Geometric Data Science

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1 Introduction

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Geometric data analysis

Geometric data, e.g. in the form of curves, surfaces, diffeomorphisms, tensors, or graphs, arise naturally in computational anatomy, brain connectivity, molecular biology, meteorology, oceanology, online navigation, social networks, and finance. Geometric datasets are increasingly publicly available, e.g. in the ADNI, HCP, and Baby connectome databases or the MPII, McGill, and CASEAR databases of human bodies. Moreover, in everyday-life applications, depth-enhanced image data is produced by time-of-flight sensors in cars, game consoles, and recently also cell phone cameras.

Figure 1.1: Geometric data arises in a variety of applications.
The configuration spaces of curves, surfaces, graphs, etc. are infinite-dimensional non-linear manifolds or stratified spaces. For example, for fixed manifolds $M$ and $N$, one may consider the space of embeddings $f: M \to N$. For any diffeomorphism $\varphi$ on $M$, the embeddings $f$ and $f \circ \varphi$ represent the same shape as they differ only by a reparameterization. Accordingly, shape space is defined as the quotient space of embeddings modulo reparameterizations. Alternatively, shapes may be encoded as diffeomorphic deformations $f = \varphi \circ f_0$ of a fixed template shape $f_0: M \to N$. This leads to the (loosely equivalent) definition of shapes as diffeomorphisms $\varphi: N \to N$ modulo the stabilizer of $f_0$.

Figure 1.2: Left: Different embeddings, same shape (mesh independence) [6]. Right: infinitesimal shape deformations corresponding to shape encodings as functions $M \to N$ or diffeomorphisms $N \to N$.

Either way, shape space is a genuine infinite-dimensional manifold even if $N$ is Euclidean. For this reason, the analysis of geometric data is a major challenge: statistics, stochastics, and machine learning have to be generalized to non-Euclidean and potentially infinite-dimensional spaces.

**Fluid dynamics**

Fluid dynamics is a collective term for hydrodynamics, aerodynamics, geodynamics, hydraulics, plasma physics, etc. There are applications in a variety of fields, including climate and ocean science, and these are of particular relevance for understanding the present rapid changes of our planet Earth.
Mathematically, fluid dynamics can be modeled via evolution equations on diffeomorphism groups: at every instant of time, the diffeomorphism encodes the current positions of all fluid particles relative to their initial position. It is commonly assumed that the dynamics are uniquely determined by the initial position and velocity of the fluid. This implies that the configuration space of fluid dynamics is (the tangent space of) a diffeomorphism group. Moreover, by physical principles, the dynamics are critical points of some energy functional on this space. In many cases, this energy functional is the geodesic distance of a Riemannian metric on the diffeomorphism group. Accordingly, the dynamics are then given by a geodesic equation. Many important fluid-dynamic equations can be understood in this way.

<table>
<thead>
<tr>
<th>Space</th>
<th>Riemannian metric</th>
<th>Geodesic equation</th>
</tr>
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<tbody>
<tr>
<td>$\text{Diff}_\mu(S^1)$</td>
<td>$L^2$</td>
<td>Incompressible Euler</td>
</tr>
<tr>
<td>$\text{Diff}(S^1)$</td>
<td>$L^2$</td>
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<tr>
<td>$\text{Diff}(S^1)$</td>
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<td>$\text{Diff}(S^1)$</td>
<td>$\mu\dot{H}^1$</td>
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<td>$\text{Rot}(S^1)\backslash\text{Diff}(S^1)$</td>
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<tr>
<td>$\text{Rot}(S^1)\backslash\text{Diff}(S^1)$</td>
<td>$\dot{H}^{1/2}$</td>
<td>mCLM</td>
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<tr>
<td>$\text{Diff}_\mu(T^2)$</td>
<td>$\dot{H}^{-1/2}$</td>
<td>SQG</td>
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<tr>
<td>$\text{Vir}(S^1)$</td>
<td>$L^2$</td>
<td>KdV</td>
</tr>
<tr>
<td>$\text{Vir}(S^1)$</td>
<td>$H^1$</td>
<td>Camassa–Holm w. disp.</td>
</tr>
</tbody>
</table>

Table 1.1: Fluid-dynamic equations as geodesic equations on diffeomorphism groups.
Riemannian geometry on mapping spaces

Riemannian geometry has established itself as a successful framework for handling the nonlinear and infinite-dimensional aspects involved in geometric data analysis and fluid dynamics. Intuitively, the Riemannian metric quantifies infinitesimal deformations of shapes and infinitesimal displacements of fluids, respectively. These interpretations go back to d’Arcy Thompson [11] and Vladimir Arnold [1]. Reparameterization-invariance of the Riemannian metric emerges as a key property from the requirement of mesh independence in shape analysis and from the Markov property in fluid dynamics. Thus, one is naturally led to the study of reparameterization-invariant Riemannian metrics on infinite-dimensional manifolds of mappings.

This setting comes with many surprises. For instance, the simplest reparameterization-invariant metric has vanishing geodesic distance. This is a purely infinite-dimensional phenomenon, which is in stark contrast to the Hopf–Rinow theorem in finite dimensions. Fortunately, this degeneracy disappears for higher-order Sobolev metrics. The corresponding geodesic initial and boundary value problems are the computational basis for statistics and machine learning on the nonlinear and infinite-dimensional configuration spaces of shapes or fluids. Moreover, the geometric interpretation allows one to relate symmetries of the Riemannian metric to conserved quantities along geodesics and has led to new well-posedness proofs of fluid-dynamic equations.

Figure 1.4: Geodesic initial and boundary value problems as a computational basis for shape registration, correspondences, interpolation, distances, means, principal components, multi-dimensional scaling, agglomerative clustering, etc.
Bibliographical notes

Bernhard Riemann mentioned the possibility of defining infinite-dimensional manifolds already in his Habilitationsschrift [10, end of section I]. The translation into English in [9] reads as follows:

There are manifoldnesses in which the determination of position requires not a finite number, but either an endless series or a continuous manifoldness of determinations of quantity. Such manifoldnesses are, for example, the possible determinations of a function for a given region, the possible shapes of a solid figure, &c.

It turns out that geometry on Banach manifolds can be developed at no extra cost compared to the finite-dimensional case [8]. Beyond Banach spaces one needs a suitable differential calculus and has to navigate around the lack of an (easy) implicit function theorem [7].

Sir D’Arcy Wentworth Thompson is often named as the founding father of shape analysis. His book on growth and form [11] introduces the paradigm of shape analysis as deformation analysis. This paradigm admits a natural Riemannian interpretation, where infinitesimal deformations are quantified by a Riemannian metric. The infinitesimal deformations are defined either on the ambient space $N$, leading to Riemannian geometry on diffeomorphism groups and the widely used large deformations diffeomorphic mapping (LDDMM) framework [13]. Alternatively, they are defined merely along the shape $f: M \to N$, leading to Riemannian geometry on spaces of immersions or embeddings and elasticity theory [3]. Both frameworks have been developed into theoretical and computational tool sets for geometric data analysis with applications in computer graphics, computer vision, computational anatomy, and bio-medical imaging [12].

Vladimir Arnold first interpreted the incompressible Euler equation of fluid dynamics as a geodesic equation on the group of volume-preserving diffeomorphisms [1]. This geometric view led to a proof of local well-posedness by Ebin and Marsden [5]. The idea is to switch from Eulerian to Lagrangian coordinates. Analytically speaking, this cancels out the highest-order derivative and allows one to view the dynamics as an ordinary differential equation. Geometrically speaking, this amounts to viewing the equation as a geodesic spray, i.e., as a vector field on the tangent space of the diffeomorphism group. Similar endeavors have subsequently been carried out for a wide range of fluid-dynamic equations [2].
Figure 1.5: A geometric framework for shape analysis and fluid dynamics.

References


2 Calculus beyond Banach spaces

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1 Locally convex spaces

Many function spaces of relevance in geometric data science are not Banach. For example, the space of smooth functions on a compact manifold is Fréchet but not Banach, and the space of smooth functions on a non-compact manifold is locally convex but not Fréchet. Working with such non-Banach function spaces is unavoidable in the context of infinite-dimensional Lie groups, as can be seen from the following theorem by Omori [18].

1.1. Theorem. [18] If a (connected) Banach–Lie group $G$ acts effectively, transitively and smoothly on a compact manifold, then $G$ must be a finite-dimensional Lie group.

A prime example are diffeomorphism groups. As these are genuinely infinite-dimensional, one to make a choice: either one models them on Banach spaces, in which case composition fails to be smooth, or one models them on Fréchet or more general locally convex vector spaces, in which case a differential calculus beyond Banach spaces is required.

1.2. Definition. Locally convex space. A topological vector space is a vector space endowed with a topology such that vector addition and scalar multiplication are continuous. A locally convex space is a topological vector space whose topology has a basis consisting of convex sets.

For example, Hilbert, Banach, and Fréchet spaces are locally convex thanks to the triangle inequality. Moreover, $L^p$ spaces are locally convex for $p \in [1, \infty]$ but not for $p \in [0, 1)$.

1.3. Definition. Seminorm. A seminorm is a nonnegative subadditive positively homogeneous function on a vector space. In formulas, $p: E \to \mathbb{R}_+$ is a seminorm on the vector space $E$ if $p(x + y) \leq p(x) + p(y)$ and $p(\lambda x) = |\lambda| p(x)$ for all $x, y \in E$ and $\lambda \in \mathbb{R}$.

1.4. Lemma. Locally convex spaces via seminorms. The initial topology of any family of seminorms is locally convex. Conversely, the topology of any locally convex space can be represented as the initial topology with respect to some family of seminorms.
A locally convex structure refers to either a locally convex topology or an associated family of seminorms. There are initial locally convex structures with respect to families of linear functions $E \to E_i$ and final locally convex structures with respect to families of surjective linear functions $E_i \to E$.

1.5. Definition. Bounded sets. A subset of a topological vector space is bounded if it can be absorbed (or swallowed) by every zero-neighborhood. In formulas, $B \subseteq E$ is bounded if for every zero-neighborhood $U$ in $E$, there exists $\lambda \geq 0$ such that $B \subseteq \lambda U$.

If the topology is generated by a family of seminorms, then boundedness of a set is equivalent to boundedness of each of these seminorms on the set. The finer the topology, the fewer bounded sets there will be; if a set is bounded in one topology, it remains so in all coarser topologies. The system of bounded sets is called a bornology. There are initial bornologies with respect to families of functions $E \to E_i$ and final bornologies with respect to families of surjective functions $E_i \to E$.

1.6. Definition. Linear and multilinear maps. The set of continuous linear functionals on a locally convex space $E$ is denoted by $E^\ast$. A function is called bounded if it maps bounded sets to bounded sets. The set of bounded linear functionals on $E$ is denoted by $E'$.

1.7. Definition. Dual pairing, compatible topologies. A dual pairing between vector spaces $E$ and $F$ is a bilinear form $\langle \cdot, \cdot \rangle : E \times F \to \mathbb{R}$ which is non-degenerate in the sense that

- $\langle x, y \rangle = 0$ for all $y \in F$, then $x = 0$, and
- $\langle x, y \rangle = 0$ for all $x \in E$, then $y = 0$.

A locally convex topology on $E$ is called compatible with the dual pairing if $E^\ast = F$.

1.8. Definition. Weak, Mackey, and strong topologies. Let $\langle \cdot, \cdot \rangle : E \times F \to \mathbb{R}$ be a dual pairing. The weak topology on $E$, denoted by $\sigma(E,F)$, is the topology of uniform convergence on finite subsets of $F$. The Mackey topology on $E$, denoted by $\mu(E,F)$, is the topology of uniform convergence on $\sigma(F,E)$-compacts in $F$. The strong topology on $E$, denoted by $\beta(E,F)$, is the topology of uniform convergence on $\sigma(F,E)$-bounded subsets of $F$.

The weak topology is coarser than the Mackey topology because finite sets are compact, and the Mackey topology is coarser than the strong topology because compact sets are bounded.

1.9. Theorem. Mackey–Arens. Let $\langle \cdot, \cdot \rangle : E \times F \to \mathbb{R}$ be a dual pairing. Then the coarsest compatible topology on $E$ is the weak topology $\sigma(E,F)$, and the finest compatible topology is the Mackey topology $\mu(E,F)$.

1.10. Theorem. Banach–Mackey. Let $\langle \cdot, \cdot \rangle : E \times F \to \mathbb{R}$ be a dual pairing. Then all compatible topologies on $E$ have the same bounded sets.

The take-away is that there is a whole range of locally convex topologies (namely, the
ones compatible with a given dual pairing) which all share the same bornology (i.e., the same system of bounded sets).

2 Fréchet and Gâteaux differentiability

In the sequel all locally convex spaces are assumed to be Hausdorff to ensure uniqueness of derivatives.

2.1. Definition. Fréchet differentiability. Let $E$ and $F$ be normed spaces. A function $f: U \to F$ defined on an open subset $U \subseteq E$ is called Fréchet differentiable at $x \in U$ with derivative $Df(x) \in L(E, F)$ if
\[
\lim_{E \setminus \{0\} \ni h \to 0} \frac{f(x + h) - f(x) - Df(x)(h)}{\|h\|} = 0.
\]
The function $f$ is called continuously Fréchet differentiable if it is Fréchet differentiable at every $x \in U$ with continuous Fréchet derivative $Df: U \to L(E, F)$.

Higher-order Fréchet derivatives, provided they exist, are defined iteratively as
\[
D^k f = D(D^{k-1} f): U \to L(E, L(E, \ldots, E; F; \ldots)),
\]
where the isomorphism is the exponential law for bounded linear maps. The function $f$ is called Fréchet smooth if it is Fréchet $C^k$ for all $k \in \mathbb{N}$.

This definition does not easily extend to more general locally convex spaces. One has to make two choices: first, as a substitute for Fréchet differentiability, one has to impose a suitable condition on the remainder $f(x + h) - f(x) - Df(x)(h)$, and second, to express the continuity of the derivative $Df$, one has to choose a locally convex structure on the space $L(E, F)$. Ideally, one would like to select a structure such that the evaluation map $ev: L(E, F) \times E \to F$ is continuous. The reason is that this would allow one to deduce continuous differentiability of $f \circ g$ from continuous differentiability of $f: E \to F$ and $g: F \to G$ via the chain rule
\[
D(f \circ g)(x) = Df(g(x)) \circ Dg(x).
\]
Unfortunately, such a locally convex structure on $L(E, F)$ does not exist unless $E$ is normable, as shown next:

2.2. Lemma. Discontinuity of the evaluation map. Let $E$ be a non-normable Hausdorff locally convex space. Then the evaluation map
\[
ev: E \times E^* \to \mathbb{R}
\]
is discontinuous for any choice of vector topology on the topological dual $E^*$. 


Proof. Assume for contradiction that the evaluation map is continuous for some vector topology on $E^\ast$. Then there are open zero-neighborhoods $U \subset E$ and $V \subset E^\ast$ with $\text{ev}(U \times V) \subset [-1,1]$. The polar set $V^\circ := \{ x \in E^\ast : |x^\ast(x)| \leq 1 \text{ for all } x^\ast \in V \}$ is a zero-neighborhood in $E$ because it contains $U$. Moreover, $V^\circ$ is bounded in $E$ with respect to the $\sigma(E,E^\ast)$-topology because for every $x^\ast \in E^\ast$, there exists $\lambda > 0$ such that $x^\ast \in \lambda V$, and consequently $x^\ast(V^\circ) \subseteq \text{ev}(V^\circ, \lambda V) \subseteq [-\lambda, \lambda]$. By the Banach–Mackey theorem, $V^\circ$ is bounded also in the original topology of $E$. To summarize, $E$ is Hausdorff and contains the convex bounded neighborhood $V^\circ$. Therefore, $E$ is normable by the gauge functional $E \ni x \mapsto \inf\{ \lambda > 0 : x \in \lambda V^\circ \} \in \mathbb{R}_+$. [9, Proposition 6.8.4], a contradiction. 

This issue can be alleviated to some extent by resorting to Gâteaux-style derivatives and by requiring the derivative to be continuous $U \times E \to F$ rather than $U \to L(E,F)$. This leads to the calculus proposed by Bastiani [2] and further developed by Keller [10].

2.3. Definition. Gâteaux differentiability. Let $E$ and $F$ be Hausdorff locally convex topological vector spaces. A function $f: U \to F$ defined on an open subset $U \subseteq E$ is called Gâteaux differentiable at $x \in U$ if for every $h \in E$ there exists $D_h f(x) \in F$ such that

$$\lim_{\mathbb{R} \setminus \{0\} \ni t \to 0} \frac{f(x + th) - f(x) - t D_h f(x)}{t} = 0.$$ 

The function $f$ is called continuously Gâteaux differentiable if it is Gâteaux differentiable at every $x \in U$ with continuous Gâteaux derivative

$$df: U \times E \ni (x,h) \mapsto D_h f(x) \in F.$$ 

Higher-order Gâteaux derivatives, provided they exist, are defined iteratively as

$$d^k f(x; h_1, \ldots, h_k) := (D_{h_k} D_{h_{k-1}} \cdots D_{h_1} f)(x): U \times E^k \to F.$$ 

The function $f$ is called Gâteaux smooth if it is Gâteaux $C^k$ for all $k \in \mathbb{N}$.

The continuity of the Gâteaux derivative in the above sense has important implications [10]. For instance, continuity of $d^k f$ implies multi-linearity of $d^k f(x, \cdot)$, which is not clear a priori. Gâteaux $C^k$ functions are Fréchet $C^{k-1}$, there is a chain rule for Gâteaux $C^k$ functions, and continuous linear functions are Gâteaux smooth. Most importantly for applications in variational calculus, the category of Gâteaux smooth functions between locally convex spaces satisfies an exponential law, to be discussed next, alas with some serious limitations.

3 Exponential law

Variational calculus studies first-order conditions of optimality along variational families of functions. This involves differential calculus on infinite-dimensional function spaces and is difficult to handle analytically. As a simplification, one typically replaces variations in a function space by functions depending on an additional variational parameter. This amounts to identifying functions $f(x)(y)$ with functions $f(x, y)$. Such an identification is called an exponential law. In modern versions of smooth calculus the exponential
law is not an assumption, which has to be verified on a case-by-case basis, but a theorem, which holds in great generality.

3.1. Definition. **Exponential law of smooth functions.** The exponential law in a category of smooth functions between vector spaces is a natural isomorphism

\[ C^\infty(E \times F, G) \cong C^\infty(E, C^\infty(F, G)), \]

which identifies functions \( f(x, y) \) with functions \( f(x)(y) \). Note that this requires the function space \( C^\infty(F, G) \) to be an object in the given category.

A typical scenario in variational calculus is that \( E = G = \mathbb{R} \), and \( F \) is Euclidean. Then the right-hand side represents variations in the space of smooth functions on \( F \), whereas the left-hand side consists simply of functions on the Euclidean space \( \mathbb{R} \times F \).

3.2. Lemma. **No exponential law for Gâteaux-smooth functions.** The exponential law fails in the category of Gâteaux-smooth functions between locally convex vector spaces.

**Proof.** Consider the setting of [Definition 3.1](#), where \( E \) is not normable, \( F = E^* \), and \( G = \mathbb{R} \). Then the inclusion \( E \to E^{**} \) is continuous linear and therefore Gâteaux-smooth. However, the exponential law would identify it with the evaluation map \( E \times E^* \to \mathbb{R} \), which is discontinuous by [Lemma 2.2](#).

The problem disappears if one is willing to assume that the space \( F \) in [Definition 3.1](#) is locally compact [1]. To gain some intuition for what goes wrong, it will be helpful to consider the exponential law in a wider context.

3.3. Definition. **Abstract exponential law.** A closed monoidal category is a category with a tensor product \( \otimes \) and an internal Hom functor \( \text{Hom} \) together with a natural isomorphism

\[ \text{Hom}(E \otimes F, G) \cong \text{Hom}(E, \text{Hom}(F, G)). \]

This isomorphism is called the exponential law. If the tensor product is the Cartesian product, the category is called Cartesian closed.

The notation stems from the category of linear functions between vector spaces, which satisfies an exponential law with respect to the tensor product of vector spaces. Similarly, the category of continuous linear maps between Banach spaces satisfies an exponential law with respect to the projective tensor product. Unfortunately, this cannot be extended to more general locally convex spaces, as shown by example in the proof of [Lemma 3.2](#).

However, this problem can be fixed by resorting to bounded instead of continuous linear functions.

3.4. Lemma. **Exponential law for bounded linear maps.** There is a natural bornological isomorphism (i.e., bounded linear map with bounded inverse)

\[ L(E, F; G) \cong L(E, L(F, G)), \]
where $L$ denotes sets of bounded linear or multilinear functions, endowed with the initial
(locally convex) topologies with respect to evaluations at points in their domain. Consequent-
ly, the exponential law is bounded bilinear
\[ \text{ev}: E \times E^* \to \mathbb{R}. \]

Proof. A map $f : E \times F \to G$ is bilinear if and only if the corresponding map $f^\vee : E \to (F \to G)$ is linear with values in the linear maps from $F$ to $G$. Thus, it remains to show boundedness. A set $A \subseteq L(E, F; G)$ is bounded if and only if $A(B \times C)$ is bounded for all bounded sets $B \subseteq E$ and $C \subseteq F$. Equivalently, $A^\vee(B)$ is contained and bounded in $L(F, G)$ for all bounded sets $B \subseteq E$. Equivalently, $A^\vee$ is contained and bounded in $L(E, L(F, G))$. This establishes the exponential law for bounded linear maps. The canonical embedding $E \to E''$ is bounded linear and is identified via the exponential law with the evaluation map, which consequently is bounded bilinear. \hfill \Box

The situation for nonlinear functions is somewhat comparable to the one for linear
functions. The exponential law holds in the category of functions between sets. More-
over, it holds in the category of continuous functions between topological spaces if $F$ is
compact and $C(F, G)$ carries the compact-open topology, i.e., the topology whose basis
are the sets $\{ f \in C(F, G) : f(K) \subseteq U \}$ with $K \subseteq F$ compact and $U \subseteq G$ open [23]
Exercise 43.1]. However, the restriction that $F$ is compact cannot be removed here.

There are several work-arounds, which we describe next. The first idea is to tinker
with the topology on the Cartesian product $E \times F$. Namely, this topology has to be
Kelleyfied, i.e., replaced by the final topology with respect to the inclusion of compact
subsets. The resulting topology is compactly generated, i.e., a set is open if and only
if its intersection with every compact subset is relatively open. This way, one obtains
Steenrod’s [21] monoidal closed category, which he called convenient:

3.5. Theorem. Exponential law for compactly generated spaces. The category
of continuous maps between compactly generated topological spaces is monoidal closed,
i.e., there is a natural homeomorphism
\[ C(k(E \times F), G) \cong C(E, C(F, G)), \]
where $k$ means Kelleyfication the function spaces carry the compact-open topology.

Alternatively, if compactness assumptions are not desired, one has to resort to non-
topological notions of convergence. Recall that on any topological space $E$, the neigh-
borhoods of any point $x \in E$ form a filter $\mathcal{F}$. More generally, following Choquet [4], one
may associate to every point $x \in E$ a family $\tau(x)$ of filters on $E$. If $\tau(x)$ is stable under
finite intersections and upward closed, then $\tau$ is called a convergence structure on $E$. A
net or filtered family $(x_i)_{i \in I}$ is said to converge to $x \in E$ if it converges with respect to
some filter $\mathcal{F} \in \tau(x)$. If the constant nets $(x)_{i \in I}$ converge to $x$, for all $x \in E$, then $\tau$ is
called a pseudo-topology on $E$.

3.6. Theorem. Exponential law for convergence spaces. The category of pseudo-
topological spaces is monoidal closed, i.e., there is a natural homeomorphism
\[ C(E \times F, G) \cong C(E, C(F, G)), \]
for suitable pseudo-topologies on the product space and the spaces of continuous functions.

If one is interested in smoothness rather than continuity, then further options are available. The key observation is that smoothness can be tested along smooth curves, i.e., a function $f$ is smooth if and only if $f \circ c$ is smooth for all smooth curves. This was discovered by Boman \cite{3} on $\mathbb{R}^2$ and was later adopted as a definition by Frölicher \cite{5,6}. Modern proofs of Boman’s theorem are available in \cite{7,12,3.2}.

3.7. Definition. Frölicher space. A Frölicher space is a set $E$ together with a set $C$ of curves $\mathbb{R} \to E$ and a set $F$ of functions $E \to \mathbb{R}$ such that

1. $f \in F$ if and only if $f \circ c \in C^\infty(\mathbb{R}, \mathbb{R})$ for all $c \in C$, and

2. $c \in C$ if and only if $f \circ c \in C^\infty(\mathbb{R})$ for all $f \in F$.

A function between Frölicher spaces is called smooth if it pushes smooth curves to smooth curves or, equivalently, if it pulls smooth functions to smooth functions.

Frölicher structures can be generated easily by imposing (1) for a given set of curves and then (2) or, alternatively, by imposing (2) for a given set of functions and then (1). Their usefulness stems from their excellent categorial properties, which follow by short and elementary arguments:

3.8. Theorem. Exponential law for Frölicher spaces. In the category of smooth functions between Frölicher spaces, arbitrary limits and colimits exist, and the exponential law holds:

$$C^\infty(E \times F, G) \cong C^\infty(E, C^\infty(F, G)).$$

Here $C^\infty(F, G)$ carries the Frölicher structure generated by the smooth functions

$$C^\infty(F, G) \xrightarrow{C^\infty(c, f)} C^\infty(\mathbb{R}, \mathbb{R}) \xrightarrow{\lambda} \mathbb{R}, \quad g \mapsto (f \circ g \circ c) \mapsto \lambda(f \circ g \circ c),$$

where $c \in C^\infty(\mathbb{R}, F)$, $f \in C^\infty(G, \mathbb{R})$, and $\lambda \in C^\infty(\mathbb{R}, \mathbb{R})'$.

Proof. Limits are formed as in the category of sets as a certain subset of the Cartesian product, and the smooth structure is generated by the smooth functions on the factors. In particular, this explains the Frölicher structure on the product $E \times F$. Colimits are formed as in the category of set as a certain quotient of the disjoint union, and the smooth functions are exactly those which induce smooth functions on the cofactors. We have the following implications:

$$\varphi^\vee : E \to C^\infty(F, G)$$

is smooth.

$\iff \varphi^\vee \circ c_E : \mathbb{R} \to C^\infty(F, G)$ is smooth for all smooth curves $c_E \in C^\infty(\mathbb{R}, E)$, by definition.

$\iff C^\infty(c_F, f_G) \circ \varphi^\vee \circ c_E : \mathbb{R} \to C^\infty(\mathbb{R}, \mathbb{R})$ is smooth for all smooth curves $c_E \in C^\infty(\mathbb{R}, E)$, $c_F \in C^\infty(\mathbb{R}, F)$, and smooth functions $f_G \in C^\infty(G, \mathbb{R})$, by definition.

$\iff f_G \circ \varphi \circ (c_E \times c_F) = f_G \circ (c_E^F \circ \varphi \circ c_E) \circ \lambda : \mathbb{R}^2 \to \mathbb{R}$ is smooth for all smooth curves $c_E$, $c_F$, and smooth functions $f_G$, by Boman’s theorem \cite{3}; see also \cite{12,3.2}.
\[ \Rightarrow \varphi : E \times F \rightarrow G \text{ is smooth, since each curve into } E \times F \text{ is of the form } (c_E, c_F) = (c_E \times c_F) \circ \Delta, \text{ where } \Delta \text{ is the diagonal mapping.} \]

\[ \Rightarrow \varphi \circ (c_E \times c_F) : \mathbb{R}^2 \rightarrow G \text{ is smooth for all smooth curves } c_E \text{ and } c_F, \text{ since the product and the composite of smooth mappings is smooth.} \]

This establishes a bijection between the function spaces on the left- and right-hand side of the exponential law. It follows by categorical arguments that the exponential law is not only a bijection but also a diffeomorphism for the Frölicher structures on the mapping spaces.

3.9. Corollary. Consequences of categorial closedness. The following canonical mappings are smooth:

\[
\begin{align*}
\text{ev} & : C^\infty(E, F) \times E \rightarrow F, \quad \text{ev}(f, x) = f(x) \\
\text{ins} & : E \rightarrow C^\infty(F, E \times F), \quad \text{ins}(x)(y) = (x, y) \\
(\ )^\wedge & : C^\infty(E, C^\infty(F, G)) \rightarrow C^\infty(E \times F, G) \\
(\ )^\lor & : C^\infty(E \times F, G) \rightarrow C^\infty(E, C^\infty(F, G)) \\
\text{comp} & : C^\infty(F, G) \times C^\infty(E, F) \rightarrow C^\infty(E, G) \\
C^\infty(\ ) & : C^\infty(F, F_1) \times C^\infty(E_1, E) \rightarrow C^\infty(C^\infty(E, F), C^\infty(E_1, F_1)) \\
\prod & : \prod C^\infty(E_i, F_i) \rightarrow C^\infty(\prod E_i, \prod F_i)
\end{align*}
\]

Proof. This follows from the exponential law by simple categorical reasoning:

The mapping associated to ev via cartesian closedness is the identity on \( C^\infty(U, F) \), which is \( C^\infty \), thus ev is also \( C^\infty \).

The mapping associated to ins via cartesian closedness is the identity on \( E \times F \), hence ins is \( C^\infty \).

The mapping associated to \( (\ )^\wedge \) via cartesian closedness is the smooth composition of evaluations \( \text{ev} \circ (\text{ev} \times \text{Id}) : (f; x, y) \mapsto f(x)(y) \).

We apply cartesian closedness twice to get the associated mapping \( (f; x; y) \mapsto f(x, y) \), which is just a smooth evaluation mapping.

The mapping associated to comp via cartesian closedness is \( (f, g; x) \mapsto f(g(x)) \), which is the smooth mapping \( \text{ev} \circ (\text{Id} \times \text{ev}) \).

The mapping associated to the one in question by applying cartesian closed is \( (f, g, h) \mapsto g \circ h \circ f \), which is (apart from permutation of the variables) the \( C^\infty \)-mapping \( \text{comp} \circ (\text{Id} \times \text{comp}) \).
Up to a flip of factors the mapping associated via cartesian closedness is the product of the evaluation mappings $C^\infty(E_i, F_i) \times E_i \to F_i$.

Frölicher spaces, without any further structure imposed, are too general for the development of infinite-dimensional differential geometry: for example, there is no notion of tangent spaces. This can be fixed by supplementing Frölicher spaces by additional structure such as parallel transport along curves \cite{11,15,19}. A more conventional way is to consider manifolds modeled on open subsets of linear Frölicher spaces. More precisely, by a linear Frölicher space we mean a locally convex space such that smoothness of curves (defined in the usual sense) can be tested by continuous or bounded linear functionals. These are precisely the Mackey complete locally convex spaces, also known as convenient spaces, to be defined next.

4 Convenient calculus

4.1. Definition. Convenient spaces. A locally convex space $E$ is called convenient if it is a Frölicher space when endowed with the following sets of “smooth” curves and functions:

1. The set of curves $c: \mathbb{R} \to E$ such that all derivatives exist and are continuous.

2. The set of functions $f: E \to \mathbb{R}$ such that $f \circ c: \mathbb{R} \to \mathbb{R}$ is smooth for all curves $c$ as above.

A function between convenient spaces is called smooth if it pushes smooth curves to smooth curves or, equivalently, if it pulls smooth functions to smooth functions.

4.2. Lemma. Convenient spaces. \cite[2.14]{12} A locally convex vector space $E$ is convenient if and only if one of the following equivalent conditions holds:

1. A curve $c: \mathbb{R} \to E$ is smooth if and only if $\lambda \circ c$ is smooth for all $\lambda \in E^*$, where $E^*$ is the set of continuous linear functionals.

2. A curve $c: \mathbb{R} \to E$ is smooth if and only if $\lambda \circ c$ is smooth for all $\lambda \in E'$, where $E'$ is the set of bounded linear functionals. (This is called scalarwise smoothness.)

3. Any Mackey-Cauchy-sequence (i.e., $t_{nm}(x_n - x_m) \to 0$ for some $t_{nm} \to \infty$ in $\mathbb{R}$) converges in $E$. (This is called Mackey completeness.)

Note that property (2) implies that smoothness is a bornological concept, i.e., it depends on the locally convex topology only via the system of bounded sets. The initial locally convex structure with respect to a family of linear maps with values in convenient spaces is again convenient. However, final locally convex structures, including quotients and inductive limits, may fail to be convenient.

4.3. Definition. $c^\infty$ topology. The $c^\infty$ topology on a locally convex space $E$ is defined as the final topology with respect to the set of smooth curves $c: \mathbb{R} \to E$. The space $E$ with this topology is denoted by $c^\infty E$. 

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In general (e.g. on the space of test functions) the $c^\infty$ topology is finer than the given locally convex topology. It is not a vector space topology, since addition is no longer jointly continuous. Namely, even $c^\infty(D \times D) \neq c^\infty D \times c^\infty D$. The finest among all locally convex topologies on $E$ which are coarser than $c^\infty E$ is the bornologification of the given locally convex topology. If $E$ is a Fréchet space, then $c^\infty E = E$.

4.4. Definition. Smooth mappings. Let $E$ and $F$ be convenient vector spaces, and let $U \subseteq E$ be $c^\infty$-open. A mapping $f: U \to F$ is called smooth, in symbols $f \in C^\infty(U,F)$, if $f \circ c \in C^\infty(\mathbb{R}, F)$ for all $c \in C^\infty(\mathbb{R}, U)$. The space $C^\infty(U,F)$ is endowed with the initial locally convex structure given by the injection

$$C^\infty(U,F) \xrightarrow{C^\infty(c,\ell)} \prod_{c \in C^\infty(\mathbb{R},U), \ell \in F^*} C^\infty(\mathbb{R},\mathbb{R}), \quad f \mapsto (\ell \circ f \circ c)_{c,\ell},$$

where $C^\infty(\mathbb{R},\mathbb{R})$ carries the topology of compact convergence in each derivative separately.

4.5. Theorem. Main properties of convenient calculus. Let $E$, $F$, and $G$ be convenient spaces, and let $U \subseteq E$ and $V \subseteq F$ be $c^\infty$-open subsets.

1. On Fréchet spaces the above notion of smoothness coincides with all other reasonable definitions.

2. Multilinear mappings are smooth iff they are bounded.

3. If $f: E \supseteq U \to F$ is smooth, then the derivative $df: U \times E \to F$ is smooth, and also $df: U \to L(E,F)$ is smooth where $L(E,F)$ denotes the space of all bounded linear mappings with the topology of uniform convergence on bounded subsets.

4. The chain rule holds.

5. The space $C^\infty(V,G)$ is convenient and the exponential law, together with all its consequences in Corollary 3.9 holds:

$$C^\infty(U, C^\infty(V,G)) \cong C^\infty(U \times V,G)$$

is a linear diffeomorphism of convenient vector spaces.

6. A linear mapping $f: E \to C^\infty(V,G)$ is smooth (by (2) equivalent to bounded) if and only if $E \xrightarrow{f} C^\infty(V,G) \xrightarrow{ev} G$ is smooth for each $v \in V$. This is called the smooth uniform boundedness theorem.

7. A mapping $f: U \to L(F,G)$ is smooth if and only if $U \xrightarrow{f} L(F,G) \xrightarrow{ev} G$ is smooth for each $v \in F$, because then it is scalarwise smooth by the classical uniform boundedness theorem.

The exponential law (for $U = \mathbb{R}$) is the main assumption of variational calculus; here it is a theorem. Beyond Fréchet spaces, as a rule, there are more smooth mappings in the convenient setting than in e.g. the Gâteaux setting due to the additional continuity requirements imposed there.
5 Pitfalls

One might argue that each serious application of infinite-dimensional calculus needs its own foundation. By a serious application one typically means some application of a hard inverse function theorem. These theorems can be proved if, by collecting enough a priori estimates, one creates enough of a Banach space situation for some modified iteration procedure to converge. Accordingly, many authors tried to build their platonic idea of a priori estimates into their differential calculus. This tends to narrow the applicability of the calculus to a specific set of problems and to hide the origin of the a priori estimates. Convenient calculus offers an alternative approach. It operates primarily in categories of smooth maps, where variational equations are easy to derive but often impossible to solve. This is highlighted by the following examples, which show that existence, uniqueness, and regularity of solutions to ordinary differential equations cannot be taken for granted beyond Banach spaces.

5.1. Example. Lack of existence. Let $E := s$ be the Fréchet space of rapidly decreasing sequences; note that by the theory of Fourier series we have $s = C^\infty(S^1, \mathbb{R})$. Consider the continuous linear operator $T : E \rightarrow E$ given by

$$T(x_0, x_1, x_2, \ldots) := (0, 1^2 x_1, 2^2 x_2, 3^2 x_3, \ldots).$$

The ordinary linear differential equation $x'(t) = T(x(t))$ with constant coefficients has no solution in $s$ for certain initial values. By recursion one sees that the general solution should be given by

$$x_n(t) = \sum_{i=0}^{n} \left( \frac{n!}{i!} \right)^2 x_i(0) \frac{t^{n-i}}{(n-i)!}.$$

If the initial value is a finite sequence, say $x_n(0) = 0$ for $n > N$ and $x_N(0) \neq 0$, then

$$x_n(t) = \sum_{i=0}^{N} \left( \frac{n!}{i!} \right)^2 x_i(0) \frac{t^{n-i}}{(n-i)!}$$

$$= \frac{(n!)^2}{(n-N)!} t^{n-N} \sum_{i=0}^{N} \left( \frac{1}{i!} \right)^2 x_i(0) \frac{(n-N)!}{(n-i)!} t^{N-i}$$

$$|x_n(t)| \geq \frac{(n!)^2}{(n-N)!} |t|^{n-N} \left( |x_N(0)| \left( \frac{1}{N!} \right)^2 - \sum_{i=0}^{N-1} \left( \frac{1}{i!} \right)^2 |x_i(0)| \frac{(n-N)!}{(n-i)!} |t|^{N-i} \right)$$

$$\geq \frac{(n!)^2}{(n-N)!} |t|^{n-N} \left( |x_N(0)| \left( \frac{1}{N!} \right)^2 - \sum_{i=0}^{N-1} \left( \frac{1}{i!} \right)^2 |x_i(0)| |t|^{N-i} \right)$$

where the first factor does not lie in the space $s$ of rapidly decreasing sequences and where the second factor is larger than $\varepsilon > 0$ for $t$ small enough. So at least for a dense set of initial values this differential equation has no local solution.

This shows also, that the theorem of Frobenius is wrong, in the following sense: The vector field $x \mapsto T(x)$ generates a 1-dimensional subbundle $E$ of the tangent bundle
on the open subset $s \setminus \{0\}$. It is involutive since it is 1-dimensional. But through points representing finite sequences there exist no local integral submanifolds ($M$ with $TM = E|M$). Namely, if $c$ were a smooth nonconstant curve with $c'(t) = f(t).T(c(t))$ for some smooth function $f$, then $x(t) := c(h(t))$ would satisfy $x'(t) = T(x(t))$, where $h$ is a solution of $h'(t) = 1/f(h(t))$.

5.2. Example. Lack of uniqueness. As next example consider $E := \mathbb{R}^N$ and the continuous linear operator $T: E \to E$ given by $T(x_0, x_1, \ldots) := (x_1, x_2, \ldots)$. The corresponding differential equation has solutions for every initial value $x(0)$, since the coordinates must satisfy the recursive relations $x_{k+1}(t) = x_k'(t)$ and hence any smooth functions $x_0 : \mathbb{R} \to \mathbb{R}$ gives rise to a solution $x(t) := (x_0^{(k)}(t))_k$ with initial value $x(0) = (x_0^{(k)}(0))_k$. So by Borel’s theorem there exist solutions to this equation for any initial value and the difference of any two functions with same initial value is an arbitrary finite function. Thus the solutions are far from being unique. Note that $\mathbb{R}^N$ is a topological direct summand in $C^\infty(\mathbb{R}, \mathbb{R})$ via the projection $f \mapsto (f(n))_n$, and hence the same situation occurs in $C^\infty(\mathbb{R}, \mathbb{R})$.

5.3. Example. Lack of analyticity. Let now $E := C^\infty(\mathbb{R}, \mathbb{R})$ and consider the continuous linear operator $T : E \to E$ given by $T(x) := x'$. Let $x : \mathbb{R} \to C^\infty(\mathbb{R}, \mathbb{R})$ be a solution of the equation $x'(t) = T(x(t))$. In terms of $\hat{x} : \mathbb{R}^2 \to \mathbb{R}$ this says $\frac{\partial}{\partial t} \hat{x}(t, s) = \frac{\partial}{\partial s} \hat{x}(t, s)$. Hence $r \mapsto \hat{x}(t - r, s + r)$ has vanishing derivative everywhere and so this function is constant, and in particular $x(t)(s) = \hat{x}(t, s) = \hat{x}(0, s + t) = x(0)(s + t)$. Thus we have a smooth solution $x$ uniquely determined by the initial value $x(0) \in C^\infty(\mathbb{R}, \mathbb{R})$ which even describes a flow for the vector field $T$. In general this solution is however not real-analytic, since for any $x(0) \in C^\infty(\mathbb{R}, \mathbb{R})$, which is not real-analytic in a neighborhood of a point $s$ the composite $ev_s \circ x = x(s+ \cdot)$ is not real-analytic around 0.

Bibliographical remarks

Section 1 is compiled from the monographs by F. Treves [22] and H. Jarchow [9]. Section 2 is adapted from the introduction of the monograph by Keller [10]. Sections 3, 4 and 5 are borrowed from the monograph of A. Kriegl and P. W. Michor [12] and from unpublished lecture notes written by P. W. Michor and M. Bruveris.

Classical calculus, based on the notion of Fréchet derivatives, works well up to and including Banach spaces [13]. During the 20-th century the demand for analysis and calculus beyond Banach spaces became stronger. Locally convex spaces were formally introduced in 1935 by John von Neumann [17], following up on investigations of non-normable topologies by Fréchet, Mazur, Orlicz, Köthe, Toeplitz, and others. Good starting points for getting acquainted with this theory are the monographs by F. Treves [22], H. Jarchow [9], Meise and Vogt [14], and Narici and Beckenstein [16]. The development of differential calculus on locally convex spaces soon met the difficulty that composition of (continuous) linear mappings ceases to be a jointly continuous operation exactly at the level of Banach spaces, for any suitable topology on spaces of linear mappings. This entails a lack of Cartesian closedness in many smooth categories which are defined using
This problem has been addressed in several different ways. Andrée Bastiani [2] proposed a continuous differential calculus based on Gâteaux style derivatives, which has been developed further by Keller [10]. The resulting smooth category is not Cartesian closed but satisfies an exponential law when restricted to finite-dimensional domains. Siegfried and Werner Gähler [8] developed a continuous differential calculus based on a non-topological notion of convergence initially proposed by Choquet [4]. Their category of pseudo-topological spaces is Cartesian closed with respect to continuous morphisms, and there is a $C^k$ calculus on these spaces. Chen, Frölicher, Sikorski, Smith, and Souriau defined various smooth categories via pre- or post-composition with test functions, thereby reducing the problem to finite dimensions; see [20] for an overview. These categories have objects which are far more general than vector spaces or manifolds, and they are Cartesian closed in the case of Frölicher and Souriau spaces. Frölicher, Kriegl, and Michor [7, 12] developed a convenient calculus, which can be seen as an application of Frölicher’s theory within the realm of locally convex spaces. The name convenient calculus is in analogy to Steenrod’s [21] convenient category for topological spaces, which is a Cartesian closed category of continuous functions between compactly generated topological spaces.

References


