On boundary discrete maximum principle in the finite element method

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Maximum principle – strong sense

- Classical formulation:

$$\begin{aligned} -\operatorname{div}(\mathcal{A}\nabla u) + \mathbf{b}\cdot\nabla u + cu = f \quad & \text{in } \Omega \\ u = g_{\mathrm{D}} \quad & \text{on } \Gamma_{\mathrm{D}} \\ \alpha u + (\mathcal{A}\nabla u)\cdot\mathbf{n} = g_{\mathrm{N}} \quad & \text{on } \Gamma_{\mathrm{N}} \end{aligned}$$

- $\Omega \subset \mathbb{R}^d, \quad \overline{\Gamma}_{\mathrm{D}} \cup \overline{\Gamma}_{\mathrm{N}} = \partial\Omega$
- $\boldsymbol{\xi}^T \mathcal{A}(x)\boldsymbol{\xi} \geq \lambda_{\min}|\boldsymbol{\xi}|^2 \quad \forall \boldsymbol{\xi} \in \mathbb{R}^d, \ \forall x \in \Omega$
- $c - \frac{1}{2}\operatorname{div}\mathbf{b} \geq 0 \quad \text{in } \Omega \quad \text{and} \quad \alpha + \frac{1}{2}\mathbf{b}\cdot\mathbf{n} \geq 0 \quad \text{on } \Gamma_{\mathrm{N}}$

Maximum principle – strong sense

- Classical formulation:

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\begin{aligned}
-\operatorname{div}(\mathcal{A}\nabla u) + \mathbf{b}\cdot\nabla u + cu &= f && \text{in } \Omega\\
u &= g_{\mathrm{D}} && \text{on } \Gamma_{\mathrm{D}}\\
\alpha u + (\mathcal{A}\nabla u)\cdot\mathbf{n} &= g_{\mathrm{N}} && \text{on } \Gamma_{\mathrm{N}}
\end{aligned}
$$

- Maximum principle (MP):

$$
f \le 0 \text{ and } g_{\mathrm{N}} \le 0 \quad \Rightarrow \quad \max_{\overline{\Omega}} u \le \max_{\Gamma_{\mathrm{D}}} \max\{0, u\}
$$

- Conservation of nonnegativity (CN):

$$
f \ge 0,\ g_{\mathrm{D}} \ge 0,\ \text{and } g_{\mathrm{N}} \ge 0 \quad \Rightarrow \quad u \ge 0
$$

- Theorem: If $c \ge 0$ and $\alpha \ge 0$ then MP $\Leftrightarrow$ CN

Maximum principle – weak sense

- Weak formulation: $u = u^0 + u^\partial$

$$u^0 \in V^0 : \quad a(u^0, v) = F(v) - a(u^\partial, v) \quad \forall v \in V^0$$

- $u^\partial \in H^1(\Omega), \quad u^\partial = g_{\mathrm{D}}$ on Γ_{D}
- $V^0 = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_{\mathrm{D}}\}$
- $a(u, v) = \int_\Omega (\mathcal{A}\nabla u) \cdot \nabla v + (\mathbf{b} \cdot \nabla u)v + cuv \,\mathrm{d}x + \int_{\Gamma_{\mathrm{N}}} \alpha uv \,\mathrm{d}s$
- $F(v) = \int_\Omega fv \,\mathrm{d}x + \int_{\Gamma_{\mathrm{N}}} g_{\mathrm{N}} v \,\mathrm{d}s$

Maximum principle – weak sense

- Weak formulation: $u = u^0 + u^\partial$

$$u^0 \in V^0: \quad a(u^0, v) = F(v) - a(u^\partial, v) \quad \forall v \in V^0$$

- Maximum principle (MP):

$$f \le 0 \text{ a.e. in } \Omega \text{ and } g_{\mathrm{N}} \le 0 \text{ a.e. on } \Gamma_{\mathrm{N}}$$
$$\Rightarrow \quad \operatorname*{ess\,sup}_{\overline{\Omega}} u \le \operatorname*{ess\,sup}_{\Gamma_{\mathrm{D}}} \max\{0, u\}$$

- Conservation of nonnegativity (CN):

$$f \ge 0 \text{ a.e. in } \Omega,\ g_{\mathrm{D}} \ge 0 \text{ a.e. on } \Gamma_{\mathrm{D}},\ \text{and } g_{\mathrm{N}} \ge 0 \text{ a.e. on } \Gamma_{\mathrm{N}}$$
$$\Rightarrow \quad u \ge 0 \text{ a.e. in } \Omega.$$

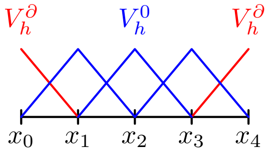
- Theorem: If $c \ge 0$ and $\alpha \ge 0$ then MP $\Leftrightarrow$ CN

Finite element method (FEM)

- hp-FEM: $\quad u_h = u_h^0 + u_h^\partial$

$$u_h^0 \in V_h^0 : \quad a(u_h^0, v_h^0) = F(v_h^0) - a(u_h^\partial, v_h^0) \quad \forall v_h^0 \in V_h^0$$

- $\mathcal{T}_h$ triangulation of Ω
- p_K polynomial degree on $K \in \mathcal{T}_h$
- $X_h = \{v_h \in H^1(\Omega) : v_h|_K \in P^{p_K}(K), K \in \mathcal{T}_h\}$
- $V_h^0 = X_h \cap V^0$
- $X_h = V_h^0 \oplus V_h^\partial$
- $u_h^\partial \in V_h^\partial, \quad u_h^\partial \approx g_\mathrm{D}$ on Γ_D



Finite element method (FEM)

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$$u_h^0 \in V_h^0 : \quad a(u_h^0, v_h^0) = F(v_h^0) - a(u_h^\partial, v_h^0) \quad \forall v_h^0 \in V_h^0$$

- $u_h^\partial \in V_h^\partial : \int_{\Gamma_\mathrm{D}} (g_\mathrm{D} - u_h^\partial) v_h^\partial \,\mathrm{d}s = 0 \quad \forall v_h^\partial \in V_h^\partial$

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- $G_{h,y}^0 \in V_h^0 \; : \quad a(v_h^0, G_{h,y}^0) = v_h^0(y) \quad \forall v_h^0 \in V_h^0, \; y \in \Omega$

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- $G_{h,y}^\partial \in V_h^\partial \; : \quad \displaystyle\int_{\Gamma_\mathrm{D}} v_h^\partial(s) G_{h,y}^\partial(s) \,\mathrm{d}s = v_h^\partial(y) - a(v_h^\partial, G_{h,y}^0) \quad \forall v_h^\partial \in V_h^\partial, \; y \in \Omega$

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- $u_h^0(y) = a(u_h^0, G_{h,y}^0)$

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- $G_{h,y}^\partial \in V_h^\partial \;:\quad \displaystyle\int_{\Gamma_\mathrm{D}} v_h^\partial(s) G_{h,y}^\partial(s) \,\mathrm{d}s = v_h^\partial(y) - a(v_h^\partial, G_{h,y}^0)$

$$\forall v_h^\partial \in V_h^\partial,\; y \in \Omega$$

- $u_h^0(y) = a(u_h^0, G_{h,y}^0) = F(G_{h,y}^0) - a(u_h^\partial, G_{h,y}^0)$

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- $$u_h^0(y) = a(u_h^0, G_{h,y}^0) = F(G_{h,y}^0) - a(u_h^\partial, G_{h,y}^0) = F(G_{h,y}^0) + \int_{\Gamma_{\mathrm{D}}} u_h^\partial(s) G_{h,y}^\partial(s) \,\mathrm{d}s - u_h^\partial(y)$$

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- $$G_{h,y}^\partial \in V_h^\partial \quad : \quad \int_{\Gamma_\mathrm{D}} v_h^\partial(s) G_{h,y}^\partial(s) \,\mathrm{d}s = v_h^\partial(y) - a(v_h^\partial, G_{h,y}^0) \quad \forall v_h^\partial \in V_h^\partial, \ y \in \Omega$$
- $$\begin{aligned} u_h^0(y) = a(u_h^0, G_{h,y}^0) &= F(G_{h,y}^0) - a(u_h^\partial, G_{h,y}^0) \\ &= F(G_{h,y}^0) + \int_{\Gamma_\mathrm{D}} g_\mathrm{D}(s) G_{h,y}^\partial(s) \,\mathrm{d}s - u_h^\partial(y) \end{aligned}$$

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- $u_h^\partial \in V_h^\partial : \int_{\Gamma_{\mathrm{D}}} (g_{\mathrm{D}} - u_h^\partial) v_h^\partial \, \mathrm{d}s = 0 \quad \forall v_h^\partial \in V_h^\partial$
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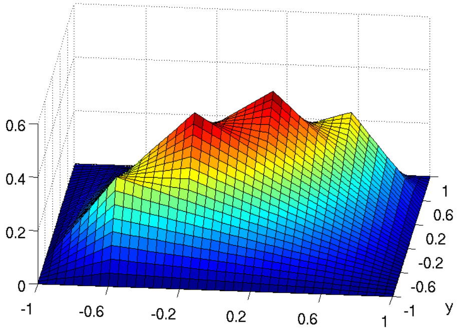
- $G_{h,y}^\partial \in V_h^\partial \ : \quad \int_{\Gamma_{\mathrm{D}}} v_h^\partial(s) G_{h,y}^\partial(s) \, \mathrm{d}s = v_h^\partial(y) - a(v_h^\partial, G_{h,y}^0)$
  $$\forall v_h^\partial \in V_h^\partial, \ y \in \Omega$$
- $$u_h^0(y) = a(u_h^0, G_{h,y}^0) = F(G_{h,y}^0) - a(u_h^\partial, G_{h,y}^0) = F(G_{h,y}^0) + \int_{\Gamma_{\mathrm{D}}} g_{\mathrm{D}}(s) G_{h,y}^\partial(s) \, \mathrm{d}s - u_h^\partial(y)$$
- $u_h(y) = \int_\Omega f \, G_{h,y}^0 \, \mathrm{d}x + \int_{\Gamma_{\mathrm{N}}} g_{\mathrm{N}} G_{h,y}^0 \, \mathrm{d}s + \int_{\Gamma_{\mathrm{D}}} g_{\mathrm{D}} G_{h,y}^\partial \, \mathrm{d}s$

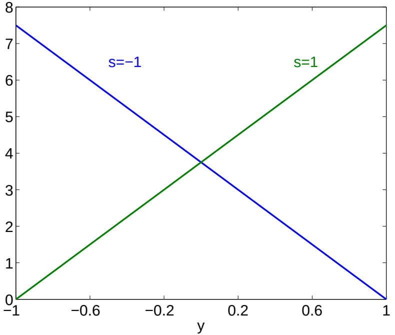
Examples of $G^0_{h,y}$ and $G^\partial_{h,y}$

$$-u'' = f \quad \text{in } (-1,1), \qquad u(0) = u(1) = g_{\mathrm{D}}$$

$G^0_{h,y}(x)$



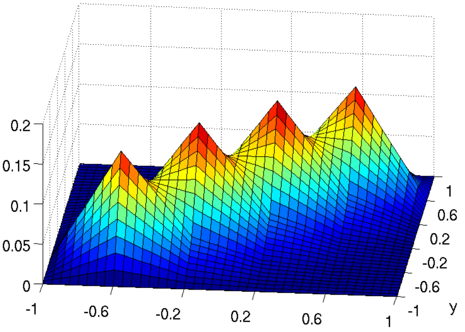
$G^\partial_{h,y}(s)$



Examples of $G^0_{h,y}$ and $G^\partial_{h,y}$

$$-u'' + 10u = f \quad \text{in } (-1,1), \qquad u(0) = u(1) = g_D$$

$G^0_{h,y}(x)$



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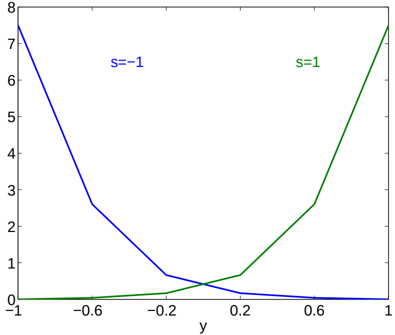

Maximum principle

- Discrete maximum principle (DMP):

  $$f \le 0 \text{ a.e. in } \Omega \text{ and } g_{\mathrm{N}} \le 0 \text{ a.e. on } \Gamma_{\mathrm{N}} \quad \Rightarrow \quad \max_{\overline{\Omega}} u_h \le \max_{\Gamma_{\mathrm{D}}} \max\{0, u_h\}$$

- Discrete conservatin of nonnegativity (DCN):

  $$f \ge 0 \text{ a.e. in } \Omega,\ g_{\mathrm{D}} \ge 0 \text{ a.e. on } \Gamma_{\mathrm{D}},\ \text{and } g_{\mathrm{N}} \ge 0 \text{ a.e. on } \Gamma_{\mathrm{N}} \quad \Rightarrow \quad u_h \ge 0 \text{ in } \Omega$$

Theorem (main)

DCN $\Leftrightarrow$ *(a)* $G^0_{h,y}(x) \ge 0 \quad \forall (x,y) \in \Omega^2$

(b) $G^\partial_{h,y}(s) \ge 0 \quad \forall (s,y) \in \Gamma_{\mathrm{D}} \times \Omega$

Proof:

$$u_h(y) = \int_\Omega f\, G^0_{h,y}\, \mathrm{d}x + \int_{\Gamma_{\mathrm{N}}} g_{\mathrm{N}}\, G^0_{h,y}\, \mathrm{d}s + \int_{\Gamma_{\mathrm{D}}} g_{\mathrm{D}}\, G^\partial_{h,y}\, \mathrm{d}s$$

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But:

(i) (DCN) $\not\Leftarrow$ (DMP)

(ii) $G^\partial_{h,y} \not\ge 0$ up to exceptional cases

Expressions for the DGF

- $\varphi_1^0, \varphi_2^0, \dots, \varphi_{N^0}^0$ basis in V_h^0
- $\varphi_1^\partial, \varphi_2^\partial, \dots, \varphi_{N^\partial}^\partial$ basis in V_h^∂
- $A \in \mathbb{R}^{N^0 \times N^0}$, $\quad A_{ij} = a(\varphi_j^0, \varphi_i^0) \quad i,j = 1,2,\dots,N^0$
- $A^\partial \in \mathbb{R}^{N^0 \times N^\partial}$, $\quad A_{ik}^\partial = a(\varphi_k^\partial, \varphi_i^0) \quad i = 1,\dots,N^0,\ k = 1,\dots,N^\partial$
- $M^\partial \in \mathbb{R}^{N^\partial \times N^\partial}$, $\quad M_{k\ell}^\partial = \int_{\Gamma_\mathrm{D}} \varphi_\ell^\partial \varphi_k^\partial \,\mathrm{d}s \quad k,\ell = 1,2,\dots,N^\partial$
- $$G_{h,y}^0(x) = \sum_{i=1}^{N^0} \sum_{j=1}^{N^0} \varphi_i^0(y)(A^{-1})_{ij} \varphi_j^0(x)$$
- $$G_{h,y}^\partial(s) = \sum_{k=1}^{N^\partial} \sum_{\ell=1}^{N^\partial} \varphi_k^\partial(s)(M^\partial)_{k\ell}^{-1} \left[\varphi_\ell^\partial(y) - \sum_{i=1}^{N^0} \sum_{j=1}^{N^0} \varphi_i^0(y)(A^{-1})_{ij} A_{j\ell}^\partial \right]$$

Maximum principle – remedy

- Discrete maximum principle (DMP):

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- Discrete conservatin of nonnegativity (DCN):

$$f \geq 0 \text{ a.e. in } \Omega,\ u_h^{\partial} \geq 0 \text{ on } \Gamma_{\mathrm{D}},\ \text{and } g_{\mathrm{N}} \geq 0 \text{ a.e. on } \Gamma_{\mathrm{N}} \quad \Rightarrow \quad u_h \geq 0 \text{ in } \Omega$$

Theorem (main)

$$DCN \quad \Leftrightarrow \quad \begin{array}{l} (a)\ G^0_{h,y}(x) \geq 0 \quad \forall (x,y) \in \Omega^2 \\ (b)\ (I - \Pi^0_h) u^{\partial}_h \geq 0 \quad \forall u^{\partial}_h \in V^{\partial}_h,\ u^{\partial}_h \geq 0 \text{ in } \Omega \end{array}$$

Elliptic projection: $\Pi^0_h : X_h \mapsto V^0_h$

$$\Pi^0_h w_h \in V^0_h \quad : \quad a(w_h - \Pi^0_h w_h, v^0_h) = 0 \quad \forall v^0_h \in V^0_h$$

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Proof:

$$u_h(y) = \int_{\Omega} f(x) G^0_{h,y}(x)\,\mathrm{d}x + \int_{\Gamma_{\mathrm{N}}} g_{\mathrm{N}}(s) G^0_{h,y}(s)\,\mathrm{d}s + (I - \Pi^0_h) u^{\partial}_h(y)$$

Maximum principle – remedy

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Theorem (main)

DCN $\Leftrightarrow$ *(a)* $G^0_{h,y}(x) \ge 0 \quad \forall (x,y) \in \Omega^2$

(b) $(I - \Pi_h^0) u_h^{\partial} \ge 0 \quad \forall u_h^{\partial} \in V_h^{\partial},\ u_h^{\partial} \ge 0$ *in* Ω

Now:

(i) DCN $\Leftrightarrow$ DMP

(ii) Condition (b) can be satisfied in nontrivial cases.

Linear FEM

Theorem

Let the basis functions be such that

$$\sum_{i=1}^{N^0} c_i^0 \varphi_i^0(x) \geq 0 \quad \forall x \in \Omega \quad \Leftrightarrow \quad c_i^0 \geq 0 \quad \forall i = 1, 2, \dots, N^0,$$

$$\sum_{\ell=1}^{N^\partial} c_\ell^\partial \varphi_\ell^\partial(x) \geq 0 \quad \forall x \in \Omega \quad \Leftrightarrow \quad c_\ell^\partial \geq 0 \quad \forall \ell = 1, 2, \dots, N^\partial.$$

Then DCN holds true if and only if

$$(a) \quad A^{-1} \geq 0 \quad and \quad (b) \quad -A^{-1}A^\partial \geq 0.$$

Proof:

$$\text{(a)} \quad G_{h,y}^0(x) = \sum_{i=1}^{N^0} \sum_{j=1}^{N^0} \varphi_i^0(y)(A^{-1})_{ij}\varphi_j^0(x) \geq 0 \quad \Leftrightarrow \quad (A^{-1})_{ij} \geq 0$$

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$$\sum_{\ell=1}^{N^\partial} c_\ell^\partial \varphi_\ell^\partial(x) \geq 0 \quad \forall x \in \Omega \quad \Leftrightarrow \quad c_\ell^\partial \geq 0 \quad \forall \ell = 1, 2, \dots, N^\partial.$$

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$$(a) \quad A^{-1} \geq 0 \quad and \quad (b) \quad -A^{-1}A^\partial \geq 0.$$

Proof:

(b) $u_h^\partial(y) = \sum_{k=1}^{N^\partial} c_k^\partial \varphi_k^\partial(y)$

$$(I - \Pi_h^0)u_h^\partial(y) = \sum_{\ell=1}^{N^\partial} c_\ell^\partial \left[\varphi_\ell^\partial(\mathbf{y}) - \sum_{i=1}^{N^0} \sum_{j=1}^{N^0} \varphi_i^0(\mathbf{y})(A^{-1})_{ij} A_{j\ell}^\partial \right]$$

Linear FEM

Theorem

Let the basis functions be such that

$$\sum_{i=1}^{N^0} c_i^0 \varphi_i^0(x) \geq 0 \quad \forall x \in \Omega \quad \Leftrightarrow \quad c_i^0 \geq 0 \quad \forall i = 1, 2, \ldots, N^0,$$

$$\sum_{\ell=1}^{N^\partial} c_\ell^\partial \varphi_\ell^\partial(x) \geq 0 \quad \forall x \in \Omega \quad \Leftrightarrow \quad c_\ell^\partial \geq 0 \quad \forall \ell = 1, 2, \ldots, N^\partial.$$

Then DCN holds true if and only if

$$(a) \quad A^{-1} \geq 0 \quad and \quad (b) \quad -A^{-1}A^\partial \geq 0.$$

Remarks:

- Conditions (a) and (b) for finite differences are due to P.G. Ciarlet, 1970.
- If $a(\varphi_i, \varphi_j) \leq 0$ for $i \neq j$ then $A^{-1} \geq 0$ and $A^\partial \leq 0$ (A is M-matrix).

Another remark

- Further modification of the definition of the DCN $\quad f \mapsto f_h$
  $$g_{\mathrm{N}} \mapsto g_{\mathrm{N}h}$$
- $\mathcal{T}_h$ fixed (V_h^0 fixed) and want $f \geq 0, \ldots \Rightarrow \quad u_h \geq 0$

  In the language of matrices:
  Want $x = A^{-1}b \geq 0$ for all $b \geq 0$ (i.e. want $A^{-1} \geq 0$)
- $f \geq 0$ fixed and want $\mathcal{T}_h$ such that $u_h \geq 0$

  In the language of matrices:
  Given $b \geq 0$ construct A such that $x = A^{-1}b \geq 0$

Thank you for your attention

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