Summary - Towards a Geometric Theory of Exact Lumpability

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Overview

In this thesis we develop a framework and study aspects of *exact lumpability* of smooth vector fields on smooth manifolds. The concept of exact lumpability, a notion mostly used in the reaction kinetics context, is concerned with the dimensional reduction of an evolution equation by means of a map that induces a unique dynamics on the target space.

Our main objectives are the development of a geometric framework for the theory of exact lumpability, its characterisation within that framework, the investigation of its relation to first integrals and the action of Lie groups, the discussion of some dynamical properties preserved under exact lumpings, the study of local lumpings generated by the flow and finally the introduction and investigation of closure measures that quantify the deviation from exactness. Some of the results have been published in [HA16] together with Fatihcan Atay.

Characterisation of Exact Lumpability

In this thesis we consider a setting, where the dynamics is defined by smooth vector fields on smooth manifolds. The lumping maps are taken to be smooth surjective submersions onto strictly lower dimensional target manifolds. We define the notion of exact lumpability in this context as follows:

Definition 1 (Exact Smooth Lumpability)**.** *Let X, Y be smooth manifolds with* $\dim X > \dim Y > 0$. *The system*

$$\frac{d}{dt}\Big|_{t=s} \Phi = v \circ \Phi_s \tag{1}$$

is called exactly smoothly lumpable (henceforth exactly lumpable) by $\pi : X \to Y$ iff there exists a smooth vector field $\tilde{v} \in \Gamma(Y, TY)$ such that the dynamics of $\Theta = \pi \circ \Phi$ is governed by

$$\frac{d}{dt}\Big|_{t=s} \Theta = \tilde{v} \circ \Theta_s \; . \tag{2}$$

We first ask about necessary and sufficient conditions for v to be exactly lumpable by π. We phrase our conditions in the framework of smooth tangent space distributions, which in our context are collections of subspaces of the tangent spaces that are spanned by locally defined smooth vector fields. One central object of our study is the *vertical distribution*, given by $\ker D\pi$.

If v is exactly lumpable by π, then local sections of $\ker D\pi$ are invariant under the Lie derivative $\mathcal{L}_v$. This is a result that confirms the intuition and we use the identity $D\pi[v, w]^a = v[(D\pi w)^a] - w[(D\pi v)^a]$ together with $w \in \ker D\pi$ and the assumption of exact lumpability to demonstrate it. The proof of the reverse direction motivates the introduction of several objects that are cursorily described in the following.

For real valued maps π the action of the Lie derivative on a pairing $\langle d\pi, w\rangle$ is $\mathcal{L}_v\langle d\pi, w\rangle = \langle \mathcal{L}_v d\pi, w\rangle + \langle d\pi, \mathcal{L}_v w\rangle$. For manifold maps this is in general not true, but with the definition of the covariant directional derivative of $D\pi$ the analogy can be made more precise. We define the derivative via its action on a test vector field w:

$$\left(\mathcal{L}_v^{\nabla} D\pi\right)\, w := \nabla_{\frac{\partial}{\partial t}}\, D(\pi \circ \Phi)\, \circ \iota(w)\Big|_{t=0}\,, \tag{3}$$

where ∇ is a Koszul connection, Φ is the flow generated by v and ι is a linear embedding of the vector field w into the appropriate space.

When one chooses ∇ to be a tensor product connection of the dual and the pullback of a torsion-free connection, respectively, then we can show that $(\, \mathcal{L}_v^{\nabla} D\pi\,)\, w = (\pi^*\bar{\nabla})_w(D\pi v)$, where $\pi^*\bar{\nabla}$ is the pullback of a torsion-free connection $\bar{\nabla}$ on TY. Therefore the analogous relation $(\pi^*\bar{\nabla})_v D\pi w = \left(\mathcal{L}_v^{\nabla} D\pi\right) w + D\pi \mathcal{L}_v w$ holds for manifold maps π. Moreover it can be seen that $\mathcal{L}_v^{\nabla} D\pi : TX \to \pi^{-1}TY$ is a vector bundle homomorphism and $\ker \mathcal{L}_v^{\nabla} D\pi$ is a smooth distribution. Its relation to exact lumpability is summarised in Theorem 1.

Another object that we introduce is a partial connection $\mathring{\nabla}^L$ on the pullback bundle $T^{-1}TY$. Its tensorial part is only defined for vectors $w \in \ker D\pi$ via:

$$\tilde{v} \mapsto \mathring{\nabla}^L_w \tilde{v} := D\pi[w, v] \tag{4}$$

such that $\tilde{v} = D\pi v$. This turns out to satisfy the requirements of a connection. We show that $\mathring{\nabla}^L$ vanishes on the pushforward of exactly lumpable vector fields (Theorem 1). We also show that it is related to the Bott connection $\mathring{\nabla}^B$ via the isomorphism $\varphi : \pi^{-1}TY \to TX/\ker D\pi$, namely $\varphi \circ \mathring{\nabla}^L = \mathring{\nabla}^B \circ \varphi$. The Bott connection is also a partial connection and plays a role in proving a topological obstruction theorem for a distribution to be homotopy equivalent to an integrable distribution.

Last but not least we introduce an object that extends the observability matrix from control theory to manifold vanlued observables and allows us to prove a manifold version of Coxson's theorem, the one that relates lumpability and observability for linear systems. We define

$$s \mapsto \mathcal{O}_2(s) := D\pi s \oplus (\mathcal{L}_v^{\nabla} D\pi)s \tag{5}$$

as the 2-Observability map and show that $\operatorname{rank} \mathcal{O}_2 = \operatorname{rank} D\pi$ iff v is exactly lumpable by π.

Theorem 1. *A vector field v is exactly lumpable by π if and only if*

1. $\Gamma_{loc}(X, \ker D\pi)$ *is invariant under* $\mathcal{L}_v$,
2. $\ker D\pi$ *is invariant under the flow of* v,
3. $\ker D\pi \subseteq \ker \mathcal{L}_v^{\nabla} D\pi$,
4. $\mathring{\nabla}^L D\pi\, v \equiv 0$,
5. *The rank of the 2-Observability map* $\mathcal{O}_2 = \binom{D\pi}{\mathcal{L}_v^{\nabla} D\pi}$ *equals the rank of* $D\pi$,
6. *Locally* $\bigwedge_{b=1}^m (D\pi)^b \wedge d\,(D\pi v)^a = 0 \qquad \forall\, a$,

for ∇ *as above.*

Aspects of Exact Lumpability

First integrals can be viewed as a special case of exact lumpings. Both are concerned with integrable distributions that are invariant under the flow of a vector field, with the only differentce that the latter has to be a section of the integrable distribution in the case of first integrals. This is discussed.

This begs the question whether symmetries are related to exact lumpings, in a similar way as for first integrals as detailed in Noether's theorem for Lagrangian dynamics. Sometimes Lie group symmetries give rise to exact lumpings and vice versa. We establish conditions in this direction for the types of Lie group actions. We say a Lie group action is v-compatible if v is closed under the action of the corresponding Lie algebra.

Theorem 2. *If there exists a Lie group with a proper and v-compatible action all of whose orbits have the same orbit type, then v is exactly lumpable by π and $\pi : X \to Y$ is a fiber bundle whose typical fiber is a homogeneous space.*

Theorem 3. *If $\pi : X \to Y$ is a fiber bundle whose typical fiber is a homogeneous space with compact isotropy group, then there exists a Lie group with a proper and v-compatible action all of whose orbits have the same orbit type.*

We investigate and illustrate the lumping phenomenon via Lie group actions. The first example concerns quaternion rotations on the 3-sphere and their projection to the 2-sphere. The second example deals with the geodesic flow on the tangent bundle of the 2-sphere.

Proposition 1. *Quaternion rotations $t \mapsto e^{tc} \star x$ on S^3 are exactly lumpable for the Hopf fibration $\pi : S^3 \to S^2$. Here $\star$ is the quaternion product and c is a pure quaternion (no real part). The lumped dynamics on S^2 is $\tilde{v}(y) = 2c \times y$.*

Proposition 2. *The geodesic flow on the unit tangent bundle of the sphere is lumpable to the sphere, not by mere projection, but via $s \mapsto (x, v) \mapsto x \times v$, where the first map is the embedding of $US^2 \hookrightarrow \mathbb{R}^3 \times \mathbb{R}^3$.*

For real-valued observables the theoretical chemists Tomlin, Li, Rabitz and Tóth have shown that exact lumpings preserve invariant sets, periodic solutions (allowing for constant solutions) and blowup solutions. We extend these results to manifold valued observables.

Finally we investigate local lumpings that are generated by the flow of hypersurfaces. We also introduce the notion of admissibility which guarantees nonintersection of the surfaces.

Theorem 4. *Let U_0 be a embedded hypersurface of X and a fibered manifold over a base B_0:*

$$B_0 \xleftarrow{\pi_0} U_0 \hookrightarrow X \ . \tag{6}$$

If U_0 is transverse to Φ, then there exists a fibered manifold $\pi : X_{\mathcal{T}} \to B_0 \times \mathcal{T}$, where $X_{\mathcal{T}} = \bigcup_{t \in \mathcal{T}} \Phi_t(U_0)$ and $\mathcal{T}$ is an admissible subset of $\mathbb{R}$. Furthermore v is exactly lumpable by π.

Closure Measures

How can one measure the deviation from exact lumpability, other than simply stating that something is or is not an exact lumping. We propose a definition for a closure measure, which captures this idea, and afterwards we put forward several measures which we demonstrate to be closure measures.

Definition 2 (Closure Measure). *Let X be a differentiable manifold and $\sigma(X)$ a sigma algebra on X. A real-valued functional $\mathfrak{C} : \mathcal{C}^\infty(X, Y) \times \mathfrak{X}(X) \times \sigma(X) \to \mathbb{R}_0^+$ is a closure measure if $\mathfrak{C}(\pi, v, \Omega) \geq 0$ for any π, v and Ω, but $\mathfrak{C}(\pi, v, \Omega) = 0$ if and only if v is exactly lumpable by π on the domain Ω.*

Suppose X and Y are endowed with Riemannian metrics g and $\tilde{g}$, then in particular they can be given the structure of a metric space with the distance δ on Y being given by the geodesic distance. One could consider a flow Ψ along the fibers and ask how the distance $\delta\Big(\pi \circ \Phi_t(x) \;\; , \;\; \pi \circ \Phi_t \circ \Psi_s(x)\Big)$ between nearby points x and $\Psi_s(x)$ on the fiber change after an evolution for time t and a subsequent projection by π. For exact lumpings this distance should vanish, but it should increase with t and s for other maps. So taking the derivative of that object in (s, t) from the positive side yields $\sqrt{\tilde{g}_{\pi(x)}\Big(\nabla_w(D\pi v)(x), \nabla_w(D\pi v)(x)\Big)}$, where $w = \frac{d}{ds}_0 \Psi_s \in \ker D\pi$. The supremum of this object along all fiber directions, averaged over Ω

$$\mathfrak{C}_{rod}(v, \pi, \Omega) := \frac{1}{|\Omega|} \int_\Omega dx \sup_{w \in \ker D\pi_x \, , \, ||w||_g = 1} \sqrt{\tilde{g}_{\pi(x)}\Big(\nabla_w D\pi v(x), \nabla_w D\pi v(x)\Big)} \tag{7}$$

is shown to be a closure measure, which we call the rate-of-divergence closure measure. We illustrate this measure for the truncation of moment equations in stochastic modeling.

We recall that v is exactly lumpable by π if and only if $\ker D\pi \subseteq \ker \mathcal{L}_v^\nabla D\pi$. Another closure measure can be obtained from this condition. We propose to measure the distance between the subspaces $\ker D\pi_x$ and $\ker \mathcal{L}_v^\nabla D\pi(x)$ pointwise and then average over all $x \in \Omega$. A convenient way to measure distances of vector spcaces of potentially different dimension involves a Grassmannian formulation and can be found in the work of Ye and Lim [YLH14]. Upon calling this 'distance' Δ we show that

$$\mathfrak{C}_{Gr}(\pi, v, \Omega) := \frac{1}{|\Omega|} \int_\Omega dx \; \Delta \left(\ker D\pi_x \, , \, \ker \mathcal{L}_v^{\bar{\nabla}} D\pi\right)(x) \tag{8}$$

is a veritable closure meausre.

References

[HA16] L. Horstmeyer and F. Atay. Characterisation of exact lumpability for vector fields on smooth manifolds. *Differ. Geom. Appl.*, 48, 2016.

[YLH14] K. Ye and Lim L.-H. Schubert varieties and distances between subspaces of different dimensions. *arXiv:1407.0900v3*, 2014.