Supplementary Material for the Manuscript "On the Implicit Bias of Adam"

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SA-1 Overview

SA-1.1. This appendix provides some omitted details and proofs.

We consider two algorithms: RMSProp and Adam, and two versions of each algorithm (with the numerical stability ε parameter inside and outside of the square root in the denominator). This means there are four main theorems: Theorem SA-2.4, Theorem SA-3.4, Theorem SA-4.4 and Theorem SA-5.4, each residing in the section completely devoted to one algorithm. The simple induction argument taken from [1], essentially the same for each of these theorems, is based on an auxiliary result whose corresponding versions are Theorem SA-2.3, Theorem SA-3.3, Theorem SA-4.3 and Theorem SA-5.3. The proof of this result is also elementary but long, and it is done by a series of lemmas in Section SA-6 and Section SA-7, culminating in Section SA-7.6. Out of these four, we only prove Theorem SA-2.3 since the other three results are proven in the same way with obvious changes.

Section SA-8 contains some details about the numerical experiments.

SA-1.2 Notation. We denote the loss of the kth minibatch as a function of the network parameters $\boldsymbol{\theta} \in \mathbb{R}^p$ by $E_k(\boldsymbol{\theta})$, and in the full-batch setting we omit the index and write $E(\boldsymbol{\theta})$. As usual, ∇E means the gradient of E, and nabla with indices means partial derivatives, e. g. $\nabla_{ijs} E$ is a shortcut for $\frac{\partial^3 E}{\partial\theta_i \partial\theta_j \partial\theta_s}$.

The letter $T > 0$ will always denote a finite time horizon of the ODEs, h will always denote the training step size, and we will replace nh with t_n when convenient, where $n \in \{0, 1, \ldots\}$ is the step number. *We will use the same notation* for the iteration of the discrete algorithm $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k\in\mathbb{Z}_{\geq 0}}$, the piecewise ODE solution $\tilde{\boldsymbol{\theta}}(t)$ and some auxiliary terms for each of the four algorithms: see Definition SA-2.1, Definition SA-

3.1, Definition SA-4.1, Definition SA-5.1. This way, we avoid cluttering the notation significantly. We are careful to reference the relevant definition in all theorem statements.

SA-2 RMSProp with ε outside the square root

Definition SA-2.1. In this section, for some $\boldsymbol{\theta}^{(0)} \in \mathbb{R}^p$, $\nu^{(0)} = \mathbf{0} \in \mathbb{R}^p$, $\rho \in (0,1)$, let the sequence of p-vectors $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k \in \mathbb{Z}_{\geq 0}}$ be defined for $n \geq 0$ by

$$\begin{aligned} \nu_j^{(n+1)} &= \rho \nu_j^{(n)} + (1-\rho)\left(\nabla_j E_n\left(\boldsymbol{\theta}^{(n)}\right)\right)^2, \\ \theta_j^{(n+1)} &= \theta_j^{(n)} - \frac{h}{\sqrt{\nu_j^{(n+1)}} + \varepsilon} \nabla_j E_n\left(\boldsymbol{\theta}^{(n)}\right). \end{aligned} \tag{SA-2.1}$$

Let $\tilde{\boldsymbol{\theta}}(t)$ be defined as a continuous solution to the piecewise ODE

$$\begin{aligned} \dot{\tilde{\theta}}_j(t) = &- \frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon} \\ &+ h\left(\frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)} - \frac{\sum_{i=1}^p \nabla_{ij} E_n\left(\tilde{\boldsymbol{\theta}}(t)\right) \frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}}{2\left(R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t)) + \varepsilon\right)} \right) \end{aligned} \tag{SA-2.2}$$

with the initial condition $\tilde{\boldsymbol{\theta}}(0) = \boldsymbol{\theta}^{(0)}$, where $\mathbf{R}^{(n)}(\boldsymbol{\theta})$, $\mathbf{P}^{(n)}(\boldsymbol{\theta})$ and $\bar{\mathbf{P}}^{(n)}(\boldsymbol{\theta})$ are p-dimensional functions with components

$$\begin{aligned} R_j^{(n)}(\boldsymbol{\theta}) &:= \sqrt{\sum_{k=0}^n \rho^{n-k}(1-\rho)\left(\nabla_j E_k(\boldsymbol{\theta})\right)^2}, \\ P_j^{(n)}(\boldsymbol{\theta}) &:= \sum_{k=0}^n \rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta}) \sum_{i=1}^p \nabla_{ij} E_k(\boldsymbol{\theta}) \sum_{l=k}^{n-1} \frac{\nabla_i E_l(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta}) + \varepsilon}, \\ \bar{P}_j^{(n)}(\boldsymbol{\theta}) &:= \sum_{k=0}^n \rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta}) \sum_{i=1}^p \nabla_{ij} E_k(\boldsymbol{\theta}) \frac{\nabla_i E_n(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta}) + \varepsilon}. \end{aligned}$$

Assumption SA-2.2.

1. For some positive constants M_1, M_2, M_3, M_4 we have

$$\begin{aligned} \sup_i \sup_k \sup_{\boldsymbol{\theta}} \left|\nabla_i E_k(\boldsymbol{\theta})\right| &\leq M_1, \\ \sup_{i,j} \sup_k \sup_{\boldsymbol{\theta}} \left|\nabla_{ij} E_k(\boldsymbol{\theta})\right| &\leq M_2, \\ \sup_{i,j,s} \sup_k \sup_{\boldsymbol{\theta}} \left|\nabla_{ijs} E_k(\boldsymbol{\theta})\right| &\leq M_3, \\ \sup_{i,j,s,r} \sup_k \sup_{\boldsymbol{\theta}} \left|\nabla_{ijsr} E_k(\boldsymbol{\theta})\right| &\leq M_4. \end{aligned}$$

2. For some $R > 0$ we have for all $n \in \{0, 1, \ldots, \lfloor T/h \rfloor\}$

$$R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) \geq R, \quad \sum_{k=0}^n \rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right)\right)^2 \geq R^2,$$

where $\tilde{\boldsymbol{\theta}}(t)$ is defined in Definition SA-2.1.

Theorem SA-2.3 (RMSProp with ε outside: local error bound)**.** *Suppose Assumption SA-2.2 holds. Then for all* $n \in \{0, 1, \ldots, \lfloor T/h \rfloor\}$

$$\left| \tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) + h \frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t_n)\right)}{\sqrt{\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right)\right)^2 + \varepsilon}} \right| \leq C_1 h^3$$

for a positive constant C_1 *depending on* ρ*.*

The proof of Theorem SA-2.3 is conceptually simple but very technical, and we delay it until Section SA-7. For now assuming it as given and combining it with a simple induction argument gives a global error bound which follows.

Theorem SA-2.4 (RMSProp with ε outside: global error bound)**.** *Suppose Assumption SA-2.2 holds, and*

$$\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\boldsymbol{\theta}^{(k)}\right)\right)^2 \geq R^2$$

for $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k \in \mathbb{Z}_{\geq 0}}$ *defined in Definition SA-2.1. Then there exist positive constants* d_1*,* d_2*,* d_3 *such that for all* $n \in \{0, 1, \ldots, \lfloor T/h \rfloor\}$

$$\|\mathbf{e}_n\| \leq d_1 e^{d_2 n h} h^2 \quad \textit{and} \quad \|\mathbf{e}_{n+1} - \mathbf{e}_n\| \leq d_3 e^{d_2 n h} h^3,$$

where $\mathbf{e}_n := \tilde{\boldsymbol{\theta}}(t_n) - \boldsymbol{\theta}^{(n)}$*. The constants can be defined as*

$$\begin{aligned} d_1 &:= C_1, \\ d_2 &:= \left[1 + \frac{M_2\sqrt{p}}{R+\varepsilon}\left(\frac{M_1^2}{R(R+\varepsilon)} + 1\right) d_1\right]\sqrt{p}, \\ d_3 &:= C_1 d_2. \end{aligned}$$

Proof. We will show this by induction over n, the same way an analogous bound is shown in [1].

The base case is $n = 0$. Indeed, $\mathbf{e}_0 = \tilde{\boldsymbol{\theta}}(0) - \boldsymbol{\theta}^{(0)} = \mathbf{0}$. Then the jth component of $\mathbf{e}_1 - \mathbf{e}_0$ is

$$\begin{aligned} [\mathbf{e}_1 - \mathbf{e}_0]_j = [\mathbf{e}_1]_j &= \tilde{\theta}_j(t_1) - \theta_j^{(0)} + \frac{h\nabla_j E_0\left(\boldsymbol{\theta}^{(0)}\right)}{\sqrt{(1-\rho)\left(\nabla_j E_0\left(\boldsymbol{\theta}^{(0)}\right)\right)^2 + \varepsilon}} \\ &= \tilde{\theta}_j(t_1) - \tilde{\theta}_j(t_0) + \frac{h\nabla_j E_0\left(\tilde{\boldsymbol{\theta}}(t_0)\right)}{\sqrt{(1-\rho)\left(\nabla_j E_0\left(\tilde{\boldsymbol{\theta}}(t_0)\right)\right)^2 + \varepsilon}}. \end{aligned}$$

By Theorem SA-2.3, the absolute value of the right-hand side does not exceed $C_1 h^3$, which means $\|\mathbf{e}_1 - \mathbf{e}_0\| \leq C_1 h^3 \sqrt{p}$. Since $C_1\sqrt{p} \leq d_3$, the base case is proven.

Now suppose that for all $k = 0, 1, \ldots, n-1$ the claim

$$\|\mathbf{e}_k\| \leq d_1 e^{d_2 k h} h^2 \quad \text{and} \quad \|\mathbf{e}_{k+1} - \mathbf{e}_k\| \leq d_3 e^{d_2 k h} h^3$$

is proven. Then

$$\begin{aligned} \|\mathbf{e}_n\| &\overset{\text{(a)}}{\leq} \|\mathbf{e}_{n-1}\| + \|\mathbf{e}_n - \mathbf{e}_{n-1}\| \leq d_1 e^{d_2(n-1)h} h^2 + d_3 e^{d_2(n-1)h} h^3 \\ &= d_1 e^{d_2(n-1)h} h^2 \left(1 + \frac{d_3}{d_1} h\right) \overset{\text{(b)}}{\leq} d_1 e^{d_2(n-1)h} h^2 (1 + d_2 h) \end{aligned}$$

$$\overset{\text{(c)}}{\leq} d_1 e^{d_2(n-1)h} h^2 \cdot e^{d_2 h} = d_1 e^{d_2 n h} h^2,$$

where (a) is by the triangle inequality, (b) is by $d_3/d_1 \leq d_2$, in (c) we used $1 + x \leq e^x$ for all $x \geq 0$.

Next, combining Theorem SA-2.3 with (SA-2.1), we have

$$\left|[\mathbf{e}_{n+1} - \mathbf{e}_n]_j\right| \leq C_1 h^3 + h \left| \frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{\sqrt{A} + \varepsilon} - \frac{\nabla_j E_n\Big(\boldsymbol{\theta}^{(n)}\Big)}{\sqrt{B} + \varepsilon} \right|, \tag{SA-2.3}$$

where to simplify notation we put

$$A := \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) \Big)^2,$$
$$B := \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \Big(\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) \Big)^2.$$

Using $A \geq R^2$, $B \geq R^2$, we have

$$\left| \frac{1}{\sqrt{A} + \varepsilon} - \frac{1}{\sqrt{B} + \varepsilon} \right| = \frac{|A - B|}{\Big(\sqrt{A} + \varepsilon\Big)\Big(\sqrt{B} + \varepsilon\Big)\Big(\sqrt{A} + \sqrt{B}\Big)} \leq \frac{|A - B|}{2R(R + \varepsilon)^2}. \tag{SA-2.4}$$

But since

$$\begin{aligned}
&\left| \Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) \Big)^2 - \Big(\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) \Big)^2 \right| \\
&\quad = \left| \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) - \nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) \right| \cdot \left| \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) + \nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) \right| \\
&\quad \leq 2M_1 \left| \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) - \nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) \right| \leq 2M_1 M_2 \sqrt{p} \left\| \tilde{\boldsymbol{\theta}}(t_k) - \boldsymbol{\theta}^{(k)} \right\|,
\end{aligned}$$

we have

$$|A - B| \leq 2M_1 M_2 \sqrt{p} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left\| \tilde{\boldsymbol{\theta}}(t_k) - \boldsymbol{\theta}^{(k)} \right\|. \tag{SA-2.5}$$

Combining (SA-2.4) and (SA-2.5), we obtain

$$\begin{aligned}
&\left| \frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{\sqrt{A} + \varepsilon} - \frac{\nabla_j E_n\Big(\boldsymbol{\theta}^{(n)}\Big)}{\sqrt{B} + \varepsilon} \right| \\
&\leq \left| \nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \right| \cdot \left| \frac{1}{\sqrt{A} + \varepsilon} - \frac{1}{\sqrt{B} + \varepsilon} \right| + \frac{\left| \nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) - \nabla_j E_n\Big(\boldsymbol{\theta}^{(n)}\Big) \right|}{\sqrt{B} + \varepsilon} \\
&\leq M_1 \cdot \frac{2M_1 M_2 \sqrt{p} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left\| \tilde{\boldsymbol{\theta}}(t_k) - \boldsymbol{\theta}^{(k)} \right\|}{2R(R+\varepsilon)^2} + \frac{M_2 \sqrt{p} \left\| \tilde{\boldsymbol{\theta}}(t_n) - \boldsymbol{\theta}^{(n)} \right\|}{R + \varepsilon} \\
&= \frac{M_1^2 M_2 \sqrt{p}}{R(R+\varepsilon)^2} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left\| \tilde{\boldsymbol{\theta}}(t_k) - \boldsymbol{\theta}^{(k)} \right\| + \frac{M_2 \sqrt{p}}{R + \varepsilon} \left\| \tilde{\boldsymbol{\theta}}(t_n) - \boldsymbol{\theta}^{(n)} \right\| \\
&\overset{\text{(a)}}{\leq} \frac{M_1^2 M_2 \sqrt{p}}{R(R+\varepsilon)^2} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) d_1 e^{d_2 k h} h^2 + \frac{M_2 \sqrt{p}}{R + \varepsilon} d_1 e^{d_2 n h} h^2,
\end{aligned} \tag{SA-2.6}$$

where in (a) we used the induction hypothesis and that the bound on $\|\mathbf{e}_n\|$ is already proven.

Now note that since $0 < \rho e^{-d_2 h} \leq \rho$, we have $\sum_{k=0}^{n} \big(\rho e^{-d_2 h}\big)^k \leq \sum_{k=0}^{\infty} \rho^k = \frac{1}{1-\rho}$, which is rewritten as

$$\sum_{k=0}^{n} \rho^{n-k}(1-\rho) e^{d_2 k h} \leq e^{d_2 n h}.$$

Then we can continue (SA-2.6):

$$\left|\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{\sqrt{A}+\varepsilon}-\frac{\nabla_j E_n\Big(\boldsymbol{\theta}^{(n)}\Big)}{\sqrt{B}+\varepsilon}\right|\le\frac{M_2\sqrt{p}}{R+\varepsilon}\left(\frac{M_1^2}{R(R+\varepsilon)}+1\right)d_1 e^{d_2 nh}h^2 \tag{SA-2.7}$$

Again using $1\le e^{d_2 nh}$, we conclude from (SA-2.3) and (SA-2.7) that

$$\|\mathbf{e}_{n+1}-\mathbf{e}_n\|\le\underbrace{\left(C_1+\frac{M_2\sqrt{p}}{R+\varepsilon}\left(\frac{M_1^2}{R(R+\varepsilon)}+1\right)d_1\right)\sqrt{p}}_{\le d_3}e^{d_2 nh}h^3,$$

finishing the induction step. □

SA-2.5 RMSProp with ε outside: full-batch. In the full-batch setting $E_k\equiv E$, the terms in (SA-2.2) simplify to

$$\begin{aligned}
R_j^{(n)}(\boldsymbol{\theta})&=\big|\nabla_j E(\boldsymbol{\theta})\big|\sqrt{1-\rho^{n+1}},\\
P_j^{(n)}(\boldsymbol{\theta})&=\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E(\boldsymbol{\theta})\sum_{i=1}^{p}\nabla_{ij}E(\boldsymbol{\theta})\sum_{l=k}^{n-1}\frac{\nabla_i E(\boldsymbol{\theta})}{\big|\nabla_i E(\boldsymbol{\theta})\big|\sqrt{1-\rho^{l+1}}+\varepsilon},\\
\bar{P}_j^{(n)}(\boldsymbol{\theta})&=\Big(1-\rho^{n+1}\Big)\nabla_j E(\boldsymbol{\theta})\sum_{i=1}^{p}\nabla_{ij}E(\boldsymbol{\theta})\frac{\nabla_i E(\boldsymbol{\theta})}{\big|\nabla_i E(\boldsymbol{\theta})\big|\sqrt{1-\rho^{n+1}}+\varepsilon}.
\end{aligned}$$

If ε is small and the iteration number n is large, (SA-2.2) simplifies to

$$\begin{aligned}
\dot{\tilde{\theta}}_j(t)&=-\operatorname{sign}\nabla_j E(\tilde{\boldsymbol{\theta}}(t))+h\frac{\rho}{1-\rho}\cdot\frac{\sum_{i=1}^{p}\nabla_{ij}E(\tilde{\boldsymbol{\theta}}(t))\operatorname{sign}\nabla_i E(\tilde{\boldsymbol{\theta}}(t))}{\Big|\nabla_j E(\tilde{\boldsymbol{\theta}}(t))\Big|}\\
&=\Big|\nabla_j E(\tilde{\boldsymbol{\theta}}(t))\Big|^{-1}\left[-\nabla_j E(\tilde{\boldsymbol{\theta}}(t))+h\frac{\rho}{1-\rho}\nabla_j\Big\|\nabla E(\tilde{\boldsymbol{\theta}}(t))\Big\|_1\right].
\end{aligned}$$

SA-3 RMSProp with ε inside the square root

Definition SA-3.1. In this section, for some $\boldsymbol{\theta}^{(0)}\in\mathbb{R}^p$, $\nu^{(0)}=\mathbf{0}\in\mathbb{R}^p$, $\rho\in(0,1)$, let the sequence of p-vectors $\Big\{\boldsymbol{\theta}^{(k)}\Big\}_{k\in\mathbb{Z}_{\ge 0}}$ be defined for $n\ge 0$ by

$$\begin{aligned}
\nu_j^{(n+1)}&=\rho\nu_j^{(n)}+(1-\rho)\Big(\nabla_j E_n\Big(\boldsymbol{\theta}^{(n)}\Big)\Big)^2,\\
\theta_j^{(n+1)}&=\theta_j^{(n)}-\frac{h}{\sqrt{\nu_j^{(n+1)}+\varepsilon}}\nabla_j E_n\Big(\boldsymbol{\theta}^{(n)}\Big).
\end{aligned}\tag{SA-3.1}$$

Let $\tilde{\boldsymbol{\theta}}(t)$ be defined as a continuous solution to the piecewise ODE

$$\begin{aligned}
\dot{\tilde{\theta}}_j(t)=&-\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}\\
&+h\left(\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big(2P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\bar{P}_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)}{2R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^3}-\frac{\sum_{i=1}^{p}\nabla_{ij}E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}}{2R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))}\right).
\end{aligned}\tag{SA-3.2}$$

with the initial condition $\tilde{\boldsymbol{\theta}}(0) = \boldsymbol{\theta}^{(0)}$, where $\mathbf{R}^{(n)}(\boldsymbol{\theta})$, $\mathbf{P}^{(n)}(\boldsymbol{\theta})$ and $\bar{\mathbf{P}}^{(n)}(\boldsymbol{\theta})$ are p-dimensional functions with components

$$
\begin{aligned}
R_j^{(n)}(\boldsymbol{\theta}) &:= \sqrt{\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\big(\nabla_j E_k(\boldsymbol{\theta})\big)^2 + \varepsilon}, \\
P_j^{(n)}(\boldsymbol{\theta}) &:= \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta}) \sum_{i=1}^{p} \nabla_{ij} E_k(\boldsymbol{\theta}) \sum_{l=k}^{n-1} \frac{\nabla_i E_l(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta})}, \\
\bar{P}_j^{(n)}(\boldsymbol{\theta}) &:= \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta}) \sum_{i=1}^{p} \nabla_{ij} E_k(\boldsymbol{\theta}) \frac{\nabla_i E_n(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta})}.
\end{aligned}
\tag{SA-3.3}
$$

Assumption SA-3.2. For some positive constants M_1, M_2, M_3, M_4 we have

$$
\begin{aligned}
&\sup_i \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_i E_k(\boldsymbol{\theta})\big| \le M_1, \\
&\sup_{i,j} \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_{ij} E_k(\boldsymbol{\theta})\big| \le M_2, \\
&\sup_{i,j,s} \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_{ijs} E_k(\boldsymbol{\theta})\big| \le M_3, \\
&\sup_{i,j,s,r} \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_{ijsr} E_k(\boldsymbol{\theta})\big| \le M_4.
\end{aligned}
$$

Theorem SA-3.3 (RMSProp with ε inside: local error bound)**.** *Suppose Assumption SA-3.2 holds. Then for all $n \in \{0, 1, \dots, \lfloor T/h \rfloor\}$*

$$
\left| \tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) + h \frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{\sqrt{\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 + \varepsilon}} \right| \le C_2 h^3
$$

for a positive constant C_2 depending on ρ, where $\tilde{\boldsymbol{\theta}}(t)$ is defined in Definition SA-3.1.

The argument is the same as for Theorem SA-2.3.

Theorem SA-3.4 (RMSProp with ε inside: global error bound)**.** *Suppose Assumption SA-3.2 holds. Then there exist positive constants d_4, d_5, d_6 such that for all $n \in \{0, 1, \dots, \lfloor T/h \rfloor\}$*

$$
\|\mathbf{e}_n\| \le d_4 e^{d_5 n h} h^2 \quad \text{and} \quad \|\mathbf{e}_{n+1} - \mathbf{e}_n\| \le d_6 e^{d_5 n h} h^3,
$$

where $\mathbf{e}_n := \tilde{\boldsymbol{\theta}}(t_n) - \boldsymbol{\theta}^{(n)}$; $\tilde{\boldsymbol{\theta}}(t)$ and $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k \in \mathbb{Z}_{\ge 0}}$ are defined in Definition SA-3.1. The constants can be defined as

$$
\begin{aligned}
d_4 &:= C_2, \\
d_5 &:= \left[1 + \frac{M_2\sqrt{p}}{\sqrt{\varepsilon}}\left(\frac{M_1^2}{\varepsilon} + 1\right) d_4\right]\sqrt{p}, \\
d_6 &:= C_2 d_5.
\end{aligned}
$$

The argument is the same as for Theorem SA-2.4.

SA-3.5 RMSProp with ε inside: full-batch. In the full-batch setting $E_k \equiv E$, the terms in (SA-3.2) simplify to

$$
R_j^{(n)}(\boldsymbol{\theta}) = \sqrt{\big|\nabla_j E(\boldsymbol{\theta})\big|^2 (1 - \rho^{n+1}) + \varepsilon},
$$

$$P_j^{(n)}(\boldsymbol{\theta}) = \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E(\boldsymbol{\theta}) \sum_{i=1}^{p} \nabla_{ij} E(\boldsymbol{\theta}) \sum_{l=k}^{n-1} \frac{\nabla_i E(\boldsymbol{\theta})}{\sqrt{|\nabla_i E(\boldsymbol{\theta})|^2(1-\rho^{l+1})+\varepsilon}},$$
$$\bar{P}_j^{(n)}(\boldsymbol{\theta}) = (1-\rho^{n+1})\nabla_j E(\boldsymbol{\theta}) \sum_{i=1}^{p} \nabla_{ij} E(\boldsymbol{\theta}) \frac{\nabla_i E(\boldsymbol{\theta})}{\sqrt{|\nabla_i E(\boldsymbol{\theta})|^2(1-\rho^{n+1})+\varepsilon}}.$$

If the iteration number n is large, (SA-3.2) rapidly becomes

$$\dot{\tilde{\theta}}_j(t) = -\frac{1}{\sqrt{|\nabla_j E(\tilde{\boldsymbol{\theta}}(t))|^2+\varepsilon}}\big(\nabla_j E(\tilde{\boldsymbol{\theta}}(t)) + \text{bias}\big), \tag{SA-3.4}$$

where

$$\text{bias} := \frac{h}{2}\left\{-\frac{2\rho}{1-\rho} + \frac{1+\rho}{1-\rho}\cdot\frac{\varepsilon}{|\nabla_j E(\tilde{\boldsymbol{\theta}}(t))|^2+\varepsilon}\right\}\nabla_j \big\|\nabla E(\tilde{\boldsymbol{\theta}}(t))\big\|_{1,\varepsilon}. \tag{SA-3.5}$$

SA-4 Adam with ε outside the square root

Definition SA-4.1. In this section, for some $\boldsymbol{\theta}^{(0)} \in \mathbb{R}^p$, $\nu^{(0)} = \mathbf{0} \in \mathbb{R}^p$, $\beta, \rho \in (0,1)$, let the sequence of p-vectors $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k\in\mathbb{Z}_{\geq 0}}$ be defined for $n \geq 0$ by

$$\begin{aligned}
\nu_j^{(n+1)} &= \rho\nu_j^{(n)} + (1-\rho)\left(\nabla_j E_n\left(\boldsymbol{\theta}^{(n)}\right)\right)^2,\\
m_j^{(n+1)} &= \beta m_j^{(n)} + (1-\beta)\nabla_j E_n\left(\boldsymbol{\theta}^{(n)}\right),\\
\theta_j^{(n+1)} &= \theta_j^{(n)} - h\frac{m_j^{(n+1)}/\left(1-\beta^{n+1}\right)}{\sqrt{\nu_j^{(n+1)}/(1-\rho^{n+1})}+\varepsilon}
\end{aligned}$$

or, rewriting,

$$\theta_j^{(n+1)} = \theta_j^{(n)} - h\frac{\frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}\beta^{n-k}(1-\beta)\nabla_j E_k\left(\boldsymbol{\theta}^{(k)}\right)}{\sqrt{\frac{1}{1-\rho^{n+1}}\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\boldsymbol{\theta}^{(k)}\right)\right)^2}+\varepsilon}. \tag{SA-4.1}$$

Let $\tilde{\boldsymbol{\theta}}(t)$ be defined as a continuous solution to the piecewise ODE

$$\begin{aligned}
\dot{\tilde{\theta}}_j(t) = &-\frac{M_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\\
&+ h\left(\frac{M_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)} - \frac{2L_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{L}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)}\right).
\end{aligned} \tag{SA-4.2}$$

with the initial condition $\tilde{\boldsymbol{\theta}}(0) = \boldsymbol{\theta}^{(0)}$, where $\mathbf{R}^{(n)}(\boldsymbol{\theta})$, $\mathbf{P}^{(n)}(\boldsymbol{\theta})$, $\bar{\mathbf{P}}^{(n)}(\boldsymbol{\theta})$, $\mathbf{M}^{(n)}(\boldsymbol{\theta})$, $\mathbf{L}^{(n)}(\boldsymbol{\theta})$, $\bar{\mathbf{L}}^{(n)}(\boldsymbol{\theta})$ are

p-dimensional functions with components

$$
\begin{aligned}
R_j^{(n)}(\boldsymbol{\theta}) &:= \sqrt{\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\big(\nabla_j E_k(\boldsymbol{\theta})\big)^2/(1-\rho^{n+1})},\\
M_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_j E_k(\boldsymbol{\theta}),\\
L_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta) \sum_{i=1}^{p} \nabla_{ij} E_k(\boldsymbol{\theta}) \sum_{l=k}^{n-1} \frac{M_i^{(l)}(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta})+\varepsilon},\\
\bar{L}_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta) \sum_{i=1}^{p} \nabla_{ij} E_k(\boldsymbol{\theta}) \frac{M_i^{(n)}(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta})+\varepsilon},\\
P_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta}) \sum_{i=1}^{p} \nabla_{ij} E_k(\boldsymbol{\theta}) \sum_{l=k}^{n-1} \frac{M_i^{(l)}(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta})+\varepsilon},\\
\bar{P}_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta}) \sum_{i=1}^{p} \nabla_{ij} E_k(\boldsymbol{\theta}) \frac{M_i^{(n)}(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta})+\varepsilon}.
\end{aligned}
\tag{SA-4.3}
$$

Assumption SA-4.2.

1. For some positive constants M_1, M_2, M_3, M_4 we have

$$
\begin{aligned}
&\sup_i \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_i E_k(\boldsymbol{\theta})\big| \le M_1,\\
&\sup_{i,j} \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_{ij} E_k(\boldsymbol{\theta})\big| \le M_2,\\
&\sup_{i,j,s} \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_{ijs} E_k(\boldsymbol{\theta})\big| \le M_3,\\
&\sup_{i,j,s,r} \sup_k \sup_{\boldsymbol{\theta}} \big|\nabla_{ijsr} E_k(\boldsymbol{\theta})\big| \le M_4.
\end{aligned}
$$

2. For some $R > 0$ we have for all $n \in \{0, 1, \dots, \lfloor T/h \rfloor\}$

$$
R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \ge R, \quad \frac{1}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 \ge R^2,
$$

   where $\tilde{\boldsymbol{\theta}}(t)$ is defined in Definition SA-4.1.

Theorem SA-4.3 (Adam with ε outside: local error bound)**.** *Suppose Assumption SA-4.2 holds. Then for all* $n \in \{0, 1, \dots, \lfloor T/h \rfloor\}$

$$
\left| \tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) + h \frac{\frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)}{\sqrt{\frac{1}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2} + \varepsilon} \right| \le C_3 h^3
$$

for a positive constant C_3 *depending on* β *and* ρ*.*

The argument is the same as for Theorem SA-2.3.

Theorem SA-4.4 (Adam with ε outside: global error bound)**.** *Suppose Assumption SA-4.2 holds, and*

$$
\frac{1}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big)\Big)^2 \ge R^2
$$

for $\Big\{\boldsymbol{\theta}^{(k)}\Big\}_{k \in \mathbb{Z}_{\ge 0}}$ *defined in Definition SA-4.1. Then there exist positive constants* d_7, d_8, d_9 *such that for all* $n \in \{0, 1, \dots, \lfloor T/h \rfloor\}$

$$
\|\mathbf{e}_n\| \le d_7 e^{d_8 nh} h^2 \quad \text{and} \quad \|\mathbf{e}_{n+1} - \mathbf{e}_n\| \le d_9 e^{d_8 nh} h^3,
$$

where $\mathbf{e}_n := \tilde{\boldsymbol{\theta}}(t_n) - \boldsymbol{\theta}^{(n)}$. *The constants can be defined as*

$$
\begin{aligned}
d_7 &:= C_3, \\
d_8 &:= \left[1 + \frac{M_2\sqrt{p}}{R+\varepsilon}\left(\frac{M_1^2}{R(R+\varepsilon)} + 1\right) d_7\right]\sqrt{p}, \\
d_9 &:= C_3 d_8.
\end{aligned}
$$

Proof. Analogously to Theorem SA-2.4, we will prove this by induction over n.

The base case is $n = 0$. Indeed, $\mathbf{e}_0 = \tilde{\boldsymbol{\theta}}(0) - \boldsymbol{\theta}^{(0)} = \mathbf{0}$. Then the jth component of $\mathbf{e}_1 - \mathbf{e}_0$ is

$$
\begin{aligned}
[\mathbf{e}_1 - \mathbf{e}_0]_j = [\mathbf{e}_1]_j &= \tilde{\theta}_j(t_1) - \theta_j^{(0)} + \frac{h\nabla_j E_0\left(\boldsymbol{\theta}^{(0)}\right)}{\left|\nabla_j E_0\left(\boldsymbol{\theta}^{(0)}\right)\right| + \varepsilon} \\
&= \tilde{\theta}_j(t_1) - \tilde{\theta}_j(t_0) + \frac{h\nabla_j E_0\left(\tilde{\boldsymbol{\theta}}(t_0)\right)}{\sqrt{\left(\nabla_j E_0\left(\tilde{\boldsymbol{\theta}}(t_0)\right)\right)^2} + \varepsilon}.
\end{aligned}
$$

By Theorem SA-4.3, the absolute value of the right-hand side does not exceed $C_3 h^3$, which means $\|\mathbf{e}_1 - \mathbf{e}_0\| \le C_3 h^3 \sqrt{p}$. Since $C_3\sqrt{p} \le d_9$, the base case is proven.

Now suppose that for all $k = 0, 1, \ldots, n-1$ the claim

$$
\|\mathbf{e}_k\| \le d_7 e^{d_8 kh} h^2 \quad \text{and} \quad \|\mathbf{e}_{k+1} - \mathbf{e}_k\| \le d_9 e^{d_8 kh} h^3
$$

is proven. Then

$$
\begin{aligned}
\|\mathbf{e}_n\| &\overset{\text{(a)}}{\le} \|\mathbf{e}_{n-1}\| + \|\mathbf{e}_n - \mathbf{e}_{n-1}\| \le d_7 e^{d_8(n-1)h} h^2 + d_9 e^{d_8(n-1)h} h^3 \\
&= d_7 e^{d_8(n-1)h} h^2 \left(1 + \frac{d_9}{d_7} h\right) \overset{\text{(b)}}{\le} d_7 e^{d_8(n-1)h} h^2 (1 + d_8 h) \\
&\overset{\text{(c)}}{\le} d_7 e^{d_8(n-1)h} h^2 \cdot e^{d_8 h} = d_7 e^{d_8 nh} h^2,
\end{aligned}
$$

where (a) is by the triangle inequality, (b) is by $d_9/d_7 \le d_8$, in (c) we used $1 + x \le e^x$ for all $x \ge 0$.

Next, combining Theorem SA-4.3 with (SA-4.1), we have

$$
\left|[\mathbf{e}_{n+1} - \mathbf{e}_n]_j\right| \le C_3 h^3 + h\left|\frac{N'}{\sqrt{D'} + \varepsilon} - \frac{N''}{\sqrt{D''} + \varepsilon}\right|, \tag{SA-4.4}
$$

where to simplify notation we put

$$
\begin{aligned}
N' &:= \frac{1}{1 - \beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_j E_k\left(\boldsymbol{\theta}^{(k)}\right), \\
N'' &:= \frac{1}{1 - \beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right), \\
D' &:= \frac{1}{1 - \rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\boldsymbol{\theta}^{(k)}\right)\right)^2, \\
D'' &:= \frac{1}{1 - \rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right)\right)^2.
\end{aligned}
$$

Using $D' \ge R^2$, $D'' \ge R^2$, we have

$$
\left|\frac{1}{\sqrt{D'} + \varepsilon} - \frac{1}{\sqrt{D''} + \varepsilon}\right| = \frac{\left|D' - D''\right|}{\left(\sqrt{D'} + \varepsilon\right)\left(\sqrt{D''} + \varepsilon\right)\left(\sqrt{D'} + \sqrt{D''}\right)} \le \frac{\left|D' - D''\right|}{2R(R+\varepsilon)^2}. \tag{SA-4.5}
$$

But since

$$\begin{aligned}
&\left|\left(\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big)\right)^2 - \left(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\right)^2\right| \\
&\quad= \left|\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\right| \cdot \left|\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) + \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\right| \\
&\quad\le 2M_1\left|\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\right| \le 2M_1M_2\sqrt{p}\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\|,
\end{aligned}$$

we have

$$\left|D' - D''\right| \le \frac{2M_1M_2\sqrt{p}}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\|. \tag{SA-4.6}$$

Similarly,

$$\begin{aligned}
\left|N' - N''\right| &\le \frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\left|\nabla_j E_k\Big(\boldsymbol{\theta}^{(k)}\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\right| \\
&\le \frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)M_2\sqrt{p}\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\|.
\end{aligned} \tag{SA-4.7}$$

Combining (SA-4.5), (SA-4.6) and (SA-4.7), we get

$$\begin{aligned}
&\left|\frac{N'}{\sqrt{D'}+\varepsilon} - \frac{N''}{\sqrt{D''}+\varepsilon}\right| \le \left|N'\right| \cdot \left|\frac{1}{\sqrt{D'}+\varepsilon} - \frac{1}{\sqrt{D''}+\varepsilon}\right| + \frac{\left|N' - N''\right|}{\sqrt{D''}+\varepsilon} \\
&\quad\le \frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)M_1 \cdot \frac{2M_1M_2\sqrt{p}}{2R(R+\varepsilon)^2(1-\rho^{n+1})} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\| \\
&\qquad+ \frac{M_2\sqrt{p}}{(R+\varepsilon)(1-\beta^{n+1})} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\| \\
&\quad= \frac{M_1^2M_2\sqrt{p}}{R(R+\varepsilon)^2(1-\rho^{n+1})} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\| \\
&\qquad+ \frac{M_2\sqrt{p}}{(R+\varepsilon)(1-\beta^{n+1})} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\left\|\boldsymbol{\theta}^{(k)} - \tilde{\boldsymbol{\theta}}(t_k)\right\| \\
&\quad\overset{\text{(a)}}{\le} \frac{M_1^2M_2\sqrt{p}}{R(R+\varepsilon)^2(1-\rho^{n+1})} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)d_7e^{d_8kh}h^2 \\
&\qquad+ \frac{M_2\sqrt{p}}{(R+\varepsilon)(1-\beta^{n+1})} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)d_7e^{d_8kh}h^2,
\end{aligned} \tag{SA-4.8}$$

where in (a) we used the induction hypothesis and that the bound on $\|\mathbf{e}_n\|$ is already proven.

Now note that since $0 < \rho e^{-d_8h} < \rho$, we have $\sum_{k=0}^{n}\left(\rho e^{-d_8h}\right)^k \le \sum_{k=0}^{n}\rho^k = \left(1-\rho^{n+1}\right)/(1-\rho)$, which is rewritten as

$$\frac{1}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)e^{d_8kh} \le e^{d_8nh}.$$

By the same logic,

$$\frac{1}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)e^{d_8kh} \le e^{d_8nh}.$$

Then we can continue (SA-4.8):

$$\left|\frac{N'}{\sqrt{D'}+\varepsilon} - \frac{N''}{\sqrt{D''}+\varepsilon}\right| \le \frac{M_2\sqrt{p}}{R+\varepsilon}\left(\frac{M_1^2}{R(R+\varepsilon)} + 1\right)d_7e^{d_8nh}h^2 \tag{SA-4.9}$$

Again using $1 \le e^{d_8 nh}$, we conclude from (SA-4.4) and (SA-4.9) that

$$\|\mathbf{e}_{n+1} - \mathbf{e}_n\| \le \underbrace{\left(C_3 + \frac{M_2\sqrt{p}}{R+\varepsilon}\left(\frac{M_1^2}{R(R+\varepsilon)} + 1\right)d_7\right)}_{\le d_9}\sqrt{p}\, e^{d_8 nh} h^3,$$

finishing the induction step. □

SA-5 Adam with ε inside the square root

Definition SA-5.1. In this section, for some $\boldsymbol{\theta}^{(0)} \in \mathbb{R}^p$, $\nu^{(0)} = \mathbf{0} \in \mathbb{R}^p$, $\beta, \rho \in (0,1)$, let the sequence of p-vectors $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k \in \mathbb{Z}_{\ge 0}}$ be defined for $n \ge 0$ by

$$\begin{aligned}
\nu_j^{(n+1)} &= \rho\nu_j^{(n)} + (1-\rho)\left(\nabla_j E_n\left(\boldsymbol{\theta}^{(n)}\right)\right)^2, \\
m_j^{(n+1)} &= \beta m_j^{(n)} + (1-\beta)\nabla_j E_n\left(\boldsymbol{\theta}^{(n)}\right), \\
\theta_j^{(n+1)} &= \theta_j^{(n)} - h\frac{m_j^{(n+1)}/\left(1-\beta^{n+1}\right)}{\sqrt{\nu_j^{(n+1)}/(1-\rho^{n+1}) + \varepsilon}}.
\end{aligned} \tag{SA-5.1}$$

Let $\tilde{\boldsymbol{\theta}}(t)$ be defined as a continuous solution to the piecewise ODE

$$\begin{aligned}
\dot{\tilde{\theta}}_j(t) = &-\frac{M_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)} \\
&+ h\left(\frac{M_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)^3} - \frac{2L_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \bar{L}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}{2R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}\right).
\end{aligned} \tag{SA-5.2}$$

with the initial condition $\tilde{\boldsymbol{\theta}}(0) = \boldsymbol{\theta}^{(0)}$, where $\mathbf{R}^{(n)}(\boldsymbol{\theta})$, $\mathbf{P}^{(n)}(\boldsymbol{\theta})$, $\bar{\mathbf{P}}^{(n)}(\boldsymbol{\theta})$, $\mathbf{M}^{(n)}(\boldsymbol{\theta})$, $\mathbf{L}^{(n)}(\boldsymbol{\theta})$, $\bar{\mathbf{L}}^{(n)}(\boldsymbol{\theta})$ are p-dimensional functions with components

$$\begin{aligned}
R_j^{(n)}(\boldsymbol{\theta}) &:= \sqrt{\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\left(\nabla_j E_k(\boldsymbol{\theta})\right)^2/(1-\rho^{n+1}) + \varepsilon}, \\
M_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}\beta^{n-k}(1-\beta)\nabla_j E_k(\boldsymbol{\theta}), \\
L_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}\beta^{n-k}(1-\beta)\sum_{i=1}^{p}\nabla_{ij}E_k(\boldsymbol{\theta})\sum_{l=k}^{n-1}\frac{M_i^{(l)}(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta})}, \\
\bar{L}_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}\beta^{n-k}(1-\beta)\sum_{i=1}^{p}\nabla_{ij}E_k(\boldsymbol{\theta})\frac{M_i^{(n)}(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta})}, \\
P_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\rho^{n+1}}\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta})\sum_{i=1}^{p}\nabla_{ij}E_k(\boldsymbol{\theta})\sum_{l=k}^{n-1}\frac{M_i^{(l)}(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta})}, \\
\bar{P}_j^{(n)}(\boldsymbol{\theta}) &:= \frac{1}{1-\rho^{n+1}}\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta})\sum_{i=1}^{p}\nabla_{ij}E_k(\boldsymbol{\theta})\frac{M_i^{(n)}(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta})}.
\end{aligned} \tag{SA-5.3}$$

Assumption SA-5.2. For some positive constants M_1, M_2, M_3, M_4 we have

$$\sup_i \sup_k \sup_{\boldsymbol{\theta}} \left|\nabla_i E_k(\boldsymbol{\theta})\right| \le M_1,$$

$$\sup_{i,j}\sup_{k}\sup_{\boldsymbol{\theta}}\left|\nabla_{ij}E_k(\boldsymbol{\theta})\right| \le M_2,$$
$$\sup_{i,j,s}\sup_{k}\sup_{\boldsymbol{\theta}}\left|\nabla_{ijs}E_k(\boldsymbol{\theta})\right| \le M_3,$$
$$\sup_{i,j,s,r}\sup_{k}\sup_{\boldsymbol{\theta}}\left|\nabla_{ijsr}E_k(\boldsymbol{\theta})\right| \le M_4.$$

Theorem SA-5.3 (Adam with ε inside: local error bound)**.** *Suppose Assumption SA-5.2 holds. Then for all* $n \in \{0, 1, \ldots, \lfloor T/h \rfloor\}$

$$\left|\tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) + h\frac{\frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}\beta^{n-k}(1-\beta)\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right)}{\sqrt{\frac{1}{1-\rho^{n+1}}\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\left(\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right)\right)^2 + \varepsilon}}\right| \le C_4 h^3$$

for a positive constant C_4 *depending on* β *and* ρ*.*

The argument is the same as for Theorem SA-2.3.

Theorem SA-5.4 (Adam with ε inside: global error bound)**.** *Suppose Assumption SA-5.2 holds for* $\left\{\boldsymbol{\theta}^{(k)}\right\}_{k\in\mathbb{Z}_{\ge 0}}$ *defined in Definition SA-5.1. Then there exist positive constants* d_{10}*,* d_{11}*,* d_{12} *such that for all* $n \in \{0, 1, \ldots, \lfloor T/h \rfloor\}$

$$\|\mathbf{e}_n\| \le d_{10}e^{d_{11}nh}h^2 \quad \textit{and} \quad \|\mathbf{e}_{n+1} - \mathbf{e}_n\| \le d_{12}e^{d_{11}nh}h^3,$$

where $\mathbf{e}_n := \tilde{\boldsymbol{\theta}}(t_n) - \boldsymbol{\theta}^{(n)}$*. The constants can be defined as*

$$d_{10} := C_4,$$
$$d_{11} := \left[1 + \frac{M_2\sqrt{p}}{\sqrt{\varepsilon}}\left(\frac{M_1^2}{\varepsilon} + 1\right)d_{10}\right]\sqrt{p},$$
$$d_{12} := C_4 d_{11}.$$

The argument is the same as for Theorem SA-4.4.

SA-6 Technical bounding lemmas

We will need the following lemmas to prove Theorem SA-2.3.

Lemma SA-6.1. *Suppose Assumption SA-2.2 holds. Then*

$$\sup_{\boldsymbol{\theta}}\left|P_j^{(n)}(\boldsymbol{\theta})\right| \le C_5, \tag{SA-6.1}$$
$$\sup_{\boldsymbol{\theta}}\left|\bar{P}_j^{(n)}(\boldsymbol{\theta})\right| \le C_6, \tag{SA-6.2}$$

with constants C_5*,* C_6 *defined as follows:*

$$C_5 := p\frac{M_1^2 M_2}{R+\varepsilon}\cdot\frac{\rho}{1-\rho},$$
$$C_6 := p\frac{M_1^2 M_2}{R+\varepsilon}.$$

Proof of Lemma SA-6.1. The proof is done in the following simple steps.

SA-6.2 Proof of (SA-6.1). This bound is straightforward:

$$\sup_{\boldsymbol{\theta}}\left|P_j^{(n)}(\boldsymbol{\theta})\right| = \sup_{\boldsymbol{\theta}}\left|\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta})\sum_{i=1}^{p}\nabla_{ij}E_k(\boldsymbol{\theta})\sum_{l=k}^{n-1}\frac{\nabla_i E_l(\boldsymbol{\theta})}{R_i^{(l)}(\boldsymbol{\theta})+\varepsilon}\right|$$
$$\leq p\frac{M_1^2M_2}{R+\varepsilon}(1-\rho)\sum_{k=0}^{n}\rho^{n-k}(n-k) \leq p\frac{M_1^2M_2}{R+\varepsilon}(1-\rho)\sum_{k=0}^{\infty}\rho^k k = C_5.$$

SA-6.3 Proof of (SA-6.2). This bound is straightforward:

$$\sup_{\boldsymbol{\theta}}\left|\bar{P}_j^{(n)}(\boldsymbol{\theta})\right| = \sup_{\boldsymbol{\theta}}\left|\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k(\boldsymbol{\theta})\sum_{i=1}^{p}\nabla_{ij}E_k(\boldsymbol{\theta})\frac{\nabla_i E_n(\boldsymbol{\theta})}{R_i^{(n)}(\boldsymbol{\theta})+\varepsilon}\right|$$
$$\leq p\frac{M_1^2M_2}{R+\varepsilon}(1-\rho)\sum_{k=0}^{n}\rho^{n-k} \leq p\frac{M_1^2M_2}{R+\varepsilon} = C_6.$$

This concludes the proof of Lemma SA-6.1. □

Lemma SA-6.4. *Suppose Assumption SA-2.2 holds. Then the first derivative of $t \mapsto \tilde{\theta}_j(t)$ is uniformly over j and $t \in [0,T]$ bounded in absolute value by some positive constant, say D_1.*

Proof. This follows immediately from $h \leq T$, (SA-6.1), (SA-6.2) and the definition of $\tilde{\boldsymbol{\theta}}(t)$ given in (SA-2.2). □

Lemma SA-6.5. *Suppose Assumption SA-2.2 holds. Then*

$$\sup_{t\in[0,T]}\sup_{j}\left|\left(\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot}\right| \leq C_7, \tag{SA-6.3}$$

$$\sup_{n,k}\sup_{t\in[t_n,t_{n+1}]}\left|\sum_{i=1}^{p}\nabla_{ij}E_k\left(\tilde{\boldsymbol{\theta}}(t)\right)\left[\dot{\tilde{\theta}}_i(t)+\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right]\right| \leq C_8 h, \tag{SA-6.4}$$

$$\sup_{k\leq n}\sup_{t\in[0,T]}\left|\sum_{i=1}^{p}\nabla_{ij}E_k\left(\tilde{\boldsymbol{\theta}}(t)\right)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(l)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right| \leq (n-k)C_9, \tag{SA-6.5}$$

$$\left|\left(P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot}\right| \leq C_{10}+C_{14}, \tag{SA-6.6}$$

$$\left|\left(\bar{P}_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))\right)^{\cdot}\right| \leq C_{15}, \tag{SA-6.7}$$

$$\left|\left(\sum_{i=1}^{p}\nabla_{ij}E_k\left(\tilde{\boldsymbol{\theta}}(t)\right)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right)^{\cdot}\right| \leq C_{13}, \tag{SA-6.8}$$

$$\left|\left(\frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}\right)^{\cdot}\right| \leq C_{17}, \tag{SA-6.9}$$

$$\left|\left(\frac{\sum_{i=1}^{p}\nabla_{ij}E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}}{2\left(R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))+\varepsilon\right)}\right)^{\cdot}\right| \leq C_{18}, \tag{SA-6.10}$$

with constants C_7, C_8, C_9, C_{10}, C_{11}, C_{12}, C_{13}, C_{14}, C_{15}, C_{16}, C_{17}, C_{18} *defined as follows:*

$$
\begin{aligned}
C_7 &:= pM_2D_1,\\
C_8 &:= pM_2\left[\frac{M_1(2C_5+C_6)}{2(R+\varepsilon)^2R}+\frac{pM_1M_2}{2(R+\varepsilon)^2}\right],\\
C_9 &:= p\frac{M_1M_2}{R+\varepsilon},\\
C_{10} &:= D_1p^2\frac{M_1M_2^2}{R+\varepsilon}\cdot\frac{\rho}{1-\rho},\\
C_{11} &:= \frac{D_1pM_1M_2}{R},\\
C_{12} &:= D_1p^2\frac{M_1M_3}{R+\varepsilon},\\
C_{13} &:= C_{12}+pM_2\left(\frac{D_1pM_2}{R+\varepsilon}+\frac{M_1}{(R+\varepsilon)^2}C_{11}\right)\\
&= \frac{D_1p^2}{R+\varepsilon}\left(M_1M_3+M_2^2+\frac{M_1^2M_2^2}{(R+\varepsilon)R}\right),\\
C_{14} &:= M_1C_{13}\frac{\rho}{1-\rho},\\
C_{15} &:= \frac{D_1p^2M_1M_2^2}{R+\varepsilon}+\frac{D_1p^2M_1^2M_3}{R+\varepsilon}+\frac{D_1p^2M_1M_2^2}{R+\varepsilon}+\frac{pM_1^2M_2C_{11}}{(R+\varepsilon)^2},\\
C_{16} &:= \frac{2C_{11}}{R(R+\varepsilon)^3}+\frac{C_{11}}{(R+\varepsilon)^4},\\
C_{17} &:= \frac{D_1pM_2\cdot(2C_5+C_6)}{2(R+\varepsilon)^2R}+\frac{M_1\big(2(C_{10}+C_{14})+C_{15}\big)}{2(R+\varepsilon)^2R}+\frac{M_1(2C_5+C_6)C_{16}}{2},\\
C_{18} &:= \frac{1}{2(R+\varepsilon)}\left(\frac{p^2D_1M_1M_3}{R+\varepsilon}+\frac{p^2D_1M_2^2}{R+\varepsilon}+\frac{pM_1M_2C_{11}}{(R+\varepsilon)^2}\right)+\frac{1}{2}\cdot\frac{pM_1M_2}{R+\varepsilon}\cdot\frac{C_{11}}{(R+\varepsilon)^2}.
\end{aligned}
$$

Proof of Lemma SA-6.5. We divide this argument in several steps.

SA-6.6 Proof of (SA-6.3). This bound is straightforward:

$$
\left|\left(\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right)^{\cdot}\right| = \left|\sum_{i=1}^{p}\nabla_{ij}E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\dot{\tilde{\theta}}_i(t)\right| \le C_7.
$$

SA-6.7 Proof of (SA-6.4). By (SA-2.2) we have for $t = t_{n+1}^-$

$$
\left|\dot{\tilde{\theta}}_j(t)+\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right| \le h\left[\frac{M_1(2C_5+C_6)}{2(R+\varepsilon)^2R}+\frac{pM_1M_2}{2(R+\varepsilon)^2}\right],
$$

giving (SA-6.4) immediately.

SA-6.8 Proof of (SA-6.5). This bound follows from the assumptions immediately.

SA-6.9 Proof of (SA-6.6). We will prove this by bounding the two terms in the expression

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \\
&\quad= \sum_{k=0}^{n}\rho^{n-k}(1-\rho)\sum_{u=1}^{p}\nabla_{ju}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\dot{\tilde{\theta}}_u(t)\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon} \qquad \text{(SA-6.11)}\\
&\qquad+\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}.
\end{aligned}$$

It is easily shown that the first term in (SA-6.11) is bounded in absolute value by C_{10}:

$$\begin{aligned}
&\left|\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\sum_{u=1}^{p}\nabla_{ju}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\dot{\tilde{\theta}}_u(t)\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right| \\
&\quad\le D_1 p^2\frac{M_1M_2^2}{R+\varepsilon}(1-\rho)\sum_{k=0}^{n}\rho^k k \\
&\quad\le D_1 p^2\frac{M_1M_2^2}{R+\varepsilon}(1-\rho)\sum_{k=0}^{\infty}\rho^k k \\
&\quad= C_{10}.
\end{aligned}$$

For the proof of (SA-6.6), it is left to show that the second term in (SA-6.11) is bounded in absolute value by C_{14}.

To bound $\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(l)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right\}$, we can use

$$\begin{aligned}
&\left|\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}\right| \\
&\quad\le\left|\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right\}\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right| \\
&\qquad+\left|\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}\right|
\end{aligned}$$

By the Cauchy-Schwarz inequality applied twice,

$$\begin{aligned}
&\left|\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right\}\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right| \\
&\quad\le\sqrt{\sum_{i=1}^{p}\sum_{s=1}^{p}\Big(\nabla_{ijs}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^2}\sqrt{\sum_{u=1}^{p}\dot{\tilde{\theta}}_u(t)^2}\sqrt{\sum_{i=1}^{p}\left|\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right|^2} \\
&\quad\le M_3 p\cdot D_1\sqrt{p}\cdot\sqrt{\sum_{i=1}^{p}\left|\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right|^2}\le(n-k)C_{12}.
\end{aligned}$$

Next, for any n and j

$$\begin{aligned}\left|\frac{\mathrm{d}}{\mathrm{d}t}R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right| &= \frac{1}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}\left|\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\dot{\tilde{\theta}}_i(t)\right| \\ &\leq \frac{1}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}D_1 p M_1 M_2\sum_{k=0}^{n}\rho^{n-k}(1-\rho) \leq C_{11}.\end{aligned} \tag{SA-6.12}$$

This gives

$$\begin{aligned}\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}\right| &\leq \frac{\left|\sum_{s=1}^{p}\nabla_{is}E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\dot{\tilde{\theta}}_s(t)\right|}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon} + \frac{\left|\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right|\cdot\left|\frac{\mathrm{d}}{\mathrm{d}t}R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right|}{\Big(R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^2} \\ &\leq \frac{D_1 p M_2}{R+\varepsilon} + \frac{M_1}{(R+\varepsilon)^2}C_{11}.\end{aligned}$$

We have obtained

$$\left|\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}\right| \leq (n-k)C_{13}. \tag{SA-6.13}$$

This gives a bound on the second term in (SA-6.11):

$$\begin{aligned}&\left|\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\left\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{l=k}^{n-1}\frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}\right| \\ &\quad\leq M_1\sum_{k=0}^{n}\rho^{n-k}(1-\rho)(n-k)C_{13} \leq C_{14},\end{aligned}$$

concluding the proof of (SA-6.6).

SA-6.10 Proof of (SA-6.7). We will prove this by bounding the four terms in the expression

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\left\{\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\frac{\nabla_i E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\} \\ &\quad= \text{Term1} + \text{Term2} + \text{Term3} + \text{Term4},\end{aligned}$$

where

$$\begin{aligned}&\text{Term1} \\ &:= \sum_{k=0}^{n}\rho^{n-k}(1-\rho)\frac{\mathrm{d}}{\mathrm{d}t}\Big\{\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big\}\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\frac{\nabla_i E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}, \\ &\text{Term2} \\ &:= \sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\sum_{i=1}^{p}\frac{\mathrm{d}}{\mathrm{d}t}\Big\{\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big\}\frac{\nabla_i E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_i^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}, \\ &\text{Term3}\end{aligned}$$

$$:= \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \frac{\frac{\mathrm{d}}{\mathrm{d}t}\Big\{\nabla_i E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big\}}{R_i^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon},$$

Term4

$$:= -\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \frac{\nabla_i E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\frac{\mathrm{d}}{\mathrm{d}t} R_i^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{\Big(R_i^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^2}.$$

To bound Term1, use $\left|\frac{\mathrm{d}}{\mathrm{d}t}\Big\{\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big\}\right| \le D_1 p M_2$, giving

$$|\text{Term1}| \le \frac{D_1 p^2 M_1 M_2^2}{R+\varepsilon} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \le \frac{D_1 p^2 M_1 M_2^2}{R+\varepsilon}.$$

To bound Term2, use $\left|\frac{\mathrm{d}}{\mathrm{d}t}\Big\{\nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big\}\right| \le D_1 p M_3$, giving

$$|\text{Term2}| \le \frac{D_1 p^2 M_1^2 M_3}{R+\varepsilon} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \le \frac{D_1 p^2 M_1^2 M_3}{R+\varepsilon}.$$

To bound Term3, use $\left|\frac{\mathrm{d}}{\mathrm{d}t}\Big\{\nabla_i E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big\}\right| \le D_1 p M_2$, giving

$$|\text{Term3}| \le \frac{D_1 p^2 M_1 M_2^2}{R+\varepsilon} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \le \frac{D_1 p^2 M_1 M_2^2}{R+\varepsilon}.$$

To bound Term4, use (SA-6.12), giving

$$|\text{Term4}| \le \frac{p M_1^2 M_2 C_{11}}{(R+\varepsilon)^2} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \le \frac{p M_1^2 M_2 C_{11}}{(R+\varepsilon)^2}.$$

SA-6.11 Proof of (SA-6.8)**.** This is proven in (SA-6.13).

SA-6.12 Proof of (SA-6.9)**.** (SA-6.12) gives

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}\right\}\right| = \frac{\left|\frac{\mathrm{d}}{\mathrm{d}t} R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right|}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^2} \le \frac{C_{11}}{R^2}, \tag{SA-6.14}$$

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right\}\right| = \frac{\left|\frac{\mathrm{d}}{\mathrm{d}t} R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right|}{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^2} \le \frac{C_{11}}{(R+\varepsilon)^2}, \tag{SA-6.15}$$

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^2}\right\}\right| = \frac{2\left|\frac{\mathrm{d}}{\mathrm{d}t} R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\right|}{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^3} \le \frac{2C_{11}}{(R+\varepsilon)^3}. \tag{SA-6.16}$$

Combining two bounds above, we have

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^{-2} R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))^{-1}\right\}\right|$$

$$\leq \frac{\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^{-2}\right\}\right|}{R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))}+\frac{\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\{R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))^{-1}\right\}\right|}{\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^2}\leq C_{16}.$$

We are ready to bound

$$\begin{aligned}
&\left|\left(\frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}\right)^{\cdot}\right| \\
&\quad\leq\left|\frac{\left(\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot}\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}\right|+ \\
&\quad+\left|\frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot}}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}\right| \\
&\quad+\left|\frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2}\right. \\
&\quad\left.\times\left(\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^{-2} R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))^{-1}\right)^{\cdot}\right|\leq C_{17}.
\end{aligned}$$

SA-6.13 Proof of (SA-6.10)**.** Since

$$\left|\sum_{i=1}^{p}\nabla_{ij}E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right|\leq\frac{pM_1M_2}{R+\varepsilon}$$

and, as we have already seen in the argument for (SA-6.7),

$$\left|\left(\sum_{i=1}^{p}\nabla_{ij}E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right)^{\cdot}\right|\leq\frac{p^2D_1M_1M_3}{R+\varepsilon}+\frac{p^2D_1M_2^2}{R+\varepsilon}+\frac{pM_1M_2C_{11}}{(R+\varepsilon)^2},$$

we are ready to bound

$$\left|\left(\frac{\sum_{i=1}^{p}\nabla_{ij}E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}}{2\left(R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))+\varepsilon\right)}\right)^{\cdot}\right|\leq C_{18}.$$

The proof of Lemma SA-6.5 is concluded. □

Lemma SA-6.14. *Suppose Assumption SA-2.2 holds. Then the second derivative of $t\mapsto\tilde{\theta}_j(t)$ is uniformly over j and $t\in[0,T]$ bounded in absolute value by some positive constant, say D_2.*

Proof. This follows from the definition of $\tilde{\boldsymbol{\theta}}(t)$ given in (SA-2.2), $h \leq T$ and that the first derivatives of all three terms in (SA-2.2) are bounded by Lemma SA-6.5. □

Lemma SA-6.15. *Suppose Assumption SA-2.2 holds. Then*

$$\left|\left(\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot\cdot}\right| \leq C_{19}, \tag{SA-6.17}$$

$$\left|\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot\cdot}\right| \leq C_{20}, \tag{SA-6.18}$$

$$\left|\left(\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^{-2}\right)^{\cdot\cdot}\right| \leq C_{21}, \tag{SA-6.19}$$

$$\left|\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)^{-1}\right)^{\cdot\cdot}\right| \leq C_{22}, \tag{SA-6.20}$$

$$\left|\left(\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon\right)^{-2} R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)^{-1}\right)^{\cdot\cdot}\right| \leq C_{23}, \tag{SA-6.21}$$

$$\left|\left(\sum_{i=1}^{p} \nabla_{ij} E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(l)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}\right)^{\cdot\cdot}\right| \leq (n-k)C_{24}, \tag{SA-6.22}$$

with constants C_{19}, C_{20}, C_{21}, C_{22}, C_{23}, C_{24} defined as follows:

$$\begin{aligned}
C_{19} &:= p^2 M_3 D_1^2 + p M_2 D_2, \\
C_{20} &:= \frac{C_{11}}{R^2} p M_1 M_2 D_1 + \frac{1}{R} p^2 M_2^2 D_1^2 + \frac{1}{R} p^2 M_1 M_3 D_1^2 + \frac{1}{R} p M_1 M_2 D_2, \\
C_{21} &:= \frac{6 C_{11}^2}{(R+\varepsilon)^4} + \frac{2 C_{20}}{(R+\varepsilon)^3}, \\
C_{22} &:= \frac{2 C_{11}^2}{R^3} + \frac{C_{20}}{R^2}, \\
C_{23} &:= \frac{C_{21}}{R} + \frac{4 C_{11}^2}{R^2 (R+\varepsilon)^3} + \frac{C_{22}}{(R+\varepsilon)^2}, \\
C_{24} &:= p \left[\frac{2 C_{11}\left(D_1 M_2^2 p + D_1 M_1 M_3 p\right)}{(R+\varepsilon)^2} + M_1 M_2 \left(\frac{2 C_{11}^2}{(R+\varepsilon)^3} + \frac{C_{20}}{(R+\varepsilon)^2} \right) \right. \\
&\quad \left. + \frac{2 D_1^2 M_2 M_3 p^2 + M_2\left(D_1^2 M_3 p^2 + D_2 M_2 p\right) + M_1\left(D_1^2 M_4 p^2 + D_2 M_3 p\right)}{R+\varepsilon} \right].
\end{aligned}$$

Proof of Lemma SA-6.15. We divide this argument in several steps.

SA-6.16 Proof of (SA-6.17). This bound is straightforward:

$$\left|\left(\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot\cdot}\right| = \left|\sum_{i=1}^{p}\sum_{s=1}^{p} \nabla_{ijs} E_n\left(\tilde{\boldsymbol{\theta}}(t)\right) \dot{\tilde{\theta}}_s(t) \dot{\tilde{\theta}}_i(t) + \sum_{i=1}^{p} \nabla_{ij} E_n\left(\tilde{\boldsymbol{\theta}}(t)\right) \ddot{\tilde{\theta}}_t(t)\right| \leq C_{19}.$$

SA-6.17 Proof of (SA-6.18). Note that

$$\begin{aligned}
\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot\cdot} &= \left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)^{-1}\right)^{\cdot} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \sum_{i=1}^{p} \nabla_{ij} E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \dot{\tilde{\theta}}_i(t) \\
&\quad + R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)^{-1} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left(\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)^{\cdot} \sum_{i=1}^{p} \nabla_{ij} E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \dot{\tilde{\theta}}_i(t)
\end{aligned}$$

$$+ R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^{-1} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \sum_{i=1}^{p} \Big(\nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^{\cdot} \dot{\tilde{\theta}}_i(t)$$
$$+ R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^{-1} \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big) \ddot{\tilde{\theta}}_i(t),$$

giving by (SA-6.14)

$$\begin{aligned}\left|\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^{\cdot\cdot}\right| &\le \frac{C_{11}}{R^2} p M_1 M_2 D_1 \sum_{k=0}^{n} \rho^{n-k}(1-\rho) + \frac{1}{R} p^2 M_2^2 D_1^2 \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \\ &\quad + \frac{1}{R} p^2 M_1 M_3 D_1^2 \sum_{k=0}^{n} \rho^{n-k}(1-\rho) + \frac{1}{R} p M_1 M_2 D_2 \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \\ &\le C_{20}.\end{aligned}$$

SA-6.18 Proof of (SA-6.19)**.** Note that

$$\left(\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \varepsilon\Big)^{-2}\right)^{\cdot\cdot} = \frac{6\left(\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^{\cdot}\right)^2}{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \varepsilon\Big)^4} - \frac{2\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^{\cdot\cdot}}{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \varepsilon\Big)^3},$$

giving by (SA-6.12) and (SA-6.18)

$$\left|\left(\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \varepsilon\Big)^{-2}\right)^{\cdot\cdot}\right| \le C_{21}.$$

SA-6.19 Proof of (SA-6.20)**.** The bound follows from (SA-6.12), (SA-6.18) and

$$\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^{-1}\Big)^{\cdot\cdot} = \frac{2\left(\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^{\cdot}\right)^2}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^3} - \frac{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)^{\cdot\cdot}}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^2}.$$

SA-6.20 Proof of (SA-6.21)**.** Putting $a := \Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \varepsilon\Big)^{-2}$, $b := R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)^{-1}$, use

$$\begin{aligned}&|a| \le \frac{1}{(R+\varepsilon)^2}, \quad |b| \le \frac{1}{R}, \\ &|\dot{a}| \le \frac{2C_{11}}{(R+\varepsilon)^3}, \quad \left|\dot{b}\right| \le \frac{C_{11}}{R^2}, \\ &|\ddot{a}| \le C_{21}, \quad \left|\ddot{b}\right| \le C_{22},\end{aligned}$$

and

$$(ab)^{\cdot\cdot} = \ddot{a}b + 2\dot{a}\dot{b} + a\ddot{b}.$$

SA-6.21 Proof of (SA-6.22)**.** Putting

$$\begin{aligned}a &:= \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big), \\ b &:= \nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t)\Big), \\ c &:= \Big(R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \varepsilon\Big)^{-1},\end{aligned}$$

we have

$$
\begin{aligned}
&|a| \le M_2, \quad |\dot{a}| \le pM_3D_1, \quad |\ddot{a}| \le p^2M_4D_1^2 + pM_3D_2,\\
&|b| \le M_1, \quad \left|\dot{b}\right| \le pM_2D_1, \quad \left|\ddot{b}\right| \le p^2M_3D_1^2 + pM_2D_2,\\
&|c| \le \frac{1}{R+\varepsilon}, \quad |\dot{c}| \le \frac{C_{11}}{(R+\varepsilon)^2}, \quad |\ddot{c}| \le \frac{2C_{11}^2}{(R+\varepsilon)^3} + \frac{C_{20}}{(R+\varepsilon)^2}.
\end{aligned}
$$

(SA-6.22) follows.

The proof of Lemma SA-6.15 is concluded. □

Lemma SA-6.22. *Suppose Assumption SA-2.2 holds. Then the third derivative of $t \mapsto \tilde{\theta}_j(t)$ is uniformly over j and $t \in [0,T]$ bounded in absolute value by some positive constant, say D_3.*

Proof. By (SA-6.5), (SA-6.13) and (SA-6.22)

$$
\begin{aligned}
&\left|\sum_{i=1}^{p} \nabla_{ij} E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(l)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon}\right| \le (n-k)C_9,\\
&\left|\left(\sum_{i=1}^{p} \nabla_{ij} E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(l)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon}\right)^{\cdot}\right| \le (n-k)C_{13},\\
&\left|\left(\sum_{i=1}^{p} \nabla_{ij} E_k\left(\tilde{\boldsymbol{\theta}}(t)\right) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(l)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon}\right)^{\cdot\cdot}\right| \le (n-k)C_{24}.
\end{aligned}
$$

From the definition of $t \mapsto P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)$, it means that its derivatives up to order two are bounded. Similarly, the same is true for $t \mapsto \bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)$.

It follows from (SA-6.19) and its proof that the derivatives up to order two of

$$
t \mapsto \left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon\right)^{-2} R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)^{-1}
$$

are also bounded.

These considerations give the boundedness of the second derivative of the term

$$
t \mapsto \frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)\left(2P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)\right)}{2\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)}
$$

in (SA-2.2). The boundedness of the second derivatives of the other two terms is shown analogously. By (SA-2.2) and since $h \le T$, this means

$$
\sup_j \sup_{t\in[0,T]} \left|\dddot{\tilde{\theta}}_j(t)\right| \le D_3
$$

for some positive constant D_3. □

SA-7 Proof of Theorem SA-2.3

Lemma SA-7.1. *Suppose Assumption SA-2.2 holds. Then for all $n \in \{0,1,\ldots,\lfloor T/h \rfloor\}$, $k \in \{0,1,\ldots,n-1\}$ we have*

$$
\left|\nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_k)\right) - \nabla_j E_k\left(\tilde{\boldsymbol{\theta}}(t_n)\right)\right| \le C_7(n-k)h \tag{SA-7.1}
$$

Proof. (SA-7.1) follows from the mean value theorem applied $n-k$ times. □

Lemma SA-7.2. *In the setting of Lemma SA-7.1, for any $l \in \{k, k+1, \dots, n-1\}$ we have*

$$\left|\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_l)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) - h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon}\right| \le \big(C_{19}/2 + C_8 + (n-l-1)C_{13}\big)h^2.$$

Proof. By the Taylor expansion of $t \mapsto \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t)\Big)$ on the segment $[t_l, t_{l+1}]$ at t_{l+1} on the left

$$\left|\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_l)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) + h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big)\dot{\tilde{\boldsymbol{\theta}}}_i\Big(t_{l+1}^-\Big)\right| \le \frac{C_{19}}{2}h^2.$$

Combining this with (SA-6.4) gives

$$\left|\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_l)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) - h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) + \varepsilon}\right| \le \big(C_{19}/2 + C_8\big)h^2. \tag{SA-7.2}$$

Now applying the mean-value theorem $n-l-1$ times, we have

$$\left|\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) + \varepsilon} - \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+2})\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_{l+2})\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_{l+2})\Big) + \varepsilon}\right| \le C_{13}h,$$

$$\dots$$

$$\left|\sum_{i=1}^{p} \nabla_{ij} E_l\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big) \frac{\nabla_i E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big) + \varepsilon} - \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon}\right| \le C_{13}h,$$

and in particular

$$\left|\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) + \varepsilon} - \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon}\right| \le (n-l-1)C_{13}h.$$

Combining this with (SA-7.2), we conclude the proof of Lemma SA-7.2. □

Lemma SA-7.3. *In the setting of Lemma SA-7.1,*

$$\left|\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) - h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon}\right| \le \left((n-k)(C_{19}/2 + C_8) + \frac{(n-k)(n-k-1)}{2}C_{13}\right)h^2.$$

Proof. Fix $n \in \mathbb{Z}_{\ge 0}$.

Note that

$$\left|\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) - h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon}\right|$$

$$
\begin{aligned}
&= \left| \sum_{l=k}^{n-1} \left\{ \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_l)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) - h \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon} \right\} \right| \\
&\leq \sum_{l=k}^{n-1} \left| \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_l)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{l+1})\Big) - h \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon} \right| \\
&\overset{\text{(a)}}{\leq} \sum_{l=k}^{n-1} (C_{19}/2 + C_8 + (n-l-1)C_{13})h^2 = \left((n-k)(C_{19}/2 + C_8) + \frac{(n-k)(n-k-1)}{2} C_{13} \right) h^2,
\end{aligned}
$$

where (a) is by Lemma SA-7.2. □

Lemma SA-7.4. *Suppose Assumption SA-2.2 holds. Then for all* $n \in \{0, 1, \ldots, \lfloor T/h \rfloor\}$

$$
\left| \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) \right)^2 - R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2 \right| \leq C_{25} h \tag{SA-7.3}
$$

and

$$
\left| \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) \right)^2 - R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2 - 2h P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \right| \leq C_{26} h^2 \tag{SA-7.4}
$$

with C_{25} *and* C_{26} *defined as follows:*

$$
\begin{aligned}
C_{25}(\rho) &:= 2M_1 C_7 \frac{\rho}{1-\rho}, \\
C_{26}(\rho) &:= M_1 |C_{19} + 2C_8 - C_{13}| \frac{\rho}{1-\rho} \\
&\quad + \left(M_1 C_{13} + |C_{19} + 2C_8 - C_{13}| C_9 + \frac{(C_{19} + 2C_8 - C_{13})^2}{4} \right) \frac{\rho(1+\rho)}{(1-\rho)^2} \\
&\quad + \left(C_{13} C_9 + \frac{C_{13}}{2} |C_{19} + 2C_8 - C_{13}| \right) \frac{\rho\big(1 + 4\rho + \rho^2\big)}{(1-\rho)^3} + \frac{C_{13}^2}{4} \cdot \frac{\rho\big(1 + 11\rho + 11\rho^2 + \rho^3\big)}{(1-\rho)^4}.
\end{aligned}
$$

Proof. Note that

$$
\begin{aligned}
&\left| \left(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) \right)^2 - \left(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \right)^2 \right| \\
&\quad \leq \left| \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) - \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \right| \cdot \left| \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) + \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \right| \\
&\quad \overset{\text{(a)}}{\leq} C_7 (n-k) h \cdot 2M_1,
\end{aligned}
$$

where (a) is by (SA-7.1). Using the triangle inequality, we can conclude

$$
\begin{aligned}
&\left| \sum_{k=0}^{n} \rho^{n-k}(1-\rho) \left(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) \right)^2 - R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2 \right| \\
&\quad \leq 2M_1 C_7 h (1-\rho) \sum_{k=0}^{n} (n-k)\rho^{n-k} = 2M_1 C_7 h (1-\rho) \sum_{k=0}^{n} k\rho^k = 2M_1 C_7 \frac{\rho}{1-\rho} h.
\end{aligned}
$$

(SA-7.3) is proven.

We continue by showing

$$\begin{aligned}
&\Bigg|\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 - \Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\Big)^2 \\
&\qquad -2\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) h \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon}\Bigg| \\
&\le 2M_1\Big((n-k)(C_{19}/2 + C_8) + \frac{(n-k)(n-k-1)}{2} C_{13}\Big) h^2 \\
&\quad + 2(n-k)C_9\Big((n-k)(C_{19}/2 + C_8) + \frac{(n-k)(n-k-1)}{2} C_{13}\Big) h^3 \\
&\quad + \Big((n-k)(C_{19}/2 + C_8) + \frac{(n-k)(n-k-1)}{2} C_{13}\Big)^2 h^4.
\end{aligned} \tag{SA-7.5}$$

To prove this, use

$$\Big|a^2 - b^2 - 2bKh\Big| \le 2|b| \cdot |a - b - Kh| + 2|K| \cdot h \cdot |a - b - Kh| + (a - b - Kh)^2$$

with

$$a := \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big), \quad b := \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big), \quad K := \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \sum_{l=k}^{n-1} \frac{\nabla_i E_l\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \varepsilon},$$

and bounding

$$\begin{aligned}
&|a - b - Kh| \overset{(a)}{\le} \Big((n-k)(C_{19}/2 + C_8) + \frac{(n-k)(n-k-1)}{2} C_{13}\Big) h^2, \\
&|b| \le M_1, \quad |K| \le (n-k)C_9,
\end{aligned}$$

where (a) is by Lemma SA-7.3. (SA-7.5) is proven.

We turn to the proof of (SA-7.4). By (SA-7.5) and the triangle inequality

$$\begin{aligned}
&\Bigg|\sum_{k=0}^{n} \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 - R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2 - 2hP_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\Bigg| \\
&\quad \le (1-\rho)\sum_{k=0}^{n} \rho^{n-k}\Big(\mathrm{Poly}_1(n-k)h^2 + \mathrm{Poly}_2(n-k)h^3 + \mathrm{Poly}_3(n-k)h^4\Big) \\
&\quad = (1-\rho)\sum_{k=0}^{n} \rho^{k}\Big(\mathrm{Poly}_1(k)h^2 + \mathrm{Poly}_2(k)h^3 + \mathrm{Poly}_3(k)h^4\Big),
\end{aligned}$$

where

$$\begin{aligned}
\mathrm{Poly}_1(k) &:= 2M_1\Big(k(C_{19}/2 + C_8) + \frac{k(k-1)}{2} C_{13}\Big) = M_1 C_{13} k^2 + M_1(C_{19} + 2C_8 - C_{13})k, \\
\mathrm{Poly}_2(k) &:= 2kC_9\Big(k(C_{19}/2 + C_8) + \frac{k(k-1)}{2} C_{13}\Big) = C_{13}C_9 k^3 + (C_{19} + 2C_8 - C_{13})C_9 k^2, \\
\mathrm{Poly}_3(k) &:= \Big(k(C_{19}/2 + C_8) + \frac{k(k-1)}{2} C_{13}\Big)^2 \\
&= \frac{C_{13}^2}{4} k^4 + \frac{C_{13}}{2}(C_{19} + 2C_8 - C_{13})k^3 + \frac{1}{4}(C_{19} + 2C_8 - C_{13})^2 k^2.
\end{aligned}$$

It is left to combine this with

$$\sum_{k=0}^{n} k\rho^k \le \sum_{k=0}^{\infty} k\rho^k = \frac{\rho}{(1-\rho)^2},$$

$$\sum_{k=0}^{n} k^2\rho^k \le \sum_{k=0}^{\infty} k^2\rho^k = \frac{\rho(1+\rho)}{(1-\rho)^3},$$
$$\sum_{k=0}^{n} k^3\rho^k \le \sum_{k=0}^{\infty} k^3\rho^k = \frac{\rho\big(1+4\rho+\rho^2\big)}{(1-\rho)^4},$$
$$\sum_{k=0}^{n} k^4\rho^k \le \sum_{k=0}^{\infty} k^4\rho^k = \frac{\rho\big(1+11\rho+11\rho^2+\rho^3\big)}{(1-\rho)^5}.$$

This gives

$$\begin{aligned}
&\left|\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 - R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2 - 2hP_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\right| \\
&\le \left(M_1C_{13}\frac{\rho(1+\rho)}{(1-\rho)^2} + M_1|C_{19}+2C_8-C_{13}|\frac{\rho}{1-\rho}\right)h^2 \\
&\quad + \left(C_{13}C_9\frac{\rho\big(1+4\rho+\rho^2\big)}{(1-\rho)^3} + |C_{19}+2C_8-C_{13}|C_9\frac{\rho(1+\rho)}{(1-\rho)^2}\right)h^3 \\
&\quad + \left(\frac{C_{13}^2}{4}\cdot\frac{\rho\big(1+11\rho+11\rho^2+\rho^3\big)}{(1-\rho)^4} + \frac{C_{13}}{2}|C_{19}+2C_8-C_{13}|\frac{\rho\big(1+4\rho+\rho^2\big)}{(1-\rho)^3}\right. \\
&\qquad \left. + \frac{1}{4}(C_{19}+2C_8-C_{13})^2\frac{\rho(1+\rho)}{(1-\rho)^2}\right)h^4 \\
&\overset{(a)}{\le} \left[M_1|C_{19}+2C_8-C_{13}|\frac{\rho}{1-\rho}\right. \\
&\quad + \left(M_1C_{13} + |C_{19}+2C_8-C_{13}|C_9 + \frac{(C_{19}+2C_8-C_{13})^2}{4}\right)\frac{\rho(1+\rho)}{(1-\rho)^2} \\
&\quad + \left(C_{13}C_9 + \frac{C_{13}}{2}|C_{19}+2C_8-C_{13}|\right)\frac{\rho\big(1+4\rho+\rho^2\big)}{(1-\rho)^3} \\
&\quad \left. + \frac{C_{13}^2}{4}\cdot\frac{\rho\big(1+11\rho+11\rho^2+\rho^3\big)}{(1-\rho)^4}\right]h^2,
\end{aligned}$$

where in (a) we used that $h < 1$. (SA-7.4) is proven. □

Lemma SA-7.5. *Suppose Assumption SA-2.2 holds. Then*

$$\left|\left(\sqrt{\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2}+\varepsilon\right)^{-1} - \Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)+\varepsilon\Big)^{-1}\right.$$
$$\left. + h\frac{P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)+\varepsilon\Big)^2 R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}\right| \le \frac{C_{25}(\rho)^2 + R^2C_{26}(\rho)}{2R^3(R+\varepsilon)^2}h^2.$$

Proof. Note that if $a \ge R^2$, $b \ge R^2$, we have

$$\begin{aligned}
&\left|\frac{1}{\sqrt{a}+\varepsilon} - \frac{1}{\sqrt{b}+\varepsilon} + \frac{a-b}{2\Big(\sqrt{b}+\varepsilon\Big)^2\sqrt{b}}\right| \\
&\quad = \frac{(a-b)^2}{2\sqrt{b}\Big(\sqrt{b}+\varepsilon\Big)\Big(\sqrt{a}+\varepsilon\Big)\Big(\sqrt{a}+\sqrt{b}\Big)}\underbrace{\left\{\frac{1}{\sqrt{b}+\varepsilon}+\frac{1}{\sqrt{a}+\sqrt{b}}\right\}}_{\le 2/R}
\end{aligned}$$

$$\leq \frac{(a-b)^2}{2R^3(R+\varepsilon)^2}.$$

By the triangle inequality,

$$\left|\frac{1}{\sqrt{a}+\varepsilon} - \frac{1}{\sqrt{b}+\varepsilon} + \frac{c}{2\Big(\sqrt{b}+\varepsilon\Big)^2\sqrt{b}}\right| \leq \frac{(a-b)^2}{2R^3(R+\varepsilon)^2} + \frac{|a-b-c|}{2\Big(\sqrt{b}+\varepsilon\Big)^2\sqrt{b}}$$
$$\leq \frac{(a-b)^2}{2R^3(R+\varepsilon)^2} + \frac{|a-b-c|}{2R(R+\varepsilon)^2}$$

Apply this with

$$a := \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2,$$
$$b := R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2,$$
$$c := 2hP_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)$$

and use bounds

$$|a-b| \leq 2M_1C_7\frac{\rho}{1-\rho}h, \quad |a-b-c| \leq C_{26}(\rho)h^2$$

by Lemma SA-7.4. □

SA-7.6. We are finally ready to prove Theorem SA-2.3.

Proof of Theorem SA-2.3. By (SA-6.9) and (SA-6.10), the first derivative of the function

$$t \mapsto \left(\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big(2P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big) + \bar{P}_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\Big)}{2\Big(R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon\Big)^2 R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)} - \frac{\sum_{i=1}^{p}\nabla_{ij}E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)\frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right)+\varepsilon}}{2\Big(R_j^{(n)}(\tilde{\boldsymbol{\theta}}(t))+\varepsilon\Big)}\right)$$

is bounded in absolute value by a positive constant $C_{27} = C_{17} + C_{18}$. By (SA-2.2), this means

$$\left|\ddot{\tilde{\theta}}_j(t) + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right)\right| \leq C_{27}h.$$

Combining this with

$$\left|\tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) - \dot{\tilde{\theta}}_j\big(t_n^+\big)h - \frac{\ddot{\tilde{\theta}}_j\big(t_n^+\big)}{2}h^2\right| \leq \frac{D_3}{6}$$

by Taylor expansion, we get

$$\left|\tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) - \dot{\tilde{\theta}}_j\big(t_n^+\big)h + \frac{h^2}{2}\cdot\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)+\varepsilon}\right)\Bigg|_{t=t_n^+}\right| \tag{SA-7.6}$$
$$\leq \left(\frac{D_3}{6} + \frac{C_{27}}{2}\right)h^3.$$

Using

$$\left|\dot{\tilde{\theta}}_j(t_n) + \frac{\nabla_j E_n\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)+\varepsilon}\right| \leq C_{28}h$$

with C_{28} defined as

$$C_{28} := \frac{M_1(2C_5 + C_6)}{2(R+\varepsilon)^2 R} + \frac{pM_1M_2}{2(R+\varepsilon)^2}$$

by (SA-2.2), and calculating the derivative, it is easy to show

$$\left| \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t)\right)}{R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t)\right) + \varepsilon} \right) \Bigg|_{t=t_n^+} - \mathrm{FrDer} \right| \le C_{29} h \tag{SA-7.7}$$

for a positive constant C_{29}, where

$$\begin{aligned}
\mathrm{FrDer} &:= \frac{\mathrm{FrDerNum}}{\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) + \varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right)} \\
\mathrm{FrDerNum} &:= \nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t_n)\right) \bar{P}_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) \\
&\quad - \left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) + \varepsilon\right) R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) \sum_{i=1}^{p} \nabla_{ij} E_n\left(\tilde{\boldsymbol{\theta}}(t_n)\right) \frac{\nabla_i E_n\left(\tilde{\boldsymbol{\theta}}(t_n)\right)}{R_i^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) + \varepsilon}, \\
C_{29} &:= \left\{ \frac{pM_2}{R+\varepsilon} + \frac{M_1^2 M_2 p}{(R+\varepsilon)^2 R} \right\} C_{28}.
\end{aligned}$$

From (SA-7.6) and (SA-7.7), by the triangle inequality

$$\left| \tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) - \dot{\tilde{\theta}}_j(t_n^+) h + \frac{h^2}{2} \mathrm{FrDer} \right| \le \left(\frac{D_3}{6} + \frac{C_{27} + C_{29}}{2} \right) h^3,$$

which, using (SA-2.2), is rewritten as

$$\begin{aligned}
&\left| \tilde{\theta}_j(t_{n+1}) - \tilde{\theta}_j(t_n) + h \frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t_n)\right)}{R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) + \varepsilon} - h^2 \frac{\nabla_j E_n\left(\tilde{\boldsymbol{\theta}}(t_n)\right) P_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right)}{\left(R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right) + \varepsilon\right)^2 R_j^{(n)}\left(\tilde{\boldsymbol{\theta}}(t_n)\right)} \right| \\
&\quad \le \left(\frac{D_3}{6} + \frac{C_{27} + C_{29}}{2} \right) h^3.
\end{aligned}$$

It is left to combine this with Lemma SA-7.5, giving the assertion of the theorem with

$$C_1 = \frac{D_3}{6} + \frac{C_{27} + C_{29}}{2} + M_1 \frac{C_{25}^2 + R^2 C_{26}}{2R^3(R+\varepsilon)^2}.$$

□

SA-8 Numerical experiments

SA-8.1 Models. We use small modifications of default Keras Resnet-50 and Resnet-101 architectures[1] for training on CIFAR-10 and CIFAR-100 (since image sizes are not the same as Imagenet), after verifying their correctness. The first convolution layer `conv1` has 3×3 kernel, stride 1 and "same" padding. Then comes batch normalization, and relu. Max pooling is removed, and otherwise `conv2_x` to `conv5_x` are as described in [2], see Table 1 there (downsampling is performed by the first convolution of each bottleneck block, same as in this original paper, not the middle one as in version 1.5[2]; all convolution layers have learned biases). After `conv5` there is global average pooling, 10 or 100-way fully connected layer (for CIFAR-10 and CIFAR-100 respectively), and softmax.

[1] https://github.com/keras-team/keras/blob/v2.13.1/keras/applications/resnet.py
[2] https://catalog.ngc.nvidia.com/orgs/nvidia/resources/resnet_50_v1_5_for_pytorch

SA-8.2 Data augmentation. We subtract the per-pixel mean and divide by standard deviation, and we use the data augmentation scheme from [3], following [2], section 4.2. We take inspiration and some code snippets from [4] (though we do not use their models). During each pass over the training dataset, each 32×32 initial image is padded evenly with zeros so that it becomes 36×36, then random crop is applied so that the picture becomes 32×32 again, and finally random (probability 0.5) horizontal (left to right) flip is used.

SA-8.3 Experiment details. In experiments whose results are reported in Figures 4 and 5 of the main paper, we train for more than 3600 epochs and stop training when the train accuracy is near-perfect (Figure SA-1) and the testing accuracy does not significantly improve (Figure SA-2). Therefore, the maximal test accuracies are the final ones reached, and the maximal perturbed one-norms, after excluding the initial fall at the beginning of training, are at peaks of the "hills" on the norm curves (Figure SA-2).

Additional evidence (for ResNet-101 on CIFAR-100 and with hyperparameters different from the ones in Figures 4 and 5) is provided in Figures SA-3 and SA-4.

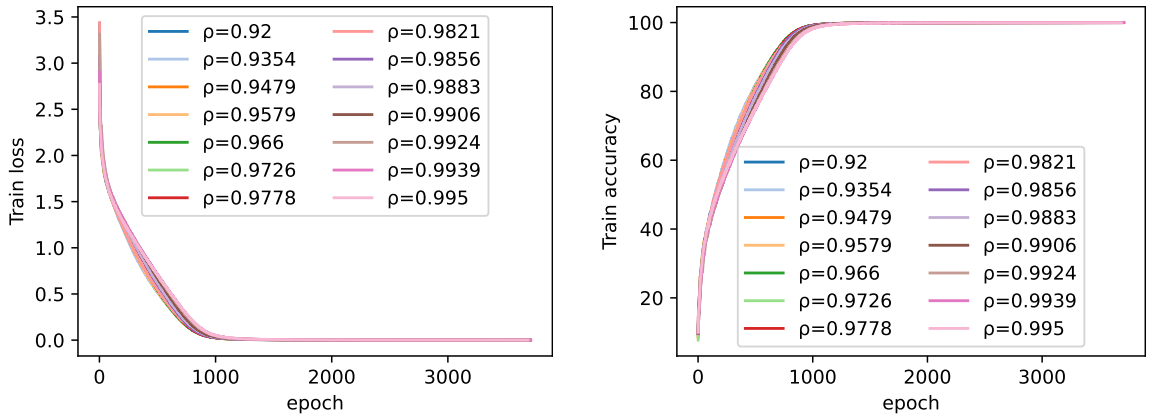

Figure SA-1: Train loss and train accuracy curves for full-batch Adam, ResNet-50 on CIFAR-10, $\beta = 0.99$, $\varepsilon = 10^{-8}$, $h = 7.5 \cdot 10^{-5}$.

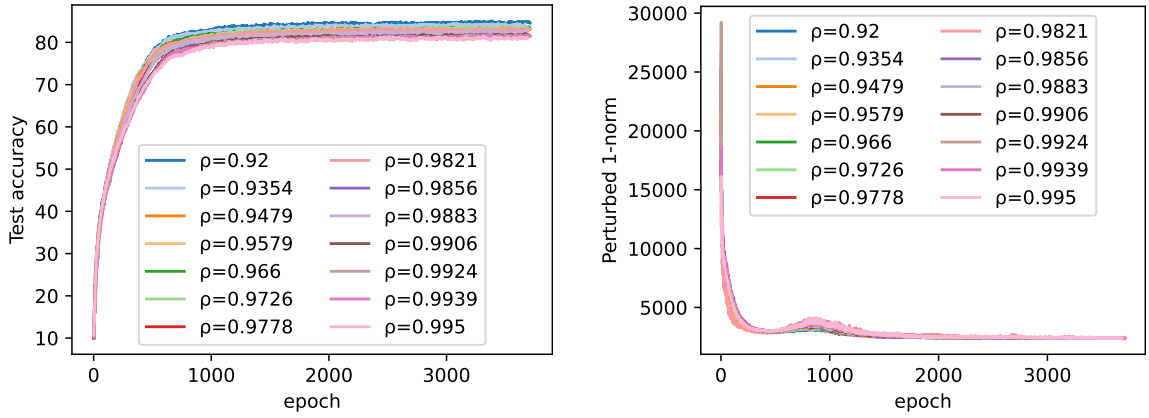

Figure SA-2: Test accuracy and $\|\nabla E\|_{1,\varepsilon}$ after each epoch. The setting is the same as in Figure SA-1.

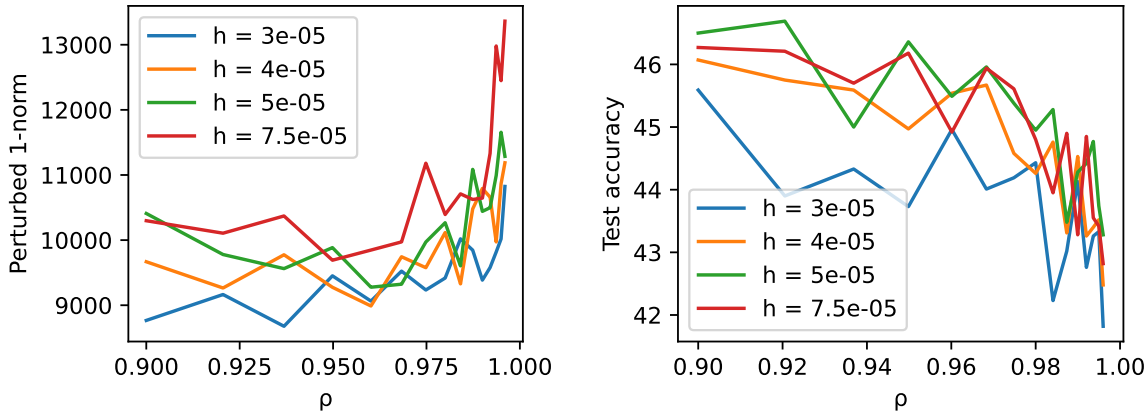

Figure SA-3: Resnet-101 on CIFAR-100 trained with full-batch Adam, $\varepsilon = 10^{-8}$, $\beta = 0.95$. As ρ increases, the perturbed one-norm seems to rise and the test accuracy seems to fall (in the stable regime of training). Both metrics are calculated as in Figures 4 and 5 of the main paper.

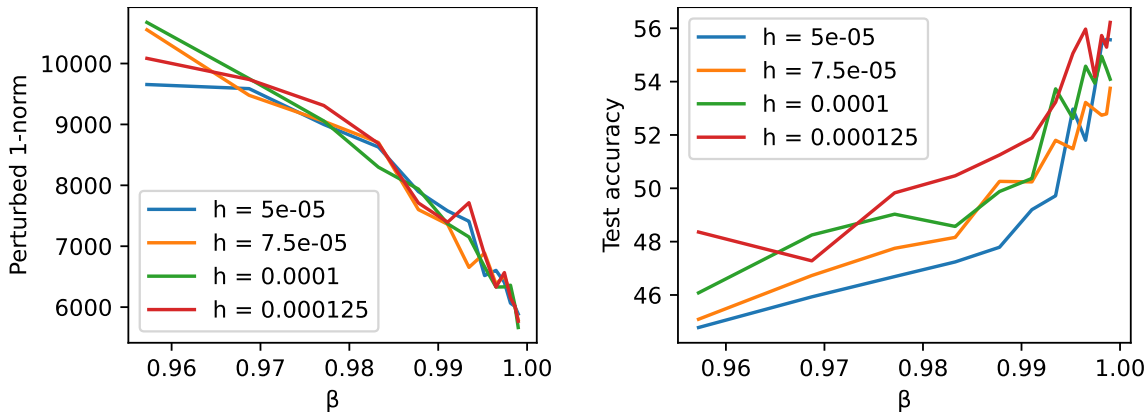

Figure SA-4: Resnet-101 on CIFAR-100 trained with full-batch Adam, $\rho = 0.99$, $\varepsilon = 10^{-8}$. The perturbed one-norm seems to fall as β increases, and the test accuracy seems to rise. Both metrics are calculated as in Figures 4 and 5 of the main paper.

SA-9 Adam with ε inside the square root: informal derivation

Result SA-9.1. *For $n \in \{0, 1, 2, \ldots\}$ we have*

$$\begin{aligned}\tilde{\theta}_j(t_{n+1}) = \tilde{\theta}_j(t_n) - h\frac{M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} \\ + h^2\left(\frac{M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^3} - \frac{L_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}\right) + O\Big(h^3\Big).\end{aligned} \tag{SA-9.1}$$

Derivation. We take

$$\tilde{\theta}_j(t_{n+1}) = \tilde{\theta}_j(t_n) - h\frac{M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} + O\Big(h^2\Big)$$

for granted. Using this and the Taylor series, we can write

$$\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)$$

$$= \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\Big\{\tilde{\theta}_i(t_{n-1}) - \tilde{\theta}_i(t_n)\Big\} + O\Big(h^2\Big)$$

$$= \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\frac{M_j^{(n-1)}\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)}{R_j^{(n-1)}\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)} + O\Big(h^2\Big)$$

$$= \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\frac{M_j^{(n-1)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n-1)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} + O\Big(h^2\Big),$$

where in the last equality we just replaced t_{n-1} with t_n in the h-term since it only affects higher-order terms. Now doing this again for step $n-1$ instead of step n, we will have

$$\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-2})\Big)$$

$$= \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big) + h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)\frac{M_j^{(n-2)}\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)}{R_j^{(n-2)}\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)} + O\Big(h^2\Big)$$

$$= \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big) + h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_{n-1})\Big)\frac{M_j^{(n-2)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n-2)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} + O\Big(h^2\Big),$$

where in the last equality we again replaced t_{n-1} with t_n since it only affects higher-order terms. Proceeding like this and adding the resulting equations, we have for $n \in \{0, 1, \ldots\}$, $k \in \{0, \ldots, n-1\}$ that

$$\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)$$

$$= \nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + h\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\sum_{l=k}^{n-1}\frac{M_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} + O\Big(h^2\Big),$$

where we ignored the fact that $n-k$ is not bounded (we will get away with this because of exponential averaging). Hence, taking the square of this formal power series,

$$\rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 = \rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\Big)^2$$

$$+ h\cdot 2\rho^{n-k}(1-\rho)\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\sum_{i=1}^{p} \nabla_{ij} E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\sum_{l=k}^{n-1}\frac{M_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} + O\Big(h^2\Big).$$

Summing up over k, we have

$$\frac{1}{1-\rho^{n+1}}\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 + \varepsilon = R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^2 + 2hP_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + O\Big(h^2\Big),$$

which, using the expression for the inverse square root $\big(\sum_{r=0}^{\infty} a_r h^r\big)^{-1/2}$ of a formal power series $\sum_{r=0}^{\infty} a_r h^r$, gives us

$$\left(\sqrt{\frac{1}{1-\rho^{n+1}}\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\Big(\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big)\Big)^2 + \varepsilon}\right)^{-1}$$

$$= \frac{1}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} - h\frac{P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^3} + O\Big(h^2\Big).$$

Similarly,

$$\begin{aligned}
&\frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}(1-\beta)\beta^{n-k}\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_k)\Big) = \frac{1}{1-\beta^{n+1}}\sum_{k=0}^{n}(1-\beta)\beta^{n-k}\nabla_j E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) \\
&\quad + \frac{h}{1-\beta^{n+1}}\sum_{k=0}^{n}(1-\beta)\beta^{n-k}\sum_{i=1}^{p}\nabla_{ij}E_k\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\sum_{l=k}^{n-1}\frac{M_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_i^{(l)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} + O\Big(h^2\Big) \\
&= M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + hL_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + O\Big(h^2\Big).
\end{aligned}$$

We conclude

$$\begin{aligned}
\tilde{\theta}_j(t_{n+1}) &= \tilde{\theta}_j(t_n) - h\Big(M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + hL_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + O\Big(h^2\Big)\Big) \\
&\quad \times \left(\frac{1}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} - h\frac{P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^3} + O\Big(h^2\Big)\right) + O\Big(h^3\Big) \\
&= \tilde{\theta}_j(t_n) - h\frac{M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)} \\
&\quad + h^2\left(\frac{M_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)P_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)^3} - \frac{L_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{R_j^{(n)}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}\right) + O\Big(h^3\Big).
\end{aligned}$$

□

Result SA-9.2. *For $t_n \le t < t_{n+1}$, the modified equation is* (SA-5.2).

Derivation. Assume that the modified flow for $t_n \le t < t_{n+1}$ satisfies $\dot{\tilde{\boldsymbol{\theta}}} = \tilde{\mathbf{f}}\Big(\tilde{\boldsymbol{\theta}}(t)\Big)$ where

$$\tilde{\mathbf{f}}(\boldsymbol{\theta}) = \mathbf{f}(\boldsymbol{\theta}) + h\mathbf{f}_1(\boldsymbol{\theta}) + O\Big(h^2\Big).$$

By Taylor expansion, we have

$$\begin{aligned}
\tilde{\boldsymbol{\theta}}(t_{n+1}) &= \tilde{\boldsymbol{\theta}}(t_n) + h\dot{\tilde{\boldsymbol{\theta}}}(t_n^+) + \frac{h^2}{2}\ddot{\tilde{\boldsymbol{\theta}}}(t_n^+) + O\Big(h^3\Big) \\
&= \tilde{\boldsymbol{\theta}}(t_n) + h\Big[\mathbf{f}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + h\mathbf{f}_1\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + O\Big(h^2\Big)\Big] \\
&\quad + \frac{h^2}{2}\Big[\nabla\mathbf{f}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\mathbf{f}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + O(h)\Big] + O\Big(h^3\Big) \\
&= \tilde{\boldsymbol{\theta}}(t_n) + h\mathbf{f}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + h^2\left[\mathbf{f}_1\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big) + \frac{\nabla\mathbf{f}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)\mathbf{f}\Big(\tilde{\boldsymbol{\theta}}(t_n)\Big)}{2}\right] + O\Big(h^3\Big).
\end{aligned} \tag{SA-9.2}$$

Using Lemma SA-9.1 and equating the terms before the corresponding powers of h in (SA-9.1) and (SA-9.2), we obtain

$$\begin{aligned}
f_j(\boldsymbol{\theta}) &= -\frac{M_j^{(n)}(\boldsymbol{\theta})}{R_j^{(n)}(\boldsymbol{\theta})}, \\
f_{1,j}(\boldsymbol{\theta}) &= -\frac{1}{2}\sum_{i=1}^{p}\nabla_i f_j(\boldsymbol{\theta})f_i(\boldsymbol{\theta}) + \frac{M_j^{(n)}(\boldsymbol{\theta})P_j^{(n)}(\boldsymbol{\theta})}{R_j^{(n)}(\boldsymbol{\theta})^3} - \frac{L_j^{(n)}(\boldsymbol{\theta})}{R_j^{(n)}(\boldsymbol{\theta})}.
\end{aligned} \tag{SA-9.3}$$

It is left to find $\nabla_i f_j(\boldsymbol{\theta})$. Using

$$\nabla_i R_j^{(n)}(\boldsymbol{\theta}) = \frac{\sum_{k=0}^{n}\rho^{n-k}(1-\rho)\nabla_{ij}E_k(\boldsymbol{\theta})\nabla_j E_k(\boldsymbol{\theta})}{(1-\rho^{n+1})R_j^{(n)}(\boldsymbol{\theta})},$$

$$\nabla_i M_j^{(n)}(\boldsymbol{\theta}) = \frac{\sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_{ij} E_k(\boldsymbol{\theta})}{1-\beta^{n+1}}$$

we have

$$\begin{aligned}
&\nabla_i \left(-\frac{M_j^{(n)}(\boldsymbol{\theta})}{R_j^{(n)}(\boldsymbol{\theta})} \right) \\
&= -\frac{\frac{R_j^{(n)}(\boldsymbol{\theta})^2}{1-\beta^{n+1}} \sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_{ij} E_k(\boldsymbol{\theta}) - \frac{M_j^{(n)}(\boldsymbol{\theta})}{1-\rho^{n+1}} \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_{ij} E_k(\boldsymbol{\theta})\nabla_j E_k(\boldsymbol{\theta})}{R_j^{(n)}(\boldsymbol{\theta})^3} \\
&= -\frac{\sum_{k=0}^{n} \beta^{n-k}(1-\beta)\nabla_{ij} E_k(\boldsymbol{\theta})}{(1-\beta^{n+1}) R_j^{(n)}(\boldsymbol{\theta})} + \frac{M_j^{(n)}(\boldsymbol{\theta}) \sum_{k=0}^{n} \rho^{n-k}(1-\rho)\nabla_{ij} E_k(\boldsymbol{\theta})\nabla_j E_k(\boldsymbol{\theta})}{(1-\rho^{n+1}) R_j^{(n)}(\boldsymbol{\theta})^3}
\end{aligned}$$

Inserting this into (SA-9.3) concludes the proof. □

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