A Theoretical Framework for Backward Error Analysis on Manifolds

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The Problem

Let $\mathcal{M}$ be a smooth manifold and let $X \in \mathfrak{X}(\mathcal{M})$ be a smooth vector field with flow map θ_t i.e.

$$\frac{d}{dt}\theta_t(p) = X_{\theta_t(p)}.$$

Let Φ_h be a numerical integrator for X i.e. Φ_h is a one-parameter family of diffeomorphisms that is smooth in h, $\Phi_0 = id$ and $\frac{d}{dh}\Big|_{h=0}\Phi_h = X$.

- Find a vector field $\widetilde{X}$ such that the flow map $\tilde{\theta}_t$ of $\widetilde{X}$ is close to the numerical solution i.e. $d(\tilde{\theta}_h(p), \Phi_h(p))$ is small for some metric d on $\mathcal{M}$.
- Determine the geometric properties of $\widetilde{X}$ from the geometric properties of Φ_h.

The Estimates

Theorem 1 *(ACH) Let $X \in \mathfrak{X}(\mathcal{M})$ and let Φ_h be a consistent integrator for X and suppose $K \subset \mathcal{M}$ is a compact and connected subset. Then,*

(i) for sufficiently small $h > 0$ there exists a family of smooth vector fields $\{X_i\}$ on $\mathcal{U}$, an open set containing K, such that for $\tilde{X}_N(h) = X_0 + hX_1 + \ldots h^N X_N$ we have

$$d(\tilde{\theta}_h(p), \Phi_h(p)) \leq C_N h^N, \qquad p \in K, \quad C_N > 0,$$

where $\tilde{\theta}_h$ is the flow map of $\tilde{X}_N(h)$ and d is some metric on $\mathcal{M}$.

(ii) if $\mathcal{M}$, X and Φ_h are analytic. Then for sufficiently small $h > 0$ there exists an analytic vector field $\tilde{X}(h)$ and $C, \gamma > 0$ such that

$$d(\Phi_h(p), \tilde{\theta}_h(p)) \leq Che^{-\gamma/h}$$

for all $p \in K$.

Preliminaries

If $\varphi : \mathcal{M} \to \mathcal{M}$ is smooth and τ is a covariant tensor field then the pull-back $\varphi^* \tau$ is given by

$$(\varphi^* \tau)_p (X_1, \ldots, X_n) = \tau_{\varphi(p)} (\varphi_* X_1, \ldots, \varphi_* X_n), \quad X_1, \ldots, X_n \in T_p \mathcal{M}.$$

Let $X \in \mathfrak{X}(\mathcal{M})$ and τ a covariant tensor field on $\mathcal{M}$. The Lie derivative of τ with respect to X is given by

$$(\mathcal{L}_X \tau)_p = \lim_{t \to 0} \frac{\theta_t^* (\tau_{\theta_t(p)}) - \tau_p}{t},$$

where θ_t is the flow map of X.

By a $k-$form we mean a smooth covariant alternating k-tensor field on $\mathcal{M}$. The set of k-forms is denoted by $\Omega^k(\mathcal{M})$.

Cartan's Subgroups

- *Diff*$(\mathcal{M})$, the group of all diffeomorphisms on $\mathcal{M}$.
- The diffeomorphisms preserving a symplectic 2-form ω on $\mathcal{M}$, that is the set of diffeomorphisms φ such that $\varphi^*\omega = \omega$.
- The diffeomorphisms preserving a volume form μ on $\mathcal{M}$, that is the set of diffeomorphisms φ such that $\varphi^*\mu = \mu$.
- The diffeomorphisms preserving a given contact 1-form α up to a scalar function, that is the set of diffeomorphisms φ such that $(\varphi^*\alpha)_p = c_\varphi(p)\alpha_p$.
- The group of diffeomorphisms preserving a given symplectic form ω up to an arbitrary constant multiple, that is the set of diffeomorphisms φ such that $\varphi^*\omega = c_\varphi\omega$.
- The group of diffeomorphisms preserving a given volume form μ up to an arbitrary constant multiple, that is the set of diffeomorphisms φ such that $\varphi^*\omega = c_\varphi\omega$.

Diff$(\mathcal{M})$ as a Lie group

Recall that $T_{id}\text{Diff}(\mathcal{M}) = \mathfrak{X}(\mathcal{M})$ i.e.

$$T_{id}\text{Diff}(\mathcal{M}) = \left\{ \frac{d}{dt}\Big|_{t=0} \theta_t : \theta_t \text{ is a flow map} \right\}.$$

Note that

$$T_{id}\text{Diff}(\mathcal{M}) = \left\{ \frac{d}{dt}\Big|_{t=0} \Phi_t : \Phi_t \text{ is a one parameter family} \right\}.$$

Definition 2 *Let $S \subset$ Diff$(\mathcal{M})$ be a set of smooth one parameter families of diffeomorphisms. Define*

$$T_{id}S = \{X \in \mathfrak{X}(\mathcal{M}) : X = \frac{d}{dt}\Big|_{t=0} \Phi_t,\ \Phi_t \in S\},$$

where $T_{id}S$ will be called the tangent space at the identity.

Subsets of $\text{Diff}(\mathcal{M})$	Subsets of $\mathfrak{X}(\mathcal{M})$
Let $\omega \in \Omega^2(\mathcal{M})$ be symplectic. $\{\varphi \in \text{Diff}(\mathcal{M}) : \varphi^*\omega = \omega\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = 0\}$
$\{\varphi \in \text{Diff}(\mathcal{M}) : \varphi^*\omega = c_\varphi\omega\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = \beta_X\omega\}$
Let $\mu \in \Omega^n(\mathcal{M})$ be a volume form. $\{\varphi \in \text{Diff}(\mathcal{M}) : \varphi^*\mu = \mu\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\mu = 0\}$
$\{\varphi \in \text{Diff}(\mathcal{M}) : \varphi^*\mu = c_\varphi\mu\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\mu = \beta_X\mu\}$
Let $\alpha \in \Omega^1(\mathcal{M})$ be a contact form. $\{\varphi \in \text{Diff}(\mathcal{M}) : (\varphi^*\alpha)_p = c_\varphi(p)\alpha_p\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : (\mathcal{L}_X\alpha)_p = \beta_X(p)\alpha_p\}$
Let $f \in C^\infty(\mathcal{M})$. $\{\varphi \in \text{Diff}(\mathcal{M}) : f \circ \varphi = f\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : f_*X = 0\}$
Let $\sigma : \text{Diff}(\mathcal{M}) \longrightarrow \text{Diff}(\mathcal{M})$ be smooth. $\{\varphi \in \text{Diff}(\mathcal{M}) : \sigma(\varphi) = \varphi^{-1}\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \sigma_*X = -X\}$

Theorem 3 *(ACH) Suppose that* $X \in A \subset \mathfrak{X}(\mathcal{M})$ *where* A *is a linear subspace. Let* $S \subset \text{Diff}(\mathcal{M})$ *be a set of smooth one parameter families of diffeomorphisms such that* S *is a semi group and that* $A = T_{id}S$*. Let* Φ_h *be an integrator for* X *and suppose also that* $\Phi_h \in S$*. Then the perturbed vector field* $\widetilde{X}(h) \in A$*.*

WARNING!!!

Note that if $A = T_{id}S$ there may exist $\tilde{S}$ such that $S \neq \tilde{S}$ and $A = T_{id}\tilde{S}$. The reason is that $\exp : \mathfrak{X}(\mathcal{M}) \to \text{Diff}(\mathcal{M})$ is not locally onto.

Example: Let ω be a symplectic 2-form on $\mathcal{M}$. Let
$A = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X \omega = 0\}$ and
$S = \{\varphi_t \in \text{Diff}(\mathcal{M}) : \varphi_t^* \omega = \omega, \varphi_t \text{ is a flowmap}\}$. Then $A = T_{id}S$.

Let $X \in A$ and let the integrator Φ_h be Euler's method applied to X and let $\tilde{S} = S \cup \Phi_h$. By consistency

$$\frac{d}{dh}\Big|_{h=0} \Phi_h = X.$$

Hence $T_{id}\tilde{S} = A$.

The Lie derivative

Note that the previous example shows that the set S in Theorem 3 must have some structure, for if we relax the semi-group hypothesis in Theorem 3 and require S only to be a set then $\tilde{S}$ is a set and $T_{id}\tilde{S} = A$ so the perturbed vector field of Euler's method would be symplectic, a contradiction.

Proposition 4 *Let Φ_t be a one parameter family of diffeomorphisms that is smooth in t and satisfies $\Phi_0 = id$. Suppose that $X \in \mathfrak{X}(\mathcal{M})$ and $\frac{d}{dt}\Big|_{t=0}\Phi_t = X$. Let τ be a smooth covariant k-tensor field. Then*

$$(\mathcal{L}_X \tau)_p = \lim_{t\to 0} \frac{\Phi_t^*\left(\tau_{\Phi_t(p)}\right) - \tau_p}{t}.$$

Corollary 5 *Let* $\tau \in \Omega^k(\mathcal{M})$ *be a smooth* k*-form. Let*

$$S_1 = \{\Phi_t : \Phi_t^* \tau = \tau\}$$

$$S_2 = \{\Phi_t : \Phi_t^* \tau = c_\Phi(t)\tau,\ c_\Phi \in C^\infty(\mathbb{R})\}$$

$$S_3 = \{\Phi_t : (\Phi_t^* \tau)_p = c_\Phi(t,p)\tau_p,\ c_\Phi \in C^\infty(\mathbb{R}, \mathcal{M})\}.$$

Also, let

$$A_1 = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X \tau = 0\}$$

$$A_2 = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X \tau = \alpha_X \tau,\ \alpha_X \text{ constant}\}$$

$$A_3 = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X \tau = \alpha_X \tau,\ \alpha_X \in C^\infty(\mathcal{M})\}.$$

Then $T_{id}S_1 = A_1, T_{id}S_2 = A_2$ *and* $T_{id}S_3 = A_3$

Corollary 6 *Let* $X \in \mathfrak{X}(\mathcal{M})$ *and* $\tau \in \Omega^k(\mathcal{M})$. *Let* Φ_h *be a numerical integrator for* X.

(i) *If* $\mathcal{L}_X\tau = 0$ *and* $\Phi_h^*\tau = \tau$, *then the perturbed vector field* $\tilde{X}(h)$ *satisfies* $\mathcal{L}_{\tilde{X}}\tau = 0$.

(ii) *If* $\mathcal{L}_X\tau = \alpha_X\tau$ *and* $\Phi_h^*\tau = c_\Phi(h)\tau$, *where* α_X *is constant and* c_Φ *is smooth, then the perturbed vector field* $\tilde{X}(h)$ *satisfies* $\mathcal{L}_{\tilde{X}}\tau = \alpha_{\tilde{X}}\tau$.

(iii) *If* $\mathcal{L}_X\tau = \alpha_X\tau$ *where* $\alpha_X \in C^\infty(\mathcal{M})$ *and* $(\Phi_h^*\tau)_p = c_\Phi(h,p)\tau_p, c_\Phi \in C^\infty(\mathbb{R}\times\mathcal{M})\}$, *then the perturbed vector field* $\tilde{X}(h)$ *satisfies* $\mathcal{L}_{\tilde{X}}\tau = \alpha_{\tilde{X}}\tau$ *where* $\alpha_X \in C^\infty(\mathcal{M})$.

Theorem 7 *(ACH) Let $X \in \mathfrak{X}(\mathcal{M})$ with corresponding flow map θ_t, and let Φ_h be a numerical integrator for X with corresponding perturbed vector field $\widetilde{X}(h)$ and flow map $\tilde{\theta}_t$. Then*

(i) if ω is a symplectic 2-form on $\mathcal{M}$ such that $\theta_t^* \omega = \omega$ and $\Phi_h^* \omega = \omega$ then the perturbed vector field $\tilde{X}(h)$ is symplectic e.g. it satisfies $\mathcal{L}_{\tilde{X}(h)} \omega = 0$, and $\tilde{\theta}_t^* \omega = \omega$.

(ii) if μ is a volume form on $\mathcal{M}$ such that $\theta_t^* \mu = \mu$ and $\Phi_h^* \mu = \mu$ then the perturbed vector field $\tilde{X}(h)$ is divergence free e.g. it satisfies div $\tilde{X}(h) = 0$, and $\tilde{\theta}_t^* \mu = \mu$.

(iii) if ω is a symplectic 2-form on $\mathcal{M}$ such that $\theta_t^* \omega = \alpha(t) \omega$ and $\Phi_h^* \omega = \beta(h) \omega$, where $\alpha, \beta : \mathbb{R} \to \mathbb{R}$ are smooth, then the perturbed vector field $\tilde{X}(h)$ satisfies $\mathcal{L}_{\tilde{X}(h)} \omega = \rho \omega$, where ρ is a real constant and $\tilde{\theta}_t^* \omega = \tilde{\alpha}(t) \omega$, where $\tilde{\alpha}$ is smooth.

(iv) if μ is a volume form on $\mathcal{M}$ such that $\theta_t^*\mu = \alpha(t)\mu$ and $\Phi_h^*\mu = \beta(h)\mu$, where $\alpha, \beta : \mathbb{R} \to \mathbb{R}$ are smooth, then the perturbed vector field $\tilde{X}(h)$ satisfies $\mathcal{L}_{\tilde{X}(h)}\mu = \rho\mu$, where ρ is a real constant and $\tilde{\theta}_t^*\mu = \tilde{\alpha}(t)\mu$, where $\tilde{\alpha}$ is smooth.

(v) if τ is a contact 1-form on $\mathcal{M}$ such that $(\theta_t^*\tau)_p = \alpha(t,p)\tau_p$ and $(\Phi_h^*\tau)_p = \beta(h,p)\tau_p$, where $\alpha, \beta \in C^\infty(\mathbb{R} \times \mathcal{M})$ then the perturbed vector field $\tilde{X}(h)$ satisfies $\mathcal{L}_{\tilde{X}(h)}\tau = \rho\tau$, where $\rho \in C^\infty(\mathcal{M})$ and $\tilde{(}\theta_t^*\tau)_p = \tilde{\alpha}(t,p)\tau_p$, where $\alpha \in C^\infty(\mathbb{R} \times \mathcal{M})$.

(vi) if $f : \mathcal{M} \to \mathbb{R}$ is a smooth function such that $f_*X = 0$ and $f \circ \Phi_h = f$. Then the perturbed vector field $\tilde{X}(h)$ satisfies $f_*\tilde{X}(h) = 0$ and $f \circ \tilde{\theta}_t = f$.

Smooth homomorphisms and their anti fixed points

Theorem 8 *(ACH) Let* $\mathcal{M}$ *be a compact manifold. Let* $X \in \mathfrak{X}(\mathcal{M})$ *with corresponding flow map* θ_t *and let* Φ_h *be a numerical integrator for* X*. Let* $\sigma : \textit{Diff}(\mathcal{M}) \to \textit{Diff}(\mathcal{M})$ *be a smooth homomorphism and define*

$$A = \{X \in \mathfrak{X}(\mathcal{M}) : \sigma_* X = -X\}, \quad S = \{\varphi \in \textit{Diff}(\mathcal{M}) : \sigma(\varphi) = \varphi^{-1}\}.$$

Suppose that $\theta_t \in S$*. If* $\Phi_h \in S$ *then the perturbed vector field* $\widetilde{X}(h) \in A$ *and* $\tilde{\theta}_t \in S$*, where* $\tilde{\theta}_t$ *is the flow map of* $\widetilde{X}(h)$*.*

Let $\rho : \mathcal{M} \to \mathcal{M}$ be a diffeomorphism. Denote the mapping $\Psi \mapsto \rho \circ \Psi \circ \rho^{-1}$ by σ. Note that this is a homomorphism on $\mathrm{Diff}(\mathcal{M})$, since $\sigma(\Psi \circ \Phi) = \sigma(\Psi) \circ \sigma(\Phi)$.

Theorem 9 *(ACH) Let $\mathcal{M}$ be a compact manifold. Let $X \in \mathfrak{X}(\mathcal{M})$ and let Φ_t be a numerical integrator for X. Suppose that σ is defined as above and that*

$$\sigma(\theta_{X,h}) = \theta_{X,h}^{-1} \quad \text{and} \quad \sigma(\Phi_h) = \Phi_h^{-1}$$

then the perturbed vector field $\tilde{X}(h)$ of Φ_h satisfies $\sigma_* \tilde{X}(h) = -\tilde{X}(h)$ and $\sigma(\tilde{\theta}_{X,t}) = \tilde{\theta}_{X,t}^{-1}$, where $\tilde{\theta}$ is the flow of $\tilde{X}(h)$.

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