On finite element discretizations of the pure Neumann problem

Pavel Bochev
University of Texas at Arlington (sabbatical visit at Sandia)
and
Rich Lehoucq
Sandia National Laboratories
Albuquerque, NM

Introduction

We consider the Neumann problem

$$\begin{aligned} -\triangle u &= f \quad \text{in } \Omega \\ \frac{\partial u}{\partial \mathbf{n}} &= 0 \quad \text{on } \Gamma \end{aligned}$$

where $\Omega \subset \mathbf{R}^N$ is a bounded open region with boundary Γ. Solutions are not unique—they are determined up to a constant value. The constraint on the source f is the *zero mean* condition

$$\int_\Omega f(x) = 0.$$

Equivalently, f is L^2 orthogonal to 1.

Standard Approach 1

A direct Galerkin discretization leads to a singular linear system

$$\mathbf{A}\mathbf{u} = \mathbf{f}.$$

Although $\mathbf{A}$ is singular, the conjugate gradient method can be used (see Axelsson 1994).

Notation:

$$\mathbf{A}_{i,j} = \mathcal{B}(\phi_j^h, \phi_i^h) = \int_\Omega \nabla\phi_i^h \cdot \nabla\phi_j^h$$

for $i, j = 1, \ldots, N$. We denote the discrete source term $\mathbf{f}$ by

$$\mathbf{f}_i = F(\phi_i^h) = \int_\Omega f\phi_i^h$$

and the basis mean vector $\mathbf{z}_i = (\phi_i^h, 1) = \int_\Omega \phi^h$.

Experiment using conjugate gradients

Set $u = cos(\pi x^2)cos(2\pi y)$, Ω be the unit square, and triangulate Ω via an unstructured mesh.

We used P1 elements on triangles, 3 point quadrature. (Number of nodes = 427, number of elements = 779, max element area $h^2/2$).

CG tolerance $= 1 \cdot 10^{-4}$ & Preconditioner = Jacobi.

Divergence is confirmed after computing $L^2(\Omega)$ and $H^1(\Omega)$ semi-norm errors of the approximate solution ($8 \cdot 10^7$ and $3 \cdot 10^1$).

Situation is worse with P2 elements.

What happened ?

Discrete source is not numerically orthogonal to the nullspace

To restore the discrete consistency of the system of the linear system, we need to orthogonalize $\mathbf{f}$ against $\mathbf{c}$:

$$(\mathbf{I} - \frac{\mathbf{z}\mathbf{c}^T}{\mathbf{z}^T\mathbf{c}})\mathbf{f}$$

where the above is formally equivalent to

$$\int_\Omega (f - \frac{\int_\Omega f \, d\Omega}{\int_\Omega d\Omega})\phi_i \, d\Omega$$

in the i-th row.

We should also worry about

$$-\nabla \cdot d(x)\nabla u = f$$

because the resulting stiffness matrix may not be singular.

Standard Approach 2

To remove the nullspace of $\mathbf{A}$, the discrete solution is specified at some nodal point and hence a degree of freedom from the linear system is removed. The system now solved is

$$(\mathbf{I}_\ell^T \mathbf{A} \mathbf{I}_\ell)\hat{\mathbf{u}} = \mathbf{I}_\ell^T \mathbf{f}$$

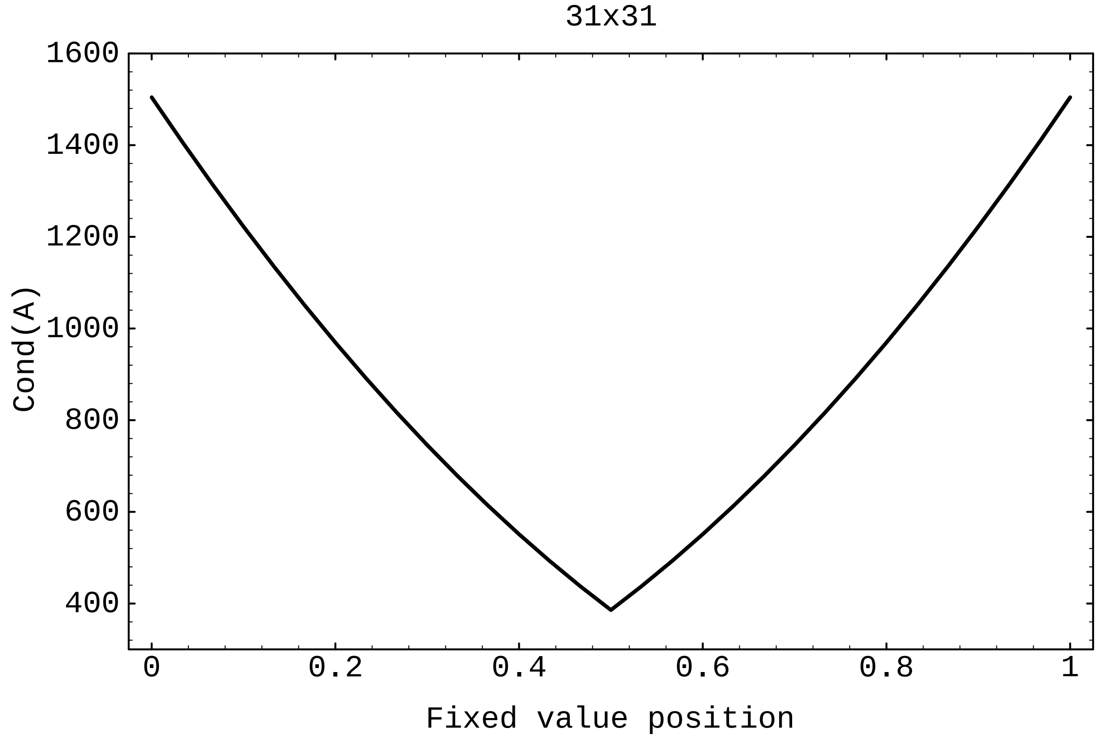
where $\mathbf{u} = \mathbf{I}_\ell \hat{\mathbf{u}}$ and

$$\mathbf{I}_\ell = \mathrm{diag}(1, \cdots, 1, 0, 1, \cdots, 1).$$

The choice of nodal point can make a dramatic difference in the condition number of the resulting stiffness matrix.

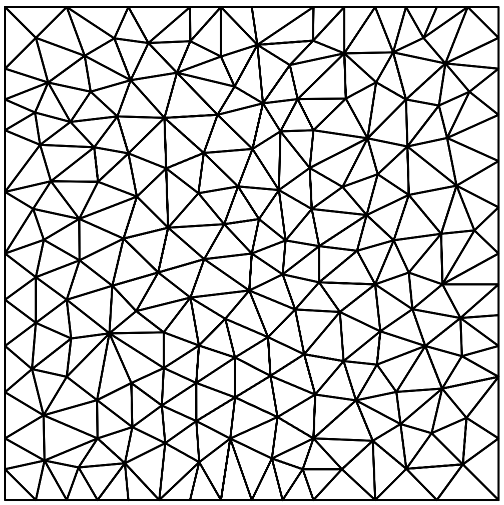
What point ? Two illustrations in the next couple of vu-graphs.

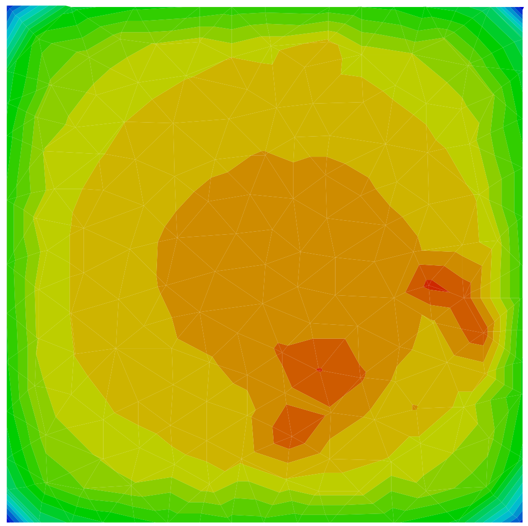
Specifying the nodal point in 1D



Condition number as a function of the specified node location for 31 points on a uniform grid in 1D using PW linears.

Specifying the nodal point in 2D





Condition number as a function of the specified node for an unstructured mesh for the unit square using P1 elements.

Motivation and Goal

- Develop a variational framework for the Neumann problem.
- Comparison of different classes of methods.
- Propose a novel penalized variational approach.
- Blend of algebraic and fem techniques.

Starting point is the quadratic functional

$$\min J(v,f) = \frac{1}{2}\int_\Omega |\nabla v|^2 dx - \int_\Omega fv dx$$

Discuss the space for the minimization and how to incorporate the constraint on the source. Three approaches are

- Lagrange multipliers
- penalization
- a subspace of $H^1(\Omega)$ functions that satisfy $(u,\omega) = \int_\Omega u\omega = 0$

Unconstrained minimization on $H^1(\Omega)/\mathbf{R}$

$$\min_{\hat{u}\in H^1(\Omega)/\mathbf{R}} J(v,f) = \frac{1}{2}\int_\Omega |\nabla v|^2 dx - \int_\Omega f v dx$$

$H^1(\Omega)/\mathbf{R}$ contains classes of functions $\hat{u}$ that differ by a constant.

Constrained minimization on $H^1(\Omega)$

Let $\omega \in H^{-1}(\Omega)$ satisfy $(\omega, 1) > 0$ and for any $u \in H^1(\Omega)$ we define the ω-mean as

$$u_\omega \equiv \frac{(u, \omega)}{(1, \omega)} = \frac{\int u\omega}{\int \omega}.$$

Consider the problem

$$\min_{u \in H^1(\Omega)} J(u, f) \quad \text{subject to} \quad u_\omega = 0.$$

Note that $\omega = 1$ implies that u_ω is the mean value of u.

A subspace of $H^1(\Omega)$—a reduced problem

Consider the space

$$H^1_\omega(\Omega) = \{u \in H^1(\Omega) \,|\, u_\omega = 0\}$$

of all functions with zero ω-mean, and the *reduced* problem

$$\min_{u \in H^1_\omega(\Omega)} J(u, f).$$

Unique minimizer $u \in H^1_\omega(\Omega)$ for every $f \in L^2(\Omega)$.

Need FE spaces that approximate $H^1_\omega(\Omega)$.

Constrain $J(u,f)$—use Lagrange multipliers

$$\min_{\substack{u \in H^1(\Omega) \\ \tau \in \mathbf{R}}} J(u,f) + \tau u_\omega$$

(Braess 1997) and the resulting optimality system: determine $u \in H^1(\Omega)$ and $\tau \in \mathbf{R}$ so that

$$\begin{array}{rcrcll} \mathcal{B}(u,v) & + & \tau v_\omega & = & F(v) & \forall v \in H^1(\Omega) \\ & & \sigma u_\omega & = & 0 & \forall \sigma \in \mathbf{R} \end{array}$$

where $v_\omega = (v,\omega)/(1,\omega)$.

Unique minimizer $u \in H^1(\Omega)$ for every $f \in L^2(\Omega)$.

Need to solve a saddle point problem.

Constrain $J(u,f)$—use penalization

$$\min_{u\in H^1(\Omega)} J(u,f) + \rho u_\omega^2 \equiv \min_{u\in H^1(\Omega)} J_\rho(u,f).$$

and the associated optimality system: seek $u \in H^1(\Omega)$ such that

$$\mathcal{B}_\rho(u,v) = F(v) \quad \forall v \in H^1(\Omega),$$

where

$$\mathcal{B}_\rho(u,v) \equiv \int_\Omega \nabla u \cdot \nabla v dx + \frac{\rho}{(1,\omega)^2} \int_\Omega u\omega dx \int_\Omega v\omega dx.$$

Unique minimizer $u \in H^1(\Omega)$ for every $f \in L^2(\Omega)$.

Remarks

Lagrangian and penalty methods can be derived from each other.

For example, the Lagrange multiplier can be eliminated by perturbing the constraint by $-\rho^{-1}(\sigma, \tau)$ and inserting into the primal equation thus eliminating the Lagrange multiplier.

Can also use a mixed method so that the natural condition becomes an essential condition. We'll not discuss this further.

No longer consider the Lagrange formulation because the resulting linear system is indefinite (saddle point problem).

Examples

1. If $\omega = 1$ then $H^1_\omega(\Omega) = H^1(\Omega) \cap L^2_0(\Omega)$. This space has been used as a setting for the Neumann problem in Brenner & Scott.

2. Recall that in one-dimension $H^1(\Omega) \subset C^0(\Omega)$ and $\delta(x_*) \in H^{-1}(\Omega)$. Then, $(u, \delta(x_*)) = u(x_*)$ and

$$H^1_\omega(\Omega) = \{u \in H^1(\Omega) \,|\, u(x_*) = 0\}.$$

This choice will give rise to a finite element method in which a solution value is specified at a given triangulation node.

Theorem

For a given $f \in L^2(\Omega)$ let u^R and u^P denote solutions of the reduced and penalized problems, respectively. Then

$$u^P_\omega = \frac{1}{\rho}(f, 1)$$

If u^R and u^P also belong to $H^2(\Omega)$, both functions solve the Neumann problem

$$-\triangle u = f - \omega \frac{(f,1)}{(\omega,1)} \quad \text{in } \Omega \quad \text{and} \quad \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on } \Gamma$$

If $f \in L^2_0(\Omega)$ then $u^P = u^R$.

FE approximation

Let P^k denote the Lagrangian space of continuous, piecewise polynomial functions with respect to a triangulation;
$P^k_\omega \equiv P^k \cap H^1_\omega(\Omega)$

$$\min_{u^h \in P^k/\mathbf{R}} J(u^h, f) \equiv \min_{\mathbf{u} \in \mathbf{R}^N/\mathbf{c}} \frac{1}{2}\mathbf{u}^T \mathbf{A}\mathbf{u} - \mathbf{u}^T \mathbf{f}$$

$$\min_{u^h \in P^k} J_\rho(u^h, f) \equiv \min_{\mathbf{u} \in \mathbf{R}^N} \frac{1}{2}\mathbf{u}^T \mathbf{A}\mathbf{u} - \mathbf{u}^T \mathbf{f} + \rho \frac{(\mathbf{u}^T \mathbf{w})^2}{(\mathbf{c}^T \mathbf{w})^2}.$$

$$\min_{u^h \in P^k_\omega} J(u^h, f) \equiv \min_{\mathbf{u} \in \mathbf{R}^{N-1}} \frac{1}{2}\mathbf{u}^T \mathbf{A}_\omega \mathbf{u} - \mathbf{u}^T \mathbf{f}_\omega,$$

Acronyms

SFEM Singular **A**

FFEM Set ω equal to a point measure in P_ω^k

RFEM Set ω equal to one in P_ω^k

PFEM Penalized formulation.

SFEM

Need to solve the singular set of equations

$$\mathbf{A}\mathbf{u} = \mathbf{f}.$$

Need $\mathbf{f}^T\mathbf{c} = \epsilon_M \|\mathbf{A}\|$. This can be done via the projection

$$(\mathbf{I} - \frac{\mathbf{z}\mathbf{c}^T}{\mathbf{z}^T\mathbf{c}})\mathbf{f}$$

Also possible to recast $\mathbf{A}\mathbf{u} = \mathbf{f}$ as a least squares problem with linear equality constraint:

$$\min_{\mathbf{B}\mathbf{u}=0} \|\mathbf{A}\mathbf{u} - \mathbf{f}\|_2.$$

There are several choices for $\mathbf{B}$ including $\mathbf{c}^T$, $\mathbf{w}^T$ and $\mathbf{e}_\ell^T$. Normal equations or a QR factorization are needed for a solution.

FE discretization of the PFEM

Given a nodal basis $\{\phi_j^h\}_{j=1}^N$ a linear system of algebraic equations whose matrix $\mathbf{A}_\rho$ has entries given by

$$\int_\Omega \nabla\phi_i^h \cdot \nabla\phi_j^h + \frac{\rho}{(1,\omega)^2}\int_\Omega \phi_i^h\omega \int_\Omega \phi_j^h\omega$$

results. Note that

$$\mathbf{A}_\rho = \mathbf{A} + \rho/(1,\omega)^2\mathbf{w}\mathbf{w}^T$$

is SPD for a conforming FEM.

Implementation of PFEM

Given a vector $\mathbf{x}$, then

$$\mathbf{A}_\rho \mathbf{x} = \mathbf{A}\mathbf{x} + \frac{\rho}{(1,\omega)^2}\mathbf{w}\mathbf{w}^T\mathbf{x} = \mathbf{A}\mathbf{x} + \frac{\rho}{(1,\omega)^2}(\mathbf{w}^T\mathbf{x})\mathbf{w}.$$

$\mathbf{A}\mathbf{x}$ is easily computed by

1. forming the vector $\mathbf{w} = \mathbf{A}\mathbf{x}$;
2. computing the scalar $\mu = \rho/(1,\omega)^2(\mathbf{w}^T\mathbf{x})$;
3. updating $\mathbf{w} + \mu\mathbf{w}$.

Matrix interpretation

Theorem Suppose that $\mathbf{A} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^T$ is an eigen-decomposition where $\mathbf{Q}\mathbf{e}_1 = \mathbf{c}$ and $\mathbf{A}\mathbf{c} = \mathbf{0}$. If

$$\mathbf{w} = \|\mathbf{w}\| \cos\phi \mathbf{c} + \mathbf{r},$$

where $\mathbf{r}^T\mathbf{c} = 0$ and ϕ measures the positive angle between $\mathbf{c}$ and $\mathbf{w}$, then

$$\|\mathbf{A}_\rho - \mathbf{Q}(\boldsymbol{\Lambda} + \rho\|\mathbf{w}\|^2 \cos^2\phi \mathbf{e}_1\mathbf{e}_1^T)\mathbf{Q}^T\| \leq \rho\|\mathbf{w}\|^2(\sin 2\phi + \sin^2\phi).$$

Set ρ to at least the smallest non-zero eigenvalue of $\mathbf{A}$ but no larger than $\|\mathbf{A}\|$.

Using $H^1_\omega(\Omega)$—FFEM and RFEM

We construct a nodal basis for P_k^ω so that the ω-weighted mean condition

$$\sum_{i=1}^{N} \alpha_i(\phi_i^h, \omega) = 0$$

Note that simply subtracting the mean value of ϕ_i^h does not work because the gradient annihilates constants.

Solving this equation for the ℓ-th term gives rise to the set of functions

$$\psi_{i,\ell}^h = \phi_i^h - \phi_\ell^h \frac{(\phi_i^h, \omega)}{(\phi_\ell^h, \omega)} \quad i = 1, \ldots, N; \quad i \neq \ell$$

The stiffness matrix $\mathbf{A}_\omega$

If $\mathbf{P}_\ell = \left(\mathbf{I} - \frac{1}{\mathbf{e}_\ell^T \mathbf{w}} \mathbf{e}_\ell \mathbf{w}^T\right) \mathbf{I}_\ell$ then

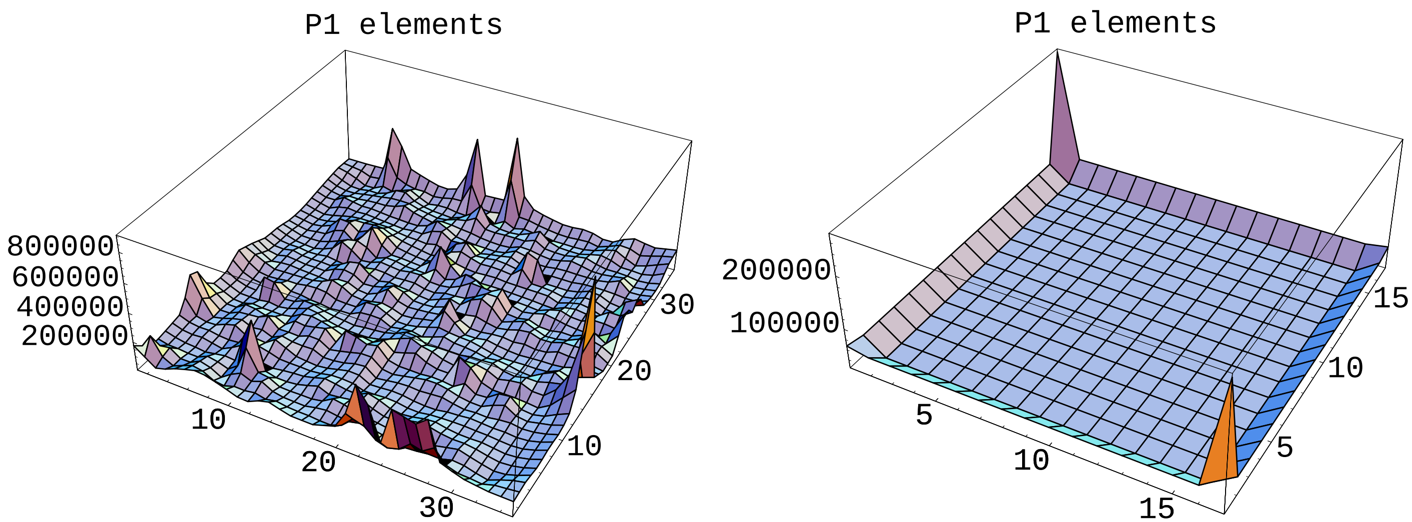
$$\mathbf{A}_\omega = \mathbf{P}_\ell^T \mathbf{A} \mathbf{P}_\ell$$

is a matrix of order $N - 1$. Note that $\mathbf{I} - \frac{1}{\mathbf{e}_\ell^T \mathbf{w}} \mathbf{e}_\ell \mathbf{w}^T$ is a projection whose Range is orthogonal to the Span($\mathbf{w}$). Postmultiplication by $\mathbf{I}_\ell$ restricts the subspace to be orthogonal to Span($\mathbf{e}_\ell$).

If $\omega = 1$ (RFEM) then $\mathbf{w} = \mathbf{z}$ and $\mathbf{I} - \frac{1}{\mathbf{e}_\ell^T \mathbf{z}} \mathbf{e}_\ell \mathbf{z}^T$ is not an orthogonal projection.

If ω is a point measure (FFEM), then $\mathbf{I} - \mathbf{e}_\ell \mathbf{e}_\ell^T$ is an orthogonal projection.

RFEM in 2D



Condition number as a function of the basis function ϕ_ℓ^h for an unstructured and structured mesh for the unit square using P1 elements.

Eigenvalues of resulting matrices

Computed the four largest and four smallest eigenvalues of $\mathbf{A}$, $\mathbf{A}_\rho$, $\mathbf{A}_{\omega=1}$ and $\mathbf{A}_{\omega=\delta}$ on the unit square using P1 on a structured mesh of triangles.

N	$\lambda_{\min}(\mathbf{A}_\rho)$	$\lambda_{\min}(\mathbf{A}_{\omega=\delta})$	$\lambda_{\max}(\mathbf{A}_{\omega=1})$
256	3.59D-02	7.78D-03	8.46D+02
1024	9.32D-03	1.61D-03	3.71D+03
4096	2.37D-03	3.41D-04	1.56D+04
16384	5.97D-04	7.39D-05	6.41D+04
65536	1.50D-04	1.63D-05	2.59D+05
262144	3.75D-05	3.65D-06	1.04D+06

Summary of computing eigenvalues

The smallest non-zero eigenvalue of $\mathbf{A}$, $\mathbf{A}_\rho$, $\mathbf{A}_{\omega=1}$ are all equal and converge at a quadratic rate. The smallest eigenvalue of $\mathbf{A}_{\omega=\delta}$ converges at a better than quadratic rate—$\log_2(4.5)$.

The largest eigenvalues of $\mathbf{A}$, $\mathbf{A}_\rho$, and $\mathbf{A}_{\omega=\delta}$ converge to the value 8. However the largest eigenvalue $\mathbf{A}_{\omega=1}$ is roughly the order of the reciprocal of the smallest eigenvalue.

PFEM produces the matrices with the smallest condition number–equivalent to the non-zero condition number of $\mathbf{A}$.

Summary

- Introduced an easy to implement penalized formulation for the Neumann problem.
- Provided an unifying framework for the Neumann problem.
- Experimental results.

Tech report nearly available.

We next want to consider Stokes problem.