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List of projects

- Symmetric Generalized Eigenvalue Problem
  - Trust-region methods on Riemannian manifolds
- Low-rank Incremental SVD methods (with Danny Sorensen)
  - Multi-pass algorithms for increased accuracy and confidence

Implicit Riemannian Trust-Region Method for the symmetric generalized eigenproblem

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`These slides and related documents are available at`

`http://www.csit.fsu.edu/∼cbaker/Publi/SGEVP_IRTR.htm`

Outline

- Review: RTR method for Extreme SGEVP.
- Review: Adaptive Model RTR.
- Implicit Riemannian Trust-Region method.
  - Description.
  - Convergence results.
- IRTR for Extreme SGEVP.
  - Algorithm details.
  - Numerical experiments.

Trust-region methods on Riemannian manifolds

1. Given: smooth manifold M; Riemannian metric g; smooth cost function f on M; retraction R from the tangent bundle TM to M; current iterate x_k.

1b. Lift up the cost function to the tangent space T_xM:

$$\hat{f}_x = f \circ R_x.$$

2. Build a model $m_k(s)$ of $\hat{f}_{x_k}$ around 0.
3. Find (up to some precision) a minimizer s_k of the model within a "trust-region", i.e., a ball of radius Δ_k around x_k.

Trust-region methods on Riemannian manifolds (cont'd)

4. Compute the ratio

$$\rho = \frac{f(x_k) - f(R_{x_k} s_k)}{m_k(0) - m_k(s_k)}$$

   to compare the actual value of the cost function at the proposed new iterate with the value predicted by the model.

5. Shrink, enlarge or keep the trust-region radius according to the value of ρ.
6. Accept or reject the proposed new iterate $R_{x_k} s_k$ according to the value of ρ.
7. Increment k and go to step 2.

Required ingredients for Riemannian TR

- Manifold M, Riemannian metric g, and cost function f on M.
- Practical expression for $T_{x_k}M$.
- Retraction $R_{x_k} : T_{x_k}M \to M$.
- Function $\hat{f}_{x_k}(s) := f(R_{x_k}(s))$.
- Gradient $\operatorname{grad} \hat{f}_{x_k}(0)$.
- Hessian $\operatorname{Hess} \hat{f}_{x_k}(0)$.

ESGEV: The optimization problem

Given: $n \times n$ pencil (A, B), $A = A^T$, $B = B^T \succ 0$,

$$Av_i = Bv_i\lambda_i, \quad i = 1, \ldots, n$$

$$v_i^T B v_j = \delta_{ij} \quad \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$$

Problem: compute the "leftmost" eigenspace

$$\mathcal{V} := \mathrm{col}(v_1, \ldots, v_p)$$

Solution: $\mathcal{V}$ satisfies

$$\mathcal{V} = \arg\min_{\mathcal{Y} \in \mathrm{Grass}(p,n)} f(\mathcal{Y}), \quad \text{where}$$

$$f : \mathrm{Grass}(p, n) \to \mathbb{R} : \mathrm{col}(Y) \mapsto \mathrm{tr}\left((Y^T BY)^{-1} Y^T AY\right).$$

Trust-region for Extreme SGEVP: principles

Ingredients of the RTR method for ESGEV [ABG06]:

1. Manifold: $M = \{p - \text{dimensional subspaces of } \mathbb{R}^n\}$ (Grassmann manifold).

2. Representations: $\mathcal{Y}$ represented by any $Y \in \mathbb{R}^{n\times p} : \mathrm{col}(Y) = \mathcal{Y}$.

3. Tangent space: formally, $T_Y M = \{Z \in \mathbb{R}^{n\times p} : Y^T B Z = 0\}$.

4. Metric: formally, $g_Y(Z_a, Z_b) = \mathrm{tr}\left((Y^T B Y)^{-1} Z_a^T Z_b\right)$.

Trust-region for Extreme SGEVP: principles (2)

5. Retraction: formally, $R_Y(Z) = (Y + Z)M$, where arbitrary M serves for normalization.

6. Cost function: formally, $f(Y) = \mathrm{tr}\left((Y^T BY)^{-1}(Y^T AY)\right)$.

Underlying fact: $\begin{bmatrix} v_1 & \dots & v_p \end{bmatrix} M$ minimizes f for all M invertible.

Trust-region for Extreme SGEVP: details

Lifted cost function:

$$\begin{aligned}
\hat{f}_Y(Z) = f(R_Y(Z)) &= \mathrm{tr}\left(\left((Y+Z)^T B (Y+Z)\right)^{-1} (Y+Z)^T A (Y+Z)\right) \\
&= \mathrm{tr}\left((Y^T BY)^{-1} Y^T AY\right) + 2\mathrm{tr}\left((Y^T BY)^{-1} Z^T AY\right) \\
&\quad + \mathrm{tr}\left((Y^T BY)^{-1} Z^T (AZ - BZ(Y^T AY))\right) + HOT \\
&= \mathrm{tr}\left((Y^T BY)^{-1} Y^T AY\right) + 2\mathrm{tr}\left((Y^T BY)^{-1} Z^T P_{BY,BY} AY\right) \\
&\quad + \mathrm{tr}\left((Y^T BY)^{-1} Z^T P_{BY,BY} (AZ - BZ(Y^T AY))\right) + HOT,
\end{aligned}$$

where $P_{BY,BY} = I - BY(Y^T B^2 Y)^{-1} Y^T B$.

Trust-region for Extreme SGEVP: details (2)

The second order approximation of $\hat{f}_Y(Z)$ is thus

$$\begin{aligned} m_Y(Z) &= f(Y) + g_Y(\operatorname{grad} f(Y), Z) + \frac{1}{2} g_Y(\mathcal{H}_Y Z, Z) \\ &= \operatorname{tr}\left((Y^T BY)^{-1} Y^T AY\right) + 2\operatorname{tr}\left((Y^T BY)^{-1} Z^T AY\right) \\ &\quad + \operatorname{tr}\left((Y^T BY)^{-1} Z^T \left(AZ - BZ(Y^T BY)^{-1} Y^T AY\right)\right). \end{aligned}$$

Compute an approximate minimizer $\tilde{Z}$ using truncated CG [CGT00]

Update: $Y_+ = R_Y(\tilde{Z}) = (Y + \tilde{Z})M$.

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A hybrid Tracemin / TR method

Collaboration with Ahmed Sameh.

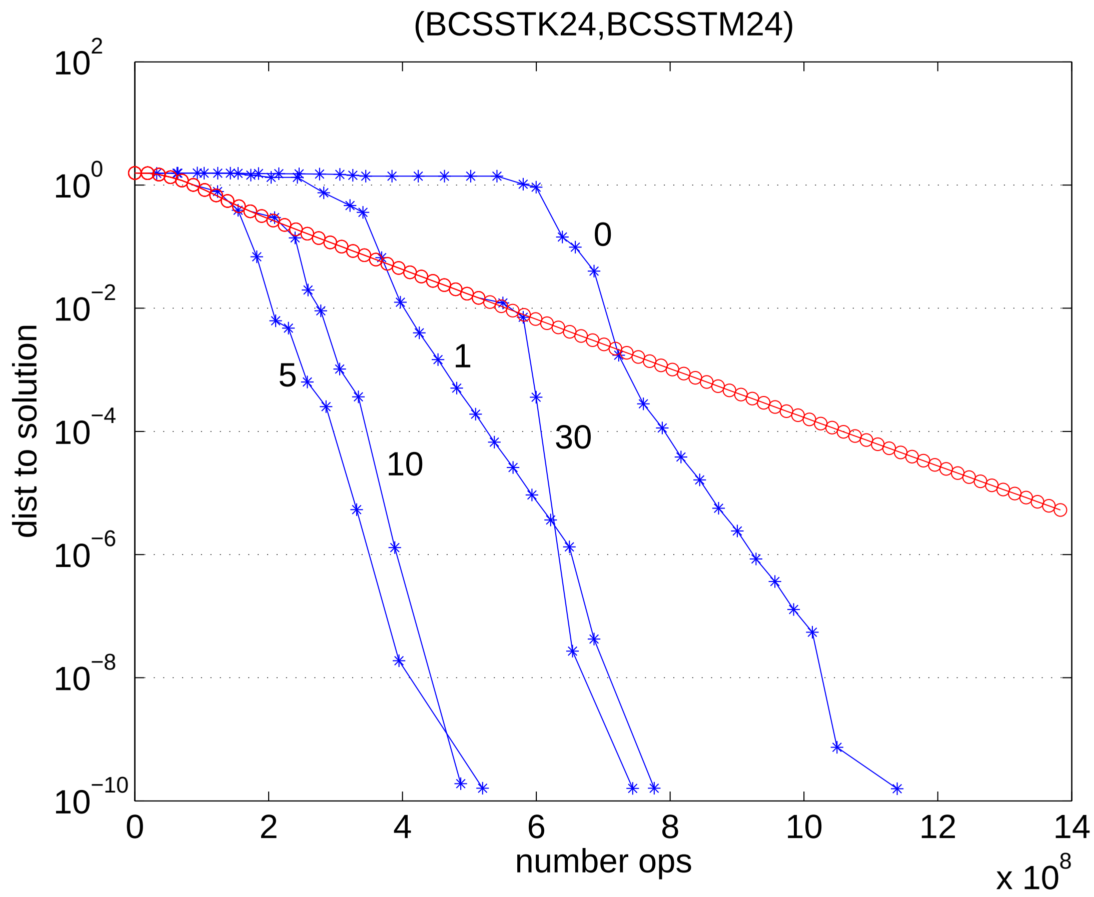
- Problem: Trust-region confinement may hamper efficient preconditioning far away from the solution.
  $\rightsquigarrow$ Use preconditioned Basic Tracemin [SW82, ST00] in Phase I.
- Problem: Close to the solution, Basin Tracemin is linear.
  $\rightsquigarrow$ Use TR method in Phase II.

Adaptive Model RTR

The method can be described in an Adaptive Model RTR framework [ABGS05].

- Phase I:
  - Use a model Hessian $P_{BX,BX} A P_{BX,BX}$
  - Set trust-region radius to infinity.
- Phase II:
  - Use model Hessian $\mathrm{Hess}\hat{f}_X[S] = P_{BX,BX}(AS - BSX^T AX)$
  - Finite trust-region radius and $\rho' \in (0,1)$.

EXP: Adaptive Model RTR



Calgary Saddledome, BCSST24; $n = 3562$; precond. with exact factorization of A after **symamd**; $p = 5$.

Adaptive Model RTR

- Method inherits the global convergence of constituent methods.
- The switching criterion affects efficiency only.
- Potential efficiency greater than constituents.
- Take-home idea: Framing the method as a model trust-region optimization allows us to choose best suited model at different points in the computation.

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Complaints Against Trust-Region Mechanism

- Trust-region radius is heuristic.
  - Radius of current trust-region based on performance of last model minimization.
  - This may constrain current model minimization.
- Iterate may be rejected.
  - Wasted time spent computing potential iterate.
  - It can take a number of outer iterations to adjust trust-region radius.

Proposal for New Trust-Region

Suggestion: Based trust-region on the current performance of the surrogate model.

New trust-region is

$$\left\{ s \in T_x M : \rho_x(s) \geq \rho' \right\}, \quad \rho' > 0.$$

ρ_x is as before:

$$\rho_x(s) = \frac{f(x) - f(R_x s)}{m_x(0) - m_x(s)}.$$

Implicit Riemannian Trust-Region (IRTR)

1. Given: smooth manifold M; Riemannian metric g; smooth cost function f on M; retraction R from the tangent bundle TM to M; current iterate x_k.

1b. Lift up the cost function to the tangent space T_xM:

$$\hat{f}_x = f \circ R_x.$$

2. Build a model $m_k(s)$ of $\hat{f}_{x_k}$ around 0.
3. Find (approximately) a minimizer s_k of the model within the new trust-region.
4. Accept $x_{k+1} = R_{x_k} s_k$.
5. Increment k and go to step 2.

Solving Model Minimization in IRTR

- Use truncated CG to solve model minimization.
- New trust-region definition requires some modifications.
- Boundary test:
  - Before: check $\|s^j\| \leq \Delta_k$
  - Now: check $\rho_{x_k}(s^j) \geq \rho'$
- If $\rho_{x_k}(s^j) < \rho'$:
  - Compute τ such that $\rho_{x_k}(s^{j-1} + \tau\delta_j) \geq \rho'$
  - This is potentially more difficult than finding $\|s^{j-1} + \tau\delta_j\| = \Delta_k$.

Required ingredients for Implicit RTR

- Manifold M, Riemannian metric g, and cost function f on M
- Practical expression for $T_{x_k}M$
- Retraction $R_{x_k} : T_{x_k}M \to M$
- Function $\hat{f}_{x_k}(s) := f(R_{x_k}(s))$
- Gradient grad $\hat{f}_{x_k}(0)$
- Hessian Hess $\hat{f}_{x_k}(0)$
- Trust-region test: $\rho_{x_k}(s)$
- Trust-region search: find τ s.t. $\rho_{x_k}(s + \tau\delta) = \rho'$

Convergence Results of IRTR

- The trust-region definition is very strong.
- As a result, standard TR global convergence results follow easily.
- Global Convergence of IRTR for ESGEV: Let $\{y_k\}$ be a sequence of iterates produced via IRTR-tCG with $\rho' \in (0,1)$. Then

$$\lim_{k \to \infty} \|\operatorname{grad} f(y_k)\|_2 = 0.$$

- The local convergence results have not yet been adapted from the RTR to the IRTR. Also, the global convergence results have yet to be adapted to a general IRTR.

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IRTR for the Extreme SGEVP

As with RTR for Extreme SGEVP:

1. Manifold: Grassman, represented as $Y \in \mathbb{R}^{n\times p}$, $Y^T BY = I$
2. Tangent space: $T_Y M = \{Z \in \mathbb{R}^{n\times p} : Y^T BZ = 0\}$.
3. Metric: $g_Y(Z_a, Z_b) = \mathrm{tr}\left(Z_a^T Z_b\right)$.
4. Retraction: $R_Y(Z) = (Y + Z)M$, M for B-orthonormalization
5. Cost function: $f(Y) = \mathrm{tr}\left((Y^T BY)^{-1}(Y^T AY)\right)$.

IRTR for the Extreme SGEVP (2)

Therefore, cost function $\hat{f}_Y$ is

$$\begin{aligned}
\hat{f}_Y(S) &= \mathrm{tr}\left((I + S^T BS)^{-1}(Y+S)^T A(Y+S)\right) \\
\mathrm{grad}\,\hat{f}_Y(0) &= P_{BY,BY}AY \\
\mathrm{Hess}\,\hat{f}_Y(0)[S] &= P_{BY}(AS - BSY^T AY)
\end{aligned}$$

Newton model of $\hat{f}_Y$ is

$$m_Y(S) = \mathrm{tr}\left(Y^T AY\right) + 2\mathrm{tr}\left(S^T AY\right) + \mathrm{tr}\left(S^T(AS - BSY^T AY)\right)$$

$\boxed{\text{Case } p = 1}$

If $p = 1$, then $\rho_y(s) = \frac{\hat{f}_y(0) - \hat{f}_y(s)}{m_y(0) - m_y(s)} = \frac{1}{1 + s^T B s}$.

- Checking trust-region inclusion requires checking $\|s\|_B$
- Solving ρ_y along a tangent vector has an analytical solution: τ s.t. $\rho_y(s + \tau\delta) = \rho'$ given by

$$\begin{aligned} \tau &= \frac{-\delta^T B s + \sqrt{(\delta^T B s)^2 + \delta^T B \delta (\Delta_{\rho'}^2 - s^T B s)}}{\delta^T B \delta} \\ \Delta_{\rho'} &= \sqrt{\frac{1}{\rho'} - 1} \end{aligned}$$

- IRTR for $p = 1$ ESGEV is straightforward.

$\boxed{\text{Implications for RTR}}$

- Implications for RTR-ESGEV when $p = 1$, $B = I$, no preconditioning.
  - In this case, TR defined by $\|s\|_2 = \|s\|_B \leq \Delta_k$
- If $\frac{1}{\sqrt{3}} < \Delta_k < \sqrt{3}$, then
  - $\rho_{y_k}(s_k) > \frac{1}{4} \Rightarrow$ iterate is acceptable!
  - $\Delta_{k+1} = \Delta_k \Rightarrow$ trust-region radius is maintained!
- Properly chosen Δ_0 guarantees model performance.

Even without preconditioner or $B \neq I$, IRTR recommended.

$$\boxed{\text{Case } p > 1}$$

$$\rho_Y(S) = \frac{\operatorname{tr}\left((I + S^T BS)^{-1}(S^T BS(Y^T AY) - 2S^T AY - S^T AS)\right)}{\operatorname{tr}\left(S^T BS(Y^T AY) - 2S^T AY - S^T AS\right)}$$

Assume that $Y^T BY = I$ and $Y^T AY = \Sigma$. Then

$$\begin{aligned} m_Y(S) &= \operatorname{tr}\left(Y^T AY + 2S^T AY + S^T(AS - BSY^T AY)\right) \\ &= \sum_{i=1}^{p} \left(\sigma_i + 2s_i^T Ay_i + s_i^T(As_i - Bs_i\sigma_i)\right) \\ &= \sum_{i=1}^{p} m_{y_i}(s_i). \end{aligned}$$

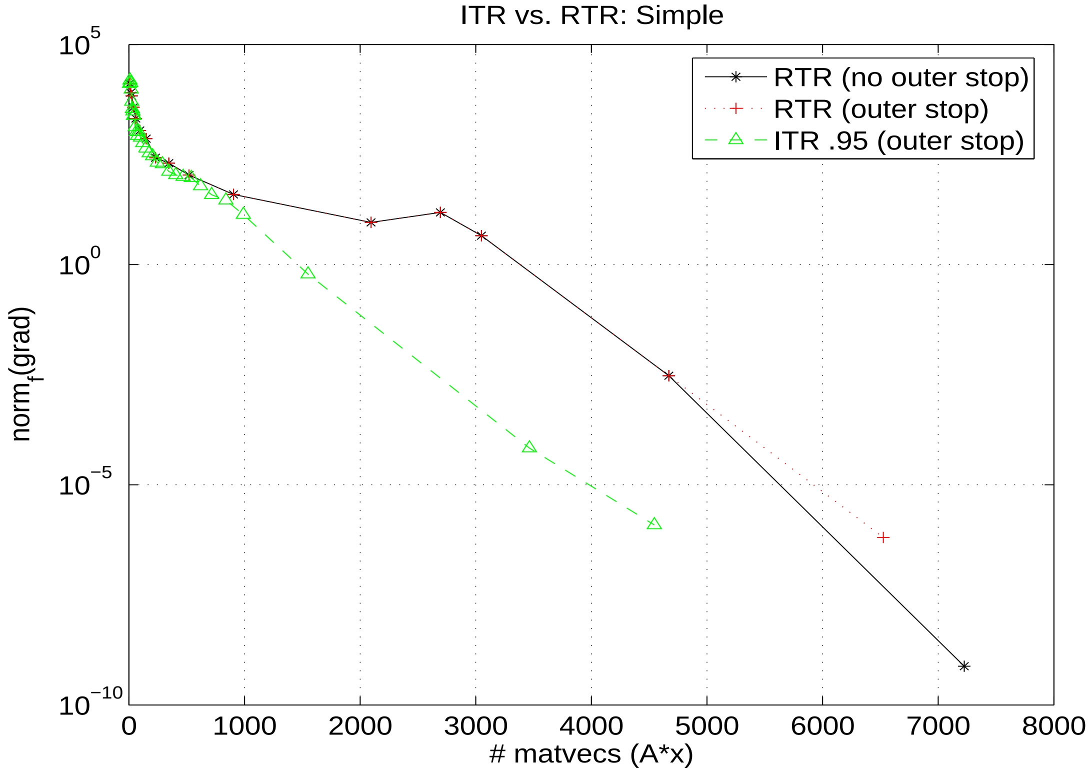
$\boxed{\text{Case } p > 1}$

- The $p > 1$ model $m_Y(S)$ can be decoupled into p "scalar" models, for which we have a formula for ρ.
- The block algorithm runs p simultaneous tCG algorithms.
- All processes are stopped if any satisfies a stopping criterion.
- Global convergence is still guaranteed.
- But $\rho_Y(S) \ngeq \rho'$: not a true IRTR!

Outer Criterion Monitoring

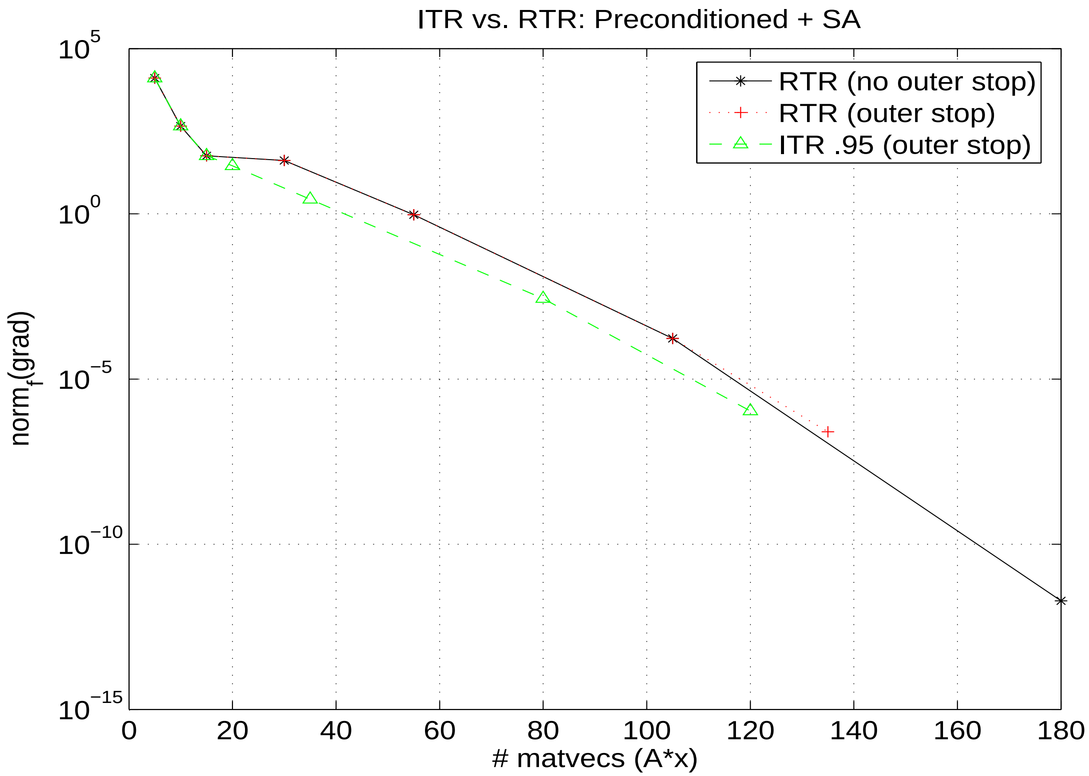
- Last call to tCG often performs more work than necessary to satisfy outer stopping criterion.
- Problem is typical for methods employing an inner iteration.
- Solution is (occasionally) compute outer residual in inner iteration, check stopping criterion.
- Similar to suggestion in [Not02], except we have no efficient formula for the residual norm.

EXP: Monitoring Outer Stopping Criterion (1)



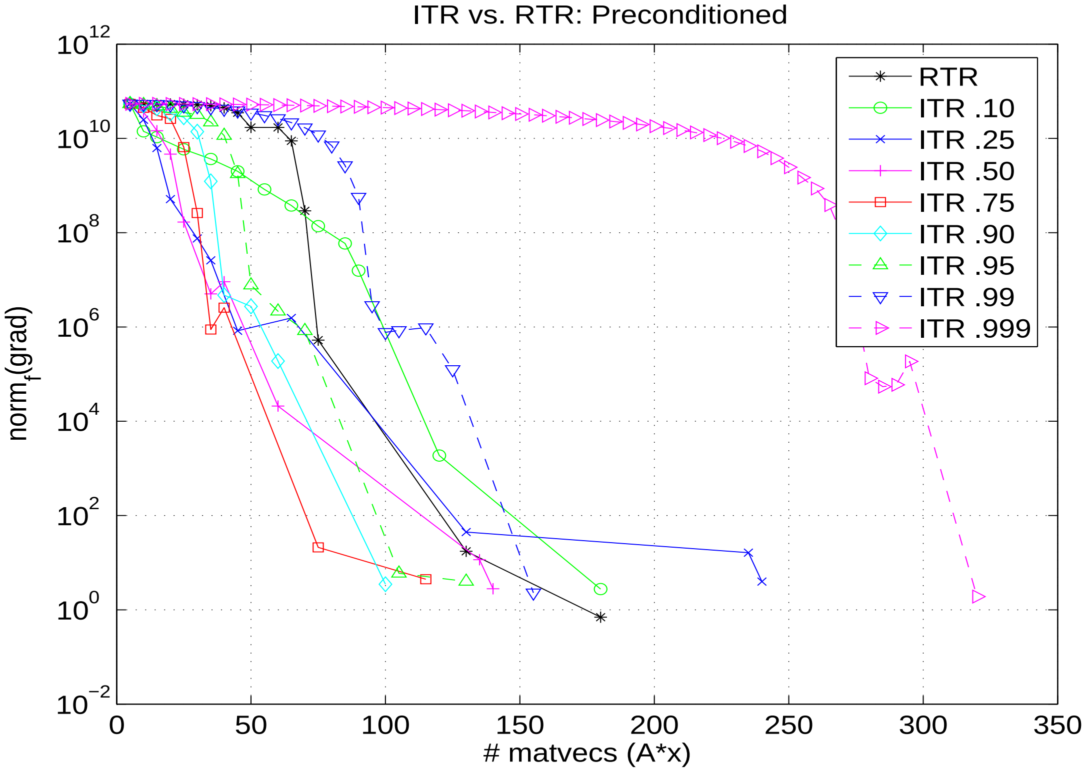
2-D Laplacian, $n = 10000$; no precond.; no subspace acceleration; $p = 5$

EXP: Monitoring Outer Stopping Criterion (2)



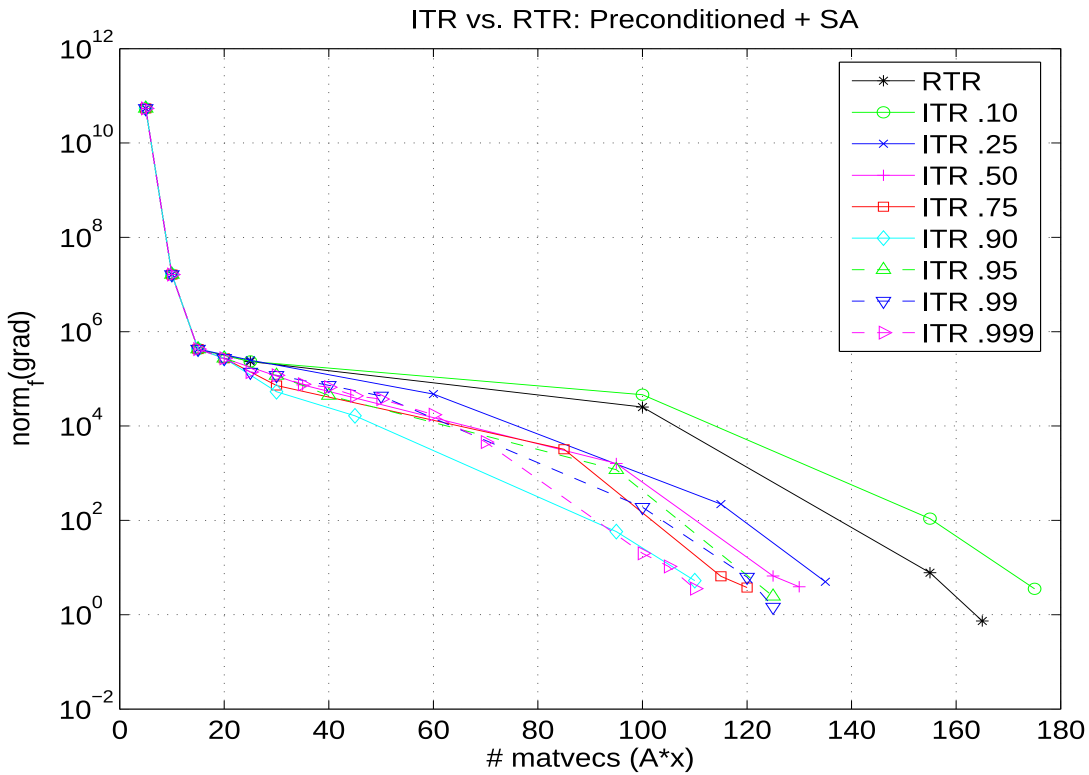
2-D Laplacian, $n = 10000$; precond. using exact factorization of A after `symamd`; 10-D subspace acceleration; $p = 5$

EXP: IRTR vs. RTR



BCSST24; precond. with exact factorization of A after `symamd`; no subspace acceleration; $p = 5$

EXP: IRTR vs. RTR



BCSST24; precond. with exact factorization of A after **symamd**; 10-D subspace acceleration; $p = 5$

Goal of IRTR

- Combined with SA, IRTR switches between optimizing on TM and M.
- Take-home idea: Break down the barrier between inner and outer iteration:
  - Outer criterion monitoring stops when iteration is ultimately satisfied; always maintain awareness of outer error
  - Base trust-region on the performance of surrogate model; always maintain awareness of cost function
- Both ideas touched on in [Not02].
- Reduce all TR parameters to one: ρ'

Future Work

- Formulation of a true block IRTR for Extreme SGEVP.
- Convergence results of IRTR for general (M, g, R, f)
- Application of IRTR to other NLA problems.
- Explore affect of ρ' parameter.
- Look at adaptive model mechanism for IRTR.

References

[ABG06] P.-A. Absil, C. G. Baker, and K. A. Gallivan, *A truncated-CG style method for symmetric generalized eigenvalue problems*, J. Comput. Appl. Math. **189** (2006), no. 1–2, 274–285.

[ABGS05] P.-A Absil, C. G. Baker, K. A. Gallivan, and A. Sameh, *Adaptive model trust region methods for generalized eigenvalue problems*, International Conference on Computational Science (Vaidy S. Sunderam, Geert Dick van Albada, and Peter M. A. Sloot, eds.), Lecture Notes in Compuer Science, vol. 3514, Springer-Verlag, 2005, pp. 33–41.

[CGT00] A. R. Conn, N. I. M. Gould, and Ph. L. Toint, *Trust-region methods*, MPS/SIAM Series on Optimization, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, and Mathematical Programming Society (MPS), Philadelphia, PA, 2000.

[Not02] Y. Notay, *Combination of Jacobi-Davidson and conjugate gradients for the partial symmetric eigenproblem*, Numer. Linear Algebra Appl. **9** (2002), no. 1, 21–44.

[ST00] A. Sameh and Z. Tong, *The trace minimization method for the symmetric generalized eigenvalue problem*, J. Comput. Appl. Math. **123** (2000), 155–175.

[SW82] A. H. Sameh and J. A. Wisniewski, *A trace minimization algorithm for the generalized eigenvalue problem*, SIAM J. Numer. Anal. **19** (1982), no. 6, 1243–1259.

THE END

Algorithm 1 (Prec. Truncated CG for IRTR)

Set $s^0 = 0$, $r_0 = \mathrm{grad}\,\hat{f}_y$, $z_0 = M^{-1} r_0$, $d^0 = -z_0$

for $j = 0, 1, 2, \ldots$

Check inner stopping criterion

Check $\delta_j^T H_y[\delta_j]$

Compute $\tau \geq 0$ *s.t.* $s = s^j + \tau \delta_j$ *satisfies* $\rho_y(s) = \rho'$; ***return*** s

Set $\alpha^j = (z_j^T r_j)/(\delta_j^T H_y[\delta_j])$

Set $s^{j+1} = s^j + \alpha_j \delta_j$

if $\rho_y(s^{j+1}) < \rho'$

Compute $\tau \geq 0$ *s.t.* $s = s^j + \tau \delta_j$ *satisfies* $\rho_y(s) = \rho'$; ***return*** s

Check outer stopping criterion

Set $r_{j+1} = r_j + \alpha^j H_y[\delta_j]$

Set $z_{j+1} = M^{-1} r_{j+1}$

Set $\beta^{j+1} = (z_{j+1}^T r_{j+1})/(z_j^T r_j)$

Set $\delta_{j+1} = -z_{j+1} + \beta^{j+1} \delta_j$

end.