

1 bLAT Layer

Definition 1. *The bi-Lipschitz affine transformation (bLAT) layer is given by the transformation, $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$, defined by*

$$f(x) = U\Sigma V^T x + b, \quad (1)$$

where $U \in \mathbb{R}^{M \times r}$, $V \in \mathbb{R}^{r \times N}$, $\Sigma \in \mathbb{R}^{r \times r}$, $b \in \mathbb{R}^M$, $r = \min(M, N)$, U and V are orthogonal matrices satisfying $U^T U = V^T V = I$, and

$$\Sigma = \text{diag} \begin{bmatrix} \sigma_1 & \dots & \sigma_r \end{bmatrix}, \quad (2)$$

where $\frac{1}{L} \leq \sigma_i \leq L$ for $i = 1, \dots, r$ and some $L \geq 1$. When $M = N$, the mapping is invertible.

$$f^{-1}(x) = V\Sigma^{-1}U^T(x - b). \quad (3)$$

Our new contribution is to include the matrix term $U\Sigma V^T$, which is written as a singular value decomposition (SVD), which exists for every matrix in $\mathbb{R}^{M \times N}$. One advantage of the bLAT layer is the following theorem.

Theorem 1. *The forward and inverse bLAT layers are both L -bi-Lipschitz.*

This follows from the fact that $\frac{1}{L} \leq \|\nabla f(x)\|_2 \leq L$ and $\frac{1}{L} \leq \|\nabla f^{-1}(x)\|_2 \leq L$. Another advantage of using the SVD is that, by construction, the evaluation of $f(x)$ and $f^{-1}(x)$ have an equivalent computational cost. In our implementation of the $M = N$ case, the orthogonal matrices of the bLAT layers are parameterized using the matrix exponential of a skew-symmetric matrix input, i.e. $U = \text{expm}(S)$, where $S = -S^T$. When $M \neq N$, the orthogonal matrices are parameterized using the Householder factorization.

2 Orthogonal/Unitary Parameterizations

2.1 Matrix Exponential

Let $S \in \mathbb{C}^{M \times M}$ be a skew symmetric matrix ($S = -S^T$), then

$$U = \text{expm}(S) \quad (4)$$

is unitary. (Note: when $S \in \mathbb{R}^{M \times M}$, then U is orthogonal.)

2.2 Householder

The notes in this section were originally written to help with implementation of code. Consider an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$. The Householder decomposition is defined by

$$Q = Q_n \dots Q_1, \quad (5)$$

$$Q^T = Q_1^T \dots Q_n^T = Q_1 \dots Q_n, \quad (6)$$

Where Q_1, \dots, Q_n are symmetric elementary orthogonal matrices defined by

$$Q_k = \begin{bmatrix} I_{N-k \times N-k} & 0 \\ 0 & F_k \end{bmatrix}, \quad F_k = I_{k \times k} - 2 \frac{v_k v_k^T}{v_k^T v_k}, \quad v_k \in \mathbb{R}^k. \quad (7)$$

We can also define Q_k using

$$Q_k = \tilde{F}_k = I_{N \times N} - 2 \frac{\tilde{v}_k \tilde{v}_k^T}{\tilde{v}_k^T \tilde{v}_k}, \quad \tilde{v}_k = \begin{bmatrix} 0 \\ v_k \end{bmatrix} \in \mathbb{R}^N. \quad (8)$$

Note that Q_k is symmetric.

$$\tilde{F}_k^T = I_{N \times N} - 2 \frac{\tilde{v}_k \tilde{v}_k^T}{\tilde{v}_k^T \tilde{v}_k} \quad (9)$$

Matrix action of Q_k :

$$Q_k y = y - 2 \frac{\tilde{v}_k \tilde{v}_k^T}{\tilde{v}_k^T \tilde{v}_k} y, \quad (10)$$

Consider $y \in \mathbb{R}^M$ $Q \in \mathbb{R}^{M \times N}$, $\tilde{v}_k \in \mathbb{R}^N$, then

$$y^T Q_k = y^T - 2 \frac{\tilde{v}_k^T}{\tilde{v}_k^T \tilde{v}_k} (y^T \tilde{v}_k). \quad (11)$$

2.3 Polcari

Orthogonal matrices can be parameterized using the Polcari decomposition, which was originally introduced in [?]. Given an orthogonal matrix, $Q \in \mathbb{R}^{N \times N}$, then Q can be decomposed as

$$Q = \Psi(w_{N-1}) \dots \Psi(w_1) S(\varphi_1, \dots, \varphi_N), \quad (12)$$

where $w_j \in \{x : x \in \mathbb{R}^j, \|x\|_2 \leq 1\}$, for $j = 1, \dots, N-1$, and $\varphi_1, \dots, \varphi_N \in \{1, -1\}$, and

$$\Psi(w_j) = \begin{bmatrix} I_j - \frac{w_j w_j^T}{1 + \sqrt{1 - w_j^T w_j}} & w_j \\ -w_j^T & \sqrt{1 - w_j^T w_j} \\ & & I_{N-j-1} \end{bmatrix}, \quad i = 1, \dots, N-1,$$

$$S(\varphi_1, \dots, \varphi_N) = \begin{bmatrix} \varphi_1 & & \\ & \ddots & \\ & & \varphi_N \end{bmatrix}.$$

Here, I_d represents a $d \times d$ identity matrix. Note that a vector, $v_j \in \mathbb{R}^i$, can be projected inside the unit ball, $w_j \in \{x : x \in \mathbb{R}^j, \|x\|_2 \leq 1\}$, using a transformation such as

$$w_j = \rho_j \frac{v_j}{\|v_j\|}, \quad \rho_j = \tanh(\|v_j\|) \in [0, 1].$$

The decomposition in (??) can be used as a parameterization to express any orthogonal matrix. Given an orthogonal matrix, $Q \in \mathbb{R}^{N \times N}$, the parameters of the Polcari decomposition can be uniquely determined. Consider the following properties.

1. $\Psi(w_j)$ for $j = 1, \dots, N-1$ and S are orthogonal matrices and therefore, by construction, the right-hand-side of (??) is orthogonal.
2. $\Psi(w_j)e_k = e_k$ for $k > j+1$, where e_k is a vector with a 1 in the k^{th} component and 0's elsewhere.
3. $P_{(k-1)N}\Psi(w_{k-1})e_k = w_{k-1}$, for $k = 2, \dots, N$, where $P_{(k-1)N}$ is an identity matrix of size $(k-1) \times N$.
4. $e_k^T \Psi(w_{k-1})e_k = \sqrt{1 - w_{k-1}^T w_{k-1}}$, for $k = 2, \dots, N$.
5. $P_{(k-1)N}\Psi(w_{k-1}) \dots \Psi(w_1)Se_k = \varphi_k w_{k-1}$, for $k = 2, \dots, N$. This follows from (2) and (3).
6. $e_k^T \Psi(w_{k-1}) \dots \Psi(w_1)Se_k = \varphi_k \sqrt{1 - w_{k-1}^T w_{k-1}}$ for $k = 2, \dots, N$. This follows from (2) and (4).

Using properties (5) and (6) for $k = N$, we have

$$P_{N-1,N}Qe_N = \varphi_N w_{N-1}, \quad e_N^T Qe_N = \varphi_N \sqrt{1 - w_{N-1}^T w_{N-1}},$$

and therefore

$$w_{N-1} = \varphi_N P_{N-1,N}Qe_N, \quad \varphi_N = \text{sign}(e_N^T Qe_N).$$

Suppose that w_k, \dots, w_{N-1} is known. We can obtain relations for w_{k-1} and φ_k using properties (5) and (6).

$$\begin{aligned} P_{(k-1)N}\Psi(w_k)^T \dots \Psi(w_{N-1})^T Qe_k &= \varphi_k w_{k-1}, \\ e_k^T \Psi(w_k)^T \dots \Psi(w_{N-1})^T Qe_k &= \varphi_k \sqrt{1 - w_{k-1}^T w_{k-1}}. \end{aligned}$$

Using this, general relations for w_k and φ_k for all k can be obtained.

$$w_k = \varphi_{k+1} P_{k,N}\Psi(w_{k+1})^T \dots \Psi(w_{N-1})^T Qe_{k+1}, \quad k = 1, \dots, N-1, \quad (13a)$$

$$\varphi_k = \text{sign}(e_k^T \Psi(w_k)^T \dots \Psi(w_{N-1})^T Qe_k), \quad k = 1, \dots, N. \quad (13b)$$

An algorithm for determining the Polcari parameters would use (??) recursively, decrementing k from N to 1. Since the Polcari parameters can be uniquely determined, the following theorem can be stated.

Theorem 2. *The decomposition given by (??) is a parameterization for any orthogonal matrix in $\mathbb{R}^{N \times N}$.*

Note that since $S(\varphi_1, \dots, \varphi_N)US(\varphi_1, \dots, \varphi_N)^T = U$, $A(\theta_A)$ is invariant to the choice of $\varphi_1, \dots, \varphi_N$. For simplicity, we choose $\varphi_1 = \dots = \varphi_N = 1$ in our parameterization, since $S(1, \dots, 1) = I$.