Structured Quasi-Newton Methods for Optimization with Orthogonality Constraints

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Outline

- Related applications
- Preliminaries on Riemannian optimization
- Adaptive regularized quasi-Newton method
- Numerical experiments

Outline

Electronic structure calculation: Kohn-Sham

- Kohn-Sham total energy minimization

$$\min_{X \in \mathbf{C}^{n\times p}} \quad E_{ks}(X) \quad \text{s.t.} \quad X^*X = I_p,$$

$$E_{ks}(X) := \frac{1}{4}\mathrm{tr}(X^*LX) + \frac{1}{2}\mathrm{tr}(X^*V_{ion}X) + \frac{1}{2}\sum_l\sum_i |x_i^* w_l|^2 + \frac{1}{4}\rho^\top L^\dagger \rho + \frac{1}{2}e^\top \epsilon_{xc}(\rho),$$

where $\rho := \rho(X) = \mathrm{diag}(XX^*)$.

- The Euclidean gradient and Hessian

$$\nabla E_{ks}(X) = H_{ks}(\rho)X, \quad \nabla^2 E_{ks}(X)[U] = H_{ks}(\rho)U + R(X)[U],$$

$$H_{ks}(\rho) := \frac{1}{2}L + V_{ion} + \sum_l w_l w_l^* + \mathrm{Diag}((\Re L^\dagger)\rho) + \mathrm{Diag}(\mu_{xc}(\rho)^* e),$$

$$R(X)[U] := \mathrm{Diag}\left((\Re L^\dagger + \frac{\partial^2 \epsilon_{xc}}{\partial \rho^2}e)(\bar{X}\odot U + X \odot \bar{U})e\right)X.$$

- First-order optimality: $H_{ks}(\rho)X = X\Lambda,\ X^*X = I_p$.

Fock exchange operator

- The operator $\mathcal{V}(\cdot) : \mathbf{C}^{n\times n} \to \mathbf{C}^{n\times n}$ is a fourth-order tensor
- For any $D_1, D_2 \in \mathbf{C}^{n\times n}$: $\langle \mathcal{V}(D_1), D_2\rangle = \langle \mathcal{V}(D_2), D_1\rangle$ and

$$\langle \mathcal{V}(D_1 + D_2), D_1 + D_2\rangle = \langle \mathcal{V}(D_1), D_1\rangle + 2\langle \mathcal{V}(D_1), D_2\rangle + \langle \mathcal{V}(D_2), D_2\rangle .$$

- Computing $\mathcal{V}(U)$ is very expensive since it needs to perform the multiplication between a $n \times n \times n \times n$ fourth-order tensor and a n-by-n matrix.
- The corresponding Fock energy is defined as

$$E_f(X) := \frac{1}{4}\langle \mathcal{V}(XX^*)X, X\rangle = \frac{1}{4}\langle \mathcal{V}(XX^*), XX^*\rangle . \tag{1}$$

Electronic structure calculation: Hartree-Fock

Hartree-Fock total energy minimization

$$\min_{X \in \mathbf{C}^{n\times p}} \quad E_{hf}(X) \quad \text{s.t.} \quad X^*X = I_p,$$

$$E_{ks}(X) := \frac{1}{4}\mathrm{tr}(X^*LX) + \frac{1}{2}\mathrm{tr}(X^*V_{ion}X) + \frac{1}{2}\sum_l \sum_i \zeta_l |x_i^* w_l|^2 + \frac{1}{4}\rho^\top L^\dagger \rho$$

$$E_{hf}(X) := E_{ks}(X) + E_f(X), \quad E_f(X) := \frac{1}{4}\langle V(D)X, X\rangle, \quad D := D(X) = XX^*$$

- The Euclidean gradient and Hessian

$$\nabla E_f(X) = V(D)X, \quad \nabla^2 E_f(X)[U] = V(D)U + V(XU^* + UX^*)X.$$

- First-order optimality

$$(H_{ks}(\rho) + V(D))X = X\Lambda, \; X^*X = I_p.$$

- $\nabla^2 E_f$ is much more expansive than $\nabla^2 E_{ks}$ due to the high computational cost of $V(D)X$.

Linear eigenvalue problem

- Linear eigenvalue problem

$$\min_{X \in \mathbb{R}^{n \times p}} f(X) := \frac{1}{2}\mathrm{tr}(X^\top (A + B)X) \quad \text{s.t.} \quad X^\top X = I_p,$$

- We assume that the multiplication of BX is much more expensive than that of AX.
- Euclidean gradient and Hessian

$$\nabla f(X) = (A + B)X, \quad \nabla^2 f(X)[U] = AU + BU.$$

Outline

Optimization with orthogonality constraints

Problem definition

$$\min_{X \in \mathbb{R}^{n \times p}} \quad f(X), \qquad \text{s.t.} \quad X^\top X = I_p,$$

where f is a differentiable function.

- The set of orthogonality matrices $\{X \in \mathbb{R}^{n \times p} \mid X^\top X = I_p\}$ is called the Stiefel manifold $\mathrm{St}(n, p)$.
- Applications: linear eigenvalue problem, electronic structure calculations, etc.

Riemannian optimization

Retraction

A retraction R on a manifold $\mathcal{M}$ at a point X is a mapping from the tangent space $T_X\mathcal{M}$ at X onto $\mathcal{M}$ satisfying

- $R_X(0_X) = X$, where 0_X denotes the zero tangent vector of $T_X\mathcal{M}$.
- $\frac{D}{dt}R_X(t\xi) = \xi$ for all $\xi \in T_X\mathcal{M}$.

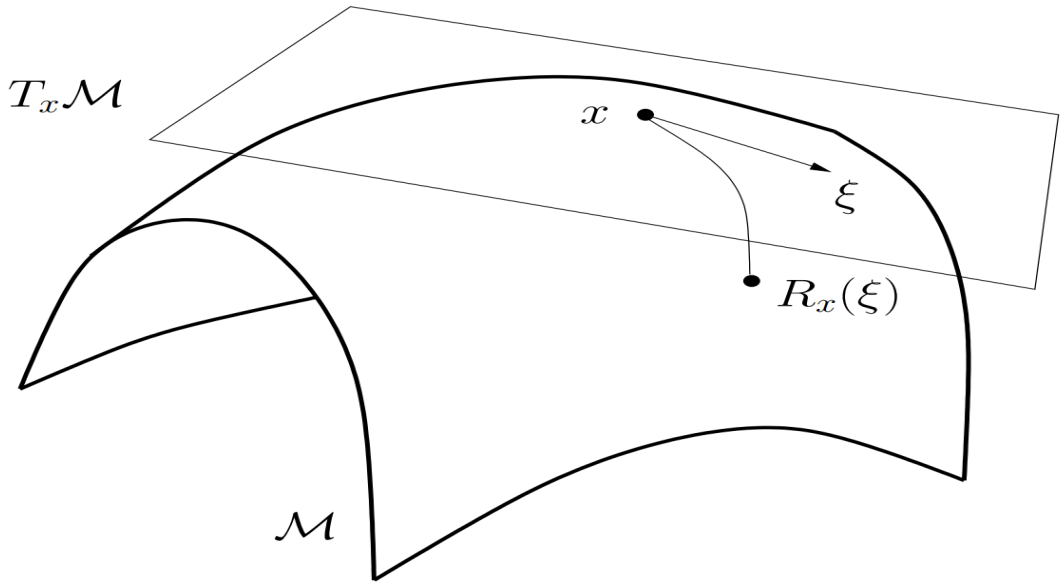


Figure: Absil et al. 2008

Riemannian optimization — Stiefel manifold

- Riemannian metric

$$\langle U, V\rangle := \mathrm{tr}(U^\top V),\ U, V \in T_X\mathcal{M}.$$

- The projection operator onto the tangent space is given by

$$\mathbf{P}_X(Z) = Z - X\mathrm{sym}(X^\top Z).$$

- Riemannian gradient and Hessian

$$\begin{aligned} \mathrm{grad} f(X) &= \mathbf{P}_X(\nabla f(X)), \\ \mathrm{Hess} f(X)[U] &= \mathbf{P}_X(\mathrm{Dgrad} f(X)[U]), \\ &= \mathbf{P}_X(\nabla^2 f(X)[U]) - U\mathrm{sym}(X^\top \nabla f(X)). \end{aligned}$$

- Riemannian optimization

$$X^{k+1} = R_{X^k}(\alpha_k \eta_k)$$

where α_k is the stepsize and $\eta_k \in T_{X^k}\mathcal{M}$ is a descent direction, e.g., $-\mathrm{grad} f(X^k)$ and $-\mathrm{Hess}^{-1} f(X^k)[\mathrm{grad} f(X^k)]$.

Outline

Existing Riemannian quasi-Newton method

- Focus on the whole approximation B^k to Riemannian Hessian

$$\mathrm{Hess} f(X^k) \ : \ T_{X^k}\mathcal{M} \to T_{X^k}\mathcal{M}.$$

- Riemannian BFGS method

$$B^{k+1} = \hat{B}^k - \frac{\hat{B}^k S^k ((\hat{B}^k)^* S^k)^\flat}{((\hat{B}^k)^* S^k)^\flat S^k} + \frac{Y^k (Y^k)^\flat}{(Y^k)^\flat S^k}, \ T_{X^{k+1}}\mathcal{M} \to T_{X^{k+1}}\mathcal{M}$$

where

$$\begin{aligned}
\hat{B}^k &= \mathbf{P}_{X^k}^{X^{k+1}} \circ B^k \circ (\mathbf{P}_{X^k}^{X^{k+1}})^{-1}, \text{change domain and range to } T_{X^{k+1}}\mathcal{M} \\
Y^k &= \beta_k^{-1} \mathrm{grad} f(X^{k+1}) - \mathbf{P}_{X^k}^{X^{k+1}} \mathrm{grad} f(X^k), \text{difference on } T_{X^{k+1}}\mathcal{M} \\
S^k &= \mathbf{P}_{X^k}^{X^{k+1}} \alpha_k \xi_k, \text{transport to } \mathrm{T}_{\mathrm{X}^{\mathrm{k+1}}}\mathcal{M}
\end{aligned}$$

with the last quasi-Newton direction $\xi_k \in T_{X^k}\mathcal{M}$ and stepsize α_k.

- $\mathbf{P}_{X^k}^{X^{k+1}} : T_{X^k}\mathcal{M} \to T_{X^{k+1}}\mathcal{M}$ is to transport the tangent vector from $T_{X^k}\mathcal{M}$ to $T_{X^{k+1}}\mathcal{M}$. β_k is a scalar (can be 1).

Existing Riemannian quasi-Newton method

- After getting B^{k+1}, the subproblem is

$$\xi_{k+1} := \arg \min_{\xi \in T_{X^{k+1}}\mathcal{M}} \quad \left\langle \operatorname{grad} f(X^{k+1}), \xi \right\rangle_{X^{k+1}} + \frac{1}{2} \left\langle B^{k+1}[\xi], \xi \right\rangle_{X^{k+1}}$$

- Do curvilinear search along xi_k to get stepsize α^k

$$X^{k+1} = R_{X^k}(\alpha_k \xi_k).$$

- To guarantee the fast local convergence
  - β_k and $\mathbf{P}_{X^k}^{X^{k+1}}$ should be chosen properly (satisfying locking condition[1]) to preserve curvature condition ($(Y^k)^\flat S^k > 0$).

[1] W. Huang, K. A. Gallivan, and P.-A. Absil, A Broyden class of quasi-Newton methods for Riemannian optimization, SIAM J. Optim., 25 (2015), pp. 16601685.

Adaptive regularized quasi-Newton method

- Riemannian Hessian of f:
  $\mathrm{Hess} f(X)[U] = \mathbf{P}_X(\nabla^2 f(X)[U]) - U\mathrm{sym}(X^\top \nabla f(X))$
- Keep the term $U\mathrm{sym}((X^k)^\top \nabla f(X^k))$ of lower computational cost, and construct an approximation B^k to expensive part $\nabla^2 f(X^k)$.
- After obtaining B^k, the subproblem is constructed as

$$\begin{cases} \min\ m_k(X) := \left\langle \nabla f(X^k), X - X^k \right\rangle + \frac{1}{2}\left\langle B^k[X - X^k], X - X^k \right\rangle + \frac{\sigma_k}{2}\|X - X^k\|^2, \\ \text{s.t. } X^T X = I_p. \end{cases}$$

- The Riemannian Hessian of $m_k(X)$ at X^k

$$\mathrm{Hess} m_k(X^k)[U] = \mathbf{P}_X(B^k[U]) - U\mathrm{sym}((X^k)^\top \nabla f(X^k)) + \sigma_k U.$$

- The vector transport is not needed since we are working the ambient Euclidean space.

Algorithm

- A modified conjugate gradient (CG) method
  Riemannian Newton equation:
  $$\mathrm{Hess} m_k(X^k)[\xi] = -\mathrm{grad} f(X^k) = \mathrm{grad}\, m_k(X^k)$$
  - Set $\xi_0 = 0, p_0 = -\mathrm{grad} f(X^k)$ and $i = 0$,
  - If negative curvature p_k is encountered, then
  $$\xi_k = \xi_{k-1} + \left\langle \mathrm{grad} f(X^k), p_j \right\rangle / \left\langle p_j, \mathrm{Hess} m_k(X^k)[p_j] \right\rangle,$$
  and return. Otherwise, do the normal truncated CG update ξ_k.
  - Do Armijo search along ξ^k to obtain a new trial point Z^k
- Choice of regularization parameter and updates
  - ratio: $\rho_k = \frac{f(Z^k) - f(X^k)}{m_k(Z^k)}$.
  - regularization parameter σ_k:

$$\sigma_{k+1} \in \begin{cases} (0, \sigma_k) & \text{if } \rho_k > \eta_2, \\ [\sigma_k, \gamma_1 \sigma_k] & \text{if } \eta_1 \le \rho_k \le \eta_2, \\ (\gamma_1 \sigma_k, \gamma_2 \sigma_k] & \text{otherwise.} \end{cases} \quad \begin{array}{l} \Rightarrow \boxed{X^{k+1} = Z^k} \\ \Rightarrow \boxed{X^{k+1} = Z^k} \\ \Rightarrow \boxed{X^{k+1} = X^k} \end{array}$$

where $0 < \eta_1 \le \eta_2 < 1$ and $1 < \gamma_1 \le \gamma_2$.

Construction of B^k with structured f

- Assume that $\nabla^2 f(X)$ takes a natural structure as

$$\nabla^2 f(X) = H^c(X) + H^e(X),$$

where the computational cost of $H^e(X)$ is much more expensive than that of $H^c(X)$.

- Quasi-Newton method with structure

$$B^k = H^c(X^k) + C^k,$$

where C^k is a quasi-Newton approximation to $H^e(X^k)$ with secant condition

$$C^k[S^k] = Y^k - H^c(X^k)[S^k],$$

where $S^k := X^k - X^{k-1}$ and $Y^k = \nabla f(X^k) - \nabla f(X^{k-1})$.

How to choose an initial quasi-Newton approximation?

- For a linear operator A of high computational cost, the limited-memory Nyström approximation[2] $\hat{A}$ is

$$\hat{A} := Y(Y^*\Omega)^\dagger Y^*,$$

  where $Y = A\Omega$ and Ω is a basis of a well-chosen subspace, e.g.,

$$\texttt{orth}(\{X^k, X^{k-1}, AX^k\}),\ \texttt{orth}(\{X^k, X^{k-1}, X^{k-2}, \ldots\}).$$

- The compressed operator $\hat{A}$ is of low rank, but consistent with A on the subspace spanned by Ω.
- Given some good approximation C_0^k of H^e, the Nyström approximation $\hat{C}_0^k$ can be utilized to further reduce the computational cost.
- More effective than the BB-type initialization (αI) in practice.

[2] Joel A Tropp, Alp Yurtsever, Madeleine Udell, and Volkan Cevher, Fixed-rank approximation of a positive-semidefinite matrix from streaming data, NIPS, 2017, pp. 1225-1234.

Application to electronic structure calculation

- Hartree-Fock total energy minimization

$$E_{hf}(X) := E_{ks}(X) + E_f(X), \quad E_f(X) := \frac{1}{4}\langle V(D)X, X\rangle .$$

- The structured update

$$H^c(X) = \nabla^2 E_{ks}(X), \quad H^e(X) = \nabla^2 E_f(X).$$

- Since $V(D^k)X^k$ can be obtained by computing the gradient $\nabla E_f(X^k)$, the Nyström approximation of V on $\{X^k\}$

$$\hat{V} := Y(Y^* X^k)^\dagger Y^*, \text{ with } Y = V(D^k)X^k.$$

- The subproblem

$$\begin{cases} \min m_k(X) := \left\langle \nabla f(X^k), X - X^k \right\rangle + \frac{1}{2}\left\langle B^k[X - X^k], X - X^k \right\rangle + \frac{\sigma_k}{2}\|X - X^k\|^2 \\ \text{s.t. } X \in \mathrm{St}(n,p). \end{cases}$$

Application to linear eigenvalue problem

- Linear eigenvalue problem

$$\min_{X\in\mathbb{R}^{n\times p}} f(X) := \frac{1}{2}\mathrm{tr}(X^\top(A+B)X) \quad \text{s.t.} \quad X^\top X = I_p,$$

- We assume that the multiplication of BX is much more expensive than that of AX.
- The structured update

$$H^c(X) = A, \quad H^e(X) = B.$$

- Limited-memory Nyström approximation of B on subspace $W^k := \mathrm{span}\{X^{k-1}, X^k\}$

$$B^k := Y(Y^\top W^k)^\dagger Y^\top, \text{ with } Y = BW^k.$$

- The subproblem

$$m_k(X) := \frac{1}{2}\mathrm{tr}(X^\top(A+B^k)X) + \frac{\sigma_k}{4}\|XX^\top - X^k(X^k)^\top\|_F^2$$

Inexact conditions for convergence

Inexact conditions for solving subproblem:

(C1) Inexact condition for global convergence:

$$m_k(Z^k) \leq -c\|\mathrm{grad} f(X^k)\|_F^2$$

with some positive constant c.

(C2) Inexact condition for local convergence:

$$\|\mathrm{grad}\, m_k(Z^k)\|_F \leq \theta^k \|\mathrm{grad} f(X^k)\|_F$$

with parameter $\theta^k := \min\left\{0.1 * \|\mathrm{grad} f(X^k)\|, \|\mathrm{grad} f(X^k)\|_F^{1+\gamma}\right\} (\gamma > 0)$.

Global convergence

Assumptions:

(A1) The gradient ∇f is Lipschitz continuous on the convex hull of the manifold $\mathrm{conv}(\mathrm{St}(n,p))$, i.e., there exists $L_f > 0$ such that

$$\|\nabla f(X) - \nabla f(Y)\| \le L_f \|X - Y\|, \quad \forall\, X, Y \in \mathrm{conv}(\mathrm{St}(n,p)).$$

(A2) There exists $\kappa_H > 0$ such that $\|B^k\| \le \kappa_H$ for all $k = 1, 2, \ldots$.

Theorem

Suppose that the assumptions (A1)–(A2) and condition (C1) hold. Then, either

$$\mathrm{grad} f(X^\ell) = 0 \ \text{ for some } \ \ell \ge 0 \quad \text{or} \quad \liminf_{k\to\infty} \|\mathrm{grad} f(X^k)\| = 0.$$

Local convergence

Assumptions:

(B1) The sequence $\{X^k\}$ converges to X_* with $\mathrm{grad} f(X_*) = 0$.

(B2) The Euclidean Hessian $\nabla^2 f$ is continuous on $\mathrm{conv}(\mathcal{M})$.

(B3) The Riemannian Hessian $\mathrm{Hess} f(X)$ is positive definite at X_*.

(B4) The Hessian approximation B^k satisfies

$$\frac{\|(B^k - \nabla^2 f(X^k))[Z^k - X^k]\|_F}{\|Z^k - X^k\|_F} \to 0, \ k \to \infty.$$

Theorem

Suppose that the assumptions (B1)-(B4) and conditions (C1)-(C2) hold. Then the sequence $\{X^k\}$ converges q-superlinearly to X_*.

Outline

Numerical results: Hartree-Fock energy minimization

Hartree-Fock total energy minimization

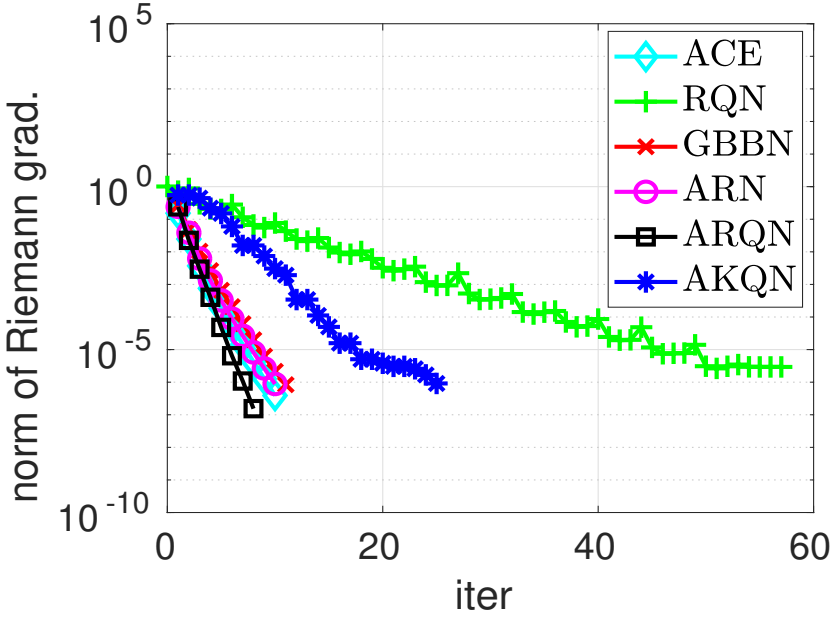
$$\min_{X \in \mathbf{C}^{n\times p}} \quad E_{hf}(X) := E_{ks}(X) + E_f(X) \quad \text{s.t.} \quad X^*X = I_p.$$

- ACE: existing two-level nested self-consistent field iteration with the Nyström approximation.
- ARQN(our method): keeps the Hessian $\nabla^2 E_{ks}$ and construct an approximation to $\nabla^2 E_f$.
- AKQN(our method): only keeps the linear operator part in $\nabla^2 E_{ks}$.
- ARN(our method): the only difference to ARQN is to set $B^k = \nabla^2 E_{ks}(X^k) + \hat{V}(D^k)$ directly, where $\hat{V}(D^k)$ is a Nyström approximation to $\nabla^2 E_f(X^k)$.
- GBBN: the only difference to ARN is that the subproblem is solved by GBB.
- RQN: Riemannian limited-memory BFGS method from Manopt

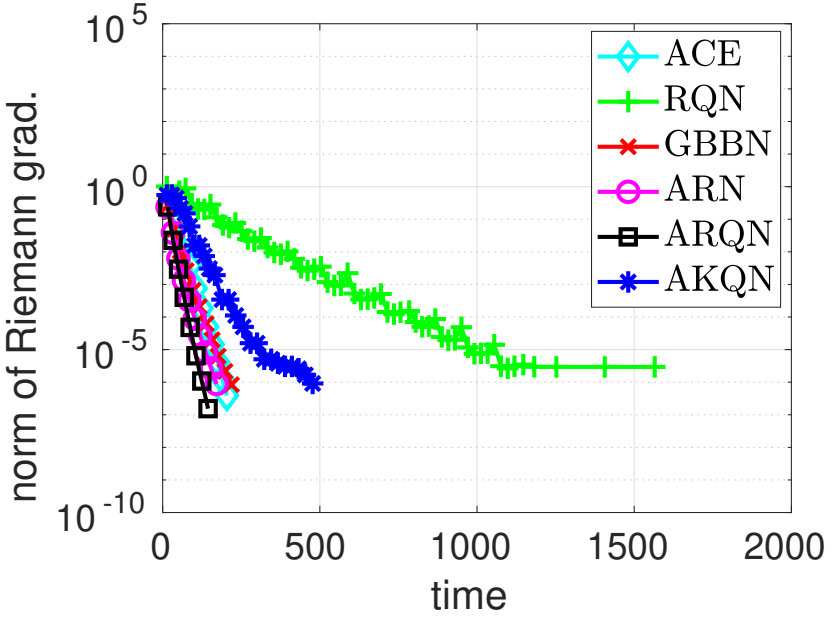
Numerical results: Hartree-Fock energy minimization

Table: Numerical results on HF total energy minimization.

Solver	fval	nrmG	its	time	fval	nrmG	its	time
	glutamine				graphene30			
ACE	-1.04525e+2	3.9e-7	10(3.0)	229.6	-1.87603e+2	8.6e-7	58(4.2)	15182.3
GBBN	-1.04525e+2	8.4e-7	11(13.3)	256.9	-1.87603e+2	8.6e-7	32(76.0)	22678.9
ARN	-1.04525e+2	8.8e-7	10(9.5)	209.5	-1.87603e+2	9.0e-7	45(35.6)	14941.2
ARQN	-1.04525e+2	1.5e-7	8(10.1)	182.9	-1.87603e+2	7.6e-7	15(26.5)	5873.2
AKQN	-1.04525e+2	9.1e-7	25(6.0)	515.7	-1.87603e+2	9.5e-7	62(7.5)	18986.5
RQN	-1.04525e+2	2.9e-6	57	1532.8	-1.87603e+2	1.5e-5	110	39057.2
	gaas				si40			
ACE	-2.93496e+2	8.8e-7	29(2.9)	343.8	-1.65698e+2	9.2e-7	29(4.5)	30256.4
GBBN	-2.93496e+2	9.3e-7	34(35.3)	659.3	-1.65698e+2	8.6e-7	24(43.9)	34846.2
ARN	-2.93496e+2	9.6e-7	31(20.4)	468.7	-1.65698e+2	8.0e-7	22(22.1)	21181.3
ARQN	-2.93496e+2	3.3e-7	10(28.0)	199.5	-1.65698e+2	2.8e-7	12(37.8)	15369.5
AKQN	-2.93496e+2	4.6e-7	22(18.4)	347.1	-1.65698e+2	9.2e-7	87(7.9)	89358.8
RQN	-2.93496e+2	1.0e-6	126	2154.1	-1.65698e+2	6.1e-6	156	181976.8



(a) norm of Riemannian gradients



(b) norm of Riemannian gradients

Figure: Comparisons of different algorithms on "glutamine" of HF total energy minimization.

Numerical results: linear eigenvalue problem

Linear eigenvalue problem

$$\min_{X\in\mathbb{R}^{n\times p}} f(X) := \frac{1}{2}\mathrm{tr}(X^\top(A+B)X) \quad \text{s.t.} \quad X^\top X = I_p, \tag{2}$$

- We assume that the multiplication of BX is much more expensive than that of AX.

- EIGS: built-in function in MATLAB.
- LOBPCG: locally optimal block preconditioned conjugate gradient method.
- ASQN (our method): keeps A but uses the limited-memory Nyström approximation of B on subspace $\mathrm{span}\{X^{k-1}, X^k\}$.
- ACE: keeps A but uses the limited-memory Nyström approximation of B on subspace $\mathrm{span}\{X^k\}$.

Numerical results: linear eigenvalue problem

Settings:

- $A = \text{randn}(n, n)$; $A = (A + A^\top)/2$;
- $B = 0.01\text{randn}(n, n)$; $B = (B + B^\top)/2$; $B = B - \lambda_{\max}(B)$;
- we compute the multiplication BX using $\frac{1}{19}\sum_{i=1}^{19} BX$

Table: Numerical results on random matrices

	AV/BV	err	time	AV/BV	err	time
n	8000			10000		
EIGS	538/538	8.7e-11	131.9	981/981	8.8e-11	327.3
LOBPCG	1996/1996	9.9e-11	336.7	2440/2440	9.7e-11	763.8
ASQN	2706/150	8.9e-11	29.8	2920/150	9.7e-11	50.2
ACE	4537/450	9.8e-11	66.3	4554/400	9.6e-11	99.4
$n = 5000$						
p	30			50		
EIGS	660/660	3.0e-11	62.8	879/879	1.6e-12	83.6
LOBPCG	4458/4458	1.0e-10	217.6	5766/5766	9.5e-11	186.7
ASQN	5315/420	9.8e-11	11.4	7879/650	9.8e-11	17.8
ACE	9701/1530	9.4e-11	23.0	21664/4450	1.0e-10	50.9

Numerical results: linear eigenvalue problem

Settings:

- $A = \text{gallery}(\text{'wathen'}, 5s, 5s)$
- $B = 0.01\text{randn}(n, n);\ B = (B + B^\top)/2;\ B = B - \lambda_{\max}(B);$

Table: Numerical results on sparse matrices

	AV/BV	err	time	AV/BV	err	time
$p = 10$						
s	11			12		
EIGS	1882/1882	1.5e-07	58.9	1463/1463	9.6e-11	65.4
LOBPCG	4282/4282	9.5e-11	136.0	4089/4089	9.9e-11	190.6
ASQN	8327/240	9.6e-11	16.7	6910/220	9.3e-11	17.5
ACE	15323/1060	9.7e-11	38.9	17907/2010	1.7e-08	65.5
$s = 12$						
p	50			60		
EIGS	1743/1743	7.3e-11	69.1	2122/2122	1.6e-11	86.7
LOBPCG	12288/12288	1.4e-09	168.4	15716/15716	1.1e-08	199.5
ASQN	21330/1300	9.3e-11	53.6	26343/1620	9.7e-11	71.8
ACE	49165/10050	2.9e-06	110.1	62668/12060	2.3e-08	134.0

Summary

- We propose a quasi-Newton method without vector transport.
- The structured update of the quasi-Newton approximation is presented by utilizing the structure of the objective f.
- The limited-memory Nyström approximation is investigated to obtain some good initial approximation for the exact Hessian.
- Numerical experiments compared with the state-of-art methods show the effectiveness of our method.
- More information can be found in `https://arxiv.org/abs/1809.00452`

Many Thanks For Your Attention!