RICE A Quadratically Constrained Eigenvalue Minimization Problem Arising from PDE of Monge-Ampère Type

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True Title

Fooling Around and Having Fun with Numerical Linear Algebra

Outline

- Motivation Monge-Ampère Equations
- \blacktriangleright FEM Discretization $~\rightarrow~$ Quadratic Min Problem
- Formulation of General Eigenvalue Constrained Quadratic Min Problem

- ► The General Secular Equation and Its Solution
- A Surprising Result Finite $\mathcal{O}(n^3)$ Complexity
- Some Numerical Results

Monge-Ampère Equations

Applications and Research Reference: BIRS Workshop (2003) on Monge-Ampère Equation http://www.birs.ca/workshops/2003/03w5067/report03w5067.pdf

Monge-Ampère Equations arise in

Riemannian Geometry Conformal Geometry CR Geometry

Example : Problem of prescribed Gauss curvature

A real-valued function K is specified on a domain Ω in \mathbb{R}^n Prescribed Gauss curvature seeks to identify a hypersurface of \mathbb{R}^{n+1} as a graph z = u(x) over $x \in \Omega$ so that the Gauss curvature is given by K(x) at every x.

Monge-Ampère Problem

Fully-Nonlinear 3D BVP (of Dirichlet type);

Find ψ such that

$$\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 = f \text{ in } \Omega, \ \psi = g \text{ on } \partial\Omega,$$

where

- Function ψ unknown; Ω is a bounded domain of \mathbb{R}^3
- ► { $\lambda_1, \lambda_2, \lambda_3$ } is the spectrum of Hessian $\mathbf{D}^2 \psi = \left(\frac{\partial^2 \psi}{\partial x_i, \partial x_j}\right)_{1 \le i,j \le 3}$
- f and g are two given functions with f > 0.

Dirichlet Problem for σ_2 -Operator

Rewrite as

$$|\nabla^2 \psi|^2 - \mathbf{D}^2 \psi : \mathbf{D}^2 \psi = 2f \text{ in } \Omega,$$

where

$$\mathbf{A} : \mathbf{B} = \sum_{1 \leq i,j \leq d} a_{ij} b_{ij} = \operatorname{trace} \mathbf{A}^T \mathbf{B}$$
 (Frobenius)

Fully nonlinear PDE becomes

$$[\operatorname{trace}\{\mathbf{D}^2\psi\}]^2 - \operatorname{trace}\{(\mathbf{D}^2\psi)^2\} = 2f.$$

Solving when σ_2 -Operator is Elliptic

Least Squares Approach:

 σ_2 -operator linearized in neighborhood of elliptic ψ gives:

$$\phi \to 2[\nabla^2 \psi \nabla^2 \phi - \mathbf{D}^2 \psi : \mathbf{D}^2 \phi].$$

Coefficient Matrix

$$2[\nabla^2\psi\mathbf{I}-\mathbf{D}^2\psi],$$

The σ_2 -operator *elliptic* in nbhd of $\psi \iff$ if Matrix is s.p.d. (or n.p.d) , i.,e.,

$$(\lambda_1+\lambda_2)(\lambda_2+\lambda_3)>0, (\lambda_1+\lambda_3)(\lambda_1+\lambda_2)>0.$$

 $\lambda_1+\lambda_2>0,\ \ \lambda_2+\lambda_3>0,\ \ \lambda_1+\lambda_3>0.$

PDE Least Squares Problem

Find
$$(\psi, \mathbf{P}) \in \mathcal{V}_g \times \mathbf{Q}_f$$
 such that $J(\psi, \mathbf{P}) \leq J(\phi, \mathbf{G}), \quad \forall (\phi, \mathbf{G}) \in \mathcal{V}_g \times \mathbf{Q}_f$, where

$$J(\phi, \mathbf{G}) = \frac{1}{2} \int_{\Omega} (\mathbf{D}^2 \phi - \mathbf{G}) : (\mathbf{D}^2 \phi - \mathbf{G}) \mathrm{d}x,$$

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with $dx = dx_1 dx_2 dx_3$.

Block Relaxation Algorithm

Given $\psi^0 \in \mathcal{V}_g$; for $k = 0, 1, 2, \dots$

- $\mathbf{P}^{k+1} = \operatorname{argmin}_{\mathbf{G} \in \mathbf{Q}_f} J(\psi^k, \mathbf{G});$
- $\psi^{k+1/2} = \operatorname{argmin}_{\phi \in \mathcal{V}_g} J(\phi, \mathbf{P}^{k+1})$;
- $\psi^{k+1} = \psi^k + \omega(\psi^{k+1/2} \psi^k);$

Relaxation Parameter: $0 < \omega < 2$ Initialization

$$\nabla^2 \psi^0 = \sqrt{3f}$$
 in Ω , ψ^0 on $\partial \Omega$.

Note that ψ^0 has the $\mathcal{H}^2(\Omega)$ -regularity if $\partial\Omega$ is 'sufficiently' smooth and/or Ω is convex.

Must solve following at the vertices of a finite element mesh:

Find
$$\mathbf{P}^{k+1}(x) \in \mathbf{E}(x)$$
, $\mathbf{j}_k(\mathbf{P}^{k+1}(x);x) \leq \mathbf{j}_k(\mathbf{A};x)$, $\forall \mathbf{A} \in \mathbf{E}(x)$,

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where
$$\mathbf{E}(x) = \{ \mathbf{A} | \mathbf{A} \in \mathbb{R}^{3 \times 3}, \ \mathbf{A} = \mathbf{A}^{T}, \\ \lambda_{1}\lambda_{2} + \lambda_{2}\lambda_{3} + \lambda_{3}\lambda_{1} = f(x), \\ \lambda_{1} + \lambda_{3} > 0, \lambda_{2} + \lambda_{3} > 0, \lambda_{3} + \lambda_{1} > 0 \}$$

and

$$\mathbf{j}_k(\mathbf{A};x) = \frac{1}{2}\mathbf{A}: \mathbf{A} - \mathbf{D}^2\psi^k(x): \mathbf{A},$$

with $\{\lambda_1, \lambda_2, \lambda_3\}$ being the spectrum of **A**.

Must solve following at the vertices of a finite element mesh: Can normalize using division by f(x).

$$\min_{\mathbf{A}\in\mathbf{E}_1}\operatorname{trace}[\mathbf{A}^{\mathcal{T}}(\mathbf{A}-2\mathbf{B})] = \min_{\mathbf{A}\in\mathbf{E}_1}\operatorname{trace}[\mathbf{A}^2-2\mathbf{A}\mathbf{B})]$$

where

$$\begin{split} \mathbf{E}_1 &= \{ \mathbf{A} | \mathbf{A} \in \mathbb{R}^{3 \times 3}, \mathbf{A} = \mathbf{A}^T, \\ &\lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1 = 1 , \\ &\lambda_1 + \lambda_3 > 0, \lambda_2 + \lambda_3 > 0, \lambda_3 + \lambda_1 > 0 \} \end{split}$$

(with $\{\lambda_1, \lambda_2, \lambda_3\}$ being the spectrum of **A**)

Minimization Problem - Matrix Form

Problem Qmin

min trace{
$$AA - 2BA$$
}
s.t.
 $\ell^T M \ell = 2$
 $M \ell \ge 0$

where

$$\mathbf{M} = \mathbf{e}\mathbf{e}^{\mathsf{T}} - \mathbf{I}, \text{ with } \mathbf{e}^{\mathsf{T}} = (1, 1, \dots, 1),$$

and

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Diagonalized Problem

Note that Problem Qmin is equivalent to

min trace{
$$\Lambda\Lambda - 2\hat{\mathbf{B}}\Lambda$$
} = min $\ell^{T}\ell - 2\mathbf{b}^{T}\ell$
s.t.
 $\ell^{T}\mathbf{M}\ell = 2$
 $\mathbf{M}\ell \ge \mathbf{0}$

where

$$\hat{\mathbf{B}} = \mathbf{Q}^T \mathbf{B} \mathbf{Q}$$
 and $\mathbf{b} = \operatorname{diag}(\hat{\mathbf{B}})$.

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Constraints for n = 3

Constraints:

$$\ell^{\mathsf{T}} \mathsf{M} \ell = 2$$
$$\mathsf{M} \ell \ge \mathbf{0}$$

$$\mathbf{M} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$
$$\ell^{T} \mathbf{M} \ell = 2 \quad \Rightarrow \quad \lambda_{1} \lambda_{2} + \lambda_{2} \lambda_{3} + \lambda_{3} \lambda_{1} = 1$$
$$\mathbf{M} \ell \ge \mathbf{0} \quad \Rightarrow \quad \begin{array}{l} \lambda_{2} + \lambda_{3} \ge 0 \\ \lambda_{1} + \lambda_{3} \ge 0 \\ \lambda_{1} + \lambda_{2} \ge 0 \end{array}$$

No Active Equality Consraint

Lemma

If the vector $\ell \in \mathbb{R}^n$ is finite and feasible, then none of the inequality constraints can be active. In other words,

$$\ell^{\mathsf{T}} \mathsf{M} \ell = 2 \quad \Rightarrow \quad \mathbf{e}_j^{\mathsf{T}} \mathsf{M} \ell > 0, \text{ for } j = 1, 2, \dots, n.$$

Proof Outline

Proof Outline: If $\lambda_2 + \lambda_3 + \dots + \lambda_n = 0$, Equality constraint $\ell^T \mathbf{M} \ell = 2$ provides $\lambda_1(\lambda_2 + \lambda_3 + \dots + \lambda_n) = 2 - \lambda_2(\lambda_3 + \lambda_4 + \dots + \lambda_n) - \lambda_3(\lambda_2 + \lambda_4 + \lambda_5 + \dots + \lambda_n)$ $\dots - \lambda_n(\lambda_2 + \lambda_3 + \dots + \lambda_{n-1}).$

It follows that

$$0 = \lambda_1(\lambda_2 + \lambda_3 + \dots + \lambda_n) = 2 + \lambda_2^2 + \lambda_3^2 \dots + \lambda_n^2 \ge 2$$

which is a contradiction.

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Lagrangian for Equality Constraint:

Lagrangian:

$$\mathcal{L}(\ell,\mu) = \ell^{\mathsf{T}}\ell - 2\mathbf{b}^{\mathsf{T}}\ell + \mu(\ell^{\mathsf{T}}\mathsf{M}\ell - 2).$$

Setting the grad of Lagrangian to zero gives:

 $(\mathbf{I} + \mu \mathbf{M})\ell = \mathbf{b}.$

If $1/\mu$ is not an eigenvalue of $-\mathbf{M}$ then the equality constraint becomes

$$\mathbf{b}^T (\mathbf{I} + \mu \mathbf{M})^{-1} \mathbf{M} (\mathbf{I} + \mu \mathbf{M})^{-1} \mathbf{b} = 2$$

Eigensystem of M

Helps to know eigensystem of $\mathbf{M} = \mathbf{e}\mathbf{e}^T - \mathbf{I}$: Eigenvalues

$$\omega_1 = n - 1$$
 and $\omega_2 = -1$, multiplicity $n - 1$

Eigenvector for ω_1 is **e**

Eigenvector Matrix

$$\mathbf{U} \equiv (\mathbf{I} - 2\mathbf{w}\mathbf{w}^T), \text{ with } \mathbf{w} = (\mathbf{e} + \sqrt{n}\mathbf{e}_1)/\|\mathbf{e} + \sqrt{n}\mathbf{e}_1\|,$$

Easily checked:

$$\mathbf{U}^{\mathsf{T}}\mathbf{M}\mathbf{U} = \mathbf{U}\mathbf{M}\mathbf{U}^{\mathsf{T}} = \mathbf{U}\mathbf{e}\mathbf{e}^{\mathsf{T}}\mathbf{U}^{\mathsf{T}} - \mathbf{I} = n\mathbf{e}_{1}\mathbf{e}_{1}^{\mathsf{T}} - \mathbf{I}.$$

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The Secular Equation

$$\frac{\beta_1^2 \omega_1}{(1+\mu\omega_1)^2} = 2 + \frac{\beta_2^2}{(1-\mu)^2}$$

where
$$(\beta_1, \mathbf{b}_2^T) = \mathbf{b}^T \mathbf{U}$$
 and $\beta_2^2 = \mathbf{b}_2^T \mathbf{b}_2$.

Note:

$$\beta_1 = \mathbf{e}^t \mathbf{b} / \sqrt{n}$$
 is invariant: $\mathbf{e}^T \mathbf{b} = \text{trace} \{ \mathbf{B} \}$

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Reciprocal Square Root Equation

Better Equivalent Form

$$\pm (1+\mu\omega_1) = \frac{(1-\mu)|\beta_1|\sqrt{\omega_1}}{\sqrt{2(1-\mu)^2+\beta_2^2}}.$$

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Algorithm: Newton's Method converges in 3 steps

Graphs of Secular Equations

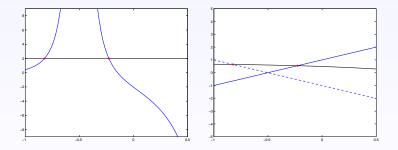


Figure: The Secular Equation for Multiplier μ (left) and the Reciprocal Square Root Secular Equation (right)

Choice of Root

Corresponding to Root μ , the vector ℓ is:

$$\ell = \mathbf{U}\mathbf{c} \text{ with } \mathbf{c}^{T} = (\frac{\beta_{1}}{(1+\mu\omega_{1})}, \frac{1}{1-\mu}\mathbf{b}_{2}^{T}).$$

Pick Solution with Positive Components:

$$0 < \mathbf{M}\ell = (\mathbf{e}\mathbf{e}^{\mathsf{T}} - \mathbf{I})\ell = \mathbf{e}(\mathbf{e}^{\mathsf{T}}\ell) - \ell$$

Suggested Alternating Min Algorithm

- **b** = diag(**B**); $\mathbf{Q} = \mathbf{I}$;
- while ('not converged'),
 - $\min_{\ell} \ell^{\mathsf{T}} \ell 2 \mathbf{b}^{\mathsf{T}} \ell$ s.t. constraints ;
 - ▶ $\min_{\mathbf{A}=\mathbf{W}\operatorname{diag}(\ell)\mathbf{W}^{\intercal}}$ trace{ $\mathbf{A}\mathbf{A} 2\mathbf{B}\mathbf{A}$ } s.t. constraints;
 - $\mathbf{b} = \operatorname{diag}(\mathbf{W}^T \mathbf{B} \mathbf{W});$

ALWAYS CONVERGED IN 2 STEPS !

Surprise Result

Suppose $\mathbf{B} = \mathbf{Q} \operatorname{diag}(\mathbf{b}) \mathbf{Q}^T$ If μ and corresponding $\ell = (\mathbf{I} + \mu \mathbf{M})^{-1} \mathbf{b}$ solve

 $\min \ell^{\mathsf{T}} \ell - 2 \mathbf{b}^{\mathsf{T}} \ell$ s.t.constraints

We have

Lemma

Let $\Lambda = \operatorname{diag}(\ell)$. Then $\mathbf{A}_{\mathbf{Q}} = \mathbf{Q} \Lambda \mathbf{Q}^{\mathsf{T}}$ solves

min trace{AA - 2BA} s.t.constraints

over all $\mathbf{A} = \mathbf{W} \wedge \mathbf{W}^T$ with $\mathbf{W}^T \mathbf{W} = \mathbf{I}$.

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Proof Outline

 $\begin{array}{l} \mbox{If } \hat{\boldsymbol{b}} = \boldsymbol{Q}^{\mathcal{T}}\boldsymbol{B}\boldsymbol{Q} \mbox{ then } \boldsymbol{W}^{\mathcal{T}}\boldsymbol{B}\boldsymbol{W} = \hat{\boldsymbol{Q}}^{\mathcal{T}}\hat{\boldsymbol{B}}\hat{\boldsymbol{Q}}. \\ \mbox{Let } \hat{\boldsymbol{b}} = \mbox{diag}(\hat{\boldsymbol{Q}}^{\mathcal{T}}\hat{\boldsymbol{B}}\hat{\boldsymbol{Q}}). \end{array}$

$$\hat{\beta}_j \equiv \hat{\mathbf{b}}(j) = \mathbf{q}_j^T \hat{\mathbf{B}} \mathbf{q}_j = \sum_{i=1}^n \beta_i \gamma_{ij}^2,$$

where $\beta_j = \mathbf{b}(j)$, $\hat{\mathbf{Q}} = (\gamma_{ij})$, $\mathbf{q}_j = \hat{\mathbf{Q}}\mathbf{e}_j$ Hence,

$$\hat{\mathbf{b}} = \mathbf{G}^T \mathbf{b}$$
, where the i, j – th entry of \mathbf{G} is γ_{ij}^2 .

We show

$$\ell^{\mathsf{T}}\ell - 2\mathbf{b}^{\mathsf{T}}\ell \leq \ell^{\mathsf{T}}\ell - 2\hat{\mathbf{b}}^{\mathsf{T}}\ell.$$

Since ℓ is fixed, sufficient to show

$$\ell^{\mathsf{T}}\hat{\mathbf{b}} - \ell^{\mathsf{T}}\mathbf{b} = \ell^{\mathsf{T}}(\hat{\mathbf{b}} - \mathbf{b}) \leq 0.$$

Proof Outline Contd.

 $\mathbf{G}\mathbf{e} = \mathbf{G}^T \mathbf{e} = \mathbf{e}$ implies

$$\hat{\mathbf{b}} - \mathbf{b} = (1 - \mu)(\mathbf{G}^{T} - \mathbf{I})\ell,$$

Therefore,

$$\ell^{\mathsf{T}}(\hat{\mathbf{b}} - \mathbf{b}) = (1 - \mu)\frac{1}{2}(\ell^{\mathsf{T}}(\mathbf{G}^{\mathsf{T}} - \mathbf{I})\ell + \ell^{\mathsf{T}}(\mathbf{G} - \mathbf{I})\ell)$$

It follows that

$$\ell^{\mathcal{T}}(\hat{\mathbf{b}}-\mathbf{b}) = -(1-\mu)\sum_{i\neq j}\gamma_{ij}^2(\lambda_j-\lambda_i)^2 \leq 0,$$

since $(1 - \mu) > 0$.

Converse

Lemma

Suppose $\mathbf{A} = \mathbf{W} \wedge \mathbf{W}^T$ solves Problem Qmin. Then there is an orthogonal $\hat{\mathbf{Q}}$ such that $\mathbf{Q} = \mathbf{W} \hat{\mathbf{Q}}$ diagonalizes \mathbf{B} and $\mathbf{A} = \mathbf{Q} \wedge \mathbf{Q}^T$. In other words, if \mathbf{A} solves Problem Qmin, then $\mathbf{A} = \mathbf{Q} \wedge \mathbf{Q}^T$ with $\mathbf{Q}^T \mathbf{B} \mathbf{Q}$ diagonal.

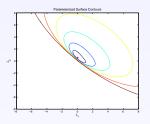
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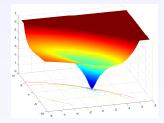
Final Algorithm

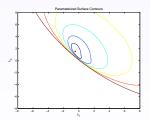
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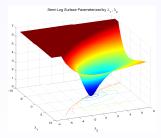
- ▶ [Q, L] = eig(B); b = diag(L)
- $\min_{\ell} \ell^{T} \ell 2 \mathbf{b}^{T} \ell$ subject to constraints
- $\mathbf{A} = \mathbf{Q} \operatorname{diag}(\ell) \mathbf{Q}^{\mathsf{T}};$

Works for ANY n









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Summary

- Monge-Ampère important to Diff Geometry
- Glowinski Dean algorithm requires MANY eigenvalue constrained min problems
- We provided a very simple and efficient method with some surprising properties.

Report:

A Quadratically Constrained Minimization Problem Arising from PDE of Monge-Ampère Type

CAAM TR08-02, DCS and R. Glowinski

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