Master Thesis Literature Study Presentation

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Conjugate Gradient Method Deflation Domain Decomposition Research

Plaxis Finite Element Method





Plaxis B.V. is a company specialized in finite element software intended for 2D and 3D analysis of deformation, stability and groundwater flow in geotechnical engineering.

Introduction

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Finite Element Method

The Finite Element Method (FEM) is a numerical technique for finding approximate solutions of partial differential equations (PDE).

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Plaxis Finite Element Method

Example



Introduction	Main Problem and Basic Iterative Methods
Conjugate Gradient Method	Conjugate Gradient Method
Deflation	Convergence of CG
Domain Decomposition	Precondtioned Conjugate Gradient Method
Research	Numerical Ilustration

Conjugate Gradient Method

Main problem

Main Problem and Basic Iterative Methods Conjugate Gradient Method Convergence of CG Precondtioned Conjugate Gradient Method Numerical Ilustration

Solve:

 $Ax = b, \tag{1}$

where $A \in \mathbb{R}^{n \times n}$ is SPD.

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Basic Iterative Methods

Let us take

$$x_{i+1} = x_i + M^{-1}(b - Ax_i)$$
(2)

Which generates a sequence with the following property

$$x_i \in x_0 + \operatorname{span}\{M^{-1}r_0, M^{-1}A(M^{-1}r_0), ..., (M^{-1}A)^{i-1}(M^{-1}r_0)\}.$$
(3)

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Conjugate Gradient Method

▶ Set M = I.

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Conjugate Gradient Method

• Set
$$M = I$$
.
• $||x - x_i||_A = \min_{y \in K^i(A;r_0)} ||x - y||_A$, for all *i*.

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Solution of the problem leads to the Conjugate Gradient Method.

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Conjugate Gradient Algorithm

Choose x_0 , set i = 0, $r_0 = b - Ax_0$. WHILE $r_k \neq 0$ DO i := i + 1IF i = 0 DO $p_1 = r_0$ ELSE $\beta_i = \frac{r_{i-1}^T r_{i-1}}{r_{i-2}^T r_{i-2}}$

 $p_i = r_{i-1} + \beta_i p_{i-1}$

ENDIF

$$\alpha_{i} = \frac{r_{i-1}^{T}r_{i-1}}{p_{i}^{T}Ap_{i}}$$

$$x_{i} = x_{i-1} + \alpha_{i}p_{i}$$

$$r_{i} = r_{i-1} - \alpha_{i}Ap_{i}$$
END WHILE

(4)

Theorem

Let A and x be the coefficient matrix and the solution of (1), and let $(x_i, i = 0, 1, 2...)$ be the sequence generated by the CG method. Then, elements of the sequence satisfy the following inequality:

$$||x - x_i||_A \le 2\left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}\right)^i ||x - x_0||_A,$$
 (5)

where $\kappa(A)$ is the condition number of A in the 2 - norm.

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Speed up? Yes, with preconditioning.

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Transform the system (1) into

$$A^*x^* = b^*, (6)$$

where $A^* = P^{-1}AP^{-T}$, $x^* = P^{-T}x$ and $b^* = P^{-1}b$, where P is a non-singular matrix. The SPD matrix M defined by $M = PP^T$ is called the preconditioner.

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Preconditioned Conjugate Gradient Algorithm

Choose
$$x_0$$
, set $i = 0$, $r_0 = b - Ax_0$.
WHILE $r_i \neq 0$ DO
 $z_i = M^{-1}r_i$
 $i := i + 1$
IF $i = 0$ DO
 $p_1 = z_0$
ELSE
 $\beta_i = \frac{r_{i-1}^T z_{i-1}}{r_{i-2}^T z_{i-2}}$
 $p_i = z_{i-1} + \beta_i p_{i-1}$
ENDIF
 $\alpha_i = \frac{r_{i-1}^T z_{i-1}}{p_i^T Ap_i}$

 $x_i = x_{i-1} + \alpha_i p_i$

$$r_i = r_{i-1} - \alpha_i A p_i$$

END WHILE

(7)

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► Jacobi, *M* - diag(A).

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► SSOR,
$$M = \frac{1}{2-\omega} (\frac{1}{\omega}D + L) (\frac{1}{\omega}D)^{-1} (\frac{1}{\omega}D + L)^T$$

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► SSOR,
$$M = \frac{1}{2-\omega} (\frac{1}{\omega}D + L) (\frac{1}{\omega}D)^{-1} (\frac{1}{\omega}D + L)^T$$

Incomplete Cholesky

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► SSOR,
$$M = \frac{1}{2-\omega} (\frac{1}{\omega}D + L) (\frac{1}{\omega}D)^{-1} (\frac{1}{\omega}D + L)^T$$

- Incomplete Cholesky
- Many, many more.

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Second Simple Problem



Figure: Second Simple Problem Representation

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Figure: Plot of log₁₀ of i-th residue

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Figure: Plot of *log*₁₀ of eigenvalues

Main idea Deflated Preconditoned Conjugate Gradient Method Deflation vector

DEFLATION

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Main idea Deflated Preconditoned Conjugate Gradient Method Deflation vector

How to get rid of unfavorable eigenvalues that deteriorate the convergence of PCG?

Main idea Deflated Preconditoned Conjugate Gradient Method Deflation vector

Split

$$x = (I - P^T)x + P^T x, \tag{8}$$

where,

P = I - AQ, $Q = ZE^{-1}Z^{T}$ $E = Z^{T}AZ$ and $Z \in \mathbb{R}^{n \times m}$. (9)

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After some transformation we get an equivalent, "deflated" system:

$$PA\bar{x} = Pb,$$
 (10)

which can be solved with CG or PCG.

Deflated Preconditioned Conjugate Gradient Algorithm

Choose
$$\bar{x}_0$$
, set $i = 0$, $\bar{r}_0 = P(b - A\bar{x}_0)$.
WHILE $\bar{r}_k \neq 0$ DO
 $i := i + 1$
IF $i = 1$ DO
 $y_0 = M^{-1}\bar{r}_0$
 $p_1 = y_0$
ELSE
 $y_{i-1} = M^{-1}\bar{r}_{i-1}$
 $\beta_i = \frac{\bar{r}_{i-1}^T y_{i-1}}{\bar{r}_{i-2}^T y_{i-2}}$
 $p_i = y_{i-1} + \beta_i p_{i-1}$
ENDIF
 $\alpha_i = \frac{\bar{r}_{i-1}^T \bar{r}_{i-1}}{p_i^T P A p_i}$
 $\bar{x}_i = \bar{x}_{i-1} + \alpha_i p_i$
 $\bar{r}_i = \bar{r}_{i-1} - \alpha_i P A p_i$
END WHILE

 $x_{orginal} = Qb + P^T \bar{x}_{last}$ (11) Konrad Kaliszka Master Thesis Literature Study Presentation

Main idea Deflated Preconditoned Conjugate Gradient Method Deflation vector

How to choose Z?

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Several choices for Z:

Approximated Eigenvector Deflation

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Several choices for Z:

- Approximated Eigenvector Deflation
- Subdomain Deflation

Main idea Deflated Preconditoned Conjugate Gradient Method Deflation vector

Several choices for Z:

- Approximated Eigenvector Deflation
- Subdomain Deflation
- Rigid Body Mode Deflation

Main Idea Schwarz Alternating Procedure Numerical Experiments

Domain Decomposition

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Definition

We will call a method a Domain Decomposition method, if its main idea will be based on the principle of divide and conquer applied on the domain of the problem.





Figure: An example of domain decomposition

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There are several ways to do it. The most known are:

- Schwarz Alternating Procedure
- Schur Complement

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Lets consider a domain as shown in the last figure with two overlapping subdomains Ω_1 and Ω_2 on which we want to solve a PDE of the following form:

$$\begin{cases} Lu = b, & \text{in } \Omega\\ u = g, & \text{on } \partial\Omega \end{cases}$$
(12)

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Schwarz Alternating Procedure

Choose u_0 WHILE no convergence DO FOR i = 1, ...s DO Solve Lu = b in Ω_i with $u = u_{ij}$ in Γ_{ij} Update u values on Γ_{ij} , $\forall j$ END FOR END WHILE

In our case, s = 2.

(13)

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Within the SAP there are two distinguished variants

- Multiplicative Schwarz Method (MSM)
- Additive Schwarz Method (ASM)

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Multiplicative Schwarz Method

$$u^{n+1/2} = u^{n} + \begin{bmatrix} A_{\Omega_{1}}^{-1} & 0\\ 0 & 0 \end{bmatrix} (b - Au^{n})$$
$$u^{n+1} = u^{n+1/2} + \begin{bmatrix} 0 & 0\\ 0 & A_{\Omega_{2}}^{-1} \end{bmatrix} (b - Au^{n+1/2})$$
(14)

where A_{Ω_i} stays for the discrete form of the operator L restricted to Ω_i

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Additive Schwarz Method

$$u^{n+1} = u^{n} + \left(\begin{bmatrix} A_{\Omega_{1}}^{-1} & 0\\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0\\ 0 & A_{\Omega_{2}}^{-1} \end{bmatrix} \right) (b - Au^{n})$$
(15)

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Additive Schwarz Method

Or in a more general:

Additive Schwarz Method

Choose u_0 , i = 0, WHILE no convergence DO $r_i = b - Au^n$ FOR i = 1, ...s DO $\delta_i = B_i r_i$ END FOR $u^{n+1} = u_n + \sum_{i=1}^s \delta_i$ i = i + 1END WHILE (16)

where
$$B_i = R_i^t A_{\Omega_i}^{-1} R_i$$

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Numerical Experiments



Figure: Domain Ω split into two subdomains, Ω_1 and Ω_2 .

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MSM



Figure: Contour plot of the log_{10} (*i*-th residue) for MSM.

Main Idea Schwarz Alternating Procedure Numerical Experiments

ASM



Figure: Contour plot of the log₁₀ (*i*-th residue) for ASM

Choice of method Test Problems Conclusions Research Goals

Research

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Choice of method Test Problems Conclusions Research Goals

Choice of the method

DPCG with Additive Schwarz as the preconditoner and physics based decomposition.

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First Simple Problem



Figure: First Simple Problem Representation

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Figure: First Simple Problem convergence behavior for PCG

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Analysis of the decomposition position



Figure: First Simple Problem distribution of error in PCG

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Second Simple Problem



Figure: Second Simple Problem Representation

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Figure: Second Simple Problem convergence behavior for PCG with 2 subdomains

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Figure: Second Simple Problem convergence behavior for PCG with 4 subdomains

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Figure: Second Simple Problem convergence behavior for PCG with 8 subdomains

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Figure: Second Simple Problem distribution of error in PCG

Choice of method Test Problems Conclusions Research Goals

▶ The choice of the method is right.

Choice of method Test Problems Conclusions Research Goals

- ▶ The choice of the method is right.
- Number and size of the subdomains matters.

Choice of method Test Problems Conclusions Research Goals

- ▶ The choice of the method is right.
- Number and size of the subdomains matters.
- Introduction of deflation.

Choice of method Test Problems Conclusions Research Goals

Research Goals

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Choice of method Test Problems Conclusions Research Goals

Research Questions

► Subdomain overlap.

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Choice of method Test Problems Conclusions Research Goals

Research Questions

- Subdomain overlap.
- Performance of Deflation.

Choice of method Test Problems Conclusions Research Goals

The End

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