Solving singularly perturbed problems using enriched finite element spaces

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Mary Immaculate College

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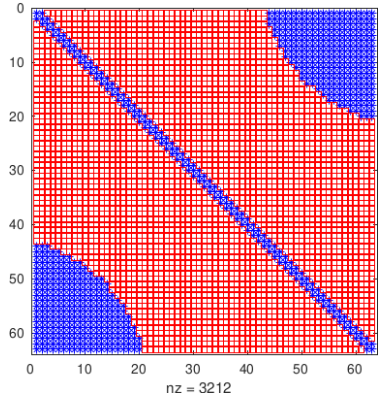
UNIVERSITY OF GALWAY



I'm interested in the numerical solution of differential equations, mainly by finite element methods (FEMs), and especially in the case where solutions exhibit boundary layers.

Solving PDEs by FEMs has three key steps:

(i) **Weak formulation**;

(ii) **Discretization**: i.e., choice of finite dimensional **approximation space**.

(iii) **Solution** of the resulting (usually) linear system.

. . . . . .

This talk is concerned with Parts (ii) and (iii), since they involve matrix theory and linear algebra, respectively.

Some model problems

In this talk, I'll mainly be concerned with the following problems:

$$-\varepsilon u'' + r(x)u = f(x) \quad \text{on} \quad \Omega := (0,1), \tag{1}$$

$$-\varepsilon \Delta u + r(x,y)u = f(x,y) \quad \text{on} \quad \Omega := (0,1)^2, \tag{2}$$

with $u|_{\partial\Omega} = 0$. We are interested in the case where $0 < \varepsilon \ll 1$.

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with $u|_{\partial\Omega} = 0$. We are interested in the case where $0 < \varepsilon \ll 1$.

$$-\varepsilon^2 u'' + r(x)u = f(x) \text{ on } \Omega := (0,1), \qquad u|_{\partial\Omega} = 0$$

Computational challenges:

(a) Solutions to this equation may exhibit boundary or interior **layers**, which are not properly captured by the numerical solution.

(b) In some cases, standard methods may provide numerical "solutions" that are not physically reasonable (e.g., the numerical solution exhibits **oscillations** that cannot be present in the true solution).

In the following set of examples, we will look at attempts to solve the problem above using a standard **finite element** method, on a uniform mesh.

A (Galerkin) **FEM** for the above problem would be:

1. Strong form of the DE: *Find* $u \in C^2(\Omega)$ *such that*

$$-\varepsilon^2 u''(x) + r(x)u(x) = f(x) \text{ on } \Omega + u(0) = u(1) = 0$$

is replaced by: *find* $u \in H_0^1(\Omega)$, *such that*

$$\underbrace{\varepsilon^2(u', v') + (ru, v)}_{B(u,v)} = \underbrace{(f, v)}_{l(v)} \text{ for all } v \in H_0^1(0,1)$$

where $(u, v) := \int_0^1 u(x)v(x)dx$.

2. Discretize: choose $\mathcal{V}_N$, a subspace of H_0^1 of dimension N, and solve: *find* $u^N \in \mathcal{V}_N$ *such that*

$$B(u^N, v) = l(v) \text{ for all } v \in \mathcal{V}_N.$$

- $B(\cdot,\cdot)$ is a symmetric, non-degenerate bilinear form, and therefore induces a norm $\|\cdot\|_B := \sqrt{B(\cdot,\cdot)}$.
- Standard analysis tells us $B(u,v) = l(v)$ has a unique solution (in both $H_0^1(\Omega)$ and $\mathcal{V}_N$).
- Choose a basis for $\mathcal{V}_N$: $\{v_1, v_2, \ldots, v_N\}$.
- We get a linear system of equations $A\widehat{\mathbf{u}} = b$, where $a_{ij} = B(v_j, v_i)$ and $b_i = l(v_i)$. The FEM solution is $u^N = \sum_{i=1}^N \mathbf{u}_i v_i$

It is elementary to show we have a "best approximation property":

$$\|u - u^N\|_B \leqslant \|u - v\|_B \text{ for all } v \in \mathcal{V}$$

This emphasises the key to the whole approach is the choice of $\mathcal{V}$.

Most typical choice for $\mathcal{V}$ is a space of piecewise polynomials on some partition (mesh) of Ω.

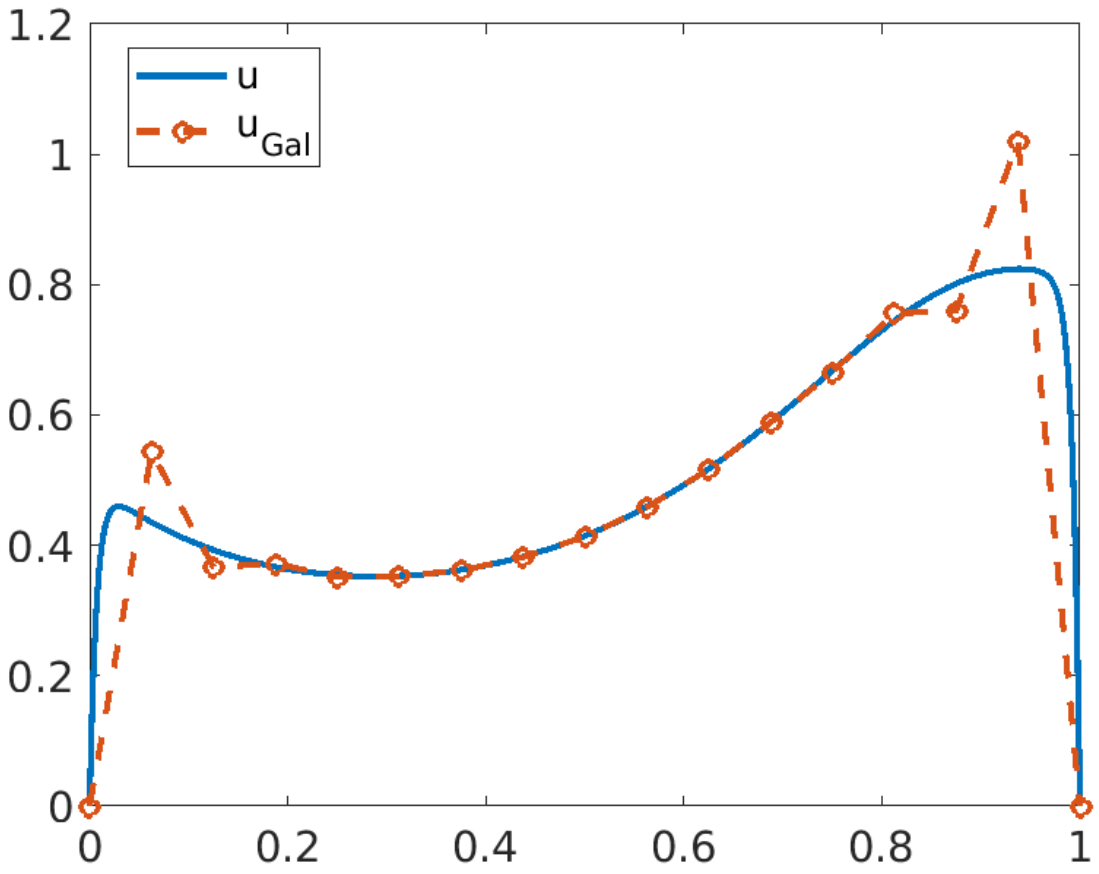
- Choose $N > 0$, and make a uniform mesh $\{x_i\}_{i=1}^{N-1}$ with $x_i = i/N$.
- Let $\mathcal{V}_N$ be the space of piecewise linear functions on that mesh, with basis of "hat functions": $\{v_i\}_{i=1}^{N-1}$.

This is the most standard approach, but is highly suboptimal when $\varepsilon \ll 1$....

Consider a simple example...

$$-\varepsilon^2 u'' + \big(2 + x + \sin(5x)\big)u = e^{x/2}, \text{ on } (0,1)$$

$$u(0) = u(1) = 0.$$



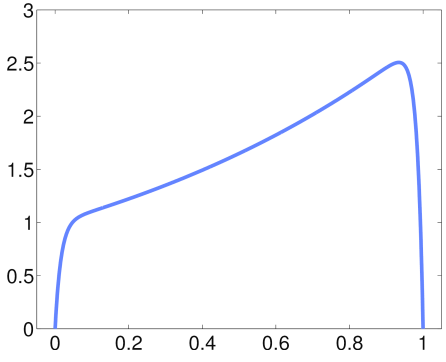
There are several problems with the numerical solution on the previous slide:

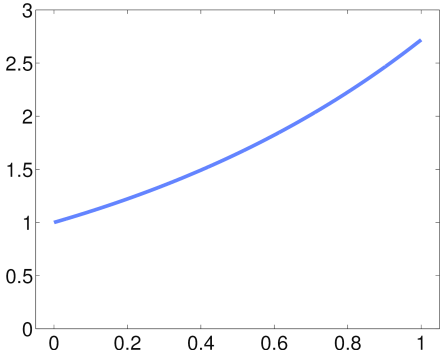
- Even at mesh points, it is not very accurate. This relates to the fact that $\|u''\|$ is $\mathcal{O}(\varepsilon^{-2})$.
- It is not resolving the boundary layers, which are the most interesting part of the true solution.
- It is not stable (in a sense that can be made precise: the differential operator satisfies a maximum principle, but the system matrix does not: it is not an M-matrix).

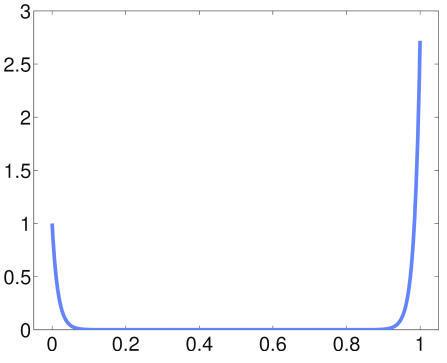
Decompose the solution of the DE as the sum of "regular" and "layer" components

$$u = \underbrace{v}_{\text{regular}} + \underbrace{w}_{\text{left and right layers}} .$$

u $=$ v $+$ $-w$







$$\|v^{(m)}\| \leqslant C\varepsilon^{(q-m)} \quad \text{and} \quad |w^{(m)}(x)| \leqslant C\varepsilon^{-m}\left(e^{-x/\epsilon} + e^{-(1-x)/\epsilon}\right).$$

Mathematical challenge: design **parameter robust methods** that yield approximations for which it can be proven that the method converges (in some norm), and at a rate that is "independent" of ε.

In the literature, these methods so by variously name, such as: **Parameter robust**, ε-robust, **Uniformly convergent**, ...

Let u^N denote a numerical approximation to u by some method. We say that u^N is an ε-robust solution (in the norm $\|\cdot\|_\star$ if

$$\|u - u^N\|_\star \leqslant CN^{-p}$$

where

- N is the mesh parameter (usually degrees of freedom, or related).
- $p > 0$ is the rate of convergence.
- C is a constant independent of ε, N and p.
- No assumption that $N = N(\varepsilon)$.

There are MANY, ε-robust methods for the problems considered so far, and their many variants.

By some distance, the most popular approaches involve applications of some standard methods on specially adapted meshes, with the meshes of Shishkin [Miller et al., 2012] and Bakhvalov [Bakhvalov, 1969] being the most popular.

Roughly, they work by apply a standard method on a mesh adapted to resolving the layer parts.

We want to take a different approach...

GOAL

When solving differential equations numerically, one frequently encounters the situation of having a priori information on the solution which one would like to incorporate into (say) a finite element solution.

We aim to develop a systematic approach for doing this.

Motivation

The idea originally emerged from studying how to incorporate information on the boundary layers in the numerical solution of singularly perturbed problems.

The basic concept exists in various forms in the literature, e.g.,

- [Hemker, 1977] FEM using a basis that combines piecewise polynomials with piecewise exponential functions for a reaction-diffusion equation.
- [Babuška and Melenk, 1995] Partition of unity FEM, again for a reaction-diffusion boundary layer problem.
- [Kellogg and Xenophontos, 2010] A polynomial space enhanced by adding boundary-layer like terms. **This is our primary reference**. One of our aims was to see how to generalise their approach.

And others, such as [Giani, 2018], and various studies of discontinuous enrichment methods (Farhat, Tezaur, and more).

Our weak formulation is $B(u, v) = l(v)$ where (for now) $B(\cdot, \cdot)$ denotes a generic non-degenerate bilinear form, l is some linear functional, and u, v belong some suitable function space, $\mathcal{H}$.

- $\mathcal{V}_N$ denotes a generic N-dimensional FEM space. Let $\mathbf{V}_N = \begin{bmatrix} v_1 & v_2 & \cdots & v_N \end{bmatrix}$ be the functions with local support spanning $\mathcal{V}_N$.
- Let $\mathcal{W}$ is a dimension k space of specially chosen global functions **encoding properties of the solution**. Typically $k \ll N$. Let $\mathbf{W} = \begin{bmatrix} w_1 & w_2 & \cdots & w_k \end{bmatrix}$ be functions spanning $\mathcal{W}$.
- Our enriched FEM space will be $\mathcal{V}_N + \mathcal{W}$.
- A function in this space can be expressed as

$$\widehat{u} = \mathbf{W}\widehat{\mathbf{w}} + \mathbf{V}_N\widehat{\mathbf{v}} \in \mathcal{W} + \mathcal{V}_N, \qquad \text{for } \widehat{\mathbf{w}} \in \mathbb{R}^k, \widehat{\mathbf{v}} \in \mathbb{R}^N.$$

Definition (Block Inner Products Forms)

Let $\mathbf{K} = \begin{bmatrix} \mathrm{k}_1 & \mathrm{k}_2 & \cdots & \mathrm{k}_\ell \end{bmatrix} \in \mathcal{H}^\ell$ be an ℓ-tuple of elements of $\mathcal{H}$. Then for $\mathrm{h} \in \mathcal{H}$ and $\mathbf{H} = \begin{bmatrix} \mathrm{h}_1 & \cdots & \mathrm{h}_\mathrm{p} \end{bmatrix} \in \mathcal{H}^\mathrm{p}$ we define

$$(\mathrm{h}, \mathbf{K})_\mathcal{H} = \begin{bmatrix} (\mathrm{h}, \mathrm{k}_1)_\mathcal{H} \\ \vdots \\ (\mathrm{h}, \mathrm{k}_\ell)_\mathcal{H} \end{bmatrix} \in \mathbb{R}^\ell$$

$$(\mathbf{H}, \mathbf{K})_\mathcal{H} = \begin{bmatrix} (\mathrm{h}_1, \mathbf{K})_\mathcal{H} & \cdots & (\mathrm{h}_\mathrm{p}, \mathbf{K})_\mathcal{H} \end{bmatrix} \in \mathbb{R}^{\ell \times \mathrm{p}}.$$

Block bilinear forms are defined similarly.

We discretize by taking $\widehat{u} = \mathbf{W}\widehat{\mathbf{w}} + \mathbf{V}_N\widehat{\mathbf{v}}$ for $\widehat{\mathbf{w}} \in \mathbb{R}^k$ and $\widehat{\mathbf{v}} \in \mathbb{R}^N$, and we solve: *Find* $\widehat{u} \in \mathcal{W} + \mathcal{V}_N$ *such that*

$$B(\widehat{u}, v) = \ell(v) \quad \text{for all} \quad v \in \widetilde{\mathcal{W}} + \widetilde{\mathcal{V}}_N$$

If we write

$$\widehat{u} = \begin{bmatrix} \mathbf{W} & \mathbf{V}_N \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{w}} \\ \widehat{\mathbf{v}} \end{bmatrix},$$

we see that we should solve the linear system

$$\begin{bmatrix} B(\mathbf{W}, \widetilde{\mathbf{W}}) & B(\mathbf{V}_N, \widetilde{\mathbf{W}}) \\ B(\mathbf{W}, \widetilde{\mathbf{V}}_N) & B(\mathbf{V}_N, \widetilde{\mathbf{V}}_N) \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{w}} \\ \widehat{\mathbf{v}} \end{bmatrix} = \begin{bmatrix} \ell\left(\widetilde{\mathbf{W}}\right) \\ \ell\left(\widetilde{\mathbf{V}}_N\right) \end{bmatrix}$$

Define

$$\mathrm{P}_{\mathcal{W}} = \mathbf{W}\mathrm{B}(\mathbf{W}, \widetilde{\mathbf{W}})^{-1}\mathrm{B}(\cdot, \widetilde{\mathbf{W}}) \quad \text{and} \quad \mathrm{S}_{\widetilde{\mathcal{W}}} = \widetilde{\mathbf{W}}\mathrm{B}(\widetilde{\mathbf{W}}, \mathbf{W})^{-1}\mathrm{B}(\cdot, \mathbf{W}).$$

Lemma

The discretization of the above problem is equivalent to approximating the solution of

$$\mathrm{B}\left((\mathrm{I} - \mathrm{P}_{\mathcal{W}})\, z, v\right) = \left(\mathrm{f}, (\mathrm{I} - \mathrm{S}_{\mathcal{W}})\, v\right)_{\mathcal{H}}$$

according to the Galerkin discretization: Find $\widehat{z} \in \mathcal{V}_{\mathrm{N}}$ *such that*

$$\mathrm{B}\left((\mathrm{I} - \mathrm{P}_{\mathcal{W}})\, \widehat{z}, v\right) = \left(\mathrm{f}, (\mathrm{I} - \mathrm{S}_{\mathcal{W}})\, v\right)_{\mathcal{H}} \quad \textit{for all} \quad v \in \mathcal{V}_{\mathrm{N}}$$

and setting $\widehat{\mathrm{u}} = (\mathrm{I} - \mathrm{P}_{\mathcal{W}})\, \widehat{z} + \mathbf{W}\mathrm{B}(\mathbf{W}, \mathbf{W})^{-1}\left(\mathrm{f}, \mathbf{W}\right)_{\mathcal{H}}$.

The above framework is somewhat unnecessarily general for our main example. We'll simplify a little:

- Let $\mathrm{B}(\cdot,\cdot)$ be symmetric and coercive.
- Galerkin: $\widetilde{\mathcal{W}} = \mathcal{W}$ and $\widetilde{\mathcal{V}}_{\mathrm{N}} = \mathcal{V}_{\mathrm{N}}$

Then our problem is:

$$\text{find } \widehat{u} \in \mathcal{W} + \mathcal{V}_{\mathrm{N}} \quad \text{such that} \quad \mathrm{B}(\widehat{u}, v) = \ell(v) \quad \forall v \in \mathcal{W} + \mathcal{V}_{\mathrm{N}}.$$

Lemma

Let $\mathrm{P}_{\mathcal{W}}$ and $\mathrm{S}_{\mathcal{W}}$ be defined above. If $\mathrm{B}(\cdot,\cdot)$ is a symmetric inner product and we have $\widetilde{\mathcal{W}} = \mathcal{W}$ and $\widetilde{\mathcal{V}}_{\mathrm{N}} = \mathcal{V}_{\mathrm{N}}$, then it follows that

- $\mathrm{P}_{\mathcal{W}} = \mathrm{S}_{\mathcal{W}}$
- $\mathrm{P}_{\mathcal{W}}$ *is the* $\mathrm{B}(\cdot,\cdot)$*-orthogonal projector onto* $\mathcal{W}$.

This can be summarised as:

Lemma

The FEM discretization of our problem is equivalent to approximating the solution of

$$\mathrm{B}\big((\mathrm{I} - \mathrm{P}_{\mathcal{W}})\, z, v \big) = (\mathrm{f}, (\mathrm{I} - \mathrm{P}_{\mathcal{W}})\, v)$$

and setting $\widehat{\mathfrak{u}} = (\mathrm{I} - \mathrm{P}_{\mathcal{W}})\, \widehat{z} + \mathbf{W}\mathrm{B}(\mathbf{W}, \mathbf{W})^{-1}\, (\mathrm{f}, \mathbf{W})$.

In practice, the method is equivalent to solving a low-rank perturbation of the original problem in $\mathcal{V}_N$, and then recovering the solution in $\mathcal{W} + \mathcal{V}_N$.

Discretization and solution of reaction-diffusion problem

- Given $\mathbf{V}_N$, $\mathbf{W}$, and $B(\cdot,\cdot)$ as described;
- Build sparse matrix $\mathbf{A}_{\mathcal{V}} = B(\mathbf{V}_N, \mathbf{V}_N)$
- Compute $B(\mathbf{W}, \mathbf{W})$, $B(\mathbf{W}, \mathbf{V}_N)$
- Build a suitable representation of the rank 2 matrix $A_{\mathcal{W}} = B(\mathbf{W}, \mathbf{V}_N)\, B(\mathbf{W}, \mathbf{W})^{-1}\, B(\mathbf{W}, \mathbf{V}_N)^T$
- Solve

$$(A_{\mathcal{V}} - A_{\mathcal{W}})\,\widehat{\mathbf{v}} = (f, \mathbf{V}_N) - B(\mathbf{W}, \mathbf{V}) B(\mathbf{W}, \mathbf{W})^{-1} (f, \mathbf{W})$$

- Recover $\widehat{\mathbf{w}} = B(\mathbf{W}, \mathbf{W})^{-1}\big((f, \mathbf{W}) - B(\mathbf{V}, \mathbf{W})\widehat{\mathbf{v}}\big)$
- Compute $\widehat{u} = \mathbf{V}_N \widehat{\mathbf{v}} + \mathbf{W}\widehat{\mathbf{w}}$

There are two formulations, which involve solving either

$$\begin{bmatrix} B(\mathbf{W},\mathbf{W}) & B(\mathbf{V}_N,\mathbf{W}) \\ B(\mathbf{W},\mathbf{V}_N) & B(\mathbf{V}_N,\mathbf{V}_N) \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{w}} \\ \widehat{\mathbf{v}} \end{bmatrix} = \begin{bmatrix} (f,\mathbf{W}) \\ (f,\mathbf{V}_N) \end{bmatrix} \tag{3}$$

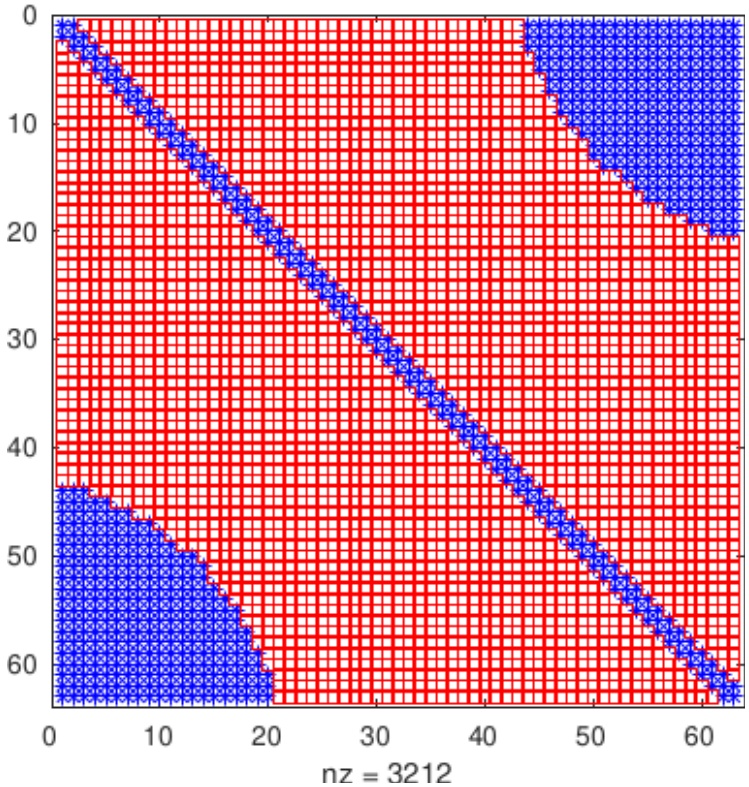
or

$$\left(\underbrace{B(\mathbf{V}_N,\mathbf{V}_N)}_{A_{\mathcal{V}}} - \underbrace{B\left(W,\mathbf{V}_N\right) B\left(\mathbf{W},\mathbf{W}\right)^{-1} B\left(\mathbf{W},\mathbf{V}_N\right)^{T}}_{A_{\mathcal{W}}} \right) \widehat{\mathbf{v}}$$

$$= (f,\mathbf{V}_N) - B(\mathbf{W},\mathbf{V}_N) B(\mathbf{W},\mathbf{W})^{-1} (f,\mathbf{W}) \tag{4}$$

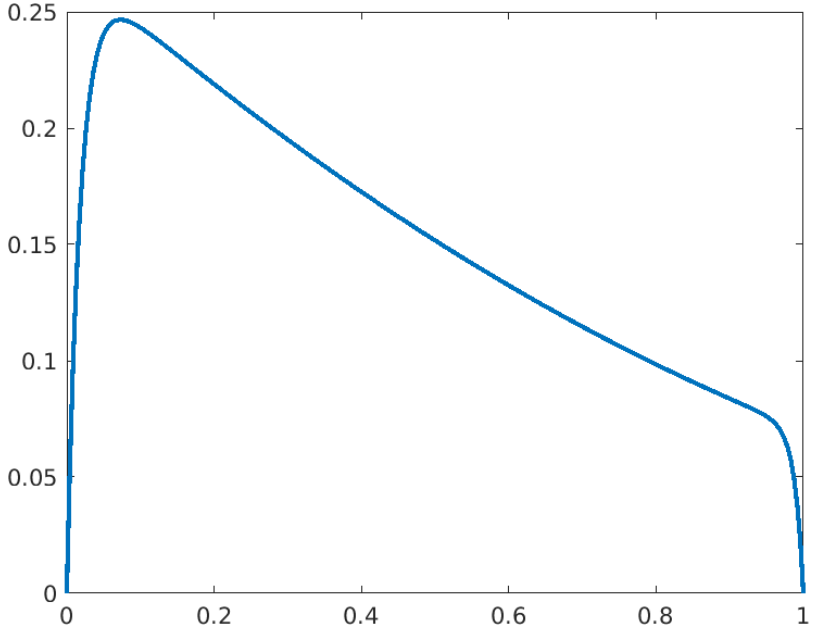
- One can show that the matrix in (3) is poorly conditioned: $\sim N^2$
- The matrix in (4) is much better conditioned (if one were to actually compute it): $\sim N$
- But $A_{\mathcal{V}} - A_{\mathcal{W}}$ is dense. In practice, it is never formed; solve (4) with a "matrix-free" type iterative method.

- Saw that solutions for the standard method, on a uniform grid, were unstable. One explanation: although $A_{\mathcal{V}}$ is SPD, it is not an M-matrix.
- Remarkably, **one can choose $\mathbf{W}$ so that** $(A_{\mathcal{V}} - A_{\mathcal{W}})^{-1} \geqslant 0$.
  This is remarkable, since this matrix is also not an M-matrix.
- Unfortunately, a general proof is still allusive.



Our linear 1D reaction-diffusion problem again

$$\mathcal{L}u := -\varepsilon u'' + r(x)u = f(x) \text{ on } \Omega := (0,1), \qquad u(0) = u(1) = 0. \tag{5}$$



As we saw earlier, the solution has a decomposition

$$u(x) \sim \underbrace{u_0(x)}_{\text{regular part}} + \underbrace{u_{\varepsilon;0}(x)}_{\text{left layer}} + \underbrace{u_{\varepsilon;1}(x)}_{\text{right layer}}.$$

Somewhat crudely, we would write

$$u(x) \sim \underbrace{u_0(x)}_{\text{regular part}} + \underbrace{e^{-\gamma_0 x/\varepsilon}}_{\text{left layer}} + \underbrace{e^{-\gamma_1(1-x)/\varepsilon}}_{\text{right layer}},$$

where

- u_0 is easily approximated using standard methods.
- $u_{\varepsilon;0}$ and $u_{\varepsilon;1}$ are more challenging to estimate, but only very locally.

We return to our earlier example

$$-\varepsilon^2 u'' + \big(2 + x + \sin(5x)\big)u = e^{x/2}, \text{ on } (0,1)$$

$$u(0) = u(1) = 0.$$

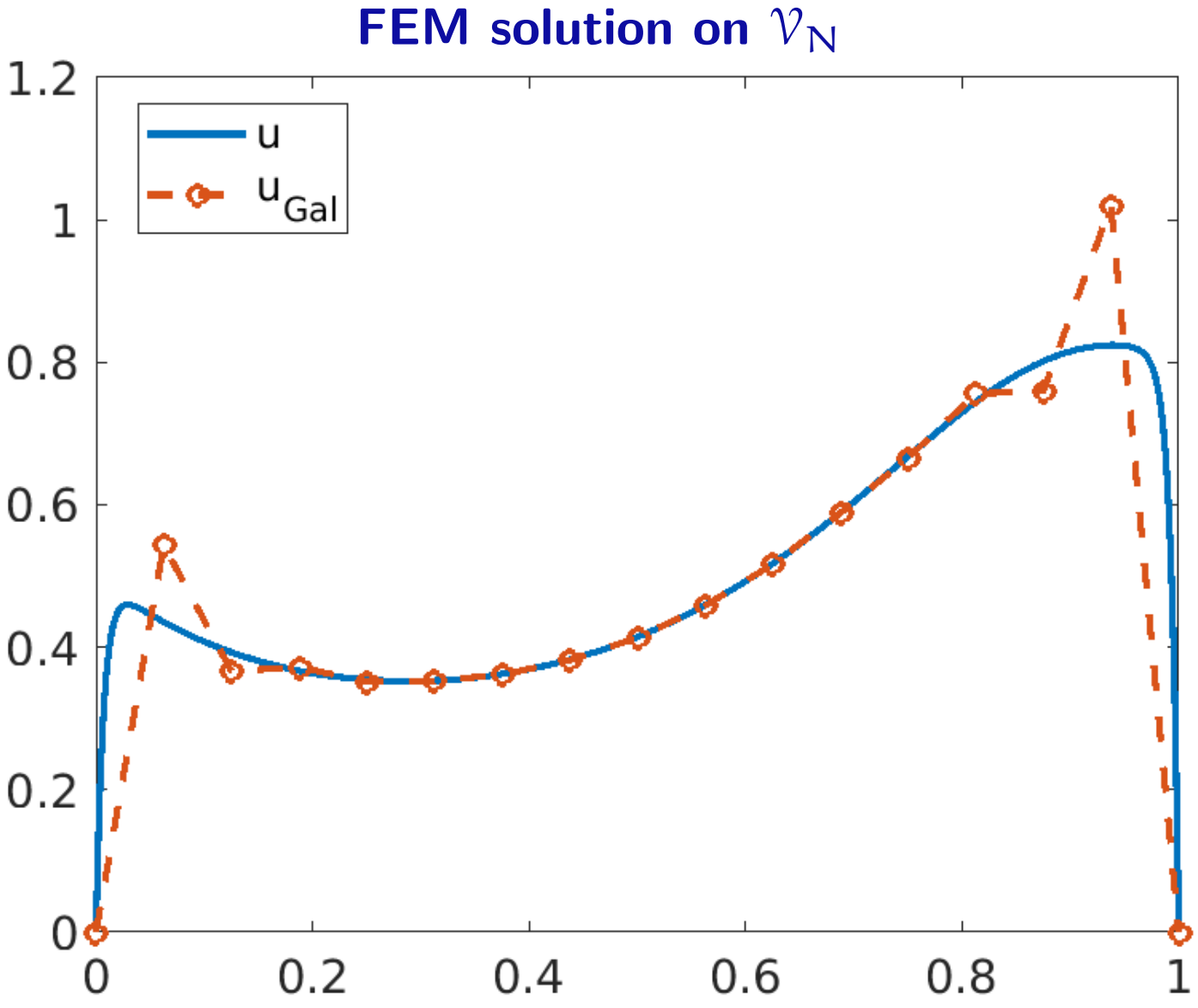
This has two boundary layers, so we'll enrich the FEM space with two functions, one for each boundary later.

That is, we take V_N to be the space of piecewise linear functions on a uniform mesh with N intervals.

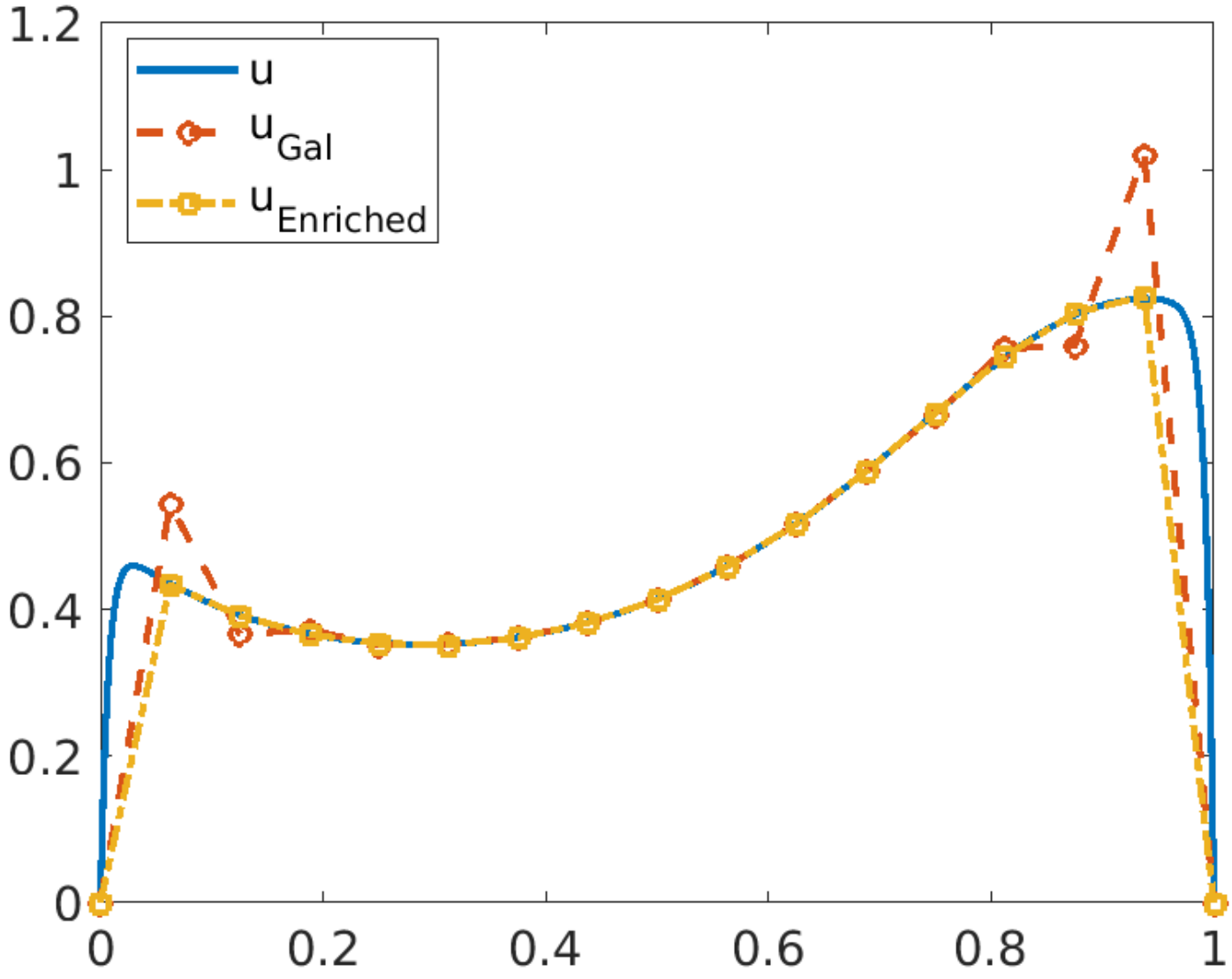
We'll take

$$w_1 = \big(1 - e^{-\gamma_0 x \varepsilon^{-1}}\big)(1-x), \qquad w_2 = \big(1 - e^{-\gamma_1 (1-x) \varepsilon^{-1}}\big)x.$$

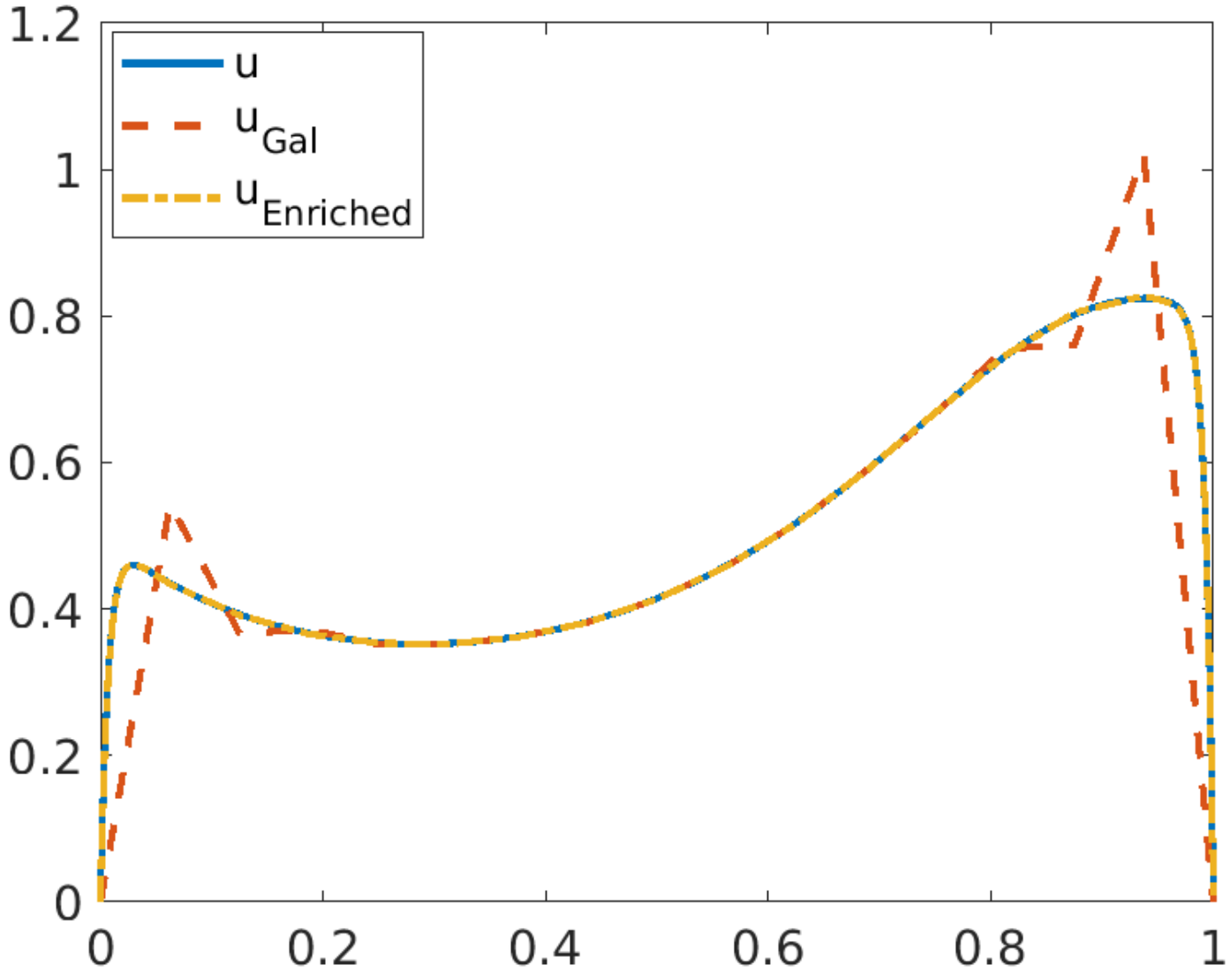
where $\gamma_0 = r(0)^{1/2}$, $\gamma_1 = r(1)^{1/2}$. We let $\mathbf{W} = [w_1\ w_2]$.


FEM solution on $\mathcal{V}_N$
u
u_Gal
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1

FEM solution on $\mathcal{W} + \mathcal{V}_N$, evaluated at mesh points



FEM solution on $\mathcal{W} + \mathcal{V}_N$, evaluated on a fine mesh



Error for standard Galerkin (max norm)

ε	N = 64	N = 128	N = 256	N = 512	N = 1024
1	5.260e-06	1.315e-06	3.288e-07	8.219e-08	2.055e-08
10^{-4}	2.184e-01	2.173e-01	2.162e-01	2.138e-01	2.053e-01
10^{-6}	2.184e-01	2.174e-01	2.169e-01	2.167e-01	2.166e-01
10^{-8}	2.184e-01	2.174e-01	2.169e-01	2.167e-01	2.166e-01
10^{-10}	2.184e-01	2.174e-01	2.169e-01	2.167e-01	2.166e-01

Error for Enriched scheme (max norm)

ε	N = 64	N = 128	N = 256	N = 512	N = 1024
1	1.970e-06	5.140e-07	1.312e-07	3.314e-08	8.326e-09
10^{-4}	2.142e-04	5.532e-05	3.438e-05	2.632e-05	1.864e-05
10^{-6}	2.011e-04	5.039e-05	1.265e-05	3.185e-06	8.066e-07
10^{-8}	2.007e-04	5.019e-05	1.255e-05	3.138e-06	7.846e-07
10^{-10}	2.007e-04	5.019e-05	1.255e-05	3.137e-06	7.843e-07

The numerical results above are just to convince one that the method works. What we can prove (at present) is that, where

$$\|u\|_\varepsilon := \left(\|u\|_0 + \varepsilon^2 \|u'\|_0\right)^{1/2},$$

then

$$\|u - \hat{u}\|_\varepsilon := C_0 N^{-2} + C_1 \varepsilon^{1/2} N^{-2} \leqslant C N^{-2}.$$

Error for Enriched scheme (energy norm)

ε	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$
1	7.781e-04	3.889e-04	1.944e-04	9.721e-05	4.860e-05
10^{-2}	9.623e-04	4.744e-04	2.175e-04	9.890e-05	4.847e-05
10^{-4}	4.601e-05	1.262e-05	2.578e-05	4.338e-06	4.558e-06
10^{-6}	4.787e-05	1.194e-05	2.978e-06	7.410e-07	1.839e-07
10^{-8}	4.794e-05	1.197e-05	2.993e-06	7.481e-07	1.870e-07
10^{-10}	4.794e-05	1.197e-05	2.993e-06	7.482e-07	1.870e-07

1. Some further work needed to investigate good choices for $\mathbf{W}$. There seems to be quite some flexibility, but also some constraints.
2. Still need a proof of that fact that $(A_{\mathcal{V}} - A_{\mathcal{W}})^{-1} \geqslant 0$.
3. Error analysis in strong norms is still open.
4. The framework developed is broadly applicable (at least to self-adjoint problems), and not restricted to the simple example given here.
5. Application to 2D problems (for example), is still in its infancy (constant coefficient problems only).
6. Opportunities for fast solvers and excellent preconditioners, e.g., via *Sherman–Morrison–Woodbury*.

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2. Still need a proof of that fact that $(A_{\mathcal{V}} - A_{\mathcal{W}})^{-1} \geqslant 0$.
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Thank you (questions?)


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