Replacing Automatic Differentiation by Sobolev Cubatures fastens Physics Informed Neural Nets and strengthens their Approximation Power

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Abstract
We present a novel class of approximations for variational losses, being applicable for the training of physics-informed neural nets (PINNs). The loss formulation reflects classic Sobolev space theory for partial differential equations and their weak formulations. The loss computation rests on an extension of Gauss-Legendre cubatures, we term Sobolev cubatures, replacing automatic differentiation (A.D.). We prove the runtime complexity of training the resulting Soblev-PINNs (SC-PINNs) to be less than required by PINNs relying on A.D. On top of one-to-two order of magnitude speed-up the SC-PINNs are demonstrated to achieve closer solution approximations for prominent forward and inverse PDE problems than established PINNs achieve.

1. Introduction
Partial differential equations (PDEs) are omnipresent mathematical models governing the dynamics and (physical) laws of complex systems (Jost, 2002; Brezis, 2011). However, analytic PDE solutions are rarely known for most of the systems being the center of current research. Therefore, there is a strong demand on efficient and accurate numerical solvers and simulations.

Machine learning methods such as: Physics-Informed GAN (Arjovsky et al., 2017), Deep Galerkin Method (Sirignano & Spiliopoulos, 2018), and Physics Informed Neural Networks (PINNs) (Raissi et al., 2019), gain big traction in the scientific computing community. In contrast to classic solvers, PINNs provide a neural net (NN) surrogate model parametrizing the solution space of the PDEs. PINN-learning is given by minimizing a variational problem, which is typically formulated in $L^2$-loss terms

$$\int_{\Omega} ||\hat{u}(x) - u(x)||^2 d\Omega \approx \frac{1}{|P|} \sum_{p \in P} ||\hat{u}(p) - u(p)||^2$$

being approximated by mean square errors (MSE) in random nodes $P$, (Yang et al., 2020),(Long et al., 2018).

However, due to the complexity of the underlying non-linear, non-convex variational problem, theoretical and computational challenges arise when demanding to guarantee convergence to PDE solutions of high accuracy.

1.1. Related Work
The importance of the present computational challenge is manifest in the large number of previous works. Consequently, an exhaustive overview of the literature cannot be given here. Instead, we restrict ourselves to mentioning those contributions that directly relate to or inspired our work.

1.1.1. Classic Numerical Methods
Main classic numerical solvers divide into: Finite Elements (Ern & Guermond, 2004); Finite Differences (LeVeque, 2007); Finite Volumes(Bernardi & Maday, 1997); Spectral Methods (Bernardi & Maday, 1997) and Particle Methods (Li & Liu, 2007). These class of methods provide solutions with high accuracy, but come with the cost of having limited flexibility with respect to the type of problems they can solve. This includes especially inverse problems, as PDE parameter inference, being a hard challenge for the aforementioned methods. In contrast, the variational formulation defining the PINN training provides the desired flexibility, but comes again with the cost of less reachable accuracy.

We focus on two recent approaches addressing the stability and accuracy of PINNs.

1.1.2. Variational PINNs (VPINNs)
VPINNs were introduced in (Kharazmi et al., 2019), (Kharazmi et al., 2020) formulating variational Sobolev

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losses for PINN-training. The approach relies on exploiting analytic integration and differentiation formulas of shallow neural networks with specified activation functions. The method is extended by using quadratures and automatic differentiation for computing the losses and complemented by a domain decomposition approach.

1.1.3. **Inverse Dirichlet Loss Balancing**

With the Inverse Dirichlet method (Maddu et al., 2021) the parameter space of the weights (and bias) \( \theta \) denotes the architecture of the hidden layers, with continuous piecewise smooth activation functions, fixing the notation used in the article. Notions of this section follow classic concepts of spectral integration and differentiation for computing the losses and complemented by a domain decomposition approach.

2. **Sobolev Cubatures**

Closer approximations of \( L^2 \)-integrals than reachable by prominent MSE approaches can be derived by applying classic Gauss-Legendre cubatures (see e.g. Stroud, 1971; 2011; Trefethen, 2017a;b; 2019) or even further extension to what we call Sobolev cubatures, presented herein. The notions of this section follow classic concepts of spectral methods (Canuto et al., 2007; Trefethen, 2019). We start by introducing fixing the notation used in the article.

2.1. **Notation**

We consider neural nets (NNs) \( \hat{u}_\theta(\cdot) \) with \( m_1, m_2 \)-dimensional input/output domain \( m_1, m_2 \in \mathbb{N} \) of fixed architecture \( \Xi_{m_1,m_2} \) (specifying number and depth of the hidden layers, with continuous piecewise smooth activation functions \( \sigma(x) \), e.g. ReLU or ELU). Further, \( \Upsilon_{m_1,m_2} \) denotes the parameter space of the weights (and bias) \( \theta = (u, b) \in W = V \times B \subseteq \mathbb{R}^K, K \in \mathbb{N}, \) see e.g. (Anthony & Bartlett, 2009; Goodfellow et al., 2016).

Throughout this article we denote with \( \Omega = [-1,1]^m \) the \( m \)-dimensional standard hypercube and with \( \|x\|_p = \left( \sum_{i=1}^m |x_i|^p \right)^{1/p}, x = (x_1, \ldots, x_m) \in \mathbb{R}^m, 1 \leq p < \infty, \|x\|_\infty = \max_{1 \leq i \leq m} |x_i| \) the \( l_p \)-norm. We recommend (Adams & Fournier, 2003; Brezis, 2011) for an excellent overview on functional analysis and the Sobolev spaces

\[
H^k(\Omega, \mathbb{R}) = \{ f \in L^2(\Omega, \mathbb{R}) : D^a f \in L^2(\Omega, \mathbb{R}) \} , \quad k \in \mathbb{N}
\]

given by all \( L^2 \)-integrable functions \( f : \Omega \to \mathbb{R} \) with existing \( L^2 \)-integrable weak derivatives \( D^a f = \partial_{x_1}^{a_1} \cdots \partial_{x_m}^{a_m} f \) up to order \( k \). In fact, \( H^k(\Omega, \mathbb{R}) \) is a Hilbert space with inner product

\[
\langle f, g \rangle_{H^k(\Omega)} = \sum_{0 \leq |\alpha| \leq k} \langle D^\alpha f, D^\alpha g \rangle_{L^2(\Omega)}
\]

and norm \( \|f\|_{H^k(\Omega)} = \langle f, f \rangle_{H^k(\Omega)}^{1/2} \), where \( H^0(\Omega, \mathbb{R}) = L^2(\Omega, \mathbb{R}) \), with \( f, g \geq L^2(\Omega) \). From the Trace Theorem (Adams & Fournier, 2003), we find furthermore that whenever \( H \subseteq R^m \) is a hyperplane of co-dimension 1, then the induced restriction

\[
g : H^k(\Omega, \mathbb{R}) \to H^{k-1/2}(\Omega \cap H, \mathbb{R})
\]

is continuous, i.e., \( \|g\|_{H^{k-1/2}(\Omega \cap H)} \leq d \|f\|_{H^k(\Omega)} \) for some \( d = d(m, \Omega) \in \mathbb{R}^+ \).

Further, \( C^k(\Omega, \mathbb{R}) \), \( k \in \mathbb{N} \cup \{ \infty \} \) denote the Banach spaces of \( k \)-times continuously differentiable functions with norm \( \|f\|_{C^k(\Omega)} = \sum_{i=0}^k \sup_{x \in \Omega, \|\alpha\|_1 \leq i} |D^\alpha f(x)| \).

\( \Pi_{m,n} = \text{span}\{x^\alpha\}_{|\alpha|_\infty \leq n} \) denotes the \( \mathbb{R} \)-vector space of all real polynomials in \( m \) variables spanned by all monomials \( x^\alpha = \prod_{i=1}^m x_i^{a_i} \) of maximum degree \( n \) \( \in \mathbb{N} \) and \( A_{m,n} = \{ \alpha \in \mathbb{N}^n : |\alpha|_\infty \leq n \} \) the corresponding multi-index set with \( |A_{m,n}| = (n+1)^m \). We order \( A_{m,n} \) with respect to the lexicographic order \( \leq \). Let \( D = (d_{i,j})_{1 \leq i,j \leq |A_{m,n}|} = (A_{m,n} \times A_{m,n}) \) be a matrix. We slightly abuse notation by writing

\[
D = (d_{\alpha,\beta})_{\alpha,\beta \in A_{m,n}},
\]

with \( d_{\alpha,\beta} \) being the \( \alpha \)-th, \( \beta \)-th entry of \( D \).

2.2. **Orthogonal Polynomials**

Let \( m, n \in \mathbb{N} \) we consider the \( m \)-dimensional Legendre grids \( P_{m,n} = \bigoplus_{l=1}^m \text{Leg}_n \subseteq \Omega \), where \( \text{Leg}_n = \{ p_0, \ldots, p_n \} \) are the \( n+1 \) Legendre nodes given by the roots of the Legendre polynomials of degree \( n+1 \) and denote \( p_\alpha = (p_{\alpha_1}, \ldots, p_{\alpha_m}) \in P_{m,n} \). It is a classic fact (Stroud, 1971; 2011; Trefethen, 2017a;b; 2019) that the Lagrange polynomials \( L_\alpha \in \Pi_{m,n}, \alpha \in A_{m,n} \) given by

\[
L_\alpha = \prod_{i=1}^m l_{\alpha_i,i} , \quad l_{j,i} = \prod_{h \neq j,h=0}^n \frac{x_i - p_h}{p_j - p_h},
\]
\[ p_h \in \text{Leg}_n \text{ satisfy } L_\alpha(p) = \delta_{\alpha,\beta}, \forall \alpha, \beta \in A_{m,n} \text{ and yield an orthogonal } L^2 \text{-basis of } \Pi_{m,n}, \text{i.e.,} \]

\[ \langle L_\alpha, L_\beta \rangle_{L^2(\Omega)} = \int_{\Omega} L_\alpha(x) L_\beta(x) d\Omega = w_\alpha \delta_{\alpha,\beta}, \]

\( \forall \alpha, \beta \in A_{m,n}, \) where \( \delta_\alpha \) denotes the Kronecker delta and

\[ w_\alpha = \| L_\alpha \|^2_{L^2(\Omega)} \quad (5) \]

the efficiently computable Gauss-Legendre cubature weight (Stroud, 1971; Trefethen, 2019). Consequently, for any polynomial \( Q \in \Pi_{m,2n+1} \) of degree \( 2n+1 \) the following cubature rule applies:

\[ \int_{\Omega} Q(x) d\Omega = \sum_{\alpha \in A_{m,n}} w_\alpha Q(p_\alpha). \quad (6) \]

Summarizing: Polynomials of degree \( 2n+1 \) can be (numerically) integrated exactly when sampled on the Legendre grid \( P_{m,n} \) of order \( n+1 \). Thanks to \( |P_{m,n}| = (n+1)^m \ll (2n+1)^m \) this makes Gauss-Legendre integration a very powerful integration scheme yielding

\[ \| Q \|^2_{L^2(\Omega)} = \int_{\Omega_m} Q(x)^2 d\Omega_m = \sum_{\alpha \in A_{m,n}} Q(p_\alpha)^2 w_\alpha. \quad (7) \]

for all \( Q \in \Pi_{m,n} \).

### 2.3. Differential Operators on \( \Pi_{m,n} \)

Based on Eq. (4) we derive exact matrix representations of differential operators on the polynomial spaces \( \Pi_{m,n} \) allowing to extend Eq. (7) to close approximations of the Sobolev norms for general Sobolev functions \( f \in H^k(\Omega, \mathbb{R}) \), \( k \in \mathbb{N} \).

For \( L_\alpha \in \Pi_{m,n} \) from Eq. (4) and \( 1 \leq i \leq m \) the computation of values \( d_{\alpha,\beta} = \partial_{x_i} L_\alpha(p) \), \( p_\beta \in P_{m,n}, \forall \beta \in A_{m,n} \) yields the Lagrange expansion

\[ \partial_{x_i} L_\alpha(x) = \sum_{\beta \in A_{m,n}} d_{\alpha,\beta} L_\beta(x). \quad (8) \]

Consequently, the matrix

\[ D_1 = (d_{\alpha,\beta})_{\alpha,\beta \in A_{m,n}} \in \mathbb{R}^{|A_{m,n}| \times |A_{m,n}|}, \quad (9) \]

represents the finite dimensional truncation of the differential operator \( \partial_{x_i} : C^1(\Omega, \mathbb{R}) \to C^0(\Omega, \mathbb{R}) \) to the polynomial space \( \Pi_{m,n} \) and for \( \beta \in \mathbb{N}^m \) we set

\[ D_\beta = \prod_{j=1}^m D_{\beta,j} \quad (10) \]

to be the approximation of \( \partial_x := \partial_{\beta,1} \ldots \partial_{\beta,m} \). As a direct consequence of Eq. (7) the following statement applies:

**Theorem 1** (Sobolev cubatures). Let \( m, n \in \mathbb{N}, A_{m,n} \subseteq \mathbb{N}^m, P_{m,n} = \{p_\alpha : \alpha \in A_{m,n}\} \), be the Legendre grid, \( W_{m,n} = \text{diag}(w_\alpha)_{\alpha \in A_{m,n}} \) be the Gauss-Legendre cubature weight matrix, and \( F_{m,n} = (f(p_\alpha))_{\alpha \in A_{m,n}} \in \mathbb{R}^{|A_{m,n}|} \). Let

\[ W_{m,n,k} = \sum_{\beta \in \mathbb{N}^m, ||\beta|| \leq k} D_\beta^T W_{m,n} D_{\beta}, \quad (11) \]

with \( D_{\beta} \) from Eq. (10) be the Sobolev cubature matrix then

\[ \| f \|^2_{H^k(\Omega)} \approx F_{m,n} W_{m,n,k} F_{m,n}, \quad (12) \]

is an exact approximation whenever \( f \in \Pi_{m,n} \).

We conclude that Theorem 1 enables to control the uniform distance \( \| f - g \|_{C^{0}(\Omega)} \) on the whole domain \( \Omega \).

**Corollary 2.** Let the assumptions of Theorem 1 be fulfilled, and \( f, g \in H^k(\Omega, \mathbb{R}), k > m/2 \) be two Sobolev functions. Assume there is \( n \in \mathbb{N} \) (large enough) such that the residuum \( f - g \in \Pi_{m,n} \) is given by a polynomial with

\[ f(p_\alpha) - g(p_\alpha) = 0, \quad \forall \alpha \in A_{m,n}. \]

Then \( f(x) - g(x) = 0 \) for all \( x \in \Omega = [-1, 1]^m \).

**Proof.** Due to Theorem 1 we deduce \( \| f - g \|_{H^k(\Omega)} = 0 \). While the Sobolev Embedding Theorem (Adams & Fournier, 2003) yields the continuous inclusion \( H^k(\Omega, \mathbb{R}) \subseteq C^0(\Omega, \mathbb{R}) \), consequently, we realize that \( \| f - g \|_{C^{0}(\Omega)} = 0 \), proving the claimed identity. \( \square \)

In light of the provided perspectives, we propose the following formalizations of classic PDE problems.

### 3. Strong and weak PDE formulations

We follow (Jost, 2002; Brezis, 2011) to restate classic (weak) PDE formulations and their Sobolev cubature approximations. For the sake of simplicity, we focus on the example of the classic Poisson equation.

#### 3.1. Poisson equation

For \( f \in C^0(\Omega, \mathbb{R}) \) the strong Poisson problem with Dirichlet boundary condition \( g \in C^0(\partial \Omega, \mathbb{R}) \) seeks for solutions \( u \in C^2(\Omega, \mathbb{R}) \) fulfilling:

\[ \begin{cases} 
-\Delta u(x) - f(x) = 0, & \forall x \in \Omega \\
\quad u(x) - g(x) = 0, & \forall x \in \partial \Omega. 
\end{cases} \quad (13) \]

We can weaken the initial regularity assumptions by demanding \( u \in H^2(\Omega, \mathbb{R}) \) to satisfy the PDE in the integral sense, yielding the strong variational formulation:

\[ \begin{cases} 
\int_{\Omega} (-\Delta u + f) \phi d\Omega = 0, & \forall \phi \in H^1(\Omega, \mathbb{R}) \\
\int_{\partial \Omega} (u - g) \phi dS = 0, & \forall \phi \in H^1(\partial \Omega, \mathbb{R}). 
\end{cases} \quad (14) \]
where $\Gamma(\Omega, \mathbb{R}) = \{ \phi \in C^\infty(\Omega, \mathbb{R}) : \| \phi \|_{C^0(\Omega)} \leq 1 \}$ denotes the space of test functions. We can weaken the regularity assumptions even more by imposing $u \in H^1(\Omega, \mathbb{R})$ to satisfy the following weak variational formulation:

$$
\int_\Omega (\nabla u \cdot \nabla \phi + f \phi) d\Omega - \int_\partial \Omega (u - g) \phi dS = 0, \\
\int_\Omega (u - g) \phi dS = 0,
$$

(15)

where we applied integration by parts and $\eta$ denotes the (piecewise smooth) normal field of $\partial \Omega$.

### 3.2. Residual loss in terms of Sobolev cubatures

We translate the introduced PDE formulations into variational optimization problems demanded to be minimized by the PINNs framework. In addition to Sobolev cubature matrix $W_{m,n,k}$ from Eq. (11) the matrices

$$
U_{m,n,k} = \sum_{\beta \in \mathbb{N}^m, \| \beta \|_1 \leq k} D_\beta W_{m,n,k},
$$

(16)

$$
V_{m-1,n,k-1/2} = \sum_{\beta \in \mathbb{N}^{m-1}, \| \beta \|_1 \leq k-1/2} D_\beta W_{m-1,n,k},
$$

relying on Theorem 1, are the key ingredient in this regard.

The strong residual loss $L_{\text{strong}} : C^2(\Omega, \mathbb{R}) \rightarrow \mathbb{R}$, relies on the residuals

$$
L_{\text{strong}}(u) = r_{\text{strong},0}(u) + s_{\text{strong},0}(u) = \| \Delta u + f \|_{L^2(\Omega)}^2 + \| \nabla u \|_{L^2(\partial \Omega)}^2 - g \|_{L^2(\partial \Omega)}^2,
$$

which we extend to $L_{\text{strong},k}, k \geq 1/2$ with

$$
L_{\text{strong},k}(u) = r_{\text{strong},k}(u) + s_{\text{strong},k}(u) = \| \Delta u + f \|_{H^k(\Omega)}^2 + \| \nabla u \|_{H^{k-1/2}(\partial \Omega)}^2 - g \|_{H^{k-1/2}(\partial \Omega)}^2,
$$

(17)

where the $H^{k-1/2}$-metric of the second residual $s_{\text{strong},k}$ reflects the Trace Theorem (Eq. (2)). We propose to approximate $L_{\text{strong},k}(u) \approx r_{\text{strong},n,k}(u) + s_{\text{strong},n,k}(u)$ by the following Sobolev cubatures:

$$
r_{\text{strong},n,k}(u) = R_{m,n}^T U_{m,n,k} R_{m,n},
$$

(18)

$$
s_{\text{strong},n,k}(u) = S_{m-1,n}^T V_{m-1,n,k-1/2} S_{m-1,n},
$$

(19)

Thereby, $V_{m-1,n,k-1/2} = W_{m-1,n}$ for $0 \leq k < 1/2$, and

$$
R_{m,n} = -D_{(2,\ldots,2)}(\hat{a}(p, x, u))_{\alpha \in \mathbb{A}_{m,n}} = F_{m,n},
$$

(20)

where $F_{m,n} = (f(p_\alpha))_{\alpha \in \mathbb{A}_{m,n}}$ and $D_{(2,\ldots,2)} = D_2^2 + \ldots + D_m^2$ denotes the polynomial approximation of the Laplacian accordingly to Eq. (9). Thus, $R_{m,n} \in \mathbb{R}^{\mathbb{A}_{m,n}}$ yields an approximation of $(\Delta u(p_\alpha) + f(p_\alpha))_{\alpha \in \mathbb{A}_{m,n}}$ by replacing automatic differentiation (Baydin et al., 2018b) with polynomial differentiation.

Moreover, by summing the residual values $S_{m-1,n}^{\pm j} = (u(p_\alpha^{\pm j}, x) - g(p_\alpha^{\pm j}))_{\alpha \in \mathbb{A}_{m-1,n}}$ over each face $\partial \Omega^{\pm j} = \{ x \in \Omega : x_j = \pm 1 \}$ of $\Omega$ we denote the boundary residual as

$$
S_{m-1,n} = \sum_{j=0}^m S_{m-1,n}^{\pm j} \in \mathbb{R}^{\mathbb{A}_{m-1,n}}.
$$

(21)

The strong variational loss $r_{\text{strong},k} : H^{2+k}(\Omega, \mathbb{R}) \rightarrow \mathbb{R}$ is given by $L_{\text{var},k}(u) = r_{\text{strong},k}(u) + s_{\text{var},k}(u)$ with

$$
r_{\text{strong},k}(u) := \sup_{\phi \in \Gamma(\Omega, \mathbb{R})} \langle -\Delta u - f, \phi \rangle_{H^k(\Omega)},
$$

(22)

$$
s_{\text{strong},k}(u) := \sup_{\phi \in \Gamma(\partial \Omega, \mathbb{R})} \langle u - g, \phi \rangle_{H^{k-1/2}(\Omega)},
$$

where the $H^{k-1/2}$-metric of the second residual reflects again the Trace Theorem (Eq. (2)). Replacing the test functions $\phi$ with the Lagrange basis $L_\alpha \in \Pi_{m,n}, \alpha \in \mathbb{A}_{m,n}$ for the Legendre nodes $p_\alpha \in \mathbb{P}_{m,n}$, from Eq. (4) yields the Sobolev cubature approximation $L_{\text{var},k}(u) \approx L_{\text{var},n,k}(u)$:

$$
r_{\text{var},n,k}(u) = R_{m,n}^T U_{m,n,k} R_{m,n},
$$

$$
s_{\text{var},n,k}(u) = S_{m-1,n}^T V_{m-1,n,k-1/2} S_{m-1,n},
$$

where $R_{m,n}$ and $S_{m-1,n}$ are as in Eq. (20). (21)

The weak variational loss $L_{\text{weak},k} : H^{1+k}(\Omega, \mathbb{R}) \rightarrow \mathbb{R}$ is given by $L_{\text{var},k} = r_{\text{weak},k}(u) + s_{\text{weak},k}(u)$ only differs in the first residual $r_{\text{weak},k}(u)$ from $L_{\text{var},k}$ by

$$
r_{\text{weak},k}(u) = \sup_{\phi \in \Gamma(\Omega, \mathbb{R})} \langle \nabla u, \nabla \phi \rangle_{H^k(\Omega)} + \langle f, \phi \rangle_{H^k(\Omega)} - \langle \nabla u \phi, \eta \rangle_{H^{k-1/2}(\Omega)},
$$

Yielding the approximations $L_{\text{weak},n,k}(u) \approx L_{\text{weak},n,k}(u)$ due to:

$$
\sup_{\phi \in \Gamma(\Omega, \mathbb{R})} \langle \nabla u, \nabla \phi \rangle_{H^k(\Omega)} \approx H_{m,n}^T U_{m,n,k} H_{m,n},
$$

$$
\sup_{\phi \in \Gamma(\partial \Omega, \mathbb{R})} \langle f, \phi \rangle_{H^k(\Omega)} \approx F_{m,n}^T U_{m,n,k} F_{m,n},
$$

$$
\sup_{\phi \in \Gamma(\partial \Omega, \mathbb{R})} \langle \nabla u \phi, \eta \rangle_{H^{k-1/2}(\partial \Omega)} \approx G_{m-1,n}^T V_{m-1,n,k-1/2} S_{m-1,n},
$$

where $H_{m,n} = \sum_{j=1}^m D_\beta^j U_{m,n,k} H_{m,n}, G_{m-1,n} = \sum_{j=1}^m D_\beta^j V_{m-1,n,k-1/2} S_{m-1,n}$, and $U_{m,n,k}, V_{m-1,n,k-1/2}$ are the Sobolev cubature matrices from Eq. (16).

Summarizing, the given notions allow to extend Corollary 2 in order to state the following result.

**Theorem 3 (Strong solution approximation).** Let $m \in \mathbb{N}$, $u \in C^2(\Omega, \mathbb{R}), u \in H^{1+k}(\Omega, \mathbb{R}), k \geq 0$, $l = 1, 2$ be a regular $m$-variate (Sobolev) function.
We conclude, that apart from the weaker regularity whenever minimization (by PINN training) reaches (optimally) adjusted weights for the proposes Sobolev loss approximations the variation in the weights.

**ii)** Denoting with \( L_{\text{strong},n,k} \), \( L_{\text{var},n,k} \), \( L_{\text{weak},n,k} \) the loss approximations of degree \( n \in \mathbb{N} \) as given above. Then for all \( \varepsilon > 0 \) there is \( n = n(\varepsilon) \) and \( u' \in \Pi_{m,n} \) with \( \| u - u' \|_{C^2(\Omega)} < \varepsilon \) such that \( L_{\text{strong},n}(u') = L_{\text{strong}}(u'), L_{\text{var},n,k}(u') = L_{\text{var},k}(u'), L_{\text{weak},n,k}(u') = L_{\text{weak},k}(u') \).

**Proof.** Statement i) reflects classic PDE theory (Jost, 2002; Brezis, 2011). ii) follows from \( H^{1+k}(\Omega, \mathbb{R}) \subseteq C^2(\Omega, \mathbb{R}) \) and the Stone-Weierstrass theorem (Weierstrass, 1885; De Branges, 1959), stating that any continuous function \( f \in C^0(\Omega, \mathbb{R}) \) can be uniformly approximated by polynomials. By a bootstrapping argument that implies that polynomials are dense in all \( C^r(\Omega, \mathbb{R}), r \in \mathbb{N} \cup \{ \infty \} \) with respect to the corresponding norms \( \| \cdot \|_{C^r(\Omega)} \). While \( C^\infty(\Omega, \mathbb{R}) \subseteq H^{1+k}(\Omega, \mathbb{R}) \) is dense (Adams & Fournier, 2003), polynomial approximations \( \| u - u' \|_{H^{1+k}(\Omega)} < \varepsilon \) exist. Due to Theorem 1 the Sobolev cubature losses \( L_{\text{strong},n}(u'), L_{\text{var},n,k}(u'), L_{\text{weak},n,k}(u') \) are exact for \( u' \in \Pi_{m,n} \) proving the statement.

We conclude, that apart from the weaker regularity assumptions on the solution \( u : \Omega \rightarrow \mathbb{R} \) required by the variational losses, Theorem 3 theoretically guarantees approximations of strong solutions whenever minimization (by PINN training) reaches \( L_{\text{strong},n,k}(u'), L_{\text{var},n,k}(u'), L_{\text{weak},n,k}(u') \approx 0 \) sufficient small losses for \( n \in \mathbb{N} \) large enough.

**4. Gradient Flow of PINN Training**

For a given PINN \( u = \hat{u}(\cdot, w) \in \Xi_{m,1} \), of fixed architecture, (optimally) adjusted weights \( w \in \Upsilon_{\Xi_{m,1}} \), are demanded, minimizing the loss. NN training is realized as a gradient descent, given by solving the gradient flow ODE

\[
\partial_t w = -\delta_w L(\hat{u}(\cdot, w(t))w_0 , \quad (23)
\]

\[
= -\nabla L(\hat{u}(\cdot, w(t)) \cdot \delta_w \hat{u}(\cdot, w(t))w_0 , \quad w(0) = w_0 ,
\]

where \( w_0 \) is given by the NN initialization and \( \delta_w \) denotes the variation in the weights.

For the proposes Sobolev loss approximations \( L_{\text{strong},n}(u'), L_{\text{var},n}(u'), L_{\text{var},n}(u') \) the gradients simplify due to the identities:

\[
\nabla_w (r_{\text{strong},n,k}(u)) = 2R^T_{m,n}W_{m,n,k} \\
\nabla_w (r_{\text{weak},n,k}(u)) = 2R^T_{m,n,k}U_{m,n,k} \\
\nabla_w (s_{\text{var},n,k}(u)) = 2H^T_{m,n} + F^T_{m,n}U_{m,n,k} + 2G^T_{m,n}V_{m-1,n,k-1/2} \ , \\
\nabla_w (s_{\text{weak},n,k}(u)) = 2R^T_{m,n}W_{m-1,n,k-1/2} ,
\]

where \( W_{m,n,k}, U_{m,n,k}, V_{m-1,n,k-1/2} \) are Sobolev cubature matrices from Eq. (11), (16).

We further investigate the Sobolev cubature properties in comparison to A.D. based PINNs below.

**5. Polynomial Differentiation vs Automatic Differentiation**

One of the main features of using the Sobolev cubatures, compared to the MSE loss, is that we can replace the problem of computing the derivatives of the PINN-surrogate, by computing them directly in the cubature. Below we present the complexity analysis for both, the normal PINN with Automatic Differentiation (A.D.) and the SC-PINN with Polynomial Differentiation (P.D.).

**Theorem 4.** For a given deep Neural Network \( \hat{u}_\theta : \Omega \rightarrow \mathbb{R} \), with architecture \( \xi_{m,1} \) consisting of \( l \) hidden layers and \( q \) neurons per layer, the complexity per epoch for computing the \( k \)-th derivative \( (\partial^k_x \hat{u}_\theta) \) in \( s \in \mathbb{N} \) training points is given by

\[
\text{i) } O(2^{k-1}lsq^2) \text{ for a PINN resting on A.D., i.e. it scales exponentially with the order of the derivative.}
\]

\[
\text{ii) } O(\max\{s^2, lsq^2\}) \text{ for the SC-PINN using P.D.}
\]

**Proof.** For proving i) we use the fact that a single backward pass required for computing the derivatives, has the same complexity as a forward pass, which is \( O(lsq^2) \) due to (Baydin et al., 2018a). Thus, for computing the first derivative at \( s \) points we need \( O(lsq^2) \) operations. Due to the chain rule, computation of the second order derivatives causes the size of the dependency graph of the A.D. to double. By recursion of this fact the factor \( 2^{k-1} \) appears as claimed.

For proving ii) we recall that the SC-PINN computes the \( k \)-th derivative by applying the pre-computed differential matrix \( \mathcal{D}^k \) at each cubature (Legendre) node \( p \in P_{m,n} \), with \( s = |P_{m,n}| \). The product has \( O(s^2) \) complexity per epoch and the evaluation \( \hat{u}_\theta(p) \), \( \forall p \in P_{m,n} \) has \( O(lsq^2) \) complexity, yielding the result. \( \square \)
Example 5. We consider a NN with architecture $\Xi_{1,1} = \{1, 50, 50, 50, 50, 1\}$ given by four hidden layers of length 50. For $s = 200$ training points computation of a 4-th order derivative computed with A.D. has a theoretical computational cost of $1.6 \cdot 10^7$ operations while P.D. requires $2 \cdot 10^6$ operations. In fact, the predicted factor-10-speed-up is achieved for the experiment in Section 6.7.

In addition to the derivative computation complexity, the SC-PINN formulation exploits the approximation power of the Gauss-Legendre cubature, as it becomes observable in the numerical experiments, Section 6.

Here, we want to point out the following insight: We consider the $m$-dimensional integral $I[f] := \int_{\Omega} f d\Omega$ of a $k$-times differentiable function once approximated by the Gauss-Legendre cubature of degree $n$, $I_n^g[f^2] := \sum_{\alpha \in A_{m,n}} f^2(p_\alpha) \omega_\alpha$ and once by the Monte Carlo approximation $I_n^M[f] := \frac{1}{N^n} \sum_{i=1}^{N^n} f^2(x_i)$, with $K \subset \mathbb{R}^m$ a set of points of size $|K| = |A_{m,n}|$. Due to (Trefethen, 2017a) the approximations rates scale as:

$$|I[f] - I_n^g[f]| = \mathcal{O}\left(\frac{1}{k(n-k)^k}\right),$$

$$|I[f] - I_n^M[f]| = \mathcal{O}\left(\frac{1}{\sqrt{K}}\right), \quad K = (n+1)^m.$$ 

Hence, for regular functions, $k \gg m$, achieving a similar accuracy with the SC-PINNs requires less points compared to applying PINNs with MSE-losses. The limitations of the Sobolev cubatures start as the dimension $m \gg 1$ of the domain becomes too high and the complexity in Theorem 4, i) is dominated by the $\mathcal{O}(s^2)$, $s = (n+1)^m$ term. We continue the comparison empirically in the next section.

6. Numerical Experiments

We designed the following experiments for validating and demonstrating our theoretical findings. All experiments were executed on the NVIDIA V100 cluster at HZDR. Precomputation of the Sobolev cubature matrices is realized in (Suraz Cardona, 2022) as a feature of the open source package (Hernandez Acosta et al., 2021), which is based on our recent work (Hecht et al., 2017; 2018; 2020; Hecht & Shalzarin, 2018). For comparison we benchmark the following schemes:

i) **Classic PINNs (PINN)** as proposed in (Raissi et al., 2019) resting on the strong $L^2$-MSE loss, Eq. (1).

ii) **Inverse Dirichlet Balancing (ID-PINNs)** with the $L^2$-MSE loss (Maddu et al., 2021), as described in the introduction.

iii) **Sobolev Cubature PINNs (SC-PINNs)** with the weak $L^2$-loss for all the experiments unless specified otherwise.

iv) **Variational PINNs (VPINNs)** with the strong $L^2$-loss with and without domain decomposition, as introduced in Section 1.1.2. While VPINNs resulted in incommensurate training effort in 2D only 1D experiments were executed.

For a given ground truth function $g : \Omega \rightarrow \mathbb{R}$ and a $\hat{u}_\theta$ approximation we measure the $l_1, l_\infty$-errors $\epsilon_1 := \|g - u\|_1, \epsilon_\infty := \|g - u\|_\infty$ by sampling on equidistant grids of size $N = 100^2$ in 2D. For (inverse) parameter inference problems we denote the parameter error with $\epsilon_\lambda = |\lambda - \lambda_{gt}|$.

All models are trained with the same number of training points regardless of their specification (random or Legendre grids).

6.1. Poisson Equation

We start by addressing the Poisson problem in dimension $m = 2$

$$\left\{ \begin{array}{l} -\Delta u(x) - f(x) = 0, \forall x \in \Omega = [-1, 1]^2 \\ u(x) - g(x) = 0, \forall x \in \partial \Omega, \end{array} \right.$$ 

described in detail Eq. (13). We choose $f(x,y) := -2\lambda^2 \cos(\lambda x) \sin(\lambda y)$ and $g(x,y) := \cos(\lambda x) \sin(\lambda y)$, with frequency $\lambda = 2\pi q$, $q = 6$, yielding $u(x,y) = g(x,y)$ to be the analytic solution.

We compare the performance of the following PINN implementations:

I) PINN and ID-PINN relying in strong mean square (MSE) loss $\mathcal{L}_{\text{MSE}}$, Eq. (1).

II) SC-PINN with strong Sobolev loss $\mathcal{L}_{\text{srong}}$, Eq. (17),

$$\mathcal{L}_{\text{strong}}(u) = r_{\text{strong},n_r,k}(u) + s_{\text{strong},n_s,l}(u)$$

for $k = 0$, $l = 2$, $n_r = 30$, $n_s = 100$, in two versions: Once computing $\Delta u$ with automatic differentiation (A.D.) and once without A.D., but with polynomial differentiation (P.D.) given in Eq. (20).

III) SC-PINN with strong variational Sobolev loss, Eq. (22)

$$\mathcal{L}_{\text{var}}^{\text{strong}}(u) = r_{\text{var},n_r,k}(u) + s_{\text{var},n_s,l}(u)$$

for $k = 0$, $l = 0$, $n_r = 30$, $n_s = 100$, without A.D., but with P.D..

All methods were implemented for fully connected feed-forward NNS, $\hat{u} \in \Xi_{2,1}$, of 5 hidden layers, each of 50 units length, unless specified otherwise. Activation functions were chosen as $\sigma(x) = \sin(x)$, which performed best compared to trials with ReLU, ELU or $\sigma(x) = \tanh(x)$. 

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All PINNs were trained by applying the Adam optimizer (Kingma & Ba, 2014) for 30000 iterations, batch size $bs = |F_{m,n}|$ for ID-PINN equals SC-PINN, and learning rate of $lr = 1e^{-3}$, whereas ID-PINN applies its dynamic gradient balancing scheme.

Approximation errors and CPU-training times $t$ are reported in Figs. 1–4. While the classic PINN approach failed to converge (reach reasonable approximations) its results are skipped.

In comparison SC-PINN reaches several orders of magnitude better approximations: SC-PINN with $L_{\text{strong}}$ and A.D. improves by one order, while replacing A.D. with P.D. even increases the accuracy by one further order. In addition the CPU runtime is reduced by three fold when executing SC-PINN with P.D. instead of A.D. The choice of $F_{\text{var}}$ improves the $\epsilon_1$ error by one order of magnitude compared to SC-PINN with $L_{\text{strong}}$ and A.D., which requires more CPU time.

We address a further prominent PDE problems to continue our empirical investigations. From here on we only use P.D. instead of A.D. for executing the experiments with the SC-PINNs.

### 6.2. Quantum Harmonic Oscillator

The time independent Quantum Harmonic Oscillator in dimension $m = 2$, corresponds to the Schrödinger equation with the linear potential $V(u(x)) := (x_1^2 + x_2^2)u(x)$, $u \in C^2(\Omega, \mathbb{R})$, see e.g. (Liboff, 1980; Griffiths & Schroeter, 2018), given by:

$$
\begin{align*}
-\Delta u(x) + V(u(x)) &= \lambda u(x) , \forall x \in \Omega \\
u(x) - g(x) &= 0 , \forall x \in \partial\Omega ,
\end{align*}
$$

We consider the eigenvalue problem $\lambda = n_1 + n_2 + 1, n_1, n_2 \in \mathbb{N}$ with eigenfunctions

$$
g(x_1, x_2) = \frac{\pi^{-1/4}}{\sqrt{2^{n_1+n_2}n_1!n_2!}} e^{-\frac{(x_1^2+x_2^2)}{2}} H_{n_1}(x_1)H_{n_2}(x_2),
$$

whereas $H_n$ denotes the $n$-th Hermite polynomial.

We keep the experimental design from Section 6.1, choose $\lambda = 15$ and report the results in Fig. 5–7: Similar to the previous experiment classic PINN failed to converge, SC-PINNs improve the accuracy up to 2 orders of magnitude in 4 fold less runtime, whereas, SC-PINN with $L_{\text{strong}}$ and P.D. performs best.

### 6.3. Poisson problems with hard transitions

We re-investigate PINN-solutions of the Poisson problem in dimension $m = 1$, whose analytic solutions include hard transitions. That is, choosing

$$f(x) := C(A\omega^2 \sin(\omega x) + 2\beta^2 \text{sech}^2(x) \tanh(\beta x)) ,$$

with boundary condition $g(x) := C(A\sin(\omega x) + \tanh(\beta x))$ yielding $u(x) = g(x)$ to be the analytic solution. Two scenarios were considered:

$$S_1 = \{ C = 0.1, A = 0.1, \beta = 30, \omega = 20\pi, bs = 100 \}$$
$$S_2 = \{ C = 0.1, A = 0.1, \beta = 5, \omega = 26.5\pi, bs = 100 \}$$
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Figure 5. ID-PINN with MSE loss and A.D., reaching $\epsilon_{\infty} = 1.46e^{-1}, \epsilon_1 = 4.78e^{-2}, t \approx 905$.

Figure 6. SC-PINN with strong Sobolev loss and P.D., reaching $\epsilon_{\infty} = 1.22e^{-2}, \epsilon_1 = 1.24e^{-3}, t \approx 165$.

Figure 7. SC-PINN with strong variational Sobolev loss and P.D., reaching $\epsilon_{\infty} = 7.27e^{-3}, \epsilon_1 = 8.16e^{-4}, t \approx 167$.

Figure 8. SC-PINN with strong Sobolev loss and P.D. (left), reaching $\epsilon_{\infty} = 3.04e^{-2}, \epsilon_1 = 7.24e^{-2}, t \approx 150$, SC-PINN with strong variational Sobolev loss and P.D. (right), reaching $\epsilon_{\infty} = 2.0e^{-3}, \epsilon_1 = 4.0e^{-4}, t \approx 151$, scenario $S_1$.

Figure 9. VPINN with $N_{el} = 1$ (left), reaching $\epsilon_{\infty} = 3.29e^{-3}, \epsilon_1 = 9.94e^{-4}, t \approx 96$, VPINN with $N_{el} = 3$ (right), reaching $\epsilon_{\infty} = 2.73e^{-3}, \epsilon_1 = 1.40e^{-3}, t \approx 191$, scenario $S_1$.

Figure 10. SC-PINN with strong variational Sobolev loss and P.D. (left), reaching $\epsilon_{\infty} = 6.50e^{-2}, \epsilon_1 = 3.40e^{-2}, t \approx 180$, scenario $S_2$.

Figure 11. ID-PINN with MSE loss, $bs = 500$ and A.D. (left), reaching $\epsilon_{\infty} = 4.74e^{-1}, \epsilon_1 = 2.50e^{-1}, t \approx 158$, ID-PINN with MSE loss without I.D., $bs = 5000$ and A.D. (right), reaching $\epsilon_{\infty} = 1.73e^{-1}, \epsilon_1 = 7.13e^{-2}, t \approx 360$, scenario $S_2$.

Up to reducing to 4 hidden layers, each of 20 units length the same NN architecture, $\hat{u} \in \Xi_{1,1}$, as prior was chosen. The degree $n \in \mathbb{N}$ of the Sobolev losses is set as the batch size $n = bs$. In addition to the previous PINN methods we consider the VPINNs, introduced in Section 1.1.2, relying on the strong variational Sobolev loss and domain decomposition specified by the number of its elements $N_{el} \in \mathbb{N}$.

Comparison of SC-PINNs and VPINNs for scenario $S_1$ is reported in Figs. 8, 9: While SC-PINN with strong Sobolev loss misses to capture the solution, SC-PINN with variational loss reaches compatible approximations compared to VPINN with 3-element decomposition $N_{el} = 3$.

For the second set of parameters $S_2$ results are reported in Fig. 10: We observe a similar behaviour as in scenario $S_1$, but SC-PINN with strong variational loss reaches one order of magnitude better (overall) $\epsilon_1$-error compared to VPINN. ID-PINN and PINN both fail to converge. We present the results only for the I.D. balancing, once for batch size $bs = 500$ and once for $bs = 5000$, are reported in Fig. 11. We, however, observe that even by increasing the batch size by a factor of 10 ID-PINN does not become compatible to SC-PINN.
6.4. 2D Poisson Inverse Problem

We will now consider the inverse problem for the 2D Poisson equation, where we want to infer \( \lambda \), that appears explicitly on the RHS \( f(x) = \lambda \cos(\omega x) \sin(\omega y) \) for \( \omega = \pi \). We used for the SC-PINN, degree 100 and 30 quadrature for the boundary and the domain respectively and the same amount of points randomly sampled for the ID-PINN and the standard PINN. The ground truth \( \lambda_{gt} = 2\omega^2 \) and the weak \( L^2 \)-loss. We test it against the standard PINN and the ID-PINN with same number of points.

![Figure 12. Solution for 2D Poisson with \( \lambda_{gt} = \pi \).](image)

| Method     | Approximation error | Runtime (s) |
|------------|---------------------|-------------|
| PINN       | \( 4.63 \cdot 10^{-1} \) | \( 1.13 \cdot 10^{-2} \) | \( t \approx 1592 \) |
| ID-PINN    | \( 2.14 \cdot 10^{-2} \) | \( 8.09 \cdot 10^{-4} \) | \( t \approx 2184 \) |
| SC-PINN    | \( 3 \cdot 10^{-4} \) | \( 5.49 \cdot 10^{-4} \) | \( t \approx 103 \) |

Table 1. Errors for 2D Poisson inverse problem

Due to Table 1, the SC-PINN recovers the parameter \( \lambda \) with one order of magnitude higher accuracy by requiring almost two orders of magnitude less runtime. even in the inverse problem setting, this shows the superiority of SC-PINN in both approximation and computational performance. To support this result, we consider the inverse problem for the time independent 2D QHO.

6.5. 2D QHO Inverse Problem

We pose the QHO eigenvalue problem for unknown eigenvalue \( \lambda_{gt} = 5 \) and seek finding the eigenvalue and the PDE solution simultaneously. In this setting we use the SC-PINN with \( L^2 \)-weak loss, and a 200 degree cubature for the boundary and use degree 50 in the domain. We compare it with the ID-PINN and the standard PINN trained with the same number of (random) training points.

![Figure 13. Solution for 2D QHO with \( \lambda_{gt} = 5 \).](image)

| Method   | Approximation error | Runtime (s) |
|----------|---------------------|-------------|
| PINN     | \( 6.01 \)         | \( 7.32 \cdot 10^{-2} \) | \( t \approx 1414 \) |
| ID-PINN  | \( 6.21 \cdot 10^{-2} \) | \( 7.51 \cdot 10^{-3} \) | \( t \approx 1346 \) |
| SC-PINN  | \( 2.18 \cdot 10^{-4} \) | \( 5.68 \cdot 10^{-4} \) | \( t \approx 192 \) |

Table 2. Errors for 2D QHO inverse problem with \( \lambda_{gt} = 5 \)

According to the results presented in Table 2 SC-PINN performs again better than the other PINN formulations by reaching 2 orders of magnitude smaller \( \epsilon_1 \)-error. However, SC-PINN is slightly slower than the other PINNs in this 1D-setting. We focus on the runtime performance in a separate experiment below.

6.6. Non-linear Burger’s Equation in 1D

We consider the time independent Burger’s equation in conservative form with Dirichlet boundary conditions given by

\[
\begin{aligned}
-\frac{d^2}{dx^2}u(x) + \frac{1}{2} \frac{d}{dx} (u(x)^2) &= f(x), \quad \forall x \in \Omega \\
u(x) - g(x) &= 0, \quad \forall x \in \partial \Omega,
\end{aligned}
\]

with \( f(x) := \frac{\omega}{2} \sin(2\omega x) + \omega^2 \sin(\omega x) \).

We solve the PDE with a 100 degree quadrature, \( \omega = 14\pi \) and the and strong variational loss for the SC-PINN norm. We test it against the PINN and the ID-PINN with same number of (random) training points.

According to the results presented in Table 3 SC-PINN performs again better than the other PINN formulations by reaching 2 orders of magnitude smaller \( \epsilon_1 \)-error. However, SC-PINN is slightly slower than the other PINNs in this 1D-setting. We focus on the runtime performance in a separate experiment below.
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As reported in Table 4 the SC-PINN recovers a more accurate solution of the 4th order ODE in one order of magnitude less runtime. This suggests that replacing A.D. by P.D. increases the efficiency, as predicted in our discussions in Section 5, Example 5.

7. Conclusion

We introduced the notion of Sobolev cubatures and gave theoretical insights in order to setup the novel Sobolev PINNs (SC-PINNs). As predicted, by the runtime complexity analysis we did, for low dimensional problems this results in a faster PDE learning scheme than PINNs relying on automatic differentiation.

Moreover, in Theorem 3 we theoretically ensured that the SC-PINNs converge to strong (smooth) PDE solutions for well posed problems. This result is complemented by the several order of magnitude higher accuracy the SC-PINNs reached when considering prominent linear, non-linear, forward, and inverse PDE problems.

Depending on the numerical experiment, the choice of the Sobolev cubature differed. While we meanwhile deepened the theoretical insights presented in this article to deliver the optimal choice beforehand these subjects are out of scope, here, and part of a follow-up study. This includes a relaxation of the Sobolev cubatures, resisting the curse of dimensionality when addressing higher dimensional problems.

Apart from these potential enhancements the class of low dimensional, \( \text{dim} = 2, 3, 4 \), real world problems is huge. Thus, the demonstrations, here, make us believe that applying the SC-PINNs might be beneficial for many scientific applications across all disciplines.

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