

A Iterative Procedure for the Inverse of i-ResNET

Let x_{t+1} in (1) be equal to x_t^0 . Then, the inverse of F_t in (1), F_t^{-1} , is given by the following procedure:

$$\begin{aligned} x_t^0 - g_t(x_t^0) &= x_t^1 \\ x_t^0 - g_t(x_t^1) &= x_t^2 \\ &\vdots \\ x_t^0 - g_t(x_t^{N-1}) &= x_t^N, \end{aligned} \tag{89}$$

where $N \in \mathbb{N}$ is the total number of iteration steps. This iterative process is called the **Banach fixed point iteration** and as $N \rightarrow \infty$, $x_t^N \rightarrow x_t$. Once we keep substituting equivalent statements for x_t^i until the N^{th} iteration:

$$\begin{aligned} x_{t+1} - g_t(x_t^0) &= x_t^1 \\ x_{t+1} - g_t[x_{t+1} - g_t(x_{t+1})] &= x_t^2 \\ \implies x_{t+1} - g_t[x_{t+1}] + g_t^2(x_{t+1}) &= x_t^2 \\ &\vdots \\ x_{t+1} + \left\{ \sum_{i=1}^N (-1)^i g_t^i \right\} (x_{t+1}) &= x_t^N \\ \implies \left\{ \sum_{i=0}^N (-1)^i g_t^i \right\} (x_{t+1}) &= x_t^N \end{aligned} \tag{90}$$

Therefore, as $N \rightarrow \infty$ in (90), the inverse, F_t^{-1} is obtained:

$$F_t^{-1}(x_{t+1}) = \lim_{N \rightarrow \infty} \left\{ \sum_{i=0}^N (-1)^i g_t^i \right\} x_{t+1} = \lim_{N \rightarrow \infty} x_t^N = x_t \tag{91}$$

It is easy to show that (91) is actually the inverse of F_t . Consider the following two series:

$$\begin{aligned} I - g_t + g_t^2 - \dots \mp g_t^N &= S_N \\ g_t - g_t^2 + \dots \mp g_t^{N+1} &= g_t S_N, \end{aligned} \tag{92}$$

where $S_N = \sum_{i=0}^N (-1)^i g_t^i$. Adding up the left and right hand sides in (92), respectively, yields:

$$I \mp g_t^{N+1} = [I + g_t] S_N \tag{93}$$

Since $Lip(g_t) < 1$, $g_t^{N+1} \rightarrow 0$ transformation as $N \rightarrow \infty$. Thus, (93) becomes:

$$I = [I + g_t] \lim_{N \rightarrow \infty} S_N \tag{94}$$

By (94), we conclude that $\lim_{N \rightarrow \infty} S_N$ is the inverse of F_t .

B Right Invariant Vector Fields & Vanishing Lie-Bracket

Let G be a connected Lie group equipped with Lie algebra $\mathfrak{g}$ and $\dim(\mathfrak{g}) = r \geq 2$. Let $\{v_1, \dots, v_r\}$ span $\mathfrak{g}$ which is isomorphic to $TG|_e$ by **Corollary 3.46** in [18], where $[v_i, v_j] \in \mathfrak{g}$ is not vanishing for any i and j . Furthermore; $v_i \in \mathcal{R}(G)$, $\forall i = 1, \dots, r$, where $\mathcal{R}(G)$ is the space of right invariant vector fields on G . By **Frobenius' theorem** (see **Lemma F.2** and **Corollary F.3** in [19]), one can always conclude that $\exists \{B_1, \dots, B_r\}$ that spans $\mathfrak{g}$ s.t. $[B_i, B_k] = 0$, $\forall i, k = 1, \dots, r$ in a small neighbourhood, U , of e . However, this is not the case for right invariant vector fields in G . Following setup is required before proving why **Frobenius' theorem** fails:

- (i) Let $R_g : G \rightarrow G$ be right translation, i.e. $R_g(h) = h \cdot g$, where $h, g \in G$.
- (ii) Suppose $\mathfrak{g} \cong \text{span}\{v_1, \dots, v_r\}|_e$ and $v_l \in \mathcal{R}(G)$, $\forall l = 1, \dots, r$ and $[v_i, v_k] \neq 0$, $\forall i \neq k$.

- (iii) Assume also $\mathfrak{g} \cong \text{span}\{B_1, \dots, B_r\}|_e$, s.t. $[B_i, B_k] = 0, \forall i, k = 1, \dots, r$ in a small neighbourhood, U , of e due to **Frobenius' theorem**.
- (iv) Following the same notation in [7], let $v_l|_g = \sum_p \eta_l^p(g) \partial_p, \forall l = 1, \dots, r$ and $\forall g \in G$.
- (v) Since $\{v_1, \dots, v_r\}$ spans $\mathfrak{g}, B_i = \sum_l \alpha_i^l(\varepsilon) v_l, \forall i, l = 1, \dots, r$, where $\alpha_i : \mathbb{R} \rightarrow \mathbb{R}^r$ are smooth functions. We are going to omit α_i^l 's arguments for brevity.
- (vi) Since G is connected, by **Proposition 1.48** in [7] $Y = v_l, \forall l = 1, \dots, r$ generates one-parameter subgroup s.t. $A(t) = \exp(tY|_e)$.
- (vii) Let $Y = v_q$ for a particular index q and g in item-(i) be equal to $\exp(t_g Y|_e)$ for a particular small $t_g \in \mathbb{R} \setminus \{0\}$, s.t. $g \in G$.

Let B_i and B_k be our two candidate vector fields for a particular pair of $(i, k) \in \{1, \dots, r\} \times \{1, \dots, r\}$. The assumption is: “**Suppose that B_i and $B_k \in \mathcal{R}(G)$** ”. Thus, we should expect: $[dR_g(B_i|_e), dR_g(B_k|_e)] = [B_i|_g, B_k|_g] = 0$, where the first equality is due to (1.32) in [7] and dR_g is the differential for R_g and is equal to:

$$dR_g(B_i|_e) = \sum_j B_i(R_g^j(e)) \partial_j = \sum_j \sum_l \alpha_i^l v_l(R_g^j(e)) \partial_j = \sum_j \sum_l \sum_p \alpha_i^l \eta_l^p(e) \frac{\partial R_g^j}{\partial x^p}(e) \partial_j, \quad (95)$$

where $\{x^p\}_{p=1}^m$ are coordinates of the Euclidean space into which G is embedded and the first equality is due to (1.23) in [7]. Since $R_g(h) = h \cdot \exp(t_g Y|_e)$:

$$R_g(h) = R_h(e) \cdot \exp(t_g Y|_e) = \exp(t_g dR_h(Y|_e)) = \exp(t_g Y(R_h(e))) = \exp(t_g Y|_h) = h + t_g \sum_p \eta_q^p(h) + \theta(t_g^2), \quad (96)$$

where the second and third equality are again due to (1.23) in [7]. Therefore, the j^{th} component function of R_g is:

$$R_g^j(h) = x^j(h) + t_g \eta_q^j(h) + \theta^j(t_g^2), \quad (97)$$

where $x^j(h) = h^j$ and $\theta^j(\cdot)$ include higher order terms. Therefore:

$$\frac{\partial R_g^j}{\partial x^p}(h) = \delta x_p^j(h) + t_g \frac{\partial \eta_q^j}{\partial x^p}(h) + \theta^j(t_g^2), \quad (98)$$

Substitute (98) into (95):

$$\begin{aligned} &= \sum_j \sum_l \sum_p \alpha_i^l \eta_l^p(e) \left(\delta x_p^j(h) + t_g \frac{\partial \eta_q^j}{\partial x^p}(h) + \theta^j(t_g^2) \right) \partial_j \\ &= \sum_j \left(\sum_l \alpha_i^l \eta_l^j(e) + t_g \sum_l \sum_p \alpha_i^l \eta_l^p(e) \frac{\partial \eta_q^j}{\partial x^p}(e) + \theta^j(t_g^2) \right) \partial_j \\ &= B_i|_e + t_g B_i(Y)|_e + \theta(t_g^2), \end{aligned} \quad (99)$$

All equations from (95) to (99) apply to B_k as well. Therefore, we may define the Lie bracket between B_i and B_k as follows:

$$\begin{aligned} [B_i|_g, B_k|_g] &= [dR_g(B_i|_e), dR_g(B_k|_e)] = [B_i|_e + t_g B_i(Y)|_e + \theta(t_g^2), B_k|_e + t_g B_k(Y)|_e + \theta(t_g^2)] \\ &= \underbrace{[B_i|_e, B_k|_e]}_{=0} + t_g [B_i|_e, B_k(Y)|_e] + t_g [B_i(Y)|_e, B_k|_e] + \underbrace{\theta(t_g^2)}_{\approx 0}, \end{aligned} \quad (100)$$

where the bilinearity property of Lie bracket is used to obtain the last equality. The first term is equal to 0 by our initial assumption; while the last term is approximately equal to 0 once we assume t_g is sufficiently small. However, the second and

the third terms may not be equal to zero in (100). Consider the second term:

$$\begin{aligned}
& t_g \left\{ \sum_{l_1} \alpha_i^{l_1} \left(\sum_{p_1} \eta(e)^{p_1}_{l_1} \right) \partial_{p_1} \left(\underbrace{\sum_{l_2} \alpha_k^{l_2} \left(\sum_{p_2} \eta(e)^{p_2}_{l_2} \partial_{p_2} \left(\sum_{p_3} \eta(e)^{p_3}_{p_3} \right) \right)}_{\omega_{l_2}|_e = \sum_{p_3} \xi(e)^{p_3}_{l_2} \partial_{p_3}} \right) \right\} - \\
& \left(\sum_{l_2} \alpha_k^{l_2} \left(\sum_{p_2} \eta(e)^{p_2}_{l_2} \partial_{p_2} \left(\sum_{p_3} \eta(e)^{p_3}_{p_3} \right) \right) \right) \sum_{l_1} \alpha_i^{l_1} \left(\sum_{p_1} \eta(e)^{p_1}_{l_1} \right) \Bigg\} \\
& = t_g \left[\sum_{l_1} \alpha_i^{l_1} \sum_{p_1} \eta(e)^{p_1}_{l_1}, \sum_{l_2} \alpha_k^{l_2} \omega_{l_2}|_e \right] = t_g \left[\sum_{l_1} \alpha_i^{l_1} v_{l_1}, \sum_{l_2} \alpha_k^{l_2} \omega_{l_2} \right] \Big|_e,
\end{aligned} \tag{101}$$

where $\omega_{l_2} \in \mathcal{R}(G)$, $\forall l_2 = 1, \dots, r$, because v_{l_2} 's action on v_q leave v_q in $\mathfrak{g}$ and not all $\omega_{l_2} = 0$ for $l_2 = 1, \dots, r$. Similarly the third term in (100) is equal to:

$$t_g \left[\sum_{l_1} \alpha_i^{l_1} \omega_{l_1}, \sum_{l_2} \alpha_k^{l_2} v_{l_2} \right] \Big|_e. \tag{102}$$

Adding (101) to (102):

$$\begin{aligned}
& t_g \left\{ \left[\sum_{l_1} \alpha_i^{l_1} v_{l_1}, \sum_{l_2} \alpha_k^{l_2} \omega_{l_2} \right] \Big|_e + \left[\sum_{l_1} \alpha_i^{l_1} \omega_{l_1}, \sum_{l_2} \alpha_k^{l_2} v_{l_2} \right] \Big|_e \right\} = \\
& t_g \left\{ \left[\sum_{l_1} \alpha_i^{l_1} v_{l_1}, \sum_{l_2} \alpha_k^{l_2} \omega_{l_2} \right] \Big|_e + \left[\sum_{l_2} \alpha_i^{l_2} \omega_{l_2}, \sum_{l_1} \alpha_k^{l_1} v_{l_1} \right] \Big|_e \right\} = \\
& t_g \left\{ \left[\sum_{l_1} \alpha_i^{l_1} v_{l_1}, \sum_{l_2} \alpha_k^{l_2} \omega_{l_2} \right] \Big|_e - \left[\sum_{l_1} \alpha_k^{l_1} v_{l_1}, \sum_{l_2} \alpha_i^{l_2} \omega_{l_2} \right] \Big|_e \right\} = \\
& t_g \sum_{l_2} \left\{ \left[\sum_{l_1} \alpha_k^{l_2} \alpha_i^{l_1} v_{l_1}, \omega_{l_2} \right] \Big|_e - \left[\sum_{l_1} \alpha_i^{l_2} \alpha_k^{l_1} v_{l_1}, \omega_{l_2} \right] \Big|_e \right\} = \\
& t_g \sum_{l_2} \left[\underbrace{\sum_{l_1} \left(\alpha_k^{l_2} \alpha_i^{l_1} - \alpha_i^{l_2} \alpha_k^{l_1} \right) v_{l_1}}_{=\beta_{l_2}}, \omega_{l_2} \right] \Big|_e,
\end{aligned} \tag{103}$$

where bilinearity of Lie bracket is used for obtaining the last two equalities and $\beta_{l_2} \in \mathcal{R}(G)$, $\forall l_2 = 1, \dots, r$, because the Lie algebra is closed under scalar multiplication and vector addition. Besides; $\beta_{l_2}|_e$ cannot be equal to the 0 vector for any $l_2 = 1, \dots, r$, because it would have implied that $\alpha_k^{l_2} B_i = \alpha_i^{l_2} B_k$, meaning that B_i and B_k were linearly dependent violating our initial assumption. Thus, (100) cannot be equal to 0 resulting in our assumption that right invariant vector fields abide by **Frobenius' theorem** is false.

C Smooth Orthonormal Global Frames for Connected Lie Groups

Let G be a connected Lie group with corresponding Lie algebra $\mathfrak{g} \cong T\mathcal{M}|_e$, where $\mathcal{M}$ is its underlying manifold in respective representation space. By **Corollary 8.39** in [33], every Lie group G has a smooth global frame, $\{X_1, \dots, X_r\}$, i.e. right (left) invariant basis at $T\mathcal{M}|_g$, $\forall g \in \mathcal{M}$ and component functions for X_j , $\forall j = 1, \dots, r$ are smooth. However, it does not mean there *always* exists an *orthonormal* smooth global frame for every Lie group. Frankly, there is none for any Lie group other than abelian ones. By **Theorem 13.4** in [33], having a global orthonormal coordinate frame implies having $\mathcal{M}$ contained in the domain of a commuting orthonormal frame $\forall g \in \mathcal{M}$, i.e. $[X_i, X_j]|_g = 0$, $\forall i, j = 1, \dots, r$ and $\forall g \in \mathcal{M}$. As discussed in

Appendix B, $[X_i, X_j]|_g \neq 0$, $\forall i \neq j$ and $\forall g \in \mathcal{M}$. Thus, we may conclude that there exists no smooth global orthonormal frame for G provided that it is not abelian. In our experiments, it also comes as no surprise when *right invariance cost* in (45) and *consistency cost* in (53) are turned off, the optimization converges to a location in parameter space where orthogonality condition at every sample point is satisfied for a particular subgroup under training.

D Right Invariance of Vector Fields in $\mathfrak{g}$ and Lie Bracket

In this section, how ensuring right invariance yields a proper Lie bracket for $\mathfrak{g}$ is discussed. It is also significant in the sense of computational efficiency, because computing Lie-bracket would have been costlier than is computing right invariance cost $\mathcal{R}\mathcal{I}$ given in (45). Besides, guaranteeing right invariance for each $X_i \in \mathfrak{g}$ implies a well-defined Lie-bracket; but not vice-versa.

Right invariance of a vector field X_i in mathematical terms equal to the following as stated in (44):

$$d\mathcal{T}_{\exp(\varepsilon X_j)}[X_i|_p] = X_i|_{\exp(\varepsilon X_j).p}, \quad \forall i, j = 1, \dots, r, \quad (104)$$

where $d\mathcal{T}_{\exp(\varepsilon X_j)}$ is the differential of group action $\mathcal{T}_j$. We tweak the LHS of (104) to suit our needs and let it be equal to $d\mathcal{T}_{\exp(\varepsilon X_j)}[X_i|_{\exp(-\varepsilon X_j).p}]$. In other words, our new smooth map is:

$$d\mathcal{T}_{\exp(\varepsilon X_j)}[\cdot|_{\exp(-\varepsilon X_j).p}] : T\mathcal{N}|_{\exp(-\varepsilon X_j).p} \rightarrow T\mathcal{N}|_p. \quad (105)$$

Note that $d\mathcal{T}_{\exp(\varepsilon X_j)}[X_i|_{\exp(-\varepsilon X_j).p}] = X_i|_p$, as we assume that $X_i \in \mathfrak{g}$, $\forall i = 1, \dots, r$ are right invariant vector fields over G . Moreover, since we assume $X_i \in \mathfrak{g}$ are smooth vector fields, the following Taylor approximations

$$d\mathcal{T}_{\exp(\varepsilon X_j)}|_p = \left[\delta_q^l + \varepsilon \frac{\partial \zeta_j^l}{\partial p^q} + \Theta(\varepsilon^2) \right]_q^l (p), \quad (106)$$

and

$$X_i|_{\exp(-\varepsilon X_j).p} = \left[\zeta_i^l - \varepsilon \sum_{k=1}^m \zeta_j^k \frac{\partial \zeta_i^l}{\partial p^k} + \Theta(\varepsilon^2) \right]_l (p) \quad (107)$$

are well-defined, where δ_q^l is the delta function and we assume that $X_{i,j}|_p = [\zeta_{i,j}^1(p), \dots, \zeta_{i,j}^l(p), \dots, \zeta_{i,j}^n(p)]^T$. Using (106) and (107), $d\mathcal{T}_{\exp(\varepsilon X_j)}[X_i|_{\exp(-\varepsilon X_j).p}]$ could be reformulated as:

$$\begin{aligned} &= \left[\zeta_i^q + \varepsilon \left(\sum_{k=1}^m \zeta_j^k \frac{\partial \zeta_j^k}{\partial p^k} - \zeta_j^k \frac{\partial \zeta_i^q}{\partial p^k} \right) + \Theta(\varepsilon^2) \right]_q (p) \\ &= [\zeta_i^q + \varepsilon [X_i, X_j]^q + \Theta(\varepsilon^2)]_q (p), \end{aligned} \quad (108)$$

where $[X_i, X_j]^q$ is the q^{th} component of the vector field generated by Lie bracket of X_i and X_j . Since $\mathfrak{g}$ is a vector space (which is closed under scalar multiplication and vector addition) and $\varepsilon > 0$, we may conclude that $[X_i, X_j] \in \mathfrak{g}$.

E The Proof of Proposition 2

Let $\mathcal{T}_j : \mathcal{P} \rightarrow \mathcal{P}$ as defined in (32) for a fixed $0 < \varepsilon^j \ll 1 \in \mathbb{R}$. To prove Proposition 2, $(X_j|_p)^n : \mathcal{P} \rightarrow \mathcal{P}$, $\forall n \geq 1$ should be treated as an *operator* acting on prolonged space $\mathcal{P}$. Let $p \in \mathcal{P}$ and $(X_j|_p)^0 \equiv p$. Then:

$$(X_j|_p)^1 = \sum_{i_1=1}^r \zeta^{i_1}(p) \partial / \partial p^{i_1}, \quad (109)$$

i.e. evaluation of vector field at that point. Defining the operator for $n = 2$ allows one to easily grasp the general iterative formula that will be given in (111):

$$(X_j|_p)^2 = \sum_{i_1=1}^r \left(\sum_{i_2=1}^r \zeta^{i_2}(p) \frac{\partial \zeta^{i_1}(p)}{\partial p^{i_2}} \right) \partial / \partial p^{i_1}. \quad (110)$$

Using the same procedure employed both in (109) and (110) which treats $X_j = \sum_{i=1}^r \zeta^i(\cdot) \partial/\partial p^i$ as an operator eating a position vector $p \in \mathcal{P}$ and spitting out a vector $v \in \mathbb{R}^m$, the $(X_j|_p)^n$ for any $n \geq 1$ becomes:

$$(X_j|_p)^n = \sum_{i_1=1}^r \left\{ \sum_{i_2=1}^r \zeta^{i_2}(p) \frac{\partial}{\partial p^{i_2}} \left\{ \dots \sum_{i_{n-2}=1}^r \zeta^{i_{n-2}}(p) \frac{\partial}{\partial p^{i_{n-2}}} \left\{ \sum_{i_{n-1}=1}^r \zeta^{i_{n-1}}(p) \frac{\partial \zeta^{i_1}}{\partial p^{i_{n-1}}}(p) \right\} \dots \right\} \right\} \partial/\partial p^{i_1}. \quad (111)$$

Now, suppose that we have two position vectors $p_1, p_2 \in \mathcal{P}$ that are sufficiently close w.r.t. Euclidean norm induced by inner product defined over $\mathbb{R}^m$. Observe that it is not necessary to define a metric on manifold, $\mathcal{N}$, for this proof, because we will use the fact that $\mathcal{T}_j$ could be rewritten in terms of X_j and $X_j: \mathcal{P} \rightarrow \mathbb{R}^m$ and $p_2 - p_1 \in \mathbb{R}^m$. From **Theorem 1** in [16], we know that the following should be satisfied:

$$\begin{aligned} \|\mathcal{T}_j \cdot p_2 - \mathcal{T}_j \cdot p_1\| &= \|p_2 - p_1 + \gamma_j(p_2, \varepsilon^j) - \gamma_j(p_1, \varepsilon^j)\| \\ &\leq \|p_2 - p_1\| + \|\gamma_j(p_2, \varepsilon^j) - \gamma_j(p_1, \varepsilon^j)\| \\ &\leq \|p_2 - p_1\| + L_j \|p_2 - p_1\| \\ &= (1 + L_j) \|p_2 - p_1\|, \end{aligned} \quad (112)$$

where $L_j < 1$ is the Lipschitz constant for $\gamma^j(\cdot, \varepsilon^j)$ and $\gamma_j(\cdot, \varepsilon^j)$ is as defined in (32). Let $\|X_j(p_2) - X_j(p_1)\| \leq K_j \|p_2 - p_1\|$, i.e. K_j is the Lipschitz constant for X_j . Then:

$$\|(X_j)^n|_{p_2} - (X_j)^n|_{p_1}\| \leq K_j \|(X_j)^{n-1}|_{p_2} - (X_j)^{n-1}|_{p_1}\| \dots \leq K_j^n \|p_2 - p_1\|. \quad (113)$$

By using the equality in (32) and the outcome from (113), (112) can be reformulated as follows:

$$\begin{aligned} \|\mathcal{T}_j \cdot p_2 - \mathcal{T}_j \cdot p_1\| &\leq \|p_2 - p_1\| + \|\gamma_j(p_2, \varepsilon^j) - \gamma_j(p_1, \varepsilon^j)\| \\ &= \|p_2 - p_1\| + \left\| \varepsilon^j (X_j|_{p_2} - X_j|_{p_1}) + \frac{(\varepsilon^j)^2}{2!} \left((X_j)^2|_{p_2} - (X_j)^2|_{p_1} \right) + \dots \right\| \\ &\leq \|p_2 - p_1\| + \left\| \varepsilon^j (X_j|_{p_2} - X_j|_{p_1}) \right\| + \left\| \frac{(\varepsilon^j)^2}{2!} \left((X_j)^2|_{p_2} - (X_j)^2|_{p_1} \right) \right\| + \dots \\ &\leq \|p_2 - p_1\| + \varepsilon^j K_j \|p_2 - p_1\| + \frac{(\varepsilon^j)^2}{2!} K_j^2 \|p_2 - p_1\| + \dots \\ &= e^{(\varepsilon^j K_j)} \|p_2 - p_1\|. \end{aligned} \quad (114)$$

Comparing (112) against (114), we can conclude that:

$$1 + L_j = e^{(\varepsilon^j K_j)} \implies L_j = e^{(\varepsilon^j K_j)} - 1. \quad (115)$$

However, since $L_j < 1$:

$$e^{(\varepsilon^j K_j)} - 1 < 1 \implies \varepsilon^j K_j < \ln(2) \implies K_j < \frac{\ln(2)}{\varepsilon^j}. \quad (116)$$

F The Order of Magnitude assoc. with the Error in Proposition 3

Our goal is to show that the following ((48) in Subsection 4.3) is equivalent to the statement in (51) in Proposition 3:

$$\Delta \bar{u}_{\bar{x}^i 1 \dots \bar{x}^i k-1} = \sum_{l=1}^d \Delta \bar{x}^l [\mathcal{T}_j \cdot p]^{u_{x^1 \dots x^i k-1} x^l} + \Theta(\|\Delta \bar{\mathcal{X}}(\Delta^q \mathcal{X}, \varepsilon^j)\|^2), \forall p \in \mathcal{N}, \quad (117)$$

where $j = 1, \dots, r$, $k = 1, \dots, O$, $\Delta \bar{\mathcal{X}} = [\Delta \bar{x}^1, \dots, \Delta \bar{x}^d]^T$, and $\Delta^q \mathcal{X} = [0, \dots, \Delta x^q, 0, \dots, 0]^T$. Assume that vector field X_j 's component functions for independent and dependent directions are as given in (50). Assume further that $|\Delta x^q|$ and $|\varepsilon^j|$ are

sufficiently small, where $q = 1, \dots, d$, $j = 1, \dots, r$, d is the dimension of the domain in which solutions reside, and $r = \dim(\mathfrak{g})$. By exploiting the fact in (49):

$$\begin{aligned}\bar{u}_{\bar{x}^1 \dots \bar{x}^{j_{k-1}}} (p + \Delta^q p, \varepsilon^j) &= u_{x^1 \dots x^{j_{k-1}}} (\mathcal{X} + \Delta^q \mathcal{X}) + \varepsilon^j \eta^{x^1 \dots x^{j_{k-1}}} (p + \Delta^q p) + \Theta \left((\varepsilon^j)^2 \right) \\ \bar{u}_{\bar{x}^1 \dots \bar{x}^{j_{k-1}}} (p, \varepsilon^j) &= u_{x^1 \dots x^{j_{k-1}}} (\mathcal{X}) + \varepsilon^j \eta^{x^1 \dots x^{j_{k-1}}} (p) + \Theta \left((\varepsilon^j)^2 \right),\end{aligned}\quad (118)$$

where $\mathcal{X} = [x^1, \dots, x^d]^T$, and $\Delta^q p$ is as defined in (52). Moreover, since we suppose that u is sufficiently smooth:

$$u_{x^1 \dots x^{j_{k-1}}} (\mathcal{X} + \Delta^q \mathcal{X}) - u_{x^1 \dots x^{j_{k-1}}} (\mathcal{X}) = \Delta^q \mathcal{X} u_{x^1 \dots x^{j_{k-1} x^q}} (\mathcal{X}) + \Theta \left(|\Delta x^q|^2 \right). \quad (119)$$

We should make good use of two equations in (118) to approximate $\Delta \bar{u}_{\bar{x}^1 \dots \bar{x}^{j_{k-1}}}$. It is simply subtracting the second equation from the first one in (118). Then substituting RHS of (119) into this result and collecting common terms yield LHS of (117) (under the assumption that our group action for $\varepsilon^j > 0$ maps nearby points $\mathcal{X}$ and $\mathcal{X} + \Delta^q \mathcal{X}$ to again nearby points $\mathcal{X}$ and $\mathcal{X} + \Delta \mathcal{X}$ respectively):

$$\Delta \bar{u}_{\bar{x}^1 \dots \bar{x}^{j_{k-1}}} = \varepsilon^j \left(\eta^{x^1 \dots x^{j_{k-1}}} (p + \Delta^q p) - \eta^{x^1 \dots x^{j_{k-1}}} (p) \right) + \Delta^q \mathcal{X} u_{x^1 \dots x^{j_{k-1} x^q}} (\mathcal{X}) + \Theta \left(|\Delta x^q|^2 \right) + \Theta \left((\varepsilon^j)^2 \right). \quad (120)$$

As for RHS of (117), observe that:

$$\begin{aligned}\bar{x}^l (p + \Delta^q p, \varepsilon^j) &= x^l + \delta_q^l \Delta x^q + \varepsilon^j \xi^{x^l} (p + \Delta^q p) + \Theta \left((\varepsilon^j)^2 \right), \\ \bar{x}^l (p, \varepsilon^j) &= x^l + \varepsilon^j \xi^{x^l} (p) + \Theta \left((\varepsilon^j)^2 \right), \text{ and} \\ [\mathcal{J}_j \cdot p]^{u_{x^1 \dots x^{j_{k-1} x^l}}} &= u_{x^1 \dots x^{j_{k-1} x^l}} (\mathcal{X}) + \varepsilon^j \eta^{x^1 \dots x^{j_{k-1} x^l}} (p) + \Theta \left((\varepsilon^j)^2 \right),\end{aligned}\quad (121)$$

by again using (49), where δ_q^l is Dirac delta function. Like in (120), to obtain $\Delta \bar{x}^l$ we subtract the second equation from the first one in (121):

$$\Delta \bar{x}^l = \delta_q^l \Delta x^q + \varepsilon^j \left(\xi^{x^l} (p + \Delta^q p) - \xi^{x^l} (p) \right) + \Theta \left((\varepsilon^j)^2 \right). \quad (122)$$

Therefore, RHS of (117) becomes:

$$\begin{aligned}& \sum_{l=1}^d \underbrace{\left(\delta_q^l \Delta x^q + \varepsilon^j \left(\xi^{x^l} (p + \Delta^q p) - \xi^{x^l} (p) \right) \right)}_{\approx \Delta \bar{x}^l} \underbrace{\left(u_{x^1 \dots x^{j_{k-1} x^l}} (\mathcal{X}) + \varepsilon^j \eta^{x^1 \dots x^{j_{k-1} x^l}} (p) \right)}_{\approx [\mathcal{J}_j \cdot p]^{u_{x^1 \dots x^{j_{k-1} x^l}}}} + \\ & \Theta \left((\varepsilon^j)^2 \right) + \Theta \left(\|\Delta \mathcal{X} (\Delta^q \mathcal{X}, \varepsilon^j)\|^2 \right).\end{aligned}\quad (123)$$

Collecting $\Theta \left((\varepsilon^j)^2 \right)$ introduced in both (120) and (123) on LHS, and doing necessary cancellations in order, we obtain:

$$\begin{aligned}& \varepsilon^j \left(\eta^{x^1 \dots x^{j_{k-1}}} (p + \Delta^q p) - \eta^{x^1 \dots x^{j_{k-1}}} (p) \right) + \Theta \left(|\Delta x^q|^2 \right) + \Theta \left((\varepsilon^j)^2 \right) = \\ & \varepsilon^j \left\{ \sum_{l=1}^d u_{x^1 \dots x^{j_{k-1} x^l}} \left[\xi^{x^l} (p + \Delta^q p) - \xi^{x^l} (p) \right] + \Delta x^q \eta^{x^1 \dots x^{j_{k-1} x^q}} (p) \right\} + \Theta \left(\|\Delta \mathcal{X} (\Delta^q \mathcal{X}, \varepsilon^j)\|^2 \right),\end{aligned}\quad (124)$$

where we introduce additional errors $\Theta \left(|\Delta x^q|^2 \right)$ and $\Theta \left((\varepsilon^j)^2 \right)$ due to approximation in (118), (119), and (121). It could be realized that as $\Delta x^q, \varepsilon^j \rightarrow 0$, equality in (124) is satisfied. On the other hand; only if $\varepsilon^j \rightarrow 0$, then the group action disappears and we are only left with (see (122) for what happens to $\Theta \left(\|\Delta \mathcal{X} (\Delta^q \mathcal{X}, \varepsilon^j)\|^2 \right)$ when $\varepsilon^j \rightarrow 0$):

$$\Theta \left(|\Delta x^q|^2 \right) = \Theta \left(|\Delta x^q|^2 \right). \quad (125)$$

Furthermore; only if $\Delta x^q \rightarrow 0$, then:

$$\Theta \left((\varepsilon^j)^2 \right) \neq 0, \quad (126)$$

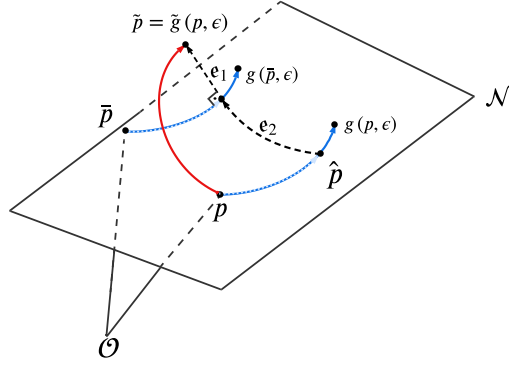


Figure 20. Numerical errors induced by translating a solution u to $\tilde{u}$ once the translation $\tilde{p} = \tilde{g}(p, \epsilon)$ is executed in prolonged space $\mathcal{P}$. Two types of error occur: (i) ϵ_1 : Diverging from solution manifold $\mathcal{N}$, which violates our constraint to stay on the manifold, and (ii) ϵ_2 : Moving away from the correct integral curve generated by true group action $g(p, \epsilon)$, which violates the translated solution's consistency with its derivatives.

is obtained. Frankly, this is the expected behaviour of this approximation scheme. Notice that the approximation errors $\Theta((\epsilon^j)^2)$ induced in (120) and (122) die out as $\Delta x^q \rightarrow 0$ regardless of the value of ϵ^j . However, the last equation in (121) has no $\Delta^q \mathcal{X}$ term involved and hence, its error term $\Theta((\epsilon^j)^2)$ is not affected by any behaviour of Δx^q .

In summary, we assume that the error terms $\Theta(|\Delta x^q|^2)$, $\Theta((\epsilon^j)^2)$, and $\Theta(\|\Delta^q \mathcal{X}(\Delta^q \mathcal{X}, \epsilon^j)\|^2)$ are *negligible* if $|\Delta x^q|$ and $|\epsilon^j|$ are sufficiently small. Thus, ignoring these error terms, we try to approximate LHS of (124) to its RHS up to a certain threshold.

G The Errors Induced by Group Actions & The Retraction Map

Due to various truncation errors, numeric errors inherent to sample dataset generation, etc.; our one-parameter group action $\tilde{g}(p, \epsilon)$ (i.e. $\mathcal{T}.p$) is not ideal. We can summarize all these errors in two broad categories: (i) Violating our constraint $\mathcal{C}_1$ in (55) and (ii) Violating our consistency cost $\mathcal{C}\mathcal{C}$ specified in (53). Both errors are depicted in Figure-20 as ϵ_1 and ϵ_2 in order. Our experiments, as discussed in 5.4, show us that the consistency of translated solution is not affected as much as constraints that enforce solutions to stay on the manifold $\mathcal{N}$, thanks to $\mathcal{C}\mathcal{C}$ introduced in (58). In fact, it could be ignored once projection onto $\mathcal{N}$ is properly done. Therefore, in this study we do not focus on fixing ϵ_2 after every translation; but rather on fixing ϵ_1 , which spirals out of control upon thousands of translations as shown in Table-2 and Table-3.

This could be mitigated by a process called “**retraction**” in differential geometry. It is an idea based on “*Whitney approximation theorem*” for functions. By **Proposition 6.25** in [33], any embedded manifold has a retraction map from its tubular neighbourhood (see Figure-10) to the manifold itself, i.e. $r : U \rightarrow \mathcal{N}$, where $U \subset \mathcal{R}^m$ is an ϵ -neighbourhood lying within tubular neighbourhood of $\mathcal{N}$. Besides, the manifolds we are interested in are embedded into $\mathcal{P}$. In the case of linear DEs, r is as simple as a projection from U to $\mathcal{N}$, i.e.:

$$r(s_k^i) = \tilde{s}_k^i = s_k^i - \langle s_k^i, \vec{n} \rangle \vec{n}, \quad (127)$$

where $\langle \cdot, \cdot \rangle$ is inner product and $\vec{n}$ is the unit normal vector for hyperplane generated by a given set of linear DEs and $i = 1, \dots, N$, and N stands for how many times group action is applied in a subsequent manner. For instance, in the case of wave equation in 2-D $\vec{n}|_p = [00 \dots 010010^{-1}/c^2]$, where c is DE constant and $p \in \mathcal{N}$. The same experiments in 5.4 are conducted with retraction map, r , included this time. At every i^{th} step, the output of group action, g_j , is subject to retraction as given below:

$$s_k^i = g_j.s_k^{i-1} \text{ then, } \tilde{s}_k^i = r(s_k^i). \quad (128)$$

Results are summarized in Table-4 and Table-5 respectively. It is obvious that retraction strives to keep points on the manifold, $\mathcal{N}$, and hence output of subsequent group actions does not diverge from $\mathcal{N}$.

Subgroup Idx (j)		C_{I_j}	CC
#g=1	2	3.391e-13	8.817e-11
	3	1.605e-13	5.143e-11
	4	1.994e-13	5.205e-12
	5	3.317e-13	1.811e-12
	6	3.081e-13	4.720e-12
	7	1.846e-13	7.727e-12
	8	2.064e-13	1.700e-15
	9	1.379e-13	3.750e-12
	10	1.757e-13	9.372e-11
	11	1.341e-13	1.831e-14
	12	1.923e-13	2.657e-13
#g=1000	2	2.619e-13	8.817e-11
	3	3.369e-13	5.143e-11
	4	2.135e-13	5.205e-12
	5	2.590e-13	1.811e-12
	6	2.119e-13	4.720e-12
	7	2.572e-13	7.727e-12
	8	1.664e-13	1.700e-15
	9	1.339e-13	3.750e-12
	10	3.230e-13	9.372e-11
	11	1.305e-13	1.831e-14
	12	3.439e-13	2.657e-13

Table 4. Quality of generalization in the case of spatial region shift with retraction, where #g stands for number of group actions applied to the initial solution. Compare this against the entries in Table-2.

Subgroup Idx (j)		C_{I_j}	CC
#g=1	2	2.950e-13	8.116e-10
	3	3.212e-13	5.136e-10
	4	3.789e-13	2.833e-11
	5	1.577e-13	3.984e-12
	6	1.984e-13	3.705e-11
	7	1.508e-13	4.608e-11
	8	2.714e-13	6.238e-14
	9	2.369e-13	2.662e-11
	10	2.571e-13	5.485e-10
	11	2.089e-13	1.049e-12
	12	2.060e-13	4.619e-12
#g=1000	2	2.738e-13	8.116e-10
	3	2.808e-13	5.136e-10
	4	1.126e-13	2.833e-11
	5	1.537e-13	3.984e-12
	6	3.508e-13	3.705e-11
	7	1.439e-13	4.608e-11
	8	2.762e-13	6.238e-14
	9	2.231e-13	2.662e-11
	10	3.249e-13	5.485e-10
	11	3.208e-13	1.049e-12
	12	3.915e-13	4.619e-12

Table 5. Quality of generalization in the case of initial condition u_{I_0} set to (87) with retraction, where #g stands for number of group actions applied to the initial solution. Compare this against the entries in Table-3.

H Algorithms

Algorithm 1: Computing $(X_j|_p)^n$ for $n \geq 2$

```
def computeVecFiAct ( $X_j|_p$ ,  $actGrad$ ) :  
    // Take inner prod. to calc. the action of  $X_j|_p$  on itself for  
    //  $k$  times, where  $k$  is the order of derivatives stored in  $actGrad$   
    for  $i$  in range(1.. $n$ ):  
         $actVF[i] \leftarrow \text{dotProd}(X_j|_p, actGrad[i]);$   
    return  $actVF$   
def computeAllOrders ( $expOrder$ ,  $p$ ,  $j$ ) :  
    global  $actionsList \leftarrow [];$   
    // The first order is equal to the evaluation of  $X_j|_p$  itself  
     $X_j|_p \leftarrow \text{iResNETBlock}(j, p);$   
     $actionsList.append(X_j|_p);$   
    for  $o$  in range(1.. $expOrder$ ):  
         $gradP[i] \leftarrow \text{grad}(actionsList[i-1], p);$   
         $(X_j|_p)^o \leftarrow \text{computeVecFiAct}(X_j|_p, gradP);$   
         $actionsList.append((X_j|_p)^o);$   
    return  $actionsList$ 
```

Algorithm 2: The cost function to be minimized for enforcing linear independence of $\{X_1, \dots, X_r\}|_p$

```
def costFuncAtPt ( $p$ ) :  
    // Extract  $X_1|_p$  and  $X_2|_p$   
     $X_1|_p \leftarrow \text{iResNETBlock}(1, p);$   
     $X_2|_p \leftarrow \text{iResNETBlock}(2, p);$   
    // To span  $\mathcal{V}_2$   
     $\mathcal{J}|_p \leftarrow \left( \frac{\langle X_1|_p, X_2|_p \rangle}{\|X_1|_p\|_2 \|X_2|_p\|_2} \right)^2;$   
    for  $i$  in range(3.. $n$ ):  
         $X_i|_p \leftarrow \text{iResNETBlock}(i, p);$   
         $X_{||i}|_p \leftarrow M_{i-1}|_p X_i|_p;$   
        // To span  $\mathcal{V}_i$  in an incremental fashion  
         $\mathcal{J}|_p \leftarrow \mathcal{J}|_p + \left( \frac{\langle X_i|_p, X_{||i}|_p \rangle}{\|X_i|_p\|_2 \|X_{||i}|_p\|_2} \right)^2;$   
    return  $\mathcal{J}|_p$ 
```

```

def nrmCost (L, R) :
     $N \leftarrow \frac{(L-R)^2}{(|L|+|R|)^2+\delta};$ 
    return N;
def measureLI (sk, Gθ, j) :
    Xj|p ← iResNETBlock (j, sk);
    X||j|p ← Mj-1Xj|p;
    linIndCost ←  $\left( \frac{\langle X_{j|p}, X_{||j|p} \rangle}{\|X_{j|p}\|_2 \|X_{||j|p}\|_2} \right)^2;$ 
    return linIndCost;
def cmpMinMax (value, minRef, maxRef) :
    if maxRef.value < 0.0 or maxRef.value < value:
        maxRef.value ← value;
    elif minRef.value < 0.0 or minRef.value > value:
        minRef.value ← value;
def trainSubgrp (Γ, Gθ, j,  $\tilde{\Gamma}$ ) :
    bestModel ← None;
    for bq ← nextBatch (Γ) :
        maxℓ1j, minℓ1j, maxℓ2j, minℓ2j ← -1.0;
        finalCostj ← zeros (|bq|);
        for sk ← nextItem (bq) :
            // no other subgroup to measure linear-ind
            if j > 0:
                ℒj|sk ← measureLI (sk, Gθ, j);
            else:
                ℒj|sk ← 0.0;
                ℓ1j|sk ← max { || $\mathcal{D}(\mathcal{T}_j.s_k)$ ||2 - κ1, 0.0 };
                cmpMinMax (ℓ1j|sk, maxℓ1j, minℓ1j);
                ℓ2j|sk ← κ2 - [σ1j, ..., σij, ..., σNjj]T|sk;
                cmpMinMax (ℓ2j|sk, maxℓ2j, minℓ2j);
                ℛℳjLHS|sk ←  $\frac{1}{m.(j-1)} \sum_{i=1}^{j-1} \sum_{q=1}^m \mathcal{R}\mathcal{S}_{ij}^{\text{LHS}q}|_{s_k};$ 
                ℛℳjRHS|sk ←  $\frac{1}{m.(j-1)} \sum_{i=1}^{j-1} \sum_{q=1}^m \mathcal{R}\mathcal{S}_{ij}^{\text{RHS}q}|_{s_k};$ 
                 $\tilde{\mathcal{R}}\mathcal{S}_j|_{s_k} \leftarrow \text{nrmCost}(\mathcal{R}\mathcal{S}_j^{\text{LHS}}|_{s_k}, \mathcal{R}\mathcal{S}_j^{\text{RHS}}|_{s_k});$ 
                ℓℓjLHS|sk ←  $\frac{1}{d} \sum_{q=1}^d \mathcal{C}\mathcal{C}_j^{\text{LHS}q}|_{s_k};$ 
                ℓℓjRHS|sk ←  $\frac{1}{d} \sum_{q=1}^d \mathcal{C}\mathcal{C}_j^{\text{RHS}q}|_{s_k};$ 
                 $\tilde{\mathcal{C}}\mathcal{C}_j|_{s_k} \leftarrow \text{nrmCost}(\mathcal{C}\mathcal{C}_j^{\text{LHS}}|_{s_k}, \mathcal{C}\mathcal{C}_j^{\text{RHS}}|_{s_k});$ 
                 $\tilde{\mathcal{J}}_j^I|_{\tilde{s}_k} \leftarrow \text{nrmCost}(\mathcal{T}_j^{-1}.\tilde{s}_k, s_k);$ 
                exℓ1j ←  $\frac{(\max_{\ell_{1j}} + \min_{\ell_{1j}})}{2.0};$ 
                exℓ2j ←  $\frac{(\max_{\ell_{2j}} + \min_{\ell_{2j}})}{2.0};$ 
                for k in range (|bq|) :
                    ℓ̄1j|sk ←  $\bar{\sigma}(\text{ex}_{\ell_{1j}}) \Upsilon(\ell_{1j}|_{s_k});$ 
                    ℓ̄2j|sk ←  $\sum_{i=1}^{N_j} \bar{\sigma}(\text{ex}_{\ell_{2j}}) \Upsilon(\ell_{2ij}|_{s_k});$ 
                    finalCostj[k] ← ℒj|sk +  $\tilde{\mathcal{R}}\mathcal{S}_j|_{s_k} + \tilde{\mathcal{J}}_j^I|_{\tilde{s}_k} + \mathcal{C}\mathcal{C}_j|_{s_k} + \tilde{\Psi}_t(\ell̄_{1j}|_{s_k}) + \tilde{\Psi}_t(\ell̄_{2j}|_{s_k});$ 
                finalCostj ← mean (finalCostj);
                finalCostj.backward();
            // end of inner for-loop
        bestModel ← validate (Gθ,  $\tilde{\Gamma}$ );
    return bestModel;
    
```

Algorithm 3: Training loop for learning symmetries (cnt.)

```
def mainLoop( $\Gamma$ ,  $\tilde{\Gamma}$ ,  $G_\theta$ , TRIES) :  
    numTries  $\leftarrow$  TRIES;  
    failed  $\leftarrow$  [];  
    grpsToTrain  $\leftarrow$   $G_\theta$ ;  
    while len (grpsToTrain) > 0 and numTries > 0:  
        for  $G_j$  in grpsToTrain:  
            setRandomSeed(j + numTries);  
            bestModel  $\leftarrow$  None;  
            for ep in range (numEpoch) :  
                bestModel  $\leftarrow$  trainSubgrp( $\Gamma$ ,  $G_\theta$ , j,  $\tilde{\Gamma}$ );  
                // Freeze its weights and finalize its training  
            if not bestModel:  
                failed.append(j);  
            else:  
                finalize( $G_\theta[j]$ );  
                // Reinitialize the entire  $G_\theta$ ; but substitute weights  
                // of subgroups which succeed to be trained  
             $G_\theta \leftarrow$  reinitialize(j, failed);  
    grpsToTrain  $\leftarrow$  failed;  
    numTries  $\leftarrow$  numTries - 1;  
    failed  $\leftarrow$  [];  
return  $G_\theta$ 
```
