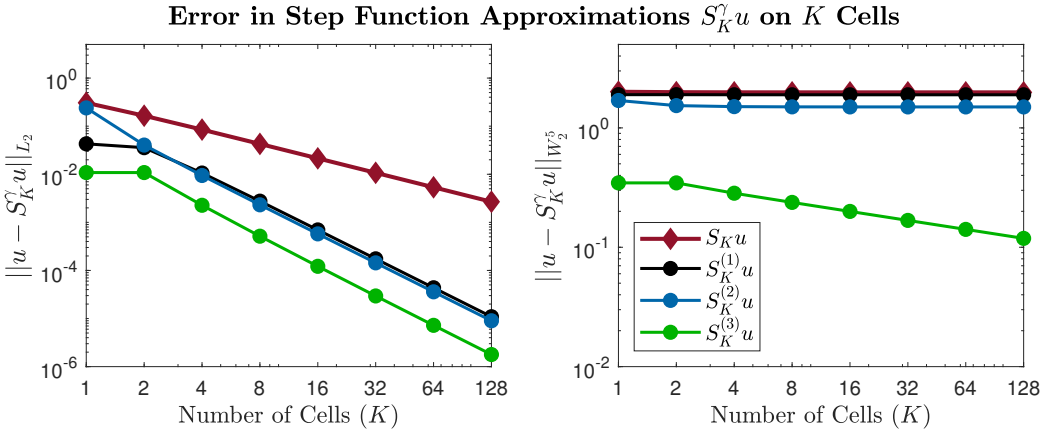

Figure 3: L_2 (left) and Sobolev (right) norms of error in step function approximations $S_K^\gamma u$ of $u \in W_2^5[-1,1]$ defined in (12), on a uniform grid of K cells. Each $S_K^\gamma u$ is computed by projecting $D^\gamma u$ onto a space spanned by K orthogonal step functions, and subsequently reconstructing an approximation of u as in (14). The error in the direct step function projection $S_K u = S_K^0 u$ is also plotted.

then construct a piecewise polynomial approximation of $\mathbf{u}$ as

$$S_K^\gamma \mathbf{u} = \sum_{0^N \leq \alpha \leq \gamma} \mathcal{G}_\alpha^\gamma S_K \left[B^{\alpha-\gamma} D^\alpha \mathbf{u} \right]. \tag{14}$$

We remark that, by expanding the derivative $D^\delta \mathbf{u} \in L_2[\Omega]$ using a basis of step functions, the proposed projection $S_K^\delta \mathbf{u} \in W_2^\delta[\Omega]$ is sufficiently smooth to capture all of the derivatives of the function $\mathbf{u} \in W_2^\delta[\Omega]$ – unlike e.g. a direct step function expansion $S_K \mathbf{u} := S_K^0 \mathbf{u} \in L_2[\Omega]$ – but will not suffer from Gibbs phenomenon – unlike e.g. a polynomial projection. In addition, the integrals $\int_{\Gamma_K^\lambda} \mathbf{v}^\alpha(s) ds$ in the step function projection are in general much easier to compute than the integrals $\int_\Omega \boldsymbol{\phi}^d(s) \mathbf{v}(s) ds$ for more complicated basis functions $\boldsymbol{\phi}^d$, such as the Legendre polynomials.

Numerical Example

Consider again the functions $u \in W_2^5[-1,1]$ and $w \in W_2^{(3,3)}[[-1,1]^2]$ defined in (12) and (13), respectively. Figure 3 shows the error in the step function approximation $S_K^\gamma u$ for increasing number of cells $K \in \mathbb{N}$, and for $\gamma \in \{0,1,3,5\}$. Similarly, Figure 4 shows the error in the step function approximation $S_K^\gamma w$ for $(K,K) \in \mathbb{N}^2$, and for $\gamma = (\gamma_0, \gamma_0)$, with $\gamma_0 = 0,1,2,3$.

The figures show that the L_2 norm of the error in the step function approximation decreases linearly on log-log scale for both functions, decaying

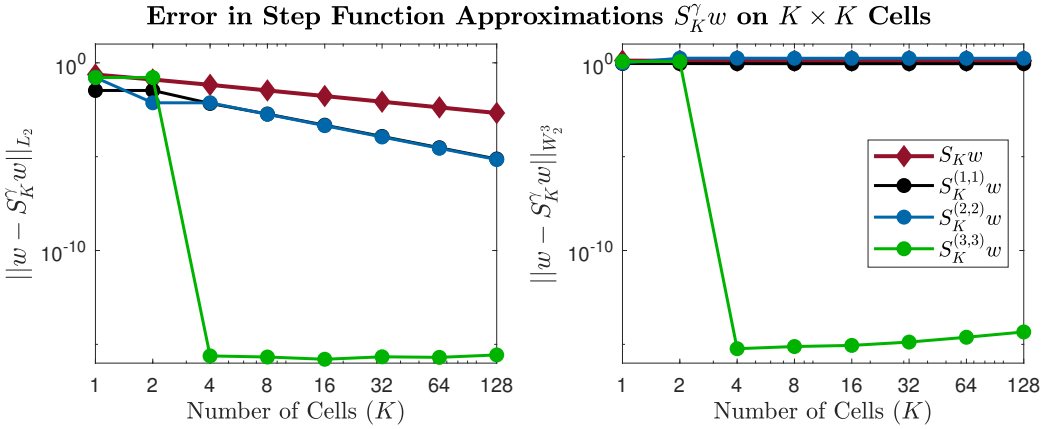

Figure 4: L_2 (left) and Sobolev (right) norms of error in step function approximations $S_K^\gamma w$ of $w \in W_2^{(3,3)}[[-1,1]^2]$ defined in (13), on a grid of $K \times K$ cells. Each $S_K^\gamma w$ is computed by projecting $D^\gamma w$ onto a space spanned by $K \times K$ orthogonal step functions, and subsequently reconstructing an approximation of w as in (14). The error in the direct step function projection $S_K w = S_K^{(0,0)} w$ is also plotted. Note that $S_K^{(3,3)} w = w$ for $K \geq 4$, since $D^{(3,3)} w$ is a piecewise constant function on 4×4 cells.

as $\mathcal{O}(K^{-2})$ when projecting a derivative of the function ($\gamma \in \{1,3,5\}$ for $S_K^\gamma u$ and $\gamma_0 \in \{1,2\}$ for $S_K^{(\gamma_0,\gamma_0)} w$), but decaying only as $\mathcal{O}(K^{-1})$ for the direct approximation $S_K = S_K^0$. However, the Sobolev norm of the error decreases only when fitting the highest-order derivative ($\gamma = 5$ for $S_K^\gamma u$ and $\gamma_0 = 3$ for $S_K^{(\gamma_0,\gamma_0)} w$) of the function, though the rate of decay is still only $\mathcal{O}(K^{-0.005})$ for the approximation $S_K^{(5)} u$. Unsurprisingly, both the L_2 and W_2^3 norms of the error in the approximation $S_K^{(3,3)} w$ drop to machine precision when $K = 4$, since the highest-order derivative $D^{(3,3)} w$ of the example function w can be exactly represented by just 4×4 step functions.

We remark that, although numerical simulation was performed only projecting using a standard basis of step functions, the proposed methodology can be readily adapted to construct a piecewise continuous approximation using any suitable basis of (discontinuous) functions. For example, better convergence results might be achieved using a complete basis of step functions $\{\boldsymbol{\psi}^d\}$ as proposed in e.g. [10], though this will again require (computationally) evaluating more complicated integrals $\int_\Omega \boldsymbol{\psi}^d(s)\mathbf{v}(s)ds$.

5. Conclusion

In this paper, we proposed a representation of a differentiable function on a N-dimensional hyperrectangle, expressing it in terms of its derivatives along lower boundaries of the domain. We proved that this representation offers a bijective map between the Sobolev space $W_2^{\delta}[\Omega]$ and a space of square-integrable functions $\mathbf{L}_2^{\delta}[\Omega]$, defined by an integral operator with polynomial kernel. Based on this map, we proposed a method for polynomial approximation of a differentiable function, by projecting its derivatives onto a space of polynomials or step functions, and then using the main theorem to reconstruct an approximation of the original function. Through numerical examples, we showed that this approach exhibits similar convergence to standard projection methods in the L_2 norm, and performed substantially better in the Sobolev norm. While the map proposed in this paper is defined only for functions on a hyperrectangle, similar maps can likely be derived for functions on more general domains, using integral operators with more general (non-polynomial) kernels.

References

[1] A. D. Polyanin, Handbook of linear partial differential equations for engineers and scientists, Chapman and Hall/CRC, 2001.

[2] C. Canuto, A. Quarteroni, Approximation results for orthogonal polynomials in Sobolev spaces, Mathematics of Computation 38 (157) (1982) 67–86.

[3] C. Canuto, M. Y. Hussaini, A. Quarteroni, T. A. Zang, Spectral methods: fundamentals in single domains, Springer Science & Business Media, 2007.

[4] D. Gottlieb, S. A. Orszag, Numerical analysis of spectral methods: theory and applications, SIAM, 1977.

[5] F. Marcellán, M. Alfaro, M. Rezola, Orthogonal polynomials on Sobolev spaces: old and new directions, Journal of Computational and Applied Mathematics 48 (1-2) (1993) 113–131.

[6] F. Marcellán, Y. Xu, On Sobolev orthogonal polynomials, Expositiones Mathematicae 33 (3) (2015) 308–352.

[7] Y. Xu, Approximation and orthogonality in Sobolev spaces on a triangle, Constructive Approximation 46 (2) (2017) 349–434.

[8] Y. Xu, Approximation by polynomials in Sobolev spaces with Jacobi weight, Journal of Fourier Analysis and Applications 24 (2018) 1438–1459.

[9] A. Díaz-González, F. Marcellán, H. Pijeira-Cabrera, W. Urbina, Discrete–continuous Jacobi–Sobolev spaces and Fourier series, Bulletin of the Malaysian Mathematical Sciences Society 44 (2021) 571–598.

[10] H. Li, D. Torney, A complete system of orthogonal step functions, Proceedings of the American Mathematical Society 132 (12) (2004) 3491–3502.