



Term Project Presentation

A Comparison of Algorithms Related to Trace Minimization to Compute a Small Number of Eigenvalues of a Real Symmetric Matrix

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Outline

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- Trace Theorem and a Proof
- Trace Minimization Method
- Trace Minimization Method as a Quasi-Newton Method
- Jacobi-Davidson / Newton with Subspace Acceleration
- Davidson-Type Trace Minimization Method
- Conclusion

Tasks

1. Detailed formulation of the problem, including proof of the trace theorem
2. Formulation of the trace minimization method as a Newton method
3. Derive TraceMin and Jacobi-Davidson algorithms and compare them

Problem Description

Compute a few of the smallest eigenvalues or eigenvectors of the large, sparse, generalized eigenvalue problem

$$Ax = \lambda Bx \quad , \quad (1)$$

where $x \in \mathbb{R}^n$, $\lambda \in \mathbb{R}$ and A, B are $n \times n$ symmetric matrices, with B being positive-definite.

- The matrix $A - \lambda B$ is called a matrix *pencil*

Theorem 1 [5]

Let A and B be symmetric $n \times n$ matrices. If B is positive-definite then there is an $n \times n$ matrix Z for which

$$Z^T B Z = I_n \quad \text{and} \quad Z^T A Z = \Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n), \quad (2)$$

where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the pencil (A, B) from problem (1) and the columns of Z are their associated eigenvectors. Furthermore, if A is positive-definite, then all of the eigenvalues λ_i are positive.

Theorem 2: The Trace Theorem [8]

Let A and B be given as in Theorem 1 and \mathcal{Y}^* be the set of all $n \times p$ matrices Y for which $Y^T B Y = I_p$. Then

$$\min_{Y \in \mathcal{Y}^*} \operatorname{tr}(Y^T A Y) = \sum_{i=1}^p \lambda_i. \quad (3)$$

In other words,

$$\min_{Y \in \mathcal{Y}^*} \operatorname{tr}(Y^T A Y) = \operatorname{tr}(X^T A X) \quad (4)$$

with

$$X^T B X = I_p \quad \text{and} \quad X^T A X = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_p), \quad (5)$$

where X corresponds to the first p columns of the matrix Z of Theorem 1.

Proof of the Trace Theorem (1/6)

Theorem 3 (*Poincaré Separation Theorem* [4, 6])

Let A be a real symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$, and let G be a semi-unitary $n \times k$ matrix ($1 \leq k \leq n$), so that $G^T G = I_k$. Then the eigenvalues $\mu_1 \leq \mu_2 \leq \dots \leq \mu_k$ of $G^T A G$ satisfy

$$\lambda_i \leq \mu_i \leq \lambda_{n-k+i} \quad (i = 1, 2, \dots, k). \quad (6)$$

Proof of the Trace Theorem (2/6)

Let A and B given as in Theorem 1, i.e., $Z \in \mathbb{R}^{n \times n}$ is the matrix for which $Z^T B Z = I_n$ and $Z^T A Z = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the pencil (A, B) .

Let $Y \in \mathcal{Y}^*$ and set $Y = ZG$ for some $G \in \mathbb{R}^{n \times p}$. $Y^T B Y = I_p \implies G$ is unitary and

$$Y^T A Y = G^T \Lambda G. \quad (7)$$

Proof of the Trace Theorem (3/6)

From Theorem 3, for the eigenvalues μ_i of $G^T \Lambda G$ it follows that $\lambda_i \leq \mu_i$ for $i = 1, \dots, p$ and thus

$$\sum_{i=1}^p \lambda_i \leq \sum_{i=1}^p \mu_i. \quad (8)$$

Proof of the Trace Theorem (4/6)

$G^T \Lambda G$ is symmetric \implies there exists a spectral decomposition [10, Theorem 4.33] of the form

$$Q^T (G^T \Lambda G) Q = \text{diag}(\mu_1, \mu_2, \dots, \mu_p), \quad (9)$$

where Q is a unitary matrix with columns q_i being the eigenvectors of $G^T \Lambda G$.

Proof of the Trace Theorem (5/6)

Consider the trace of the spectral decomposition in Eq. (9):

$$\operatorname{tr}(\mathbf{Q}^T (\mathbf{G}^T \mathbf{\Lambda} \mathbf{G}) \mathbf{Q}) = \operatorname{tr}(\mathbf{Q} \mathbf{Q}^T (\mathbf{G}^T \mathbf{\Lambda} \mathbf{G})) = \operatorname{tr}(\mathbf{G}^T \mathbf{\Lambda} \mathbf{G}) = \sum_{i=1}^p \mu_i. \quad (10)$$

From Eqs. (7), (8) and (10) it follows that

$$\sum_{i=1}^p \lambda_i \leq \operatorname{tr}(\mathbf{Y}^T \mathbf{A} \mathbf{Y}). \quad (11)$$

Proof of the Trace Theorem (6/6)

By the the spectral decomposition [10, Theorem 4.33] equality holds if $\mathbf{Y} = \mathbf{Z}_p = [z_1, \dots, z_p]$, where the columns z_i are the eigenvectors of the pencil (\mathbf{A}, \mathbf{B}) .

\mathbf{Z}_p hence diagonalizes the matrix \mathbf{A} from problem (1) and thus leads to

$$\mathbf{Z}_p^T \mathbf{A} \mathbf{Z}_p = \text{diag}(\lambda_1, \dots, \lambda_p).$$



The Trace Minimization Method [8, 7]

Trace Minimization (TRACEMIN): Use trace theorem (Theorem 2) and treat problem (1) as the quadratic minimization problem

$$\begin{aligned} & \text{minimize} && \text{tr}(\mathbf{Y}^T \mathbf{A} \mathbf{Y}) \\ & \text{subject to} && \mathbf{Y}^T \mathbf{B} \mathbf{Y} = \mathbf{I}_p. \end{aligned} \tag{12}$$

The Trace Minimization Method [8, 7]

Idea is to compute a correction term Δ_k that is chosen as to

$$\begin{aligned} & \text{minimize} && \text{tr}((\mathbf{Y}_k - \Delta_k)^T \mathbf{A}(\mathbf{Y}_k - \Delta_k)) \\ & \text{subject to} && \mathbf{Y}_k^T \mathbf{B} \Delta_k = \mathbf{0}. \end{aligned} \tag{13}$$

The Trace Minimization Method [8, 7]

Next iterate \mathbf{Y}_{k+1} is formed by B -orthonormalizing $\mathbf{Y}_k - \mathbf{\Delta}_k$. By also enforcing $\mathbf{Y}_k^T \mathbf{B} \mathbf{\Delta}_k = \mathbf{0}$ in the minimization problem (13) it guarantees that

$$\operatorname{tr}(\mathbf{Y}_{k+1}^T \mathbf{A} \mathbf{Y}_{k+1}) \leq \operatorname{tr}((\mathbf{Y}_k - \mathbf{\Delta}_k)^T \mathbf{A} (\mathbf{Y}_k - \mathbf{\Delta}_k)) \leq \operatorname{tr}(\mathbf{Y}_k^T \mathbf{A} \mathbf{Y}_k). \quad (14)$$

The Trace Minimization Method [8, 7]

Solution of the minimization problem (13) can be obtained by solving the saddle-point problem

$$\begin{pmatrix} \mathbf{A} & \mathbf{B}\mathbf{Y}_k \\ \mathbf{Y}_k^T \mathbf{B} & 0 \end{pmatrix} \begin{pmatrix} \Delta_k \\ \mathbf{L}_k \end{pmatrix} = \begin{pmatrix} \mathbf{A}\mathbf{Y}_k \\ 0 \end{pmatrix} \quad (15)$$

where \mathbf{L}_k represents the Lagrange multipliers

The Trace Minimization Method [8, 7]

The saddle-point problem is further reduced to the following positive-semidefinite system

$$(PAP)\Delta_k = PAY_k, \quad Y_k^T B \Delta_k = 0 \quad (16)$$

where

$$P = I - BY_k(Y_k^T B^2 Y_k)^{-1} Y_k^T B \quad (17)$$

is the orthogonal projector onto the space B -orthogonal to Y_k , which guarantees that $Y_k^T B \Delta_k = 0$.

The Trace Minimization Method [8, 7]

If the projected system in Eq. (16) is solved exactly at each iteration step, TRACEMIN is mathematically equiv. to inverse iteration.

- Inherits robust global convergence property
- Also inherits linear convergence rate
 - TRACEMIN can be accelerated by using shifting strategies

Trace Minimization Method as a Quasi-Newton Method

Newton's method: Solve

$$F(\mathbf{x}) = \mathbf{0}. \quad (18)$$

Newton step: Use $F(\mathbf{x}) = \text{grad } f(\mathbf{x})$, then:

$$\mathbf{p}_k = -\text{Hess}_f(\mathbf{x}_k)^{-1} \text{grad } f(\mathbf{x}_k). \quad (19)$$

Quasi-Newton step:

$$\mathbf{p}_k = -\mathbf{B}_k^{-1} \text{grad } f(\mathbf{x}_k), \quad (20)$$

with \mathbf{B}_k being an approximation of the true Hessian $\text{Hess}_f(\mathbf{x}_k)$.

Trace Minimization Method as a Quasi-Newton Method

TRACEMIN's objective function is given by

$$f : \mathbb{R}_*^{n \times p} \rightarrow \mathbb{R} : \mathbf{Y} \mapsto \text{tr}((\mathbf{Y}^T \mathbf{B} \mathbf{Y})^{-1} (\mathbf{Y}^T \mathbf{A} \mathbf{Y})), \quad (21)$$

where $\mathbb{R}_*^{n \times p}$ denotes the set of full-rank $n \times p$ matrices.

Trace Minimization Method as a Quasi-Newton Method

A second-order expansion of f around $\Delta_k = \mathbf{0}$ gives:

$$\begin{aligned}
 f(\mathbf{Y}_k + \Delta_k) &= \text{tr}((\mathbf{Y}_k^T \mathbf{B} \mathbf{Y}_k)^{-1} (\mathbf{Y}_k^T \mathbf{A} \mathbf{Y}_k)) \\
 &+ \text{tr}((\mathbf{Y}_k^T \mathbf{B} \mathbf{Y}_k)^{-1} \Delta_k^T \mathbf{2} \mathbf{A} \mathbf{Y}_k) \\
 &+ \frac{1}{2} \text{tr}((\mathbf{Y}_k^T \mathbf{B} \mathbf{Y}_k)^{-1} \Delta_k^T \mathbf{2} (\mathbf{A} \Delta_k \\
 &- \mathbf{B} \Delta_k (\mathbf{Y}_k^T \mathbf{B} \mathbf{Y}_k)^{-1} \mathbf{Y}_k^T \mathbf{A} \mathbf{Y}_k)) + H.O.T.
 \end{aligned} \tag{22}$$

Trace Minimization Method as a Quasi-Newton Method

Introduce $P = I - BY_k(Y_k^T B^2 Y_k)^{-1} Y_k^T B$ as the orthogonal projector onto the space B -orthogonal to Y_k

Further, introduce the inner product [1, 3]

$$\langle Z_1, Z_2 \rangle := \text{tr}((Y_k^T B Y_k)^{-1} Z_1^T Z_2), \quad Z_1, Z_2 \text{ } B\text{-orthogonal to } Y_k. \quad (23)$$

Trace Minimization Method as a Quasi-Newton Method

Now rewrite second-order expansion as

$$f(\mathbf{Y}_k + \Delta_k) = f(\mathbf{Y}_k) + \langle \Delta_k, 2P\mathbf{A}\mathbf{Y} \rangle + \frac{1}{2} \langle \Delta_k, 2P(\mathbf{A}\Delta_k - \mathbf{B}\Delta_k(\mathbf{Y}_k^T \mathbf{B}\mathbf{Y}_k)^{-1} \mathbf{Y}_k^T \mathbf{A}\mathbf{Y}_k) \rangle + H.O.T. \quad (24)$$

Identify $2P\mathbf{A}\mathbf{Y}$ to be the gradient of f at $\Delta_k = \mathbf{0}$ and the operator

$$\text{Hess}_f : \Delta_k \mapsto 2P(\mathbf{A}\Delta_k - \mathbf{B}\Delta_k(\mathbf{Y}_k^T \mathbf{B}\mathbf{Y}_k)^{-1} \mathbf{Y}_k^T \mathbf{A}\mathbf{Y}_k) \quad (25)$$

to be the Hessian of f at $\Delta_k = \mathbf{0}$ [1, 3]

Trace Minimization Method as a Quasi-Newton Method

Newton correction equation now becomes

$$P(A\Delta_k - B\Delta_k(Y_k^T B Y_k)^{-1} Y_k^T A Y_k) = -PAY. \quad (26)$$

Substitute the Hessian of f with the approximate Hessian $2PAP$ and the correction equation becomes

$$(PAP)\Delta_k = -PAY, \quad Y_k^T B \Delta_k = \mathbf{0}, \quad (27)$$

which is the same as Eq. (16) solved in the TRACEMIN method [3, § 4.3.2].

Trace Minimization Method as a Quasi-Newton Method

Important to mention: further calculations needed to capture TRACEMIN's global convergence theory; see [3, § 4.3.2] for further details.

Nonetheless, TRACEMIN can be described as inexact, quasi-Newton method.

- Method yields linear (instead of quadratic) convergence rate due to the usage of approx. Hessian
- Authors of TRACEMIN knew this result due to relationship between TRACEMIN and inverse iteration

Trace Minimization Method as a Quasi-Newton Method

In [1], the authors present a two-phase algorithm using a Riemannian trust-region algorithm:

1. Use basic TRACEMIN far away from solution, i.e. use approximate Hessian
2. When a switching criterion is satisfied (i.e. algorithm is close to solution), continue calculations with exact Hessian

Result: superlinear convergence.

Jacobi-Davidson [9, 2]

The Jacobi-Davidson (JD) method calculates the eigenvectors and eigenvalues of the pencil (A, B) by constructing a correction, for a given eigenvector approximation, in a subspace orthogonal to the given approximation.

Name follows from two basic principles:

1. Jacobi's idea: compute orthogonal corrections
2. Davidson approach: Computation of the correction in a given subspace different from Krylov subspaces

Jacobi-Davidson: Newton with Subspace Acceleration [9, 2]

Derive a Newton update from the generalized Rayleigh quotient

$$\rho(\mathbf{x}) = \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{B} \mathbf{x}}, \quad \forall \mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}. \quad (28)$$

The Newton equation $\text{Hess}_\rho(\mathbf{x}_k) \mathbf{t}_k = -\text{grad } \rho(\mathbf{x}_k)$ becomes

$$\begin{aligned} \left(\mathbf{I} - \frac{2}{\mathbf{x}_k^T \mathbf{B} \mathbf{x}_k} \mathbf{B} \mathbf{x}_k \mathbf{x}_k^T \right) (\mathbf{A} - \rho(\mathbf{x}_k) \mathbf{B}) \left(\mathbf{I} - \frac{2}{\mathbf{x}_k^T \mathbf{B} \mathbf{x}_k} \mathbf{x}_k \mathbf{x}_k^T \mathbf{B} \right) \\ = -(\mathbf{A} \mathbf{x}_k - \mathbf{B} \mathbf{x}_k \rho(\mathbf{x}_k)). \end{aligned} \quad (29)$$

Problem: Hessian is always singular when \mathbf{x} is an eigenvector, because then $\text{Hess}_\rho(\mathbf{x}) \mathbf{x} = -F(\mathbf{x}) = \mathbf{0}$ [2]

Jacobi-Davidson: Newton with Subspace Acceleration [9, 2]

Apply the Newton method instead to

$$F(\mathbf{x}, \lambda) := \begin{pmatrix} (\mathbf{A} - \lambda \mathbf{B})\mathbf{x} \\ \mathbf{x}^T \mathbf{B} \mathbf{x} - 1 \end{pmatrix}. \quad (30)$$

New Newton step:

$$\begin{pmatrix} \mathbf{A} - \lambda_k \mathbf{B} & \mathbf{B} \mathbf{x}_k \\ \mathbf{x}_k^T \mathbf{B} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{t}_k \\ \epsilon_k \end{pmatrix} = \begin{pmatrix} -\mathbf{r}_k \\ 0 \end{pmatrix}, \quad (31)$$

Note: Is only singular if $(\mathbf{x}_k, \lambda_k)$ is an eigenpair of the pencil (\mathbf{A}, \mathbf{B}) with λ_k being a multiple eigenvalue [2]

Jacobi-Davidson: Newton with Subspace Acceleration [9, 2]

Davidson's approach: consecutive corrections \mathbf{t}_k are now used to build the search space.

- Solution \mathbf{t}_k of the Jacobian correction equation is appended to \mathbf{V}_k , resulting in $\mathbf{V}_{k+1} = [\mathbf{V}_k, \mathbf{t}_k]$
- Speeds up convergence by increasing dimension of trial space by one

Block JD approx. l eigenvalues simultaneously. Further, the trial space dimension is increased by l .

Davidson-Type Trace Minimization Method [7]

Problems of block JD:

1. Shifting strategy forces algorithm to converge to eigenvalues closest to Ritz values (often far away from desired eigenvalues at the beginning)
2. Subspace expanding decreases Ritz values; block JD is forced to converge to smallest eigenpairs
3. Ill-conditioning when Ritz value approaches multiple eigenvalue or cluster of eigenvalues

Davidson-Type Trace Minimization Method [7]

Solution:

1. Use multiple dynamic shifting strategy
2. Use implicit deflation technique ($\mathbf{Y}^T \mathbf{B} \mathbf{d}_{k,i} = 0$)
3. Use dynamic stopping strategy for accuracy when solving inner system

Conclusion

- Proof of trace theorem using Poincaré separation theorem
- Trace minimization characterization as quasi-Newton more difficult than expected (requires background in differential geometry)
- Block JD and TRACEMIN are quite similar
- Although JD has better convergence rate in some cases, it still depends on a good starting subspace
 - Davidson-type TRACEMIN is not affected; is more robust

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