Characterization of the Critical Sets of Quantum Unitary Control Landscapes

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Abstract

This work considers various families of quantum control landscapes (i.e. objective functions for optimal control) for obtaining target unitary transformations as the general solution of the controlled Schrödinger equation. We examine the critical topology of the kinematic landscapes $J_F(U) = \| (U - W) A \|^2$ and $J_P(U) = \| A \|^4 - |\text{Tr}(AA^\dagger W^\dagger U)|^2$ defined on the unitary group $\text{U}(N)$. The parameter matrix $A$ is allowed to be completely arbitrary, yielding an objective function that measures the difference in the actions of $U$ and the target $W$ on a subspace of state space. The analysis of this function includes a description of the structure of the critical sets of these kinematic landscapes and characterization of the critical points as maxima, minima, and saddles. In addition, we consider the question of whether these landscapes are Morse-Bott functions on $\text{U}(N)$. These results are then used to deduce properties of the critical set of the corresponding dynamical landscapes. Finally, landscapes based on the intrinsic (geodesic) distance on $\text{U}(N)$ and the projective unitary group $\text{PU}(N)$ are considered.

1 Introduction

An important application of quantum optimal control theory is the generation of target quantum logic gates for quantum information processing. The goal of such optimal control is to arrange the dynamics such that the desired logical gate is realized as the final time unitary evolution operator, which is the general solution of the controlled Schrödinger equation. Additionally, there may not be a single target gate, but a family of them. For example, since the global phase is not observable, the goal may be any unitary operator that is equivalent to the target gate up to global phase. Likewise, in some cases only a subspace of the Hilbert space of states may be used for the quantum register, so that any unitary propagator should be acceptable that acts as the target gate on that subspace. In contrast to other quantum control problems, for example
the maximization of a quantum mechanical observable, there is no unique or natural choice for the objective function against which the optimization is performed. Indeed, any smooth function \( J : U(\mathbb{N}) \to \mathbb{R} \) with a global minimum at the target unitary gate or gates is a candidate objective for the unitary problem. But, as we will see, some choices may have more favorable convergence and other properties.

Let \( \mathbb{K} \) denote the space of admissible control functions. For the present analysis, \( \mathbb{K} \) will be \( L^2(\mathbb{R}_+; \mathbb{R}) \), where \( T \) is some fixed final time over which the controlled dynamics take place. Let \( \mathbb{C}^{N \times N} \) possess the real Hilbert-Schmidt inner product \( \langle A, B \rangle = \Re \text{Tr}(A^\dagger B) \), and let \( U(\mathbb{N}) \subset \mathbb{C}^{N \times N} \) denote the \( N \times N \) unitary group endowed with the Riemannian metric induced by this inner product. Also let \( V_T : \mathbb{K} \to U(\mathbb{N}) \) denote the map, defined implicitly by the Schrödinger equation in the dipole approximation

\[
\frac{i \hbar}{\text{d}t} U(t, t_0) = (H_0 - \mu E(t)) U(t, t_0) \quad U(t_0, t_0) = I,
\]

(1)

such that \( V_T(E) = U(T, 0)[E] \) is the unitary propagator at time \( T \) for the control field \( E \). Finally, for any candidate objective function \( J : U(\mathbb{N}) \to \mathbb{R} \) (the “kinematic landscape”), let \( \tilde{J} : \mathbb{K} \to \mathbb{R} \) (the “dynamical landscape”) be the composition \( \tilde{J} = J \circ V_T \). Then

\[
\text{grad } \tilde{J}(E) = (d_E V_T)^* \left( \text{grad } J(V_T(E)) \right),
\]

(2)

where \( (d_E V_T)^* \) is the operator adjoint of the differential \( d_E V_T \). Much of the important information about the nature of the gradient flow of \( \tilde{J} \) is embodied in the critical points of this landscape, i.e. those fields \( E \in \mathbb{K} \) for which \( \text{grad } \tilde{J}(E) = 0 \). Any \( E \in \mathbb{K} \) such that \( d_E V_T \) is full rank and \( \text{grad } J(V_T(E)) = 0 \) (so-called “regular” critical points) will satisfy the condition. There may be other critical points where \( d_E V_T \) is rank-deficient and \( \text{grad } J(V_T(E)) \) may or may not be zero (“singular” points). Consideration of such singular points is important for a complete understanding on the dynamical control landscape. However, since \( V_T \) is a highly nonlinear map from an infinite dimensional space to a finite dimensional space, singular points are expected to be rare and will not be considered in the present analysis. Singular points and their role in quantum control landscapes have only recently begun to be analyzed \[3, 21\].

The critical points of the kinematic landscape having been identified, they may then be characterized as local maxima, local minima, and saddles. As has been demonstrated for other classes of kinematic quantum control landscapes \[8, 11, 12, 16, 19, 22, 23\], the landscapes considered in this work will turn out to have global maxima and minima, but no other local extrema. Moreover, the critical sets will be shown generally to comprise disjoint submanifolds, and these submanifolds are nondegenerate in the Morse-Bott sense. In other words, the null space of the Hessian of \( J \) and the tangent space of the critical submanifold coincide at each critical point \( U \in U(\mathbb{N}) \). This condition identifies the kinematic landscape as a Morse-Bott function, which is interesting for at least two reasons. First, certain results about the convergence of the gradient flow may be proved for Morse-Bott functions, in particular that (on a compact manifold) the gradient flow always converges to a critical point \[1\]. Second, the identification of the null space of the Hessian and the tangent space of the critical submanifold is important for certain numerical methods, such as second order D-MORPH \[2\], that are designed to explore the critical sets.
Several classes of landscapes for generating target unitary transformations will be considered. They include $J_F(U) = \|(U-W)A\|^2$ and $J_P(U) = \|A\|^4 - \|\text{Tr}(AA^\dagger W^\dagger U)\|^2$ for some fixed target $W \in \text{U}(N)$ and some arbitrary fixed $A \in \mathbb{C}^{N \times N}$, as well as the corresponding landscapes using the intrinsic (geodesic) distance on the unitary group $\text{U}(N)$ and the projective unitary group $\text{PU}(N)$, rather than the norm (Euclidean) distance in $J_F$ and $J_P$. Landscapes of the form $J_F$ and $J_P$ have been studied in the past [3,11,17]. The present paper extends these various works by broadening the families of landscapes under consideration, describing the structure of the critical submanifolds, and directly addressing the issue of Morse-Bott nondegeneracy of the critical submanifolds.

The paper is organized as follows. Sections 2 and 3 describe the critical points of the kinematic landscapes $J_F$ and $J_P$. In Section 4 these results are related back to the dynamical landscapes. The two additional landscapes based on geodesic distance are presented and analyzed in Section 5. The overall results are summarized in Section 6. Two appendices are included which provide a proof of the infinite Fréchet differentiability of the control-to-propagator map $V_T$ and a derivation of the gradient of the geodesic distance landscape on $\text{U}(N)$.

## 2  Kinematic Critical Point Analysis of $J_F(U) = \|(U-W)A\|^2$  

For now we put aside the dynamical component of the map and focus just on the critical point analysis of the kinematic map $J_F(U) = \|(U-W)A\|^2 = 2\|A\|^2 - 2\Re \text{Tr}(AA^\dagger W^\dagger U)$. In contrast to the landscape $J_P$ that will be the subject of the next section, the value of $J_F(U)$ depends upon the global phase of $U$. However, if $AA^\dagger$ has a null space, then $J_F(U)$ is invariant to the action of $U$ on that null space. This freedom allows for the possibility that $A$ is a projection matrix as discussed in [15].

### 2.1 Critical Point Identification

Let $D \in \text{U}(N)$ be a unitary matrix that diagonalizes $AA^\dagger$ such that $D^\dagger AA^\dagger D = \Omega^2$ with $\Omega^2_{jj} = \omega_j^2$ and $\omega_1^2 \geq \omega_2^2 \geq \cdots \geq \omega_k^2$. Let $\tilde{\omega}_1^2 > \cdots > \tilde{\omega}_k^2 > \tilde{\omega}_0^2 = 0$ denote the distinct eigenvalues of $AA^\dagger$, and let $\{n_1, \ldots, n_\kappa, n_0\}$ be the degeneracies of these eigenvalues. While $n_1, \ldots, n_\kappa$ are all strictly positive integers, $n_0$ may be either positive or zero. This distinction is made due to the special significance of the zero eigenvalues of $AA^\dagger$ in the analysis that follows. Suppose that $\tilde{D} \in \text{U}(N)$ is any unitary matrix such that $\tilde{D}\Omega^2\tilde{D}^\dagger = AA^\dagger = D\Omega^2D^\dagger$. Then $(D^\dagger \tilde{D})\Omega^2(D^\dagger \tilde{D})^\dagger = \Omega^2$, so that $D^\dagger \tilde{D}$ lies in the stabilizer subgroup of $\Omega^2$, i.e. $D^\dagger \tilde{D} \in \mathcal{G} := \text{U}(n_1) \oplus \cdots \oplus \text{U}(n_\kappa) \oplus \text{U}(n_0) \subset \text{U}(N)$ and $\tilde{D} \in D\mathcal{G}$. In other words, $D\mathcal{G}$ is the set of all unitary matrices $\{\tilde{D}\}$ such that $D^\dagger AA^\dagger \tilde{D} = \Omega^2$.

Now, the differential of $J_F$, $d_U J_F : T_U \text{U}(N) \to \mathbb{R}$, is given by

$$
d_U J_F(\delta U) = -2\Re \text{Tr}(AA^\dagger W^\dagger \delta U) = \langle UAA^\dagger W^\dagger U - WAA^\dagger, \delta U \rangle, \quad (3)$$

where the last step included a projection of $-2WAA^\dagger$ into the tangent space $T_U \text{U}(N)$. Therefore,

$$
\text{grad } J_F(U) = UAA^\dagger W^\dagger U - WAA^\dagger \quad (4)
$$
and a critical point of \( J_F \) is a \( U \) such that \( UAA^\dagger W^\dagger U = WAA^\dagger \). Let \( X = W^\dagger U \in U(N) \), and let \( \hat{X} = D^\dagger XD \). Then the critical point condition becomes \( \hat{X}^\dagger \Omega^2 = \Omega^2 \hat{X} \). This result also implies that \( \hat{X}^\dagger = \Omega^\dagger \hat{X} \). Hence for any \( i \) and \( j \), if \( \omega_{ij}^2 \neq \omega_{ji}^2 \) then \( \hat{X}_{ij} = 0 \), and if \( \omega_{ij}^2 = \omega_{ji}^2 \neq 0 \) then \( \hat{X}_{ij} = \hat{X}_{ji}^* \). So, \( \hat{X} \) is unitary and block-diagonal with block sizes \( \{ n_1, \ldots, n_\kappa, n_0 \} \) and the first \( \kappa \) blocks are Hermitian. In particular, this implies that \( [\hat{X}, AA^\dagger] = 0 \), so that \( \hat{X} \) and \( AA^\dagger \) may be simultaneously diagonalized by some \( \Gamma \in D \). Every critical \( X \) can then be written as \( X = D(\tilde{\Gamma} \Lambda \tilde{\Gamma}^\dagger + \tilde{X}_0) \), where \( \tilde{X}_0 = \sum_{\nu} \nu^2 \hat{X}_0 \), \( \nu \) is a critical point of \( \hat{X}_0 \), \( \nu \leq 0 \), \( \nu \leq n_i \), and \( \tilde{X}_0 \in U(n_0) \). Only the number \( \nu \) of negative 1’s is important in defining \( \Lambda \). Therefore if \( X \) is a critical point of \( J_F \) with critical value \( J_F(U) = 4 \sum_{\nu=i}^\kappa \nu^2 \). Thus, the set of all critical points is

\[
\text{Crit}(J_F) = \left\{ U = WD(\tilde{\Gamma} \Lambda \tilde{\Gamma}^\dagger + \tilde{X}_0) \right\}.
\]

Let \( \Phi : \mathcal{G} \times U(N) \to U(N) \) be the Lie group action \( \Phi(\Gamma, V) = \Gamma V(\tilde{\Gamma} \tilde{\Gamma}^\dagger + \tilde{X}_0) \). For a fixed \( V \in U(N) \), the set of all matrices reached by the action is the orbit through \( V \) in \( U(N) \). Similarly, for a fixed \( V \in U(N) \), the set of all \( \Gamma \)'s in \( G \) that keep \( V \) fixed is called the stabilizer (or isotropy) subgroup of \( \mathcal{G} \): \( \text{Stab}_\mathcal{G}(V) = \{ \Gamma \in \mathcal{G} : \Phi(\Gamma, V) = V \} \). Since \( \mathcal{G} \) is a compact Lie group, \( \text{Orb}_\mathcal{G}(V) \) is an embedded submanifold of \( U(N) \) for each \( V \in U(N) \). Furthermore, \( \text{Orb}_\mathcal{G}(V) \) is diffeomorphic to the connected differentiable manifold \( \mathcal{G}/\text{Stab}_\mathcal{G}(V) \). In particular, \( \dim(\text{Orb}_\mathcal{G}(V)) = \dim(\mathcal{G}) - \dim(\text{Stab}_\mathcal{G}(V)) \). Details on this orbit-stabilizer result may be found, for example, in [13] or [3, Ch. II, Ex. C.5].

For a given \( \Lambda = -I_{n_1} \oplus I_{n_1-n_\nu} \cdots \oplus -I_{n_\kappa} \oplus I_{n_\kappa-n_\nu} \), let us now characterize \( \text{Orb}_\mathcal{G}(\Lambda \oplus I_{n_0}) \). Observe that \( \text{Stab}_\mathcal{G}(\Lambda \oplus I_{n_0}) = U(\nu_1) \oplus U(n_1 - \nu_1) \oplus \cdots \oplus U(\nu_\kappa) \oplus U(n_\kappa - \nu_\kappa) \oplus I_{n_0} \). The dimension of \( \mathcal{G} \) is \( \dim(\mathcal{G}) = \sum_{i=0}^\kappa n_i^2 \), while the dimension of \( \text{Stab}_\mathcal{G}(\Lambda \oplus I_{n_0}) \) is \( \dim(\text{Stab}_\mathcal{G}(\Lambda \oplus I_{n_0})) = \sum_{i=1}^\kappa \nu_i^2 + (n_i - \nu_i)^2 \). Hence, we obtain

\[
\begin{align*}
\text{Orb}_\mathcal{G}(\Lambda \oplus I_{n_0}) & \simeq \frac{U(n_1) \oplus \cdots \oplus U(n_\kappa) \oplus U(n_0)}{U(\nu_1) \oplus U(n_1 - \nu_1) \oplus \cdots \oplus U(\nu_\kappa) \oplus U(n_\kappa - \nu_\kappa) \oplus I_{n_0}} \quad (6a) \\
& \simeq \text{Gr}_{\nu_1}(\mathbb{C}^{n_1}) \oplus \cdots \oplus \text{Gr}_{\nu_\kappa}(\mathbb{C}^{n_\kappa}) \oplus U(n_0) \quad (6b) \\
\dim(\text{Orb}_\mathcal{G}(\Lambda \oplus I_{n_0})) & = n_0^2 + \sum_{i=1}^\kappa n_i^2 - \nu_i^2 - (n_i - \nu_i)^2 = n_0^2 + 2 \sum_{i=1}^\kappa \nu_i(n_i - \nu_i), \quad (6c)
\end{align*}
\]

where \( \text{Gr}_{\nu_i}(\mathbb{C}^n) \) denotes the complex Grassmannian manifold of \( \nu \)-dimensional complex subspaces of \( \mathbb{C}^n \).

Therefore if \( AA^\dagger \) has \( \kappa \) distinct non-zero eigenvalues with degeneracies \( \{ n_1, \ldots, n_\kappa \} \), then \( J_F \) has exactly \( M = \prod_{i=1}^\kappa (n_i + 1) \) connected critical submanifolds. Note that in the case of complete degeneracy of \( AA^\dagger \) (e.g. \( A = I \)), \( \kappa = 1 \) and \( n_1 = N \), implying that there are \( N + 1 \) critical submanifolds with dimensions \( 0, 2(N - 1), 4(N - 2), 6(N - 3), \ldots \) for \( \nu_1 = 0, 1, 2, 3, \ldots \). In the case of complete non-degeneracy and non-singularity of \( AA^\dagger \), \( \kappa = N \) and \( n_i = 1 \) for all \( i \), so there are \( 2^N \) critical submanifolds, all of dimension 0, i.e. isolated points.
2.2 Hessian Analysis

Turning to the question of the signatures of these critical points, we extend the gradient vector field grad $J_F$ in the obvious way to all of $\mathbb{C}^{N \times N}$ and differentiate to find $d_U \text{grad} J_F(\delta U) = \delta U AA^1 W^1 U + UAA^1 W^1 \delta U$. Projecting this onto the tangent bundle of $U(N)$ gives

$$\text{Hess}_{J_F,U}(\delta U) := \nabla_{\delta U} \text{grad} J_F(U)$$

(7a)

$$= \frac{1}{2}(\delta U AA^1 W^1 U - WAA^1 \delta U^1 U + UAA^1 W^1 \delta U - U \delta U^1 WAA^1)$$

(7b)

$$= \frac{1}{2}(\delta U AA^1 W^1 U + WAA^1 \delta U^1 U + UAA^1 W^1 \delta U + U \delta U^1 WAA^1),$$

(7c)

using the fact that any tangent vector $\delta U \in T_UU(N)$ satisfies $\delta U^1 = -U^1 \delta U U^1$, and where $\nabla_{\delta U}$ denotes the covariant derivative in the direction $\delta U$. At a critical point, grad $J_F(U) = 0$, so that $W^1 U$ and $U^1 W$ both commute with $AA^1$, and also $W^1 UAA^1 = AA^1 W^1 U = D\Omega^2(\hat{\Gamma} \Lambda \hat{\Gamma} + \hat{\lambda}_0) D^\dagger = D\Omega^2(\hat{\Gamma} \Lambda \hat{\Gamma} + 0) D^\dagger = U^1 WAA^1 = AA^1 U^1 W$. Then the Hessian becomes

$$\text{Hess}_{J_F,U}(\delta U) = \delta U AA^1 W^1 U + UAA^1 W^1 \delta U.$$  

(8)

Suppose that $U \in U(N)$ is a critical point of $J_F$, i.e. $U = WD(\hat{\Gamma} \Lambda \hat{\Gamma} + \hat{\lambda}_0) D^\dagger$ for some $\hat{\Gamma} \in \hat{G}$ and $\Lambda = -I_{\nu_1} \oplus I_{n_1 - \nu_1} \cdots \oplus -I_{\nu_\kappa} \oplus I_{n_\kappa - \nu_\kappa}$ and $\hat{\lambda}_0 \in U(n_0)$. Furthermore, let $Y := (\hat{\Gamma} \Lambda \hat{\Gamma} + \hat{\lambda}_0) D^\dagger \delta U D(\hat{\Gamma} \Lambda \hat{\Gamma} + \hat{\lambda}_0)$ so that $Y$ is skew-Hermitian. Then $\text{Hess}_{J_F}(\delta U) = \gamma \delta U$ if and only if $Y \Omega^2(\Lambda \oplus I_{n_0}) + \Omega^2(\Lambda \oplus I_{n_\kappa}) Y = \gamma Y$.

For the null space of $\text{Hess}_{J_F}$, we want to solve this equation for $\gamma = 0$. This equation is solved in $\mathfrak{u}(N)$ if and only if $Y$ is of the form

$$Y = \begin{bmatrix}
0 & Q_1 & & \\
-\bar{Q}_1^\dagger & 0 & & \\
& \cdots & \\
& & 0 & Q_\kappa \\
& & -\bar{Q}_\kappa^\dagger & 0 \\
& & & 0 & Q_0
\end{bmatrix},$$

(9)

where $Q_i \in \mathbb{C}^{n_i \times (n_i - \nu_i)}$ for $i = 1, \ldots, \kappa$ and $Q_0 \in \mathfrak{u}(n_0)$ are arbitrary. These $Y$’s span a dimension $d = n_0^2 + 2 \sum \nu_i(n_i - \nu_i)$ (real) subspace of $\mathfrak{u}(N)$. Hence the nullity of $\text{Hess}_{J_F}$ is $\mathcal{N}_0 = n_0^2 + 2 \sum \nu_i(n_i - \nu_i)$. Since this is the same as the dimension of the corresponding critical submanifold, and since the tangent space of the critical submanifold must lie in the null space of the Hessian, these two subspaces of $T_UU(N)$ must be identical. Therefore $J_F$ is Morse-Bott for all $A$ matrices.

To conclude this kinematic analysis, we can compute the numbers of positive and negative eigenvalues (i.e. $\mathcal{N}_+$ and $\mathcal{N}_-$, respectively) of $\text{Hess}_{J_F}$ at a critical point $U$. Let $\hat{\lambda}_i = \Lambda_{ii}$ for $i = 1, \ldots, N - n_0$ and $\hat{\lambda}_i = 1$ for $i = N - n_0 + 1, \ldots, N$. Then $Y \Omega^2(\Lambda \oplus I_{n_0}) + \Omega^2(\Lambda \oplus I_{n_\kappa}) Y = \gamma Y$ can be expressed as $(\omega_j^2 \hat{\lambda}_i + \omega_i^2 \hat{\lambda}_i - \gamma) Y_{ij} = 0$ for $1 \leq i, j \leq N$. Then $\gamma$ is an eigenvalue of $\text{Hess}_{J_F}$ if and only if $\gamma = \omega_j^2 \hat{\lambda}_j + \omega_i^2 \hat{\lambda}_i$ for some $i$ and $j$. Now, $\omega_j^2 \hat{\lambda}_j + \omega_i^2 \hat{\lambda}_i < 0$ whenever:

5
\[ \hat{\lambda}_i = \hat{\lambda}_j = -1, \text{ which happens for } (\sum_{l=1}^{\kappa} \nu_l)^2 \text{ ordered pairs } (i, j), \]

\[ \hat{\lambda}_i = -1, \hat{\lambda}_j = +1 \text{ and } \omega_i^2 > \omega_j^2, \text{ which happens for } \sum_{k>l}^{\kappa} \nu_k(n_l - \nu_l) + n_0 \sum_{i=1}^{\kappa} \nu_i \text{ ordered pairs } (i, j), \]

or

\[ \hat{\lambda}_i = +1, \hat{\lambda}_j = -1 \text{ and } \omega_i^2 < \omega_j^2, \text{ which happens for } \sum_{1 \leq k < l}^{\kappa} \nu_k(n_l - \nu_l) + n_0 \sum_{i=1}^{\kappa} \nu_i \text{ ordered pairs } (i, j). \]

Since each ordered pair \((i, j)\) contributes one (real) degree of freedom in \(Y\), there are \(N_- = (\sum_{i=1}^{\kappa} \nu_i)^2 + 2 \sum_{k>l}^{\kappa} \nu_k(n_l - \nu_l) + n_0 \sum_{i=1}^{\kappa} \nu_i\) negative eigenvalues of \(\text{Hess}_{J_P}\). Likewise, \(\omega_i^2 \hat{\lambda}_j + \omega_j^2 \hat{\lambda}_i > 0\) whenever

\[ \hat{\lambda}_i = \hat{\lambda}_j = +1 \text{ and at least one of } \omega_i^2 \text{ and } \omega_j^2 \text{ is nonzero, which happens for } \]

\[ (N - n_0 - \sum_{i=1}^{\kappa} \nu_i)^2 + 2n_0 (N - n_0 - \sum_{k=1}^{\kappa} \nu_k) \text{ ordered pairs } (i, j), \]

\[ \hat{\lambda}_i = -1, \hat{\lambda}_j = +1 \text{ and } \omega_i^2 < \omega_j^2, \text{ which happens for } \sum_{1 \leq k < l}^{\kappa} \nu_k(n_l - \nu_l) \text{ ordered pairs } (i, j), \]

or

\[ \hat{\lambda}_i = +1, \hat{\lambda}_j = -1 \text{ and } \omega_i^2 > \omega_j^2, \text{ which happens for } \sum_{k>l}^{\kappa} \nu_k(n_l - \nu_l) = \sum_{1 \leq k < l}^{\kappa} \nu_k(n_l - \nu_l) \text{ ordered pairs } (i, j). \]

Therefore, the positive eigenvalues number

\[
N_+ = \left( N - n_0 - \sum_{i=1}^{\kappa} \nu_i \right)^2 + 2n_0 \left( N - n_0 - \sum_{k=1}^{\kappa} \nu_k \right) + 2 \sum_{1 \leq k < l}^{\kappa} \nu_k(n_l - \nu_l) \quad (10a)
\]

\[
= N^2 - n_0^2 + \left( \sum_{i=1}^{\kappa} \nu_i \right)^2 - 2N \sum_{i=1}^{\kappa} \nu_i + 2 \sum_{1 \leq k < l}^{\kappa} \nu_k(n_l - \nu_l). \quad (10b)
\]

It is easy to see that \(N_- + N_+ + N_0 = N^2\) as expected. Furthermore, we find that \(N_+ = 0\) if and only if \(\nu_i = n_i\) for all \(i = 1, \ldots, \kappa\), i.e. only at the global maximum \(\{U = -WD(I \oplus \hat{X}_0)D\dagger : \hat{X}_0 \in U(n_0)\}\). Likewise \(N_- = 0\) if and only if \(\nu_i = 0\) for all \(i = 1, \ldots, \kappa\), i.e. only at the global minimum \(\{U = WD(I \oplus \hat{X}_0)D\dagger : \hat{X}_0 \in U(n_0)\}\). So, there are no local traps in the kinematic landscape, and the remaining \(\prod_{i=1}^{\kappa} (n_i + 1) - 2\) critical submanifolds are all saddles.

3 Kinematic Critical Point Analysis of Phase-Invariant Landscapes

Now consider the phase-invariant kinematic landscape \(J_P(U) := \|A\|^4 - |\text{Tr}(AA\dagger WU)|^2\). Since \(J_P\) is phase-invariant, there exists a well-defined function \(\hat{J}_P : \text{PU}(N) \to \mathbb{R}\) such that \(J_P = \hat{J}_P \circ \pi\), where \(\text{PU}(N)\) is the projective unitary group \(U(N)/U(1)\) and \(\pi : U(N) \to \text{PU}(N)\) is the natural projection map depicted in Figure 1. One can then lift \(\hat{J}_P\) to \(\hat{J}_P : SU(N) \to \mathbb{R}\) on \(SU(N)\), the universal covering space of \(\text{PU}(N)\), by the covering map \(p : SU(N) \to \text{PU}(N)\). Here, \(J_P\) is just the restriction to \(SU(N)\) of \(\hat{J}_P\), and it is easily verified that \(\text{grad} \hat{J}_P(U) = \text{grad} J_P(U)\) and \(\text{Hess}_{J_P,U} = \text{Hess}_{J_P,U} |_{T_U SU(N)}\) for \(U \in SU(N)\). Many components of the critical set of \(\hat{J}_P\) will admit exactly \(N\) disconnected images in the critical set of \(J_P\). Choosing one representative such image for each connected component of \(\hat{J}_P\) permits simplifying the analysis below.
3.1 Distance Metric on $PU(N)$

There are various ways of deriving a phase-invariant landscape like $J_P$ from one that is phase-dependent like $J_F$. A simple approach is to observe that

$$\min_{\phi \in U(1)} \|(U - \phi W)A\|^2 = 2\|A\|^2 - 2|\text{Tr}(AA^\dagger WU)|.$$  

This provides a means to define a quotient metric on the projective unitary group $PU(N)$ from the metric $d(U,W) = \| (U - W)A \|^2$ on $U(N)$.

Another approach involves the adjoint representation of the unitary group, $\text{Ad} : U(N) \to \text{Aut} \left( \text{u}(N) \right) \subset \text{GL}(\text{u}(N)) \cong \text{GL}(N^2; \mathbb{R})$, which is given by $\text{Ad}(A) = UAU^\dagger$ for any $A \in \text{u}(N)$, and where $\text{Aut} (\text{u}(N))$ is the group of Lie algebra automorphisms on $\text{u}(N)$ [14, 20]. With $\text{u}(N)$ given the Hilbert-Schmidt inner product, $\langle \text{Ad}(U)A, \text{Ad}(U)B \rangle = \langle UAU^\dagger, UBU^\dagger \rangle = \langle A, B \rangle$, so that for each $U \in PU(N)$, $\text{Ad}(U)$ is an orthogonal operator on $\text{u}(N)$. Furthermore, if $W$ and $U$ differ only by a global phase, i.e. $W = e^{i\theta}U$, then $\text{Ad}(U) = \text{Ad}(W)$. Moreover, the kernel of $\text{Ad}$, i.e. $\text{Ad}^{-1}(\text{id})$, is the center of $U(N)$ [6, Cor. 5.2, pg. 129][20, Thm. 3.50] which is $Z(U(N)) = \{ e^{i\theta} \mid \theta \in \mathbb{R} \}$ . Then $\text{Ad}(U) = \text{Ad}(W)$ if and only if $W = e^{i\theta}U$, so the image of $\text{Ad}$ is a faithful representation of $PU(N)$ and $\text{Ad}$ may be thought of as playing a role similar to the projection $\pi : U(N) \to PU(N)$.

Consider some target $W \in U(N)$ and some $B \in \text{GL}(\text{u}(N))$ and define

$$J(U) = \| (\text{Ad}(U) - \text{Ad}(W)) \circ B \|^2_{HS},$$  

where $\| \cdot \|_{HS}$ is the Hilbert-Schmidt norm on $\text{End} \left( \text{u}(N) \right) \cong \mathbb{R}^{N^2 \times N^2}$, the space of all linear operators on $\text{u}(N)$. Let $\{ \Omega_j \}$ be the orthonormal basis for $\text{u}(N)$ (with the Hilbert-Schmidt inner product), with the elements $i|p\rangle\langle p|$ for $p = 1, \ldots, N$; $\frac{1}{\sqrt{2}}(|p\rangle\langle q| + |q\rangle\langle p|)$ for $1 \leq p < q \leq N$; and $\frac{1}{\sqrt{2}}(|p\rangle\langle q| - |q\rangle\langle p|)$ for $1 \leq p < q \leq N$, where $\{|p\rangle\}$ is the canonical basis for $\mathbb{R}^N$. Then,

$$J(U) = 2 \text{Tr}(B^* \circ B) - 2 \text{Tr} \left( B^* \circ \text{Ad}(W)^* \circ \text{Ad}(U) \circ B \right)$$

$$= 2 \text{Tr}(B^* \circ B) - 2 \sum_j \langle B(\Omega_j), \text{Ad}(W^\dagger U)B(\Omega_j) \rangle.$$  

Let $A \in GL(\mathbb{C}^N)$ be an arbitrary $N \times N$ matrix, and let $B$ be defined by $B(\Omega) = A\Omega A^\dagger$. Then $\langle B(\Omega_j), \text{Ad}(W^\dagger U)B(\Omega_j) \rangle$ can be computed for each of the basis elements as in Table [1] We find that

![Figure 1: U(N) and SU(N) as fibre bundles over PU(N).](image-url)
Now, the differential of
Consequently, the kinematic landscape
\[ J(U) = 2 \text{Tr}(B^*B) - 2 \sum_j \langle B(\Omega_j), \text{Ad}(U^†W)B(\Omega_j) \rangle \]
\[ = 2 \text{Tr}(B^*B) - 2 \sum_{p=1}^{N} |\langle p|A^†W^†UA|p \rangle|^2 \]
\[ - 2 \sum_{p<q} \Re(\langle p|A^†W^†UA|q \rangle \langle q|A^†U^†WA|q \rangle + \langle q|A^†W^†UA|q \rangle \langle p|A^†U^†WA|q \rangle) \]
\[ - 2 \sum_{p<q} \Re(\langle p|A^†W^†UA|q \rangle \langle q|A^†U^†WA|q \rangle - \langle q|A^†W^†UA|q \rangle \langle p|A^†U^†WA|q \rangle) \]
\[ = 2 \text{Tr}(B^*B) - 2 \sum_{p=1}^{N} |\langle p|A^†W^†UA|p \rangle|^2 - 2 \sum_{p\neq q} \langle p|A^†W^†UA|p \rangle \langle q|A^†U^†WA|q \rangle \]
\[ = 2 \text{Tr}(B^*B) - 2 \sum_{p=1}^{N} \sum_{q=1}^{N} \langle p|A^†W^†UA|p \rangle \langle q|A^†U^†WA|q \rangle \]
\[ = 2 \sum_j \langle B(\Omega_j), B(\Omega_j) \rangle - 2 |\text{Tr}(A^†W^†UA)|^2 \]
\[ = 2\|A\|^4_{HS} - 2 |\text{Tr}(AA^†W^†U)|^2 = 2J_P(U). \]

\[ J_P(U) = \|A\|^4 - |\text{Tr}(AA^†W^†U)|^2 \] on \( U(N) \) is equivalent to the weighted Hilbert-Schmidt distance function on the subgroup of \( \text{SO}(N^2) \) given by \( \text{Im(Ad)} \simeq \text{PU}(N) \).

3.2 Critical Point Identification

Now, the differential of \( J_P \) at \( U \in U(N) \), \( d_UJ_P : T_UU(N) \to \mathbb{R} \) is given by

\[ d_UJ_P(\delta U) = - \text{Tr}(AA^†W^†U \delta U) \text{Tr}(U^†W AA^†) - \text{Tr}(AA^†W^†U) \text{Tr}(\delta U^†W AA^†) \]
\[ = \langle T(U^†W AA^†)UAA^†W^†U - \text{Tr}(AA^†W^†U)W AA^†, \delta U \rangle \]

so that

\[ \text{grad } J_P(U) = \text{Tr}(U^†W AA^†)UAA^†W^†U - \text{Tr}(AA^†W^†U)W AA^†. \]
For $J_P(U) < \|A\|^2$, $\text{Tr}(U^\dagger W A A^\dagger) \neq 0$, so $\text{grad} J_P(U) = 0$ if and only if $A A^\dagger Z = Z^\dagger A A^\dagger$, where $Z = \frac{\text{Tr}(U^\dagger W A A^\dagger)}{\|\text{Tr}(U^\dagger W A A^\dagger)\|} W U \in U(N)$. Using the notation from the previous section, $D \in U(N)$ is such that $D^\dagger A A^\dagger D = \Omega^2$ with $\Omega^2_{ij} = \omega^2_i$ and $\omega^2_i \geq \cdots \geq \omega^2_N$; additionally, $\omega^2_1 > \cdots > \omega^2_N > 0$ denote the distinct eigenvalues of $A A^\dagger$, with $\{n_1, \ldots, n_k, n_0\}$ being the multiplicities of these eigenvalues. Then $A A^\dagger Z = Z^\dagger A A^\dagger$ can be rewritten $\Omega^2 Z = \tilde{Z}^\dagger \Omega^2$ where $\tilde{Z} = D^\dagger Z D$. This same condition was considered in section 2 (and 3), where it was shown to imply that $[Z, A A^\dagger] = 0$ and $\tilde{Z} = \tilde{\Gamma} A^\dagger \oplus \tilde{Z}_0$ where $\tilde{\Gamma} \in \hat{\mathcal{G}} = U(n_1) \oplus \cdots \oplus U(n_k)$, $\Lambda = \Lambda_1 \oplus \cdots \oplus \Lambda_k$, $\Lambda_i = (-I_{n_i}) \oplus I_{n_i-n_i} \in U(n_i)$, $0 \leq n_i \leq n_1$, and $\tilde{Z}_0 \in U(n_0).

Drawing on the material above, we find that any critical point $U$ of $J_P$ with $J_P(U) < \|A\|^2$ can be written as $U = \frac{\text{Tr}(A A^\dagger W U)}{\|\text{Tr}(U^\dagger W A A^\dagger)\|} W D(\tilde{\Gamma} A^\dagger \oplus \tilde{Z}_0) D^\dagger$. This characterization is complicated by the presence of $U$ on both sides of the equation, especially with regard to the phase factor on the right-hand side. We may write $U = e^{i\theta} W D(\tilde{\Gamma} A^\dagger \oplus \tilde{Z}_0) D^\dagger$ for any $\theta \in \mathbb{R}$, $\tilde{\Gamma} \in \hat{\mathcal{G}}$, $\Lambda = -I_{n_1} \oplus I_{n_1-n_1} \oplus \cdots \oplus -I_{n_k} \oplus I_{n_k-n_k}$, and $\tilde{Z}_0 \in U(n_0)$. Then $[U^\dagger W, A A^\dagger] = [W^\dagger U, A A^\dagger] = 0$ and $U^\dagger W A A^\dagger = (A A^\dagger W U)^\dagger = e^{-2i\theta} A A^\dagger U W$, so that $\text{grad} J_P(U) = 0$. Hence, every such $U$ is a critical point of $J_P$, and they comprise connected critical sets

$$C_{\Lambda} := \{U = e^{i\theta} W D(\tilde{\Gamma} A^\dagger \oplus \tilde{Z}_0) D^\dagger : e^{i\theta} \in U(1), \tilde{\Gamma} \in \hat{\mathcal{G}}, \tilde{Z}_0 \in U(n_0)\}$$

(16)

$$U = WD([e^{i\theta} \tilde{\Gamma} A^\dagger] \oplus \tilde{Z}_0) D^\dagger : e^{i\theta} \in U(1), \tilde{\Gamma} \in \hat{\mathcal{G}}, \tilde{Z}_0 \in U(n_0)$$

(17)

for $\Lambda = -I_{n_1} \oplus I_{n_1-n_1} \oplus \cdots \oplus -I_{n_k} \oplus I_{n_k-n_k}$ such that $\text{Tr}(\Omega^2(\Lambda \oplus I_{n_n})) > 0$ (hence $J_P(U) < \|A\|^2$). Such a critical submanifold $C_{\Lambda}$ has the critical value $J_P(U) = \text{Tr}(\Omega^2)^2 - \text{Tr}(\Omega^2(\Lambda \oplus I_{n_n})) = (\sum_{i=1}^{\kappa} n_i \omega^2_i)^2 - (\sum_{i=1}^{\kappa} (n_i - 2n_i) \omega^2_i)^2 = 4(\sum_{i=1}^{\kappa} n_i \omega^2_i)(\sum_{i=1}^{\kappa} (n_i - n_i) \omega^2_i)$ for every $U \in C_{\Lambda}$. Consider the set $R := \{e^{i\theta} \tilde{\Gamma} A^\dagger : e^{i\theta} \in U(1) \text{ and } \tilde{\Gamma} \in \hat{\mathcal{G}} \} \subset U(N - n_0)$ for this same fixed $\Lambda$. An element of $R$ has determinant $e^{i(N-n_0)\theta}(1)\sum \nu_i$, so for it to lie in $R \cap SU(N - n_0)$, we must have that $\theta = \pi(2k + \sum \nu_i)/(N - n_0)$ for some $k$. Thus, $R \cap SU(N - n_0)$ is a covering of $N - n_0$ distinct connected components, each one being the image of the projection of $R$ into $PU(N - n_0)$. Let $\theta$ be any of the $N - n_0$ admissible phases above. Then $\hat{R} := \{e^{i\theta} \tilde{\Gamma} A^\dagger : \tilde{\Gamma} \in \hat{\mathcal{G}}\}$ is one of the connected components of $R \cap SU(N - n_0)$, and $R = \pi^{-1}(p(\hat{R}))$, where $p$ and $\pi$ are the projections from Figure 1. The projection $p$ is a covering map and therefore is necessarily also a local diffeomorphism, and since it is a bijection on $\hat{R}$, it is a diffeomorphism between $\hat{R}$ and $p(\hat{R})$. The fact that $\hat{R}$ is a dimension $d = \sum_{i=1}^{\kappa} (n_i^2 - \nu_i^2 - (n_i - \nu_i)^2) = 2 \sum_{i=1}^{\kappa} \nu_i (n_i - \nu_i)$ manifold diffeomorphic to

$$U(n_1) \oplus \cdots \oplus U(n_\kappa) \oplus U(n_1 - \nu_1) \oplus \cdots \oplus U(n_\kappa - \nu_\kappa) \simeq \text{Gr}_{\nu_1}(C^{n_1}) \oplus \cdots \oplus \text{Gr}_{\nu_\kappa}(C^{n_\kappa})$$

(18)

implies the same about $p(\hat{R})$. Then, since the projection $\pi : U(N - n_0) \to PU(N - n_0)$ is a surjective submersion, $R = \pi^{-1}(p(\hat{R}))$ is a dimension $1 + 2 \sum_{i=1}^{\kappa} \nu_i (n_i - \nu_i)$ submanifold of $U(N - n_0)$. Moreover, $R$ is a $U(1)$ principal fibre bundle over $\text{Gr}_{\nu_1}(C^{n_1}) \oplus \cdots \oplus \text{Gr}_{\nu_\kappa}(C^{n_\kappa})$. Then $R \oplus U(n_0)$ is a dimension $1 + n_0^2 + 2 \sum_{i=1}^{\kappa} \nu_i (n_i - \nu_i)$ submanifold of $U(N)$, and since conjugation and left translation are both diffeomorphisms on $U(N)$, $C_{\Lambda} \cong R \oplus U(n_0)$ is also a dimension $1 + n_0^2 + 2 \sum_{i=1}^{\kappa} \nu_i (n_i - \nu_i)$ submanifold of $U(N)$. 
### 3.3 Hessian Analysis

Given the form of the gradient of $J_P$ in (13), by again extending the gradient vector field to $\mathbb{C}^{N \times N}$ and differentiating, it is found that

$$
d_U \text{grad } J_P(dU) = \text{Tr}(\delta U^\dagger W AA^\dagger) UAA^\dagger W^\dagger U + \text{Tr}(U^\dagger W AA^\dagger) \delta UAA^\dagger W^\dagger U$$

$$+ \text{Tr}(U^\dagger W AA^\dagger) UAA^\dagger W^\dagger \delta U - \text{Tr}(AA^\dagger W^\dagger \delta U) W AA^\dagger,
$$

(19)

whence by projection onto the tangent bundle of $U(N)$,

$$
\text{Hess}_{J_P,U}(dU) = \nabla_{dU} \text{grad } J_P = -\text{Tr}(AA^\dagger W^\dagger \delta U) W AA^\dagger + \text{Tr}(\delta U^\dagger W AA^\dagger) UAA^\dagger W^\dagger U$$

$$+ \frac{1}{2} \left\{ \text{Tr}(U^\dagger W AA^\dagger) \delta UAA^\dagger W^\dagger U + \text{Tr}(AA^\dagger W^\dagger U) WAA^\dagger \delta U W U^\dagger \right\}$$

$$+ \text{Tr}(U^\dagger W AA^\dagger) UAA^\dagger W^\dagger \delta U + \text{Tr}(AA^\dagger W^\dagger U) U^\dagger \delta U W AA^\dagger \right\}.
$$

(20)

On one of the critical submanifolds $C_{\Lambda}$, the Hessian is given by

$$
\text{Hess}_{J_P,U}(dU) = \text{Tr}(AA^\dagger W^\dagger U) \delta U U^\dagger W AA^\dagger + \text{Tr}(AA^\dagger W^\dagger U) WAA^\dagger U^\dagger \delta U$$

$$- 2 \text{Tr}(AA^\dagger W^\dagger U) W AA^\dagger.
$$

(21)

Since $U = e^{i\theta} WD(\tilde{\Gamma} \Lambda \dagger \oplus \tilde{Z}_0) D^\dagger$ can also be written $U = (-e^{i\theta}) WD(\tilde{\Gamma} (\Lambda \oplus \tilde{Z}_0) D^\dagger$, we can choose to always write such a critical $U$ such that $\text{Tr}(\Omega^2 (\Lambda \oplus \tilde{Z}_0)) \geq 0$. We seek an eigenvalue decomposition of $\text{Hess}_{J_P,U}$, and find that $\gamma U = \text{Hess}_{J_P,U}(dU)$ if and only if

$$\gamma Y = \text{Tr}(\Omega^2 \Lambda)(Y \Omega^2 \Lambda + \Omega^2 \Lambda Y) - 2 \text{Tr}(\Omega^2 \Lambda Y) \Omega^2 \Lambda
$$

(22)

where $Y = (\tilde{\Gamma} \oplus I_{n_0}) D^\dagger U D(\tilde{\Gamma} \oplus I_{n_0}) \in u(N)$ and $\Lambda = \Lambda \oplus I_{n_0}$. We begin by looking at the null space of $\text{Hess}_{U,J_P}$, where $2 \text{Tr}(\Omega^2 \Lambda Y) \Omega^2 \Lambda = \text{Tr}(\Omega^2 \Lambda)(Y \Omega^2 \Lambda + \Omega^2 \Lambda Y)$. Then $\text{Tr}(\Omega^2 \Lambda)(\lambda_\Lambda \omega^2 + \hat{\lambda}_\Lambda \omega^2) Y_{ij} = 2 \text{Tr}(\Omega^2 \Lambda Y) \lambda_\Lambda \omega^2 \delta_{ij}$. For $i \neq j$, and since $\text{Tr}(\Omega^2 \Lambda) \neq 0$ by assumption ($J_P(U) = \|A\|^2$), this implies that either $\lambda_\Lambda \omega^2 + \hat{\lambda}_\Lambda \omega^2 = 0$ or $Y_{ij} = 0$. For $i = j$, we get $\text{Tr}(\Omega^2 \Lambda \omega^2) Y_{ii} = \text{Tr}(\Omega^2 \Lambda Y) \omega^2_i$, implying that the diagonal elements of $Y$ are all identical where $\omega^2_i \neq 0$. So $Y = (iyd I_{N-n_0}) \oplus 0_{n_0} + \tilde{Y}$, where $yd \in \mathbb{R}$ and $\tilde{Y}$ is of the block diagonal form shown in (9). Hence the nullity of $\text{Hess}_{J_P,U}$ is $N_0 = 1 + n_0^2 + 2 \sum \nu_i (n_i - \nu_i)$.

For the remaining eigenvalues $\gamma \neq 0$, we have $\gamma Y - \text{Tr}(\Omega^2 \Lambda)(Y \Omega^2 \Lambda + \Omega^2 \Lambda Y) = -2 \text{Tr}(\Omega^2 \Lambda Y) \Omega^2 \Lambda$ or $\gamma Y_{ij} - \text{Tr}(\Omega^2 \Lambda)(\lambda_\Lambda \omega^2 + \hat{\lambda}_\Lambda \omega^2) Y_{ij} = -2 \text{Tr}(\Omega^2 \Lambda Y) \omega^2_i \lambda_\Lambda \delta_{ij}$. Since the right hand side is diagonal, when $i \neq j$ either $\gamma = \text{Tr}(\Omega^2 \Lambda)(\lambda_\Lambda \omega^2 + \hat{\lambda}_\Lambda \omega^2)$, or $Y_{ij} = 0$. Since we chose $\Lambda$ such that $\text{Tr}(\Omega^2 \Lambda) > 0$, $\gamma < 0$ if $\lambda_\Lambda \omega^2 + \hat{\lambda}_\Lambda \omega^2 < 0$ for $i \neq j$, i.e. whenever

- $\lambda_\Lambda = \hat{\lambda}_\Lambda = -1$, which happens for $(\sum_{i=1}^{\kappa} \nu_i)(\sum_{i=1}^{\kappa} \nu_i - 1)$ ordered pairs $(i,j)$,
- $\lambda_\Lambda = -1, \hat{\lambda}_\Lambda = +1$ and $\omega^2_i > \omega^2_j$, which happens for $\sum_{k \geq 1} \nu_k (n_k - \nu_k) + n_0 \sum_{i=1}^{\kappa} \nu_i$ ordered pairs $(i,j)$, or
- $\lambda_\Lambda = +1, \hat{\lambda}_\Lambda = -1$ and $\omega^2_i < \omega^2_j$, which happens for $\sum_{1 \leq k < l}(n_k - \nu_k) \nu_l + n_0 \sum_{i=1}^{\kappa} \nu_i = \sum_{k \geq 1} \nu_k (n_k - \nu_k) + n_0 \sum_{i=1}^{\kappa} \nu_i$ ordered pairs $(i,j)$. 


Likewise, $\gamma > 0$ if $\lambda_i \omega_i^2 + \lambda_j \omega_j^2 < 0$ for $i \neq j$, i.e. whenever

- $\lambda_i = \lambda_j = +1$ and at most one of $\omega_i^2$ and $\omega_j^2$ is zero, which happens for $(N - n_0 - \sum_{l=1}^\kappa \nu_l)(N - n_0 - 1 - \sum_{l=1}^\kappa \nu_l) + 2n_0(N - n_0 - \sum_{k=1}^\kappa \nu_k)$ ordered pairs $(i,j)$,

- $\lambda_i = -1$, $\lambda_j = +1$ and $\omega_i^2 < \omega_j^2$, which happens for $\sum_{k=1}^\kappa \nu_k(n_1 - \nu_l)$ ordered pairs $(i,j)$, or

- $\lambda_i = +1$, $\lambda_j = -1$ and $\omega_i^2 > \omega_j^2$, which happens for $\sum_{k=1}^\kappa (n_k - \nu_k)\nu_l = \sum_{k=1}^\kappa \nu_k(n_1 - \nu_l)$ ordered pairs $(i,j)$.

On the other hand, when $i = j$, we get $\gamma Y_i - 2 \text{Tr}(\Omega^2 \Lambda) \lambda_i \omega_i^2 Y_i = -2 \text{Tr}(\Omega^2 \Lambda Y) \lambda_i \omega_i^2$. If $\gamma = 2 \text{Tr}(\Omega^2 \Lambda) \lambda_i \omega_i^2 = 2 \text{Tr}(\Omega^2 \Lambda) \lambda_i \omega_i^2$, and $Y = \frac{1}{\sqrt{2}} (|j\rangle \langle j| - |k\rangle \langle k|)$, then $\text{Tr}(\Omega^2 \Lambda Y) = 0$ and $\gamma Y_{jj} + 2 \text{Tr}(\Omega^2 \Lambda) \lambda_j \omega_j^2 Y_{jj} = 2 \text{Tr}(\Omega^2 \Lambda Y) \lambda_j \omega_j^2$. This accounts for an additional $\sum_{i=1}^\kappa \max(\nu_i - 1, 0) = \sum_{i=1}^\kappa \nu_i - \#\{j : 1 \leq j \leq \kappa \text{ and } \nu_j > 0\}$ eigenvectors for $\gamma < 0$ and $\sum_{i=1}^\kappa \max(n_i - \nu_i - 1, 0) = N - n_0 - \sum_{i=1}^\kappa \nu_i - \#\{j : 1 \leq j \leq \kappa \text{ and } \nu_j < n_j\}$ eigenvectors for $\gamma > 0$. Finally, consider the case where $Y$ is diagonal and $\text{Tr}(\Omega^2 \Lambda Y) \neq 0$. Then $(\gamma - 2 \text{Tr}(\Omega^2 \Lambda) \lambda_j \omega_j^2) Y = \text{Tr}(\Omega^2 \Lambda Y) \lambda_j \omega_j^2$, so for $\gamma \neq -2 \text{Tr}(\Omega^2 \Lambda) \lambda_j \omega_j^2$ for all $j$, $Y = \frac{-2 \text{Tr}(\Omega^2 \Lambda Y) \lambda_j \omega_j^2}{2 \text{Tr}(\Omega^2 \Lambda Y) \lambda_j \omega_j^2}$.

This yields $\text{Tr}(\Omega^2 \Lambda Y) = \text{Tr}(\Omega^2 \Lambda Y) \text{Tr} \left( \frac{2 \omega_i^4}{2 \text{Tr}(\Omega^2 \Lambda)^2 \omega_i^2 - \gamma} \right)$ and since we assume that $\text{Tr}(\Omega^2 \Lambda Y) \neq 0$, it follows that $\gamma$ must satisfy

$$f(\gamma) := \text{Tr} \left( \frac{2 \omega_i^4}{2 \text{Tr}(\Omega^2 \Lambda)^2 \omega_i^2 - \gamma} \right) = \frac{2 \omega_i^4}{2 \text{Tr}(\Omega^2 \Lambda)^2 \omega_i^2 - \gamma} = 1. \quad (23)$$

If there are $l$ distinct values $\eta_1 < \cdots < \eta_l$ of $2 \text{Tr}(\Omega^2 \Lambda) \lambda_i \omega_i^2$ with $\omega_i^2 \neq 0$, the function $f$ has $l$ solutions $f(\gamma) = 1$: $\gamma_1 < \eta_1$ and $\eta_{k-1} < \gamma_k < \eta_k$ for $k = 2, \ldots, l$. Note that $\gamma_k = 0$ is one of these solutions, but should be neglected since we have already characterized the null space of $\text{Hess}_{J_p, U}$. Letting $Y = \frac{2 \omega_i^4 \Lambda}{2 \text{Tr}(\Omega^2 \Lambda)^2 \omega_i^2 - \gamma}$, where $\alpha > 0$ is a normalizing factor, we see that $\text{Tr}(\Omega^2 \Lambda Y) = i \alpha \neq 0$, $\text{Tr}(Y) = 0$, and that $Y$ is a diagonal eigenvector of $\text{Hess}_{J_p, U}$ with positive eigenvalue $\gamma_k$. The number of eigenvectors with negative eigenvalue contributed in this way is equal to $\#\{j : 1 \leq j \leq \kappa \text{ and } \nu_j > 0\}$, while the number of eigenvectors with positive eigenvalue is equal to $\#\{j : 1 \leq j \leq \kappa \text{ and } \nu_j < n_j\} - 1$.

To summarize, away from the global maximum, the function $J_p$ has connected critical submanifolds

$$C_A := \{ U = e^{i\theta} W D(\tilde{\Gamma} \Lambda \Gamma \tilde{\Lambda} \tilde{\Gamma}) \tilde{Z}_0 | \tilde{D} \} : e^{i\theta} \in U(1), \tilde{\Gamma} \in \tilde{G}, \text{ and } \tilde{Z}_0 \in U(n_0) \} \quad (24)$$

for $\Lambda = - I_{n_1} \oplus I_{n_1 - \nu_1} \oplus \cdots \oplus - I_{\nu_\kappa} \oplus I_{\nu_\kappa - \nu_\kappa}$ such that $\text{Tr}(\Omega^2 \Lambda \oplus I_{n_0}) > 0$ (hence $J_p(U) < ||A||^2$). Such a critical submanifold has dimension $d_A = 1 + n_0^2 + 2 \sum_{i=1}^\kappa (n_i - \nu_i)$, which is identical to the nullity $N_0$ of the Hessian on $C_A$. Tallying up the dimensions of the negative and positive Hessian eigenspaces, we find $\mathcal{N}_- = (\sum_{i=1}^\kappa \nu_i)^2 + 2 \sum_{k=1}^\kappa \nu_k(n_k - \nu_k) + 2n_0 \sum_{i=1}^\kappa \nu_i$ and $\mathcal{N}_+ = (N - n_0 - \sum_{i=1}^\kappa \nu_i)^2 + 2n_0(N - n_0 - \sum_{k=1}^\kappa \nu_k) + 2 \sum_{1 \leq k < 1}^{\kappa} \nu_k(n_k - \nu_k) - 1$. As a result, $\mathcal{N}_- = 0$ if and only if $\nu_k = 0$ for all $i = 1, \ldots, \kappa$, i.e. only at the global minimum $\{ U = e^{i\theta} W D(I \oplus \tilde{Z}_0) | \tilde{Z}_0 \in U(n_0) \text{ and } \theta \in [0, 2\pi) \}$. Furthermore, $\mathcal{N}_+$ can be zero for such a critical point only if $\omega_i^2 > \sum_{i=2}^\kappa \omega_i^2$, $n_0 = 0$, and $\Lambda = 1 + \oplus I_{n_0}$. The critical value of such a point is $||A||^4 - (\omega_i^2 - \sum_{i=2}^\kappa \omega_i^2)^2 < ||A||^4$, so in this very special circumstance, there exists a local maximum submanifold distinct from the global maximum set $\{ U : J_p(U) = ||A||^4 \}$. Since the intended use of this function is for minimization, such a local maximum submanifold does not act as a “trap”.
3.4 Global Maximum Set

Finally, consider the global maximum set \( \{ U : J_F(U) = ||A||^4 \} = \{ U : \text{Tr}(AA^\dagger W^\dagger U) = 0 \} \). This set does not admit analysis by the methods used thus far, so a different approach is required. Let \( F : U(N) \to \mathbb{R}^2 \) be given by \( F_1 := \Re \text{Tr}(AA^\dagger W^\dagger U) \) and \( F_2 := \Im \text{Tr}(AA^\dagger W^\dagger U) \). Then,

\[
d_U F_1(\delta U) = \Re \text{Tr}(AA^\dagger W^\dagger \delta U) = \frac{1}{2}(WAA^\dagger - UAA^\dagger W^\dagger U, \delta U) \tag{25a}
\]

\[
d_U F_2(\delta U) = \Im \text{Tr}(AA^\dagger W^\dagger \delta U) = \frac{1}{2}(iWAA^\dagger + iUAA^\dagger W^\dagger U, \delta U) \tag{25b}
\]

so that the gradients are given by

\[
\begin{align*}
\text{grad } F_1(U) &= \frac{1}{2}(WAA^\dagger - UAA^\dagger W^\dagger U) \tag{26a} \\
\text{grad } F_2(U) &= \frac{i}{2}(WAA^\dagger + UAA^\dagger W^\dagger U). \tag{26b}
\end{align*}
\]

Thus, \( dF \) is surjective except where there exists \((\alpha, \beta) \neq 0 \in \mathbb{R}^2\) such that \( \alpha \text{ grad } F_1(U) = \beta \text{ grad } F_2(U) \), i.e. where

\[
\cos(\alpha)U^\dagger WAA^\dagger = e^{-i\beta} AA^\dagger W^\dagger U, \tag{27}
\]

where \( e^{i\beta} = (\alpha-i\beta)/|\alpha+i\beta| \). As we have already seen, this equation implies that \( U = e^{i\beta} W D(\tilde{\Lambda} \tilde{\Gamma} \tilde{\Lambda}^\dagger \oplus \tilde{Z}_0) D^\dagger \). For such a \( U \), \( \text{Tr}(AA^\dagger W^\dagger U) = e^{i\beta} \text{Tr}(\Omega^2 \tilde{\Lambda}) \), so the only way for \( \text{Tr}(AA^\dagger W^\dagger U) \) to be zero is if \( \Omega^2 \) is orthogonal to one of the possible \( \tilde{\Lambda} \)'s. This means that for a given \( N \) and \( n_0 \), \( \Omega^2 \) would have to lie in the union of the \( 2^{N-n_0-1} \) hyperplanes which form the orthogonal spaces of the \( \tilde{\Lambda} \)'s within the space of real diagonal matrices. For a given \( N \) and \( n_0 \), the collection of all \( A \)'s for which \( dF \) is surjective at \( F(U) = 0 \) [hence \( \{ U : F(U) = 0 \} \) forms a codimension 2 submanifold of \( U(N) \)] corresponds to an open dense subset of \( \mathbb{C}^{N \times N} \). Now, at a point \( U \) such that \( \text{Tr}(AA^\dagger W^\dagger U) = 0 \),

\[
\text{Hess}_{J_F,U}(\delta U) = -\text{Tr}(AA^\dagger W^\dagger \delta U)WAA^\dagger + \text{Tr}(\delta U^\dagger WAA^\dagger)UAA^\dagger W^\dagger U \tag{28a}
\]

\[
= - \left[ \Re \text{Tr}(AA^\dagger W^\dagger \delta U) + i\Re \text{Tr}(-iAA^\dagger W^\dagger \delta U) \right] WAA^\dagger
+ \left[ \Re \text{Tr}(\delta U^\dagger WAA^\dagger) + i\Re \text{Tr}(-i\delta U^\dagger WAA^\dagger) \right] UAA^\dagger W^\dagger U \tag{28b}
\]

\[
= - \frac{1}{2} \left[ (WAA^\dagger - UAA^\dagger W^\dagger U, \delta U) + i(WAA^\dagger + iUAA^\dagger W^\dagger U, \delta U) \right] WAA^\dagger
+ \frac{1}{2} \left[ (WAA^\dagger - UAA^\dagger W^\dagger U, \delta U) - i(WAA^\dagger + iUAA^\dagger W^\dagger U, \delta U) \right] UAA^\dagger W^\dagger U \tag{28c}
\]

\[
= - \frac{1}{2} \left\{ (WAA^\dagger - UAA^\dagger W^\dagger U, \delta U)(WAA^\dagger - UAA^\dagger W^\dagger U)
+ (WAA^\dagger + iUAA^\dagger W^\dagger U, \delta U)(WAA^\dagger + iUAA^\dagger W^\dagger U) \right\} \tag{28d}
\]

so that the Hessian is rank 2 except where there exists \((\alpha, \beta) \neq 0 \in \mathbb{R}^2\) such that \( \alpha(WAA^\dagger - UAA^\dagger W^\dagger U) = \beta(iWAA^\dagger + iUAA^\dagger W^\dagger U) \). This is exactly the condition just considered for the surjectivity of \( dF \), so that the Hessian is rank 2 if and only if \( dF \) is surjective. So, on the open dense set of \( A \)'s for which this happens,
the maximum set is a nondegenerate (in the Morse-Bott sense), codimension 2 submanifold of $U(N)$. Since the other critical points also comprise nondegenerate submanifolds, we conclude that for these $A$’s, $J_P$ is a Morse-Bott function. In the particular case that $AA^\dagger$ is fully degenerate (e.g., $A = I$), it is found that the maximum set of $J_P$ is a nondegenerate submanifold if and only if $N$ is odd. However, when $N$ is even, arbitrarily small perturbations of $A$ about $I$ are sufficient to obtain a Morse-Bott function.

4 Dynamical Critical Point Analysis

Now that we have elucidated the structure of the critical sets of the kinematic landscapes $J_F$ and $J_P$, we return to the problem of characterizing the critical set of the dynamical landscapes $\tilde{J} = J \circ V_T$. Let $\mathcal{M} \subset U(N)$ be one of the critical submanifolds identified in the previous sections. It can be proved (see Appendix A) that $V_T : K \to U(N)$ is $C^\infty$. In addition, since $U(N)$ is finite-dimensional, if $V_T(\mathcal{E}) \in \mathcal{M}$ then $(d_{\mathcal{E}} V_T)^{-1}(T_{V_T(\mathcal{E})}\mathcal{M})$ has finite codimension, so is closed and has a closed complement (i.e., it “splits”). Therefore, away from singular points of $V_T$ (i.e., those $\mathcal{E} \in K$ such that $d_{\mathcal{E}} V_T$ is rank-deficient), $V_T$ is transversal to $\mathcal{M}$ and by the transversal mapping theorem [1], $V_T^{-1}(\mathcal{M})$ is a Hilbert submanifold of $K$, $T_{\mathcal{E}}(V_T^{-1}(\mathcal{M})) = (d_{\mathcal{E}} V_T)^{-1}(T_{V_T(\mathcal{E})}\mathcal{M})$, and codim $(V_T^{-1}(\mathcal{M})) = \text{codim}(\mathcal{M})$.

Let $\mathcal{E} \in K$ be a regular critical point of $\tilde{J}$, i.e. such that grad $\tilde{J}(\mathcal{E}) = 0$ and $d_{\mathcal{E}} V_T$ is full rank. It may be seen that at such a point, the Hessian of $\tilde{J}$ is given by $\text{Hess}_{\tilde{J},\mathcal{E}} = (d_{\mathcal{E}} V_T)^* \circ \text{Hess}_{J,V_T(\mathcal{E})} \circ (d_{\mathcal{E}} V_T)$. Let $A_{\mathcal{E}}$ be the linear operator on $T_{V_T(\mathcal{E})} U(N)$ given by

$$A_{\mathcal{E}} = (d_{\mathcal{E}} V_T \circ (d_{\mathcal{E}} V_T)^*)^{\frac{1}{2}} \circ \text{Hess}_{J,V_T(\mathcal{E})} \circ (d_{\mathcal{E}} V_T \circ (d_{\mathcal{E}} V_T)^*)^{\frac{1}{2}}.$$ (29)

Since $d_{\mathcal{E}} V_T$ is assumed to have full rank, we may apply Sylvester’s law of inertia [9] to conclude that $A_{\mathcal{E}}$ and $\text{Hess}_{J,V_T(\mathcal{E})}$ have the same numbers of positive, negative, and zero eigenvalues. Let $\{(\eta_j, V_j)\}$ for $j = 1, \ldots, N^2$ be the eigenvalues and eigenvectors of $A_{\mathcal{E}}$, and let $Z_j = (d_{\mathcal{E}} V_T)^* \circ (d_{\mathcal{E}} V_T \circ (d_{\mathcal{E}} V_T)^*)^{\frac{1}{2}} V_j$. Then

$$\text{Hess}_{\tilde{J},\mathcal{E}} Z_j = (d_{\mathcal{E}} V_T)^* \circ \text{Hess}_{J,V_T(\mathcal{E})} \circ (d_{\mathcal{E}} V_T \circ (d_{\mathcal{E}} V_T)^*)^{\frac{1}{2}} V_j$$ (30a)

$$= \eta_j (d_{\mathcal{E}} V_T)^* \circ (d_{\mathcal{E}} V_T \circ (d_{\mathcal{E}} V_T)^*)^{\frac{1}{2}} V_j = \eta_j Z_j$$ (30b)

so that $\{(\eta_j, Z_j)\}$ for $j = 1, \ldots, N^2$ are eigenvalues and eigenvectors of $\text{Hess}_{\tilde{J},\mathcal{E}}$. Since $\text{Hess}_{\tilde{J},\mathcal{E}}$ is self-adjoint, any other eigenvector $Z$ must be orthogonal to the $\{Z_j\}$. Also, note that since the $\{V_j\}$ span $T_{V_T(\mathcal{E})} U(N)$, the $\{Z_j\}$ span $\text{Range} ((d_{\mathcal{E}} V_T)^*)$. Then, for any $X \in T_{V_T(\mathcal{E})} U(N)$, $0 = \langle Z, (d_{\mathcal{E}} V_T)^*(X) \rangle = \langle d_{\mathcal{E}} V_T(Z), X \rangle$, so that $d_{\mathcal{E}} V_T(Z) = 0$ and therefore $\text{Hess}_{\tilde{J},\mathcal{E}} Z = 0$. Thus, $\text{Hess}_{\tilde{J},\mathcal{E}}$ has infinitely many eigenvalues; $N^2$ of them are identical to the eigenvalues of $A_{\mathcal{E}}$, and the remaining infinite number of eigenvalues are all zero. Since $J$ has no local traps, we can conclude that $\tilde{J}$ has no local traps among the regular critical points. From the transversal mapping theorem we find that $T_{\mathcal{E}}(V_T^{-1}(\mathcal{M})) = (d_{\mathcal{E}} V_T)^{-1}(T_{V_T(\mathcal{E})}\mathcal{M})$, implying that for any
\[ f \in K, \text{ we have} \]
\[
\begin{align*}
\text{Hess}_{J,E}(f) = (d_F V_T) \circ \text{Hess}_{J,V_T(E)} \circ (d_F V_T)(f) = 0 & \iff d_F V_T(f) \in \ker \text{Hess}_{J,E} \quad (31a) \\
& \iff d_F V_T(f) \in T_{V_T(E)} \mathcal{M} \quad (31b) \\
& \iff f \in (d_F V_T)^{-1}(T_{V_T(E)} \mathcal{M}) \quad (31c) \\
& \iff f \in T_{E}(V_T^{-1}(\mathcal{M})). \quad (31d)
\end{align*}
\]

Hence, the null space of \( \text{Hess}_{J,E} \) is identical to \( T_{E}(V_T^{-1}(\mathcal{M})) \), the tangent space to the critical submanifold.

In the case where the Hamiltonian takes the dipole form \( H(t) = H_0 - \mathcal{E}(t)\mu \) for any \( \mathcal{E} \in L^2(\mathbb{R}_+; \mathbb{R}) \), the Fréchet derivative of \( V_T \) is given by \( d_F V_T(\delta \mathcal{E}) = \frac{\delta}{\mathbb{R}} V_T(\mathcal{E}) \int_0^T V_1^T(\mathcal{E}) \mu V_1(\mathcal{E}) d\mathcal{E}(t) dt \). Then the adjoint operator of the derivative is \( d_F V_T^*(A)(t) = -\Im \text{Tr} (A^1 V_T(\mathcal{E}) V_1^T(\mathcal{E}) \mu V_1(\mathcal{E})) \) for any \( A \in T_{V_T(E)} U(N) \), and the operator norm of this adjoint is uniformly bounded by \( ||d_F V_T^*|| \leq \sqrt{T}\|\mu\| \). For any smooth ‘kinematic’ function \( g : U(N) \rightarrow \mathbb{R} \), let \( \tilde{g} = g \circ V_T \) be the corresponding ‘dynamical’ function on \( L^2(\mathbb{R}_+; \mathbb{R}) \). Then \( \text{grad} \tilde{g}(\mathcal{E}) = d_F V_T(\text{grad} g(V_T(\mathcal{E}))) \) and \( ||\text{grad} \tilde{g}(\mathcal{E})|| \leq ||d_F V_T^*|| ||\text{grad} g(V_T(\mathcal{E}))|| \leq \sqrt{T}\|\mu\| ||\text{grad} g(V_T(\mathcal{E}))|| \).

Since \( g \) is smooth, \( ||\text{grad} g|| \) is continuous over \( U(N) \), so that since \( U(N) \) is compact, \( ||\text{grad} g|| \) is uniformly bounded. Therefore, \( ||\text{grad} \tilde{g}|| \) is uniformly bounded over \( L^2(\mathbb{R}_+; \mathbb{R}) \). For any dynamical quantum control landscape constructed in this way, the slope of the landscape is uniformly bounded by some constant.

## 5 Landscapes Based on Intrinsic (Geodesic) Distance

The kinematic landscapes \( J_F \) and \( J_P \) considered above are based on the Euclidean (or norm) distance on \( U(N) \) and \( PU(N) \), respectively. We now describe two additional distance measures based on the intrinsic distance between operators in \( U(N) \) and \( PU(N) \) under the Riemannian metric induced by the real Hilbert-Schmidt inner product on \( \mathbb{C}^{N \times N} \).

The first of these distance measures is quite simple to define. Since the chosen Riemannian metric is bi-invariant on \( U(N) \), any geodesic starting at \( U \in U(N) \) is of the form \( \gamma(s) = U e^{A{s}} \) for some \( A \in \mathfrak{u}(N) \). To find a geodesic joining \( U \) to some target \( W \in U(N) \), let \( U e^A = \gamma(1) = W \), so that \( e^A = U^\dagger W \) and \( A = \log(U^\dagger W) \). This matrix logarithm is not uniquely defined, but the length of the geodesic \( \gamma \) defined on the interval \([0, 1]\) is given by \( L[\gamma] = \int_0^1 ||\gamma'(s)|| ds = ||A|| \). The minimum such length is obtained by taking \( A = \log(U^\dagger W) \) from the principal branch of the logarithm so that all eigenvalues lie in \( (-i\pi, i\pi) \). We then define the landscape as \( J_G(U) := \frac{1}{2} ||\log(U^\dagger W)||^2 \). Then the gradient of \( J_G \) is given by (see Appendix B)

\[
\text{grad} J_G(U) = -U \log(U^\dagger W).
\]

As most numerical matrix logarithm routines (e.g., the \texttt{logm} function in MATLAB) compute the principal branch, they provide a ready means to obtain both the landscape value and the gradient. Since the norm of \( \text{grad} J_G \) is the distance to the target, this vector field is only zero at the target, i.e. the global minimum of the landscape. Hence, there are no traps or saddles. The gradient field has the property that it is
discontinuous and multiply defined at the cut loci of $U(N)$ (where the spectrum of $U^{\dagger}W$ contains $-1$), but this is not a problem for an optimal control algorithm since the matrix logarithm routine will have to choose one from among the possible solutions, all of which describe minimal geodesics to the target that are equally satisfactory.

A phase-invariant version of $J_G$ may be constructed analogously by considering minimal geodesics on the projective unitary group $PU(N) \simeq U(N)/U(1)$, or equivalently by defining $J_{GP}(U) := \min_{k} \frac{1}{2} \| \log(e^{i\theta}U^{\dagger}W) \|^2$ on $U(N)$. It may be shown that

$$J_{GP} = \min_{k \in \mathbb{Z}_N} \frac{1}{2} \| \log \left( e^{\frac{2\pi i k}{N}} \det(U^{\dagger}W)^{-\frac{1}{N}} U^{\dagger}W \right) \|^2$$

(33a)

$$\text{grad} \ J_{GP}(U) = -U \left\{ \log \left( e^{\frac{2\pi i k}{N}} \det(U^{\dagger}W)^{-\frac{1}{N}} U^{\dagger}W \right) - \frac{1}{N} \text{Tr} \left[ \log \left( e^{\frac{2\pi i k}{N}} \det(U^{\dagger}W)^{-\frac{1}{N}} U^{\dagger}W \right) \right] 1 \right\},$$

(33b)

where $k$ in (33b) is the minimizer from (33a). With this minimizing $k$, the trace in (33b) will be zero, so that

$$\text{grad} \ J_{GP}(U) = -U \log \left( e^{\frac{2\pi i k}{N}} \det(U^{\dagger}W)^{-\frac{1}{N}} U^{\dagger}W \right).$$

(34)

As with $J_G$, the norm of grad $J_{GP}$ is the distance to the target, and this vector field is only zero at the target, i.e. the global minimum of the landscape. Hence, there are no traps or saddles. One downside to this landscape is that it appears that all $N$ possible values of $k$ must be tried in order to find the minimizer of (33a). This behavior has a topological interpretation on $PU(N)$. Since the fundamental group of $PU(N)$ is $\pi_1(\text{PU}(N)) \cong \mathbb{Z}_N = \mathbb{Z}/N\mathbb{Z}$, there are exactly $N$ homotopy classes of paths connecting $\pi(U)$ to the target $\pi(W)$. Within each of these classes is a unique minimal geodesic, and these $N$ minimal geodesics are identified by the vectors $U \left\{ \log \left( e^{\frac{2\pi i k}{N}} \det(U^{\dagger}W)^{-\frac{1}{N}} U^{\dagger}W \right) - \frac{1}{N} \text{Tr} \left[ \log \left( e^{\frac{2\pi i k}{N}} \det(U^{\dagger}W)^{-\frac{1}{N}} U^{\dagger}W \right) \right] 1 \right\}$ indexed by $k$.

A distance metric based on intrinsic distance could in principle be applied to the case where only some of the states are important, analogous to $J_F$ and $J_P$ where $A$ is rank deficient (e.g. where $A$ is a projector). This is equivalent to computing the geodesic distance between points on the Stiefel manifold $V_k(\mathbb{C}^N) \simeq U(N)/\mathbb{I}_k \oplus U(N-k)$ or on its projective cousin $V_k(\mathbb{C}^N)/U(1)$. However, the two-point geodesics on these spaces are non-trivial to compute. The problem requires solution of a boundary value problem or an optimization problem to find each minimal geodesic. For that reason, these intrinsic distance metrics may not be practical for this scenario.

6 Summary

This work presented an expanded analysis of landscapes $J_F$ and $J_P$, which are based on the Euclidean distances between unitary operators in $U(N)$ and $PU(N)$, respectively. The expansion appears in several ways. First, additional freedom has been allowed in the landscape functions themselves, by admitting $A$
matrices that are rank-deficient. Landscapes based on these rank-deficient $A$ matrices measure the distance between unitary operators by their action on a subspace of the full state space. This can be the desired objective for designing a quantum information processor, for example, where only this subspace of the state space is to be used for the quantum register. This additional freedom in defining the landscape is consistent with the principal finding of earlier work on landscapes of this form: they have no suboptimal minima (i.e., “traps”) that could impede a deterministic optimal control algorithm (such as gradient descent) from reaching the global minimum.

In addition to broadening the families of landscapes for consideration, we have provided more detail on the structure of the critical sets and the behavior of the landscape functions at these critical sets. The critical sets were shown to generally be disjoint unions of critical submanifolds and we have described the structure of these submanifolds, either as products of Grassmannians and a unitary group in the case of $J_F$, or as a $U(1)$ principal fibre bundle over such a product in the case of $J_P$. Furthermore, we have shown that these critical submanifolds are generally nondegenerate in the Morse-Bott sense, so that the kinematic landscapes are generally Morse-Bott functions.

These results were related back to the corresponding dynamical landscapes through the control-to-propagator map $V_T$, implicitly defined by the Schrödinger equation, that takes a control function as input and returns the final time unitary evolution operator. This map was shown to be infinitely Fréchet differentiable, leading to the conclusion that, away from the singular points of $V_T$, the level sets and critical sets of the dynamical landscapes are $C^\infty$ smooth, finite codimension submanifolds of the infinite dimensional control space $K = L^2(R_+;R)$. Also, the number of positive and negative Hessian eigenvalues (and therefore the characterization as a minimum, maximum, or saddle) was shown to be identical for a kinematic critical point and a regular point of $V_T$ that maps to it. This behavior implies that no traps exist in the dynamical landscape among the set of regular points of $V_T$. Furthermore, Morse-Bott nondegeneracy of the critical set is also preserved away from singular points of $V_T$, which can be important for certain numerical landscape exploration methods such as second order D-MORPH [2].

Finally, two additional landscapes were introduced that are based on the intrinsic or geodesic distance between operators in $U(N)$ and $PU(N)$, respectively, rather than Euclidean distance. These kinematic landscapes have the desirable property of having no critical points except at the target. These landscapes may allow for more efficient performance of optimal control algorithms over $J_F$ and $J_P$, since the latter have many saddle points where the gradient is zero.

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\section*{A Differentiability of $U(T, 0)$ With Respect to the Control}

Let $\mathbb{M}(N) \subset \mathbb{C}^{N \times N}$ denote the space of $N \times N$ Hermitian matrices endowed with the real Hilbert-Schmidt inner product $\langle A, B \rangle_{HS} = \Re \text{Tr}(A^\dagger B)$, and let $\mathbb{H}(N) = L^2(\mathbb{R}_+; \mathbb{M}(N))$ denote the space of all $N \times N$ square-integrable time-dependent Hamiltonians with inner product $\langle H_1, H_2 \rangle_{L^2} = \int_0^\infty \Re \text{Tr}[H_1^\dagger(t)H_2(t)] \, dt$. Let $Z_T : \mathbb{H}(N) \to U(N)$ be the map, defined implicitly through the Schrödinger equation, that takes a time-dependent Hamiltonian $H(\cdot) \in \mathbb{H}(N)$ and produces the corresponding unitary time-evolution operator at time $T$: $U(T, 0) \in U(N)$. This map is well-defined over the entire domain because of the absolute convergence of the Dyson series over $\mathbb{H}(N)$:

$$Z_T(H) = I + \left( -\frac{i}{\hbar} \right) \int_0^T dt_1 H(t_1) + \left( -\frac{i}{\hbar} \right)^2 \int_0^T dt_1 H(t_1) \int_0^{t_1} dt_2 H(t_2) + \ldots . \tag{35}$$

In this appendix, we will prove that $Z_T$ is well-defined and infinitely Fréchet differentiable over $\mathbb{H}(N)$. A corollary is that the map $V_T : \mathbb{K} \to U(N)$ defined in the body of the paper is infinitely Fréchet differentiable over all of $\mathbb{K} = L^2(\mathbb{R}_+; \mathbb{R})$.

\textbf{Lemma 1.} If $f : [a, b] \to \mathbb{R}$ is integrable, then

$$\int_a^b dt_1 f(t_1) \int_a^{t_1} dt_2 f(t_2) \cdots \int_a^{t_{n-1}} dt_n f(t_n) = \frac{1}{n!} \left( \int_a^b f(t) \, dt \right)^n . \tag{36}$$

\textbf{Proof.} Note first that (36) holds trivially for $n = 1$. Suppose that it holds for $n = m$. Then

$$\int_a^b dt_1 f(t_1) \int_a^{t_1} dt_2 f(t_2) \cdots \int_a^{t_m} dt_{m+1} f(t_{m+1})$$

$$= \frac{1}{m!} \int_a^b f(t_1) \left( \int_a^{t_1} f(t) \, dt \right)^m \, dt_1 \tag{37a}$$

$$= \frac{1}{m!} \int_a^b \frac{d}{dt_1} \left[ \frac{1}{m+1} \left( \int_a^{t_1} f(t) \, dt \right)^{m+1} \right] \, dt_1 \tag{37b}$$

$$= \frac{1}{(m+1)!} \left( \int_a^b f(t) \, dt \right)^{m+1} \tag{37c}$$

and the lemma follows for arbitrary $n \in \mathbb{N}$ by induction. \hfill \square

\textbf{Definition 1.} For integrable matrix functions $A_i : [0, T] \to \mathbb{C}^{N \times N}$ and for integrable real-valued functions $a_i : [0, T] \to \mathbb{R}$, we will use the following short-hand notation for the Dyson-esque terms

$$\Upsilon_T[A_1, A_2, \ldots, A_n] := \int_0^T dt_1 A_1(t_1) \int_0^{t_1} dt_2 A_2(t_2) \cdots \int_0^{t_{n-1}} dt_n A_n(t_n) \quad \text{and} \tag{38a}$$

$$\Upsilon_T[a_1, a_2, \ldots, a_n] := \int_0^T dt_1 a_1(t_1) \int_0^{t_1} dt_2 a_2(t_2) \cdots \int_0^{t_{n-1}} dt_n a_n(t_n) . \tag{38b}$$
Lemma 2. If $g_1, \ldots, g_m \in L^2(\mathbb{R}_+; \mathbb{R}_+)$ are non-negative square-integrable functions on $[0, \infty)$, then
\begin{equation}
\mathcal{Y}_T[g_1, g_2, \cdots, g_m] \leq T^{m/2} \|g_1\|_{L^2} \cdots \|g_m\|_{L^2} \tag{39}
\end{equation}

Proof. Since the $g_i$'s are non-negative functions, we get the inequalities
\begin{align*}
\mathcal{Y}_T[g_1, g_2, \cdots, g_m] &= \int_0^T dt_1 g_1(t_1) \int_0^{t_1} dt_2 g_2(t_2) \cdots \int_0^{t_{m-1}} dt_m g_m(t_m) \tag{40a} \\
&\leq \int_0^T dt_1 g_1(t_1) \int_0^T dt_2 g_2(t_2) \cdots \int_0^T dt_m g_m(t_m) \tag{40b} \\
&\leq T^{m/2} \left( \int_0^T dt_1 g_1^2(t_1) \right)^{\frac{1}{2}} \left( \int_0^T dt_2 g_2^2(t_2) \right)^{\frac{1}{2}} \cdots \left( \int_0^T dt_m g_m^2(t_m) \right)^{\frac{1}{2}} \tag{40c} \\
&\leq T^{m/2} \|g_1\|_{L^2} \cdots \|g_m\|_{L^2} \tag{40d}
\end{align*}
by extension of the integrals out to the interval $[0,T]$, followed by application of the Cauchy-Schwarz inequality, and finally extension out to $[0,\infty)$.

Lemma 3. If $f, g_1, \ldots, g_m \in L^2(\mathbb{R}_+; \mathbb{R}_+)$ are non-negative square-integrable functions on $[0, \infty)$, then
\begin{equation}
\mathcal{Y}_T[f, f, g_1, \ldots, f, f, g_2, \ldots, f, f, \ldots, g_m, f, \ldots, f, f, \ldots, f] \leq \frac{T^{1/2} \sum \beta_i}{\prod_{i=0}^{m} \beta_i} \|f\|_{L^2} \mathcal{Y}_T[g_1, g_2, \cdots, g_m] \tag{41}
\end{equation}

Proof. Let $\sigma_i = \beta_0 + \cdots + \beta_i + i + 1$ for $i = 0, \ldots, m$. Then, using Fubini’s theorem, we may rearrange the order of integration as follows:
\begin{align*}
\mathcal{Y}_T[f, f, g_1, \ldots, f, f, g_2, \ldots, f, f, \ldots, g_m, f, \ldots, f, f, \ldots, f] &= \int_0^T dt_1 f(t_1) \cdots \int_0^{t_{\sigma_0-2}} dt_{\sigma_0-1} f(t_{\sigma_0-1}) \int_0^{t_{\sigma_0-1}} dt_{\sigma_0} g_1(t_{\sigma_0}) \int_0^{t_{\sigma_0}} dt_{\sigma_0+1} f(t_{\sigma_0+1}) \cdots \tag{42a} \\
&\quad \cdots \int_0^{t_{\sigma_m-2}} dt_{\sigma_m-1} f(t_{\sigma_m-1}) \int_0^{t_{\sigma_m-1}} dt_{\sigma_m} g_m(t_{\sigma_m}) \times \int_0^{t_{\sigma_m-2}} dt_{\sigma_m-1} f(t_{\sigma_m-1}) \cdots \int_0^{t_{\sigma_m-1}} dt_{\sigma_m-2} f(t_{\sigma_m-2}) \times \cdots \\
&= \frac{1}{\prod_{i=0}^{m} \beta_i} \int_0^T dt_0 g_1(t_0) \int_0^{t_{\sigma_0}} dt_{\sigma_1} g_2(t_{\sigma_1}) \cdots \int_0^{t_{\sigma_m-1}} dt_{\sigma_m-1} g_m(t_{\sigma_m-1}) \times \int_0^{t_{\sigma_m-1}} dt_{\sigma_m-1} f(t_{\sigma_m-1}) \cdots \int_0^{t_{\sigma_m-2}} dt_{\sigma_m-2} f(t_{\sigma_m-2}) \times \cdots \tag{42b}
\end{align*}
where the last step follows from Lemma 1. Then, since \( f \) is a non-negative function, we get the inequality

\[
\mathcal{Y}_T[f, \ldots, f, g_1, f, \ldots, f, g_2, \ldots, f, g_m, \ldots, f] 
\leq \frac{1}{\prod_{i=0}^{n} \beta_i!} \left( \int_0^T f(t) \, dt \right)^{\sum_{i=0}^{n} \beta_i} \int_0^T \, dt_1 \cdot \int_0^{t_1} \, dt_2 \cdot \cdots \cdot \int_0^{t_{m-1}} \, dt_m \cdot g_m(t_m) 
\leq \frac{T^{\sum \beta_i}}{\prod_{i=0}^{n} \beta_i!} \left\| f \right\|_{L^2} \sum \beta_i \mathcal{Y}_T[g_1, g_2, \ldots, g_m] 
\] (43a)

by first extending the \( f \) integrals to the interval \([0, T]\), and then invoking the Cauchy-Schwarz inequality. □

**Lemma 4.**

\[
\sum_{c_1 + \cdots + c_r = p} \frac{1}{\prod_{i=1}^{r} c_i!} = \frac{r^p}{p!}. 
\] (44)

**Proof.** First, observe that for any \( \alpha > 0 \),

\[
\sum_{c_j = 1}^{p - \sum_{i=1}^{j-1} c_i} \frac{\alpha^{p - \sum_{i=1}^{j} c_i}}{c_j! (p - \sum_{i=1}^{j} c_i)!} = \frac{1}{\left( p - \sum_{i=1}^{j} c_i \right)!} \sum_{c_j = 0}^{p - \sum_{i=1}^{j-1} c_i} \left( p - \sum_{i=1}^{j-1} c_i \right) \alpha^{p - \sum_{i=1}^{j} c_i} 
\] (45a)

\[
= \frac{(\alpha + 1)^{p - \sum_{i=1}^{j-1} c_i}}{\left( p - \sum_{i=1}^{j-1} c_i \right)!}. 
\] (45b)

Then it follows that

\[
\sum_{c_1 + \cdots + c_r = p} \frac{1}{\prod_{i=1}^{r} c_i!} = \sum_{c_1 = 0}^{p-c_1} \sum_{c_2 = 0}^{p-c_1-c_2} \cdots \sum_{c_r = 0}^{p-c_1-c_2-\cdots-c_{r-1}} \frac{1}{c_1! \cdots c_{r-1}! \left( p - \sum_{i=1}^{r-1} c_i \right)!} 
\] (46a)

\[= \sum_{c_1 = 0}^{p} \left( \frac{(r-1)^{p-c_1}}{c_1!(p-c_1)!} \right) 
\] (46c)

\[= \frac{r^p}{p!}. 
\] (46d)
Definition 2. For $m = 0, 1, 2, \ldots$, let $\mathcal{B}^m(\mathbb{T}(N); \mathbb{C}^{N \times N})$ denote the space of bounded $m$-multilinear operators from $(\mathbb{T}(N))^m = \mathbb{T}(N) \times \mathbb{T}(N) \times \cdots \times \mathbb{T}(N)$ to $\mathbb{C}^{N \times N}$, with the norm
\[
\|A\| = \sup_{\{\|\delta H\| \neq 0\}} \frac{\|A(\delta H_1, \ldots, \delta H_m)\|}{\|\delta H_1\| \cdots \|\delta H_m\|}
\]
for each $A \in \mathcal{B}^m(\mathbb{T}(N); \mathbb{C}^{N \times N})$. Then let $\Phi_{T,m}: \mathbb{H} \to \mathcal{B}^m(\mathbb{T}(N); \mathbb{C}^{N \times N})$ be defined by
\[
\Phi_{T,m}(H)(\delta H_1, \delta H_2, \ldots, \delta H_m) := \sum_{n=m}^{\infty} \sum_{a_0 + \cdots + a_m = n-m} \sum_{\pi \in S_m} \left(\frac{i}{\hbar}\right)^n \times
\]
\[
\times \Upsilon \left[ H, \ldots, H, \delta H_{\pi(1)}, H, \ldots, H, \delta H_{\pi(2)}, H, \ldots, H, \delta H_{\pi(m)}, H, \ldots, H \right],
\]
where $S_m$ denotes the symmetric group on $m$ elements (i.e., the group of permutations of $m$ elements). For $m, q = 0, 1, 2, \ldots$, let $\Psi_{T,m,q}: \mathbb{H} \oplus \mathbb{T}(N) \to \mathcal{B}^m(\mathbb{T}(N); \mathbb{C}^{N \times N})$ be defined by
\[
\Psi_{T,m,q}(H, \delta H)(\delta H_1, \delta H_2, \ldots, \delta H_m) := \sum_{n=m+q}^{\infty} \sum_{a_0 + \cdots + a_{m+q} = n-m-q} \sum_{b_0 + \cdots + b_{m+q} = q} \sum_{\pi \in S_m} \left(\frac{i}{\hbar}\right)^n \times
\]
\[
\times \Upsilon \left[ H, \ldots, H, A_1, H, \ldots, H, A_2, H, \ldots, H, A_{m+q}, H, \ldots, H \right],
\]
where
\[
\{A_1, A_2, \ldots, A_{m+q}\} = \left\{ \delta H, \ldots, \delta H, \delta H_{\pi(1)}, \delta H, \ldots, \delta H_{\pi(2)}, \delta H, \ldots, \delta H_{\pi(m)}, \delta H, \ldots, \delta H \right\}
\]
Lemma 5. $\Phi_{T,m}$ and $\Psi_{T,m,q}$ are well-defined since their defining sums converge absolutely, and for each $H \in \mathbb{H}$ and $\delta H \in \mathbb{T}(N)$, $\Phi_{T,m}(H)$ and $\Psi_{T,m,q}(H)(\delta H)$ are bounded $m$-multilinear operators.

Proof. Let $f(t) = \|H(t)\|, g_i(t) = \|A_i(t)\|, h_j(t) = \|\delta H_j(t)\|$, and $h(t) = \|\delta H(t)\|$. Then
\[
\|\Upsilon \left[ H, \ldots, H, A_1, H, \ldots, H, A_2, H, \ldots, H, A_{m+q}, H, \ldots, H \right]\|
\leq \Upsilon \left[ f, \ldots, f, g_1, f, \ldots, f, g_2, f, \ldots, f, g_{m+q}, f, \ldots, f \right]
\leq \frac{T^{n-m-q}}{\prod_{i=0}^{m+q} a_i} \|f\|_{L^2}^{n-m-q} \Upsilon \left[ g_1, g_2, \ldots, g_{m+q} \right]
\leq \frac{T^{n-m-q}}{\prod_{i=0}^{m+q} a_i} \|H\|_{L^2}^{n-m-q} \Upsilon \left[ h, \ldots, h, h_{\pi(1)}, h, \ldots, h, h_{\pi(2)}, h, \ldots, h, h_{\pi(m)}, h, \ldots, h \right]
\]

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Theorem 1. \(Z_T\) is infinitely Fréchet differentiable, i.e. \(C^\infty\), everywhere on \(\mathbb{H}\). 

Proof. We begin by establishing that \(\Phi_{T,m}\) is Fréchet differentiable for each \(m = 0, 1, 2, \ldots\), with derivative \(\Phi_{T,m+1}\). Observe that 

\[
\Phi_{T,m+1}(H)(\delta H_1, \ldots, \delta H_m, \delta H) = \Psi_{T,m,1}(H, \delta H)(\delta H_1, \ldots, \delta H_m)
\]

and that since the defining sum for \(\Phi_{T,m}(H + \delta H)\) converges absolutely, it may be rearranged as 

\[
\Phi_{T,m}(H + \delta H)(\delta H_1, \ldots, \delta H_m) = \sum_{q=0}^{\infty} \Psi_{T,m,q}(H, \delta H)(\delta H_1, \ldots, \delta H_m).
\]
Then by appealing to the bound of $\Psi_{T,m,q}$ in (52c), we get

$$\|\Phi_{T,m}(H + \delta H) - \Phi_{T,m}(H) - \Phi_{T,m+1}(H)(\ldots, \delta H)\|$$

$$= \sup_{\|\delta H\| = 1} \left\| \Phi_{T,m}(H + \delta H)(\delta H_1, \ldots, \delta H_m) - \Phi_{T,m}(H)(\delta H_1, \ldots, \delta H_m) \right\|$$

$$= \sup_{\|\delta H\| = 1} \left\| \sum_{q=2}^{\infty} \Psi_{T,m,q}(H, \delta H)(\delta H_1, \ldots, \delta H_m) \right\|$$

$$\leq \sup_{\|\delta H\| = 1} \sum_{q=2}^{\infty} \|\Psi_{T,m,q}(H, \delta H)(\delta H_1, \ldots, \delta H_m)\|$$

$$\leq \sum_{q=2}^{\infty} \frac{m!T^{m+q}}{h^{m+q} q!} \exp \left( \frac{(m + q + 1)\sqrt{T}}{h} \right) \|\delta H\| L^2$$

$$\leq \sum_{q=2}^{\infty} \frac{m!T^{m+q}}{h^{m+q} (q - 2)!} \exp \left( \frac{(m + q + 1)\sqrt{T}}{h} \right) \|\delta H\| L^2$$

$$= \frac{m!T^{m+2}}{h^{m+2}} \exp \left( \frac{(m + 3)\sqrt{T}}{h} \right) \|\delta H\| L^2 \exp \left( \frac{\sqrt{T}}{h} \|\delta H\| L^2 \right) \|\delta H\| L^2.$$ (56f)

Hence,

$$\lim_{\|\delta H\| \to 0} \frac{\|\Phi_{T,m}(H + \delta H) - \Phi_{T,m}(H) - \Phi_{T,m+1}(H)(\ldots, \delta H)\|}{\|\delta H\|} = 0$$ (57)

and therefore $\Phi_{T,m}$ is Fréchet differentiable with derivative $\Phi_{T,m+1}$. Since $Z_T = \Phi_{T,0}$, this implies that $Z_T$ is infinitely Fréchet differentiable, and that the $m$th derivative of $Z_T$ is $\Phi_{T,m}$.

\[\Box\]

**Lemma 6.** Let $\hat{H} : \mathbb{K} \to \mathbb{H}(N)$ be defined by $\hat{H}(\mathcal{E})(t) = H_0 - \mu \mathcal{E}(t)$ for some fixed $N \times N$ Hermitian matrices $H_0$ and $\mu$. Then $\hat{H}$ is infinitely Fréchet differentiable, i.e. $C^\infty$.

**Proof.** Let $\zeta : \mathbb{K} \to \mathcal{B}(\mathbb{T}_N \mathbb{H}(N))$ be defined by $\zeta(\mathcal{E})(\delta \mathcal{E})(t) = -\mu \delta \mathcal{E}(t)$. For each $\mathcal{E} \in \mathbb{K}$, $\zeta(\mathcal{E})$ is linear, and $\|\zeta(\mathcal{E})(\delta \mathcal{E})\|_{L^2} = \|\mu\|_{HS} \|\delta \mathcal{E}\|_{L^2}$, so $\zeta(\mathcal{E})$ is bounded. Now,

$$\lim_{\|\delta \mathcal{E}\| \to 0} \frac{\|\hat{H}(\mathcal{E} + \delta \mathcal{E}) - \hat{H}(\mathcal{E}) - \zeta(\mathcal{E})(\delta \mathcal{E})\|}{\|\delta \mathcal{E}\|} = 0$$ (58)

so that $\zeta$ is the Fréchet derivative of $\hat{H}$. Since $\zeta$ is constant (i.e., $\zeta(\mathcal{E})$ is the same linear operator regardless of which $\mathcal{E} \in \mathbb{K}$ is input), the higher Fréchet derivatives also exist and are all equal to zero. \[\Box\]

**Theorem 2.** $V_T = Z_T \circ \hat{H} : \mathbb{K} \to U(N)$ is a composition of $C^\infty$ maps and therefore is itself a $C^\infty$ map.
Several steps in Section 5 require differentiation of expressions involving the matrix logarithm. Since the expressions to be differentiated are all similar, this appendix will demonstrate the computation of the gradient of the kinematic landscape $J_G$, as the other variations follow along the same lines. To this end, we fix some target $W \in \mathbf{U}(N)$ and $U \in \mathbf{U}(N)$ and define the following maps:

- $f : \mathfrak{u}(N) \rightarrow \mathbb{R}$, with $f(A) = \frac{1}{2} \text{Tr}(A^\dagger A) = \frac{1}{2} \langle A, A \rangle = \frac{1}{2} \|A\|^2$.
- $g : \mathbf{U}(N) \rightarrow \mathfrak{u}(N)$, with $g(V) = \log(V)$.
- $h : \mathbf{U}(N) \rightarrow \mathbf{U}(N)$, with $h(U) = U^\dagger W$.

Then $J_G = f \circ g \circ h$. To compute $\text{grad} J_G$, we will determine the various pieces of the differential

$$d_U J_G(\delta U) = d_{g(h(U))} f \circ d_{h(U)} g \circ d_U h(\delta U)$$

and then recombine them as

$$\text{grad} J_G(U) = d_U h^* \circ d_{h(U)} g^* \circ \text{grad} f(g(h(U))).$$

First, let us examine $f(a) = \frac{1}{2} \langle A, A \rangle$. Because of the bilinearity and symmetry of the inner product, we can easily establish that the differential $d_A f : \mathfrak{u}(N) \rightarrow \mathbb{R}$ is given by $d_A f(\delta A) = \langle A, \delta A \rangle$. Hence, by the definition of the gradient,

$$\text{grad} f(A) = A.$$  

For $h(U) = U^\dagger W$, it is easy to see that

$$d_U h(\delta U) = \delta U^\dagger W = -U^\dagger \delta U U^\dagger W.$$  

Then to compute the adjoint of $d_U h$, we write for an arbitrary $\delta V \in T_{U^\dagger} \mathbf{U}(N)$ and $\delta V \in T_{h(U)} \mathbf{U}(N)$

$$\langle d_U h^* (\delta V), \delta U \rangle = \langle \delta V, d_U h(\delta U) \rangle = \langle \delta V, -U^\dagger \delta U U^\dagger W \rangle = \langle -U \delta V W^\dagger U, \delta U \rangle.$$  

Since $\delta V \in T_{U^\dagger W} \mathbf{U}(N)$, it can be written as $\delta V = AU^\dagger W$ for some $A \in \mathfrak{u}(N)$, so that $-U \delta V W^\dagger U = -UA \in T_{U} \mathbf{U}(N)$. Therefore $d_U h^* : T_{h(U)} \mathbf{U}(N) \rightarrow T_{U^\dagger} \mathbf{U}(N)$ is given by

$$d_U h^* (\delta V) = -U \delta V W^\dagger U.$$  

Consider now the differentiation of $g(V) = \log(V)$, which needs to take into account that the $N \times N$ matrices form a non-commutative algebra. We begin by rewriting the definition of $g$ as $\exp \circ g = \text{id}$, and differentiating both sides. Using the discussion of Kronecker sums in [1], we get

$$\delta V = \int_0^1 \exp \left( g(V) s \right) d_V g(\delta V) \exp \left( g(V) (1 - s) \right) ds$$

$$= \nu^* \circ \left( \int_0^1 \exp \left( g(V)^T (1 - s) \right) \otimes \exp \left( g(V) s \right) ds \right) \nu(d_V g(\delta V)).$$
that (70) has a unique solution, and therefore

\[ d_V g(\delta V) = \nu^* \circ \left( \int_0^1 \exp(g(V)^T (1 - s)) \otimes \exp(g(V)s) \, ds \right)^{-1} \nu(\delta V) \]  

where we have defined the linear operator \( \nu : \mathbb{C}^{N \times N} \to \mathbb{C}^{N^2} \) to be the operator that takes a square matrix and stacks the columns to create a vector. If we let \( \mathbb{C}^{N \times N} \) and \( \mathbb{C}^{N^2} \) both be real Hilbert spaces with respective inner products \( \langle A, B \rangle = \Re \text{Tr}(A^\dagger B) \) and \( \langle x, y \rangle = \Re(x^\dagger y) \), then we can find the adjoint of \( \nu \):

\[ \langle \nu^*(x), A \rangle = \langle x, \nu(A) \rangle = \Re \sum_{k=1}^{2^n} \bar{x}_k \nu_k(A) = \Re \sum_{i,j=1}^{2^n} \bar{x}_{i+j-1}\nu_{i+j-1}(A) = \Re \sum_{i,j} \nu^{-1}(\bar{x}^\dagger_{ij} A_{ij}) = \Re \text{Tr}(\nu^{-1}(x)^\dagger, A) = \langle \nu^{-1}(x), A \rangle \]

for a given \( x \in \mathbb{C}^{2N} \) and all \( A \in \mathbb{C}^{2N \times 2N} \). Hence \( \nu^* = \nu^{-1} \) is the “matrixization” operator that cuts the vector up and arranges the pieces as the columns of matrix.

By construction, \( g(V) \) will be skew-Hermitian and have imaginary eigenvalues in the (imaginary) interval \( (-i\pi, i\pi) \). It may be shown that as long as the spectrum of \( V \) does not contain the eigenvalue \(-1\) (which holds with probability 1), the inverse operator in (67b) is well-defined.

Applying these differentials to our problem, we find that

\[ \text{grad } J_G(U) = d_U h^* \circ d_{h(U)} g^* \circ \text{grad } f(h(h(U))) = d_U h^* \circ d_{h(U)} g^* (g(h(U))). \]

Now,

\[ d_V g^*(g(V)) = \nu^* \circ \left( \int_0^1 \exp(-g(V)^T (1 - s)) \otimes \exp(-g(V)s) \, ds \right)^{-1} \nu(g(V)) \]

is the matrix solution \( A \) to the problem \( \int_0^1 \exp(-g(V)s) \ A \exp(-g(V)(1-s)) \, ds = g(V) \). If we assume temporarily that \( A \) commutes with \( g(V) \), then we find that \( A = Vg(V) \) is one solution to this equation. Under the assumption that the spectrum of \( Q \) does not contain \(-1\), the inverse operator in (70) is well-defined, so that (70) has a unique solution, and therefore

\[ d_V g^*(g(V)) = Vg(V). \]

Hence,

\[ \text{grad } J_G(U) = d_U h^*(h(U)g(h(U))) = -Uh(U)g(h(U)) W^\dagger U \]

\[ = -W \log(U^\dagger W) W^\dagger U = -U(U^\dagger W \log(U^\dagger W) W^\dagger U) \]

\[ = -U \log(U^\dagger W). \]
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