Convergence of 4th Runge-Kutta method on Least Square problem

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First draft : September 3, 2020
Last update : October 22, 2020

Setup

- Given $\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{b} \in \mathbb{R}^m$, find $\mathbf{x} \in \mathbb{R}^n$ by solving

$$(\mathcal{P}) \quad : \quad \min_{\mathbf{x}} f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2.$$

- We solve $(\mathcal{P})$ by the 4th-order Runge Kutta method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \frac{h}{6}\Big(\mathbf{s}_1 + 2\mathbf{s}_2 + 2\mathbf{s}_3 + \mathbf{s}_4\Big)$$

where

$$\begin{aligned}
\mathbf{s}_1 &= \nabla f(\mathbf{x}_k) \\
\mathbf{s}_2 &= \nabla f\big(\mathbf{x}_k + \tfrac{h}{2}\mathbf{s}_1\big) \\
\mathbf{s}_3 &= \nabla f\big(\mathbf{x}_k + \tfrac{h}{2}\mathbf{s}_2\big) \\
\mathbf{s}_4 &= \nabla f(\mathbf{x}_k).
\end{aligned}$$

The RK4 update on least square

- After lots of algebra, the RK4 update on least square problem $(\mathcal{P})$ is

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \left(h\mathbf{I} - \frac{h^2}{2}\mathbf{Q} + \frac{h^3}{6}\mathbf{Q}^2 - \frac{h^4}{24}\mathbf{Q}^3\right)(\mathbf{Q}\mathbf{x}_k - \mathbf{p}),$$

  where $\mathbf{Q} = \mathbf{A}^\top\mathbf{A}$, $\mathbf{p} = \mathbf{A}^\top\mathbf{b}$.

- The update can also be expressed as

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{H}\nabla f(\mathbf{x}_k),$$

  with

$$\mathbf{H} = h\mathbf{I} - \frac{h^2}{2}\mathbf{Q} + \frac{h^3}{6}\mathbf{Q}^2 - \frac{h^4}{24}\mathbf{Q}^3.$$

- This document: discuss the convergence of this update.

Convergence of RK4 update

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \Big(h\mathbf{I} - \frac{h^2}{2}\mathbf{Q} + \frac{h^3}{6}\mathbf{Q}^2 - \frac{h^4}{24}\mathbf{Q}^3\Big)(\mathbf{Q}\mathbf{x}_k - \mathbf{p}).$$

- Let $\mathbf{x}^*$ be the minimizer. The 1st-order optimality condition $\nabla f(\mathbf{x}^*) = 0$ gives $\mathbf{p} = \mathbf{Q}\mathbf{x}^*$, so

$$\begin{aligned}
\mathbf{x}_{k+1} - \mathbf{x}^* &= \mathbf{x}_k - \Big(h\mathbf{I} - \frac{h^2}{2}\mathbf{Q} + \frac{h^3}{6}\mathbf{Q}^2 - \frac{h^4}{24}\mathbf{Q}^3\Big)(\mathbf{Q}\mathbf{x}_k - \mathbf{p}) - \mathbf{x}^* \\
&= \mathbf{x}_k - \mathbf{x}^* - \Big(h\mathbf{I} - \frac{h^2}{2}\mathbf{Q} + \frac{h^3}{6}\mathbf{Q}^2 - \frac{h^4}{24}\mathbf{Q}^3\Big)\mathbf{Q}(\mathbf{x}_k - \mathbf{x}^*) \\
&= \Big(\mathbf{I} - h\mathbf{Q} + \frac{h^2}{2}\mathbf{Q}^2 - \frac{h^3}{6}\mathbf{Q}^3 + \frac{h^4}{24}\mathbf{Q}^4\Big)(\mathbf{x}_k - \mathbf{x}^*) \\
\|\mathbf{x}_{k+1} - \mathbf{x}_k\|_2 &= \left\|\Big(\mathbf{I} - h\mathbf{Q} + \frac{h^2}{2}\mathbf{Q}^2 - \frac{h^3}{6}\mathbf{Q}^3 + \frac{h^4}{24}\mathbf{Q}^4\Big)(\mathbf{x}_k - \mathbf{x}^*)\right\|_2 \\
&\overset{(*)}{\leq} \left\|\mathbf{I} - h\mathbf{Q} + \frac{h^2}{2}\mathbf{Q}^2 - \frac{h^3}{6}\mathbf{Q}^3 + \frac{h^4}{24}\mathbf{Q}^4\right\|_2 \|\mathbf{x}_k - \mathbf{x}^*\|_2
\end{aligned}$$

  (*) : $\|\mathbf{M}\mathbf{x}\|_2 \leq \|\mathbf{M}\|_2 \|\mathbf{x}\|_2$

- The update converges if

$$\left\|\mathbf{I} - h\mathbf{Q} + \frac{h^2}{2}\mathbf{Q}^2 - \frac{h^3}{6}\mathbf{Q}^3 + \frac{h^4}{24}\mathbf{Q}^4\right\|_2 < 1.$$

Convergence of RK4 update

- Let $\mathbf{V}\mathbf{\Sigma}\mathbf{V}^\top$ be the eigendecomposition of $\mathbf{Q}$. As norm is invariant to orthogonal transform, we have
$$\left\| \mathbf{I} - h\mathbf{\Sigma} + \frac{h^2}{2}\mathbf{\Sigma}^2 - \frac{h^3}{6}\mathbf{\Sigma}^3 + \frac{h^4}{24}\mathbf{\Sigma}^4 \right\|_2 < 1. \tag{1}$$
- The matrix in (1) is diagonal, so (1) is true if the largest absolute value of the diagonal matrix is smaller than 1. This translates as follows. Let $\phi_i(h, \lambda_i) = 1 - h\lambda_i + \frac{h^2}{2}\lambda_i^2 - \frac{h^3}{6}\lambda_i^3 + \frac{h^4}{24}\lambda_i^4$,
$$\text{RK4 update converges} \iff \max_i |\phi_i(h, \lambda_i)| < 1.$$
Furthermore, we can pick h by minimizing this value as
$$h = \min_h \max_i |\phi_i(h, \lambda_i)|.$$
- In general, h can be complex-valued. For $\mathbf{Q} = \mathbf{A}^\top \mathbf{A}$ that is positive definite (i.e., $\mathbf{A}$ is full rank), h reduces to real value because eigenvalues of $\mathbf{A}^\top A$ are real.

Convergence rate of RK4 update

- To derive (asymptotic) convergence rate of the RK4 method, we go back to the form
$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{H}\nabla f(\mathbf{x}_k). \tag{2}$$
By looking at (2), we have to consider variable metric: the weighted norm with respect to a symmetric positive definite matrix $\mathbf{U}$ is defined as
$$\|\mathbf{x}\|_{\mathbf{U}} = \langle \mathbf{x}, \mathbf{U}\mathbf{x}\rangle^{\frac{1}{2}}.$$
- We now derive the convergence rate: first, assume $\mathbf{H}(h)$ is non-singular (so $\mathbf{H}^{-1}$ exists), from (2) we have
$$\begin{aligned} \|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} &\overset{(2)}{=} \|\mathbf{x}_k - \mathbf{H}\nabla f(\mathbf{x}_k) - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} \\ &= \|(\mathbf{x}_k - \mathbf{x}^*) - \mathbf{H}\nabla f(\mathbf{x}_k)\|^2_{\mathbf{H}^{-1}}. \end{aligned}$$
Simplifying notation: let $\mathbf{g}_k = \nabla f(\mathbf{x}_k)$, then
$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} = \|(\mathbf{x}_k - \mathbf{x}^*) - \mathbf{H}\mathbf{g}_k\|^2_{\mathbf{H}^{-1}}.$$

$$
\begin{aligned}
\|\mathbf{x}_{k+1}-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2 &= \|(\mathbf{x}_k-\mathbf{x}^*)-\mathbf{H}\mathbf{g}_k\|_{\mathbf{H}^{-1}}^2 \\
&= \Big\langle (\mathbf{x}_k-\mathbf{x}^*)-\mathbf{H}\mathbf{g}_k,\ \mathbf{H}^{-1}\Big((\mathbf{x}_k-\mathbf{x}^*)-\mathbf{H}\mathbf{g}_k\Big)\Big\rangle \\
&= \big\langle (\mathbf{x}_k-\mathbf{x}^*)-\mathbf{H}\mathbf{g}_k,\ \mathbf{H}^{-1}(\mathbf{x}_k-\mathbf{x}^*)-\mathbf{g}_k\big\rangle \\
&= \|\mathbf{x}_k-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2+\|\mathbf{g}_k\|_{\mathbf{H}}^2-2\langle\mathbf{g}_k,\mathbf{x}_k-\mathbf{x}^*\rangle.
\end{aligned}
$$

As f is convex, its first-order Taylor approximation is an global under estimator: for any $\mathbf{y},\mathbf{x}\in$dom$f$, then $f(\mathbf{y})\geq f(\mathbf{x})+\langle\nabla f(\mathbf{x}),\mathbf{y}-\mathbf{x}\rangle$. Put $\mathbf{y}=\mathbf{x}^*$ and $\mathbf{x}=\mathbf{x}_k$ gives $f(\mathbf{x}^*)\geq f(\mathbf{x}_k)+\langle\mathbf{g}_k,\mathbf{x}^*-\mathbf{x}_k\rangle$, rearrange gives

$$
-\langle\mathbf{g}_k,\mathbf{x}_k-\mathbf{x}^*\rangle\leq-(f(\mathbf{x}_k)-f(\mathbf{x}^*)).
$$

So $\|\mathbf{x}_{k+1}-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2\leq\|\mathbf{x}_k-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2+\|\mathbf{g}_k\|_{\mathbf{H}}^2-2(f(\mathbf{x}_k)-f(\mathbf{x}^*))$.
Rearrange again gives

$$
f(\mathbf{x}_k)-f(\mathbf{x}^*)\leq\frac{1}{2}\|\mathbf{x}_k-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2-\frac{1}{2}\|\mathbf{x}_{k+1}-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2+\frac{1}{2}\|\mathbf{g}_k\|_{\mathbf{H}}^2.
$$

Simplify notation, let $f^*=f(\mathbf{x}^*)$ and $f_k=f(\mathbf{x}_k)$

$$
f_k-f^*\leq\frac{1}{2}\|\mathbf{x}_k-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2-\frac{1}{2}\|\mathbf{x}_{k+1}-\mathbf{x}^*\|_{\mathbf{H}^{-1}}^2+\frac{1}{2}\|\mathbf{g}_k\|_{\mathbf{H}}^2.
$$

Convergence rate of RK4 update

Take iteration counter from k to 0:

$$
\begin{array}{rcccccc}
f_k - f^* & \leq & \frac{1}{2}\|\mathbf{x}_k - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & - & \frac{1}{2}\|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & + & \frac{1}{2}\|\mathbf{g}_k\|^2_{\mathbf{H}} \\
f_{k-1} - f^* & \leq & \frac{1}{2}\|\mathbf{x}_{k-1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & - & \frac{1}{2}\|\mathbf{x}_{k} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & + & \frac{1}{2}\|\mathbf{g}_{k-1}\|^2_{\mathbf{H}} \\
f_{k-2} - f^* & \leq & \frac{1}{2}\|\mathbf{x}_{k-2} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & - & \frac{1}{2}\|\mathbf{x}_{k-1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & + & \frac{1}{2}\|\mathbf{g}_{k-2}\|^2_{\mathbf{H}} \\
\vdots & & & & & & \\
f_0 - f^* & \leq & \frac{1}{2}\|\mathbf{x}_0 - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & - & \frac{1}{2}\|\mathbf{x}_{1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}} & + & \frac{1}{2}\|\mathbf{g}_0\|^2_{\mathbf{H}}
\end{array}
$$

Sum all the inequalities

$$
\begin{aligned}
\sum_{i=0}^{k}\left(f_i - f^*\right) &\leq \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}}}{2} - \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}}}{2} + \frac{1}{2}\sum_{i=0}^{k}\|\mathbf{g}_i\|^2_{\mathbf{H}} \\
&\leq \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}}}{2} + \frac{1}{2}\sum_{i=0}^{k}\|\mathbf{g}_i\|^2_{\mathbf{H}}.
\end{aligned}
$$

Convergence rate of RK4 update

We have

$$\sum_{i=0}^{k}\left(f_i - f^*\right) \quad \le \quad \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|_{\mathbf{H}^{-1}}^2}{2} + \frac{1}{2}\sum_{i=0}^{k}\|\mathbf{g}_i\|_{\mathbf{H}}^2.$$

Since

$$(k+1)\left(f_i^{\text{best}} - f^*\right) \le \sum_{i=0}^{k}\left(f_i - f^*\right)$$

we arrive

$$f_i^{\text{best}} - f^* \le \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|_{\mathbf{H}^{-1}}^2}{2(k+1)} + \frac{1}{2(k+1)}\sum_{i=0}^{k}\|\mathbf{g}_i\|_{\mathbf{H}}^2.$$

If $\sum_{i=0}^{k}\|\mathbf{g}_i\|_{\mathbf{H}}^2$ grows slower than k, the term $\sum_{i=0}^{k}\|\mathbf{g}_i\|_{\mathbf{H}}^2 \to 0$ we have convergence rate $\dfrac{1}{k}$.

Convergence of Projected RK4 update

- We now consider a general problem: let $\mathcal{C} \subset \mathbb{R}^n$ be a convex set

$$(\mathcal{P}_{\mathcal{C}}) \;\; : \;\; \min_{\mathbf{x} \in \mathcal{C}} f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2.$$

- We solve it by the projected RK4 (pRK4):

$$\mathbf{x}_{k+1} = P_{\mathcal{C}}\Big(\mathbf{x}_k - \mathbf{H}\nabla f(\mathbf{x}_k)\Big), \tag{3}$$

  where $P_{\mathcal{C}}$ is the projection.

- The previous convergence analysis still holds for pRK4. The proof starts with the non-expansive property of projection

$$\begin{aligned} \|\mathbf{x}_{k+1} - \mathbf{x}^*\|_{\mathbf{H}^{-1}}^2 &\overset{(3)}{=} \|P_{\mathcal{C}}\Big(\mathbf{x}_k - \mathbf{H}\nabla f(\mathbf{x}_k)\Big) - P_{\mathcal{C}}(\mathbf{x}^*)\|_{\mathbf{H}^{-1}}^2 \\ &\leq \|\mathbf{x}_k - \mathbf{H}\nabla f(\mathbf{x}_k) - \mathbf{x}^*\|_{\mathbf{H}^{-1}}^2, \end{aligned}$$

  and then proceed.

Last page - summary

- Given $\mathbf{A} \in \mathbb{R}^{m\times n}, \mathbf{b} \in \mathbb{R}^m$, find $\mathbf{x} \in \mathbb{R}^n$ by solving

$$(\mathcal{P}) \quad : \quad \min_{\mathbf{x}} f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2.$$

- We solve $(\mathcal{P})$ by the 4th-order Runge Kutta method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \frac{h}{6}\Big(\mathbf{s}_1 + 2\mathbf{s}_2 + 2\mathbf{s}_3 + \mathbf{s}_4\Big)$$

$$\begin{array}{lllllll} \mathbf{s}_1 & = & \nabla f(\mathbf{x}_k) & \qquad & \mathbf{s}_2 & = & \nabla f\big(\mathbf{x}_k + \frac{h}{2}\mathbf{s}_1\big) \\ \mathbf{s}_3 & = & \nabla f\big(\mathbf{x}_k + \frac{h}{2}\mathbf{s}_2\big) & & \mathbf{s}_4 & = & \nabla f(\mathbf{x}_k). \end{array}$$

- Convergence

$$f_i^{\text{best}} - f^* \leq \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2_{\mathbf{H}^{-1}}}{2(k+1)} + \frac{1}{2(k+1)}\sum_{i=0}^{k}\|\mathbf{g}_i\|^2_{\mathbf{H}}.$$

If $\sum_{i=0}^{k}\|\mathbf{g}_i\|^2_{\mathbf{H}}$ grows slower than k, the term $\sum_{i=0}^{k}\|\mathbf{g}_i\|^2_{\mathbf{H}} \to 0$ we have convergence rate $\frac{1}{k}$.

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