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A POSTERIORI ERROR ESTIMATION FOR ARBITRARY ORDER FEM APPLIED TO SINGULARLY PERTURBED ONE-DIMENSIONAL REACTION-DIFFUSION PROBLEMS

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Cordially dedicated to Michal Křížek on occasion of his 60th birthday

Abstract. FEM discretizations of arbitrary order r are considered for a singularly perturbed one-dimensional reaction-diffusion problem whose solution exhibits strong layers. A posteriori error bounds of interpolation type are derived in the maximum norm. An adaptive algorithm is devised to resolve the boundary layers. Numerical experiments complement our theoretical results.

Keywords: reaction-diffusion problem; singular perturbation; mesh adaptation

MSC 2010: 65L10, 65L50, 65L60

1. Introduction

Consider the boundary value problem of finding u such that

$$\mathcal{L}u := -\varepsilon^2 u'' + cu = f \quad \text{in } (0,1), \quad u(0) = u(1) = 0 \tag{1.1}$$

with functions $c, f\colon [0,1] \to \mathbb{R}$. The coefficient c is assumed to be piecewise continuous with a finite number of discontinuities. Furthermore, let c be strictly positive, i.e., $c \geqslant \gamma^2$ on $[0,1]$ with some constant $\gamma > 0$.

Its solution exhibits two layers of width $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ at the two endpoints of the domain. If the right-hand side f or the reaction coefficient c possesses a discontinuity at a point $d \in (0,1)$, then an interior layer of the same width will form at d. Because of the presence of these layers, special measures are required to efficiently obtain good numerical approximations. Modern literature [15] favours the use of meshes that are a priori adapted to the layer structure, for example Bakhvalov meshes [1] or Shishkin meshes [16].

In many cases, convergence of the FEM for (1.1) is studied in the energy norm naturally associated with its weak formulation: $|||v||| := \varepsilon|v|_1 + \|v\|_0$. Melenk [12] analyses high-order FEM. He establishes exponential convergence in the energy norm. A posteriori error bounds for (1.1) in this norm have been derived by Kunert [9]. A drawback of the energy norm is its failure to capture the afore mentioned layers. They are of $\mathcal{O}(\varepsilon^{1/2})$ in that norm. In the recent paper [14] an idea is presented for studying convergence in a differently weighted H^1-norm: $|||v|||_* := \varepsilon^{1/2}|v|_1 + \|v\|_0$, a norm that captures the layers in (1.1).

Here our focus is on a posteriori error bounds in the maximum norm. This norm captures the layers and often is the norm of choice for singularly perturbed problems like (1.1). For some classical problems, i.e. problems without layers, various a posteriori error estimators in the maximum are available. For example, in [13], Nochetto et al. studied finite element methods of arbitrary order for the semilinear problem $-\Delta u + r(\cdot, u) = 0$ in more dimensions. The crucial point—and often also the main difficulty—in singular perturbations is to carefully monitor the dependence of any constants on the perturbation parameter(s).

We remark that a standard linearization technique allows to extend the results to semilinear differential equations $-\varepsilon^2 u'' + c(\cdot, u) = 0$ with $c_u > \gamma^2$; see for example [5].

The analysis is easily adapted for systems of reaction-diffusion equations using the technique in [10, §6.2.3.4]. Furthermore, the results can be used as a building block in the a posteriori error estimation for parabolic problems in the context of [4], [7], [6]. This is one of the main motivations for the present study.

The outline of the paper is as follows. In Section 2 we introduce a finite element discretization of (1.1) and summarize our theoretical results for this method. Section 3 contains our a posteriori error analysis, while in the final Section 4 an adaptive mesh-movement strategy is studied which is based on the a posteriori error estimator of Section 3.

2. Summary

The variational formulation of (1.1) is: Find $u \in H_0^1(0,1)$ such that

$$a(u,v) := \varepsilon^2(u',v') + (cu,v) = (f,v) \quad \forall v \in H_0^1(0,1) \tag{2.1}$$

with the L_2 scalar product $(w,v) := \int_0^1 w(x)v(x)\,\mathrm{d}x$.

Let the discretization mesh $\overline{\omega} = \{x_i\}_{i=0}^N$ be given by the mesh nodes

$$0 = x_0 < x_1 < \ldots < x_N = 1.$$

The mesh intervals and mesh sizes are denoted by $J_i := [x_{i-1}, x_i]$ and $h_i := x_i - x_{i-1}$, $i = 1, \dots, N$.

We shall discretize (2.1) using piecewise polynomials of highest degree $r \in \mathbb{N}^+$. To this end let

$$C_0[0,1] := \{v \in C[0,1]\colon\ v(0) = v(1) = 0\}$$

and

$$V_r := \{v \in C_0[0,1]\colon\ v|_{J_i} \in \Pi_r,\ i = 1, \dots, N\} \subset H_0^1(0,1),$$

where Π_r is the space of polynomials of degree r or less.

A first discretization of (2.1) would be: Find $u_\omega \in V_r$ such that

$$a(u_\omega, v) = (f, v) \quad \forall v \in V_r. \tag{2.2}$$

However, in general, the integrals involved cannot be evaluated exactly. Therefore, we shall consider a discretization which involves the use of quadrature.

Let $t_j = j/r$, $j = 0, 1, \dots, r$. Then, for any function $v \in C_0[0,1]$, an interpolant $I_r^L v \in V_r$ is uniquely defined by

$$I_r^L v(x_{i-t_j}) = v(x_{i-t_j}), \quad i = 1, \dots, N,\ j = 0, \dots, r,$$

where for $t \in [0,1]$ we have set $x_{i-t} := x_i - t h_i$. For example, $x_{i-1/2}$ is the midpoint of the mesh interval J_i. For any function $g \in C[0,1]$, we shall also use the notation $g_{i-t} := g(x_{i-t})$.

Replacing the L_2 scalar product (w, v) in (2.2) by its discrete version $(w, v)_{\overline{\omega}} := (I_r^L w, v)$, we arrive at the FEM: Find $u_\omega \in V_r$ such that

$$a_{\overline{\omega}}(u_\omega, v) := \varepsilon^2(u_\omega', v') + (c u_\omega, v)_{\overline{\omega}} = (f, v)_{\overline{\omega}} \quad \forall v \in V_r. \tag{2.3}$$

Remark 1. If the data c or f are discontinuous at a point $d \in (0,1)$ then the mesh points must be chosen to cover this discontinuity, i.e., $d \in \overline{\omega}$. Furthermore, appropriate one sided limits have to be taken in the definition of the interpolation operator I_r^L.

In Section 3 the following a posteriori error bound will be derived (Theorem 1):

$$\begin{aligned} \|u - u_\omega\|_\infty \leqslant{} & \left\| \frac{q - I_r^L q}{c} \right\|_\infty \\ & + \max_{i=1,\dots,N} \frac{h_i^{r+1}}{\varepsilon^2} \Big(\frac{\alpha_r}{(2r)!} |D_+^{r-1} q_i + D_-^{r-1} q_i| + \frac{2\beta_r h_i}{(2r+1)!} |D_0^r q_i| \Big) \end{aligned} \tag{2.4}$$

with certain constants α_r and β_r, and $q := f - cu_\omega$. Here and throughout we denote by $\|\cdot\|_{\infty,\Omega}$ the supremum/maximum norm in $L_\infty(\Omega)$. If $\Omega = (0,1)$, then we drop Ω from the notation.

The first term on the right-hand side of (2.4) captures the data oscillations and inevitably requires sampling of c and f, i.e., the data has to be evaluated at a (potentially large) number of points that do not coincide with mesh points or points used in the definition of the discrete L_2 scalar product $(w,v)_{\overline{\omega}}$. For details how this can be done, see Section 3.4.

The difference operators D_+^{r-1}, D_-^{r-1} and D_0^r represent approximations of derivatives of order $r-1$ and r, respectively. They will be defined in Section 3.3. In particular, $|D_0^r q_i| \leqslant r(|D_+^{r-1} q_i| + |D_-^{r-1} q_i|)/h_i$. Thus,

$$\|u - u_\omega\|_\infty \leqslant \left\| \frac{q - I_r^L q}{c} \right\|_\infty + \frac{\kappa_r}{\varepsilon^2} \max_{i=1,\dots,N} h_i^{r+1} (|D_+^{r-1} q_i| + |D_-^{r-1} q_i|), \tag{2.5}$$

with another constant κ_r.

In view of the differential equation (1.1) we have $q = f - cu_\omega \approx f - cu = -\varepsilon^2 u''$. Therefore, the term $\varepsilon^{-2}(|D_+^{r-1} q_i| + |D_-^{r-1} q_i|)$ corresponds to an approximation of the derivative of order $r+1$ of u_ω. Estimates with a similar structure are well known for the interpolation error:

$$\|w - I_r^L w\|_\infty \leqslant C \max_{i=1,\dots,N} h_i^{r+1} \|w^{(r+1)}\|_{\infty,J_i}.$$

Therefore, we call (2.5) an a posteriori error bound of interpolation type.

3. A posteriori error bounds

Our error analysis is based on a representation of the error by means of Green's function $\mathcal{G}$ associated with the differential operator $\mathcal{L}$ and the point $x \in (0,1)$:

$$(u - u_\omega)(x) = a(u - u_\omega, \mathcal{G}(x)) = (f, \mathcal{G}(x)) - a(u_\omega, \mathcal{G}(x)),$$

by (2.1).

3.1. Properties of Green's function. In the sequel we shall use Green's function $\mathcal{G}\colon [0,1]^2 \to \mathbb{R}$ associated with $a(\cdot,\cdot)$—or $\mathcal{L}$—to represent the error of the FEM. For arbitrary but fixed $x \in (0,1)$, $\Gamma := \mathcal{G}(x,\cdot)$ satisfies $\Gamma \in H_0^1(0,1)$ and

$$a(w, \Gamma) = w(x) \quad \text{for all } w \in H_0^1(0,1). \tag{3.1}$$

We have assumed that c is piecewise continuous with a finite number of points of discontinuity. Hence, $\Gamma \in C^2(\Delta \setminus \{x\}) \cap C^1((0,1) \setminus \{x\}) \cap C[0,1]$, where $\Delta \subset (0,1)$ is the set of points where c is continuous. Furthermore, Γ satisfies

$$\text{(3.1}'\text{)} \quad \mathcal{L}\Gamma = 0 \text{ in } \Delta \setminus \{x\}, \quad \Gamma(0) = \Gamma(1) = 0 \quad \text{and} \quad \Gamma'(x-0) - \Gamma'(x+0) = \varepsilon^{-2}.$$

We quote bounds on Green's function from [10, §3.3.1.1]. First, the comparison principle gives $0 \leqslant \Gamma(\xi) \leqslant (2\varepsilon)^{-1/2} \mathrm{e}^{-\gamma|\xi - x|/\varepsilon}$ because $\mathcal{L}$ is inverse monotone. Next, $\Gamma \geqslant 0$ on $[0,1]$ implies $\Gamma'(1) \leqslant 0$ and $\Gamma'(0) \geqslant 0$. Integrating (3.1′) over $(0,1)$, we get

$$0 \leqslant \int_0^1 (c\Gamma)(\xi)\,\mathrm{d}\xi = 1 + \varepsilon^2(\Gamma'(1) - \Gamma'(0)) \leqslant 1.$$

Thus

$$\text{(3.2a)} \qquad \|c\Gamma\|_{L_1(0,1)} \leqslant 1.$$

The positivity of Γ'' on Δ, which follows from the differential equation in (3.1′), and the jump condition for Γ' at x yield

$$\text{(3.2b)} \qquad \|\Gamma''\|_{L_1} \leqslant 2\varepsilon^{-2}.$$

3.2. Preliminaries. A special interpolation operator $I_r^M \colon C_0[0,1] \to V_r$, which will turn out to be particularly suitable for our analysis, is defined via moments. For $i = 1, \ldots, N$ it satisfies

$$\text{(3.3a)} \qquad I_r^M v(x_{i-1}) = v(x_{i-1}), \quad I_r^M v(x_i) = v(x_i),$$

and

$$\text{(3.3b)} \qquad \int_{J_i} \pi(\xi) I_r^M v(\xi)\,\mathrm{d}\xi = \int_{J_i} \pi(\xi) v(\xi)\,\mathrm{d}\xi, \quad \forall \pi \in \Pi_{r-2}.$$

The following polynomial $p_{r,i}$ will be central in our analysis:

$$\begin{aligned} p_{r,i}(\xi) &:= ((\xi - x_i)(\xi - x_{i-1}))^r = \left((\xi - x_{i-1/2})^2 - \left(\frac{h_i}{2}\right)^2\right)^r \\ &= \sum_{k=0}^{r} (-1)^k \binom{r}{k} (\xi - x_{i-1/2})^{2(r-k)} \left(\frac{h_i}{2}\right)^{2k}. \end{aligned}$$

Proposition 1.

$$\int_{J_i} \frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi^{r-1}}(p_{r,i}(\xi)\varrho(\xi))\pi(\xi)\,\mathrm{d}\xi = 0 \quad \forall \pi \in \Pi_{r-2},\ \varrho \in \Pi.$$

P r o o f. The polynomial $p_{r,i}\varrho$ possesses zeros of multiplicity r at x_{i-1} and x_i. Thus, its derivatives up to and including order $r-1$ also vanish at x_{i-1} and x_i. Therefore, integrating by parts $r-1$ times, we obtain

$$\int_{J_i} \frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi^{r-1}}(p_{r,i}(\xi)\varrho(\xi))\pi(\xi)\,\mathrm{d}\xi = (-1)^{r-1}\int_{J_i}(p_{r,i}(\xi)\varrho(\xi))\pi^{(r-1)}(\xi)\,\mathrm{d}\xi.$$

The proposition follows because $\pi^{(r-1)} \equiv 0$ for all $\pi \in \Pi_{r-2}$. □

Proposition 2. *There exist polynomials* $\pi_1, \pi_2 \in \Pi_{r-2}$ *such that*

$$p_{r,i}^{(r+1)}(\xi) = (-1)^r\frac{(2r)!}{(r-1)!}(\xi - x_{i-1/2})^{r-1} + \pi_1(\xi) \tag{3.4a}$$

and

$$\frac{\mathrm{d}^{r+1}}{\mathrm{d}\xi^{r+1}}(p_{r,i}(\xi)(\xi - x_{i-1/2})) = (-1)^r\frac{(2r+1)!}{r!}(\xi - x_{i-1/2})^r + \pi_2(\xi). \tag{3.4b}$$

P r o o f. These identities readily follow from the definition of $p_{r,i}$. □

Lemma 1. *Let* $\Gamma = \mathcal{G}(x,\cdot)$ *be Green's function associated with the operator* $\mathcal{L}$ *and the point* $x \in (0,1)$*. Then*

$$\int_{J_i} \pi'(\xi)(\Gamma - I_r^M\Gamma)'(\xi)\,\mathrm{d}\xi = 0 \quad \forall \pi \in \Pi_r, \tag{3.5a}$$

$$\int_{J_i}(\xi - x_{i-1/2})^k(\Gamma - I_r^M\Gamma)(\xi)\,\mathrm{d}\xi = 0 \quad \textit{for } k = 0,\dots,r-2, \tag{3.5b}$$

$$\int_{J_i}(\xi - x_{i-1/2})^{r-1}(\Gamma - I_r^M\Gamma)(\xi)\,\mathrm{d}\xi = (-1)^{r+1}\frac{(r-1)!}{(2r)!}\int_{J_i} p_{r,i}^{(r-1)}(\xi)\Gamma''(\xi)\,\mathrm{d}\xi \tag{3.5c}$$

and

$$\begin{aligned}\int_{J_i}&(\xi - x_{i-1/2})^r(\Gamma - I_r^M\Gamma)(\xi)\,\mathrm{d}\xi \\ &= (-1)^{r+1}\frac{r!}{(2r+1)!}\int_{J_i}\frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi^{r-1}}(p_{r,i}(\xi)(\xi - x_{i-1/2}))\Gamma''(\xi)\,\mathrm{d}\xi\end{aligned} \tag{3.5d}$$

for $i = 1,\dots,N$.

P r o o f. Fix any $i \in \{1, \ldots, N\}$.

(i) First, we verify (3.5a). Integration by parts gives

$$\int_{J_i} \pi'(\xi)(\Gamma - I_r^M \Gamma)'(\xi)\,\mathrm{d}\xi$$
$$= \pi'(\xi)(\Gamma - I_r^M \Gamma)(\xi)\big|_{\xi=x_{i-1}}^{x_i} - \int_{J_i} \pi''(\xi)(\Gamma - I_r^M\Gamma)(\xi)\,\mathrm{d}\xi = 0,$$

by (3.3).

(ii) Equation (3.5b) immediately follows from (3.3b).

(iii) Next, (3.3b) and (3.4a) give

$$\begin{aligned} T &:= \int_{J_i} (\xi - x_{i-1/2})^{r-1}(\Gamma - I_r^M\Gamma)(\xi)\,\mathrm{d}\xi \\ &= (-1)^r \frac{(r-1)!}{(2r)!} \int_{J_i} p_{r,i}^{(r+1)}(\xi)(\Gamma - I_r^M\Gamma)(\xi)\,\mathrm{d}\xi. \end{aligned}$$

Integrate by parts and use (3.3a) to obtain

$$T = (-1)^{r+1} \frac{(r-1)!}{(2r)!} \int_{J_i} p_{r,i}^{(r)}(\xi)(\Gamma - I_r^M\Gamma)'(\xi)\,\mathrm{d}\xi.$$

Once again, integrate by parts. We get

$$T = (-1)^r \frac{(r-1)!}{(2r)!} \int_{J_i} p_{r,i}^{(r-1)}(\xi)(\Gamma - I_r^M\Gamma)''(\xi)\,\mathrm{d}\xi,$$

because $p_{r,i}^{(r-1)}$ vanishes at x_{i-1} and x_i. Proposition 1 with $\pi = (I_r^M\Gamma)''$ yields (3.5c).

The proof of (3.5d) is similar. □

3.3. Error analysis. Let $x \in (0,1)$ be arbitrary, but fixed. Set $q := f - cu_\omega$. With Green's function $\Gamma := \mathcal{G}(x,\cdot)$ associated with $\mathcal{L}$ and x we have

$$\begin{aligned} (u - u_\omega)(x) &= a(u - u_\omega, \Gamma) = (f, \Gamma) - a(u_\omega, \Gamma) \\ &= (f,\Gamma) - (f, I_r^M\Gamma)_{\varpi} - a(u_\omega, \Gamma) + a_{\varpi}(u_\omega, I_r^M\Gamma)_{\varpi} = (q,\Gamma) - (q, I_r^M\Gamma)_{\varpi} \end{aligned}$$

where we have used (2.1), (3.1), (2.3) and (3.5a). We get the error representation

$$(u - u_\omega)(x) = (q - I_r^L q, \Gamma) - (I_r^L q, \Gamma - I_r^M\Gamma). \tag{3.6}$$

The first term on the right-hand side can be bounded as follows using (3.2a):

$$|(q - I_r^L q, \Gamma)| \leqslant \left\| \frac{q - I_r^L q}{c} \right\|_\infty. \tag{3.7}$$

The second term on the right-hand side of (3.6) will be bounded using Lemma 1. We have

$$(I_r^L q)(\xi) = \sum_{j=0}^{r} \frac{(I_r^L q)_{i-1/2}^{(j)}}{j!} (\xi - x_{i-1/2})^j \quad \text{for } \xi \in \overline{J}_i,\ i = 1, \ldots, N.$$

For arbitrary $i \in \{1, \ldots, N\}$, application of Lemma 1 yields

$$\begin{aligned}
&\int_{J_i} (I_r^L q)(\xi)(\Gamma - I_r^M \Gamma)(\xi)\,\mathrm{d}\xi \\
&\quad = (-1)^{r+1} \int_{J_i} \Bigg[\frac{(I_r^L q)_{i-1/2}^{(r-1)}}{(2r)!} p_{r,i}^{(r-1)}(\xi) \\
&\qquad\qquad + \frac{(I_r^L q)_{i-1/2}^{(r)}}{(2r+1)!} \frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi^{r-1}} (p_{r,i}(\xi)(\xi - x_{i-1/2})) \Bigg] \Gamma''(\xi)\,\mathrm{d}\xi \\
&\quad = (-1)^{r+1} \int_{J_i} \Bigg[\frac{p_{r,i}^{(r-1)}(\xi)}{(2r)!} \psi_{r,i}(\xi) + \frac{r-1}{(2r+1)!} p_r^{(r-2)}(\xi) (I_r^L q)_{i-1/2}^{(r)} \Bigg] \Gamma''(\xi)\,\mathrm{d}\xi
\end{aligned}$$

with

$$\psi_{r,i}(\xi) := (I_r^L q)_{i-1/2}^{(r-1)} + \frac{(I_r^L q)_{i-1/2}^{(r)}}{2r+1} (\xi - x_{i-1/2}).$$

Note that $\psi \in \Pi_1$. Hence it attains its maximum and minimum on $\overline{J}_i$ at the end-points of the interval. Consequently,

$$\|\psi_{r,i}\|_{\infty,J_i} = \max \left\{ \left| (I_r^L q)_{i-1/2}^{(r-1)} \pm \frac{h_i (I_r^L q)_{i-1/2}^{(r)}}{2(2r+1)} \right| \right\}. \tag{3.8}$$

Introducing constants

$$\alpha_r := 2 \max_{\xi \in [0,1]} \left| \frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi^{r-1}} (\xi^r (\xi - 1)^r) \right|$$

and

$$\beta_r := \frac{2(r-1)}{2r+1} \max_{\xi \in [0,1]} \left| \frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi^{r-1}} (\xi^r (\xi - 1)^r (\xi - 1/2)) \right|,$$

we estimate as follows:

$$\begin{aligned}
&\left| \int_{J_i} (I_r^L q)(\xi)(\Gamma - I_r^M \Gamma)(\xi)\,\mathrm{d}\xi \right| \\
&\qquad \leqslant \frac{1}{2(2r)!} \{ \alpha_r h_i^{r+1} \|\psi_{r,i}(\xi)\|_{\infty,J_i} + \beta_r h_i^{r+2} |(I_r^L q)_{i-1/2}^{(r)}| \} \int_{J_i} |\Gamma''(\xi)|\,\mathrm{d}\xi.
\end{aligned} \tag{3.9}$$

R e m a r k 2. For small values of r, the constants α_r and β_r can be computed exactly. Otherwise, the constants can be approximated numerically with arbitrary accuracy.

Next, we derive alternative expressions for $(I_r^L q)_{i-1/2}^{(r-1)}$ and $(I_r^L q)_{i-1/2}^{(r)}$. To this end, let $i = 1, \dots, N$ be arbitrary. Recall that $t_j = j/r$, $j = 0, 1, \dots, r$, and

$$x_{i-t} := x_i - t h_i \quad \text{and} \quad q_{i-t} := q(x_{i-t}), \quad t \in [0, 1].$$

Then, using the Lagrangian basis to represent I_r^L, we obtain

$$(I_r^L q)^{(r-1)}(x) = \sum_{l=0}^{r} q_{i-(r-l)/r} \prod_{\substack{j=0 \\ j \neq l}}^{r} \frac{(r-1)!}{(t_l - t_j) h_i} \sum_{\substack{j=0 \\ j \neq l}}^{r} (x - t_j h_i - x_{i-1}), \quad x \in J_i,$$

and

$$(I_r^L q)^{(r)}(x) = \sum_{l=0}^{r} q_{i-(r-l)/r} \prod_{\substack{j=0 \\ j \neq l}}^{r} \frac{r!}{(t_l - t_j) h_i}, \quad x \in J_i.$$

Set

$$D_-^{r-1} q_i := \left(\frac{r}{h_i}\right)^{r-1} \sum_{j=0}^{r-1} \binom{r-1}{j} (-1)^j q_{i-(r-j)/r}, \quad i = 1, \dots, N$$

and

$$D_+^{r-1} q_i := \left(\frac{r}{h_i}\right)^{r-1} \sum_{j=0}^{r-1} \binom{r-1}{j} (-1)^j q_{i-j/r}, \quad i = 1, \dots, N.$$

These are standard difference quotients of order $r-1$ with evenly distributed knots with distance h_i/r. A straightforward calculation yields

$$(I_r^L q)_{i-1/2}^{(r-1)} = \frac{D_+^{r-1} q_i + D_-^{r-1} q_i}{2} \quad \text{and} \quad (I_r^L q)_{i-1/2}^{(r)} = D_0^r q_i := \frac{r(D_+^{r-1} q_i - D_-^{r-1} q_i)}{h_i}.$$

Substituting these two expressions into (3.8), we obtain

$$\|\psi_{r,i}\|_{\infty, J_i} = \max\{|D_+^{r-1}|, |D_-^{r-1}|\}, \quad i = 1, \dots, N.$$

These representations are inserted into (3.9). Then summation for $i = 1, \dots, N$, (3.6), the Hölder inequality and (3.2b) yield our a posteriori error bound which we summarize as follows.

Theorem 1. *Let u be the solution of the boundary-value problem* (1.1) *and u_ω its numerical approximation from V_r, $r \in \mathbb{N}^+$ obtained by* (2.3). *Then,*

$$\|u - u_\omega\|_\infty \leqslant \eta_I + \eta_D \tag{3.10}$$

with

$$\eta_I := \left\| \frac{q - I_r^L q}{c} \right\|_\infty$$

and

$$\eta_D := \max_{i=1,\dots,N} \Big[\frac{h_i^{r+1}}{(2r)!\varepsilon^2} (\alpha_r \max\{|D_+^{r-1} q_i|, |D_-^{r-1} q_i|\} + r\beta_r |D_+^{r-1} q_i - D_-^{r-1} q_i|) \Big].$$

R e m a r k 3. For $r = 1$, we recover the result from [11], [10]:

$$\|u - u_\omega\|_\infty \leqslant \left\| \frac{q - I_1^L q}{c} \right\|_\infty + \max_{i=1,\dots,N} \Big[\frac{h_i^2}{4\varepsilon^2} \max\{|q_{i-1}|, |q_i|\} \Big].$$

R e m a r k 4. In *hp*- and *hpr*-FEM, polynomials of different degrees may be used on each subinterval. Our analysis easily extends to these methods.

Let $\mathbf{r} \in (\mathbb{N}^+)^N$ and $V_\mathbf{r} := \{v \in C_0[0,1] \colon v|_{J_i} \in \Pi_{r_i},\ i = 1, \dots, N\}$. For $v \in C_0[0,1]$, the interpolant $I_\mathbf{r}^L v \in V_\mathbf{r}$ is uniquely defined by

$$I_\mathbf{r}^L v(x_i - jh_i/r_i) = v(x_i - jh_i/r_i), \quad j = 0, \dots, r_i,\ i = 1, \dots, N.$$

Then, our *hpr*-FEM is: Find $u_\omega \in V_\mathbf{r}$ such that

$$a_*(u_\omega, v) := \varepsilon^2 (u_h', v') + (cu_\omega, v)_* = (f, v)_* \quad \forall v \in V_\mathbf{r},$$

with $(w, v)_* := (I_\mathbf{r}^L w, v)$.

Imitating the above argument, we obtain (3.10) with

$$\eta_I := \max_{i=1,\dots,N} \left\| \frac{q - I_{r_i}^L q}{c} \right\|_{\infty, J_i}$$

and

$$\eta_D := \max_{i=1,\dots,N} \Big[\frac{h_i^{r_i+1}}{(2r_i)!\varepsilon^2} (\alpha_{r_i} \max\{|D_+^{r_i-1} q_i|, |D_-^{r_i-1} q_i|\} + r_i \beta_{r_i} |D_+^{r_i-1} q_i - D_-^{r_i-1} q_i|) \Big].$$

3.4. Numerical results. Consider the test problem

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x)u(x) = \mathrm{e}^{-x}, \quad x \in (0,1),\ u(0) = u(1) = 0. \tag{3.11}$$

Its exact solution is unknown. Therefore, we approximate the errors in u_ω by comparison with the numerical solution u_{ω^*} on a mesh ω^* obtained by uniformly bisecting the original mesh twice, i.e., a mesh that is four times as fine:

$$\|u - u_\omega\|_\infty \approx \|u_{\omega^*} - u_\omega\|_\infty.$$

We are left with determining the maximum difference of two polynomials of potentially high degree, which again can be done approximately only. We use the following approximation:

$$\|u - u_\omega\|_\infty \approx \|u_{\omega^*} - u_\omega\|_\infty \approx \chi_\omega := \max_{i=1,\dots,N} \|u_{\omega^*} - u_\omega\|_{\widehat{\infty},J_i}$$

with

$$\|\varphi\|_{\widehat{\infty},J_i} := \max_{k=0,\dots,4r} |\varphi(x_{i-k/(4r)})|, \quad i = 1,\dots,N.$$

Thus, on each mesh interval $\overline{J}_i$, $i = 1,\dots,N$, we use $4r+1$ evenly distributed points to approximate the maximum errors. Note that for computing the the discrete L_2 scalar product $(w,v)_{\varpi}$, only $r+1$ points are used.

Similarly, the term η_I appearing in the error estimator cannot be computed exactly because it involve the data c and f of the problem which can be computed in a finite number of points only. Therefore, we approximate η_I:

$$\left\|\frac{q - I_r^L q}{c}\right\|_{\infty,J_i} \approx \left\|\frac{q - I_r^L q}{c}\right\|_{\widehat{\infty},J_i},$$

i.e., on each mesh interval J_i we compute the difference $(q - I_r^L q)/c$ in $4r+1$ points. Then we take the maximum.

We use a Bakhvalov mesh [1] with N mesh intervals. This mesh is designed to resolve the layers in the solution. Its mesh nodes are given by $x_i = \mu(i/N)$, $i = 0,\dots,N$, with the mesh generating function

$$\mu(\zeta) = \begin{cases} \vartheta(\zeta) := \dfrac{\sigma\varepsilon}{\gamma} \ln \dfrac{\alpha}{\alpha - \zeta}, & \zeta \in [0, \zeta^*], \\ \vartheta(\zeta^*) + \vartheta'(\zeta^*)(\zeta - \zeta^*), & \zeta \in [\zeta^*, 1/2], \\ 1 - \mu(1-\zeta), & \zeta \in [1/2, 1]. \end{cases}$$

The transition point ζ^* satisfies $(1 - 2\zeta^*)\vartheta'(\zeta^*) = 1 - 2\vartheta(\zeta^*)$, which implies $\mu \in C^1[0,1]$. The mesh parameters are chosen as $\sigma = r+1$ and $\alpha = 1/4$. It is well known that the parameter σ should be chosen to be equal to or greater than the formal order of the method [10]. Other layer-adapted meshes, for example Shishkin's piecewise uniform mesh [16], have been tested too. The results are comparable.

In our experiments, we fix the perturbation parameter as $\varepsilon = 10^{-8}$. This is a sufficiently small value to bring out the singular-perturbation nature of the problem. Almost identical results are obtained for other values of ε, thus illustrating the robustness of the method with respect to the perturbation parameter.

Tables 1 and 2 display the results of our tests for elements of order $r = 5$ and $r = 10$. The first column contains the number of mesh intervals N followed by the maximum-norm error (estimated as above by χ_ω), by the rate of convergence and by the two components η_I and η_D of the error estimator. The last two columns contain the full error estimator η and the effectivity index η/χ_ω. Clearly, $\eta/\chi_\omega \geqslant 1$, and the smaller this ratio the less the overestimation of the error.

N	χ_ω	rate	η_I	η_D	η	η/χ_ω
2^8	2.753e-12	5.99	8.512e-19	1.104e-11	1.104e-11	4.012
2^9	4.344e-14	5.99	1.331e-20	8.824e-14	8.824e-14	2.031
2^{10}	6.820e-16	6.00	2.081e-22	1.375e-15	1.375e-15	2.015
2^{11}	1.068e-17	6.00	3.252e-24	2.144e-17	2.144e-17	2.007
2^{12}	1.671e-19	6.00	5.082e-26	3.348e-19	3.348e-19	2.003
2^{13}	2.613e-21	6.00	7.941e-28	5.229e-21	5.229e-21	2.001
2^{14}	4.084e-23	6.00	1.241e-29	8.169e-23	8.169e-23	2.001
2^{15}	6.382e-25	6.00	1.939e-31	1.276e-24	1.276e-24	2.000
2^{16}	9.972e-27	—	3.029e-33	1.994e-26	1.994e-26	2.000

Table 1. The FEM on a Bakhvalov mesh for (3.11), $r = 5$.

N	χ_ω	rate	η_I	η_D	η	η/χ_ω
2^8	1.566e-21	10.96	2.918e-28	1.493e-20	1.493e-20	9.538
2^9	7.840e-25	10.98	1.462e-31	7.469e-24	7.469e-24	9.527
2^{10}	3.877e-28	10.99	7.228e-35	3.691e-27	3.691e-27	9.522
2^{11}	1.905e-31	11.00	3.552e-38	1.813e-30	1.813e-30	9.520
2^{12}	9.330e-35	11.00	1.740e-41	8.881e-34	8.881e-34	9.518
2^{13}	4.563e-38	11.00	8.509e-45	4.343e-37	4.343e-37	9.518
2^{14}	2.230e-41	11.00	4.158e-48	2.122e-40	2.122e-40	9.517
2^{15}	1.089e-44	11.00	2.031e-51	1.037e-43	1.037e-43	9.517
2^{16}	5.319e-48	—	9.920e-55	5.062e-47	5.062e-47	9.517

Table 2. The FEM on a Bakhvalov mesh for (3.11), $r = 10$.

In both tables the errors reduce as expected with order $r + 1$. The convergence is uniform in the perturbation parameter. Furthermore, we observe a strong linear correlation of actual errors and of the error estimator η. The error overestimation is moderate: close to 2 for $r = 5$, and less than 10 for $r = 10$.

The dominant component of the error estimator is η_D. In both tables it is significantly larger than η_I. This is more pronounced on a Shishkin mesh where $\eta_I \sim N^{-(r+1)}$, while both the actual error and η_D behave like $(N^{-1}\ln N)^{r+1}$, i.e., η_I converges faster to zero than η_D.

4. An adaptive algorithm

Using the a posteriori estimates of the preceding section an adaptive algorithm can be devised. It is based on an idea by de Boor [3] and uses an equidistribution principle. Its convergence in connection with an error estimator for the second order central difference scheme was recently studied by Kopteva and Chadha [2].

The idea is to adaptively design a mesh for which the local contributions to the a posteriori error estimator (incorporating sampling of the data as in Section 3.4)

$$\begin{aligned}\nu_i(u_\omega,\omega) := {}& \left\|\frac{q - I_r^L q}{c}\right\|_{\widehat{\infty},J_i} \\ &+ \frac{h_i^{r+1}}{(2r)!\varepsilon^2}(\alpha_r \max\{|D_+^{r-1}|,|D_-^{r-1}|\} + r\beta_r|D_+^{r-1}q_i - D_-^{r-1}q_i|)\end{aligned}$$

are the same on each mesh interval, i.e., $\nu_{i-1}(u_\omega,\omega) = \nu_i(u_\omega,\omega)$ for $i = 1,\ldots,N$. This is equivalent to

$$Q_i(u_\omega,\omega) = \frac{1}{N}\sum_{j=1}^{N} Q_j(u_\omega,\omega), \quad Q_i(u_\omega,\omega) := \nu_i(u_\omega,\omega)^{1/(r+1)}. \tag{4.1}$$

However, de Boor's algorithm, which we are going to describe now, becomes numerically unstable when the equidistribution principle (4.1) is enforced strongly. Instead, the algorithm is stopped as proposed in [2], [8] when

$$\widetilde{Q}_i(u_\omega,\omega) \leqslant \frac{\gamma}{N}\sum_{j=1}^{N}\widetilde{Q}_j(u_\omega,\omega)$$

for some user chosen constant $\gamma > 1$. Here we have also modified Q_i by choosing

$$\widetilde{Q}_i(u_\omega,\omega) := h_i + \nu_i(u_\omega,\omega)^{1/(r+1)}.$$

Adding this positive constant to ν_i avoids mesh starvation and smoothes the convergence of the adaptive mesh algorithm.

4.1. Adaptive mesh-movement algorithm.

(1) Fix N, r and a constant $\gamma > 1$. The initial mesh $\omega^{[0]}$ is uniform with mesh size $1/N$.

(2) For $k = 0, 1, \ldots$, given the mesh $\omega^{[k]}$, compute the FEM solution $u_{\omega^{[k]}}^{[k]}$ on this mesh. Set $h_i^{[k]} = x_i^{[k]} - x_{i-1}^{[k]}$ for each i. Compute the piecewise-constant function $M^{[k]}$ defined by

$$M^{[k]}(x) := \widetilde{Q}_i^{[k]} := \widetilde{Q}_i(u_{\omega^{[k]}}^{[k]}, \omega^{[k]}) \quad \text{for } x \in (x_{i-1}^k, x_i^k).$$

The total integral of the monitor function is

$$I^{[k]} := \int_0^1 M^{[k]}(t)\,\mathrm{d}t = \sum_{j=1}^{N} h_j^{[k]} \widetilde{Q}_j^{[k]}.$$

(3) Test mesh: If $h_j^{[k]} \widetilde{Q}_j^{[k]} \leqslant \gamma I^{[k]} N^{-1}$ for $j = 1, \ldots, N$, then go to Step 5. Otherwise, continue to Step 4.

(4) Generate a new mesh by equidistributing $M^{[k]}$, i.e., choose the new mesh $\omega^{[k+1]}$ such that

$$\int_{x_{i-1}^{[k+1]}}^{x_i^{[k+1]}} M^{[k]}(t)\,\mathrm{d}t = \frac{I^{[k]}}{N}, \quad i = 1, \ldots, N.$$

Return to Step 2.

(5) Set $\omega = \omega^{[k]}$ and $u_\omega = u_{\omega^{[k]}}^{[k]}$ then stop.

4.2. Numerical results. We consider a modification of (3.11):

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x) u(x) = x^{3/2} + \mathrm{e}^{-x}, \quad x \in (0,1),\ u(0) = u(1) = 0. \tag{4.2}$$

Because of the term $x^{3/2}$ on the right-hand side, the second derivative of the reduced solution $u_0 = f/c$ has a singularity at $x = 0$.

Consequently, a mesh that resolves the layers only, but not the singularity, will give unsatisfactory approximations. This is confirmed by Table 3. The error estimator correctly reflects this behaviour. Note that for this example the actual errors and the values of η_I are (almost) identical. This indicates that the data is not sufficiently well approximated.

In contrast, the FEM with adaptive mesh movement according to the algorithm of Section 4.1 preserves the high order of the method; see Table 4. Both the errors and their a posteriori bounds are converging with order close to $r + 1$, although the errors converge a bit faster. This implies that the effectivity index worsens with N.

The results of the experiments are promising. However, more systematic numerical investigations are required, as is a rigorous theoretical justification for the adaptive algorithm.

N	χ_ω	rate	η_I	η_D	η	η/χ_ω
2^8	2.943e-07	1.52	2.943e-07	6.343e-06	6.637e-06	22.548
2^9	1.028e-07	1.53	1.028e-07	2.115e-06	2.218e-06	21.569
2^{10}	3.555e-08	1.56	3.555e-08	6.881e-07	7.236e-07	20.357
2^{11}	1.205e-08	1.61	1.205e-08	2.160e-07	2.280e-07	18.920
2^{12}	3.949e-09	1.69	3.949e-09	6.438e-08	6.833e-08	17.304
2^{13}	1.220e-09	1.84	1.220e-09	1.780e-08	1.902e-08	15.594
2^{14}	3.418e-10	2.06	3.418e-10	4.411e-09	4.752e-09	13.903
2^{15}	8.203e-11	2.40	8.203e-11	9.300e-10	1.012e-09	12.338
2^{16}	1.555e-11	—	1.555e-11	1.549e-10	1.704e-10	10.959

Table 3. The FEM on a Bakhvalov mesh for (4.2), $r = 7$.

N	χ_ω	rate	η_I	η_D	η	η/χ_ω	K
2^8	9.130e-16	5.91	1.467e-16	4.606e-15	4.753e-15	5.205	16
2^9	1.522e-17	11.41	4.000e-18	1.076e-16	1.116e-16	7.333	7
2^{10}	5.587e-21	8.77	1.031e-19	2.827e-20	1.314e-19	23.511	8
2^{11}	1.279e-23	8.05	2.273e-21	5.604e-23	2.329e-21	182.163	8
2^{12}	4.816e-26	4.98	1.769e-23	6.188e-25	1.831e-23	380.143	9
2^{13}	1.528e-27	10.60	8.918e-27	9.763e-27	1.868e-26	12.224	12
2^{14}	9.817e-31	7.03	1.398e-28	9.326e-30	1.491e-28	151.906	11
2^{15}	7.537e-33	9.43	1.230e-30	1.178e-31	1.347e-30	178.792	11
2^{16}	1.094e-35	—	3.463e-33	7.680e-35	3.540e-33	323.458	12
ave. rate		8.27	7.32	8.21	7.53		

Table 4. The FEM for (4.2) using adaptive mesh movement, $r = 7$, $\gamma = 2$.

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