An implicit trust-region method on Riemannian manifolds[§]

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Abstract

We propose and analyze an "implicit" trust-region method in the general setting of Riemannian manifolds. The method is implicit in that the trust-region is defined as a superlevel set of the ρ ratio of the actual over predicted decrease in the objective function. Since this method potentially requires the evaluation of the objective function at each step of the inner iteration, we do not recommend it for problems where the objective function is expensive to evaluate. However, we show that on some instances of a very structured problem—the extreme symmetric eigenvalue problem, or equivalently the optimization of the Rayleigh quotient on the unit sphere—the resulting numerical method outperforms state-of-the-art algorithms. Moreover, the new method inherits the detailed convergence analysis of the generic Riemannian trust-region method.

Keywords. optimization on manifolds, trust-region methods, Newton's method, symmetric generalized eigenvalue problem

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1 Introduction

Trust-region methods are widely used in the unconstrained optimization of smooth functions. Much of the reason for their popularity is the superposition of strong global convergence, fast local convergence, and ease of implementation. In (Pow70), Powell helped to establish a following for this family of methods. In addition to proving global convergence of the method under mild conditions, the work showed that the method was competitive with state-of-the-art algorithms for unconstrained optimization. This launched a period of great interest in the methods (see (CGT00) and references therein).

Similar to Euclidean trust-region methods, the Riemannian Trust-Region method (see (ABG06c)) ensures strong global convergence properties while allowing superlinear local convergence. The trust-region mechanism is a heuristic, whereby the performance of the last update dictates the constraints on the next update. The trust-region mechanism makes it possible to disregard the (potentially expensive) objective function during the inner iteration by relying instead on a model restricted to a trust region, i.e., a region where the model is tentatively trusted to be a sufficiently accurate approximation of the objective function. A downside lies in the difficulty of adjusting the trust-region size. When the trust-region radius is too large, valuable time may be spent proposing a new iterate that may be rejected. Alternatively, when the trust-region radius is too small, the algorithm progresses unnecessarily slowly.

The inefficiencies resulting from the trust-region mechanism can be addressed by disabling the trust-region mechanism in such a way as to preserve the desired convergence properties. In (GST05), the authors describe a filter-trust-region method, where a modified acceptance criterion seeks to encourage convergence to first-order critical points. Other approaches adjust the trust-region radius according to dynamic measures such as objective function improvement and step size lengths (see (CGT00)).

Instead of relaxing the acceptance criterion, this paper proposes that the trust-region be identified as that set of points that would have been accepted under the classical mechanism. Therefore, as long as the update returned from the model minimization is feasible, i.e., it belongs to the trust-region, then acceptance is automatic. In addition to avoiding the discarding of valuable updates, this method eliminates the explicit trust-region radius and its heuristic mechanism, in place of a meaningful measure of performance.

The description of the algorithm and the analysis of convergence consider the optimization of a smooth real function f whose domain is a differentiable manifold M with Riemannian metric g. Briefly, we exploit the intrinsic property of the manifold known as the tangent plane at the current iterate y, denoted by T_yM.

This space, coupled with g_y, is an abstract vector space where most of the effort of the solution occurs via a mapping R_y from T_yM to M (called a retraction). The Riemannian setting is beneficial because many interesting problems are very easily described in terms of optimizing a smooth function on a manifold (e.g., the eigenvalue problem studied in this paper). Furthermore, as this is a more general setting than that of unconstrained Euclidean optimization, all of the material here is immediately applicable to the latter. By identifying $M = \mathbb{R}^d$ along with the canonical identification $T_yM = \mathbb{R}^d$, and choosing g as the canonical Euclidean dot product and $R_y(\eta) = (y + \eta)$, the approach described in this paper results in an implicit trust-region method for functions defined on $\mathbb{R}^d$.

Section 2 reviews the workings of the RTR and describes the IRTR modification. Section 3 presents the global and local convergence properties for the IRTR method. Section 4 shows the feasibility of the IRTR method for the symmetric generalized eigenvalue problem, and Section 5 presents numerical results illustrating the benefit of this approach.

2 Implicit Riemannian Trust-Region Method

This section briefly reviews the workings of the Riemannian Trust-Region (RTR) method and introduces the Implicit Riemannian Trust-Region (IRTR) method. The attempt is made to limit the amount of background material from differential geometry and Euclidean optimization. Interested readers are recommended to see (Boo75; dC92) for theory on Riemannian manifolds. Trust-region information can be found in most books on unconstrained optimization, for example (CGT00; NW99). Readers interested in optimization on Riemannian manifolds and the RTR are recommended (ABG06c) and the upcoming (AMS07).

The goal of the IRTR, like that of the RTR, is to find a local minimizer of the objective function

$$f : M \to \mathbb{R},$$

where M is a differentiable manifold and g is a Riemannian metric on M. Together, (M, g) describes a Riemannian manifold. The RTR method, like Euclidean trust-region methods, computes iterates by solving a minimization problem on a model of the objective function. However, the RTR performs this model minimization, not on the manifold M, but on the tangent bundle TM. This is achieved through the use of a mapping called a <u>retraction</u>. The retraction maps the tangent bundle TM to the manifold. More specifically, a retraction R maps a tangent vector $\xi \in T_yM$ to an element $R_y(\xi) \in M$. The retraction is used to define a "lifted" cost function

$$\hat{f} = f \circ R : TM \to \mathbb{R}.$$

At a single point $y \in M$, we can restrict the domain of $\hat{f}$ to yield $\hat{f}_y = f \circ R_y : T_yM \to \mathbb{R}$.

The benefit of this is that the tangent plane, coupled with the Riemannian metric g, is an abstract Euclidean space, and therefore a more familiar and convenient arena for conducting numerical optimization. The RTR method follows the example of Euclidean trust-region methods by constructing a model m_y of $\hat{f}_y$ and solving the trust-region subproblem using m_y:

$$\text{minimize } m_y(\xi), \quad \text{subject to } g_y(\xi, \xi) \leq \Delta^2, \tag{1}$$

where Δ is the trust-region radius. We assume through the paper that the model m_y is a quadratic model of $\hat{f}_y$ which approximates $\hat{f}_y$ to at least the first order:

$$m_y(\xi) = \hat{f}_y(0_y) + g_y\left(\xi, \operatorname{grad} \hat{f}_y(0_y)\right) + \frac{1}{2} g_y(\xi, \mathscr{H}_y[\xi]), \tag{2}$$

where $\mathscr{H}_y[\xi]$ is a symmetric operator on T_yM and 0_y is the additive identity in T_yM.

The tangent vector ξ is used to generate a new iterate, which is accepted depending on the value of the quotient

$$\rho_y(\xi) = \frac{\hat{f}_y(0_y) - \hat{f}_y(\xi)}{m_y(0_y) - m_y(\xi)}. \tag{3}$$

The value of $\rho_y(\xi)$ is also used to expand or shrink the trust-region radius. The RTR algorithm is stated in Algorithm 2.1.

Algorithm 2.1. ***Require:*** *Complete Riemannian manifold* (M, g)*; scalar field* f *on* M*; retraction* R *from* TM *to* M.

Input: $\bar{\Delta} > 0$, $\Delta_0 \in (0, \bar{\Delta})$, *and* $\rho' \in [0, \frac{1}{4})$, *initial iterate* $y_0 \in M$.

Output: *Sequences of iterates* $\{y_k\}$.

```
for k = 0, 1, 2, ... do
    Model-based Minimization
    Obtain η_k by approximately solving (1)
    Evaluate ρ_k = ρ_{y_k}(η_k) as in (3)
    Adjust trust region
    if ρ_k < 1/4 then
        Set Δ_{k+1} = (1/4) Δ_k
    else if ρ_k > 3/4 and ||η_k|| = Δ_k then
        Set Δ_{k+1} = min(2Δ_k, Δ̄)
    else
        Set Δ_{k+1} = Δ_k
    end if
```

Compute next iterate
    if $\rho_k > \rho'$ ***then***
        Set $y_{k+1} = R_{y_k}(\eta_k)$
    else
        Set $y_{k+1} = y_k$
    end if
end for

The general algorithm does not state how (1) should be solved. We have previously advocated the use of the truncated conjugate gradient method of Steihaug and Toint (see (Ste83) or (Toi81) or (CGT00)). This method has the benefit of requiring very little memory and returning a point inside the trust-region. It can also exploit a preconditioner in solving the model minimization. Algorithm 2.2 states a preconditioned truncated conjugate gradient method for solving the model minimization on the tangent plane.

Algorithm 2.2. ***Input:*** *Iterate* $y \in M$, grad $f(y) \neq 0$*; trust-region radius* Δ*; convergence criteria* $\kappa \in (0,1)$, $\theta > 0$*; model* m_y *as in 2; symmetric/positive definite preconditioner* $M : T_yM \to T_yM$

Set $\eta_0 = 0_y$, $r_0 = \text{grad}\, f(y)$, $z_0 = M^{-1}r_0$, $d_0 = -z_0$
for $j = 0,1,2,\ldots$ ***do***
    Check κ/θ ***stopping criterion***
    if $\|r_j\| \leq \|r_0\| \min\left\{\kappa, \|r_0\|^\theta\right\}$ ***then***
        return η_j
    end if
    Check curvature of current search direction
    if $g_y(\mathscr{H}_y[d_j], d_j) \leq 0$ ***then***
        Compute $\tau > 0$ *such that* $\eta = \eta_j + \tau d_j$ *satisfies* $\|\eta\| = \Delta$
        return η
    end if
    Set $\alpha_j = g_y(z_j, r_j)/g_y(\mathscr{H}_y[d_j], d_j)$
    Generate next inner iterate
    Set $\eta_{j+1} = \eta_j + \alpha_j d_j$
    Check trust-region
    if $\|\eta_{j+1}\| > \Delta$ ***then***
        Compute $\tau > 0$ *such that* $\eta = \eta_j + \tau d_j$ *satisfies* $\|\eta\| = \Delta$
        return η
    end if
    Use CG recurrences to update residual and search direction
    Set $r_{j+1} = r_j + \alpha_j \mathscr{H}_y[d_j]$
    Set $z_{j+1} = M^{-1} r_{j+1}$

Set $\beta_{j+1} = g_y(z_{j+1}, r_{j+1}) / g_y(z_j, r_j)$
Set $d_{j+1} = -z_{j+1} + \beta_{j+1} d_j$
end for

The classical trust-region mechanism has many favorable features, including global convergence to a critical point, stable convergence only to local minimizers, and superlinear local convergence (depending on the choice of quadratic model)(see (ABG06c)). The trust-region heuristic is self-tuning, such that an appropriate trust-region radius will eventually be discovered by the algorithm. In practice, however, this adjustment can result in wasted iterations, as proposed iterates are rejected do to poor scores under ρ.

We propose a modification to the trust-region method. This modification bypasses the step size heuristic and directly addresses the model performance. The implicit trust-region is defined as a superlevel set of ρ:

$$\left\{ \xi \in T_y M : \rho_y(\xi) \geq \rho' \right\}. \tag{4}$$

The model minimization now consists of

$$\text{minimize } m_y(\xi), \quad \text{subject to } \rho_y(\xi) \geq \rho'. \tag{5}$$

The implicit trust-region contains exactly those points that would have been accepted by the classical trust-region mechanism. The result is that there is no trust-region radius to adjust and no rejections. The IRTR algorithm is stated in Algorithm 2.3.

Algorithm 2.3. ***Require:*** *Complete Riemannian manifold* (M, g)*; scalar field* f *on* M*; retraction* R *from* TM *to* M*.*
Input: $\bar{\Delta} > 0$, $\Delta_0 \in (0, \bar{\Delta})$, *and* $\rho' \in (0, 1)$, *initial iterate* $y_0 \in M$.
Output: *Sequences of iterates* $\{y_k\}$.
for $k = 0, 1, 2, \ldots$ ***do***
Model-based Minimization
Obtain η_k *by approximately solving* (5)
Compute next iterate
Set $y_{k+1} = R_{y_k}(\eta_k)$
end for

The new trust-region definition modifies the model minimization, and these modifications must be reflected in the truncated conjugate gradient solver. The trust-region definition occurs in the solver in two cases: when testing that the CG iterates remain inside the trust-region, and when moving along search direction to the edge of the trust-region. The updated truncated conjugate gradient algorithm is displayed in Algorithm 2.4.

Algorithm 2.4. ***Input:*** *Iterate* $y \in M$, grad $f(y) \neq 0$*; trust-region parameter* $\rho' \in (0,1)$*; convergence criteria* $\kappa \in (0,1)$, $\theta > 0$*; model* m_y *as in 2; symmetric/positive definite preconditioner* $M : T_yM \to T_yM$

Set $\eta_0 = 0_y$, $r_0 = \text{grad}\, f(y)$, $z_0 = M^{-1}r_0$, $d_0 = -z_0$
for $j = 0,1,2,\ldots$ ***do***
  Check κ/θ ***stopping criterion***
  if $\|r_j\| \leq \|r_0\| \min\left\{\kappa, \|r_0\|^{\theta}\right\}$ ***then***
    return η_j
  end if
  Check curvature of current search direction
  if $g_y(\mathscr{H}_y[d_j], d_j) \leq 0$ ***then***
    Compute $\tau > 0$ *such that* $\eta = \eta_j + \tau d_j$ *satisfies* $\boxed{\rho_y(\eta) = \rho'}$
    return η
  end if
  Set $\alpha_j = g_y(z_j, r_j) / g_y(\mathscr{H}_y[d_j], d_j)$
  Generate next inner iterate
  Set $\eta_{j+1} = \eta_j + \alpha_j d_j$
  Check trust-region
  if $\boxed{\rho_y(\eta_{j+1}) < \rho'}$ ***then***
    Compute $\tau > 0$ *such that* $\eta = \eta_j + \tau d_j$ *satisfies* $\boxed{\rho_y(\eta) = \rho'}$
    return η
  end if
  Use CG recurrences to update residual and search direction
  Set $r_{j+1} = r_j + \alpha_j \mathscr{H}_y[d_j]$
  Set $z_{j+1} = M^{-1} r_{j+1}$
  Set $\beta_{j+1} = g_y(z_{j+1}, r_{j+1}) / g_y(z_j, r_j)$
  Set $d_{j+1} = -z_{j+1} + \beta_{j+1} d_j$
end for

The benefit of the classical trust-region definition is that trust-region membership is easily determined, requiring only a norm calculation. The implicit trust-region, on the other hand, requires checking the value of the update vector under ρ. Furthermore, there are two occasions in the truncated CG method that require following a search direction to the edge of the trust-region. In the case of the implicit trust-region, this will not in general admit an analytical solution, and may require a search of ρ along the direction of interest. Each evaluation of ρ will require evaluating the objective function f, which will be unallowable in many applications. However, we show in Section 4 that in a specific but very important application—the symmetric eigenvalue problem—the IRTR algorithm can be implemented in a remarkably efficient way, and yields an algorithm that outperforms state-of-the-art methods on certain instances of the problem. In addition to providing an efficient application of the IRTR, this analysis will provide a new look at an existing eigensolver, the trace minimization method. Before this, Section 3 will show that the IRTR inherits all of the convergence properties of the RTR.

3 Convergence Analysis for IRTR

The mechanisms of the IRTR method are sufficiently different from those of the RTR method that we must construct a separate convergence theory, albeit one that is readily adapted from the classical trust-region theory. Section 3.1 describes conditions that guarantee global convergence to first-order critical points. Section 3.2 describes the local convergence behavior of the IRTR.

In the discussion that follows, (M,g) is a complete Riemannian manifold of dimension d and R is a retraction on M, as defined in (ABG06c). We assume that the domain of R is the whole of TM. We define

$$\hat{f} : TM \to \mathbb{R} : \xi \mapsto f(R(\xi)) \;, \tag{6}$$

and denote by $\hat{f}_x$ the restriction of $\hat{f}$ to T_xM, with gradient $\operatorname{grad} \hat{f}_x(0_x)$ abbreviated $\operatorname{grad} \hat{f}_x$. Recall from (2) that m_x has the form

$$m_x(\xi) = \hat{f}_x(0_x) + g_x\left(\xi, \operatorname{grad} \hat{f}_x\right) + \frac{1}{2} g_x\left(\xi, \mathscr{H}_x[\xi]\right) \;,$$

with a direction of steepest descent at the origin given by

$$p_x^{\mathrm{S}} = -\frac{\operatorname{grad} \hat{f}_x}{\|\operatorname{grad} \hat{f}_x\|} \;. \tag{7}$$

Similar to the convergence proofs for RTR, we will utilize the concept of a radially Lipschitz continuously differentiable function. This concept is defined here.

Definition 3.1 (Radially L-C^1 Function)**.** *Let $\hat{f} : TM \to \mathbb{R}$ be as in* (6)*. We say that $\hat{f}$ is radially Lipschitz continuously differentiable if there exist reals $\beta_{\mathrm{RL}} > 0$ and $\delta_{\mathrm{RL}} > 0$ such that, for all $x \in M$, for all $\xi \in T_xM$ with $\|\xi\| = 1$, and for all $t < \delta_{\mathrm{RL}}$, it holds*

$$\left| \frac{d}{d\tau} \hat{f}_x(\tau\xi) \,|_{\tau=t} - \frac{d}{d\tau} \hat{f}_x(\tau\xi) \,|_{\tau=0} \right| \leq \beta_{\mathrm{RL}} t \;. \tag{8}$$

3.1 Global Convergence Analysis

The main effort here regards the concept of the Cauchy point (see (NW99)). The Cauchy point is defined as the point inside the current trust-region which minimizes the quadratic model m_x along the direction of steepest descent of m_x. In trust-region methods employing a spherical or elliptical definitions of the trust-region, the Cauchy point is easily computed. This follows from the fact that moving along a tangent vector (in this case, the gradient of m_x) will cause you exit the trust-region only once and never re-enter it. However, for the IRTR method, depending on the function ρ_x, it may be possible to move along a tangent vector, exiting and re-entering the trust-region numerous times. Therefore, it may be difficult to compute the Cauchy point; in some cases, the Cauchy point may not even exist.

One solution is to restrict consideration to a local trust region. Definition 3.2 defines the relevant segment along the direction of steepest descent, and Definition 3.3 defines the local Cauchy point. Theorem 3.4 describes the form of the local Cauchy point, while Theorem 3.5 gives a bound on its decrease under the model m_x. All of these results are analogous to theorems and concepts from classical trust-region theory (see (CGT00; NW99)).

Definition 3.2 (Local Trust-Region)**.** *Consider an iterate $x \in M$, $\operatorname{grad} \hat{f}_x \neq 0$, and a model m_x as in* (2)*. Let ρ_x be defined as in* (3) *and let p_x^{S} be the direction of steepest descent of m_x, given in* (7)*. The local trust-region along p_x^{S} is given by the following set:*

$$\left\{ \tau p_x^{\mathrm{S}} : 0 < \tau \le \Delta_x \right\},$$

where Δ_x specifies the distance to the edge of the trust-region along p_x^{S}, given by

$$\Delta_x = \inf \left\{ \tau > 0 : \rho_x \left(\tau p_x^{\mathrm{S}} \right) < \rho' \right\} . \tag{9}$$

The local Cauchy point will fulfill the same role as the Cauchy point, except that it is confined to the local trust-region instead of the entirety of the trust-region. The formal definition follows.

Definition 3.3 (Local Cauchy Point)**.** *Consider an iterate $x \in M$, $\operatorname{grad} \hat{f}_x \neq 0$, and a model m_x. The local Cauchy point p_x^{L} is the point*

$$p_x^{\mathrm{L}} = \tau_x p_x^{\mathrm{S}} , \tag{10}$$

where

$$\tau_x = \operatorname*{argmin}_{0 \le \tau \le \Delta_x} m_x(\tau p_x^{\mathrm{S}}) ,$$

and where Δ_x and p_x^{S} are from Definition 3.3.

The local Cauchy point is easily computed without leaving the trust-region. This makes it an attractive target when solving the trust-region subproblem using a feasible point method (such as the truncated conjugate gradient method discussed in this paper). As such, the global convergence result for IRTR will require that every solution to the trust-region subproblem produce at least as much decrease in m_x as the local Cauchy point. Therefore, we wish to describe this decrease. Before that, we present some helpful properties of the local Cauchy point.

Theorem 3.4. *Consider an iterate $x \in M$, $\operatorname{grad} \hat{f}_x \neq 0$, and $\rho' \in (0,1)$. Then the local Cauchy point takes the form*

$$p_x^{\mathrm{L}} = \tau_x p_x^{\mathrm{S}},$$

where

$$\begin{aligned} \tau_x &= \begin{cases} \Delta_x, & \textit{if } \gamma_x \leq 0 \\ \min\left\{\Delta_x, \frac{\|\operatorname{grad} \hat{f}_x\|^3}{\gamma_x}\right\} & \textit{otherwise} \end{cases} \\ \gamma_x &= g_x\left(\operatorname{grad} \hat{f}_x, \mathscr{H}_x[\operatorname{grad} \hat{f}_x]\right) . \end{aligned}$$

Furthermore, if $\hat{f}_x$ is bounded below, then $\tau_x < \infty$.

Proof. Assume first that $\gamma_x \leq 0$. Then m_x monotonically decreases as we move along p_x^{S}, so that the minimizer along p_x^{S} inside $[0, \Delta_x]$ is $\tau_x p_x^{\mathrm{S}} = \Delta_x p_x^{\mathrm{S}}$.

Assume instead that $\gamma_x > 0$. Then m_x has a global minimizer along p_x^{S} at $\tau_* p_x^{\mathrm{S}}$, where

$$\tau_* = \frac{g_x\left(-p_x^{\mathrm{S}}, \operatorname{grad} \hat{f}_x\right)}{g_x\left(p_x^{\mathrm{S}}, \mathscr{H}_x[p_x^{\mathrm{S}}]\right)} = \frac{\|\operatorname{grad} \hat{f}_x\|^3}{\gamma_x} .$$

If $\tau_* \in (0, \Delta_x)$, then $\tau_x = \min\{\Delta_x, \tau_*\} = \tau_*$ is the minimizer of m_x along p_x^{S} in the local trust-region, and $\tau_x p_x^{\mathrm{S}}$ is the local Cauchy point. Otherwise, $\Delta_x \leq \tau_*$. Note that m_x monotonically decreases along p_x^{S} between $[0, \tau_*]$, so that the minimizer of m_x along p_x^{S} between $[0, \Delta_x]$ occurs at $\Delta_x = \min\{\Delta_x, \tau_*\} = \tau_x$, and $\tau_x p_x^{\mathrm{S}}$ is the local Cauchy point.

Assume now that $\hat{f}$ is bounded below. We will show that $\tau_x < \infty$. First consider when $\gamma > 0$. We have that $\tau_x = \min\{\tau_*, \Delta_x\}$. But τ_* is finite, so that τ_x is finite as well.

Consider now that $\gamma \leq 0$. Assume for the purpose of contradiction that $\tau_* = \infty$. Then $\Delta_x = \infty$, and for all $\tau > 0$, $\rho_x(\tau p_x^{\mathrm{S}}) \geq \rho'$. Then

$$\begin{aligned} \lim_{\tau\to\infty} \hat{f}_x(0) - \hat{f}_x(\tau p_x^{\mathrm{S}}) &= \lim_{\tau\to\infty} \rho_x(\tau p_x^{\mathrm{S}})\left(m_x(0) - m_x(\tau p_x^{\mathrm{S}})\right) \\ &\geq \lim_{\tau\to\infty} \rho'\left(m_x(0) - m_x(\tau p_x^{\mathrm{S}})\right) \\ &= \infty. \end{aligned}$$

But this contradicts the assumption that $\hat{f}$ is bounded below. Therefore, our initial assumption is false and τ_* is finite. $\square$

The next theorem concerns the decrease in m_x associated with the local Cauchy point, as described above. The proof is a straightforward modification of the classical result; see (ABG06c).

Theorem 3.5. *Take an iterate $x \in M$, $\operatorname{grad} \hat{f}_x \neq 0$, and $\rho' \in (0,1)$. Then the local Cauchy point p_x^{L} (as given in Theorem 3.4) has a decrease in m_x satisfying*

$$m_x(0) - m_x(p_x^{\mathrm{L}}) \geq \frac{1}{2} \|\operatorname{grad} \hat{f}_x\| \min \left\{ \Delta_x, \frac{\|\operatorname{grad} \hat{f}_x\|}{\|\mathscr{H}_x\|} \right\} .$$

The last result needed before presenting the global convergence result proves that, under the radially Lipschitz continuous assumption on $\hat{f}$, our local trust-region in the direction of steepest descent always maintains a certain size. The following lemmas guarantee this.

Lemma 3.6. *Assume that $\hat{f}$ is radially L-C^1. Assume that there exists $\beta_{\mathscr{H}} \in (0,\infty)$ such that $\|\mathscr{H}_x\| \leq \beta_{\mathscr{H}}$ for all $x \in M$. Then for all $\rho' \in (0,1)$, there exists a $\beta_\Delta > 0$ such that, for all $x \in M$, $\operatorname{grad} \hat{f}_x \neq 0$, and all $t \in (0,1]$,*

$$\rho_x\left(t \min\left\{\beta_\Delta \|\operatorname{grad} \hat{f}_x\|, \delta_{\mathrm{RL}}\right\} p_x^{\mathrm{S}}\right) \geq \rho'.$$

Proof. As a consequence of the radially L-C^1 property, we have that

$$\left| \hat{f}_x(\xi) - \hat{f}_x(0) - g_x\left(\operatorname{grad} \hat{f}_x, \xi\right) \right| \leq \frac{1}{2} \beta_{\mathrm{RL}} \|\xi\|^2 , \tag{11}$$

for all $x \in M$ and all $\xi \in T_x M$ such that $\|\xi\| \leq \delta_{\mathrm{RL}}$.

Note that

$$\rho_x(\xi) = \frac{\hat{f}_x(0) - \hat{f}_x(\xi)}{m_x(0) - m_x(\xi)} = 1 - \frac{\hat{f}_x(\xi) - m_x(\xi)}{m_x(0) - m_x(\xi)}.$$

Let $t \in (0,1]$. Let ξ be defined

$$\xi = t \min\left\{\beta_\Delta \|\operatorname{grad} \hat{f}_x\|, \delta_{\mathrm{RL}}\right\} p_x^{\mathrm{S}} .$$

Then

$$\rho_x(\xi) = 1 - \frac{\hat{f}_x(\xi) - m_x(\xi)}{m_x(0) - m_x(\xi)} . \tag{12}$$

Since

$$\hat{f}_x(\xi) - m_x(\xi) = \hat{f}_x(\xi) - \hat{f}_x(0) - g_x\left(\operatorname{grad} \hat{f}_x, \xi\right) - \frac{1}{2} g_x\left(\xi, \mathscr{H}_x[\xi]\right)$$

it follows from (11) and from the bound on $\|\mathscr{H}_x\|$ that

$$\left|\hat{f}_x(\xi)-m_x(\xi)\right| \le \frac{1}{2}\beta_{\mathrm{RL}}t^2\min{}^2\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\} + \frac{1}{2}\beta_{\mathscr{H}}t^2\min{}^2\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}\ . \tag{13}$$

Also note that

$$m_x(0)-m_x(\xi) = t\min\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}\|\operatorname{grad}\hat{f}_x\| - g_x(\xi,\mathscr{H}_x[\xi])$$

and

$$|m_x(0)-m_x(\xi)| \ge t\min\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}\|\operatorname{grad}\hat{f}_x\| - t^2\min{}^2\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}\beta_{\mathscr{H}}\ . \tag{14}$$

Then combining (13) and (14), we have

$$\begin{aligned}\frac{\left|\hat{f}_x(\xi)-m_x(\xi)\right|}{|m_x(0)-m_x(\xi)|} &\le \frac{1}{2}\frac{(\beta_{\mathrm{RL}}+\beta_{\mathscr{H}})t\min\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}}{\|\operatorname{grad}\hat{f}_x\|-t\min\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}\beta_{\mathscr{H}}}\\ &\le \frac{1}{2}\frac{(\beta_{\mathrm{RL}}+\beta_{\mathscr{H}})\beta_\Delta\|\operatorname{grad}\hat{f}_x\|}{\|\operatorname{grad}\hat{f}_x\|-\beta_\Delta\|\operatorname{grad}\hat{f}_x\|\beta_{\mathscr{H}}}\\ &= \frac{1}{2}\frac{(\beta_{\mathrm{RL}}+\beta_{\mathscr{H}})\beta_\Delta}{1-\beta_\Delta\beta_{\mathscr{H}}}\ ,\end{aligned}$$

because $t\min\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\} \le \beta_\Delta\|\operatorname{grad}\hat{f}_x\|$. Then it is easy to see that there exists $\beta_\Delta > 0$ such that

$$\frac{1}{2}\frac{(\beta_{\mathrm{RL}}+\beta_{\mathscr{H}})\beta_\Delta}{1-\beta_\Delta\beta_{\mathscr{H}}} < 1-\rho'\ .$$

□

Corollary 3.7 (Bound on Δ_x)**.** *It follows from Lemma 3.6 that, under the conditions required for the lemma,* $\Delta_x \ge \min\left\{\beta_\Delta\|\operatorname{grad}\hat{f}_x\|,\delta_{\mathrm{RL}}\right\}$.

The convergence theory of the RTR method (see (ABG06c)) provides two results on global convergence. The stronger of these results states that the accumulation points of any series generated by the algorithm are critical points of the objective function. Theorem 3.8 proves this for the IRTR method described in Algorithm 2.3.

Theorem 3.8 (Global Convergence)**.** *Let $\{x_k\}$ be a sequence of iterates produced by Algorithm 2.3, each* $\operatorname{grad} \hat{f}_x \neq 0$*, with $\rho' \in (0,1)$. Suppose that there exists $\beta_{\mathscr{H}} \in (0,\infty)$ such that each $\|\mathscr{H}_{x_k}\| \leq \beta_{\mathscr{H}}$. Suppose that each $\hat{f}_{x_k}$ is C^1, and that $\hat{f}$ is radially L-C^1 and bounded below on the level set*

$$\{x : f(x) \leq f(x_0)\}.$$

Further suppose that each update η_k produces at least as much decrease in m_{x_k} as a fixed fraction of the local Cauchy point. That is, for some constant $c_1 > 0$,

$$m_{x_k}(0) - m_{x_k}(\eta_k) \geq c_1 \|\operatorname{grad} \hat{f}_{x_k}\| \min\left\{\Delta_{x_k}, \frac{\|\operatorname{grad} \hat{f}_{x_k}\|}{\beta_{\mathscr{H}}}\right\},$$

where the terms in this inequality are from Theorem 3.5.

Then

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

Proof. Assume for the purpose of contradiction that the theorem does not hold. Then there exists $\varepsilon > 0$ such that, for all $K > 0$, there exists $k \geq K$ such that

$$\|\operatorname{grad} f(x_k)\| > \varepsilon.$$

From the workings of Algorithm 2.3,

$$\begin{aligned}
f(x_k) - f(x_{k+1}) &= \hat{f}_{x_k}(0) - \hat{f}_{x_k}(\eta_k) = \rho_{x_k}(\eta_k)\,(m_{x_k}(0) - m_{x_k}(\eta_k)) \\
&\geq \rho'\,(m_{x_k}(0) - m_{x_k}(\eta_k)) \\
&\geq \rho' c_1 \|\operatorname{grad} \hat{f}_{x_k}\| \min\left\{\Delta_{x_k}, \frac{\|\operatorname{grad} \hat{f}_{x_k}\|}{\beta_{\mathscr{H}}}\right\} \\
&\geq \rho' c_1 \|\operatorname{grad} \hat{f}_{x_k}\| \min\left\{\beta_\Delta \|\operatorname{grad} \hat{f}_x\|, \delta_{\mathrm{RL}}, \frac{\|\operatorname{grad} \hat{f}_{x_k}\|}{\beta_{\mathscr{H}}}\right\},
\end{aligned}$$

where the last inequality results from Corollary 3.7. Then for all $K > 0$, there exists $k \geq K$ such that

$$f(x_k) - f(x_{k+1}) \geq \rho' c_1 \varepsilon \min\left\{\beta_\Delta \varepsilon, \delta_{\mathrm{RL}}, \frac{\varepsilon}{\beta_{\mathscr{H}}}\right\} > 0.$$

But because f is bounded below and decreases monotonically with the iterates produced by the algorithm, we know that

$$\lim_{k\to\infty} (f(x_k) - f(x_{k+1})) = 0,$$

and we have reached a contradiction. Hence, our original assumption must be false, and the desired result is achieved. □

3.2 Local Convergence Analysis

The local convergence results for the IRTR require significantly less modification from the RTR than did the global convergence results. For the sake of brevity, only original proofs will be provided. Neglected proofs may be found in (ABG06c; ABG06a).

First, we ask one additional constraint be placed upon the retraction, in addition to the definition of retraction from (ABG06c). This is that that there exists some $\mu > 0$ and δ_μ such that

$$\|\xi\| \geq \mu d(x, R_x(\xi)), \quad \text{for all } x \in M, \text{ for all } \xi \in T_x M, \|\xi\| \leq \delta_\mu. \tag{15}$$

For the exponential retraction, (15) is satisfied as an equality, with $\mu = 1$. The bound is also satisfied when R is smooth and M is compact.

We will state a few preparatory lemmas before moving on the to local convergence results.

Lemma 3.9 (Taylor)**.** *Let $x \in M$, let V be a normal neighborhood of x, and let ζ be a C^1 tangent vector field on M. Then, for all $y \in V$,*

$$P_\gamma^{0\leftarrow 1}\zeta_y = \zeta_x + \nabla_\xi \zeta + \int_0^1 \left(P_\gamma^{0\leftarrow\tau}\nabla_{\gamma'(\tau)}\zeta - \nabla_\xi\zeta\right) d\tau,$$

where γ is the unique minimizing geodesic satisfying $\gamma(0) = x$ and $\gamma(1) = y$, and $\xi = \mathrm{Exp}_x^{-1} y = \gamma'(0)$.

Lemma 3.10. *Let $v \in M$ and let f be a C^2 cost function such that* $\operatorname{grad} f(v) = 0$ *and* $\operatorname{Hess} f(v)$ *is positive definite with maximal and minimal eigenvalues $\lambda_{\max}$ and $\lambda_{\min}$. Then, given $c_0 < \lambda_{\min}$ and $c_1 > \lambda_{\max}$, there exists a neighborhood V of v such that, for all $x \in V$, it holds that*

$$c_0 \mathit{dist}(v,x) \leq \|\operatorname{grad} f(x)\| \leq c_1 \mathit{dist}(v,x).$$

The first local convergence result states that the nondegenerate local minima are attractors of Algorithm 2.3/2.4. This theorem is unmodified from the same result for the RTR.

Theorem 3.11 (Local Convergence to Local Minimima)**.** *Consider Algorithm 2.3/2.4– i.e., the Implicit Riemannian Trust-Region algorithm where the trust-region subproblem* (1) *is solved using the modified truncated CG algorithm–with all the assumptions of Theorem 3.8 (Global Convergence). Let v be a nondegenerate local minimizer of f, i.e.,* $\operatorname{grad} f(v) = 0$ *and* $\operatorname{Hess} f(v)$ *is positive definite. Assume that $x \to \|\mathscr{H}_x^{-1}\|$ is bounded on a neighborhood of v and that* (15) *holds for some $\mu > 0$ and $\delta_\mu > 0$. Then there exists a neighborhood V of v such that, for all $x_0 \in V$, the sequence $\{x_k\}$ generated by Algorithm 2.3/2.4 converges to v.*

Now we study the order of convergence of the sequences that converge to a nondegenerate local minimizer. This result is the same as for the RTR, though the proof is modified somewhat. The new effort concerns the proof that the trust-region eventually becomes inactive as a stopping condition on the truncated CG.

Theorem 3.12 (Order of Local Convergence)**.** *Consider Algorithm 2.3/2.4. Suppose that R is C^2 retraction, that f is a C^2 cost function on M, and that*

$$\|\mathscr{H}_{x_k} - \operatorname{Hess}\hat{f}_{x_k}(0_{x_k})\| \leq \beta_{\mathscr{H}} \|\operatorname{grad} f(x_k)\|, \tag{16}$$

that is, $\mathscr{H}_{x_k}$ is a sufficiently good approximation of $\operatorname{Hess}\hat{f}_{x_k}(0_{x_k})$. Let $v \in M$ be a nondegenerate local minimizer of f, (i.e., $\operatorname{grad} f(v) = 0$ and $\operatorname{Hess} f(v)$ is positive definite). Further assume that $\operatorname{Hess}\hat{f}_x(0_x)$ is Lipschitz-continuous at 0_x uniformly in a neighborhood of v, i.e., there exist β_{L2}, $\delta_1 > 0$ and $\delta_2 > 0$ such that, for all $x \in B_{\delta_1}(v)$ and all $\xi \in B_{\delta_2}(0_x)$, there holds

$$\|\operatorname{Hess}\hat{f}_x(\xi) - \operatorname{Hess}\hat{f}_x(0_x)\| \leq \beta_{\mathrm{L2}}\|\xi\|. \tag{17}$$

Then there exists $c \geq 0$ such that, for all sequences $\{x_k\}$ generated by the algorithm converging to v, there exists $K > 0$ such that for all $k > K$,

$$dist(x_{k+1}, v) \leq c\,(dist(x_k, v))^{\min\{\theta+1,2\}}.$$

Proof. We will show below that there exist $\tilde{\Delta}$, c_0, c_1, c_2, c_3, c_3', c_4, and c_5 such that, for all sequences $\{x_k\}$ satisfying the conditions asserted, all $x \in M$, all ξ with $\|\xi\| \leq \tilde{\Delta}$, and all k greater than some K, there holds

$$c_0 \operatorname{dist}(v, x_k) \leq \|\operatorname{grad} f(x_k)\| \leq c_1 \operatorname{dist}(v, x_k), \tag{18}$$

$$\|\eta_k\| \leq c_4 \|\operatorname{grad} m_{x_k}(0_{x_k})\| \leq \tilde{\Delta}, \tag{19}$$

$$\|\operatorname{grad} f(R_{x_k}(\xi))\| \leq c_5 \|\operatorname{grad} \hat{f}_{x_k}(\xi)\|, \tag{20}$$

$$\|\operatorname{grad} m_{x_k}(\xi) - \operatorname{grad} \hat{f}_{x_k}(\xi)\| \leq c_3\|\xi\|^2 + c_3'\|\operatorname{grad} f(x_k)\|\|\xi\|, \tag{21}$$

$$\|\operatorname{grad} m_{x_k}(\eta_k)\| \leq c_2 \|\operatorname{grad} m_{x_k}(0)\|^{\theta+1}, \tag{22}$$

where $\{\eta_k\}$ is the sequence of update vectors corresponding to $\{x_k\}$. With these results at hand, the proof is concluded as follows. For all $k > K$, it follows from (18) that

$$c_0 \operatorname{dist}(v, x_{k+1}) \leq \|\operatorname{grad} f(x_{k+1})\| = \|\operatorname{grad} f(R_{x_k}(\eta_k))\|,$$

and from (20) that

$$\|\operatorname{grad} f(R_{x_k}(\eta_k))\| \leq c_5 \|\operatorname{grad} \hat{f}_{x_k}(\eta_k)\|,$$

and from (19) and (21) and (22) that

$$\begin{aligned}\|\operatorname{grad}\hat{f}_{x_k}(\eta_k)\| &\le \|\operatorname{grad} m_{x_k}(\eta_k)-\operatorname{grad}\hat{f}_{x_k}(\eta_k)\|+\|\operatorname{grad} m_{x_k}(\eta_k)\|\\ &\le (c_3c_4^2+c_3'c_4)\|\operatorname{grad} m_{x_k}(0)\|^2+c_2\|\operatorname{grad} m_{x_k}(0)\|^{\theta+1},\end{aligned}$$

and from (18) that

$$\|\operatorname{grad} m_{x_k}(0)\| = \|\operatorname{grad} f(x_k)\| \le c_1\operatorname{dist}(v,x_k).$$

Consequently, taking K larger if necessary so that $\operatorname{dist}(v,x_k)<1$ for all $k>K$, it follows that

$$\begin{aligned}c_0\operatorname{dist}(v,x_{k+1}) &\le \|\operatorname{grad} f(x_{k+1})\|\\ &\le c_5(c_3c_4^2+c_3'c_4)\|\operatorname{grad} f(x_k)\|^2+c_5c_2\|\operatorname{grad} f(x_k)\|^{\theta+1}\\ &\le c_5((c_3c_4^2+c_3'c_4)c_1^2(\operatorname{dist}(v,x_k))^2+c_2c_1^{\theta+1}(\operatorname{dist}(v,x_k))^{\theta+1})\\ &\le c_5((c_3c_4^2+c_3'c_4)c_1^2+c_2c_1^{\theta+1})(\operatorname{dist}(v,x_k))^{\min\{2,\theta+1\}}\end{aligned}$$

for all $k>K$, which is the desired result. It remains to prove the bounds (18)-(22).

Equation (18) comes from Lemma 3.10 and is due to the fact that v is a nondegenerate critical point. Equations (19)-(21) are proved in (ABG06c).

It remains only to prove (22). Let γ_k denote $\|\operatorname{grad} f(x_k)\|$. It follows from the definition of ρ_k that

$$\rho_k-1=\frac{m_{x_k}(\eta_k)-\hat{f}_{x_k}(\eta_k)}{m_{x_k}(0_{x_k})-m_{x_k}(\eta_k)}. \tag{23}$$

From Taylor's theorem (3.9), there holds

$$\hat{f}_{x_k}(\eta_k)=\hat{f}_{x_k}(0_{x_k})+g_{x_k}(\operatorname{grad} f(x_k),\eta_k)+\int_0^1 g_{x_k}\left(\operatorname{Hess}\hat{f}_{x_k}(\tau\eta_k)[\eta_k],\eta_k\right)(1-\tau)d\tau.$$

It follows that

$$\begin{aligned}\left|m_{x_k}(\eta_k)-\hat{f}_{x_k}(\eta_k)\right| &= \left|\int_0^1\left(g_{x_k}(\mathscr{H}_{x_k}[\eta_k],\eta_k)-g_{x_k}\left(\operatorname{Hess}\hat{f}_{x_k}(\tau\eta_k)[\eta_k],\eta_k\right)\right)(1-\tau)d\tau\right|\\ &\le \int_0^1\left|g_{x_k}\left((\mathscr{H}_{x_k}-\operatorname{Hess}\hat{f}_{x_k}(0_{x_k}))[\eta_k],\eta_k\right)\right|(1-\tau)d\tau\\ &\quad+\int_0^1\left|g_{x_k}\left((\operatorname{Hess}\hat{f}_{x_k}(0_{x_k})-\operatorname{Hess}\hat{f}(\tau\eta_k))[\eta_k],\eta_k\right)\right|(1-\tau)d\tau\\ &\le \frac{1}{2}\beta_{\mathscr{H}}\gamma_k\|\eta_k\|^2+\frac{1}{6}\beta_{\mathrm{L2}}\|\eta_k\|^3.\end{aligned}$$

It then follows from (23), using the bound on the Cauchy decrease, that

$$\|\rho_k-1\| \le \frac{(3\beta_{\mathscr{H}}\gamma_k+\beta_{\mathrm{L2}}\|\eta_k\|)\|\eta_k\|^2}{6\gamma_k\min\{\Delta_k,\gamma_k/\beta\}},$$

where β is an upper bound on the norm of $\mathscr{H}_{x_k}$. Since $\Delta_k \geq \min\{\beta_\Delta \gamma_k, \delta_{\mathrm{RL}}\}$ (Corollary 3.7) and $\lim_{k\to\infty} \gamma_k = 0$ (in view of Theorem 3.8), we can choose K large enough that $\Delta_k \geq \beta_\Delta \gamma_k$, for all $k > K$. This and $\|\eta_k\| \leq c_4 \gamma_k$ yield

$$\|\rho_k - 1\| \leq \frac{(3\beta_{\mathscr{H}} + \beta_{\mathrm{L2}} c_4) c_4^2 \gamma_k^3}{6 \min\left\{\beta_\Delta, \frac{1}{\beta}\right\} \gamma_k^2}.$$

Since $\lim_{k\to\infty} \gamma_k = 0$, it follows that $\lim_{k\to\infty} \rho_k = 1$.

Therefore, the trust-region eventually becomes inactive as a stopping criterion for the truncated CG. Furthermore, because $\{x_k\}$ converges to v and $\operatorname{Hess} f(v)$ is positive definite, it follows that $\mathscr{H}_{x_k}$ is positive definite for all k greater than a certain K. This eliminates negative curvature of the Hessian as a stopping criterion for truncated CG.

This means that the truncated CG loop terminates only after sufficient reduction has been made in $\|\operatorname{grad} m_{x_k}(\eta_k)\|$ with respect to $\|\operatorname{grad} m_{x_k}(0_{x_k})\|$:

$$\|\operatorname{grad} m_{x_k}(\eta_k)\| \leq \|\operatorname{grad} m_{x_k}(0_{x_k})\|^{\theta+1},$$

(choosing K large enough that $\|\operatorname{grad} m_{x_k}(0_{x_k})\|^{\theta} < \kappa$ for all $k > K$), or the model minimization has been solved exactly, in which case $\operatorname{grad} m_{x_k}(\eta_k) = 0$. In either case, we have satisfied (22). □

4 Application: Extreme Symmetric Generalized Eigenspaces

We will demonstrate the applicability of IRTR for the solution of generalized eigenvalue problems. Given two $n \times n$ matrices, λ is an eigenvalue if there exists a non-zero vector v such that

$$Av = Bv\lambda.$$

If A is symmetric and B is symmetric/positive definite then the generalized eigenvalue problem is said to be symmetric/positive definite. In this case, the eigenvalues are all real and the eigenvectors are B-orthogonal (and can be chosen B-orthonormal).

Let the eigenvalues of the pencil (A, B) be $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. Consider the p leftmost eigenvalues, $\lambda_1, \ldots, \lambda_p$, and corresponding eigenvectors $v_1, \ldots, v_p$. We will assume below, though it is not strictly necessary, that $\lambda_p < \lambda_{p+1}$. It is known that the $n \times p$ matrix containing the leftmost eigenvectors is a global minimizer of the generalized Rayleigh quotient

$$f : \mathbb{R}_*^{n\times p} \to \mathbb{R} : Y \mapsto \operatorname{trace}\left((Y^T BY)^{-1}(Y^T AY)\right),$$

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

It is easily shown that the generalized Rayleigh quotient depends only on $\mathrm{colsp}(Y)$. Therefore, f induces a real-valued function on the set of p-dimensional subspaces of $\mathbb{R}^n$. This set is the Grassmann manifold $\mathrm{Grass}(p,n)$, and it can be endowed with a Riemannian structure. The Riemannian trust-region method has previously been applied to finding extreme eigenspaces of a symmetric/positive definite matrix pencil (in (ABG06b; ABG06c; ABGS05; BAG06)). The manifold optimization problem is stated as follows.

As in (ABG06c; AMS04), we will treat the Grassman manifold $\mathrm{Grass}(p,n)$ as the quotient manifold $\mathbb{R}_*^{n\times p}/\mathrm{GL}_p$ of the non-compact Stiefel by the set of transformations that preserves column space. In this approach, a subspace in $\mathrm{Grass}(p,n)$ is represented by any $n \times p$ matrix whose columns span the subspace. A real function h on $\mathrm{Grass}(p,n)$ is thereby represented by its lift $h_\uparrow(Y) = h(\mathrm{colsp}(Y))$. To represent a tangent vector ξ to $\mathrm{Grass}(p,n)$ at a point $\mathscr{Y} = \mathrm{colsp}(Y)$, we will define a horizontal space H_Y. Then ξ is uniquely represented by its horizontal lift $\xi_{\uparrow Y}$, which is in turn defined by the following conditions: (i) $\xi_{\uparrow Y} \in H_Y$ and (ii) $\mathrm{D}h(\mathscr{Y})[\xi] = Dh_\uparrow(Y)[\xi_{\uparrow Y}]$ for all real functions h on $\mathrm{Grass}(p,n)$. In this way, the horizontal space H_Y represents the tangent space $T_\mathscr{Y}\mathrm{Grass}(p,n)$. For more information, see (ABG06c; AMS04).

To simplify the derivation of the gradient and Hessian of the Rayleigh cost function, we define the horizontal space as

$$H_Y = \left\{ Z \in \mathbb{R}^{n\times p} : Z^T BY = 0 \right\}. \tag{24}$$

We will employ a (non-canonical) Riemannian metric g defined as

$$g_\mathscr{Y}(\xi,\zeta) = \mathrm{trace}\left((Y^T BY)^{-1} \xi_{\uparrow Y}^T \zeta_{\uparrow Y} \right), \tag{25}$$

and a retraction chosen as

$$R_\mathscr{Y}(\xi) = \mathrm{colsp}(Y + \xi_{\uparrow Y}) \tag{26}$$

The objective function is the the generalized Rayleigh quotient, defined from this point forward as follows:

$$f : \mathrm{Grass}(p,n) \to \mathbb{R} : \mathrm{colsp}(Y) \mapsto \mathrm{trace}\left((Y^T BY)^{-1}(Y^T AY) \right). \tag{27}$$

The retraction is used to lift this function from the manifold to the tangent plane, yielding

$$\hat{f} : T\mathrm{Grass}(p,n) \to \mathbb{R} : \xi \mapsto f(R(\xi)), \tag{28}$$

and, as before, $\hat{f}_\mathscr{Y}$ is this function restricted to $T_\mathscr{Y}\mathrm{Grass}(p,n)$.

We denote by $P_{BY} = I - BY(Y^TB^2Y)^{-1}Y^TB$ the orthogonal projector onto the horizontal space H_Y. An expansion of $\hat{f}_{\mathscr{Y}}$ yields:

$$\begin{aligned}\hat{f}_{\mathscr{Y}}(\xi) &= \operatorname{trace}\left(\left((Y+\xi_{\uparrow Y})^T B(Y+\xi_{\uparrow Y})\right)^{-1}(Y+\xi_{\uparrow Y})^T A(Y+\xi_{\uparrow Y})\right)\\ &= \operatorname{trace}\left((Y^TBY)^{-1}Y^TAY\right) + 2\operatorname{trace}\left((Y^TBY)^{-1}\xi_{\uparrow Y}^T AY\right)\\ &\quad + \operatorname{trace}\left((Y^TBY)^{-1}\xi_{\uparrow Y}^T\left(A\xi_{\uparrow Y} - B\xi_{\uparrow Y}(Y^TBY)^{-1}Y^TAY\right)\right) + HOT\\ &= \operatorname{trace}\left((Y^TBY)^{-1}Y^TAY\right) + 2\operatorname{trace}\left((Y^TBY)^{-1}\xi_{\uparrow Y}^T P_{BY}AY\right)\\ &\quad + \operatorname{trace}\left((Y^TBY)^{-1}\xi_{\uparrow Y}^T P_{BY}\left(A\xi_{\uparrow Y} - B\xi_{\uparrow Y}(Y^TBY)^{-1}Y^TAY\right)\right) + HOT,\end{aligned} \tag{29}$$

where the introduction of the projectors does not modify the expression since $P_{BY}\xi_{\uparrow Y} = \xi_{\uparrow Y}$. Then using the Riemannian metric (25), we can make the following identifications:

$$(\operatorname{grad} f(\mathscr{Y}))_{\uparrow Y} = \left(\operatorname{grad} \hat{f}_{\mathscr{Y}}(0_{\mathscr{Y}})\right)_{\uparrow Y} = 2P_{BY}AY, \tag{30}$$

$$\left(\operatorname{Hess} \hat{f}_{\mathscr{Y}}(0_{\mathscr{Y}})[\xi]\right)_{\uparrow Y} = 2P_{BY}\left(A\xi_{\uparrow Y} - B\xi_{\uparrow Y}(Y^TBY)^{-1}Y^TAY\right). \tag{31}$$

An efficient implementation of the implicit RTR requires an understanding of the improvement ratio ρ, repeated here:

$$\rho_{\mathscr{Y}}(\xi) = \frac{\hat{f}_{\mathscr{Y}}(0_{\mathscr{Y}}) - \hat{f}_{\mathscr{Y}}(\xi)}{m_{\mathscr{Y}}(0_{\mathscr{Y}}) - m_{\mathscr{Y}}(\xi)},$$

where $m_{\mathscr{Y}}$ is the quadratic model chosen to approximate $\hat{f}_{\mathscr{Y}}$:

$$m_{\mathscr{Y}}(\xi) = f(\mathscr{Y}) + g_{\mathscr{Y}}(\operatorname{grad} f(\mathscr{Y}), \xi) + \frac{1}{2} g_{\mathscr{Y}}(\mathscr{H}_{\mathscr{Y}}[\xi], \xi). \tag{32}$$

Note that the model Hessian $\mathscr{H}_{\mathscr{Y}}$ has been left unspecified, as its effect on $m_{\mathscr{Y}}$, and therefore on $\rho_{\mathscr{Y}}$, may cause us to prefer one form over another. In the discussion that follows, we will examine two choices for the model Hessian.

4.1 Case 1: TRACEMIN Model

We assumed above the matrices A and B are both symmetric and that B is positive definite. Consider the case now where A is positive semi-definite, and that we have chosen for the model Hessian the operator

$$(\mathscr{H}_{\mathscr{Y}}[\xi])_{\uparrow Y} = 2P_{BY}AP_{BY}\xi_{\uparrow Y}.$$

Note that this operator is symmetric/positive definite, so that the model minimization problem is well-defined. Assume also that the basis Y representing $\mathscr{Y}$ is B-orthonormal (this is easily enforced in the retraction). This assumption simplifies many of the formulas. Take some update vector $\eta \in T_{\mathscr{Y}}\text{Grass}(p,n)$ produced by (approximately) minimizing $m_{\mathscr{Y}}$. We assume nothing of η except that it does produces a decrease in $m_{\mathscr{Y}}$, i.e. $m_{\mathscr{Y}}(0_{\mathscr{Y}}) - m_{\mathscr{Y}}(\eta) > 0$.

Consider the form of ρ:

$$\rho_{\mathscr{Y}}(\eta) = \frac{f(\mathscr{Y}) - f(R_{\mathscr{Y}}(\eta))}{m_{\mathscr{Y}}(0_{\mathscr{Y}}) - m_{\mathscr{Y}}(\eta)} = \frac{f(\mathscr{Y}) - f(R_{\mathscr{Y}}(\eta))}{f(\mathscr{Y}) - m_{\mathscr{Y}}(\eta)}. \tag{33}$$

The following developments allow us to say more about the value $\rho_{\mathscr{Y}}(\eta)$:

$$\begin{aligned} f(R_{\mathscr{Y}}(\eta)) &= f(\text{colsp}(Y + \eta_{\uparrow Y})) = f_{\uparrow}(Y + \eta_{\uparrow Y}) \\ &= \text{trace}\left(\left((Y + \eta_{\uparrow Y})^T B (Y + \eta_{\uparrow Y}) \right)^{-1} (Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y}) \right) \\ &= \text{trace}\left((I + \eta_{\uparrow Y}^T B \eta_{\uparrow Y})^{-1} (Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y}) \right). \end{aligned} \tag{34}$$

$$\begin{aligned} m_{\mathscr{Y}}(\eta) &= f(\text{colsp}(Y)) + g_{\mathscr{Y}}\left(\text{grad}\, f(\mathscr{Y}), \eta\right) + \frac{1}{2} g_{\mathscr{Y}}\left(\mathscr{H}_{\mathscr{Y}}[\eta], \eta\right) \\ &= \text{trace}\left(Y^T A Y\right) + 2\text{trace}\left(\eta_{\uparrow Y}^T A Y\right) + \text{trace}\left(\eta_{\uparrow Y}^T A \eta_{\uparrow Y}\right) \\ &= \text{trace}\left((Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y})\right). \end{aligned} \tag{35}$$

Because B is symmetric/positive definite, then $I + \eta_{\uparrow Y}^T B \eta_{\uparrow Y}$ is also symmetric/positive definite with eigenvalues greater than or equal to one. Then $(I + \eta_{\uparrow Y}^T B \eta_{\uparrow Y})^{-1}$ is symmetric/positive definite with eigenvalues less than or equal to one. Since A is symmetric/positive semi-definite, then $(Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y})$ is symmetric/positive semi-definite. Then we know that

$$\text{trace}\left((I + \eta_{\uparrow Y}^T B \eta_{\uparrow Y})^{-1} (Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y})\right) \le \text{trace}\left((Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y})\right).$$

This, along with (34) and (35), yields:

$$f(R_{\mathscr{Y}}(\eta)) \le m_{\mathscr{Y}}(\eta). \tag{36}$$

Substituting this result back into (33), we obtain the following:

$$\rho_{\mathscr{Y}}(\eta) = \frac{f(\mathscr{Y}) - f(R_{\mathscr{Y}}(\eta))}{f(\mathscr{Y}) - m_{\mathscr{Y}}(\eta)} \ge 1.$$

This means that for any $\rho' \in (0,1)$ and any tangent vector $\eta \in T_{\mathscr{Y}}\text{Grass}(p,n)$ which produces a decrease in the model (35), we have that $\rho_{\mathscr{Y}}(\eta) \ge 1 > \rho'$, i.e., η is in the implicit trust-region.

The truncated CG iteration (Algorithm 2.4) computes iterates which are monotonically decreasing under the quadratic model. Therefore, these iterates are all member of the trust-region. This, combined with the positive definiteness of the chosen Hessian, ensures that the truncated CG will terminate only after reaching the desired residual decrease. It is, in effect, an inexact Newton iteration with an approximate Hessian.

The resulting algorithm is nearly identical to the trace minimization algorithm (see (ST00; SW82)). TRACEMIN computes the leftmost eigenpairs of a symmetric/positive definite matrix pencil $(A,B))$ by minimizing the function

$$\operatorname{trace}(Y^T AY)$$

for $Y^T BY = I_p$. The proposed iteration selects Y_{k+1} as a B-orthonormal basis for $Y_k - \Delta$, where Δ (approximately) solves the following:

$$\text{minimize } (Y_k - \Delta)^T A(Y_k - \Delta), \quad \text{subject to } Y_k^T B\Delta = 0. \tag{37}$$

The significant difference between TRACEMIN and the RTR/IRTR algorithm described above involves the solution of the model minimizations (32) and (37), and this difference illustrates an easily overlooked characteristic of the IRTR/truncated CG approach: while the model minimization for the chosen representation can be written as a system of simultaneous linear equations

$$P_{BY}AP_{BY}\eta_{\uparrow Y} = -P_{BY}AY,$$

the RTR/IRTR computes a solution using a single-vector iteration. This is equivalent to applying CG to solving the linear system

$$\begin{bmatrix} P_{BY}AP_{BY} & & & \\ & P_{BY}AP_{BY} & & \\ & & \ddots & \\ & & & P_{BY}AP_{BY} \end{bmatrix} \begin{bmatrix} \eta_{\uparrow Y}e_1 \\ \eta_{\uparrow Y}e_2 \\ \vdots \\ \eta_{\uparrow Y}e_p \end{bmatrix} = - \begin{bmatrix} P_{BY}AYe_1 \\ P_{BY}AYe_2 \\ \vdots \\ P_{BY}AYe_p \end{bmatrix}.$$

This is because the $n \times p$ <u>matrix</u> $\eta_{\uparrow Y}$ represents a tangent <u>vector</u> η. This should be contrasted against the p independent equations solved in TRACEMIN.

Another consequence of the Hessian choice $(\mathscr{H}_{\mathscr{Y}}[\xi])_{\uparrow Y} = 2P_{BY}AP_{BY}\xi_{\uparrow Y}$ is that it does not adequately approximate the actual Hessian of $\hat{f}$. As a result, the method yields only a linear rate of convergence. This result was known by the authors of TRACEMIN, due to the relationship between optimal TRACEMIN and the subspace iteration method (see (ST00; SW82)). The approach in the following subsection addresses the slow convergence by using a more accurate model Hessian.

4.2 Case 2: Newton Model

Consider the case where the quadratic model $m_{\mathscr{Y}}$ is chosen as the Newton model, i.e., the quadratic Taylor expansion of $\hat{f}_{\mathscr{Y}}$:

$$m_{\mathscr{Y}}(\xi) = f(\mathscr{Y}) + g_{\mathscr{Y}}(\text{grad} f(\mathscr{Y}), \xi) + \frac{1}{2} g_{\mathscr{Y}} \left(\text{Hess} \hat{f}_{\mathscr{Y}}(0_{\mathscr{Y}})[\xi], \xi\right).$$

We wish to perform an analysis of $\rho_{\mathscr{Y}}$ for the Newton model just as we did for the TRACEMIN model. Assume as before that $\mathscr{Y}$ is represented by a B-orthonormal basis, i.e. $Y^T BY = I$. Take some tangent vector $\eta \in T_{\mathscr{Y}}\text{Grass}(p,n)$. Consider the denominator of $\rho_{\mathscr{Y}}(\eta)$:

$$\begin{aligned} m_{\mathscr{Y}}(0_{\mathscr{Y}}) - m_{\mathscr{Y}}(\eta) &= -g_{\mathscr{Y}}(\text{grad} f(\mathscr{Y}), \eta) - \frac{1}{2} g_{\mathscr{Y}}(\mathscr{H}_{\mathscr{Y}}[\eta], \eta) \\ &= -2\text{trace}\left(\eta_{\uparrow Y}^T AY\right) - \text{trace}\left(\eta_{\uparrow Y}^T A \eta_{\uparrow Y} - \eta_{\uparrow Y}^T B \eta_{\uparrow Y} Y^T AY\right) \\ &= \text{trace}\left(\eta_{\uparrow Y}^T B \eta_{\uparrow Y} Y^T AY - 2\eta_{\uparrow Y}^T AY - \eta_{\uparrow Y}^T A \eta_{\uparrow Y}\right) \\ &= \text{trace}\left(\hat{M}\right), \end{aligned} \tag{38}$$

for $\hat{M} = \eta_{\uparrow Y}^T B \eta_{\uparrow Y} Y^T AY - 2\eta_{\uparrow Y}^T AY - \eta_{\uparrow Y}^T A \eta_{\uparrow Y}$. Consider the numerator:

$$\begin{aligned} \hat{f}_{\mathscr{Y}}(0_{\mathscr{Y}}) - \hat{f}_{\mathscr{Y}}(\eta) &= f(\text{colsp}(Y)) - f(\text{colsp}(Y + \eta_{\uparrow Y})) \\ &= \text{trace}\left(Y^T AY - \left((Y + \eta_{\uparrow Y})^T B (Y + \eta_{\uparrow Y})\right)^{-1} (Y + \eta_{\uparrow Y})^T A (Y + \eta_{\uparrow Y})\right) \\ &= \text{trace}\left(\left(I + \eta_{\uparrow Y}^T B \eta_{\uparrow Y}\right)^{-1} \left(\eta_{\uparrow Y}^T B \eta_{\uparrow Y} Y^T AY - 2\eta_{\uparrow Y}^T AY - \eta_{\uparrow Y}^T A \eta_{\uparrow Y}\right)\right) \\ &= \text{trace}\left((I + \eta_{\uparrow Y}^T B \eta_{\uparrow Y})^{-1} \hat{M}\right). \end{aligned} \tag{39}$$

This formula, to our knowledge, does not in general admit any useful information about $\rho_{\mathscr{Y}}(\eta)$. However, in the specific case of $p = 1$, we see that

$$\rho_{\mathscr{Y}}(\eta) = \frac{1}{1 + \eta_{\uparrow Y}^T B \eta_{\uparrow Y}}. \tag{40}$$

This formula for $\rho_{\mathscr{Y}}$ enables the two actions required to efficiently implement the IRTR: an efficient method for evaluating $\rho_{\mathscr{Y}}(\eta)$; and the ability to efficiently move along a search direction to the edge of the trust-region. The result is an inexact Newton iteration along with stopping criterion that ensure strong global convergence results and a fast rate of local convergence.

This technique, like that resulting from applying the RTR to this problem, has many similarities to the Jacobi-Davidson method (see, for example, (SV96)).

In (Not02), the author developed an analysis which (inexpensively) provides knowledge of the residual of the outer (eigenvalue) iteration based on the conjugate gradient coefficients used to solve the Jacobi-Davidson correction equation. Notay suggests exploiting this information as a stopping criterion for the inner iteration. His suggestion involves stopping the inner iteration when the marginal decrease in the outer residual is less than some fraction of the marginal decrease in the inner residual. The implicit trust-region, on the other hand, is comprised of strictly those points where the decrease under the objective function is some fraction of the decrease of the quadratic model. In this regard, both approaches strive to stop the inner iteration when it becomes inefficient or irrelevant with regard to the outer iteration, though the IRTR does this in a way that yields strong global convergence results.

The next section examines the performance of the IRTR for computing the leftmost eigenpair of a symmetric/positive definite matrix pencil.

5 Numerical Results

This section illustrates the potential efficiency of the IRTR method over the RTR method for the problem of computing the leftmost eigenpair of a symmetric/positive definite matrix pencil. The IRTR is also compared against the LOBPCG method from (Kny01), as implemented in (HL06). This method was chosen because it implements a state-of-the-art optimization-oriented, CG-based eigensolver. Both methods were implemented in the Anasazi eigensolver package of the Trilinos package (see (BHLT05) and (HBH$^+$03)). Tests were conducted using a single processor, on a PowerMac with dual 2.5 GHz G5 processors and 8 GB of memory.

The pencil used for experimentation derives from a finite element discretization (with linear basis functions) of a one-dimensional Laplacian. The parameter n refers to the number of elements in the discretization. The parameter ρ' is the acceptance parameter. IRTR was evaluated for multiple values of ρ', to illustrate the effect of the parameter on the efficiency of the method. Table 1 lists the results of the comparison.

This testing shows that the IRTR has the potential to exceed the performance of the RTR, while maintaining competitiveness against methods designed specifically for solving this class of problems.

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Table 1: Experimental comparison of IRTR, RTR and LOBPCG methods. n denotes the problem size, while the numbers in the table indicate runtime in seconds. The parameter to RTR and IRTR denotes the value of ρ'.

n	RTR(.1)	IRTR(.1)	IRTR(.45)	IRTR(.90)	LOBPCG
100	0.040	0.038	**0.027**	0.031	0.103
500	0.227	0.448	0.298	**0.185**	2.414
1,000	0.524	0.596	0.592	**0.383**	1.794
10,000	36.38	54.36	**27.66**	42.25	130.3
50,000	**850**	2985	1221	1202	3819

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