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Analysis Of Momentum Methods

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Abstract

Gradient descent-based optimization methods underpin the parameter training which results in the impressive results now found when testing neural networks. Introducing stochasticity is key to their success in practical problems, and there is some understanding of the role of stochastic gradient descent in this context. Momentum modifications of gradient descent such as Polyak's Heavy Ball method (HB) and Nesterov's method of accelerated gradients (NAG), are also widely adopted. In this work our focus is on understanding the role of momentum in the training of neural networks, concentrating on the common situation in which the momentum contribution is fixed at each step of the algorithm; to expose the ideas simply we work in the deterministic setting. We show that, contrary to popular belief, standard implementations of fixed momentum methods do no more than act to rescale the learning rate. We achieve this by showing that the momentum method converges to a gradient flow, with a momentum-dependent time-rescaling, using the method of modified equations from numerical analysis. Furthermore we show that the momentum method admits an exponentially attractive invariant manifold on which the dynamics reduces to a gradient flow with respect to a modified loss function, equal to the original one plus a small perturbation.

Keywords: Optimization, Machine Learning, Deep Learning, Gradient Flows, Momentum Methods, Modified Equation, Invariant Manifold

1. Introduction

1.1 Background and Literature Review

At the core of many machine learning tasks is solution of the optimization problem

$$\arg\min_{u \in \mathbb{R}^d} \ \Phi(u) \tag{1}$$

where $\Phi : \mathbb{R}^d \to \mathbb{R}$ is an objective (or loss) function that is, in general, non-convex and differentiable. Finding global minima of such objective functions is an important and challenging task with a long history, one in which the use of stochasticity has played a prominent role for many decades, with papers in the early development of machine learning Geman and

Geman (1987); Styblinski and Tang (1990), together with concomitant theoretical analyses for both discrete Bertsimas et al. (1993) and continuous problems Kushner (1987); Kushner and Clark (2012). Recent successes in the training of deep neural networks have built on this older work, leveraging the enormous computer power now available, together with empirical experience about good design choices for the architecture of the networks; reviews may be found in Goodfellow et al. (2016); LeCun et al. (2015). Gradient descent plays a prominent conceptual role in many algorithms, following from the observation that the equation

$$\frac{du}{dt} = -\nabla\Phi(u) \tag{2}$$

will decrease Φ along trajetories. The most widely adopted methods use stochastic gradient decent (SGD), a concept introduced in Robbins and Monro (1951); the basic idea is to use gradient decent steps based on a noisy approximation to the gradient of Φ. Building on deep work in the convex optimization literature, momentum-based modifications to stochastic gradient decent have also become widely used in optimization. Most notable amongst these momentum-based methods are the Heavy Ball Method (HB), due to Polyak (1964), and Nesterov's method of accelerated gradients (NAG) Nesterov (1983). To the best of our knowledge, the first application of HB to neural network training appears in Rumelhart et al. (1986). More recent work, such as Sutskever et al. (2013), has even argued for the indispensability of such momentum based methods for the field of deep learning.

From these two basic variants on gradient decent, there have come a plothera of adaptive methods, incorporating momentum-like ideas, such as Adam Kingma and Ba (2014), Adagrad Duchi et al. (2011), and RMSProp Tieleman and Hinton (2012). There is no consensus on which method performs best and results vary based on application. The recent work of Wilson et al. (2017) argues that the rudimentary, non-adaptive schemes SGD, HB, and NAG result in solutions with the greatest generalization performance for supervised learning applications with deep neural network models.

There is a natural physical analogy for HB methods, namely that they relate to a damped second order Hamiltonian dynamic with potential Φ:

$$m\frac{d^2u}{dt^2} + \gamma(t)\frac{du}{dt} + \nabla\Phi(u) = 0. \tag{3}$$

This persective was introduced in Qian (1999) although no proof was given. For NAG, the work of Su et al. (2014) shows that the method approximates a damped Hamiltonian system of precisely this form, with a time-dependent damping coefficient. The analysis holds when the momentum factor is step-dependent and choosen as in the original work of Nesterov (1983). However this is not the way that NAG is usually used for machine learning applications, especially for deep learning: in many situations the method is employed with a constant momentum factor. In fact, popular books on the subject such as Goodfellow et al. (2016) introduce the method in this way, and popular articles, such as He et al. (2016) to name one of many, simply state the value of the constant momentum factor used in their experiments. Widely used deep learning libraries such as Tensorflow Abadi et al. (2015) and PyTorch Paszke et al. (2017) implement the method with a fixed choice of momentum factor.

Momentum based methods, as practically implemented in many machine learning optimization tasks, with fixed momentum, have not been carefully analyzed. We will undertake such an analysis, using ideas from numerical analsysis, and in particular the concept of modified equations Griffiths and Sanz-Serna (1986); Chartier et al. (2007) and from the theory of attractive invariant manifolds Hirsch et al. (2006); Wiggins (2013). Both ideas are explained in the text Stuart and Humphries (1998).

1.2 Our Contribution

We study momentum-based optimization algorithms for the minimization task (1), with fixed momentum, focussing on deterministic methods for clarity of exposition. We make the following contributions to their understanding.

- We show that momentum-based methods as used by machine learning practitioners, with fixed momentum, satisfy, in the continuous-time limit, a rescaled version of the gradient flow equation (2).
- We show that such methods also approximate a damped Hamiltonian system of the form (3), with small mass m (on the order of the learning rate) and constant damping $\gamma(t) = \gamma$; this approximation has the same order of accuracy as the approximation of the rescaled equation (2) but can provide a better qualitative approximation.
- Furthermore, for the approximate Hamiltonian system, we show that the dynamics admit an exponentially attractive invariant manifold which is locally representable as a graph mapping co-ordinates to their velocities. The map generating this graph describes a gradient flow in a potential which is a small (on the order of the learning rate) perturbation of Φ.
- On the invariant manifold, we show that momentum methods are approximated by the perturbed gradient flow (18) to second order accuracy.
- We provide numerical experiments which illustrate the foregoing considerations.

Taken together our results are interesting because they demonstrate that the popular belief that (fixed) momentum methods resemble the dynamics induced by (3) is misleading. Whilst it is true, the mass in the approximating equation is small and as a consequence understanding the dynamics as gradient flows (2), with modified potential, is more instructive. In fact, in the first application of HB to neural networks by Rumelhart et al. (1986), the authors state that “[their] experience has been that [one] get[s] the same solutions by setting [the momentum factor to zero] and reducing the size of [the learning rate].” While our analysis is confined to the non-stochastic case to simplify the exposition, the results will, with some care, extend to the stochastic setting using ideas from averaging and homogenization Pavliotis and Stuart (2008) as well as continuum analyses of SGD as in Li et al. (2017); Feng et al. (2018). Furthermore we also confine our analysis to fixed learning rate, and impose global bounds on the relevant derivatives of Φ; this further simplifies the exposition of the key ideas, but is not essential to them; with considerably more analysis the ideas exposed in this paper will transfer to adaptive time-stepping methods.

The paper is organized as follows. Section 2 introduces the optimization procedures and states the convergence result to a rescaled gradient flow. In section 3 we derive the modified, second-order equation and state convergence of the schemes to this equation. Section 4 asserts the existence of an attractive invariant manifold, demonstrating that it results in a gradient flow with respect to a small perturbation of Φ. We conclude in section 5. All proofs of theorems are given in the appendices so that the ideas of the theorems can be presented clearly within the main body of the text.

1.3 Notation

We use $|\cdot|$ to denote the Euclidean norm on $\mathbb{R}^d$. We define $f : \mathbb{R}^d \to \mathbb{R}^d$ by $f(u) \coloneqq -\nabla\Phi(u)$ for any $u \in \mathbb{R}^d$. Given parameter $\lambda \in [0, 1)$ we define $\bar{\lambda} \coloneqq (1-\lambda)^{-1}$.

For two Banach spaces A, B, and A_0 a subset in A, we denote by $C^k(A_0; B)$ the set of k-times continously differentiable functions with domain A_0 and range B. For a function $u \in C^k(A_0; B)$, we let $D^j u$ denote its j-th (total) Fréchet derivative for $j = 1, \dots, k$. For a function $u \in C^k([0, \infty), \mathbb{R}^d)$, we denote its derivatives by $\frac{du}{dt}, \frac{d^2u}{dt^2}$, etc. or equivalently by $\dot{u}, \ddot{u}$, etc.

To simplify our proofs, we make the following assumption about the objective function.

Assumption 1 *Suppose $\Phi \in C^3(\mathbb{R}^d; \mathbb{R})$ with uniformly bounded derivatives. Namely, there exist constants $B_0, B_1, B_2 > 0$ such that*

$$\|D^{j-1}f\| = \|D^j\Phi\| \leq B_{j-1}$$

for $j = 1, 2, 3$ where $\|\cdot\|$ denotes any appropriate operator norm.

Finally we observe that the nomenclature "learning rate" is now prevalent in machine learning, and so we use it in this paper; it refers to the object commonly refered to as "time-step" in the field of numerical analysis.

2. Momentum Methods and Convergence to Gradient Flow

In subsection 2.1 we state Theorem 2 concerning the convergence of a class of momentum methods to a rescaled gradient flow. Subsection 2.2 demonstrates that the HB and NAG methods are special cases of our general class of momentum methods, and gives intuition for proof of Theorem 2; the proof itself is given in Appendix A. Subsection 2.3 contains a numerical illustration of Theorem 2.

2.1 Main Result

The standard Euler discretization of (2) gives the discrete time optimization scheme

$$\mathsf{u}_{n+1} = \mathsf{u}_n + hf(\mathsf{u}_n), \quad n = 0, 1, 2, \dots . \tag{4}$$

Implementation of this scheme requires an initial guess $\mathsf{u}_0 \in \mathbb{R}^d$. For simplicity we consider a fixed learning rate $h > 0$. Equation (2) has a unique solution $u \in C^3([0, \infty); \mathbb{R}^d)$ under Assumption 1 and for $u_n = u(nh)$

$$\sup_{0 \leq nh \leq T} |\mathsf{u}_n - u_n| \leq C(T)h;$$

see Stuart and Humphries (1998), for example.

In this section we consider a general class of momentum methods for the minimization task (1) which can be written in the form, for some $a \geq 0$ and $\lambda \in (0,1)$,

$$\begin{aligned} \mathsf{u}_{n+1} &= \mathsf{u}_n + \lambda(\mathsf{u}_n - \mathsf{u}_{n-1}) + hf(\mathsf{u}_n + a(\mathsf{u}_n - \mathsf{u}_{n-1})), \quad n = 0,1,2,\dots, \\ \mathsf{u}_1 &= \mathsf{u}_0 + hf(\mathsf{u}_0)\,. \end{aligned} \tag{5}$$

Again, implementation of this scheme requires an an initial guess $\mathsf{u}_0 \in \mathbb{R}^d$. The parameter choice $a = 0$ gives HB and $a = \lambda$ gives NAG. In Appendix A we prove the following:

Theorem 2 *Suppose Assumption 1 holds and let $u \in C^3([0,\infty);\mathbb{R}^d)$ be the solution to*

$$\begin{aligned} \frac{du}{dt} &= -(1-\lambda)^{-1}\nabla\Phi(u) \\ u(0) &= \mathsf{u}_0 \end{aligned} \tag{6}$$

with $\lambda \in (0,1)$. For $n = 0,1,2,\dots$ let u_n be the sequence given by (5) and define $u_n := u(nh)$. Then for any $T \geq 0$, there is a constant $C = C(T) > 0$ such that

$$\sup_{0 \leq nh \leq T} |u_n - \mathsf{u}_n| \leq Ch.$$

Note that (6) is simply a sped-up version of (2): if v solves (2) and w solves (6) then $v(t) = w((1-\lambda)t)$ for any $t \in [0,\infty)$. This demonstrates that introduction of momentum in the form used within both HB and NAG results in numerical methods that do not differ substantially from gradient descent.

2.2 Link to HB and NAG

The HB method is usually written as a two-step scheme taking the form (Sutskever et al. (2013))

$$\begin{aligned} \mathsf{v}_{n+1} &= \lambda\mathsf{v}_n + hf(\mathsf{u}_n) \\ \mathsf{u}_{n+1} &= \mathsf{u}_n + \mathsf{v}_{n+1} \end{aligned}$$

with $\mathsf{v}_0 = 0$, $\lambda \in (0,1)$ the momentum factor, and $h > 0$ the learning rate. We can re-write this update as

$$\begin{aligned} \mathsf{u}_{n+1} &= \mathsf{u}_n + \lambda\mathsf{v}_n + hf(\mathsf{u}_n) \\ &= \mathsf{u}_n + \lambda(\mathsf{u}_n - \mathsf{u}_{n-1}) + hf(\mathsf{u}_n) \end{aligned}$$

hence the method reads

$$\begin{aligned} \mathsf{u}_{n+1} &= \mathsf{u}_n + \lambda(\mathsf{u}_n - \mathsf{u}_{n-1}) + hf(\mathsf{u}_n) \\ \mathsf{u}_1 &= \mathsf{u}_0 + hf(\mathsf{u}_0). \end{aligned} \tag{7}$$

Similarly NAG is usually written as (Sutskever et al. (2013))

$$\begin{aligned} \mathsf{v}_{n+1} &= \lambda\mathsf{v}_n + hf(\mathsf{u}_n + \lambda\mathsf{v}_n) \\ \mathsf{u}_{n+1} &= \mathsf{u}_n + \mathsf{v}_{n+1} \end{aligned}$$

with $\mathsf{v}_0 = 0$. Define $\mathsf{w}_n \coloneqq \mathsf{u}_n + \lambda \mathsf{v}_n$ then

$$\begin{aligned}\mathsf{w}_{n+1} &= \mathsf{u}_{n+1} + \lambda \mathsf{v}_{n+1} \\ &= \mathsf{u}_{n+1} + \lambda(\mathsf{u}_{n+1} - \mathsf{u}_n)\end{aligned}$$

and

$$\begin{aligned}\mathsf{u}_{n+1} &= \mathsf{u}_n + \lambda \mathsf{v}_n + hf(\mathsf{u}_n + \lambda \mathsf{v}_n) \\ &= \mathsf{u}_n + (\mathsf{w}_n - \mathsf{u}_n) + hf(\mathsf{w}_n) \\ &= \mathsf{w}_n + hf(\mathsf{w}_n).\end{aligned}$$

Hence the method may be written as

$$\begin{aligned}\mathsf{u}_{n+1} &= \mathsf{u}_n + \lambda(\mathsf{u}_n - \mathsf{u}_{n-1}) + hf(\mathsf{u}_n + \lambda(\mathsf{u}_n - \mathsf{u}_{n-1})) \\ \mathsf{u}_1 &= \mathsf{u}_0 + hf(\mathsf{u}_0).\end{aligned} \tag{8}$$

It is clear that (7) and (8) are special cases of (5) with $a = 0$ giving HB and $a = \lambda$ giving NAG. To intuitively understand Theorem 2, re-write (6) as

$$\frac{du}{dt} - \lambda \frac{du}{dt} = f(u).$$

If we discretize the du/dt term using forward differences and the $-\lambda du/dt$ term using backward differences, we obtain

$$\frac{u(t+h) - u(t)}{h} - \lambda \frac{u(t) - u(t-h)}{h} \approx f(u(t)) \approx f\left(u(t) + ha\frac{u(t) - u(t-h)}{h}\right)$$

with the second approximate equality coming from the Taylor expansion of f. This can be rearragned as

$$u(t+h) \approx u(t) + \lambda(u(t) - u(t-h)) + hf(u(t) + a(u(t) - u(t-h)))$$

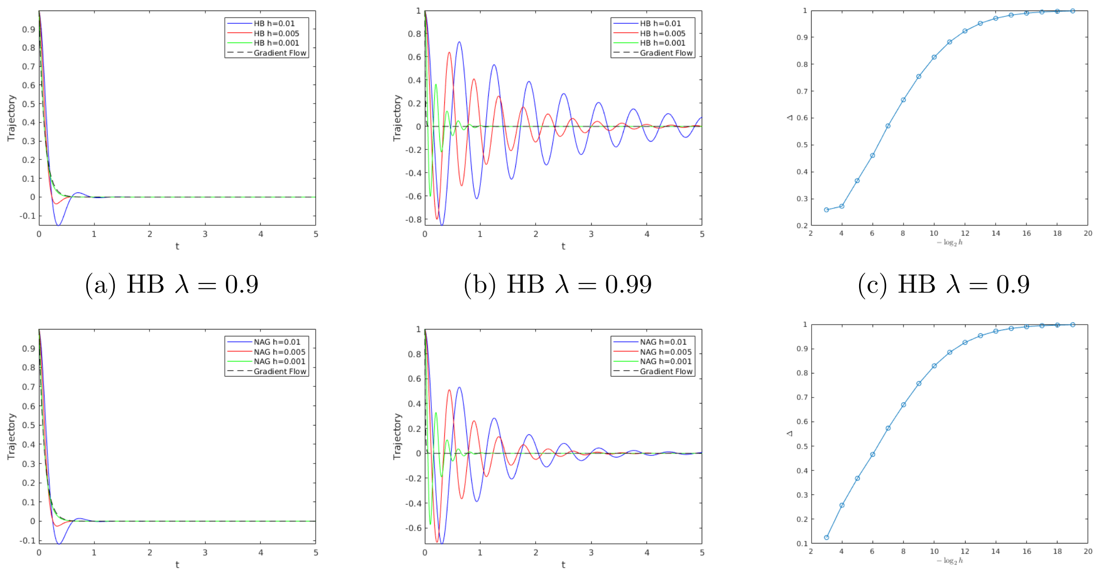
which has the form of (5) with the identification $\mathsf{u}_n \approx u(nh)$.

2.3 Numerical Illustration

Figure 1 compares trajectories of the momentum numerical method (5) with the rescaled gradient flow (6), for the one-dimensional problem $\Phi(u) = \frac{1}{2}u^2$. Panels (a) and (d) show that, for fixed $\lambda = 0.9$, the trajectories of the numerical method match those of the gradient flow increasingly well as the learning rate is decreased; however some initial transient oscillations are present. The same phenomenon is clear in Panels (b) and (e), but becasue λ is increased to 0.99, the transient oscillations are more pronounced; however convergence to the gradient flow is still apparent as the learning rate is decreased. Panels (c) and (f) estimate the rate of convergence, as a function of h, which is defined as

$$\Delta = \log_2 \frac{\|\mathsf{u}^{(h)} - u\|_\infty}{\|\mathsf{u}^{(h/2)} - u\|_\infty}$$

where $\mathsf{u}^{(\alpha)}$ is the numerical solution using timestep α and show that it is close to 1, as predicted by our theory. In summary the behaviour of the momentum methods is precisely that of a rescaled gradient flow, but with initial transient oscillations which capture momentum effects, but disappear as the learning rate is decreased. We model these oscillations in the next section via use of a modified equation.



(a) HB $\lambda = 0.9$ (b) HB $\lambda = 0.99$ (c) HB $\lambda = 0.9$

(d) NAG $\lambda = 0.9$ (e) NAG $\lambda = 0.99$ (f) NAG $\lambda = 0.9$

Figure 1: Comparison of trajectories for HB and NAG with the gradient flow (6) on the one dimensional problem $\Phi(u) = \frac{1}{2}u^2$. Panels (a),(b),(d),(e) show sample trajectories for different choices of λ and h. Panels (c),(f) show the numerical order of convergence as a function of the step size h.

3. Modified Equations

The previous section demonstrates how the momentum methods approximate a time rescaled version of the gradient flow (2). In this section we show how the same methods may also be viewed as approximations of the damped Hamiltonian system (3), with mass m on the order of the learning rate, using the method of modified equations. In subsection 3.1 we state and discuss the main result of the section, Theorem 3. Subsection 3.2 gives intuition for proof of Theorem 3; the proof itself is given in Appendix B. And the section also contains comments on generalizing the idea of modified equations. In subsection 3.3 we describe a numerical illustration of Theorem 3.

3.1 Main Result

The main result of this section quantifies the sense in which momentum methods do, in fact, approximate a damped Hamiltonian system; it is proved in Appendix B.

Theorem 3 *Fix $\lambda \in (0,1)$ and assume that $a \geq 0$ is chosen so that $\alpha := \frac{1}{2}(1+\lambda-2a(1-\lambda))$ is strictly positive. Suppose Assumption 1 holds and let $u \in C^4([0,\infty);\mathbb{R}^d)$ be the solution to*

$$\begin{aligned} &h\alpha\frac{d^2u}{dt^2} + (1-\lambda)\frac{du}{dt} = -\nabla\Phi(u) \\ &u(0) = \mathsf{u}_0, \quad \frac{du}{dt}(0) = \mathsf{u}_0' \end{aligned} \tag{9}$$

Suppose futher that $h \leq (1-\lambda)^2/2\alpha B_1$. *For* $n = 0, 1, 2, \dots$ *let* u_n *be the sequence given by* (5) *and define* $u_n := u(nh)$. *Then for any* $T \geq 0$, *there is a constant* $C = C(T) > 0$ *such that*

$$\sup_{0 \leq nh \leq T} |u_n - \mathsf{u}_n| \leq Ch.$$

Theorem 2 demonstrates the same order of convergence, namely $\mathcal{O}(h)$, to the rescaled gradient flow equation (6), obtained from (9) simply by setting $h = 0$. In the standard method of modified equations the limit system (here (6)) is perturbed by small terms (in terms of the assumed small learning rate) and an increased rate of convergence is obtained to the modified equation (here (9)). In our setting however, because the small modification is to a higher derivative (here second) than appears in the limit equation (here first order), an increased rate of convergence is not obtained. This is due to the nature of the modified equation, whose solution has derivatives that are inversely proportional to powers of h; this fact is quantified in Lemma 8 from Appendix B. It is precisely because the modified equation does not lead to a higher rate of convergence that the initial parameter u'_0 is arbitrary; the same rate of convergence is obtain no matter what value it takes.

It is natural to ask, therefore, what is learned from the convergence result in Theorem 3. The answer is that, although the modified equation (9) is approximated at the same order as the limit equation (6), it actually contains considerably more qualitative information about the dynamics of the system, particularly in the early transient phase of the algorithm; this will be illustrated in subsection 3.3. Indeed we will make a specific choice of u'_0 in our numerical experiments, namely

$$\frac{du}{dt}(0) = \frac{1-2\alpha}{2\alpha - \lambda + 1} f(\mathsf{u}_0), \tag{10}$$

to better match the transient dynamics.

3.2 Intuition and Wider Context

3.2.1 Idea Behind The Modified Equations

In this subsection, we show that the scheme (5) exhibits momentum, in the sense of approximating a momentum equation, but the size of the momentum term is on the order of the step size h. To see this intuitively, we add and subtract $\mathsf{u}_n - \mathsf{u}_{n-1}$ to the right hand size of (5) then we can rearange it to obtian

$$h\frac{\mathsf{u}_{n+1} - 2\mathsf{u}_n + \mathsf{u}_{n-1}}{h^2} + (1-\lambda)\frac{\mathsf{u}_n - \mathsf{u}_{n-1}}{h} = f(\mathsf{u}_n + a(\mathsf{u}_n - \mathsf{u}_{n-1})).$$

This can be seen as a second order central difference and first order backward difference discretization of the momentum equation

$$h\frac{d^2u}{dt^2} + (1-\lambda)\frac{du}{dt} = f(u)$$

noting that the second derivative term has size of order h.

3.2.2 Higher Order Modified Equations For HB

We will now show that, for HB, we may derive higher order modified equations that are consistent with (7). Taking the limit of these equations yields an operator that agrees with with our intuition for discretizing (6). To this end, suppose $\Phi \in C_b^\infty(\mathbb{R}^d, \mathbb{R})$ and consider the ODE(s),

$$\sum_{k=1}^{p} \frac{h^{k-1}(1+(-1)^k\lambda)}{k!}\frac{d^k u}{dt^k} = f(u) \tag{11}$$

noting that $p=1$ gives (6) and $p=2$ gives (9). Let $u \in C^\infty([0,\infty), \mathbb{R}^d)$ be the solution to (11) and define $u_n \coloneqq u(nh)$, $u_n^{(k)} \coloneqq \frac{d^k u}{dt^k}(nh)$ for $n = 0, 1, 2, \dots$ and $k = 1, 2, \dots, p$. Taylor expanding yields

$$u_{n\pm 1} = u_n + \sum_{k=1}^{p} \frac{(\pm 1)^k h^k}{k!} u_n^{(k)} + h^{p+1} I_n^{\pm}$$

where

$$I_n^{\pm} = \frac{(\pm 1)^{p+1}}{p!} \int_0^1 (1-s)^p \frac{d^{p+1}u}{dt^{p+1}}((n \pm s)h) ds.$$

Then

$$\begin{aligned} u_{n+1} - u_n - \lambda(u_n - u_{n-1}) &= \sum_{k=1}^{p} \frac{h^k}{k!} u_n^{(k)} + \lambda \sum_{k=1}^{p} \frac{(-1)^k h^k}{k!} u_n^{(k)} + h^{p+1}(I_n^+ - \lambda I_n^-) \\ &= h \sum_{k=1}^{p} \frac{h^{k-1}(1+(-1)^k\lambda)}{k!} u_n^{(k)} + h^{p+1}(I_n^+ - \lambda I_n^-) \\ &= h f(u_n) + h^{p+1}(I_n^+ - \lambda I_n^-) \end{aligned}$$

showing consistency to order $p+1$. As is the case with (9) however, the $I_n^{\pm}$ terms will be inversely proportional to powers of h hence global accuracy will not improve.

We now study the differential operator on the l.h.s. of (11) as $p \to \infty$. Define the sequence of differential operators $T_p : C^\infty([0,\infty), \mathbb{R}^d) \to C^\infty([0,\infty), \mathbb{R}^d)$ by

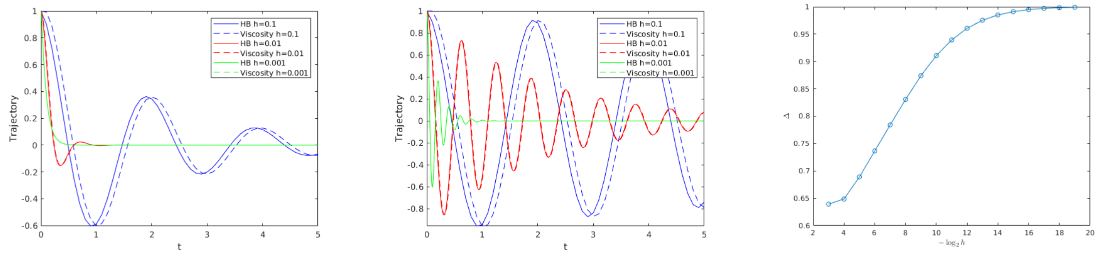
$$T_p u = \sum_{k=1}^{p} \frac{h^{k-1}(1+(-1)^k\lambda)}{k!}\frac{d^k u}{dt^k}, \quad \forall u \in C^\infty([0,\infty), \mathbb{R}^d).$$

Taking the Fourier transform yields

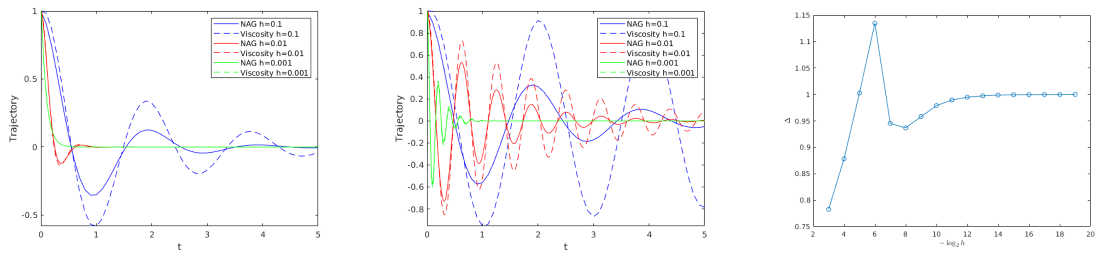
$$\mathcal{F}(T_p u)(\omega) = \sum_{k=1}^{p} \frac{h^{k-1}(1+(-1)^k\lambda)(i\omega)^k}{k!} \mathcal{F}(u)(\omega)$$

where $i = \sqrt{-1}$ denotes the imaginary unit. Suppose there is a limiting operator $T_p \to T$ as $p \to \infty$ then taking the limit yields

$$\mathcal{F}(Tu)(\omega) = \frac{1}{h}(e^{ih\omega} + \lambda e^{-ih\omega} - \lambda - 1)\mathcal{F}(u)(\omega).$$



(a) HB $\lambda = 0.9$ (b) HB $\lambda = 0.99$ (c) HB $\lambda = 0.9$



(d) NAG $\lambda = 0.9$ (e) NAG $\lambda = 0.99$ (f) NAG $\lambda = 0.9$

Figure 2: Comparison of trajectories for HB and NAG with the momentum equation (9) on the one dimensional problem $\Phi(u) = \frac{1}{2}u^2$. Figures (a),(b),(d),(e) show sample trajectories for different choices of λ and h. Figures (c),(f) show the numerical order of convergence as a function of the step size h.

Taking the inverse transform and using the convolution theorem, we obtain

$$\begin{aligned}
(Tu)(t) &= \frac{1}{h}\mathcal{F}^{-1}(e^{ih\omega} + \lambda e^{-ih\omega} - \lambda - 1)(t) * u(t) \\
&= \frac{1}{h}\left(-(1+\lambda)\delta(t) + \lambda\delta(t+h) + \delta(t-h)\right) * u(t) \\
&= \frac{1}{h}\int_{-\infty}^{\infty} \left(-(1+\lambda)\delta(t-\tau) + \lambda\delta(t-\tau+h) + \delta(t-\tau-h)\right) u(\tau)\, d\tau \\
&= \frac{1}{h}\left(-(1+\lambda)u(t) + \lambda u(t-h) + u(t+h)\right) \\
&= \frac{u(t+h) - u(t)}{h} - \lambda\left(\frac{u(t) - u(t-h)}{h}\right)
\end{aligned}$$

where $\delta(\cdot)$ denotes the Dirac-delta distribution and we abuse notation by writing its action as an integral. The above calculation does not prove convergence of T_p to T, but simply confirms our intuition that (7) is a forward and backward discretization of (6).

3.3 Numerical Illustration

Figure 2 shows trajectories of (5) and (9) for different values of a, λ, and h on the one-dimensional problem $\Phi(u) = \frac{1}{2}u^2$. We make the specific choice of u_0' implied by the initial condition (10). Panels (c),(f) shows the numerical order of convergence as a function of h, as defined in Section 2.3, which is near 1, matching our theory. We note that the oscillations in

HB are captured well by (9) expect for a slight shift when h is large. This is due to our choice of initial condition which cancels the maximum number of terms in the Taylor expansion initially, but the overall rate of convergence remains $\mathcal{O}(h)$ due to Lemma 8. Other choices of u_0' also result in $\mathcal{O}(h)$ convergence and can be picked on a case-by-case basis to obtain consistency with different qualitative phenomena of interest in the dynamics. Note also that $\alpha|_{a=\lambda} < \alpha|_{a=0}$. As a result the transient oscillations in (9) are more quickly damped in the NAG case than in the HB case; this is consistent with the numerical results. Indeed panels (d),(e) show that (9) is not able to adequately capture the oscillations of NAG when h is relatively large.

4. Invariant Manifold

The key lessons of the previous two sections are that the momentum methods approximate a rescaled gradient flow of the form (2) and a damped Hamiltonian system of the form (3), with small mass m which scales with the learning rate, and constant damping γ. Both approximations hold with the same order of accuracy, in terms of the learning rate, and numerics demonstrate that the Hamiltonian system is particularly useful in providing intuition for the transient regime of the algorithm. In this section we link the two theorems from the two preceding sections by showing that the Hamiltonian dynamics with small mass from section 3 has an exponentially attractive invariant manifold on which the dynamics is, to leading order, a gradient flow. That gradient flow is a small, in terms of the learning rate, perturbation of the time-rescaled gradient flow from section 2.

4.1 Main Result

Define

$$\mathsf{v}_n := (\mathsf{u}_n - \mathsf{u}_{n-1})/h \tag{12}$$

noting that then (5) becomes

$$\mathsf{u}_{n+1} = \mathsf{u}_n + h\lambda \mathsf{v}_n + hf(\mathsf{u}_n + ha\mathsf{v}_n)$$

and

$$\mathsf{v}_{n+1} = \frac{\mathsf{u}_{n+1} - \mathsf{u}_n}{h} = \lambda \mathsf{v}_n + f(\mathsf{u}_n + ha\mathsf{v}_n).$$

Hence we can re-write (5) as

$$\begin{aligned} \mathsf{u}_{n+1} &= \mathsf{u}_n + h\lambda \mathsf{v}_n + hf(\mathsf{u}_n + ha\mathsf{v}_n) \\ \mathsf{v}_{n+1} &= \lambda \mathsf{v}_n + f(\mathsf{u}_n + ha\mathsf{v}_n). \end{aligned} \tag{13}$$

Note that if $h = 0$ then (13) shows that $\mathsf{u}_n = \mathsf{u}_0$ is constant in n, and that v_n converges to $(1-\lambda)^{-1} f(\mathsf{u}_0)$. This suggests that, for h small, there is an invariant manifold which is a small perturbation of the relation $\mathsf{v}_n = \bar{\lambda} f(\mathsf{u}_n)$ and is representable as a graph. Motivated by this, we look for a function $g : \mathbb{R}^d \to \mathbb{R}^d$ such that the manifold

$$\mathsf{v} = \bar{\lambda} f(\mathsf{u}) + hg(\mathsf{u}) \tag{14}$$

is invariant for the dynamics of the numerical method:

$$\mathsf{v}_n = \bar{\lambda} f(\mathsf{u}_n) + hg(\mathsf{u}_n) \Longleftrightarrow \mathsf{v}_{n+1} = \bar{\lambda} f(\mathsf{u}_{n+1}) + hg(\mathsf{u}_{n+1}). \tag{15}$$

We will prove the existence of such a function g by use of the contraction mapping theorem to find fixed point of mapping T defined in subsection 4.2 below. We seek this fixed point in set Γ which we now define:

Definition 4 *Let $\gamma, \delta > 0$ be as in Lemmas 9, 10. Define $\Gamma \coloneqq \Gamma(\gamma, \delta)$ to be the closed subset of $C(\mathbb{R}^d; \mathbb{R}^d)$ consisting of γ-bounded functions:*

$$\|g\|_\Gamma \coloneqq \sup_{\xi \in \mathbb{R}^d} |g(\xi)| \leq \gamma, \quad \forall g \in \Gamma$$

that are δ-Lipshitz:

$$|g(\xi) - g(\eta)| \leq \delta |\xi - \eta|, \quad \forall g \in \Gamma, \xi, \eta \in \mathbb{R}^d.$$

Theorem 5 *Fix $\lambda \in (0,1)$. Suppose that h is chosen small enough so that Assumption 11 holds. For $n = 0, 1, 2, \ldots$, let u_n, v_n be the sequences given by (13). Then there is a $\tau > 0$ such that, for all $h \in (0, \tau)$, there is a unique $g \in \Gamma$ such that (15) holds. Furthermore,*

$$|\mathsf{v}_n - \bar{\lambda} f(\mathsf{u}_n) - hg(\mathsf{u}_n)| \leq (\lambda + h^2 \lambda \delta)^n |\mathsf{v}_0 - \bar{\lambda} f(\mathsf{u}_0) - hg(\mathsf{u}_0)|$$

where $\lambda + h^2 \lambda \delta < 1$.

The statement of Assumption 11, and the proof of the preceding theorem, are given in Appendix C. The assumption appears somewhat involved at first glance but inspection reveals that it simply places an upper bound on the learning rate h, as detailed in Lemmas 9, 10. The proof of the theorem rests on the Lemmas 13, 14 and 15 which establish that the operator T is well-defined, maps Γ to Γ, and is a contraction on Γ. The operator T is defined, and expressed in a helpful form for the purposes of analysis, in the next subsection.

In the next subsection we obtain the leading order approximation for g, given in equation (29). Theorem 5 implies that the large-time dynamics are governed by the dynamics on the invariant manifold. Substituting the leading order approximation for g into the invariant manifold (14) and using this expression in the definition (12) shows that

$$\mathsf{v}_n = -(1-\lambda)^{-1} \nabla \left(\Phi(\mathsf{u}_n) + \frac{1}{2} h \bar{\lambda} (\bar{\lambda} - a) |\nabla \Phi(\mathsf{u}_n)|^2 \right), \tag{16a}$$

$$\mathsf{u}_n = \mathsf{u}_{n-1} - h(1-\lambda)^{-1} \nabla \left(\Phi(\mathsf{u}_n) + \frac{1}{2} h \bar{\lambda} (\bar{\lambda} - a) |\nabla \Phi(\mathsf{u}_n)|^2 \right). \tag{16b}$$

Setting

$$c = \bar{\lambda} \left(\bar{\lambda} - a + \frac{1}{2} \right) \tag{17}$$

we see that for large time the dynamics of momentum methods, including HB and NAG, are approximately those of the modified gradient flow

$$\frac{du}{dt} = -(1-\lambda)^{-1} \nabla \Phi_h(u) \tag{18}$$

with

$$\Phi_h(u) = \Phi(u) + \frac{1}{2}hc|\nabla\Phi(u)|^2. \tag{19}$$

To see this we proceed as follows. Note that from (18)

$$\frac{d^2u}{dt^2} = -\frac{1}{2}(1-\lambda)^{-2}\nabla|\nabla\Phi(u)|^2 + \mathcal{O}(h)$$

then Taylor expansion shows that, for $u_n = u(nh)$,

$$\begin{aligned} u_n &= u_{n-1} + h\dot{u}_n - \frac{h^2}{2}\ddot{u}_n + \mathcal{O}(h^3) \\ &= u_{n-1} - h\bar{\lambda}\left(\nabla\Phi(u_n) + \frac{1}{2}hc\nabla|\nabla\Phi(u_n)|^2\right) + \frac{1}{4}h^2\bar{\lambda}^2\nabla|\nabla\Phi(u_n)|^2 + \mathcal{O}(h^3) \end{aligned}$$

where we have used that

$$Df(u)f(u) = \frac{1}{2}\nabla\left(|\nabla\Phi(u)|^2\right).$$

Choosing $c = \bar{\lambda}(\bar{\lambda} - a + 1/2)$ we see that

$$u_n = u_{n-1} - h(1-\lambda)^{-1}\nabla\left(\Phi(u_n) + \frac{1}{2}h\bar{\lambda}(\bar{\lambda}-a)|\nabla\Phi(u_n)|^2\right) + \mathcal{O}(h^3) \tag{20}$$

Notice that comparison of (16b) and (20) shows that, on the invariant manifold, the dynamics are to $\mathcal{O}(h^2)$ the same as the equation (18); this is because the truncation error between (16b) and (20) is $\mathcal{O}(h^3)$.

Thus we have proved:

Theorem 6 *Suppose that the conditions of Theorem 5 hold. Then for initial data started on the invariant manifold and any $T \geq 0$, there is a constant $C = C(T) > 0$ such that*

$$\sup_{0\leq nh\leq T} |u_n - \mathsf{u}_n| \leq Ch^2,$$

where $\mathsf{u}_n = \mathsf{u}(nh)$ solves the modified equation (18) with $c = \bar{\lambda}(\bar{\lambda} - a + 1/2)$.

4.2 Intuition

We will define mapping $T : C(\mathbb{R}^d;\mathbb{R}^d) \to C(\mathbb{R}^d;\mathbb{R}^d)$ via the equations

$$\begin{aligned} p &= \xi + h\lambda\big(\bar{\lambda}f(\xi) + hg(\xi)\big) + hf\Big(\xi + ha\big(\bar{\lambda}f(\xi) + hg(\xi)\big)\Big) \\ \bar{\lambda}f(p) + h(Tg)(p) &= \lambda\big(\bar{\lambda}f(\xi) + hg(\xi)\big) + f\Big(\xi + ha\big(\bar{\lambda}f(\xi) + hg(\xi)\big)\Big). \end{aligned} \tag{21}$$

A fixed point of the mapping $g \mapsto Tg$ will give function g so that, under (21), identity (15) holds. Later we will show that, for g in Γ and all h sufficiently small, ξ can be found from (21a) for every p, and that thus (21b) defines a mapping from $g \in \Gamma$ into $Tg \in C(\mathbb{R}^d;\mathbb{R}^d)$. We will then show that, for h sufficiently small, $T : \Gamma \mapsto \Gamma$ and is a contraction.

For any $g \in C(\mathbb{R}^d;\mathbb{R}^d)$ and $\xi \in \mathbb{R}^d$ define

$$w_g(\xi) := \bar{\lambda} f(\xi) + hg(\xi) \tag{22}$$

$$z_g(\xi) := \lambda w_g(\xi) + f\big(\xi + haw_g(\xi)\big). \tag{23}$$

With this notation the fixed point mapping (21) for g may be written

$$\begin{aligned} p &= \xi + hz_g(\xi), \\ \bar{\lambda} f(p) + h(Tg)(p) &= z_g(\xi). \end{aligned} \tag{24}$$

Then, by Taylor expansion,

$$\begin{aligned} f\Big(\xi + ha\big(\bar{\lambda} f(\xi) + hg(\xi)\big)\Big) &= f\big(\xi + haw_g(\xi)\big) \\ &= f(\xi) + ha\int_0^1 Df\big(\xi + shaw_g(\xi)\big)w_g(\xi)ds \\ &= f(\xi) + haI_g^{(1)}(\xi) \end{aligned} \tag{25}$$

where the last line defines $I_g^{(1)}$. Similarly

$$\begin{aligned} f(p) &= f(\xi + hz_g(\xi)) \\ &= f(\xi) + h\int_0^1 Df\big(\xi + shz_g(\xi)\big)z_g(\xi)ds \\ &= f(\xi) + hI_g^{(2)}(\xi), \end{aligned} \tag{26}$$

where the last line now defines $I_g^{(2)}$. Then (21b) becomes

$$\bar{\lambda}\big(f(\xi) + hI_g^{(2)}(\xi)\big) + h(Tg)(p) = \lambda\bar{\lambda} f(\xi) + h\lambda g(\xi) + f(\xi) + haI_g^{(1)}(\xi)$$

and we see that

$$(Tg)(p) = \lambda g(\xi) + aI_g^{(1)}(\xi) - \bar{\lambda} I_g^{(2)}(\xi).$$

In this light, we can rewrite the defining equations (21) for T as

$$p = \xi + hz_g(\xi), \tag{27}$$

$$(Tg)(p) = \lambda g(\xi) + aI_g^{(1)}(\xi) - \bar{\lambda} I_g^{(2)}(\xi). \tag{28}$$

for any $\xi \in \mathbb{R}^d$.

Perusal of the above definitions reveals that, to leading order in h,

$$w_g(\xi) = z_g(\xi) = \bar{\lambda} f(\xi), I_g^{(1)}(\xi) = I_g^{(2)}(\xi) = \bar{\lambda} Df(\xi)f(\xi).$$

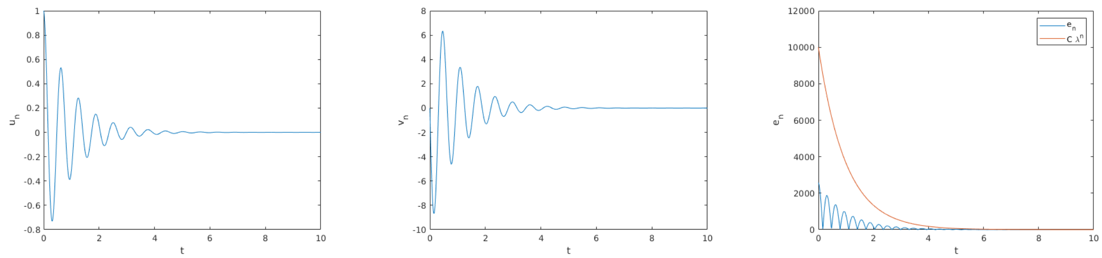
Thus setting $h = 0$ in (27), (28) shows that, to leading order in h,

$$g(p) = \bar{\lambda}^2(a - \bar{\lambda})Df(p)f(p). \tag{29}$$

Note that since $f(p) = -\nabla\Phi(p)$, Df is the negative Hessian of Φ and is thus symmetric. Hence we can write g in gradient form, leading to

$$g(p) = \frac{1}{2}\bar{\lambda}^2(a - \bar{\lambda})\nabla\big(|\nabla\Phi(p)|^2\big). \tag{30}$$

Remark 7 *This modified potential* (19) *also arises in the construction of Lyapunov functions for the one-stage theta method – see Corollary 5.6.2 in Stuart and Humphries (1998).*



(a) u_n given by (13). (b) v_n given by (13). (c) e_n given by (32).

Figure 3: Invariant manifold for NAG with $h = 0.01$ and $\lambda = 0.99$ on the one dimensional problem $\Phi(u) = \frac{1}{2}u^2$.

4.3 Numerical Illustration

In Figure 3 panels (a) and (b), we plot the components u_n and v_n found by solving (13) with initial conditions $\mathsf{u}_0 = 1$ and $\mathsf{v}_n = 0$ in the case where $\Phi(u) = \frac{1}{2}u^2$. These initial conditions correspond to initializing the map off the invariant manifold. To leading order in h the invariant manifold is given by (see equation (16))

$$v = -(1-\lambda)^{-1}\nabla\left(\Phi(u) + \frac{1}{2}h\bar{\lambda}(\bar{\lambda}-a)|\nabla\Phi(u)|^2\right). \tag{31}$$

To measure the distance of the trajectory shown in panels (a), (b) from the invariant manifold we define

$$\mathsf{e}_n = \left|\mathsf{v}_n + (1-\lambda)^{-1}\nabla\left(\Phi(\mathsf{u}_n) + \frac{1}{2}h\bar{\lambda}(\bar{\lambda}-a)|\nabla\Phi(\mathsf{u}_n)|^2\right)\right|. \tag{32}$$

Panel (c) shows the evolution of e_n as well as the (approximate) bound on it found from substituing the leading order approximation of g into the following upper bound from Theorem 5:

$$(\lambda + h^2\lambda\delta)^n|\mathsf{v}_0 - \bar{\lambda}f(\mathsf{u}_0) - hg(\mathsf{u}_0)|.$$

5. Conclusion

Together, equations (6), (9) and (18) describe the dynamical systems which are approximated by momentum methods, when implemented with fixed momentum, in a manner made precise by the four theorems in this paper. The insight obtained from these theorems sheds light on how momentum methods perform optimization tasks.

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Appendix A

Proof [of Theorem 2] Taylor expanding yields

$$u_{n+1} = u_n + h\bar{\lambda}f(u_n) + \mathcal{O}(h^2)$$

and

$$u_n = u_{n-1} + h\bar{\lambda}f(u_n) + \mathcal{O}(h^2).$$

Hence

$$(1+\lambda)u_n - \lambda u_{n-1} = u_n + h\lambda\bar{\lambda}f(u_n) + \mathcal{O}(h^2).$$

Subtracting the third identity from the first, we find that

$$u_{n+1} - ((1+\lambda)u_n - \lambda u_{n-1}) = hf(u_n) + \mathcal{O}(h^2)$$

by noting $\bar{\lambda} - \bar{\lambda}\lambda = 1$. Similarly,

$$a(u_n - u_{n-1}) = ha\bar{\lambda}f(u_n) + \mathcal{O}(h^2)$$

hence Taylor expanding yields

$$\begin{aligned} f(u_n + a(u_n - u_{n-1})) &= f(u_n) + aDf(u_n)(u_n - u_{n-1}) \\ &\quad + a^2 \int_0^1 (1-s)D^2 f(u_n + sa(u_n - u_{n-1}))[u_n - u_{n-1}]^2 ds \\ &= f(u_n) + ha\bar{\lambda}Df(u_n)f(u_n) + \mathcal{O}(h^2). \end{aligned}$$

From this, we conclude that

$$hf(u_n + a(u_n - u_{n-1})) = hf(u_n) + \mathcal{O}(h^2)$$

hence

$$u_{n+1} = (1+\lambda)u_n - \lambda u_{n-1} + hf(u_n + a(u_n - u_{n-1})) + \mathcal{O}(h^2).$$

Define the error $e_n := u_n - \mathsf{u}_n$ then

$$\begin{aligned} e_{n+1} &= (1+\lambda)e_n - \lambda e_{n-1} + h\left(f(u_n + a(u_n - u_{n-1})) - f(\mathsf{u}_n + a(\mathsf{u}_n - \mathsf{u}_{n-1}))\right) + \mathcal{O}(h^2) \\ &= (1+\lambda)e_n - \lambda e_{n-1} + h\mathsf{M}_n((1+a)e_n - ae_{n-1}) + \mathcal{O}(h^2) \end{aligned}$$

where, from the mean value theorem, we have

$$\mathsf{M}_n = \int_0^1 Df\Big(s\big(u_n + a(u_n - u_{n-1})\big) + \big(1-s\big)\big(\mathsf{u}_n + a(\mathsf{u}_n - \mathsf{u}_{n-1})\big)\Big)ds.$$

Now define the concatenation $E_{n+1} := [e_{n+1}, e_n] \in \mathbb{R}^{2d}$ then

$$E_{n+1} = A^{(\lambda)}E_n + hA_n^{(a)}E_n + \mathcal{O}(h^2)$$

where $A^{(\lambda)}, A_n^{(a)} \in \mathbb{R}^{2d\times 2d}$ are the block matricies

$$A^{(\lambda)} := \begin{bmatrix} (1+\lambda)I & -\lambda I \\ I & 0I \end{bmatrix}, \quad A_n^{(a)} := \begin{bmatrix} (1+a)\mathsf{M}_n & -a\mathsf{M}_n \\ 0I & 0I \end{bmatrix}$$

with $I \in \mathbb{R}^{d\times d}$ the identity. We note that $A^{(\lambda)}$ has minimal polynomial

$$\mu_{A^{(\lambda)}}(z) = (z-1)(z-\lambda)$$

and is hence diagonalizable. Thus there is a norm on $\|\cdot\|$ on $\mathbb{R}^{2d}$ such that its induced matrix norm $\|\cdot\|_m$ satifies $\|A^{(\lambda)}\|_m = \rho(A^{(\lambda)})$ where $\rho : \mathbb{R}^{2d\times 2d} \to \mathbb{R}_+$ maps a matrix to its spectral radius. Hence, since $\lambda \in (0,1)$, we have $\|A^{(\lambda)}\|_m = 1$. Thus

$$\|E_{n+1}\| \leq (1 + h\|A_n^{(a)}\|_m)\|E_n\| + \mathcal{O}(h^2).$$

Then, by finite dimensional norm equivalence, there is a constant $\alpha > 0$, independent of h, such that

$$\begin{aligned}\|A_n^{(a)}\|_m &\leq \alpha \left\| \begin{bmatrix} 1+a & -a \\ 0 & 0 \end{bmatrix} \otimes \mathsf{M}_n \right\|_2 \\ &= \alpha\sqrt{2a^2+2a+1}\|\mathsf{M}_n\|_2\end{aligned}$$

where $\|\cdot\|_2$ denotes the spectral 2-norm. Using Assumption 1, we have

$$\|\mathsf{M}_n\|_2 \leq B_1$$

thus, letting $c := \alpha\sqrt{2a^2+2a+1}B_1$, we find

$$\|E_{n+1}\| \leq (1+hc)\|E_n\| + \mathcal{O}(h^2).$$

Then, by Grönwall lemma,

$$\begin{aligned}\|E_{n+1}\| &\leq (1+hc)^n\|E_1\|_n + \frac{(1+hc)^{n+1}-1}{ch}\mathcal{O}(h^2) \\ &= (1+hc)^n\|E_1\|_n + \mathcal{O}(h)\end{aligned}$$

noting that the constant in the $\mathcal{O}(h)$ term is bounded above in terms of T, but independently of h. Finally, we check the initial condition

$$E_1 = \begin{bmatrix} u_1 - \mathsf{u}_1 \\ u_0 - \mathsf{u}_0 \end{bmatrix} = \begin{bmatrix} h(\bar{\lambda}-1)f(\mathsf{u}_0) + \mathcal{O}(h^2) \\ 0 \end{bmatrix} = \mathcal{O}(h)$$

as desired. ■

Appendix B

Proof [of Theorem 3] Taylor expanding yields

$$u_{n\pm 1} = u_n \pm h\dot{u}_n + \frac{h^2}{2}\ddot{u}_n \pm \frac{h^3}{2}I_n^{\pm}$$

where

$$I_n^{\pm} = \int_0^1 (1-s)^2 \dddot{u}((n\pm s)h)ds.$$

Then using equation (9)

$$
\begin{aligned}
u_{n+1} - u_n - \lambda(u_n - u_{n-1}) &= h(1-\lambda)\dot{u}_n + \frac{h^2}{2}(1+\lambda)\ddot{u}_n + \frac{h^3}{2}(I_n^+ - \lambda I_n^-) \\
&= hf(u_n) + h^2 a(1-\lambda)\ddot{u}_n + \frac{h^3}{2}(I_n^+ - \lambda I_n^-).
\end{aligned} \tag{33}
$$

Similarly

$$
a(u_n - u_{n-1}) = ha\dot{u}_n - \frac{h^2}{2}a\ddot{u}_n + \frac{h^3}{2}aI_n^-
$$

hence

$$
f(u_n + a(u_n - u_{n-1})) = f(u_n) + haDf(u_n)\dot{u}_n - Df(u_n)\left(\frac{h^2}{2}a\ddot{u}_n - \frac{h^3}{2}aI_n^-\right) + I_n^f
$$

where

$$
I_n^f = a^2\int_0^1 (1-s)D^2 f(u_n + sa(u_n - u_{n-1}))[u_n - u_{n-1}]^2 ds.
$$

Differentiating (9) yields

$$
h\alpha\frac{d^3u}{dt^3} + (1-\lambda)\frac{d^2u}{dt^2} = Df(u)\frac{du}{dt}
$$

hence

$$
\begin{aligned}
hf(u_n + a(u_n - u_{n-1})) &= hf(u_n) + h^2 a\left(h\alpha\dddot{u}_n + (1-\lambda)\ddot{u}_n\right) - Df(u_n)\left(\frac{h^3}{2}a\ddot{u}_n - \frac{h^4}{2}aI_n^-\right) + hI_n^f \\
&= hf(u_n) + h^2 a(1-\lambda)\ddot{u}_n + h^3 a\alpha\dddot{u}_n - Df(u_n)\left(\frac{h^3}{2}a\ddot{u}_n - \frac{h^4}{2}aI_n^-\right) + hI_n^f.
\end{aligned}
$$

Rearranging this we obtain an expression for $hf(u_n)$ which we plug into equation (33) to yield

$$
u_{n+1} - u_n - \lambda(u_n - u_{n-1}) = hf(u_n + a(u_n - u_{n-1})) + \mathrm{LT}_n
$$

where

$$
\mathrm{LT}_n = \underbrace{\frac{h^3}{2}(I_n^+ - \lambda I_n^-)}_{\mathcal{O}\left(h\exp\left(-\frac{(1-\lambda)}{2\alpha}n\right)\right)} - \underbrace{h^3 a\alpha\dddot{u}_n}_{\mathcal{O}\left(h\exp\left(-\frac{(1-\lambda)}{2\alpha}n\right)\right)} + \underbrace{Df(u_n)\left(\frac{h^3}{2}a\ddot{u}_n - \frac{h^4}{2}aI_n^-\right)}_{\mathcal{O}(h^2)} - \underbrace{hI_n^f}_{\mathcal{O}(h^3)}.
$$

The bounds (in braces) on the four terms above follow from employing Assumption 1 and Lemma 8. From them we deduce the existence of constants $K_1, K_2 > 0$ independent of h such that

$$
|\mathrm{LT}_n| \leq hK_1\exp\left(-\frac{(1-\lambda)}{2\alpha}n\right) + h^2 K_2.
$$

We proceed similarly to the proof of Theorem 2, but with a different truncation error structure, and find the error satsifies

$$
\|E_{n+1}\| \leq (1+hc)\|E_n\| + hK_1\exp\left(-\frac{(1-\lambda)}{2\alpha}n\right) + h^2 K_2
$$

where we abuse notation and continue to write K_1, K_2 when, in fact, the constants have changed by use of finite-dimensional norm equivalence. Define $K_3 := K_2/c$ then summing this error, we find

$$\begin{aligned}\|E_{n+1}\| &\leq (1+hc)^n\|E_1\| + hK_3((1+hc)^{n+1}-1) + hK_1\sum_{j=0}^{n}(1+hc)^j \exp\left(-\frac{(1-\lambda)}{2\alpha}(n-j)\right)\\ &= (1+hc)^n\|E_1\| + hK_3((1+hc)^{n+1}-1) + hK_1 S_n.\end{aligned}$$

where

$$S_n = \exp\left(-\frac{(1-\lambda)}{2\alpha}n\right)\left(\frac{(1+hc)^{n+1}\exp\left(\frac{(1-\lambda)}{2\alpha}(n+1)\right)-1}{(1+hc)\exp\left(\frac{1-\lambda}{2\alpha}\right)-1}\right).$$

Let $T = nh$ then

$$\begin{aligned}S_n &\leq \frac{(1+hc)^{n+1}\exp\left(\frac{1-\lambda}{2\alpha}\right)}{(1+hc)\exp\left(\frac{1-\lambda}{2\alpha}\right)-1}\\ &\leq \frac{2\exp\left(cT+\frac{1-\lambda}{2\alpha}\right)}{\exp\left(\frac{1-\lambda}{2\alpha}\right)-1}\end{aligned}$$

From this we deduce that

$$\|E_{n+1}\| \leq (1+hc)^n\|E_1\| + \mathcal{O}(h)$$

noting that the constant in the $\mathcal{O}(h)$ term is bounded above in terms of T, but independently of h. For the initial condition, we check

$$u_1 - \mathsf{u}_1 = h(\mathsf{u}_0' - f(\mathsf{u}_0)) + \frac{h^2}{2}\ddot{u}_0 + \frac{h^3}{2}I_0^+$$

which is $\mathcal{O}(h)$ by Lemma 8. Putting the bounds together we obtain

$$\sup_{0\leq nh\leq T}\|E_n\| \leq C(T)h.$$

■

Lemma 8 *Suppose Assumption 1 holds and let* $u \in C^3([0,\infty);\mathbb{R}^d)$ *be the solution to*

$$\begin{aligned}h\alpha\frac{d^2u}{dt^2} + (1-\lambda)\frac{du}{dt} &= f(u)\\ u(0) = \mathsf{u}_0, \quad \frac{du}{dt}(0) &= \mathsf{v}_0\end{aligned}$$

for some $\mathsf{u}_0, \mathsf{v}_0 \in \mathbb{R}^d$ *and* $\alpha > 0$ *independent of* h. *Suppose* $h \leq (1-\lambda)^2/2\alpha B_1$ *then there are constants* $C^{(1)}, C_1^{(2)}, C_2^{(2)}, C_1^{(3)}, C_2^{(3)} > 0$ *independent of* h *such that for any* $t \in [0,\infty)$,

$$\begin{aligned}|\dot{u}(t)| &\leq C^{(1)},\\ |\ddot{u}(t)| &\leq \frac{C_1^{(2)}}{h}\,\mathit{exp}\left(-\frac{(1-\lambda)}{2h\alpha}t\right) + C_2^{(2)},\\ |\dddot{u}(t)| &\leq \frac{C_1^{(3)}}{h^2}\,\mathit{exp}\left(-\frac{(1-\lambda)}{2h\alpha}t\right) + C_2^{(3)}.\end{aligned}$$

One readily verifies that the result of Lemma 8 is tight by considering the one-dimensional case with $f(u) = -u$. This implies that the result of Theorem 3 cannot be improved without further assumptions.

Proof [of Lemma 8] Define $v \coloneqq \dot{u}$ then

$$\dot{v} = -\frac{1}{h\alpha}\left((1-\lambda)v - f(u)\right).$$

Define $w \coloneqq (1-\lambda)v - f(u)$ hence $\dot{v} = -(1/h\alpha)w$ and $\dot{u} = v = \bar{\lambda}(w + f(u))$. Thus

$$\begin{aligned}
\dot{w} &= (1-\lambda)\dot{v} - Df(u)\dot{u} \\
&= -\frac{(1-\lambda)}{h\alpha}w - Df(u)(\bar{\lambda}(w + f(u))).
\end{aligned}$$

Hence we find

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}|w|^2 &= -\frac{(1-\lambda)}{h\alpha}|w|^2 - \bar{\lambda}\langle w, Df(u)w\rangle - \bar{\lambda}\langle w, Df(u)f(u)\rangle \\
&\leq -\frac{(1-\lambda)}{h\alpha}|w|^2 + \bar{\lambda}|\langle w, Df(u)w\rangle| + \bar{\lambda}|\langle w, Df(u)f(u)\rangle| \\
&\leq -\frac{(1-\lambda)}{h\alpha}|w|^2 + \bar{\lambda}B_1|w|^2 + \bar{\lambda}B_0B_1|w| \\
&\leq -\frac{(1-\lambda)}{h\alpha}|w|^2 + \frac{(1-\lambda)}{2h\alpha}|w|^2 + \bar{\lambda}B_0B_1|w| \\
&= -\frac{(1-\lambda)}{2h\alpha}|w|^2 + \bar{\lambda}B_0B_1|w|
\end{aligned}$$

by noting that our assumption $h \leq (1-\lambda)^2/2\alpha B_1$ implies $\bar{\lambda}B_1 \leq (1-\lambda)/2h\alpha$. Hence

$$\frac{d}{dt}|w| \leq -\frac{(1-\lambda)}{2h\alpha}|w| + \bar{\lambda}B_0B_1$$

so, by Grönwall lemma,

$$\begin{aligned}
|w(t)| &\leq \exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right)|w(0)| + 2h\bar{\lambda}^2\alpha B_0B_1\left(1 - \exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right)\right) \\
&\leq \exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right)|w(0)| + h\beta_1
\end{aligned}$$

where we define $\beta_1 \coloneqq 2\bar{\lambda}^2\alpha B_0B_1$. Hence

$$\begin{aligned}
|\ddot{u}(t)| &= |\dot{v}(t)| \\
&= \frac{1}{h\alpha}|w(t)| \\
&\leq \frac{1}{h\alpha}\exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right)|w(0)| + \frac{\beta_1}{\alpha} \\
&= \frac{|(1-\lambda)\mathsf{v}_0 - f(\mathsf{u}_0)|}{h\alpha}\exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right) + \frac{\beta_1}{\alpha}
\end{aligned}$$

thus setting $C_1^{(2)} = |(1-\lambda)\mathsf{v}_0 - f(\mathsf{u}_0)|/\alpha$ and $C_1^{(2)} = \beta_1/\alpha$ gives the desired result. Further,

$$\begin{aligned}|\dot{u}(t)| &= |v(t)| \\ &\leq \bar{\lambda}(|w(t)| + |f(u(t))|) \\ &\leq \bar{\lambda}(|w(0)| + h\beta_1 + B_0)\end{aligned}$$

hence we deduce the existence of $C^{(1)}$. Now define $z \coloneqq \dot{w}$ then

$$\dot{z} = -\frac{(1-\lambda)}{h\alpha}z - \bar{\lambda}Df(u)z + G(u,v,w)$$

where we define $G(u,v,w) \coloneqq -\bar{\lambda}(Df(u)(Df(u)v) + D^2f(u)[v,w] + D^2f(u)[Df(u)v, f(u)])$. Using Assumption 1 and our bounds on w and v, we deduce that there is a constant $C > 0$ independent of h such that

$$|G(u,v,w)| \leq C$$

hence

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}|z|^2 &= -\frac{(1-\lambda)}{h\alpha}|z|^2 - \bar{\lambda}\langle z, Df(u)z\rangle + \langle z, G(u,v,w)\rangle \\ &\leq -\frac{(1-\lambda)}{h\alpha}|z|^2 + \bar{\lambda}B_1|z|^2 + C|z| \\ &\leq -\frac{(1-\lambda)}{2h\alpha}|z|^2 + C|z|\end{aligned}$$

as before. Thus we find

$$\frac{d}{dt}|z| \leq -\frac{(1-\lambda)}{2h\alpha}|z| + C$$

so, by Grönwall lemma,

$$|z(t)| \leq \exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right)|z(0)| + h\beta_2$$

where we define $\beta_2 \coloneqq 2\bar{\lambda}\alpha C$. Recall that

$$\dddot{u} = \ddot{v} = -\frac{1}{h\alpha}\dot{w} = -\frac{1}{h\alpha}z$$

and note

$$|z(0)| \leq \frac{(1-\lambda)|(1-\lambda)\mathsf{v}_0 - f(\mathsf{u}_0)|}{h\alpha} + B_1|\mathsf{v}_0|$$

hence we find

$$|\dddot{u}(t)| \leq \left(\frac{(1-\lambda)|(1-\lambda)\mathsf{v}_0 - f(\mathsf{u}_0)}{h^2\alpha^2} + \frac{B_1|\mathsf{v}_0|}{h\alpha}\right)\exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right) + \frac{\beta_2}{\alpha}.$$

Thus we deduce that there is a consant $C_1^{(3)} > 0$ independent of h such that

$$|\dddot{u}(t)| \leq \frac{C_1^{(3)}}{h^2}\exp\left(-\frac{(1-\lambda)}{2h\alpha}t\right) + C_2^{(3)}$$

as desired where $C_2^{(3)} = \beta_2/\alpha$. ■

Appendix C.

For the results of Section 4 we make the following assumption on the size of h. Recall first that by Assumption 1 there are constants $B_0, B_1, B_2 > 0$ such that

$$\|D^{j-1} f\| = \|D^j \Phi\| \leq B_{j-1}$$

for $j = 1, 2, 3$.

Lemma 9 *Suppose $h > 0$ is small enough such that*

$$\lambda + hB_1(a + \lambda\bar{\lambda}) < 1$$

then there is a $\tau_1 > 0$ such that for any $\gamma \in [\tau_1, \infty)$

$$(\lambda + hB_1(a + \lambda\bar{\lambda}))\gamma + \bar{\lambda}B_0B_1(a + \bar{\lambda}) \leq \gamma. \tag{34}$$

Using Lemma 9 fix $\gamma \in [\tau_1, \infty)$ and define the constants

$$\begin{aligned}
K_1 &:= \bar{\lambda}B_0 + h\gamma \\
K_3 &:= B_0 + \lambda K_1 \\
\alpha_2 &:= h^2(\lambda + haB_1), \\
\alpha_1 &:= \lambda - 1 + h\left(B_1(\bar{\lambda} + a(1 + h\bar{\lambda}B_1)) + \lambda\bar{\lambda}(B_1 + hB_2K_3) + ha(aB_2K_1 + B_1\bar{\lambda}(B_1 + hB_2K_3)\right), \\
\alpha_0 &:= aB_2K_1(1 + ha\bar{\lambda}B_1) + \bar{\lambda}(aB_1^2 + B_2K_3) + \bar{\lambda}^2B_1(1 + haB_1)(B_1 + hB_2K_3).
\end{aligned} \tag{35}$$

Lemma 10 *Suppose $h > 0$ is small enough such that*

$$\alpha_1^2 > 4\alpha_2\alpha_0, \quad \alpha_1 < 0$$

then there are $\tau_2^{\pm} > 0$ such that for any $\delta \in (\tau_2^-, \tau_2^+]$

$$\alpha_2\delta^2 + \alpha_1\delta + \alpha_0 \leq 0. \tag{36}$$

Using Lemma 10 fix $\delta \in (\tau_2^-, \tau_2^+]$. We make the following assumption on the size of the learning rate h which is achievable since $\lambda \in (0, 1)$.

Assumption 11 *Let Assumption 1 hold and suppose $h > 0$ is small enough such that the assumptions of Lemmas 9, 10 hold. Define $K_2 := \bar{\lambda}B_1 + h\delta$ and suppose $h > 0$ is small enough such that*

$$c := h(\lambda K_2 + B_1(1 + haK_2)) < 1. \tag{37}$$

Define constants

$$\begin{aligned}
Q_1 &:= \lambda\delta + a(B_1K_2 + B_2K_1(1 + haK_2)) + \bar{\lambda}((B_1 + hB_2K_3)(\lambda K_2 + B_1(1 + haK_2)) + B_2K_3), \\
Q_2 &:= h(a(B_1 + haB_2K_1) + \bar{\lambda}(\lambda + haB_1)(B_1 + hB_2K_3)), \\
Q_3 &:= h(\lambda K_2 + B_1(1 + haK_2)), \\
\mu &:= \lambda + Q_2 + \frac{h^2(\lambda + haB_1)Q_1}{1 - Q_3}.
\end{aligned} \tag{38}$$

Suppose $h > 0$ is small enough such that

$$Q_3 < 1, \quad \mu < 1. \tag{39}$$

Lastly assume $h > 0$ is small enough such that

$$\lambda + h^2 \lambda \delta < 1. \tag{40}$$

Proof [of Lemma 9.] Since $\lambda + hB_1(a + \lambda\bar{\lambda}) < 1$ and $\bar{\lambda}B_0B_1(a + \bar{\lambda}) > 0$ the line defined by

$$(\lambda + hB_1(a + \lambda\bar{\lambda}))\gamma + \bar{\lambda}B_0B_1(a + \bar{\lambda})$$

will intersect the identity line at a positive γ and lie below it thereafter. Hence setting

$$\tau_1 = \frac{\bar{\lambda}B_0B_1(a + \bar{\lambda})}{1 - \lambda + hB_1(a + \lambda\bar{\lambda})}$$

completes the proof. ■

Proof [of Lemma 10.] Note that since $\alpha_2 > 0$, the parabola defined by

$$\alpha_2\delta^2 + \alpha_1\delta + \alpha_0$$

is upward-pointing and has roots

$$\zeta_\pm = \frac{-\alpha_1 \pm \sqrt{\alpha_1^2 - 4\alpha_2\alpha_0}}{2\alpha_2}.$$

Since $\alpha_1^2 > 4\alpha_2\alpha_0$, $\zeta_\pm \in \mathbb{R}$ with $\zeta_+ \neq \zeta_-$. Since $\alpha_1 < 0$, $\zeta_+ > 0$ hence setting $\tau_2^+ = \zeta_+$ and $\tau_2^- = \max\{0, \zeta_-\}$ completes the proof. ■

The following proof refers to four lemmas whose statement and proof follow it.

Proof [of Theorem 5.] Define $\tau > 0$ as the maximum h such that Assumption 11 holds. The contraction mapping principle together with Lemmas 13, 14, and 15 show that the operator T defined by (27) and (28) has a unique fixed point in Γ. Hence, from its definition and equation (21b), we immediately obtain the existence result. We now show exponential attractivity. Recall the definition of the operator T namely equations (27), (28):

$$p = \xi + hz_g(\xi)$$
$$(Tg)(p) = \lambda g(\xi) + aI_g^{(1)}(\xi) - \bar{\lambda}I_g^{(2)}(\xi).$$

Let $g \in \Gamma$ be the fixed point of T and set

$$p = \mathsf{u}_n + hz_g(\mathsf{u}_n)$$
$$g(p) = \lambda g(\mathsf{u}_n) + aI_g^{(1)}(\mathsf{u}_n) - \bar{\lambda}I_g^{(2)}(\mathsf{u}_n).$$

Then

$$\begin{aligned}|\mathsf{v}_{n+1} - \bar{\lambda} f(\mathsf{u}_{n+1}) - hg(\mathsf{u}_{n+1})| &\leq |\mathsf{v}_{n+1} - \bar{\lambda} f(\mathsf{u}_{n+1}) - hg(p)| + h|g(p) - g(\mathsf{u}_{n+1})| \\ &\leq |\mathsf{v}_{n+1} - \bar{\lambda} f(\mathsf{u}_{n+1}) - hg(p)| + h\delta|p - \mathsf{u}_{n+1}|\end{aligned}$$

since $g \in \Gamma$. Since, by definition,

$$\mathsf{v}_{n+1} = \lambda \mathsf{v}_n + f(\mathsf{u}_n + ha\mathsf{v}_n)$$

we have,

$$\begin{aligned}|\mathsf{v}_{n+1} - \bar{\lambda} f(\mathsf{u}_{n+1}) - hg(p)| &= |\lambda \mathsf{v}_n + f(\mathsf{u}_n + ha\mathsf{v}_n) - \bar{\lambda} f(\mathsf{u}_{n+1}) - h(\lambda g(\mathsf{u}_n) + aI_g^{(1)}(\mathsf{u}_n) - \bar{\lambda} I_g^{(2)}(\mathsf{u}_n))| \\ &= \lambda|\mathsf{v}_n - \bar{\lambda} f(\mathsf{u}_n) - hg(\mathsf{u}_n)|\end{aligned}$$

by noting that

$$\begin{aligned}&f(\mathsf{u}_n + ha\mathsf{v}_n) = f(\mathsf{u}_n) + haI_g^{(1)}(\mathsf{u}_n) \\ &f(\mathsf{u}_{n+1}) = f(\mathsf{u}_n) + hI_g^{(2)}(\mathsf{u}_n).\end{aligned}$$

From definition,

$$\mathsf{u}_{n+1} = \mathsf{u}_n + h\lambda \mathsf{v}_n + hf(\mathsf{u}_n + ha\mathsf{v}_n)$$

thus

$$\begin{aligned}|p - \mathsf{u}_{n+1}| &= |\mathsf{u}_n + hz_g(\mathsf{u}_n) - \mathsf{u}_n - h\lambda \mathsf{v}_n - hf(\mathsf{u}_n + ha\mathsf{v}_n)| \\ &= h|\lambda(\bar{\lambda} f(\mathsf{u}_n) + hg(\mathsf{u}_n)) + f(\mathsf{u}_n + ha\mathsf{v}_n) - \lambda \mathsf{v}_n - f(\mathsf{u}_n + ha\mathsf{v}_n)| \\ &= h\lambda|\mathsf{v}_n - \bar{\lambda} f(\mathsf{u}_n) - hg(\mathsf{u}_n)|.\end{aligned}$$

Hence

$$|\mathsf{v}_{n+1} - \bar{\lambda} f(\mathsf{u}_{n+1}) - hg(\mathsf{u}_{n+1})| \leq (\lambda + h^2\lambda\delta)|\mathsf{v}_n - \bar{\lambda} f(\mathsf{u}_n) - hg(\mathsf{u}_n)|$$

as desired. By Assumption 11, $\lambda + h^2\lambda\delta < 1$. ■

The following lemma gives basic bounds which are used in the proof of Lemmas 13, 14, 15.

Lemma 12 *Let $g, q \in \Gamma$ and $\xi, \eta \in \mathbb{R}^d$ then the quantities defined by* (22), (23), (25), (26) *satisfy the following:*

$$\begin{aligned}
|w_g(\xi)| &\leq K_1, \\
|w_g(\xi) - w_g(\eta)| &\leq K_2|\xi - \eta|, \\
|w_g(\xi) - w_q(\xi)| &\leq h|g(\xi) - q(\xi)|, \\
|z_g(\xi)| &\leq K_3, \\
|z_g(\xi) - z_g(\eta)| &\leq (\lambda K_2 + B_1(1 + haK_2))|\xi - \eta|, \\
|z_g(\xi) - z_q(\xi)| &\leq h(\lambda + haB_1)|g(\xi) - q(\xi)|, \\
|I_g^{(1)}(\xi)| &\leq B_1 K_1, \\
|I_g^{(1)}(\xi) - I_g^{(1)}(\eta)| &\leq (B_1 K_2 + B_2 K_1(1 + haK_2))|\xi - \eta|, \\
|I_g^{(1)}(\xi) - I_q^{(1)}(\xi)| &\leq h(B_1 + haB_2 K_1)|g(\xi) - q(\xi)|, \\
|I_g^{(2)}(\xi)| &\leq B_1 K_3 \\
|I_g^{(2)}(\xi) - I_g^{(2)}(\eta)| &\leq ((B_1 + hB_2K_3)(\lambda K_2 + B_1(1 + haK_2)) + B_2 K_3)|\xi - \eta|, \\
|I_g^{(2)}(\xi) - I_q^{(2)}(\xi)| &\leq h(\lambda + hB_1 a)(B_1 + hB_2 K_3)|g(\xi) - q(\xi)|.
\end{aligned}$$

Proof These bounds relay on applications of the triangle inequality together with boundedness of f and its derivatives as well as the fact that functions in Γ are bounded and Lipschitz. To illustrate the idea, we will prove the bounds for $w_g, w_q, I_g^{(1)}$, and $I_q^{(1)}$. To that end,

$$\begin{aligned}
|w_g(\xi)| &= |\bar{\lambda} f(\xi) + hg(\xi)| \\
&\leq \bar{\lambda}|f(\xi)| + h|g(\xi)| \\
&\leq \bar{\lambda} B_0 + h\gamma \\
&= K_1
\end{aligned}$$

establishing the first bound. For the second,

$$\begin{aligned}
|w_g(\xi) - w_g(\eta)| &\leq \bar{\lambda}|f(\xi) - f(\eta)| + h|g(\xi) - g(\eta)| \\
&\leq \bar{\lambda} B_1|\xi - \eta| + h\delta|\xi - \eta| \\
&= K_2|\xi - \eta|
\end{aligned}$$

as desired. Finally,

$$\begin{aligned}
|w_g(\xi) - w_q(\xi)| &= |\bar{\lambda} f(\xi) + hg(\xi) - \bar{\lambda} f(\xi) - hq(\xi)| \\
&= h|g(\xi) - q(\xi)|
\end{aligned}$$

as desired. We now turn to the bounds for $I_g^{(1)}, I_q^{(1)}$,

$$\begin{aligned}
|I_g^{(1)}(\xi)| &\leq \int_0^1 |Df(\xi + shaw_g(\xi))||w_g(\xi)|ds \\
&\leq \int_0^1 B_1 K_1 ds \\
&= B_1 K_1
\end{aligned}$$

establishing the first bound. For the second bound,

$$\begin{aligned}
|I_g^{(1)}(\xi) - I_g^{(1)}(\eta)| &\le \int_0^1 |Df(\xi + shaw_g(\xi))w_g(\xi) - Df(\eta + shaw_g(\eta))w_g(\xi)|ds \\
&\quad + \int_0^1 |Df(\eta + shaw_g(\eta))w_g(\xi) - Df(\eta + shaw_g(\eta))w_g(\eta)|ds \\
&\le K_1 B_2 \int_0^1 (|\xi - \eta| + sha|w_g(\xi) - w_g(\eta)|)ds + B_1|w_g(\xi) - w_g(\eta)| \\
&\le K_1 B_2 (|\xi - \eta| + haK_2|\xi - \eta|) + B_1 K_2 |\xi - \eta| \\
&= (B_1 K_2 + B_2 K_1 (1 + haK_2))|\xi - \eta|
\end{aligned}$$

as desired. Finally

$$\begin{aligned}
|I_g^{(1)}(\xi) - I_q^{(1)}(\xi)| &\le \int_0^1 |Df(\xi + shaw_g(\xi))w_g(\xi) - Df(\xi + shaw_g(\xi))w_q(\xi)|ds \\
&\quad + \int_0^1 |Df(\xi + shaw_g(\xi))w_q(\xi) - Df(\xi + shaw_q(\xi))w_q(\xi)|ds \\
&\le B_1 \int_0^1 |w_g(\xi) - w_q(\xi)|ds + K_1 B_2 \int_0^1 |\xi + shaw_g(\xi) - \xi - shaw_q(\xi)|ds \\
&\le hB_1|g(\xi) - q(\xi)| + h^2 a B_2 K_1 |g(\xi) - q(\xi)| \\
&= h(B_1 + haB_2K_1)|g(\xi) - q(\xi)|
\end{aligned}$$

as desired. The bounds for $z_g, z_q, I_g^{(2)}$, and $I_q^{(2)}$ follow similarly. ■

We also need the following three lemmas:

Lemma 13 *Suppose Assumption 11 holds. For any $g \in \Gamma$ and $p \in \mathbb{R}^d$ there exists a unique $\xi \in \mathbb{R}^d$ satisfying* (27).

Lemma 14 *Suppose Assumption 11 holds. The operator T defined by* (28) *satisfies $T : \Gamma \to \Gamma$.*

Lemma 15 *Suppose Assumption 11 holds. For any $g_1, g_2 \in \Gamma$, we have*

$$\|Tg_1 - Tg_2\|_\Gamma \le \mu \|g_1 - g_2\|_\Gamma$$

where $\mu < 1$.

Now we prove these three lemmas.

Proof [of Lemma 13.] Consider the iteration of the form

$$\xi^{k+1} = p - hz_g(\xi^k).$$

For any two sequences $\{\xi^k\}$, $\{\eta^k\}$ generated by this iteration we have, by Lemma 12,

$$\begin{aligned}
|\xi^{k+1} - \eta^{k+1}| &\le h|z_g(\eta^k) - z_g(\xi^k)| \\
&\le h(\lambda K_2 + B_1(1 + haK_2))|\xi^k - \eta^k| \\
&= c|\xi^k - \eta^k|
\end{aligned}$$

which is a contraction by (37). ■

Proof [of Lemma 14.] Let $g \in \Gamma$ and $p \in \mathbb{R}^d$ then by Lemma 13 there is a unique $\xi \in \mathbb{R}^d$ such that (27) is satisfied. Then

$$\begin{aligned}
|(Tg)(p)| &\le \lambda |g(\xi)| + a|I_g^{(1)}(\xi)| + \tilde{\lambda}|I_g^{(2)}(\xi)| \\
&\le \lambda\gamma + aB_1(\tilde{\lambda}B_0 + h\gamma) + \tilde{\lambda}B_1(\lambda(\tilde{\lambda}B_0 + h\gamma) + B_0) \\
&= (\lambda + hB_1(a + \lambda\tilde{\lambda}))\gamma + \tilde{\lambda}B_0B_1(a + \tilde{\lambda}) \\
&\le \gamma
\end{aligned}$$

with the last inequality following from (34).

Let $p_1, p_2 \in \mathbb{R}^d$ then, by Lemma 13, there exist $\xi_1, \xi_2 \in \mathbb{R}^d$ such that (27) is satisfied with $p = \{p_1, p_2\}$. Hence, by Lemma 12,

$$\begin{aligned}
|(Tg)(p_1) - (Tg)(p_2)| &\le \lambda|g(\xi_1) - g(\xi_2)| + a|I_g^{(1)}(\xi_1) - I_g^{(1)}(\xi_2)| + \tilde{\lambda}|I_g^{(2)}(\xi_1) - I_g^{(2)}(\xi_2)| \\
&\le K|\xi_1 - \xi_2|
\end{aligned}$$

where we define

$$K \coloneqq \lambda\delta + a(B_1K_2 + B_2K_1(1 + haK_2)) + \tilde{\lambda}((B_1 + hB_2K_3)(\lambda K_2 + B_1(1 + haK_2)) + B_2K_3).$$

Now, using (27) and the proof of Lemma 13,

$$\begin{aligned}
|\xi_1 - \xi_2| &\le |p_1 - p_2| + h|z_g(\xi_1) - z_g(\xi_2)| \\
&\le |p_1 - p_2| + c|\xi_1 - \xi_2|.
\end{aligned}$$

Since $c < 1$ by (37), we obtain

$$|\xi_1 - \xi_2| \le \frac{1}{1-c}|p_1 - p_2|$$

thus

$$|(Tg)(p_1) - (Tg)(p_2)| \le \frac{K}{1-c}|p_1 - p_2| \le \delta|p_1 - p_2|.$$

To see the last inequality, we note that

$$\frac{K}{1-c} \le \delta \iff K - \delta(1-c) \le 0$$

and $K - \delta(1-c) = \alpha_2\delta^2 + \alpha_1\delta + \alpha_0$ by (35) hence (36) gives the desired result. ■

Proof [of Lemma 15.] By Lemma 13, for any $p \in \mathbb{R}^d$ and $g_1, g_2 \in \Gamma$, there are $\xi_1, \xi_2 \in \mathbb{R}^d$ such that

$$\begin{aligned}
p &= \xi_j + hz_{g_j}(\xi_j) \\
(Tg_j)(p) &= \lambda g_j(\xi_j) + aI_{g_j}^{(1)}(\xi_j) - \tilde{\lambda}I_{g_j}^{(2)}(\xi_j)
\end{aligned}$$

for $j = 1, 2$. Then

$$|(Tg_1)(p) - (Tg_2)(p)| \leq \lambda |g_1(\xi_1) - g_2(\xi_2)| + a|I^{(1)}_{g_1}(\xi_1) - I^{(1)}_{g_2}(\xi_2)| + \tilde{\lambda}|I^{(2)}_{g_1}(\xi_1) - I^{(2)}_{g_2}(\xi_2)|.$$

Note that

$$\begin{aligned} |g_1(\xi_1) - g_2(\xi_2)| &= |g_1(\xi_1) - g_2(\xi_2) - g_2(\xi_1) + g_2(\xi_1)| \\ &\leq |g_1(\xi_1) - g_2(\xi_1)| + \delta|\xi_1 - \xi_2|. \end{aligned}$$

Similarly, by Lemma 12,

$$\begin{aligned} |I^{(1)}_{g_1}(\xi_1) - I^{(1)}_{g_2}(\xi_2)| &= |I^{(1)}_{g_1}(\xi_1) - I^{(1)}_{g_2}(\xi_2) - I^{(1)}_{g_2}(\xi_1) + I^{(1)}_{g_2}(\xi_1)| \\ &\leq |I^{(1)}_{g_1}(\xi_1) - I^{(1)}_{g_2}(\xi_1)| + |I^{(1)}_{g_2}(\xi_1) - I^{(1)}_{g_2}(\xi_2)| \\ &\leq h(B_1 + haB_2K_1)|g_1(\xi_1) - g_2(\xi_1)| + (B_1K_2 + B_2K_1(1 + haK_2))|\xi_1 - \xi_2| \end{aligned}$$

Finally,

$$\begin{aligned} |I^{(2)}_{g_1}(\xi_1) - I^{(2)}_{g_2}(\xi_2)| &= |I^{(2)}_{g_1}(\xi_1) - I^{(2)}_{g_2}(\xi_2) - I^{(2)}_{g_2}(\xi_1) + I^{(2)}_{g_2}(\xi_1)| \\ &\leq |I^{(2)}_{g_1}(\xi_1) - I^{(2)}_{g_2}(\xi_1)| + |I^{(2)}_{g_2}(\xi_1) - I^{(2)}_{g_2}(\xi_2)| \\ &\leq h(\lambda + hB_1a)(B_1 + hB_2K_3)|g_1(\xi_1) - g_2(\xi_1)| + \\ &\quad + ((B_1 + hB_2K_3)(\lambda K_2 + B_1(1 + haK_2)) + B_2K_3)|\xi_1 - \xi_2| \end{aligned}$$

Putting these together and using (38), we obtain

$$|(Tg_1)(p) - (Tg_2)(p)| \leq (\lambda + Q_2)|g_1(\xi_1) - g_2(\xi_1)| + Q_1|\xi_1 - \xi_2|.$$

Now, by Lemma 12,

$$\begin{aligned} |\xi_1 - \xi_2| &\leq h|z_{g_1}(\xi_1) - z_{g_2}(\xi_2) - z_{g_2}(\xi_1) + z_{g_2}(\xi_1)| \\ &\leq h(|z_{g_1}(\xi_1) - z_{g_2}(\xi_1)| + |z_{g_2}(\xi_1) - z_{g_2}(\xi_2)|) \\ &\leq h^2(\lambda + haB_1)|g_1(\xi) - g_2(\xi_1)| + h(\lambda K_2 + B_1(1 + haK_2))|\xi_1 - \xi_2| \\ &= h^2(\lambda + haB_1)|g_1(\xi) - g_2(\xi_1)| + Q_3|\xi_1 - \xi_2| \end{aligned}$$

using (38). Since, by (39), $Q_3 < 1$, we obtain

$$|\xi_1 - \xi_2| \leq \frac{h^2(\lambda + haB_1)}{1 - Q_3}|g_1(\xi_1) - g_2(\xi_1)|$$

and thus

$$\begin{aligned} |(Tg_1)(p) - (Tg_2)(p)| &\leq \left(\lambda + Q_2 + \frac{h^2(\lambda + haB_1)Q_1}{1 - Q_3}\right)|g_1(\xi_1) - g_2(\xi_1)| \\ &= \mu|g_1(\xi_1) - g_2(\xi_1)| \end{aligned}$$

by (38). Taking the supremum over ξ_1 then over p gives the desired result. Since $\mu < 1$ by (39), we obtain that T is a contraction on Γ. ■

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