Multigrid method based on Finite Elements on Metric Graphs

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Objective

- Solve elliptic partial differential equations (PDE) on network like structures
- explain network structure with metric graphs

Multigrid method used to solve the system of equations arising from the PDE

Metric graphs

Combinatorial graph:

- $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ consisting of set of vertices $\mathcal{V} = \{v_1, v_2, \ldots, v_n\}$ and set of edges $\mathcal{E} = \{e_1, e_2, \ldots, e_m\}$
- $\mathcal{E}_v$ denotes set of edges adjacent to vertex $v \in \mathcal{V}$

Coordinates on edges:

- Assign length $\ell_e < \infty$ and interval $[0, \ell_e]$ to each edge $e \in \mathcal{E}$ of $\mathcal{G}$
- Each point on edge e corresponds to a coordinate $x \in [0, \ell_e]$

$\rightsquigarrow$ metric graph $\Gamma = (\mathcal{V}, \mathcal{E}, \ell_{\mathcal{E}})$, where $\ell_{\mathcal{E}} = \{\ell_e\}_{e \in \mathcal{E}}$

Function spaces on metric graphs:

- Lebesgue space $L_2(\Gamma) := \bigoplus_{e \in \mathcal{E}} L_2(e)$, with $L_2(e)$ Lebesgue space on interval $[0, \ell_e]$
- Sobolev space $H^1(\Gamma) := \bigoplus_{e \in \mathcal{E}} H^1(e) \cap C^0(\Gamma)$

Additional condition $C^0(\Gamma)$ necessary to guarantee continuity on vertices

Formulation of the problem

For given $f \in L_2(\Gamma)$, find solution u of:

$$-\frac{d^2u}{dx^2}(x) + \nu u(x) = f \quad \text{for } x \in \Gamma \text{ and constant potential } \nu \geq 0$$

with Neumann-Kirchhoff conditions: $\sum_{e \in \mathcal{E}_v} \frac{du}{dx}(v) = 0$ for all vertices $v \in \mathcal{V}$

and u continuous on all vertices: $u \in C^0(\Gamma)$.

Weak formulation:

Find $u \in H^1(\Gamma)$, such that

$$\mathfrak{h}(u, g) = \sum_{e \in \mathcal{E}} \left\{ \int_e \frac{du}{dx}\frac{dg}{dx}\,dx + \int_e \nu u g\, dx \right\} = \sum_{e \in \mathcal{E}} \int_e f g\, dx =: F(g) \quad \text{for all } g \in H^1(\Gamma) \tag{1}$$

bilinear form $\mathfrak{h}$ fulfills requirements of the Lax-Milgram theorem

$\rightsquigarrow$ existence of a unique solution of (1)

Discretization

Discretization of edges:

- Standard finite element discretization on each edge
- Divide interval $[0, \ell_e]$ on edge $e \in \mathcal{E}$ into n_e subintervals of length $h_e = \frac{1}{n_e}$

$\rightsquigarrow$ internal vertices $\mathscr{V}_e = \{x_j^e\}_{j=1}^{n_e-1}$ (discretization points)

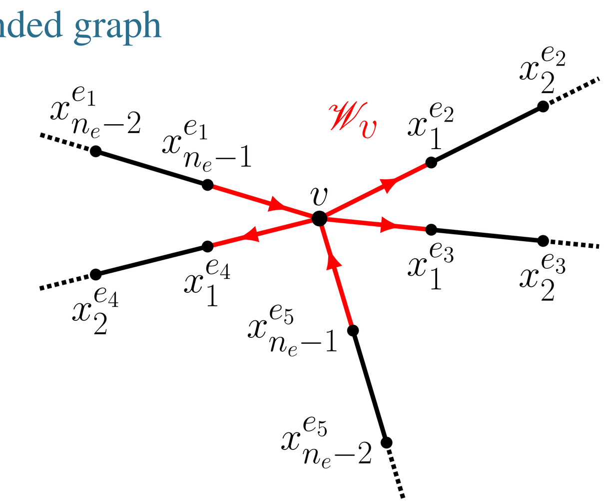
Extended graph:

Sequence $v_{\text{out}} < x_1^e < x_2^e < \ldots < x_{n_e-1}^e < v_{\text{in}}$ forms connected sequence of vertices and edges, on edge $e = \{v_{\text{out}}, v_{\text{in}}\} \in \mathcal{E}$

$\rightsquigarrow$ discretized metric graph is again a metric graph $\mathscr{G}$ called extended graph

Neighbourhood of vertex v:

Neighbouring set $\mathscr{W}_v$ of vertex $v \in \mathcal{V}$ contains all adjacent subintervals to vertex v:



$$\mathscr{W}_v := \left\{ \bigcup_{e \in \{e \in \mathcal{E}_v : v^e_{\text{in}} = v\}} [v, x_1^e] \right\} \cup \left\{ \bigcup_{e \in \{e \in \mathcal{E}_v : v^e_{\text{out}} = v\}} [x^e_{n_e-1}, v] \right\}$$

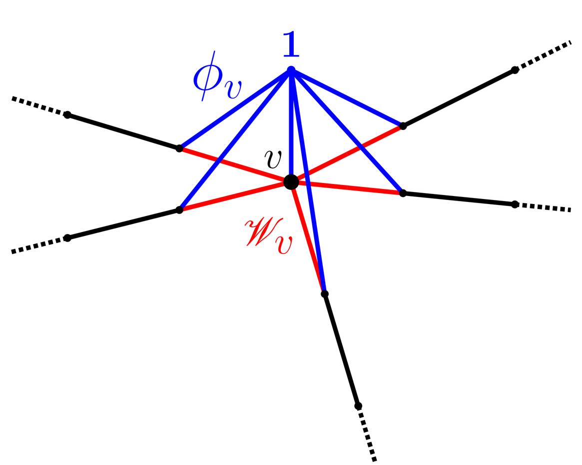
Hat function basis:

Basis of hat functions centred around internal vertices:

$$\psi_j^e(x) = \begin{cases} 1 - \frac{|x_j^e - x|}{h_e} & \text{, if } x_{j-1}^e \leq x \leq x_{j+1}^e \\ 0 & \text{, else} \end{cases}$$

$\rightsquigarrow \left\{\psi_j^e\right\}_{j=1}^{n_e-1}$ form basis of the space

$$V_{h_e}^e = \left\{ w \in H_0^1(e) : w|_{[x_j^e, x_{j+1}^e]} \text{ linear function }, j = 0, \ldots, n_e - 1 \right\}$$



Basis functions centred around vertices given by vertex hat functions:

$$\phi_v(x)|_{\mathscr{W}_v \cap e} = \begin{cases} 1 - \frac{|x_v^e - x|}{h_e} & \text{, if } x \in \mathscr{W}_v \cap e \text{ and } e \in \mathcal{E}_v \\ 0 & \text{, else} \end{cases}$$

Approximation space: $V_h(\Gamma) \subset C^0(\Gamma)$, $\quad V_h(\Gamma) := \left(\bigoplus_{e \in \mathcal{E}} V_{h_e}^e \right) \oplus \text{span}\{\phi_v\}_{v \in \mathcal{V}}$

Discretization of the weak form

Solution of the weak form in $V_h(\Gamma)$:

- $u_h \in V_h(\Gamma)$ solution of the weak form (1) in the approximation space
- Written as linear combination of basis functions:

$$u_h(x) = \sum_{e \in \mathcal{E}} \sum_{j=1}^{n_e-1} u_j^e \psi_j^e(x) + \sum_{v \in \mathcal{V}} u_v \phi_v(x) \tag{2}$$

System of equations:

Testing with basis functions in the bilinear form $\rightsquigarrow$ system of equations:

$$\mathbf{H} \begin{bmatrix} \mathbf{u}_{\mathcal{E}} \\ \mathbf{u}_{\mathcal{V}} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{\mathcal{E}\mathcal{E}} & \mathbf{H}_{\mathcal{E}\mathcal{V}} \\ \mathbf{H}_{\mathcal{E}\mathcal{V}}^T & \mathbf{H}_{\mathcal{V}\mathcal{V}} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathcal{E}} \\ \mathbf{u}_{\mathcal{V}} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{\mathcal{E}} \\ \mathbf{f}_{\mathcal{V}} \end{bmatrix},$$

where

$$\mathbf{u}_{\mathcal{E}} = \begin{bmatrix} \mathbf{u}^1 \\ \vdots \\ \mathbf{u}^m \end{bmatrix}, \text{ with } \mathbf{u}^e = \begin{bmatrix} u_1^e \\ \vdots \\ u_{n_e-1}^e \end{bmatrix}, \text{ and } \mathbf{u}_{\mathcal{V}} = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix},$$

vectors with coefficients from the linear combination (2).

Vectors $\mathbf{f}_{\mathcal{E}}$ and $\mathbf{f}_{\mathcal{V}}$ given by

$$\mathbf{f}_{\mathcal{E}} = \begin{bmatrix} \mathbf{f}^1 \\ \vdots \\ \mathbf{f}^m \end{bmatrix}, \text{ with } \mathbf{f}^e = \begin{bmatrix} f_1^e \\ \vdots \\ f_{n_e-1}^e \end{bmatrix} \text{ and } \mathbf{f}_{\mathcal{V}} = \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \text{ such that } f_k^e = \int_{\text{supp}(\psi_k^e)} f \psi_k^e dx \text{ and } f_v = \int_{\mathscr{W}_v} f \phi_v dx$$

Properties of $\mathfrak{h}$ imply: $\mathbf{H}$ is symmetric positive definite

- $\mathbf{H}_{\mathcal{E}\mathcal{E}} \in \mathbb{R}^{\tilde{n} \times \tilde{n}}$, $\quad \tilde{n} := \sum_{e \in \mathcal{E}} n_e - 1$
  describes overlap of supports of $(only)$ $\psi_j^e \rightsquigarrow$ block-tridiagonal-matrix (one block per edge)
- $\mathbf{H}_{\mathcal{E}\mathcal{V}} \in \mathbb{R}^{\tilde{n} \times \tilde{n}}$; overlap of supports of both ψ_j^e and ϕ_v
- $\mathbf{H}_{\mathcal{V}\mathcal{V}} \in \mathbb{R}^{n \times n}$; overlap of supports of $\phi_v \rightsquigarrow$ diagonal matrix

Multigrid method on graphs

- Use hierarchical discretization on edges $\rightsquigarrow$ divide edges into 2^J subintervals, $J = 1, \ldots, J_{\max}$
- Use intergrid operators to transport solution between level J and $J+1$ of dicretization

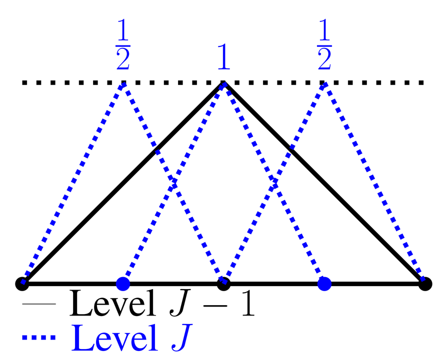
Restriction operators on edge:

- Standard hat functions at internal nodes $\rightsquigarrow$ refinement relation:

$$\psi_i^{e,J-1}(x) = \frac{1}{2}\psi_{i-1}^{e,J}(2x) + \psi_i^{e,J}(2x) + \frac{1}{2}\psi_{i+1}^{e,J}(2x) \tag{3}$$

- Vertex hat functions at vertices $\rightsquigarrow$ adjusted refinement relation:

$$\phi_{v_{\text{in}}}^{J-1}(x) = \phi_{v_{\text{in}}}^{J}(2x) + \frac{1}{2}\psi_1^{e,J}(2x) \tag{4}$$



$\rightsquigarrow$ Restriction operator $\mathbf{r}$ and prolongation operator $\mathbf{p} = \mathbf{r}^T$ defined by refinement relations

Restriction operators on the graph:

$$\mathbf{r} = \begin{pmatrix} \mathbf{r}_{\mathcal{E}\mathcal{E}} & \mathbf{0} \\ \mathbf{r}_{\mathcal{V}\mathcal{E}} & \mathbf{r}_{\mathcal{V}\mathcal{V}} \end{pmatrix}$$

- $\mathbf{r}_{\mathcal{E}\mathcal{E}}$: edgewise application of refinement relation (3) to functions ψ_j^e
- $\mathbf{r}_{\mathcal{V}\mathcal{E}}$ and $\mathbf{r}_{\mathcal{V}\mathcal{V}}$: edgewise application of refinement relation (4)
  $\rightsquigarrow$ for $e \in \mathcal{E}_v$ edgewise application of (4) on vertex hat functions

Multigrid method k-th cycle $(MG(J, \mathbf{u}_J^{(k)}, \nu_1, \nu_2, \mu))$:

J level of refinement, $\mathbf{u}_J^{(k)}$ approximation of solution $\mathbf{u}_J$,
$\nu_{1/2}$ number of a priori/posteriori smoothing steps, μ parameter for recursive call of MG

1. A priori smoothing: $\mathbf{u}_J^{(k,1)} := (\mathcal{S}(\mathbf{u}_J^{(k)}))^{\nu_1}$
2. Coarse grid correction:
   residual $\mathbf{d}_J = \mathbf{f}_J - \mathbf{H}_J \mathbf{u}_J^{(k,1)}$ and restriction $\mathbf{f}_{J-1} = \mathbf{r}\,\mathbf{d}_J$
   restriction $\mathbf{H}_{J-1} = \mathbf{r}\,\mathbf{H}_J\,\mathbf{r}^T$
   solve $\mathbf{H}_{J-1}\mathbf{v}_{J-1} = \mathbf{f}_{J-1}$
   If $J = J_{\min}$ solve problem exactly
   If $J > J_{\min}$ find approximation by performing μ steps of $MG(J-1, \mathbf{u}_{J-1}^{(0)} = \mathbf{0}, \nu_1, \nu_2, \mu)$
3. Prolongation: Set $\mathbf{u}_J^{(k,2)} := \mathbf{u}_J^{(k,1)} + \mathbf{r}^T \mathbf{v}_{J-1}$
4. A posteriori smoothing: $\mathbf{u}_J^{(k,3)} = (\mathcal{S}(\mathbf{u}_J^{(k,2)}))^{\nu_2}$

Set $\mathbf{u}_J^{(k+1)} := \mathbf{u}_J^{(k,3)}$

Choice of smoother:

$\mathcal{S}$ chosen as Jacobi smoother; balance between computational cost and convergence improvement

Numerical results on convergence

- Test problem on graph obtained using Barabási-Albert model: 2000 vertices, 25909 edges
- Discretization with 256 subintervals on each edge of length $\ell_e = 1$ ($\sim J_{\max} = 8$)
  $\rightsquigarrow$ size of $\mathbf{H}_{\mathcal{E}\mathcal{E}}$: 6606795×6606795
- Stopping criteria: error accuracy of 10^{-8}; f edgewise defined by $f^{e_k}(x) = cos(2\pi\, x\, k)$
- Convergence rate measured as quotient of norm of consecutive residual on vertices and edges

Numerical convergence rate for V-cycle ($\mu = 1$) and W-cycle ($\mu = 2$):

convergence rate on edges
convergence rate on vertices

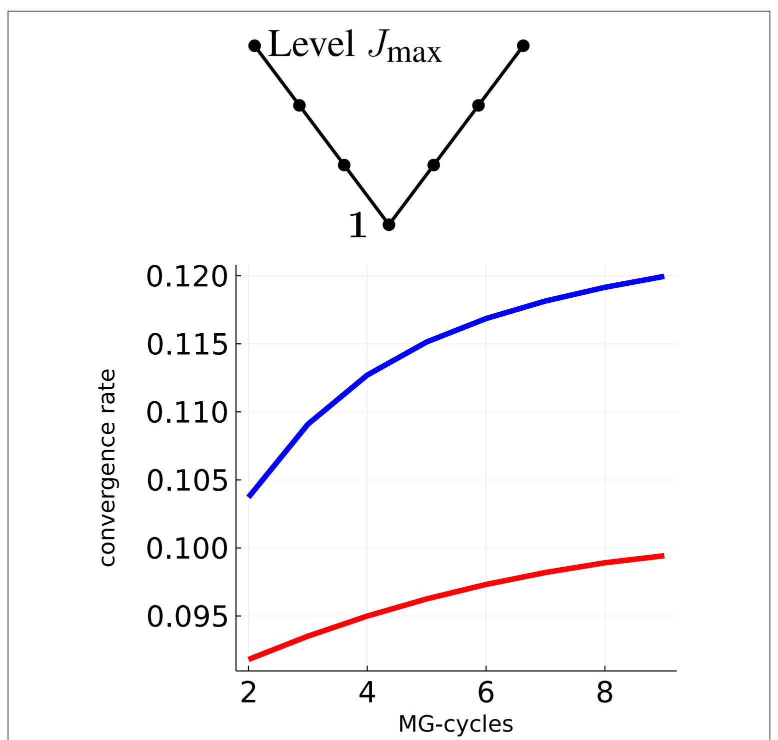


Figure 1: smoothing parameters $\nu_1 = 2$, $\nu_2 = 2$

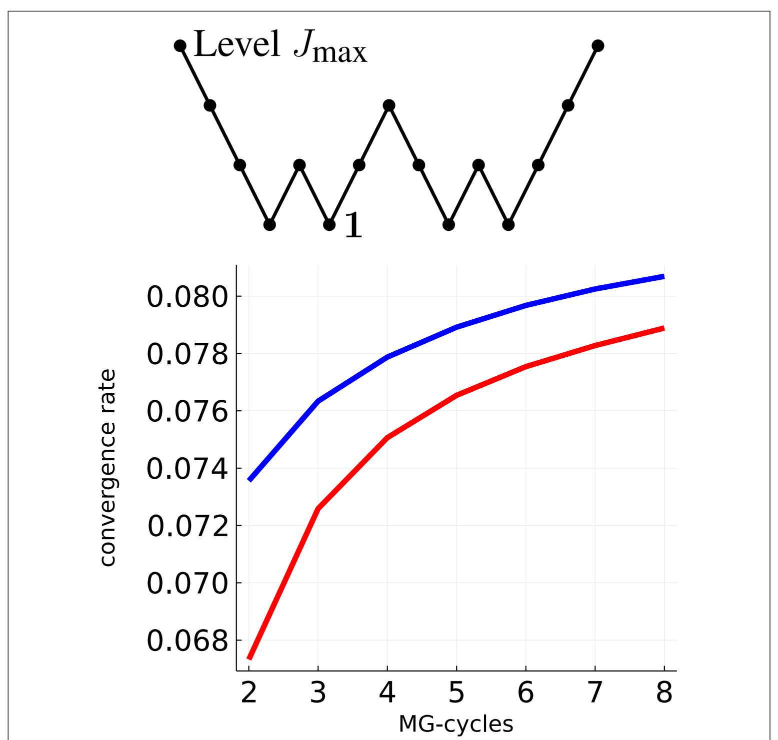


Figure 3: smoothing parameters $\nu_1 = 2$, $\nu_2 = 2$

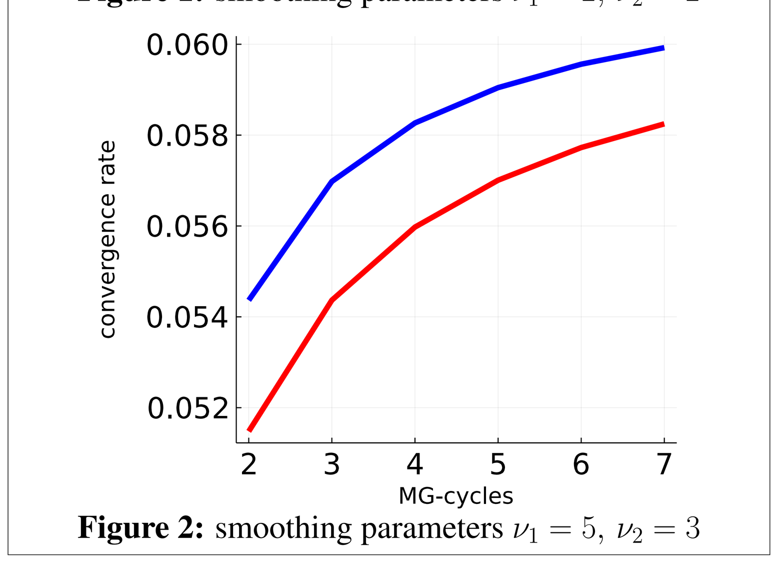


Figure 2: smoothing parameters $\nu_1 = 5$, $\nu_2 = 3$

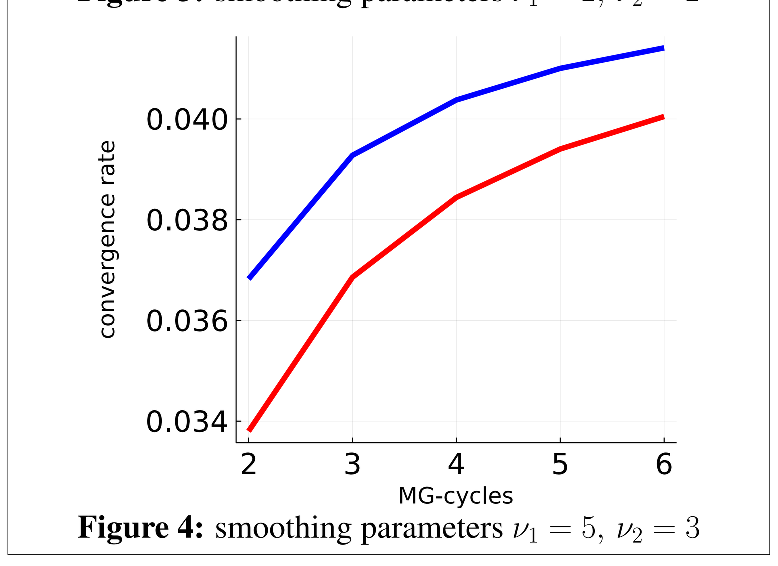


Figure 4: smoothing parameters $\nu_1 = 5$, $\nu_2 = 3$

References

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