Minimal Positive Stencils in Meshfree Finite Difference Methods for Linear Elliptic PDEs

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Outline

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Introduction to Elliptic Equations

Main goal: Solve the second-order linear elliptic equations in non-divergence form

$$\begin{cases} -Lu(\boldsymbol{x}) := -\sum_{i,j=1}^{d} a^{ij}(\boldsymbol{x})\partial_{ij}u(\boldsymbol{x}) = f(\boldsymbol{x}) & \boldsymbol{x} \in \Omega \\ u(\boldsymbol{x}) = g(\boldsymbol{x}) & \boldsymbol{x} \in \partial\Omega \end{cases},$$

for an open bounded domain $\Omega \in \mathbb{R}^d$. The matrix $A(\boldsymbol{x}) = (a^{ij}(\boldsymbol{x}))_{i,j=1}^{d}$ is assumed to be symmetric and positive definite satisfying the uniform ellipticity condition

$$\lambda|\boldsymbol{\xi}|^2 \leq \boldsymbol{\xi}^T A(\boldsymbol{x})\boldsymbol{\xi} \leq \Lambda|\boldsymbol{\xi}|^2 \qquad \forall \boldsymbol{\xi} \in \mathbb{R}^d$$

for positive constants λ, Λ with ratio $\lambda/\Lambda \leq 1$.
Denote $M(\boldsymbol{x}) := (A(\boldsymbol{x}))^{1/2}$.

Nonlocal Relaxation to Elliptic Equations

When $A(\boldsymbol{x}) = I$, we get the Laplace operator:

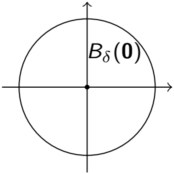
$$\Delta u(\boldsymbol{x}) = \sum_{i=1}^{d} \partial_{ii} u(\boldsymbol{x}).$$

The nonlocal Laplace operator[1] is given by

$$\tilde{\mathcal{L}}_\delta u(\boldsymbol{x}) = \int_{B_\delta(\mathbf{0})} \frac{1}{\delta^{d+2}} \gamma\left(\frac{|\boldsymbol{y}|}{\delta}\right) \left(u(\boldsymbol{x}+\boldsymbol{y}) - u(\boldsymbol{x})\right) d\boldsymbol{y},$$

where γ is a nonnegative kernel with

$$\int_{B_1(\mathbf{0})} |\boldsymbol{y}|^2 \gamma(|\boldsymbol{y}|)\, d\boldsymbol{y} = 2d.$$



[1] [Du et al., 2012] and [Silling, 2000]

Nonlocal Relaxation to Elliptic Equations

$$\tilde{\mathcal{L}}_\delta u(\boldsymbol{x}) = \int_{B_\delta(\boldsymbol{0})} \frac{1}{\delta^{d+2}} \gamma \left(\frac{|\boldsymbol{y}|}{\delta} \right) \left(u(\boldsymbol{x}+\boldsymbol{y}) - u(\boldsymbol{x}) \right) d\boldsymbol{y},$$

It can be shown that

$$\tilde{\mathcal{L}}_\delta u(\boldsymbol{x}) \to \Delta u(\boldsymbol{x}) \qquad \text{as} \quad \delta \to 0.$$

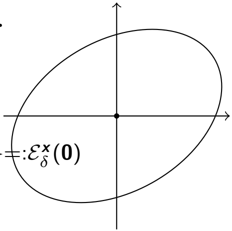
Nonlocal Relaxation to Elliptic Equations

For general $A(\boldsymbol{x})$, the nonlocal elliptic operator[2] can be defined as

$$\mathcal{L}_\delta u(\boldsymbol{x}) = \int_{B_\delta(\mathbf{0})} \frac{1}{\delta^{d+2}} \gamma\left(\frac{|\boldsymbol{z}|}{\delta}\right) \left(u(\boldsymbol{x} + M(\boldsymbol{x})\boldsymbol{z}) - u(\boldsymbol{x})\right) d\boldsymbol{z}$$

$$= \int_{\mathcal{E}_\delta^{\boldsymbol{x}}(\mathbf{0})} \frac{1}{\delta^{d+2}} \gamma\left(\frac{|M(\boldsymbol{x})^{-1}\boldsymbol{y}|}{\delta}\right) \det(M(\boldsymbol{x}))^{-1} \left(u(\boldsymbol{x}+\boldsymbol{y}) - u(\boldsymbol{x})\right) d\boldsymbol{y}$$

$$:= \int_{\mathcal{E}_\delta^{\boldsymbol{x}}(\mathbf{0})} \rho_\delta(\boldsymbol{x}, \boldsymbol{y}) \left(u(\boldsymbol{x}+\boldsymbol{y}) - u(\boldsymbol{x})\right) d\boldsymbol{y}.$$



[2] [Nochetto and Zhang, 2018]

Nonlocal Relaxation to Elliptic Equations

$$
\begin{aligned}
\mathcal{L}_\delta u(\boldsymbol{x}) &= \int_{B_\delta(\mathbf{0})} \frac{1}{\delta^{d+2}} \gamma\left(\frac{|\boldsymbol{z}|}{\delta}\right) \left(u(\boldsymbol{x} + M(\boldsymbol{x})\boldsymbol{z}) - u(\boldsymbol{x})\right) d\boldsymbol{z} \\
&= \int_{\mathcal{E}_\delta^{\boldsymbol{x}}(\mathbf{0})} \frac{1}{\delta^{d+2}} \gamma\left(\frac{|M(\boldsymbol{x})^{-1}\boldsymbol{y}|}{\delta}\right) \det(M(\boldsymbol{x}))^{-1} \left(u(\boldsymbol{x}+\boldsymbol{y}) - u(\boldsymbol{x})\right) d\boldsymbol{y} \\
&:= \int_{\mathcal{E}_\delta^{\boldsymbol{x}}(\mathbf{0})} \rho_\delta(\boldsymbol{x},\boldsymbol{y}) \left(u(\boldsymbol{x}+\boldsymbol{y}) - u(\boldsymbol{x})\right) d\boldsymbol{y}.
\end{aligned}
$$

It can be shown that

$$
\mathcal{L}_\delta u(\boldsymbol{x}) \to Lu(\boldsymbol{x}) \qquad \text{as} \quad \delta \to 0.
$$

Why Minimal Positive Stencil

Lax equivalence theorem states that

$$\text{Consistency} \; + \; \text{Stability} \; \to \; \text{Convergence.}$$

We usually use **truncation error** to analyze the consistency of a method. Then if the method also satisfies the **discrete maximum principle**, according to the Lax equivalence theorem, we will have a convergent method.

Why Minimal Positive Stencil

We aim to obtain a **positive** stencil, because a positive stencil automatically satisfies the discrete maximum principle.

In formula

$$\mathcal{L}_\delta^h u(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_j \in \mathcal{N}(\boldsymbol{x}_i)} \beta_{j,i} \Big(u(\boldsymbol{x}_j) - u(\boldsymbol{x}_i) \Big)$$

where $\mathcal{N}(\boldsymbol{x}_i)$ is some neighborhood of $\boldsymbol{x}_i$,
we need $\beta_{j,i} \geq 0$ for all j.

Why Minimal Positive Stencil

Minimal stencils are beneficial for the sparsity of the linear system matrix, resulting in a lower memory consumption and a faster solution of a linear system.

In formula

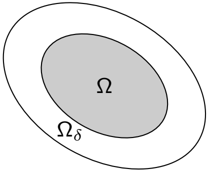
$$\mathcal{L}_\delta^h u(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_j \in \mathcal{N}(\boldsymbol{x}_i)} \beta_{j,i} \Big(u(\boldsymbol{x}_j) - u(\boldsymbol{x}_i) \Big)$$

we need a small $\#\{j : \beta_{j,i} > 0\}$.

Outline

To Find a Stencil

Let Ω_δ be the extended domain.
Point cloud $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_M\} \subset \Omega_\delta$ be given. Meshfree just means that no information about connection of points is provided.



Point cloud contains two types of points:

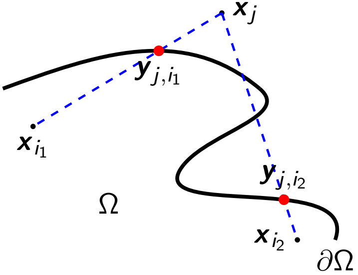
1. Interior points $\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ (in Ω),
2. Boundary points $\{\boldsymbol{x}_{N+1}, \dots, \boldsymbol{x}_M\}$ (in $\Omega_\delta \setminus \Omega$).

For each interior point, two steps are needed:

1. Define which points are its neighbors (vary for $A(\boldsymbol{x})$),
2. Select a stencil (using a minimization problem).

Proper Point Cloud

We consider each boundary point $\boldsymbol{x}_j$ around $\boldsymbol{x}_i$ as the closest projection $\boldsymbol{y}_{j,i}$ from $\boldsymbol{x}_j$ to $\boldsymbol{x}_i$ at the boundary.



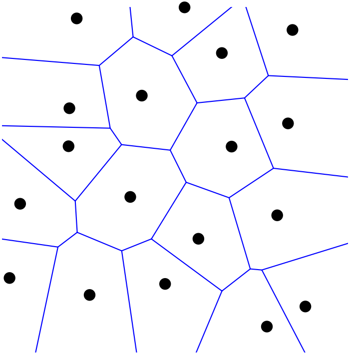
Then apply the boundary condition to these mapped boundary points to proceed.

Proper Point Cloud

Fill Distance[3]:

$$h = \inf \left\{ h : \overline{\Omega_\delta} \subseteq \bigcup_{i=1}^{M} \overline{B_h(\boldsymbol{x}_i)} \right\}$$
$$= \sup_{\boldsymbol{x}\in\overline{\Omega_\delta}} \min_{1\leq i\leq M} |\boldsymbol{x} - \boldsymbol{x}_i|.$$

Use **Voronoi diagram**.



[3] [Wendland, 2004]

Proper Point Cloud

When we say a point cloud is proper, we mean

1. Fill distance is small enough;
2. Separation between interior points is large enough;
3. Proportional to the fill distance, there are no interior points too close to the boundary.

In short, we want the points in the point cloud to be as evenly distributed as possible (each point is not too far away from or too close to its neighbors).

The Minimization Problem

We use the following minimization problem[4] to select a unique stencil for interior point $\boldsymbol{x}_i$ and p the order of the polynomial space:

$$\{\beta_{j,i}\} = \underset{\{\beta_{j,i}\}\in S_{\delta,h,p}}{\arg\min} \sum_j \frac{\beta_{j,i}}{\rho_\delta(\boldsymbol{x}_i, \boldsymbol{x}_j - \boldsymbol{x}_i)},$$

where

$$S_{\delta,h,p} := \left\{\{\beta_{j,i}\} : \beta_{j,i} \geq 0 \text{ and } \mathcal{L}_\delta^h u(\boldsymbol{x}_i) = \mathcal{L}_\delta u(\boldsymbol{x}_i) \ \forall u \in \mathcal{P}_p(\mathbb{R}^d)\right\},$$

$$\mathcal{L}_\delta^h u(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_j \in \mathcal{E}_\delta^{\boldsymbol{x}_i}(\boldsymbol{x}_i)} \beta_{j,i}(u(\boldsymbol{x}_j) - u(\boldsymbol{x}_i)).$$

[4] [Seibold, 2008] and [Trask et al., 2019]

The Minimization Problem

$$\{\beta_{j,i}\} = \arg\min_{\{\beta_{j,i}\}\in S_{\delta,h,p}} \sum_j \frac{\beta_{j,i}}{\rho_\delta(\boldsymbol{x}_i, \boldsymbol{x}_j - \boldsymbol{x}_i)},$$

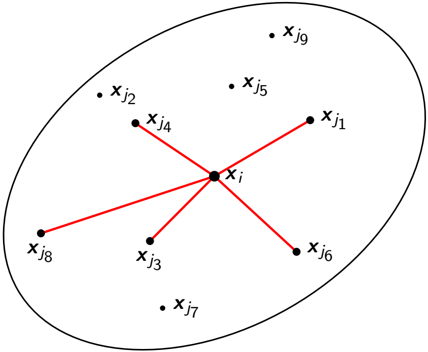
Recall:

$$\rho_\delta(\boldsymbol{x}_i, \boldsymbol{x}_j - \boldsymbol{x}_i) = \frac{1}{\delta^{d+2}}\gamma\left(\frac{|M(\boldsymbol{x}_i)^{-1}(\boldsymbol{x}_j - \boldsymbol{x}_i)|}{\delta}\right)\det(M(\boldsymbol{x}_i))^{-1},$$

$$\mathcal{L}_\delta u(\boldsymbol{x}_i) = \int_{\mathcal{E}_\delta^{\boldsymbol{x}_i}(\boldsymbol{0})} \rho_\delta(\boldsymbol{x}_i, \boldsymbol{y})(u(\boldsymbol{x}_i + \boldsymbol{y}) - u(\boldsymbol{x}_i))\, d\boldsymbol{y}.$$

The Minimization Problem

$$\{\beta_{j,i}\} = \underset{\{\beta_{j,i}\}\in S_{\delta,h,p}}{\arg\min} \sum_j \frac{\beta_{j,i}}{\rho_\delta(\boldsymbol{x}_i, \boldsymbol{x}_j - \boldsymbol{x}_i)},$$



The Minimization Problem

To include the projection for all boundary points, define

$$\boldsymbol{y}_{j,i} = \begin{cases} \boldsymbol{x}_j & , \boldsymbol{x}_j \in \overline{\Omega} \\ \text{projection from } \boldsymbol{x}_j \text{ to } \boldsymbol{x}_i \text{ at } \partial\Omega & , \boldsymbol{x}_j \in \Omega_\delta \setminus \overline{\Omega} \end{cases}$$

and

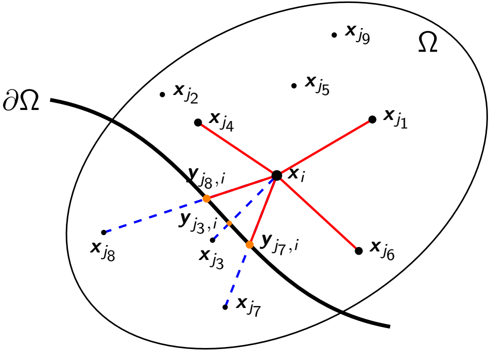
$$\overline{S}_{\delta,h,p} := \left\{ \{\beta_{j,i}\} : \beta_{j,i} \geq 0 \text{ and } \mathcal{L}^h_{\delta,\Omega} u(\boldsymbol{x}_i) = \mathcal{L}_\delta u(\boldsymbol{x}_i) \ \forall u \in \mathcal{P}_p(\mathbb{R}^d) \right\},$$

$$\mathcal{L}^h_{\delta,\Omega} u(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_j \in \mathcal{E}_\delta^{\boldsymbol{x}_i}(\boldsymbol{x}_i)} \beta_{j,i}(u(\boldsymbol{y}_{j,i}) - u(\boldsymbol{x}_i)).$$

The Minimization Problem

Then the minimization problem becomes

$$\{\beta_{j,i}\} = \underset{\{\beta_{j,i}\}\in\overline{S}_{\delta,h,p}}{\arg\min} \sum_j \frac{\beta_{j,i}}{\rho_\delta(\boldsymbol{x}_i, \boldsymbol{y}_{j,i} - \boldsymbol{x}_i)},$$



Error Using Discrete Operator

Lemma 1 (Ye-Tian, 2022)

Assume $\overline{S}_{\delta,h,p}$ is not empty and $C > 0$ is a generic constant.

1. *If $p \geq 2$ and $u \in C^2(\overline{\Omega})$, then $|\mathcal{L}^h_{\delta,\Omega} u(\boldsymbol{x}_i) - Lu(\boldsymbol{x}_i)| \to 0$ as $\delta \to 0$ for all $\boldsymbol{x}_i \in \Omega$.*
2. *If $p \geq 2$ and $u \in C^{2,\alpha}(\overline{\Omega})$ for $\alpha \in (0,1]$, then $|\mathcal{L}^h_{\delta,\Omega} u(\boldsymbol{x}_i) - Lu(\boldsymbol{x}_i)| \leq C|u|_{C^{2,\alpha}(\overline{\Omega})}\delta^{\alpha}$ for all $\boldsymbol{x}_i \in \Omega$.*
3. *If $p \geq 3$ and $u \in C^{3,\alpha}(\overline{\Omega})$ for $\alpha \in (0,1]$, then $|\mathcal{L}^h_{\delta,\Omega} u(\boldsymbol{x}_i) - Lu(\boldsymbol{x}_i)| \leq C|u|_{C^{3,\alpha}(\overline{\Omega})}\delta^{1+\alpha}$ for all $\boldsymbol{x}_i \in \Omega$.*

Nonempty Feasible Set Condition

Theorem 2 (Ye-Tian, 2022)

In $d = 2$, there exists a constant $C > 0$ such that if

$$h \leq C\delta\sqrt{\lambda/\Lambda}$$

then $S_{\delta,h,2}$ and $\overline{S}_{\delta,h,2}$ are not empty.

Error Estimate

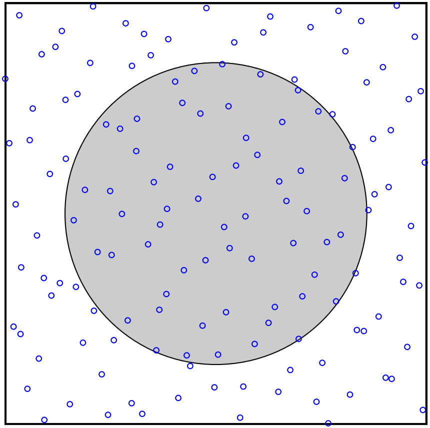
Theorem 3 (Ye-Tian, 2022)

In $d = 2$, assume $\overline{S}_{\delta,h,p}$ is not empty, let u be the real solution and u_δ^h be the solution solved by the discrete operator and $C > 0$ is a generic constant.

1. *If $p \geq 2$ and $u \in C^{2,\alpha}(\overline{\Omega})$ for $\alpha \in (0,1]$, then*
$$\max_{\boldsymbol{x}_i \in \Omega} \left| u(\boldsymbol{x}_i) - u_\delta^h(\boldsymbol{x}_i) \right| \leq C |u|_{C^{2,\alpha}(\overline{\Omega})} \left(\sqrt{\lambda / \Lambda} \right)^{-\alpha} h^\alpha$$
2. *If $p \geq 3$ and $u \in C^{3,\alpha}(\overline{\Omega})$ for $\alpha \in (0,1]$, then*
$$\max_{\boldsymbol{x}_i \in \Omega} \left| u(\boldsymbol{x}_i) - u_\delta^h(\boldsymbol{x}_i) \right| \leq C |u|_{C^{3,\alpha}(\overline{\Omega})} \left(\sqrt{\lambda / \Lambda} \right)^{-(1+\alpha)} h^{1+\alpha}$$

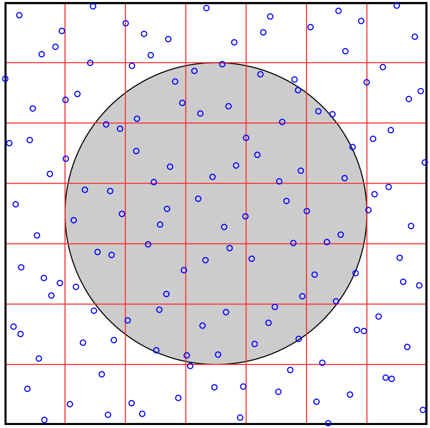
Outline

Generate Point Cloud



Use **Quasi-Monte Carlo method**.

Generate Voxels

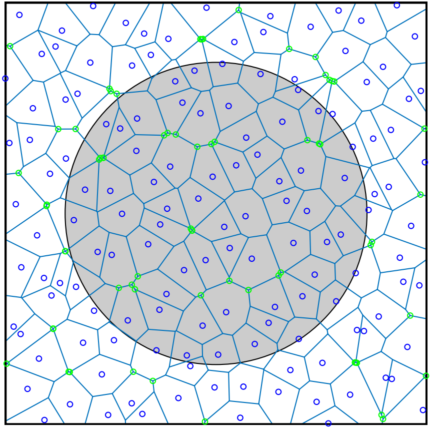


Divide points into small blocks.

Adjust the Point Cloud

Step 1:

Add points to decrease the fill distance

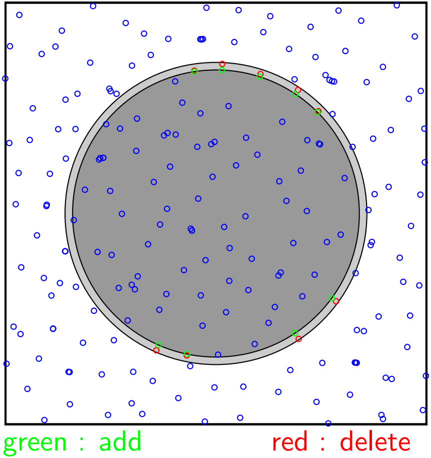


green : add red : delete

Adjust the Point Cloud

Step 2:

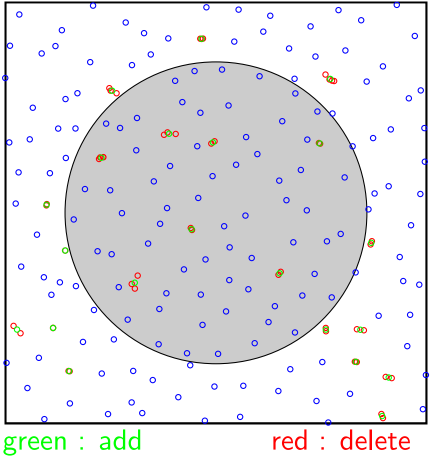
Map points to increase the minimum distance from interior points to the boundary



Adjust the Point Cloud

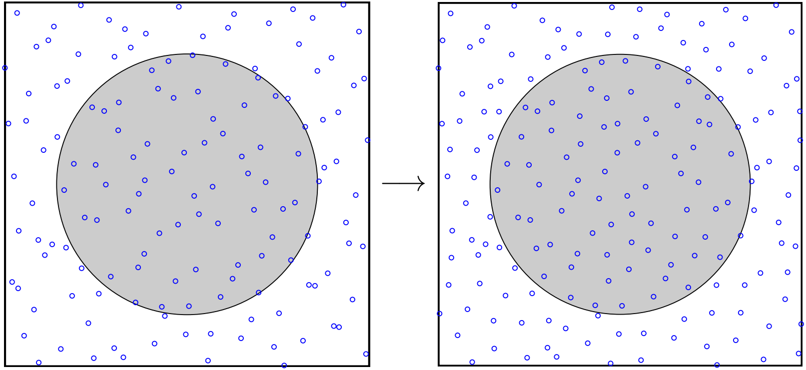
Step 3:

Merge points to increase the separation between interior points



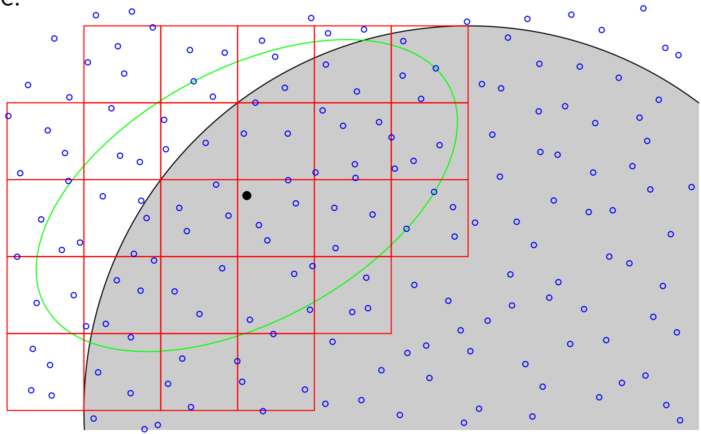
Adjust the Point Cloud

Repeat steps 1-3 until the point cloud is proper or the process exceeds the maximum number of iterations.



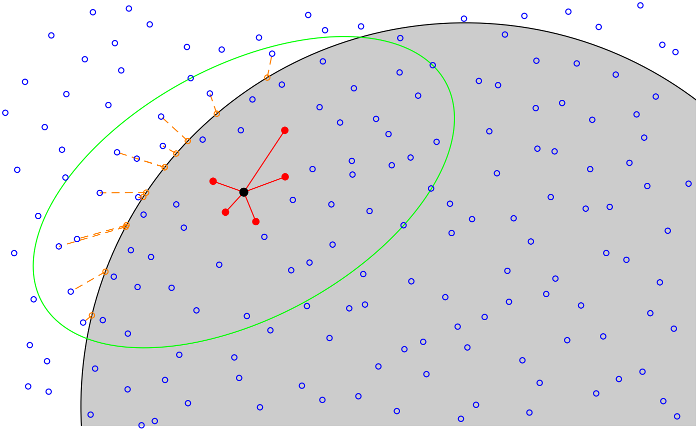
Find Neighbors

Use the voxels to find the neighbors of an interior point inside ellipse.



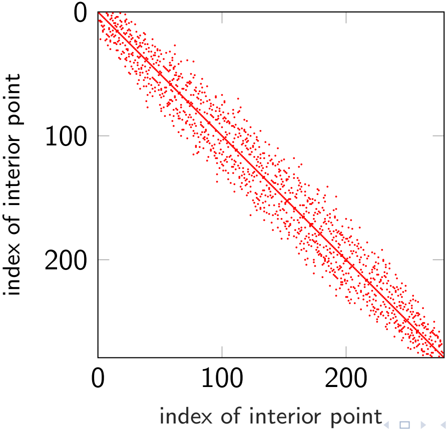
Solve the Linear Minimization Problem

Use the **simplex method**.



Assemble the Matrix

Reindex the interior points, we get the following matrix represents the nonzero relations between interior points:



Outline

Parameter Matrices

We tested for the following $A(\boldsymbol{x})$ in $d = 2$, $p = 2$:

Name	Matrix	λ/Λ for $\boldsymbol{x} \in [-1,1]^2$
$A_1(x_1, x_2)$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	1.0000
$A_2(x_1, x_2)$	$\begin{bmatrix} 12-6\lvert x_1\rvert & 0 \\ 0 & 3+3\lvert x_2\rvert \end{bmatrix}$	0.2500
$A_3(x_1, x_2)$	$\begin{bmatrix} 12-6\lvert x_1\rvert & 3 \\ 3 & 3+3\lvert x_2\rvert \end{bmatrix}$	0.1459
$A_4(x_1, x_2)$	$\begin{bmatrix} 100(12-6\lvert x_1\rvert) & 0 \\ 0 & 3+3\lvert x_2\rvert \end{bmatrix}$	0.0025

Error Graph I

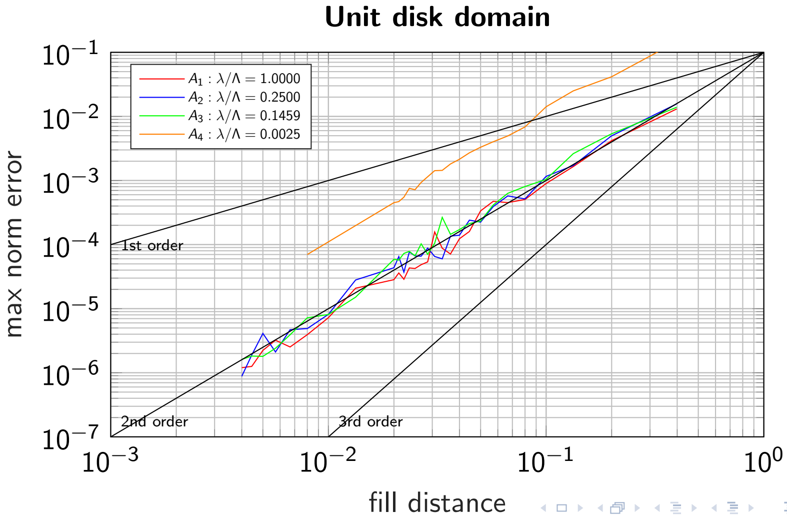
Solve for the following equation:

$$u(x_1, x_2) = x_1 x_2 + \cos(x_1)\exp(x_2)$$

by

$$\begin{cases} \mathcal{L}^h_{\delta,\Omega} u^h_\delta = \sum_{i,j=1}^{2} a^{ij}(\boldsymbol{x})\partial_{ij} u(\boldsymbol{x}) & \boldsymbol{x} \in \Omega \\ u^h_\delta(\boldsymbol{x}) = u(\boldsymbol{x}) & \boldsymbol{x} \in \partial\Omega \end{cases}.$$

Error Graph I



Error Graph II

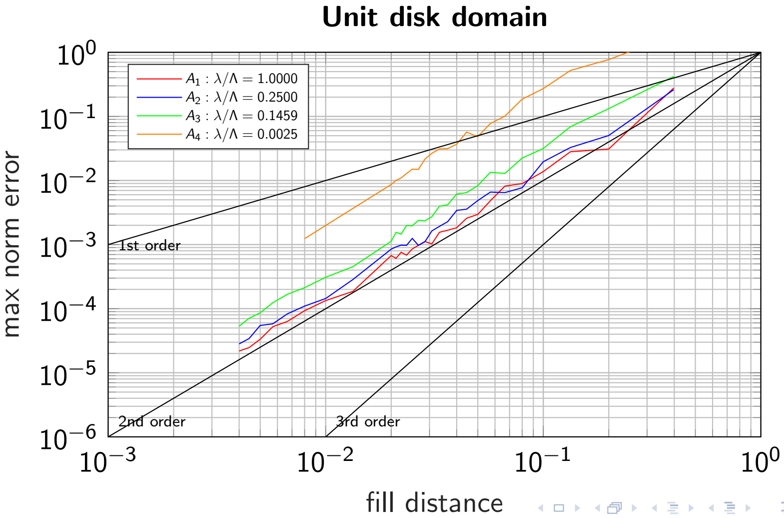
Solve for the following equation:

$$u(x_1, x_2) = (x_1 + x_2)^4 \cos(x_1(x_1 + 2x_2))$$

by

$$\begin{cases} \mathcal{L}^h_{\delta,\Omega} u^h_\delta = \sum_{i,j=1}^{2} a^{ij}(\boldsymbol{x}) \partial_{ij} u(\boldsymbol{x}) & \boldsymbol{x} \in \Omega \\ u^h_\delta(\boldsymbol{x}) = u(\boldsymbol{x}) & \boldsymbol{x} \in \partial\Omega \end{cases}.$$

Error Graph II



Thank you

Thank you for listening!
Questions?

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