Index theorems for graph-parametrized optimal control problems

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Abstract

In this paper we prove Morse index theorems for a big class of constrained variational problems on graphs. Such theorems are useful in various physical and geometric applications. Our formulas compute the difference of Morse indices of two Hessians related to two different graphs or two different sets of boundary conditions. Some applications such as the iteration formulas and lower bounds for the index are proved.

1 Introduction

1.1 Motivation

The aim of this paper is to derive effective ways of computing the Morse index of second variation of constrained variational problems on graphs. Such problems can be conveniently formulated as optimal control problems. The results of this article can be used to study minimality and stability in a variety of geometrically and physically interesting problems.

Let us start with some examples which motivate the overall set-up in which we are working. Given three points a, b, c on a plane $\mathbb{R}^2$, place a point $d \in \mathbb{R}^2$ such that the sum of the distances between d and each of the points a, b, c is minimal. It is well known that d should be placed at the Fermat point. In particular, each of the angles $\angle adb$, $\angle adc$, $\angle bdc$ should be of $120°$.

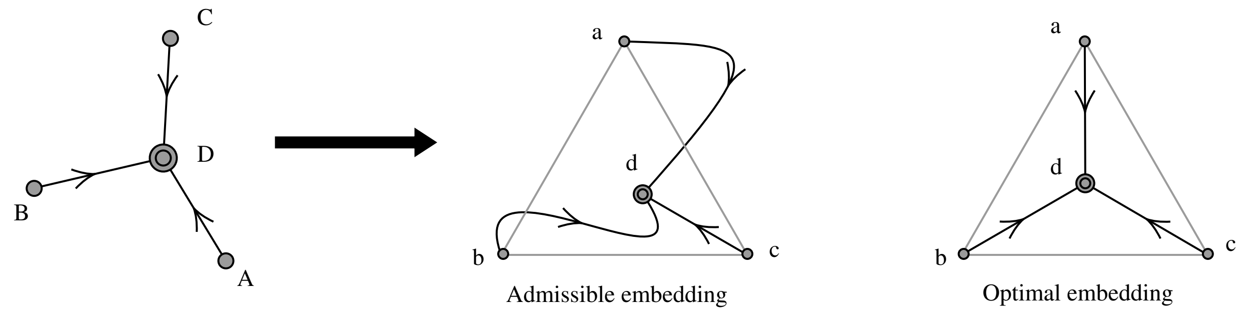

Figure 1: The graph $\mathcal{G}$ associated to the Fermat problem and two possible embeddings in $\mathbb{R}^2$.

We can formulate the same problem in a slightly different but equivalent way. Consider the tree graph $\mathcal{G}$ in Figure 1 and denote by $\mathcal{G}_0 = \{A, B, C, D\}$ the set of its vertices and by $\mathcal{G}_1$ the set of its edges. We can parametrize each edge by the interval $[0, 1]$, an operation which also assigns orientations to each of them. Then the goal is to find a continuous map $F : \mathcal{G} \to \mathbb{R}^2$ with smooth restrictions to each edge such that

$$F(A) = a,$$
$$F(B) = b,$$
$$F(C) = c$$

and

$$\sum_{e \in \mathcal{G}_1} l(F(e)) \to \min,$$

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where l is the Euclidean length. So, we have reformulated our problem as a minimal immersion of the graph $\mathcal{G}$ into the Euclidean subspace $\mathbb{R}^2$.

Let us consider another example. Assume that we have a set of elastic rods and rigid beams soldered together to form a graph-like structure. Some vertices of this graph are assumed to be fixed, while others are free. What shapes can it take? This question arises often in civil engineering, for example in the construction of bridges, towers and various other structures (Figure 2). Such structures have some parts firmly fixed on the ground, which correspond to fixed vertices, while others are free to move in the space. It is known that the elastic rods are extremal curves in certain constrained variational problems and stable configurations correspond to local minimizers of the bending energy [14].

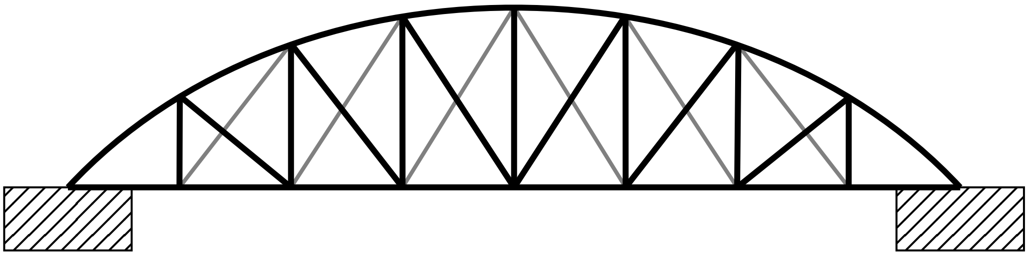

Figure 2: An example of a truss bridge, which can be viewed as a number of connected elastic beams forming a graph.

We can generalize the previous examples in several ways in order to encompass a great variety of situations commonly encountered in applications. For example, we can consider more general metric graphs $\mathcal{G}$, a manifold M instead of $\mathbb{R}^2$, we can choose a different functional to minimize and, most importantly, we can assume that each edge satisfies a differential constraint.

In this reformulation the following well-known notion plays a central role.

Definition 1. A metric graph is a graph $\mathcal{G} = (\mathcal{G}_0, \mathcal{G}_1)$, where $\mathcal{G}_0$ is the set of vertices and $\mathcal{G}_1$ is the set of parametrized edges. Each edge $e \in \mathcal{G}_1$ is parametrized either by a finite interval $[0, l_e]$ for some $l_e > 0$ or by $[0, +\infty)$.

In this paper we will discuss necessary optimality conditions for the following class of problems:

Definition 2. Given a metric graph $\mathcal{G} = (\mathcal{G}_0, \mathcal{G}_1)$ and a manifold M, consider the following data:

1. *Control constraints* U_e, $e \in \mathcal{G}_1$, which are subsets $U_e \subset \mathbb{R}^{k_e}$ for some $k_e \in \mathbb{N}$;
2. *Families of time-dependent complete vector fields* $f^e_{t,u} \in Vec(M)$, where $e \in \mathcal{G}_1$ and $u \in U_e$;
3. *Lagrangians* $\ell^e : [0, l_e] \times M \times U_e \to \mathbb{R}$, where $e \in \mathcal{G}_1$.
4. *Boundary conditions* given by a subset $N \subset M^{|\mathcal{G}_0|}$.

A graph-parametrized optimal control problem is the problem of finding a control u and a continuous map $q : \mathcal{G} \to M$ with almost everywhere differentiable restrictions to edges $q_e : [0, l_e] \to M$, such that it minimizes the following functional

$$\varphi[u] = \sum_{e \in \mathcal{G}_1} \int_0^{l_e} \ell^e(q_e(t), u_e(t))dt \to \min \tag{1}$$

subject to constraints

$$\dot{q}_e = f^e_{t,u_e(t)}(q_e), \qquad u_e \in L^\infty([0, l_e], U_e), \tag{2}$$

$$(q(v_1), q(v_2), \dots, q(v_{|\mathcal{G}_0|}) \in N. \tag{3}$$

where $v_1, \dots, v_{|\mathcal{G}_0|}$ are vertices in $\mathcal{G}_0$.

Let us illustrate the definition with another interesting example coming from quantum mechanics. A quantum graph is a metric graph $\mathcal{G}$ with a possibly non-linear Schrödinger equation defined on it. A ground state $\psi : \mathcal{G} \to \mathbb{C}$ of a quantum graph is a global minimizer of the functional

$$\sum_{e \in \mathcal{G}_1} \int_0^{l_e} \frac{|\dot{\psi}_e|^2}{2} - \frac{|\psi_e|^\alpha}{\alpha} dt \to \min, \tag{4}$$

under the constraint of fixed total mass μ:

$$\sum_{e\in\mathcal{G}_1}\int_0^{l_e}|\psi_e|^2dt=\mu, \tag{5}$$

together with a regularity condition $\psi\in H^1(\mathcal{G})$:

$$\sum_{e\in\mathcal{G}_1}\int_0^{l_e}|\psi_e|^2+|\dot\psi_e|^2dt<\infty, \tag{6}$$

and certain boundary condition on the value of ψ at the vertices $\mathcal{G}_0$ which are usually taken to be Dirichlet, Neumann or Kirkchoff (or a combination of the above). Here ψ_e are restrictions of ψ to the edge e, l_e is the length of edge and $2\le\alpha\le 6$ is a constant.

We can reformulate it as an optimal control parametrized by $\mathcal{G}$ taking as cost

$$\sum_{e\in\mathcal{G}_1}\int_0^{l_e}\frac{|u_e|^2}{2}-\frac{|\psi_e|^\alpha}{\alpha}dt\to\min$$

under the differential constraints

$$\begin{cases}\dot\psi_e=u_e,\\ \dot m_e=|\psi_e|^2,\end{cases}$$

with additional condition at the boundary

$$\sum_{e\in\mathcal{G}_1}m_e(l_e)=\mu,$$

and the same continuity conditions for values of ψ_e at the vertices. In Section 2.5 we study numerically some critical points of the NLS energy on binary trees in greater detail.

There is an extensive literature concerning quantum graphs. In particular regarding existence of global minimizers for the NLS energy with fixed total mass, see for example [5], [6], [4], [22] (or [20] and [2] for overviews of the results) and references therein. Or [19, 3, 35] for more recent result and variations of the problem. Situation that do not fit in our current framework have been investigated too, see for example [27] where the same problem is discussed on a graph with an infinite number of edges. For the linear case, i.e. when $\alpha=2$, see [18].

Another important application comes from quantum physics. In the perturbative approach to quantum mechanics and quantum field theory via the path integral method, a formal analogue of the stationary phase method is used. This formula requires to know the index and a suitable generalization of the determinant of the second variation at a critical point [29, 32]. The index is computed in the current paper, while the determinant is investigated in [16].

1.2 General setting and problem statement

All of the examples from Section 1.1 can be formulated as graph-parametrized optimal control problems. The goal of this article is to study the second variation of such minimization problems and characterize local minimizers. Local minimizers play an important role in modelling various physical phenomena, since they usually correspond to stable configurations observable in nature, which makes them relevant even if there are no global minima. In order to transmit better the ideas and simplify the proofs we will make several technical assumptions, starting with the following ones.

Assumption 1. 1. The graph $\mathcal{G}$ has a finite number of edges;

2. N is an embedded submanifold;
3. $U_e=\mathbb{R}^k$ for some $k\in\mathbb{N}$ and all $e\in\mathcal{G}_1$;
4. Vector fields f^e_u and functions ℓ^e are jointly smooth in the space variables q and in the control variables u, piecewise smooth in t for all $e\in\mathcal{G}_1$.

We can reformulate a graph-parametrized optimal control problem (1)-(3) as an equivalent standard optimal control problem with non-fixed boundary conditions of the form:

$$\dot q=f^t_{u(t)}(q),\qquad q\in M,\qquad u\in L^\infty([0,1],\mathbb{R}^k); \tag{7}$$

$$(q(0),q(1))\in N\subset M\times M; \tag{8}$$

$$\varphi[u] = \int_0^1 \ell(t, q(t), u(t))dt \to \min. \tag{9}$$

We will show the precise algorithm to reformulate problem (1)-(3) as problem (7)-(9) later on, in Subsection 2.1. Note that (7)-(9) by itself is a special case of a graph-parametrized optimal control problem where the metric graph $\mathcal{G}$ is the interval $[0, 1]$.

We recall now some definitions concerning problem (7)-(9).

Definition 3. 1. Let $u \in L^\infty([0, 1], \mathbb{R}^k)$ be a control and $q' \in M$. We say that (q', u) is admissible if the solution to the Cauchy problem:

$$\begin{cases} \dot{q} = f^t_{u(t)}(q), \\ q(0) = q' \end{cases} \tag{10}$$

is defined up to time $t = 1$.

2. We say that a curve $\gamma : [0, 1] \to M$ is admissible if there exists a control u such that $(\gamma(0), u)$ is admissible, i.e.:

$$\dot{\gamma} = f^t_{u(t)}(\gamma), \qquad \text{for } a.e.\, t \in [0, 1].$$

3. Suppose that (q', u) is admissible and define the map $(q', u) \mapsto q_u(t)$, where $q_u(t)$ is the solution of (10) evaluated at time $t \in [0, 1]$. We will refer to this map as *Evaluation map* and denote it by $F^t(q', u)$ when final time is implicit. We will call the restriction of F^1 to $\{(q', u) : q' = q_0\}$ for a fixed $q_0 \in M$ the *Endpoint map* and denote it by E_{q_0}.

4. An admissible curve γ is said to be an admissible variation if it satisfies the boundary conditions $(\gamma(0), \gamma(1)) \in N$. In terms of the Evaluation map, admissible variations are elements of the set $(F^0 \times F^1)^{-1}(N)$.

Denote by $\mathcal{U}$ the collection of admissible controls (q_0, u). It is an open set of $M \times L^\infty([0, 1], \mathbb{R}^k)$ (see for instance [13, 10]). Moreover, it is a smooth Banach manifold modelled over $\mathbb{R}^{\dim(M)} \times L^\infty([0, 1], \mathbb{R}^k)$. It turns out that the map $(q', u) \mapsto q_u(1)$ defined on $\mathcal{U}$ is smooth and a submersion. On the contrary, the differential of the *Endpoint map* may fail to be surjective.

Admissible curves are, in particular, Lipschitz continuous under Assumption 1. Thus, the space of admissible curves is the subset of Lipschitz paths γ satisfying $\dot{\gamma}_t \in \cup_{u \in U} f^t_u(\gamma)$ for almost every $t \in [0, 1]$.

When an admissible curve $\gamma = q_u$, satisfying $(\gamma(0), \gamma(1)) \in N$ is fixed and the differential of the Endpoint map E_{q_0} at u is surjective, the space $(F^0 \times F^1)^{-1}(N)$ admits a structure of Banach manifold. In particular we can talk about its tangent space $\mathcal{V}$, which is a finite codimension subspace of $\mathbb{R}^{\dim(M)} \times L^\infty([0, 1], \mathbb{R}^k)$.

Let us turn now to our minimization problem. The usual approach for identifying local minimizers can be roughly described as follows. First one applies first order minimality conditions and identifies critical points of the functional φ. These critical points are called *extremal curves*.

They have a relatively simple characterisation, known as the Ponrtyagin maximum principle (PMP). In order to describe the PMP in this setting we introduce a family of Hamiltonian functions on T^*M

$$h^t_u(\lambda) = \langle \lambda, f^t_u(q) \rangle - \nu \ell^t(q, u), \qquad q = \pi(\lambda),$$

where $\nu \in \{0, 1\}$ and $u \in \mathbb{R}^k$. For any submanifold $N \subseteq M \times M$ define

$$A(N) = \{(\lambda_0, \lambda_1) \in T^*M \times T^*M : \langle \lambda_0, X_0 \rangle = \langle \lambda_1, X_1 \rangle, \forall (X_0, X_1) \in T_{\pi(\lambda_0, \lambda_1)} N\}, \tag{11}$$

called the annihilator of N.

Theorem. Suppose that $u \in L^\infty([0, 1], \mathbb{R}^k)$ is an optimal control and let $q : [0, 1] \to M$ the corresponding trajectory. Then, there exists a curve $\lambda : [0, 1] \to T^*M$ and $\nu \geq 0$ such that for almost all $t \in [0, 1]$

1. the curve q is the projection of λ:
$$q(t) = \pi(\lambda(t));$$

2. λ satisfies the following Hamiltonian system:
$$\frac{d\lambda}{dt} = \vec{h}^t_{u(t)}(\lambda); \tag{12}$$

3. the control u is determined by the maximum condition:
$$h^t_{u(t)}(\lambda(t)) = \max_{u \in \mathbb{R}^k} h^t_u(\lambda(t));$$

4. the non-triviality condition holds: $(\lambda(t), \nu) \neq (0, 0)$;

5. and the transversality conditions holds:

$$(\lambda(0), \lambda(1)) \in A(N). \tag{13}$$

A solution to the Hamiltonian system (12) is called an *extremal*. It is known that extremal curves in optimal control problems can have very different behaviour. They are usually separated into several classes, such as regular, singular, bang-bang and others [37, 34, 15, 12].

After critical points are identified, one proceeds to study second order conditions.

Definition 4. Suppose that (q_0, u) is a critical point of the functional φ restricted to $(F^0 \times F^1)^{-1}(N)$. Suppose that the differential of the Endpoint map E_{q_0} is surjective at u. The Hessian (or the second variation) is a quadratic form Q defined on the tangent space $\mathcal{V}$ to the space of admissible variations. It is given by the (intrinsic) second derivative of the functional φ (see section 3.2 and equation (37) for an explicit representation).

Often, in constrained variational problems, the space of admissible variations is not a manifold. For this reason we have to make additional assumptions on the Endpoint map in order to guarantee that this space is at least locally smooth, in a neighbourhood of a critical point.

The quadratic form Q encodes information about minimality of a given extremal curve through the dimension of its kernel and its negative inertia index $\operatorname{ind}^- Q$. In the classical theory of calculus of variations, a necessary and sufficient condition for an extremal curve to be a local minimizer is $\operatorname{ind}^- Q = 0$, whenever the second variation is non-degenerate. Note that this is not always true for constrained variational problems. Sometimes a critical point stops being a local minimizer only when the inertia index of Q exceeds a certain threshold (see [11, Theorem 20.3]). Thus we need to find good algorithms for computing $\operatorname{ind}^- Q$. This paper provides several efficient ways of doing this in the context of graph-parametrized problems.

We will now list the last pair of assumptions that will allow us to focus on a rather broad class of extremals for which a good geometric description of the second variation is possible.

Assumption 2. The maximized Hamiltonian

$$H^t(\lambda) = \max_{u \in U} h_u^t(\lambda), \qquad \lambda \in T^*M$$

is well-defined and C^2 on $T^*M \times [0,1]$.

Assumption 3. If $\lambda : [0,1] \to T^*M$ is an extremal satisfying PMP with control $u \in L^\infty([0,1], \mathbb{R}^k)$, then it satisfies the *strong Legendre condition*. Which means that there exists a constant $c > 0$ such that

$$\left.\frac{\partial^2 h_u^t}{\partial u^2}(v, v)\right|_{u=u(t)} \leq -c\|v\|^2. \tag{14}$$

Assumption 2 allows us to state the results in a simple form using the Hamiltonian flow of $\vec{H}^t$, while Assumption 3 guarantees that the quadratic form Q in Definition 4 has finite negative index, and that small arcs of a given extremal curve are local minimizers [11, Theorem 20.1].

1.3 Main results and structure of the paper

We are now ready to formulate and discuss the main results of this paper. Consider an extremal λ of an optimal control problem (7)-(9), which satisfies a Hamiltonian system

$$\dot{\lambda} = \vec{H}^t(\lambda) \tag{15}$$

under the Assumption 2. $\vec{H}^t$ generates the flow $\Psi_t : T^*M \to T^*M$. Denote by

$$\Gamma(\Psi_t) = \{(\lambda, \Psi_t(\lambda)) : \lambda \in T^*M\} \subset T^*M \times T^*M$$

its graph, which is a smooth submanifold of the product space $T^*M \times T^*M$. We will simply write $\Gamma(\Psi)$ to denote $\Gamma(\Psi_1)$. We have the following main index theorem for the optimal control problem on the interval.

Theorem 1. Let $\lambda : [0,1] \to T^*M$ be an extremal for (7), (9) and simultaneously for two different boundary conditions N and $\tilde{N}$ in (8). Let Q_N and $Q_{\tilde{N}}$ be the two quadratic forms for the second variation corresponding to the two boundary conditions. Denote $\underline{\lambda} = (\lambda(0), \lambda(1))$. Then, under the Assumptions 1-3, the negative inertia indices $\operatorname{ind}^- Q_N$, $\operatorname{ind}^- Q_{\tilde{N}}$ are finite and

$$\operatorname{ind}^- Q_{\tilde{N}} - \operatorname{ind}^- Q_N = i\big(T_{\underline{\lambda}}A(N), T_{\underline{\lambda}}\Gamma(\Psi), T_{\underline{\lambda}}A(\tilde{N})\big) + \dim(T_{\underline{\lambda}}N \cap T_{\underline{\lambda}}\tilde{N}) - \dim T_{\underline{\lambda}}N + k_0 \tag{16}$$

where $k_0 = \dim(T_{\underline{\lambda}}A(N) \cap T_{\underline{\lambda}}\Gamma(\Psi)) - \dim(T_{\underline{\lambda}}A(N) \cap T_{\underline{\lambda}}\Gamma(\Psi) \cap T_{\underline{\lambda}}A(\tilde{N}))$.

Only one term on the right hand-side still requires an explanation. The term $i(T_{\underline{\lambda}}A(N), T_{\underline{\lambda}}\Gamma(\Psi), T_{\underline{\lambda}}A(\tilde{N}))$ denotes the negative Maslov index of the triple of Lagrangian subspaces. Roughly speaking this number measures the relative position of three Lagrangian subspaces of a common symplectic space, in this case the symplectic space is $T_{\lambda(0)}(T^*M) \times T_{\lambda(1)}(T^*M)$ with the form $\big(-\sigma_{\lambda(0)}\big) \oplus \sigma_{\lambda(1)}$. A precise definition of Lagrangian spaces and of the Maslov index can be found in Appendix A.2. For now it is enough to know that it is a certain symplectic invariant of the triple of subspaces, which can be computed in an explicit algebraic way.

A relevant example to keep in mind is when $N \subset \tilde{N}$. In this case if λ satisfies the transversality conditions for $\tilde{N}$, then it satisfies the transversality conditions for N too. In particular, N can be just the product of two points $N = \{q_0\} \times \{q_1\}$, for which transversality conditions are trivially satisfied.

Theorem 1 has many interesting applications and allows us to have a fresh view on some classical results. When we consider a graph-parametrized problem (1)-(3) and reformulate it as problem on an interval (7)-(9), the structure of the graph $\mathcal{G}$ is completely encoded in the boundary conditions N. It is often the case that a single critical point satisfies two graph-parametrized problems with different boundary constraints or even with different underlying graphs.

For example, we can introduce an extra vertex on an edge of a graph, and assume that this vertex is free. This obviously does not change the possible critical points. However, now, we can compare it to a problem where the new vertex is fixed. A possible (and simple) application of this technique would be to consider a fixed boundary optimal control problem on an interval (1)-(3) with $N = \{q_0\} \times \{q_1\}$. Then introduce several free vertices in the interior of the interval and compare it with a problem where each one of the vertices is fixed, as depicted in Figure 3.

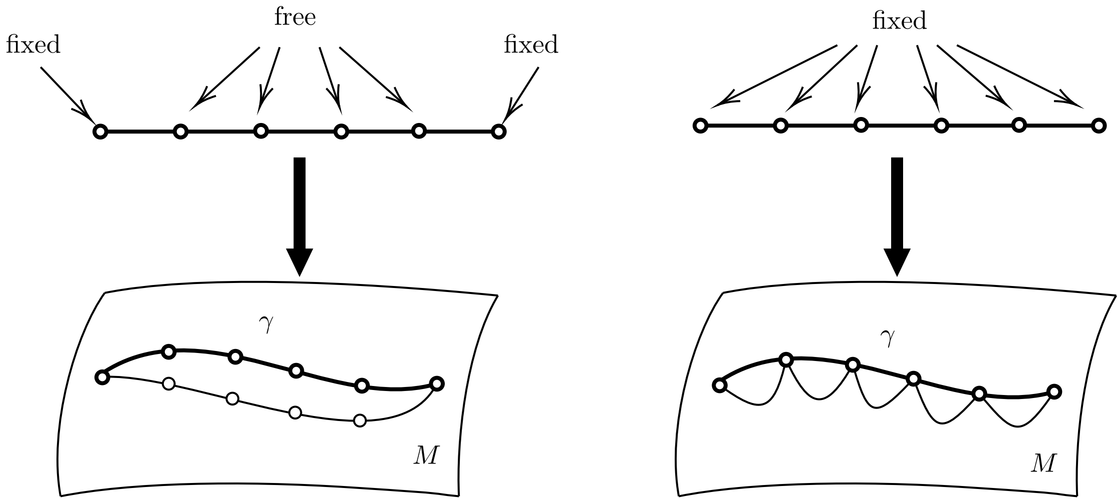

Figure 3: Variation of γ in the original problem and a problem with extra fixed vertices.

In order to formulate the next result, we need the definition of conjugate times and conjugate points. Given $\mu \in T^*M$, denote by $\Pi_\mu := T_\mu(T^*_{\pi(\mu)}M)$, the tangent space to the fibre over $\pi(\mu)$. We will often refer to it as the *vertical subspace*.

Definition 5. Given an extremal $\lambda : [0,1] \to T^*M$ of an optimal control problem (7)-(9), we say that $t \in [0,1]$ is a *conjugate time* if the linear map

$$\pi_* \circ (\Psi_t)_*|_{\Pi_{\lambda(0)}}$$

has a kernel. The corresponding point $q(t) = \pi(\lambda(t))$ is said to be a *conjugate point*.

To simplify notation we will denote by $\Theta_t = (\Psi_t)_*$ the differential of the extremal flow. It is straightforward to check that the tangent space $T_{\underline{\lambda}}\Gamma(\Psi)$ is actually the graph of the linear map $\Theta_t : T_\lambda T^*M \to T_{\Psi_t(\lambda)}T^*M$. We will denote by $\Gamma(\Theta_t)$ said graph and by $\Gamma(\Theta)$ the graph at time $t = 1$.

A consequence of Theorem 1 is the following result.

Theorem 2 (Discretization)**.** Let $\lambda : [0,1] \to T^*M$ be an extremal for (7)-(9) with $N = \{q_0\} \times \{q_1\}$ and let $\Xi = \{t_0, \dots, t_n\}$ be a partition of $[0,1]$. Denote by $\Theta_{i+1,i}$ the restriction to the interval $[t_i, t_{i+1}]$ of the differential of the extremal flow in (15). The following formula holds:

$$\operatorname{ind}^- Q \geq \sum_{i=0}^{n-1} i\big(\Theta_{i+1,i}^{-1}(\Pi_{i+1}), \Pi_i, \Theta_{i,i-1} \circ \dots \circ \Theta_{1,0}(\Pi_0)\big), \tag{17}$$

where $\Pi_i = T_{\lambda(t_i)}(T^*_{\pi(\lambda(t_i))}M) \simeq T^*_{\pi(\lambda(t_i))}M$. Moreover, equality holds if $\max_i |t_{i+1} - t_i|$ is sufficiently small and no t_i is a conjugate time.

As previously discussed a necessary condition for minimality under Assumptions 1-3 is $\operatorname{ind}^- Q = 0$. For this reason a necessary condition for minimality of a critical point is that the right hand side of (17) equals zero. In practice, this allows us to determine non-optimal solutions and greatly reduce the number of candidates for the minimal solution.

Another example of this type is given by the k-th iterate γ^k of a periodic extremal trajectory γ. If γ has period T, we can view γ^k as a periodic trajectory of period kT. Hence it is a graph-parametrized problem with the graph having one edge of length kT and a single vertex. We can add k more equispaced vertices and compare the problem to the k copies of smaller circle graphs which correspond to γ as depicted in Figure 4. We denote by Θ the linearization of the flow given in equation (15) along γ at $t = T$. Again an application of

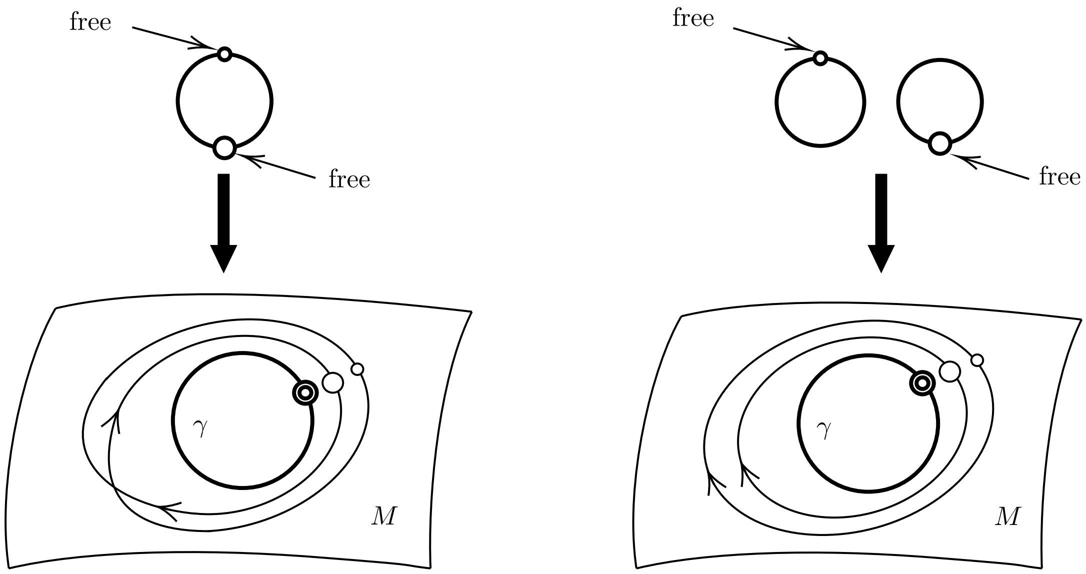

Figure 4: Variations of a periodic extremal trajectory γ as a periodic trajectory ran twice (left) and as two separate periodic trajectory (right).

Theorem 1 gives us the following iteration formulae:

Theorem 3 (Iteration Formulae)**.** Let $k > 1$ and γ be an extremal curve for the problem (7)-(9) with $N = \Delta$, where $\Delta \subset M \times M$ is the diagonal of M. It holds:

$$\begin{aligned} \operatorname{ind}^- Q_{\gamma^k} - k \operatorname{ind}^- Q_\gamma &= \sum_{j=1}^{k} i\big(\Gamma(\Theta^{j-1}), T_{\underline{\lambda}} A(\Delta), \Gamma(\Theta^j)\big) - \dim(M) + \dim(\ker(\Theta^{j-1} - 1)) \qquad (18) \\ &= \sum_{j=1}^{k-1} \dim(M) - \dim(\ker(\Theta - \omega^j)) - i\big(\Gamma(\Theta), T_{\underline{\lambda}} A(\Delta), \Gamma(\omega^j \Theta)\big). \qquad (19) \end{aligned}$$

Where ω is a primitive k-th root of unity.

Equality 18 is much in the spirit of [25] and [28]. Formula 19 is obtained using a complexified version of Maslov index described in Appendix A.2, yielding a result very similar to Bott's original approach given in [21].

The theorems above are examples of index formulas, which try to encode the information about the index of the second variation of variational problems in terms of geometric quantities such as the Maslov index. In the context of variational problems on 1D objects such as curves or graphs, it is possible to reduce the problem of studying index of a linear operator on an infinite-dimensional space to the study of non-autonomous linear ODEs in finite dimensional spaces. There exist various analogues of this result. For example, in the context of classical calculus of variations an infinite-dimensional version of Morse index formulas was proven by several groups in works [28, 38, 23, 24]. In the case of strongly indefinite problems the index formulas are replaced by spectral flow theorems, which are valid both in finite [33, 30, 39] and infinite dimensions [36]. There are also various approaches to infinite-dimensional Morse homology [1]. A very general index theorem for optimal control problems was proven by the first and third author in [9], which encompasses many separate classical constructions for various types of extremals [37, 34, 15, 12, 8].

A variant of Theorem 1 was proven by Baryshnikov in [17]. His formula is true in the generic case for graph-parametrized problems in classical calculus of variations with separated boundary conditions. In the generic picture, the various intersection terms in (16) disappear. Our formula holds without the genericity assumption and extends to a large class of optimal control problems with arbitrary boundary conditions. The authors of [31] study the Morse index of Schrödinger operators on graphs. After reducing the problem to an interval, they provide a Morse index formula involving intersection theory. The Morse index is computed as the Maslov index of a curve in a Lagrangian Grassmanian of a sufficiently big dimension. Instead our formulas separate the contribution to the index coming from varying the edges and the contribution to index coming from varying vertices. This allows us to perform various manipulations on graphs to reduce dimensions and simplify final formulas.

The paper has the following structure. In Section 2 we focus on applications for the graph-parametrized problems. We prove our main applications, Theorems 2 and 3, as well as a formula to reduce the dimensionality in Theorem 1 using a filtration of the vertices. In Section 2.5 we discuss some numerical application of our formula to NLS equation on graphs. This section relies only on Theorem 1 and properties of the Maslov index. The reader who only wants to understand how to compute the index and apply the main theorems can focus just on Section 2 and Appendix A, which contains all the necessary information regarding symplectic geometry, Lagrangian spaces and Maslov index. In Section 3 we prove Theorem 1.

2 Applications and proofs of Theorem 2 and Theorem 3

2.1 Reduction of the problem on a graph to a problem on an interval

It will be convenient to assume that, in problem (1)-(3), all edges are parametrized on the interval $[0,1]$. When $l_e < +\infty$, we can rescale time appropriately. If $l_e = +\infty$ we can compactify the semi-line $[0,+\infty)$ via a suitable change of coordinates in the time variable, provided that the compactification satisfies Assumption 3, fact that may depend on the choice of change of variables. This will merely change the Lagrangians ℓ^e and the vector fields $f^e_{t,u}$ which can be redefined accordingly.

Let us ignore for the moment the boundary conditions (3) and treat the restriction of the optimal control problem to every edge as an independent problem. Define the map $\pi_e : M^{\mathcal{G}_1} \to M_e$ as the projection onto the copy of M relative to edge e. The functional $J[u]$ and the control system can be seen as an optimal control problem on $M^{\mathcal{G}_1}$. We define the new Lagrangian $\ell : [0,1] \times M^{\mathcal{G}_1} \times (\mathbb{R}^k)^{\mathcal{G}_1}$ as

$$\ell(t,q,u) = \sum_{e\in\mathcal{G}_1} \ell^e(t,q_e,u_e)$$

and a new family of time dependent vector fields $f^t_u \in Vec(M^{\mathcal{G}_1})$ such that for a fixed edge $e \in \mathcal{G}_1$

$$(\pi_e)_*(f^t_u) = f^e_{t,u_e}.$$

Let us consider the boundary conditions (3). In order to make this construction cleaner, we need the following definitions.

Definition 6. Let $I = \{i_1, i_2, \dots, i_m\}$ be a finite set and W an arbitrary set. A *I-parametrized direct product of W* is

$$W^I = W_{i_1} \times \cdots \times W_{i_m},$$

where $W_{i_j} = W$ for all $j = 1,\dots,m$.

Since we use I as an index set, for a given subset $J \subset I$ we can define the projection map

$$\pi_J : W^I \to W^J$$

by forgetting the copies of W indexed by the elements of $I \setminus J$.

Definition 7. Let I, J be two finite index sets, W an arbitrary set and $f : I \to J$ a surjective map. Then the *pull-back product* $f^*(W^J)$ is a subset of W^I characterized by the property that for every $j \in J$

$$\pi_{f^{-1}(j)}(f^*(W^J)) = \left\{(q,q,\dots,q) \in W^{f^{-1}(j)} : q \in W_j\right\}.$$

Similarly if $X \subset W^J$, then the pull-back $f^*(X)$ is a subset of W^I defined by the property that for every $j \in J$.

$$\pi_{f^{-1}(j)}(f^*(X)) = \left\{(q,q,\dots,q) \in W^{f^{-1}(j)} \,:\, q \in \pi_j(X)\right\}.$$

Let us look at an example when $I = \{1,2\}$ and $J = \{1\}$ and $f(1) = f(2) = 1$. In this case the preimage of 1 is all of I, hence

$$f^*(W^J) = \pi_{f^{-1}(1)}(f^*(W^J)) = \{(q,q) \in W^I : q \in W\},$$

which is just the diagonal. Similarly, if $X \subset W$ then $f^*(X)$ is the intersection of the diagonal with $X \times X \subset W \times W$.

Now we can describe the reduction procedure. The idea is intuitive. We want to use the orientations on edges of $\mathcal{G}$ and pull-back the set of boundary constraints N, a priori defined just on the vertex set $\mathcal{G}_0$, to a new manifold embedded in $(M \times M)^{\mathcal{G}_1}$. This allows us to separate the dynamic on each edge from the boundary conditions, exactly as we did a few lines above.

Saying that each edge $e \in \mathcal{G}_1$ is oriented is equivalent to having source and target maps $s, t : \mathcal{G}_1 \to \mathcal{G}_0$. The image of the source and the target of an edge e are

$$(q_e(0), q_e(1)) \in M_e \times M_e \simeq M \times M.$$

Taking a product indexed by $\mathcal{G}_1$ we obtain that

$$(q(0), q(1)) \in (M \times M)^{\mathcal{G}_1} \simeq M^{\mathcal{G}_1 \sqcup \mathcal{G}_1},$$

where $\mathcal{G}_1 \sqcup \mathcal{G}_1$ is a disjoint union of two copies of $\mathcal{G}_1$. The source and the target maps induce a surjective map $s \sqcup t : \mathcal{G}_1 \sqcup \mathcal{G}_1 \to \mathcal{G}_0$. This allows us to pull-back the boundary conditions to

$$\tilde{N} = (s \sqcup t)^*(N).$$

Hence we have reduced the optimal control problem (1)-(3) to an optimal control problem (7)-(9) with the configuration space $M^{\mathcal{G}_1}$ and the boundary conditions $(s \sqcup t)^*(N)$, which encode all the information about the graph structure.

The final remark concerns the symplectic form on $(T^*M \times T^*M)^{\mathcal{G}_1}$ that will be used for the calculation of the Maslov index. We will assume that each copy of T^*M corresponding to a source vertex carries *minus* the standard symplectic form $-\sigma$, while every target copy T^*M carries σ, the standard one.

2.2 Discretization

In this subsection we prove Theorem 2. Fix a partition $\Xi = \{t_i : t_0 = 0, t_n = 1, t_i < t_{i+1}\}$ of the unit interval.

We will work with an optimal control problem and Assumptions 1–3. In particular, Assumption 3, ensures that the Morse index is finite and that the conjugate points form a discrete set. This will guarantee that, under mild conditions and after enough successive refinements of the partition, formula (17) will give exactly the Morse index of the extremal.

Let us first prove the formula when only one extra vertex is introduced. Let $\gamma = \pi(\lambda)$ be an extremal curve in a problem with fixed end-points. Take a point $t^* \in (0,1)$. Let us call $\gamma_1 = \gamma|_{[0,t^*]}$ and $\gamma_2 = \gamma|_{[t^*,1]}$ the restrictions. Q_{γ_i} will denote the second variation of the segment as an extremal curve with fixed points. Recall that $\Pi_i = T_{\lambda(t_i)}(T^*_{\pi(\lambda(t_i))}M) \simeq T^*_{\pi(\lambda(t_i))}M$ is the vertical subspace over the point $\gamma(t_i)$.

Proposition 1. *The index of the second variation Q_γ satisfies:*

$$\operatorname{ind}^- Q_\gamma = \operatorname{ind}^- Q_{\gamma_1} + \operatorname{ind}^- Q_{\gamma_2} + i\big(\Theta_2^{-1}(\Pi_2), \Pi_1, \Theta_1(\Pi_0)\big) + k, \tag{20}$$

where $k = \dim(\Theta_2(\Pi_1) \cap \Pi_2) + \dim(\Theta_1(\Pi_0) \cap \Pi_1) - \dim(\Theta_2^{-1}(\Pi_2) \cap \Pi_1 \cap \Theta_1(\Pi_0))$.

Proof. Let us consider the following three points in M:

$$q_0 = \gamma(0), \quad q_1 = \gamma(t^*), \quad q_2 = \gamma(1).$$

Variations of γ as a curve from q_0 to q_2 do not necessarily pass through the point q_1 at time t^*. They satisfy a continuity condition instead. We perform the reduction to a single interval as discussed in Subsection 2.1. To do this we break up $[0,1]$ in two intervals and consider the dynamics separately (i.e. duplicate the variables). The new boundary conditions which allow us to glue the two pieces together are of the form:

$$(\gamma_1(0), \gamma_2(t^*), \gamma_1(t^*), \gamma_2(1)) \in \{q_0\} \times \Delta \times \{q_2\} = \{(q_0, q_1, q_1, q_2) | \, q_1 \in M\}.$$

Now we are going to compare the following two problems. The first one prescribes *fixed end-points*, we impose that the curve starts from (q_0, q_1) and arrives to (q_1, q_2). The second one prescribes the constraints given by the manifold $N = \{q_0\} \times \Delta \times \{q_2\}$ defined above.

Recall that γ is a projection of a solution $\lambda : [0,1] \to T^*M$ of the Hamiltonian system. Let us consider the tangent space to the annihilator of N at the point $\underline{\lambda} = (\lambda(0), \lambda(1), \lambda(1), \lambda(2))$. Fix a system of coordinates, which determines a complement to the subspace $\ker \pi_* = \Pi_1$ which we call B. In these coordinates the annihilator reads:

$$T_{\underline{\lambda}}A(N) = \left\{ \begin{pmatrix} \nu_1 \\ \alpha + X \\ \alpha + X \\ \nu_2 \end{pmatrix} \,:\, \alpha, \nu_i \in \Pi_1,\ X \in B \right\}.$$

The other space appearing is the graph of the two symplectomorphisms Θ_1 and Θ_2 coming from the Hamiltonian flows of PMP on intervals $[0,t^*]$ and $[t^*,1]$. It will be denoted by $\Gamma(\Theta_1 \times \Theta_2)$.

Let us look at the subspace on which the Maslov form m is defined, $(T_{\underline{\lambda}}A(N) + \Pi^4) \cap \Gamma(\Theta_1 \times \Theta_2)$, where $\Pi^4 = \Pi_0 \times \Pi_1^2 \times \Pi_2$. This is defined by the following equations,

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \Theta_1(\xi_1) \\ \Theta_2(\xi_2) \end{pmatrix} = \begin{pmatrix} \nu_1 \\ \alpha + X \\ \alpha + X \\ \nu_2 \end{pmatrix} + \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \end{pmatrix} \iff \xi_1 \in \Pi_0, \Theta_2(\xi_2) \in \Pi_2,\ \xi_2 - \Theta_1(\xi_1) \in \Pi_1,$$

where α, ν_i, for $i = 1,2$ and μ_j for $j = 1, \dots 4$ lie in the vertical subspace over the respective points, whereas $X \in B$ is in the horizontal space. In particular Maslov form reads:

$$m(\xi_1, \xi_2) = \sigma(\mu_3 - \mu_2, X) = \sigma(\Theta_1(\xi_1) - \xi_2, \xi_2) = \sigma(\Theta_1(\xi_1), \xi_2) = \sigma(\xi_2, -\Theta_1(\xi_1)).$$

So, if we call $\eta = \Theta_2(\xi_2) \in \Pi_2$ and $\xi = \xi_1$ then we have $\xi \in \Pi_0, \eta \in \Pi_2$ and $\Theta_2^{-1}(\eta) - \Theta_1(\xi) \in \Pi_1$ and:

$$m(\Pi^4, \Gamma(\Theta_1 \times \Theta_2), T_{\underline{\lambda}}A(N)) = m(\Theta_2^{-1}(\Pi_2), \Pi_1, \Theta_1(\Pi_0)).$$

The additional terms popping up in Theorem 1 are

$$\dim(\Gamma(\Theta_1 \times \Theta_2) \cap \Pi^4) = \dim(\Theta_1(\Pi_0) \cap \Pi_1) + \dim(\Theta_2^{-1}(\Pi_2) \cap \Pi_1)$$

and

$$\dim(\Gamma(\Theta_1 \times \Theta_2) \cap \Pi^4 \cap T_{\underline{\lambda}}A(N)) = \dim(\Theta_2^{-1}(\Pi_2) \cap \Theta_1(\Pi_0) \cap \Pi_1)$$

as a quick calculation shows. □

We can now prove Theorem 2.

Prood of Theorem 2. The statement follows from Proposition 1. First of all notice that in equation (20) all terms are positive, hence $\operatorname{ind}^- Q \geq i\big(\Theta_2^{-1}(\Pi), \Pi, \Theta_1(\Pi)\big)$ when the partition is $\Xi = \{0, t^*, 1\}$. For a general Ξ apply Proposition 1 iteratively to $\{0, t_{j-1}, t_j\}$ where j runs from 2 to n. This allows to express the index of the second variation of $\gamma|_{[0,t_j]}$ as the sum of the index of the second variation of $\gamma|_{[0,t_{j-1}]}$ and $\gamma_j := \gamma|_{[t_{j-1},t_j]}$ plus other terms.

Iteratively replacing the terms $\operatorname{ind}^- Q_{\gamma|_{[0,t_j]}}$ we obtain the following formula:

$$\operatorname{ind}^- Q_\gamma = \sum_{j=0}^{n-1} \operatorname{ind}^- Q_{\gamma_j} + i\big(\Theta_{j+1,j}^{-1}(\Pi_{j+1}), \Pi_j, \Theta_{j,j-1} \circ \cdots \circ \Theta_{1,0}(\Pi_0)\big)$$
$$+ \dim(\Theta_{j,0}(\Pi_0) \cap \Pi_j) + \dim(\Theta_{j+1,j}(\Pi_j) \cap \Pi_{j+1}) - \dim(\Theta_{j,0}(\Pi_0) \cap \Pi_j \cap \Theta_{j+1,j}^{-1}(\Pi_{j+1})).$$

Here as described in the statement the maps $\Theta_{j,j-1}$ are the linearisation of the Hamiltonian flow of equation (15). The notation comes from the composition law of non autonomous flows, we have $\Theta_{j,k} \circ \Theta_{k,l} = \Theta_{j,l}$.

The index is presented as sum of three positive terms: the first one $\operatorname{ind}^- Q_{\gamma_i}$ is zero when each segment $\gamma|_{[t_i,t_{i+1}]}$ is minimizing [11, Theorem 21.3]. Under Assumption 3 this is the case when $\sup_i |t_i - t_{i-1}|$ is small enough (see [11] for instance). The same goes for $\dim(\Theta_{i+1,i}(\Pi_i) \cap \Pi_{i+1}) - \dim(\Theta_{i,0}(\Pi_0) \cap \Pi_i \cap \Theta_{i+1,i}^{-1}(\Pi_{i+1}))$. Moreover $\dim(\Theta_{i,0}(\Pi_0) \cap \Pi_i)$ is zero precisely when t_i is not a conjugate time for γ.

Thus equality holds exactly when our hypotheses on the partition are satisfied. □

Remark 1. The hypothesis on the partition Ξ can be weakened if we change a bit our way of counting. If we add to the dimension of the negative space the dimension of the null space of the Maslov form we can essentially forget about avoiding conjugate points of γ.

You can see that the correction term k in Proposition 1 is in fact the dimension of the kernel of the Maslov form $m\big(\Theta_2^{-1}(\Pi_2), \Pi_1, \Theta_1(\Pi_1)\big)$. The quantity $\sum_{i=1}^{n-1} (\operatorname{ind}^- + \ker)\Big(m\big(\Theta_{i+1,i}^{-1}(\Pi_{i+1}), \Pi_i, \Theta_{i,i-1} \circ \cdots \circ \Theta_{1,0}(\Pi_0)\big)\Big)$ still approximates from below the negative index and includes the contribution of conjugate points of γ that are possibly present in the partition.

Remark 2. If we combine Theorem 1 and Theorem 2 we can obtain a formula for the index involving just the Maslov index i and dimension of intersections for arbitrary boundary conditions.

2.3 Filtration formula

In the previous subsection we have proven a discretization formula for the fixed end-point problem on an interval. The idea was to introduce extra vertices inside the single edge and apply an iterative procedure consisting in fixing each of the new vertices one by one. Note that, if we had fixed all of the vertices at the same time, a direct application of (16) would have resulted in a computation of the Maslov index in a very big symplectic space. Instead, the recursive nature of the proof allows us to reduce greatly the dimensionality of the problem.

A way of reducing the dimensionality in formula (16) for problems with separated boundary conditions is discussed in [17]. The argument works when all of the Lagrangian spaces in the final formula are transversal. We can reproduce this argument in a greater generality using Theorem 1.

Assume that each vertex $v \in \mathcal{G}_0$ is constrained to lie on a separate submanifold $N_v \subset M$. We denote by N the boundary conditions, which are obtained after the reduction of the problem to an interval. We can introduce a filtration of vertices

$$\emptyset = \mathcal{G}_0^0 \subset \mathcal{G}_0^1 \subset \dots \subset \mathcal{G}_0^{|\mathcal{G}_0|} = \mathcal{G}_0,$$

such that

$$|\mathcal{G}_0^j| = |\mathcal{G}_0^{j-1}| + 1, \qquad i = 1, \dots, |\mathcal{G}_0|.$$

To each set $\mathcal{G}_0^j$ we associate boundary conditions $N_j \subset N$ in the following way. We assume that vertices $v \in \mathcal{G}_0^j$ vary on N_v, while vertices $v \in \mathcal{G}_0 \setminus \mathcal{G}_0^j$ are assumed to be fixed. Thus we activate variations of each individual vertex at a time and track how the index changes as we do so.

We now apply Theorem 1 to compute $\operatorname{ind}^- Q_{N_{j+1}} - \operatorname{ind}^- Q_{N_j}$. Let us introduce some simplifying notations. Recall that $s, t : \mathcal{G}_1 \to \mathcal{G}_0$ are the source and the target maps. Let $v_j \in \mathcal{G}_0^{j+1} \setminus \mathcal{G}_0^j$ be the activated vertex. We introduce a separate notation for the set of edges that are incident to v_j:

$$\mathcal{G}_1^j = s^{-1}(v_j) \cup t^{-1}(v_j).$$

A naive guess would be that, when we activate a vertex, the only relevant contributions come from the edges incident to a given vertex. Thus we define forgetful projections $\pi_{\mathcal{G}_1^j}$ which forget all the edges except the ones incident to v_j:

$$\pi_{\mathcal{G}_1^j} : T_{\bar\lambda}(T^*M)^{\mathcal{G}_1} \times T_{\bar\lambda}(T^*M)^{\mathcal{G}_1} \to T_{\bar\lambda}(T^*M)^{\mathcal{G}_1^j} \times T_{\bar\lambda}(T^*M)^{\mathcal{G}_1^j}.$$

Subspaces $T_{\bar\lambda}A(N_{j-1})$ and $T_{\bar\lambda}A(N_j)$ can have a big intersection. For sure this intersection contains the subset $V_j = \pi^{-1}_{\mathcal{G}_1^j}(0)$, which is an isotropic subspace. This means that we can perform a symplectic reduction to the space $V_j^\perp / V_j$. Let

$$\pi_j : T_{\bar\lambda}(T^*M)^{|\mathcal{G}_1|} \times T_{\bar\lambda}(T^*M)^{|\mathcal{G}_1|} \to V_j^\perp / V_j$$

be the projection maps for each $j = 1, \dots, |\mathcal{G}_1|$. We can then define shortened notations for the images:

$$\begin{aligned} A^j_{j-1} &= \pi_j(T_{\bar\lambda}A(N_{j-1})), \\ A^j_j &= \pi_j(T_{\bar\lambda}A(N_j)), \\ \Gamma(\Theta_j) &= \pi_j(\Gamma(\Theta)). \end{aligned}$$

By property (54), we can factor out V_j in the definition of the Maslov index and get

$$i(T_{\bar\lambda}A(N_{j-1}), \Gamma(\Theta), T_{\bar\lambda}A(N_j)) = i(A^j_{j-1}, \Gamma(\Theta_j), A^j_j)$$

and for the same reason

$$\dim\left(T_{\bar\lambda}A(N_{j-1}) \cap \Gamma(\Theta)\right) - \dim\left(T_{\bar\lambda}A(N_j) \cap \Gamma(\Theta) \cap T_{\bar\lambda}A(N_{j-1})\right) = \dim\left(A^j_{j-1} \cap \Gamma(\Theta_j)\right) - \dim\left(A^j_{j-1} \cap \Gamma(\Theta_j) \cap A^j_j\right).$$

Finally, since $N_{j-1} \subset N_j$, we have that

$$\dim(T_{\pi(\bar\lambda)}N_{j-1} \cap T_{\pi(\bar\lambda)}N_j) - \dim(T_{\pi(\bar\lambda)}N_{j-1}) = 0.$$

Now we collect all of the terms and sum by the index $j = 1, \dots, |\mathcal{G}_0|$. As a result, we obtain a formula that expresses the difference between the index of the second variation Q of the original problem with the index of the second variation $Q_0 := Q_{N_0}$ of the problem with the same graph and fixed vertices:

$$\begin{aligned} \operatorname{ind}^- Q - \operatorname{ind} Q_0 &= \sum_{j=1}^{|\mathcal{G}_0|} \operatorname{ind}^- Q_{N_j} - \operatorname{ind}^- Q_{N_{j-1}} = \\ &= \sum_{j=1}^{|\mathcal{G}_0|} i(A^j_{j-1}, \Gamma(\Theta_j), A^j_j) + \dim\left(A^j_{j-1} \cap \Gamma(\Theta_j)\right) - \dim\left(A^j_{j-1} \cap \Gamma(\Theta_j) \cap A^j_j\right). \end{aligned}$$

This is the same formula as in [17] modulo terms containing dimensions of intersections.

We end this subsection with a couple of remarks regarding this formula. First of all, in practice, the dimensions are reduced even more because $A^j_{j-1} \cap A^j_j \neq \emptyset$. Nevertheless further reductions depend on the structure of the graph and the filtration chosen. Secondly, at first sight it may seem that the formula is a sum of local contributions, because we have used only edges incident to a given vertex in the derivation. However, this is not the case. The non-locality is hidden in the reduced space $V_j^{\perp}/V_j$ and the corresponding projection π_j.

For example, in the case when $\mathcal{G}_1$ is a tree, we can define a partial order $\leq$ on $\mathcal{G}_0$ by saying that $v \leq w$ if the minimal path from v to the root crosses less or equal number of vertices than the minimal path from w to the root. If we choose a filtration, which orders vertices one by one compatible with the partial ordering, one can identify the set $\mathcal{G}_0^j$ with a sub-tree of $\mathcal{G}$. Then the formula for the indices $i(A^j_{j-1}, \Gamma(\Theta_j), A^j_j)$ will contain terms involving symplectomorphisms of all of the edges in the sub-tree determined by $\mathcal{G}_0^j$ and not only of the incident edges. This can be checked via a long but straightforward calculation.

2.4 Iteration Formulae

Now we prove Theorem 3. For clarity we prove separately the two formulas since the strategies in the two cases are a bit different.

Suppose that γ is a closed periodic extremal trajectory. It is straightforward to see that iterations (i.e. concatenation of γ with itself) are still critical points.

We will use the following notation: γ^k will denote the $k-$th iteration of γ whereas $\operatorname{ind}^- Q_\gamma$ and $\operatorname{ind}^- Q_{\gamma^k}$ the Morse index of γ and γ^k respectively as periodic trajectories. We want to compute the difference $\operatorname{ind}^- Q_{\gamma^k} - k \operatorname{ind}^- Q_\gamma$.

First of all we compute the difference $\operatorname{ind}^- Q_{\gamma^k} - \operatorname{ind}^- Q_{\gamma^{k-1}}$. Let us consider the following manifolds of constraints:

$$\Delta^{\circlearrowleft} := \{(q_1, q_2, q_2, q_1) : q_i \in M, \} \subset M^2 \times M^2,$$
$$\Delta^2 = \{(q_1, q_2, q_1, q_2) : q_i \in M\} \subset M^2 \times M^2.$$

When we restrict to variations satisfying the boundary conditions given by $\Delta^{\circlearrowleft}$, we consider variations of γ^k as a periodic trajectory, whereas when we take boundary conditions Δ^2, we consider independent variations of γ^{k-1} and γ as periodic trajectories. See Figure 4 for a visual explanation. Now we prove the following lemma:

Lemma 1. *Let $\Gamma^j = \Gamma(\Theta^j)$ the graph of Θ^j. Then:*

$$\operatorname{ind}^- Q_{\gamma^k} - \operatorname{ind}^- Q_{\gamma^{k-1}} = \operatorname{ind}^- Q_\gamma + i\big(\Gamma^{k-1}, T_{\underline{\lambda}} A(\Delta), \Gamma^k\big) - \dim(M) + \dim\big(\ker(\Theta^{k-1} - 1)\big).$$

Proof. The statements follows applying Theorem 1. We take as $N_1 = \Delta^{\circlearrowleft}$ and as $N_2 = \Delta^2$. The part coming from the dimension is straightforward, the intersection of the tangent spaces has dimension $\dim(M)$ while the dimension of Δ^2 is $2\dim(M)$. So we get a $-\dim(M)$.

For the part concerning the intersection between annihilators and graphs, one can check that $T_{(\lambda(0),\lambda(0))}A(\Delta^2) \cap \Gamma(\Theta^{k-1} \times \Theta)$ is isomorphic to the sum $\ker(\Theta^{k-1} - 1) \oplus \ker(\Theta - 1)$. The triple intersection consists of $\ker(\Theta - 1)$ and thus the term in the statement.

From the definitions it follows that, when we impose the boundary conditions Δ^2, we have $\operatorname{ind}^- Q_{N_2} = \operatorname{ind}^- Q_{\gamma^{k-1}} + \operatorname{ind}^- Q_\gamma$, so the only thing to check is the Maslov index part.

The equation defining the subspace are the following:

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \Theta^{k-1}(\xi_1) \\ \Theta(\xi_2) \end{pmatrix} = \begin{pmatrix} X_1 + Y_1 \\ X_2 + Y_2 \\ X_2 + Y_1 \\ X_1 + Y_2 \end{pmatrix} \quad X_i, Y_i, \xi_i \in T_{\lambda(0)}(T^*M).$$

By subtracting the second and the third equations, and then the first and the fourth we find

$$\xi_2 - \Theta^{k-1}(\xi_1) = Y_2 - Y_1,$$
$$\Theta^{k-1}(\xi_1) - \Theta^k(\xi_2) = \Theta^{k-1}(Y_1 - Y_2).$$

Changing coordinates and setting $\eta = \Theta^{k-1}(\xi_1)$, $Y_1 - Y_2 = \eta_1$ and $\eta_2 = \xi_2$ we get:

$$(\eta, \eta) \in T_{\underline{\lambda}} A(\Delta) \cap (\Gamma^{k-1} + \Gamma^k) \iff \begin{pmatrix} \eta \\ \eta \end{pmatrix} = \begin{pmatrix} \eta_1 + \eta_2 \\ \Theta^{k-1}(\eta_1) + \Theta^k(\eta_2) \end{pmatrix}$$

So the Maslov form reduces to a form on $\Delta \cap (\Gamma^{k-1} + \Gamma^k)$. It reads:

$$\begin{aligned} m(\xi_1, \xi_2) = \sigma(X_2, Y_1 - Y_2) - \sigma(X_1, Y_1 - Y_2) = \sigma(\xi_2 - \Theta(\xi_2), Y_1 - Y_2) \\ = \sigma(\eta_2 - \Theta(\eta_2), \eta_1) \\ = \sigma(\eta_2, \eta_1) - \sigma(\Theta(\eta_2), \eta_1) \\ = -\sigma(\eta_1, \eta_2) + \sigma(\Theta^{k-1}(\eta_1), \Theta^k(\eta_2)). \end{aligned}$$

Which is exactly $m(\Gamma^{k-1}, T_{\underline{\lambda}}A(\Delta), \Gamma^k)$ in the coordinates just introduced. And thus the formula is proved. $\square$

The first iteration formula is now a direct consequence of the Lemma just proved:

Theorem (Iteration Formulae I)**.** The index of the $k-$th iteration of γ as a periodic trajectory satisfies:

$$\operatorname{ind}^- Q_{\gamma^k} - k \operatorname{ind}^- Q_\gamma = \sum_{j=1}^{k} i\big(\Gamma(\Theta^{j-1}), T_{\underline{\lambda}}A(\Delta), \Gamma(\Theta^j)\big) - \dim(M) + \dim(\ker(\Theta^{j-1} - 1)). \tag{21}$$

Proof. We will use an inductive procedure in a similar spirit as in the proof of Theorem 2. First we will look at γ^k as the concatenation of γ^{k-1} and γ and express the difference $\operatorname{ind}^- Q_{\gamma^k} - \operatorname{ind}^- Q_\gamma$ in terms of $\operatorname{ind}^- Q_{\gamma^{k-1}}$.

This is the first step of the scheme and was proved in Lemma 1. Then, we apply the argument iteratively to obtain (21). $\square$

Now we prove the second iteration formula.

Theorem (Iteration Formulae II)**.** The index of the $k-$th iteration of γ as a periodic trajectory satisfies:

$$\operatorname{ind}^- Q_{\gamma^k} - k \operatorname{ind}^- Q_\gamma = \sum_{j=1}^{k-1} \dim(M) - \dim(\ker(\Theta - \omega^j)) - i(\Gamma(\Theta), \Delta, \Gamma(\omega^j\Theta)). \tag{22}$$

Where ω is a primitive $k-$th root of the unity.

Proof. We work on the space $M^k = M \times \cdots \times M$. The first set of boundary conditions we are going to consider is the following:

$$\Delta^{\circlearrowleft} := \{(q_1, \dots, q_k, r_1 \dots r_k) : r_i, q_i \in M, q_i = r_{i-1}\} \subset M^k \times M^k.$$

Set $q_0 = \gamma(0) = \gamma(1)$. Any curve satisfying the boundary conditions $\Delta^{\circlearrowleft}$ gives a variation of the $k-$th iterate of γ seen as periodic trajectory.

The other sets of constraints we are going to introduce are the following:

$$\begin{aligned} \Delta^k &= \{(q_1, \dots, q_k, q_1, \dots, q_k) : q_i \in M\} \subset M^k \times M^k, \\ \underline{q}_0 &= \{(q_0, \dots, q_0) : q_0 = \gamma(0) = \gamma(1)\}. \end{aligned}$$

The first boundary condition is the product of $2k$ copies of the diagonal. Any curve satisfying this set of constraints at point $(q_0, \dots, q_0)$ is a variation of γ^k as k independent periodic trajectories γ. The second boundary condition corresponds to k copies of a single point q_0. Variations of γ^k satisfying these latter conditions are k independent variations of γ as a trajectory with fixed points.

To simplify notation, set $\Delta^k = T_{\underline{\lambda}}A(\Delta^k)$, $\Delta^{\circlearrowleft} = T_{\underline{\lambda}}A(\Delta^{\circlearrowleft})$ and $\Gamma = \Gamma(\Theta \times \cdots \times \Theta)$ to be the product of k copies of $\Gamma(\Theta)$. We have $T_{\underline{\lambda}}A(\underline{q}_0) = \Pi^{2k}_{\lambda(0)} = \Pi^{2k}$ where $\lambda(0)$ is the initial covector of the lift to the cotangent bundle.

First of all we compute directly $\operatorname{ind}^- Q_{\gamma^k}$ using Theorem 1, comparing with the fixed endpoints problem. We get:

$$\operatorname{ind}^- Q_{\gamma^k} = k \operatorname{ind}^- Q_0 + i\big(\Pi^{2k}, \Gamma, \Delta^{\circlearrowleft}\big) + \dim(\Gamma \cap \Pi^{2k}) - \dim(\Gamma \cap \Pi^{2k} \cap A(\Delta^{\circlearrowleft})).$$

Here the notation $\operatorname{ind}^- Q_0$ stands for the index of Q at γ seen as a trajectory with fixed end points. We analyse first the term $i\big(\Pi^{2k}, \Gamma, \Delta^{\circlearrowleft}\big)$. To compute it, we present the Maslov form as the direct sum of k forms defined on a $\dim(M)-$dimensional subspace. This is done in Lemma 2, where we use the *complexified* version of Maslov index. The term $i\big(\Pi^{2k}, \Gamma, \Delta^{\circlearrowleft}\big)$ is thus the sum of contributions of the type $i\big(\Pi^2, \Gamma(\omega^j\Theta), \Delta\big)$ where ω is a primitive root of unity.

$$i\big(\Pi^{2k}, \Gamma, \Delta^{\circlearrowleft}\big) = \sum_{j=0}^{k-1} i\big(\Pi^2, \Gamma(\omega^j\Theta), \Delta\big).$$

Now we apply Theorem 1 to the second set of boundary conditions, i.e. Δ^k. We find that:

$$k \operatorname{ind}^- Q_\gamma = k \operatorname{ind}^- Q_0 + i\big(\Pi^{2k}, \Gamma, \Delta^k\big) + \dim(\Gamma \cap \Pi^{2k}) - \dim(\Gamma \cap \Pi^{2k} \cap \Delta^k).$$

Exactly as in the previous case the piece $i\big(\Pi^{2k},\Gamma,\Delta^k\big)$ splits as a sum. But this time the reason is more apparent: we are considering independent variation on each iteration. It follows that $i\big(\Pi^{2k},\Gamma,\Delta^k\big) = k\, i\big(\Pi^2,\Gamma(\Theta),\Delta\big)$

Now we subtract the two equations and we are left with the following expression for $\operatorname{ind}^- Q_{\gamma^k} - k \operatorname{ind}^- Q_\gamma$:

$$\operatorname{ind}^- Q_{\gamma^k} - k \operatorname{ind}^- Q_\gamma = \sum_{j=0}^{k-1}\Big(i\big(\Pi^2,\Gamma(\omega^j\Theta),\Delta^{\circlearrowleft}\big) - i\big(\Pi^2,\Gamma(\Theta),\Delta\big)\Big) + \dim(\Gamma\cap\Pi^{2k}\cap\Delta^k) - \dim(\Gamma\cap\Pi^{2k}\cap\Delta^{\circlearrowleft}).$$

Let's rewrite the term involving the intersections. It is straightforward to see that $\dim(\Gamma\cap\Pi^{2k}\cap\Delta^k) = k\dim(\Gamma(\Theta)\cap\Pi^2\cap\Delta)$. In turn, this rewrites as $k\dim(\ker(\Theta-1)\cap\Pi)$.

For the second piece it holds that:

$$\dim(\Gamma\cap\Pi^k\cap\Delta^{\circlearrowleft}) = \sum_{j=0}^{k-1}\dim(\ker(\Theta-\omega^j)\cap\Pi).$$

We prove this below, in Proposition 2. Putting all together we get:

$$\dim(\Gamma\cap\Pi^{2k}\cap\Delta^k) - \dim(\Gamma\cap\Pi^k\cap\Delta^{\circlearrowleft}) = \sum_{j=0}^{k-1}\dim(\Gamma(\Theta)\cap\Pi^2\cap\Delta) - \dim(\ker(\Theta-\omega^j)\cap\Pi). \tag{23}$$

Now we can use the cocycle property given in equation (55) with the subspaces $\Pi,\Gamma(\omega^j\Theta),\Gamma(\Theta)$ and Δ to rewrite the difference of Maslov indexes using the subspaces $\Gamma(\omega^j\Theta)$ and Δ. These computations are collected in Proposition 2. What we find is that:

$$\begin{aligned} i\big(\Pi^2,\Gamma(\omega^j\Theta),\Delta\big) - i\big(\Pi^2,\Gamma(\Theta),\Delta\big) &= -i\big(\Gamma(\Theta),\Delta,\Gamma(\omega^j\Theta)\big) + \dim(M)\\ &\quad - \dim(\ker(\Theta-1)\cap\Pi) + \dim(\ker(\Theta-\omega^{-j})\cap\Pi) - \dim\ker(\Theta-\omega^{-j}). \end{aligned}$$

Since we are summing over $j=0,\dots,k-1$ and ω is a primitive k-th root of unity, we have that $\sum_{j=0}^{k-1}\dim(\ker(\Theta-\omega^{-j})\cap\Pi) = \sum_{j=0}^{k-1}\dim(\ker(\Theta-\omega^j)\cap\Pi)$ and thus the intersection of the eigenspaces with the fibre cancel out with the part coming from triple intersection given in equation (23). Summing up we finally obtain (21). $\square$

Lemma 2. *Let $\omega\in\mathbb{C}$ be a primitive $k-$th root of the unity. The Maslov form $m(\Pi^{2k},\Gamma,\Delta^{\circlearrowleft}) = \bigoplus_{i=0}^{k-1} m_i$ where:*

$$m_i = m(\Pi^2,\Gamma(\omega^i\Theta),\Delta).$$

Proof. We will use the Hermitian version of Maslov index. Any real subspace V appearing in the proof will stand for its complexification $V\otimes\mathbb{C}$ without any mention to the tensor product operation. Let us write down the equation defining the space $(\Pi^{2k}+\Delta^{\circlearrowleft})\cap\Gamma$.

$$v\in\Gamma \iff v = (\xi_1,\dots,\xi_k,\Theta(\xi_1),\dots,\Theta(\xi_k)),\quad \xi_j\in T_{\lambda_0}(T^*_{q_0}M).$$

On the other hand belonging to $\Pi^{2k}+\Delta^{\circlearrowleft}$ means:

$$v\in\Pi^{2k}+\Delta^{\circlearrowleft} \iff v = (\mu_1,\dots,\mu_k,\nu_1,\dots,\nu_k),\quad \mu_{i+1}-\nu_i\in\Pi,$$

where $\mu_{k+1}=\mu_1$. So the space $(\Pi^{2k}+\Delta^{\circlearrowleft})\cap\Gamma$ is given by $\{(\xi_1,\dots,\xi_k) : \xi_{i+1}-\Theta(\xi_i)\in\Pi\}$.

Maslov form is computed in the following way. Let

$$\begin{aligned}\xi_i &= X_i+\alpha_i,\\ \Theta(\xi_i) &= X_{i+1}+\beta_i,\end{aligned}$$

where $\alpha_i,\beta_i\in\Pi$, $X_i\in T_{\lambda_0}(T^*M)$. Then we have

$$\begin{aligned} m(\underline{\xi}) &= \sum_{i=1}^k -\sigma(\bar\alpha_i,X_i)+\sigma(\bar\beta_i,X_{i+1}) = \sum_{i=1}^k -\sigma(\bar\alpha_i,X_i)+\sigma(\bar\beta_{i-1},X_i) = \sum_{i=1}^k \sigma(-\bar\alpha_i+\bar\beta_{i-1},X_i)\\ &= \sum_{i=1}^k \sigma(-\bar\alpha_i+\bar\beta_{i-1},\xi_i) = \sum_{i=1}^k \sigma(\Theta(\bar\xi_{i-1})-\bar\xi_i,\xi_i) = \sum_{i=1}^k \sigma(\Theta(\bar\xi_{i-1}),\xi_i)-\sigma(\bar\xi_i,\xi_i). \end{aligned}$$

Where in the third equality we simply shifted the second index cyclically.

Suppose that ω is a primitive $k-$th root of the identity and make the following change of variables.

$$\underline{\xi} = (\xi_1, \ldots, \xi_k) \mapsto \left(\sum_{i=1}^{k} \xi_i, \ldots, \sum_{i=1}^{k} \omega^{j(i-1)} \xi_i, \ldots, \sum_{i=1}^{k} \omega^{(k-1)(i-1)} \xi_i \right) =: \underline{\eta},$$

which, essentially, is just the Kronecker product of the identity with the transpose of Vandermonde's matrix obtained with $\{1, \omega, \ldots, \omega^{k-1}\}$. In the new coordinates the equation reads:

$$\begin{aligned}
\eta_l - \omega^{l-1}\Theta(\eta_l) &= \sum_{i=1}^{k} \omega^{(l-1)(i-1)} \xi_i - \sum_{i=1}^{k} \omega^{(l-1)i} \Theta(\xi_i) \\
&= \sum_{i=1}^{k} \omega^{(l-1)i} \xi_{i+1} - \omega^{(l-1)i}\Theta(\xi_i) \\
&= \sum_{i=1}^{k} \omega^{(l-1)i} (\xi_{i+1} - \Theta(\xi_i)) \in \Pi.
\end{aligned}$$

So in the new coordinates the space $(\Pi^{2k} + \Delta^{\circlearrowleft}) \cap \Gamma$ splits as the direct sum $\bigoplus_{l=1}^{k} \{\eta \,:\, \eta - \omega^l \Theta(\eta) \in \Pi\}$.
The inverse transformation is given by the following rule:

$$\xi_i = \frac{1}{k} \sum_{l=1}^{k} \omega^{-(i-1)(l-1)} \eta_l.$$

If we plug it in the second term of the Maslov form we have:

$$\sum_{i=1}^{k} \sigma(\Theta(\overline{\xi_i}), \xi_{i+1}) = \frac{1}{k^2} \sum_{i,l,s=1}^{k} \sigma(\Theta(\omega^{(i-1)(s-1)} \bar{\eta}_s), \omega^{-i(l-1)} \eta_l)$$

$$= \frac{1}{k^2} \sum_{i,l,s=1}^{k} \omega^{i(s-l)} \omega^{-(s-1)} \sigma(\Theta(\bar{\eta}_s), \eta_l) = \frac{1}{k^2} \sum_{l,s=1}^{k} \Big(\sum_{i=1}^{k} (\omega^{i(s-l)}) \omega^{1-s} \sigma(\Theta(\bar{\eta}_s), \eta_l) \Big).$$

In particular, the only non zero terms are those for which $s = l$ since the sum of powers of any primitive root (up to k) is zero.

We can handle similarly the first term. In this way we find that the Maslov form on our subspace splits in the following way:

$$m(\underline{\eta}) = \frac{1}{k} \sum_{s=1}^{k} \sigma(\overline{\omega^{s-1}\Theta(\eta_s)}, \eta_s) - \sigma(\bar{\eta}_s, \eta_s).$$

The factor $\frac{1}{k}$ is irrelevant for us and comes just from the change of coordinates. The last step is to identify the summands with $m(\Pi^2, \Gamma(\omega^{s-1}\Theta), \Delta)$. Let's write down the kernel for these forms. The space we have to look at is $(\Pi^2 + \Delta) \cap \Gamma(\omega^{s-1}\Theta)$. It is defined by:

$$\eta = \alpha + X \quad \omega^{s-1}\Theta(\eta) = \beta + X \quad \alpha, \beta \in \Pi.$$

By the definition the Maslov form is given by

$$m(\eta) = -\sigma(\bar{\alpha}, X) + \sigma(\bar{\beta}, X) = \sigma(\overline{\omega^{s-1}\Theta(\eta)} - \bar{\eta}, \eta).$$

□

Proposition 2. *The following relation holds:*

$$i\big(\Pi^2, \Gamma(\omega^j\Theta), \Delta\big) - i\big(\Pi^2, \Gamma(\Theta), \Delta\big) = -i\big(\Gamma(\Theta), \Delta, \Gamma(\omega^j\Theta)\big) + \dim(M) + d_j, \tag{24}$$

where $d_j = -\dim(\ker(\Theta - 1) \cap \Pi) + \dim(\ker(\Theta - \omega^{-j}) \cap \Pi) - \dim\ker(\Theta - \omega^{-j})$. *Moreover the space* $\Gamma \cap \Pi^{2k} \cap \Delta^{\circlearrowleft}$ *splits as a direct sum and its dimension is given by:*

$$\dim(\Gamma \cap \Pi^{2k} \cap \Delta^{\circlearrowleft}) = \sum_{j=0}^{k-1} \dim(\ker(\Theta - \omega^j) \cap \Pi).$$

Proof. The second part can be deduced by the proof of Lemma 2. In fact the space $\Pi^{2k} \cap \Gamma \cap \Delta^{\circlearrowleft}$ is isomorphic to $\bigoplus_i \ker(\Theta - \omega^i) \cap \Pi$. This can be either directly computed from the definition of the spaces or deduced in the following way.

Let P represent the standard $k-$cycle which maps $\xi_i \to \xi_{i+1}$ and $\xi_k \to \xi_1$. A direct calculation shows that $\Delta^{\circlearrowleft} = \Gamma(P)$. Thus any element of $\Delta^{\circlearrowleft} \cap \Gamma$ can be written as

$$\begin{pmatrix} \xi \\ P\xi \end{pmatrix} = \begin{pmatrix} \xi \\ diag(\Theta)(\xi) \end{pmatrix} \iff P^{-1} diag(\Theta)(\xi) = \xi \iff diag(\Theta)P^{-1}(\eta) = \eta, \text{ where } \eta = P\xi.$$

i.e. an eigenvalue problem.

The core of the proof of Lemma 2 consisted in the diagonalization of the following matrix:

$$\begin{pmatrix} \Theta & & \\ & \ddots & \\ & & \Theta \end{pmatrix} P^{-1} \sim \begin{pmatrix} \omega^0\Theta & & \\ & \ddots & \\ & & \omega^{k-1}\Theta \end{pmatrix}$$

with the remaining elements understood to be zero. The transformation diagonalizing the matrix we used preserves the fibre. So it follows that $\Pi^{2k} \cap \Gamma \cap \Delta^{\circlearrowleft}$ is the sum of the eigenspaces $\ker(\Theta - \omega^j)$ intersected with the fibre Π.

Now we prove the first part of the proposition. Let us apply the cocycle property to $\Pi^2, \Gamma(\omega^j\Theta), \Gamma(\Theta)$ and Δ.

$$\begin{aligned} i\big(\Pi^2, \Gamma(\omega^j\Theta), \Delta\big) - i\big(\Pi^2, \Gamma(\Theta), \Delta\big) &= i\big(\Gamma(\Theta), \Pi^2, \Gamma(\omega^j\Theta)\big) \\ &\quad - i\big(\Gamma(\Theta), \Delta, \Gamma(\omega^j\Theta)\big) + c_i, \\ c_i = \dim(\Theta(\Pi) \cap \Pi) &- \dim(\ker(\Theta - 1) \cap \Pi) + \dim(\ker(\Theta - \omega^{-j}) \cap \Pi) + \\ &- \dim\ker(\Theta - \omega^{-j}). \end{aligned}$$

The formula is almost the one given in the statement except for the terms $\dim(\Theta(\Pi) \cap \Pi)$ and $i\big(\Gamma(\Theta), \Pi^2, \Gamma(\omega^j\Theta)\big)$ and a lacking $\dim(M)$.

We can compute the Maslov index term in the following way. Notice that $\Gamma(\omega^j\Theta)$ and $\Gamma(\omega^l\Theta)$ are transversal if the index j is different form l. It follows that the space on which the form is defined is Π^2. Moreover the equations are $\xi_1 + \xi_2 = \nu_1 \in \Pi$ and $\Theta(\xi_1 + \omega^j\xi_2) = \nu_2 \in \Pi$. Thus Maslov form reads:

$$m(\nu_1, \nu_2) = -\sigma(\bar{\xi}_1, \xi_2) + \omega^j\sigma(\Theta(\bar{\xi}_1), \Theta(\xi_2)) = (\omega^j - 1)\sigma(\bar{\xi}_1, \xi_2).$$

We can invert the equations to write them on Π^2. We get $\xi_2 = \frac{1}{1-\omega^j}(\nu_1 - \Theta^{-1}(\nu_2))$ and $\xi_1 = \frac{1}{1-\omega^j}(\Theta^{-1}(\nu_2) - \omega^j\nu_1)$ and thus the form is equivalent to:

$$m(\nu_1, \nu_2) = \frac{1}{\bar{\omega}^j - 1}(\sigma(\bar{\nu}_2, \Theta(\nu_1)) + \omega^{-j}\sigma(\bar{\nu}_1, \Theta^{-1}(\nu_2))).$$

This form has zero signature and kernel isomorphic to two copies of $\Theta(\Pi) \cap \Pi$. This is a general fact and can be seen as follow. Suppose the matrix representing the quadratic form has the following expression:

$$\mathcal{M} = \begin{pmatrix} 0 & X \\ \bar{X}^* & 0 \end{pmatrix} \quad m(\nu_1, \nu_2) = \langle \bar{\nu}_1, X\nu_2 \rangle + \langle \bar{\nu}_2, \bar{X}^*\nu_1 \rangle.$$

Let be Q and R unitary matrices which gives the singular values decomposition for X, i.e. $QXR = D$ for $D = diag(d_i^2)$, diagonal and with non negative entries.

Apply the following change of coordinates to $\mathcal{M}$:

$$\begin{pmatrix} Q & 0 \\ 0 & \bar{R}^* \end{pmatrix} \begin{pmatrix} 0 & X \\ \bar{X}^* & 0 \end{pmatrix} \begin{pmatrix} \bar{Q}^* & 0 \\ 0 & R \end{pmatrix} = \begin{pmatrix} 0 & D \\ D & 0 \end{pmatrix}.$$

And then apply another change:

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & D \\ D & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} -2D & 0 \\ 0 & 2D \end{pmatrix}.$$

Thus the non zero eigenvalues of the matrix $\mathcal{M}$ are $\pm d_i^2$, where $d_i^2 > 0$ are the positive singular values of X. The kernel of $\mathcal{M}$ has dimension $2\dim\ker(X)$.

This is precisely our situation: fix a Lagrangian complement to the fibre Π, and consider the matrices associated to Θ and $\frac{\omega^{-j}}{\omega^{-j}-1}J\Theta^{-1}$. In blocks they can be written as:

$$\Theta = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad J\Theta^{-1} = \begin{pmatrix} C^* & -A^* \\ D^* & -B^* \end{pmatrix}, \quad J\Theta = \begin{pmatrix} -C & -D \\ A & B \end{pmatrix}.$$

We are using coordinates in which the fibre Π is the span of the first n coordinates. Thus the block we have to consider is always the upper left one. Our form, with this conventions, is written as:

$$m(\nu_1,\nu_2)=\left\langle \bar\nu_2, \frac{1}{1-\omega^{-j}}C\nu_1\right\rangle+\left\langle \bar\nu_1,\frac{\omega^{-j}}{\omega^{-j}-1}C^*\nu_2\right\rangle.$$

So for us $X=\frac{\omega^{-j}}{1-\omega^{-j}}C^*$. Thus our form has zero signature, is defined on a $2\dim(M)$ dimensional vector space and the kernel is isomorphic to two copies of the kernel of X. The latter is easily seen to be $\Theta(\Pi)\cap\Pi$.

Thus it follows that $i\big(\Gamma(\Theta),\Pi^2,\Gamma(\omega^j\Theta)\big)=\dim(M)-\dim(\Theta(\Pi)\cap\Pi)$. Inserting above we get (24). □

In order to give a complete discussion, we consider the function $\mathbb{S}^1\ni z\mapsto i(\Gamma(\Theta),\Delta,\Gamma(z\Theta))$ and study its properties. We give an explicit description in terms of the monodromy matrix Θ and its spectrum. These ideas are collected in the following proposition.

Proposition 3. *The number $i\left(\Gamma(\Theta),\Delta,\Gamma(\omega^j\Theta)\right)$ corresponds to the number of negative eigenvalues of the following matrix:*

$$M_{\omega^j}=\frac{1}{1-\omega^{-j}}J\Big(\omega^{-j}+1-\omega^{-j}\Theta-\Theta^{-1}\Big).$$

If we consider the function $\mathbb{S}^1\ni z\mapsto i\big(\Gamma(\Theta),\Delta,\Gamma(z\Theta)\big)$, it is locally constant with at most $2n$ jumps at eigenvalues of Θ. Moreover the jumps are bounded in amplitude by $\dim(\ker(\Theta-z))$ where $z\in\mathbb{S}^1$.

Proof. The first part is just a straightforward computation. Take for any $\alpha\in\mathbb{S}^1$:

$$\begin{pmatrix}\xi_1\\ \Theta(\xi_1)\end{pmatrix}+\begin{pmatrix}\xi_2\\ \alpha\Theta(\xi_2)\end{pmatrix}=\begin{pmatrix}X\\ X\end{pmatrix}\Rightarrow\begin{cases}(1-\alpha)\xi_2=X-\Theta^{-1}(X),\\ (\alpha-1)\xi_1=\alpha X-\Theta^{-1}(X).\end{cases}$$

If $\alpha\neq 1$ the two graphs are always transversal and the Maslov quadratic form can be written in terms of the variable X:

$$\begin{aligned}m(X)&=-\sigma(\bar\xi_1,\xi_2)+\alpha\sigma(\Theta(\bar\xi_1),\Theta(\xi_2))=(\alpha-1)\sigma(\bar\xi_1,\xi_2)\\&=\frac{1}{1-\bar\alpha}\sigma\Big(\bar\alpha\bar X-\Theta^{-1}(\bar X),X-\Theta^{-1}(X)\Big)\\&=\frac{\bar\alpha+1}{1-\bar\alpha}\sigma(\bar X,X)-\frac{1}{1-\bar\alpha}\sigma((\bar\alpha\Theta+\Theta^{-1})(\bar X),X).\end{aligned}$$

It follows that the kernel is $M_\alpha=\frac{1}{1-\bar\alpha}J\Big(\bar\alpha+1-\bar\alpha\Theta-\Theta^{-1}\Big)$.

For the second part notice that the map $\alpha\mapsto M_\alpha$ is continuous away from 1 with values in the space of Hermitian matrices.

A change of index can occur only at those points in which the determinant of M_z is zero, thus at most $2n$ times. Moreover the jumps are the following:

$$\det(M_\alpha)=0\iff\det(\bar\alpha+1-\bar\alpha\Theta-\Theta^{-1})=0,\ \alpha\neq1.$$

In particular, notice that Θ and Θ^{-1} can be put in the same block triangular form. For example one can choose to put Θ in its Jordan form. On the diagonal, at a block corresponding to eigenvalue λ of Θ, the elements are $\bar\alpha+1-\bar\alpha\lambda-\frac{1}{\lambda}$. This quantity is zero if and only if $\alpha=\frac{\lambda}{|\lambda|^2}$ i.e. if α is an eigenvalue of Θ that lies on the circle.

Thus the jumps are at most $2n$. The part on the bound follows by this observation: take a Jordan block of Θ with eigenvalue λ. Then the corresponding block of Θ^{-1} will have $\bar\lambda$ on the diagonal and $(-1)^k\bar\lambda^{k+1}$ on the $k-$th upper diagonal. This implies that on the first upper diagonal of the λ block of $\bar\lambda\Theta+\Theta^{-1}$ we considered you end up with $-\bar\lambda+\bar\lambda^2$, which is different from zero. Thus each $\lambda-$block contributes with a single eigenvalue and so the jumps are controlled by $\dim(\ker(\Theta-\lambda))$. □

2.5 Numerical study of NLS on trees

Formulas (16), (17), (18) and (19) are used to determine whether a given extremal is a local minimum. These formulas can be difficult to apply because of a complicated parametrization of critical points or a complex graph structure. Nevertheless, we can always use them to construct reliable numerical algorithms for studying stability or testing theoretical hypothesis. In this subsection we illustrate this claim by examining numerically solutions of the NLS on a symmetric rooted tree graph with a finite number of edges.

More precisely, consider a rooted tree whose finite edges have all length l. Each vertex is of degree d except the root, and there are d^s vertices in total. We denote such a tree by $\mathcal{T}_{l,d,s}$. We look for a minimizer of the functional (4) under the constraints (5) and (6) with $\mathcal{G}_1 = \mathcal{T}_{l,d,s}$ and Neumann condition at the root. This problem has a discrete symmetry given by exchanging various branches. Hence a very natural question is to understand whether the global minima have this symmetry as well. If this is the case, then the value of a minimizer at a given point only depends on the distance to the root. We call such minimizers *symmetric*. It is known that for the tree with only one branching the minimizers are indeed symmetric [5, Theorem 2.7]. For trees with several branchings this is unknown. Let us consider numerically the local minimality of an asymmetric critical point in the simplest case with the non-linearity power $\alpha = 4$ and a rooted tree with $s = 2$ and $d = 2$ depicted in Figure 5.

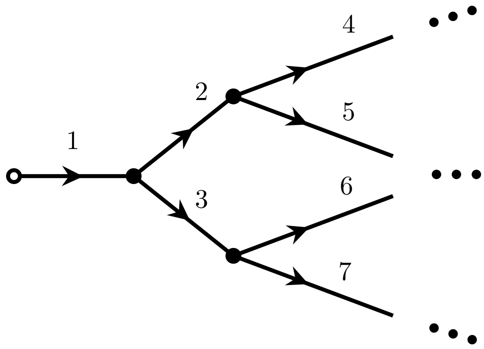

Figure 5: Symmetric tree $\mathcal{T}_{l,2,2}$. Numbers correspond to the numbering of the edges in the text.

The algorithm follows the following steps, which are universal for any graph-parametrized problem:

Step 1: Reformulate the considered problem on a graph as an optimal control problem on a subset of the line;

Step 2: Write down the Hamiltonian system for each edge and transeversality conditions;

Step 3: Identify an extremal of interest using numerical integration;

Step 4: Linearize the Hamiltonian system and integrate it numerically to obtain the graph of the flow Ψ_t. One needs to integrate it until the end of the edge or the first conjugate point, i.e., until $\Psi_t(\Pi) \cap \Pi \neq \emptyset$. One can encode this condition as vanishing of the determinant of a submatrix of Ψ_t.

Step 5: If there are no internal conjugate points, write down the Maslov form from (16) and compute numerically its eigenvalues.

In Step 1 we transform the problem (4), (5), (6) into an optimal control problem by introducing new variables:

$$q_e = \psi_e, \qquad u_e = \dot{q}_e, \qquad m_e(t) = \int_0^t |\psi_e(s)|^2 ds.$$

This gives us the functional

$$\sum_{e=1}^{7} \int_0^{l_e} \frac{|u_e|^2}{2} - \frac{|q_e|^4}{4} dt \to \min,$$

and differential constraints

$$\begin{cases} \dot{q}_e = u_e, \\ \dot{m}_e = |q_e|^2. \end{cases}$$

Usually ψ_e are taken to be complex-valued. However, it is known that the minimizer can be assumed to be real [5]. For this reason we minimize only among real-valued functions and avoid writing the absolute values any further. In addition (5) is equivalent to

$$\sum_{e=1}^{7} m_e(l_e) = \mu, \tag{25}$$

equation (6) implies that $q_e(\infty) = 0$ for the infinite edges $e = 4, 5, 6, 7$ of the tree and the Neumann condition at the root is equivalent to assuming that the value of $q_1(0)$ is free. Finally we have the continuity condition of q at each vertex.

Next we apply the Pontryagin maximum principle and deduce that at each edge restrictions of a critical point must satisfy the Hamiltonian system

$$\begin{cases} \dot{q}_e = p_e, \\ \dot{m}_e = q_e^2, \\ \dot{p}_e = -2\lambda_e q_e - q_e^3, \\ \dot{\lambda}_e = 0. \end{cases} \tag{26}$$

The transversality conditions gives us conditions on p_e and λ_e at various vertices. From (25) we get that all λ_e must be equal to some fixed λ, that at the root $p_1(0) = 0$, and that

$$\begin{aligned} p_1(l) &= p_2(0) + p_3(0), \\ p_2(l) &= p_4(0) + p_5(0), \\ p_3(l) &= p_6(0) + p_7(0). \end{aligned} \tag{27}$$

Those are just the standard Kirkchoff boundary conditions. Finally, if we are interested in minimizers in $H^1(\mathcal{T}_{l,2,2})$, we need to put an extra condition that $p_e(\infty) = 0$ for infinite edges of the graph.

Now we can start constructing possible extremal solutions. The phase portrait of (26) is depicted in Figure 6 and qualitatively it is the same for all negative λ.

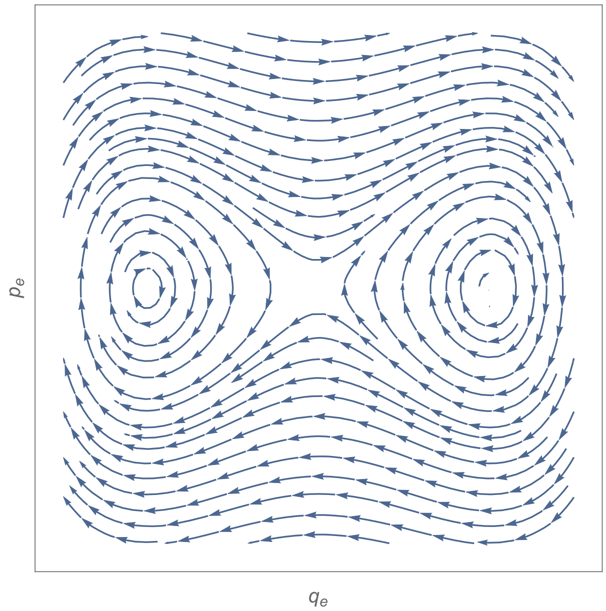

Figure 6: Phase portrait of the subsystem (q_e, p_e) of (26).

Since $p_e(\infty) = q_e(\infty) = 0$, the restrictions to the last edge are either trivial or pieces of the separatrix solution also called the soliton. For positive λ there are no soliton solutions. In [5] the authors prove, using the decreasing rearrangement technique, that at the very last branching the solitons must be symmetric, i.e. $p_e(0)$ of the two edges attached to one of the last vertices must coincide. Hence we need to choose values of q for each soliton piece at the final vertices.

After those values are chosen, we solve numerically equations (26) backward in time for each edge using Kirkchoff conditions (27). Unfortunately, the solutions may fail to satisfy the Neumann condition at the root and continuity conditions at other vertices. We need to find the initial values of the solitons that would guarantee that those conditions are met. This can be done using any quasi-Newtonian method. There are always symmetric critical points. However, one can also find some asymmetric candidates. Figure 7 shows the plot of such a critical point as a multivalued function for $\lambda = -1$ and $l = 1$. In this case the two inital values of q of the soliton are approximately 1.77094 and 0.243391.

Once an extremal solution is found, we linearize system (26) and add them to the original system. This gives

$$\begin{cases} \dot{q}_e = p_e, \\ \dot{m}_e = q_e^2, \\ \dot{p}_e = -2\lambda_e q_e - q_e^3, \\ \dot{\lambda}_e = 0. \end{cases} \qquad \begin{cases} \dot{X}_e = Y_e, \\ \dot{M}_e = 2q_e X_e, \\ \dot{Y}_e = -2\lambda_e X_e - 2\Lambda_e q_e - 3q_e^2 X_e, \\ \dot{\Lambda}_e = 0. \end{cases} \tag{28}$$

From here we can compute numerically the fundamental solution Ψ_t of the linearized system for each edge and check that the minimum candidate depicted in Figure 7 do not contain conjugate points.

Remark 3. One should be careful when integrating (28) along the soliton. It is difficult to follow numerically the separatrix solution for long times, since a small error will result in a solution inside or outside the region bounded by this solution. Thus one should take only a finite piece of a soliton, where the numerical error is sufficiently small.

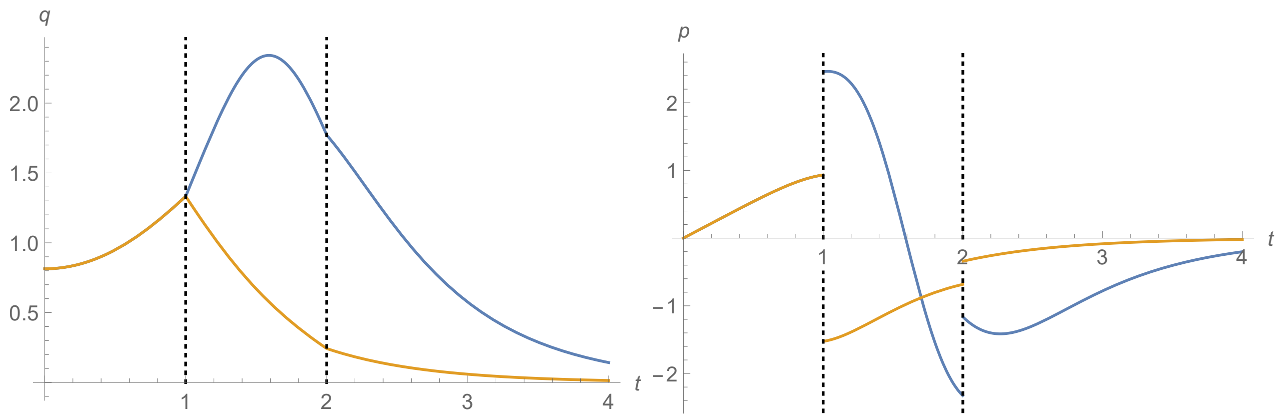

Figure 7: Graphs of $q(t)$ and $p(t)$ of an assymetric extremal point as the distance to the root. The dotted lines indicate branchings .

It only remains to check whether the index of the Maslov form in (16) is positive. Now we explain in detail how to write down explicitly its associated symmetric matrix. The symplectic form is the standard symplectic form on the double space $\mathbb{R}^4 \times \mathbb{R}^4$. We denote its matrix by J. We write down the two orthogonal projectors π_Π and π_{TN}, where the first one is the projector to the vertical space and π_{TN} is the projector to the tangent space of the boundary constraints. Note that the whole projector to the tangent of the annihilator is not needed, because the vertical part cancels out due to the skew-symmetry of the symplectic form. Now we need to find the vectors which lie in the intersection $(T_{\underline{\lambda}}A(N) + \Pi) \cap T_{\underline{\lambda}}\Gamma(\Psi)$. We can do this by using the previously defined orthogonal projections. In order to do this, find numerically the kernel of $(1 - \pi_\Pi - \pi_{TN})\Psi$. From here we can construct the projector π_{mas} onto the domain of the Maslov form. The matrix of the Maslov is now the symmetrization of the matrix $(\pi_\Pi \circ \Psi \circ \pi_{mas})^T J(\pi_{TN} \circ \Psi \circ \pi_{mas})$.

For our example depicted in Figure 7, when we take the length of the soliton piece to be equal to one, one of the eigenvalues is equal to -0.544933. Hence this critical point is not a local minimum. In exactly the same manner one can study local minimality of any other critical state of the NLS on a rooted tree.

3 Index formulas and proof of Theorem 1

3.1 Reduction to a variational problem with fixed end-points

In this section we prove Theorem 1. We will consider first the case in which the boundary constraints in (8) are separated. This means that we look for a minimizer γ with initial point $\gamma(0)$ in N_0 and final point $\gamma(1)$ in N_1, where $N_0, N_1 \subset M$ are embedded submanifolds. The general case will be reduced to this one.

Given an extremal trajectory γ of the optimal control problem (7)-(9) with $N = N_0 \times N_1$, we will now construct a new optimal control problem with fixed end-points and interpret γ as the restriction of an extremal $\hat{\gamma}$. Moreover, we will show that the two problems are locally equivalent.

Denote $q_i = \gamma(i) \in N_i$ for $i = 0, 1$. We want to construct an extended control system in such a way that all admissible curves $\hat{\alpha}$, connecting q_0 with q_1 and sufficiently close to γ, are concatenations $\hat{\alpha} = \alpha_1 * \alpha * \alpha_0$, where α_i are curves inside N_i and α connects N_0 to N_1.

To do so, fix neighbourhoods $\mathcal{O}(q_i) \subset M$, of the points q_i. If $\mathcal{O}(q_i)$ are sufficiently small, we can construct regular foliations of $\mathcal{O}(q_i)$ such that $N_i \cap \mathcal{O}(q_i)$ are leaves passing through q_i. Consider the union of all tangent space to each leaf of the foliation. This gives two integrable distributions D_0 and D_1 in each neighbourhood. After shrinking the neighbours if necessary, we can choose a set of vector fields f_i^j, $j = 1, \dots, \dim N_i$ defined on $\mathcal{O}(q_i)$, which generate these distributions:

$$\operatorname{span}\left\{ f_i^j(q),\, j = 1, \dots, \dim N_i \right\} = D_i(q), \quad \forall q \in \mathcal{O}(q_i), \quad i = 0, 1.$$

Using these vector fields, we extend our control system on $[-1, 2]$, adding a part linear in the controls for $t \in [0, 1]^c$. Namely:

$$\hat{f}_u^t(q) = \begin{cases} f_0(q)u_0 := \sum_{j=1}^{\dim N_0} f_0^j(q)u_{0j}, & \text{if } t < 0, \\ f_u^t(q), & \text{if } t \in [0, 1], \\ f_1(q)u_1 := \sum_{j=1}^{\dim N_1} f_1^j(q)u_{1j}, & \text{if } t > 1. \end{cases}$$

where $u_0 \in \mathbb{R}^{\dim N_0}$ and $u_1 \in \mathbb{R}^{\dim N_1}$. The space of the extended controls (u_0, u, u_1) is isomorphic to $\hat{\mathcal{U}} = \mathbb{R}^{\dim N_0} \oplus L^\infty([0,1], \mathbb{R}^k) \oplus \mathbb{R}^{\dim N_1}$ and can be identified with functions which are constant on $[-1,0]$ and on $[1,2]$ with values in $\mathbb{R}^{\dim N_0}$ and $\mathbb{R}^{\dim N_1}$ respectively.

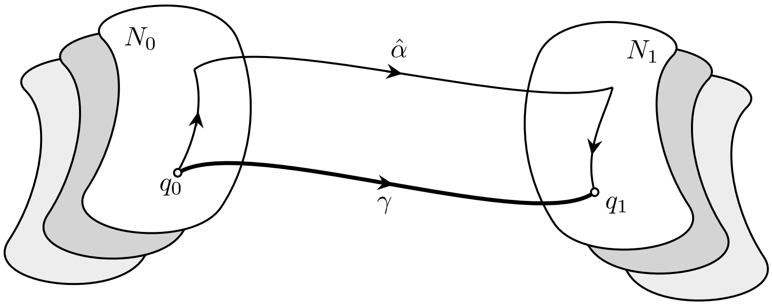

Figure 8: An admissible extended variation $\hat{\alpha}$ of an extremal curve γ

In Figure 8 the construction is explained visually. The local foliations are depicted in grey scale with the white surfaces being N_0 and N_1. An admissible curve $\hat{\alpha}$ of an extended system is confined to the leaf of the starting point up to time 0, evolves with the law prescribed by the initial system and then continues inside the leaf reached at time 1. In particular, if we restrict a curve $\hat{\alpha}$ connecting q_0 and q_1 to $[0,1]$, then we get a curve that connect N_0 to N_1.

We define the new optimal control problem as

$$\dot{q} = \hat{f}^t_{\hat{u}(t)}(q), \qquad \hat{u} \in \mathbb{R}^{\dim N_0} \oplus L^\infty([0,1], \mathbb{R}^k) \oplus \mathbb{R}^{\dim N_1}, \tag{29}$$

$$q(-1) = q_0, \quad q(2) = q_1, \tag{30}$$

$$\min_{\hat{u} \in \hat{\mathcal{U}}} \hat{\varphi}(\hat{u}) = \min_{\hat{u} \in \hat{\mathcal{U}}} \int_0^1 \ell(t, u(t), q_u(t))dt. \tag{31}$$

where $u = \hat{u}|_{[0,1]}$.

Lemma 3. *Optimal control problems* (7)-(9) *with* $N = N_0 \times N_1$ *and* (29)-(31) *are locally equivalent.*

Proof. Suppose that α is an admissible curve of the original control system. Let u be its control and assume that $\alpha(i) \in \mathcal{O}(q_i) \cap N_i$ for $i = 0, 1$. Then, α can be lifted to an admissible curve of the new system connecting q_0 and q_1. Indeed, take the unique controls u_i for which

$$\exp\left(f_0(\cdot)u_0\right) q_0 = \alpha(0), \qquad \exp\left(f_1(\cdot)u_1\right) \alpha(1) = q_1,$$

where exp denotes the flow of the vector field inside the brackets at time $t = 1$. Hence, the lift $\hat{\alpha}$ is defined as

$$\hat{\alpha}(t) = \begin{cases} \exp\left(tf_0(\cdot)u_0\right) q_0, & \text{if } t < 0, \\ \alpha(t), & \text{if } t \in [0,1], \\ \exp\left(tf_1(\cdot)u_1\right) \alpha(1), & \text{if } t > 1, \end{cases} \qquad \hat{u}(t) = \begin{cases} u_0, & \text{if } t < 0, \\ u(t), & \text{if } t \in [0,1], \\ u_1, & \text{if } t > 1. \end{cases}$$

Conversely, if we have an admissible curve $\hat{\alpha}$ such that $\hat{\alpha}(-1) = q_0$, $\hat{\alpha}(2) = q_1$ and $\alpha(i) \in \mathcal{O}(q_i)$, then its restriction $\alpha = \hat{\alpha}|_{[0,1]}$ is a curve connecting N_0 to N_1. Thus we obtain a local bijection between the two spaces of admissible curves.

Lastly, notice that $\hat{\varphi}(\hat{u}) = \varphi(u)$. Hence, the two problems are locally equivalent. □

3.2 Computation of first and second variation of the extended problem

Let $\lambda : [0,1] \to T^*M$ be an extremal satisfying PMP for the problem (7)-(9) with $N = N_0 \times N_1$. Denote by $\tilde{u}$ the corresponding control and by $\gamma(t) = \pi(\lambda(t))$, $t \in [0,1]$ the extremal curve on the manifold M. As discussed in the proof of Lemma 3, we can extend γ to an admissible curve of (29)-(31) as

$$\hat{\gamma} = \begin{cases} q_0, & \text{if } t < 0, \\ \gamma(t), & \text{if } t \in [0,1], \\ q_1, & \text{if } t > 1, \end{cases} \qquad \hat{\tilde{u}}(t) = \begin{cases} 0, & \text{if } t < 0, \\ \tilde{u}(t), & \text{if } t \in [0,1], \\ 0, & \text{if } t > 1. \end{cases}$$

In order to simplify slightly the notations, we will omit in the future the hat symbol for $\hat{\tilde{u}}$ by essentially identifying $\tilde{u}$ with $(0, \tilde{u}, 0)$.

In this section we compute the first and second variations of the problem (29)-(31) at a critical point $\tilde{u}$. In order to so this, we use the already existing formulas for the fixed end-point problem which can be found in several references such as [11].

For the reader's convenience, we recall here the main ideas behind this differentiation process. The first differential of E_{q_0} at a point u has an integral expression. This comes from an *asymptotic expansion* for flows, known as Volterra series, used in Chronological Calculus [11]. Namely, assume that X_t is a smooth and complete vector field. Its flow can be characterized using a differential or integral equation:

$$\begin{cases} \dot{P}_t = X_t \circ P_t \\ P_0 = I \end{cases} \iff P_t = 1 + \int_0^t X_\tau d\tau + \int_0^t \int_0^\tau X_\tau \circ X_s d\tau ds + \dots$$

When the vector field X_t depends on a parameter ϵ we can use this expansion to compute the derivative with respect to the parameter ϵ. Without loss generality set X_t^ϵ and $X_t = X_t^0$ and let P_t^ϵ be the flow of X_t^ϵ. Define $g_t^\epsilon := (P_t)_*^{-1}(X_t^\epsilon - X_t) \circ P_t$ and let Ψ_t^ϵ be its flow. One can check that $P_t \circ \Psi_t^\epsilon = P_t^\epsilon$. Differentiating this expression with respect to ϵ and using Volterra expansion yields:

$$\partial_\epsilon P_t^\epsilon|_{\epsilon=0} = (P_t)_* \circ \int_0^t (P_\tau^{-1})_* \partial_\epsilon X_\tau^\epsilon|_{\epsilon=0} \circ P_\tau d\tau$$

Remark 4. We use g_t^ϵ to differentiate the Endpoint map mainly for two reasons. The first one is that, since g_t^0 is zero, only finitely many terms of the expansion appear. The second one is that, in this way, all the integrals are performed in a fixed tangent space.

We can apply this procedure to the Endpoint map of our system at $u = \tilde{u}$. Let P_t be the flow generated by $f_{\tilde{u}}^t(q)$ and $q_t = P_t(q_0)$. As usual we denote $P := P_1$. We obtain the following integral expression for the first derivative:

$$d_{\tilde{u}} E_{q_0}(v) = P_* \int_0^1 (P_t^{-1})_* \partial_u f_{\tilde{u}}^t(q_t) v(t) dt. \tag{32}$$

Differentiating twice yields an expression for the second derivative:

$$d_{\tilde{u}}^2 E_{q_0}(v, w) = P_* \left(\int_0^1 (P_t^{-1})_* \partial_u^2 f_{\tilde{u}}^t(q_t)(v(t), w(t)) dt + \int_0^1 \int_0^t \big((P_\tau^{-1})_* \partial_u f_{\tilde{u}}^\tau(q_\tau) w(\tau)\big) \circ \big((P_t^{-1})_* \partial_u f_{\tilde{u}}^t(q_t) v(t)\big) d\tau dt \right). \tag{33}$$

Remark 5. Notice that in (33) we have a *quadratic mapping* (i.e. vector valued). Moreover this expression is coordinate dependent, unlike equation (32). The invariant second derivative of a smooth mapping $F : M \to N$ is defined only at critical points, with values in the cokernel of the differential. Namely:

$$d_p^2 F : \ker dF \subseteq T_p M \to T_{F(p)} N / \operatorname{im}(dF).$$

Recall now our setting. We have a smooth map E_{q_0}, the Endpoint map, defined on a open subset of $L^\infty([0,1], \mathbb{R}^k)$. We are assuming that the control $\tilde{u}$ is a regular point of E_{q_0}. Hence, $E_{q_0}^{-1}(q_1)$ is smooth around $\tilde{u}$. We are looking for local minima of a functional φ on the level set $E_{q_0}^{-1}(q_1)$. If $\tilde{u}$ is a critical point, we formulate second order optimality conditions in terms of the Hessian of the cost φ. To get an expression for this quadratic form restricted to $T_{\tilde{u}} E_{q_0}^{-1}(q_1) = \ker d_{\tilde{u}} E_{q_0}$, we differentiate a suitable modification of the Endpoint map. We extend the state space to $M \times \mathbb{R}$ and we look for critical points of the Endpoint map of the following system:

$$X_u^t(q, x) = \begin{pmatrix} f_u^t(q) \\ \ell(t, u, q) \end{pmatrix}.$$

This is essentially the same idea behind Lagrange multipliers rule. Since we are assuming that $d_{\tilde{u}} E_{q_0}$ is surjective, there exists a unique covector (up to multiples) (λ, ν) such that $\lambda d_{\tilde{u}} E_{q_0} + \nu d_{\tilde{u}} \varphi = 0$ and $\nu \neq 0$. We take ν to be negative since we are looking for minima and normalize it to -1. We obtain:

$$d_{\tilde{u}} \varphi(v) = \lambda d_{\tilde{u}} E_{q_0}(v), \quad \forall v \in L^\infty([0,1], \mathbb{R}^k).$$

Thus the kernel of the new Endpoint map coincides with the kernel of the old one. Now we can apply equation (33) to get an expression for the second derivative of the Endpoint map and then project onto $\mathbb{R}$ using the covector (λ, ν) (recall that the second derivative is well defined only as a map with values in the cokernel). We will need a little bit of symplectic geometry to simplify the expression above. Denote by $\bar{P}_t$ the flow generated by $X^t_{\tilde{u}(t)}(q,x)$. Set $\eta_0 := \bar{P}^*(\lambda,\nu)$, the pull back of (λ,ν). One can check that η_0 and (λ,ν) lie on the same solution of the Hamiltonian system generated by the Hamiltonian

$$\bar{h}^t_{\tilde{u}}(\lambda,\nu) = \langle(\lambda,\nu), X^t_{\tilde{u}(t)}\rangle = \langle\lambda, f^t_{\tilde{u}(t)}\rangle + \nu\ell(t,\tilde{u}(t),q),$$
$$\bar{h}^t_{\tilde{u}}(\lambda,\nu) = \bar{h}^t_u(\lambda,\nu)|_{u=\tilde{u}(t)}, \quad \bar{h}^t_u(\lambda,\nu) = \langle\lambda, f^t_u\rangle + \nu\ell(t,u,q).$$

We denote the Hamiltonian flow by $\bar{\Phi}_t$.

Notice that, if we project $M\times\mathbb{R}$, the $\bar{h}^t_u(\lambda,\nu)$ are precisely the Hamiltonians appearing in PMP. Using these conventions, the first term in (33) reads:

$$\eta_0\int_0^1 (\bar{P}_t^{-1})_*\partial^2_u X^t_{\tilde{u}}(q_t)(v(t),w(t)) = \int_0^1 \partial^2_u\bar{h}_{\tilde{u}}((\bar{P}_t^{-1})^*\eta_0)(v(t),w(t))dt = \int_0^1 \partial^2_u\bar{h}_{\tilde{u}}\circ\bar{\Phi}_t(\eta_0)(v(t),w(t))dt.$$

For the second one we have to work a little more. First of all one has the following identity for all $v,w\in\ker d_{\tilde{u}}E_{q_0}$:

$$\eta_0\int_0^1\int_0^t \left((\bar{P}_\tau^{-1})_*\partial_u X^\tau_{\tilde{u}}(q_\tau)w(\tau)\right)\circ\left((\bar{P}_t^{-1})_*\partial_u X^t_{\tilde{u}}(q_t)v(t)\right)d\tau dt =$$
$$= \int_0^1\int_0^t \langle\eta_0, \left[(\bar{P}_\tau^{-1})_*\partial_u X^\tau_{\tilde{u}}(q_\tau)w(\tau), (\bar{P}_t^{-1})_*\partial_u X^t_{\tilde{u}}(q_t)v(t)\right]\rangle d\tau dt.$$

We also have an useful identity, valid on all cotangent bundles, involving functions linear on fibres of the form $h_X(\eta) = \langle\eta, X\rangle$, for a smooth vector field X. It holds:

$$\langle\lambda,[X,Y]\rangle = \sigma(\vec{h}_X,\vec{h}_Y).$$

We can modify the integrand using this formula. Let us substitute the commutators with the symplectic pairing of Hamiltonian fields of $\partial_u(\bar{h}^t_{\tilde{u}}\circ\bar{P}_t)v(t)$ and $\partial_u(\bar{h}^\tau_{\tilde{u}}\circ\bar{P}_\tau)w(\tau)$. We obtain:

$$\int_0^1\int_0^t \sigma_{\eta_0}(\partial_u(\vec{\bar{h}}^\tau_{\tilde{u}}\circ\bar{P}_\tau)w(\tau), \partial_u(\vec{\bar{h}}^t_{\tilde{u}}\circ\bar{P}_t)v(t))dt d\tau.$$

The expression of the second derivative of the Endpoint map now involves just the functions $\bar{h}^t_u(\lambda,\nu)$ and their derivatives. It is not hard to check that we can forget the $\mathbb{R}$ component and work on M directly. For more details we always refer to [11, Chapter 2 and Section 20.3].

Remark 6. The quadratic form coincides indeed with $d^2_{\tilde{u}}\varphi$ restricted to $\ker d_{\tilde{u}}E_{q_0}$. For a detailed discussion on this equivalence and further reference one can check [11, Section 20.1] or [9]

Now, we specialize the formulas for the derivatives of the Endpoint mapping to the extended system (29)-(31). The Hamiltonian of PMP, which is everything needed to compute the derivatives. It is given by:

$$\hat{h}^t_{\tilde{u}}(\lambda) = \begin{cases}\langle\lambda, f_0u_0\rangle =: h_0u_0, & \text{if } t<0,\\ \langle\lambda, f^t_u(\pi(\lambda))\rangle - \ell(t,u,\pi(\lambda)), & \text{if } t\in[0,1],\\ \langle\lambda, f_1u_1\rangle =: h_1u_1, & \text{if } t>1.\end{cases}$$

According to PMP a minimal control must maximize $\hat{h}^t_{\tilde{u}}(\lambda)$. Given an extremal $\hat{\lambda}:[-1,2]\to T^*M$, let λ_0 and λ_1 be its restrictions to the intervals $[-1,2]$ and $[0,1]$. Since this family is linear in u_0 and u_1, λ_i must lie in the annihilators $A(N_i)$. In particular, if $\lambda:[0,1]\to T^*M$ was an extremal of the original problem such that $\gamma(t) = \pi(\lambda(t))$, $\forall t\in[0,1]$, we can extend λ to an extremal $\hat{\lambda}$ of problem (29)-(31) exactly as before:

$$\hat{\lambda}(t) = \begin{cases}\lambda(0), & \text{if } t<0,\\ \lambda(t), & \text{if } t\in[0,1],\\ \lambda(1), & \text{if } t>1.\end{cases}$$

Denote by $\hat{\Phi}_t$ the flow generated by $\hat{h}^t_{\tilde{u}}$, or more precisely

$$\hat{\Phi}_t = \begin{cases}\mathbb{I}, & \text{if } t<0,\\ \Phi_t, & \text{if } t\in[0,1],\\ \Phi_1 =: \Phi, & \text{if } t>1.\end{cases}$$

Since the vector field associated to $\tilde{u}$ is zero on $[-1,0]\cup[1,2]$ the flow is a constant transformation. Composing the Hamiltonian with the flow $\hat{\Phi}_t$ gives us

$$\hat{b}^t_{\hat{u}}(\lambda) = \left(\hat{h}_{\hat{u}} - \hat{h}_{\tilde{u}(t)}\right) \circ \hat{\Phi}_t(\lambda) = \begin{cases} \langle \lambda, f_0 u_0 \rangle, & \text{if } t < 0, \\ b^t_u(\lambda), & \text{if } t \in [0,1], \\ \langle \cdot\,, f_1 u_1 \rangle \circ \hat{\Phi}_1(\lambda), & \text{if } t > 1. \end{cases}$$

Then we can define

$$\hat{Z}_t = \partial_{\hat{u}} \overrightarrow{\hat{b}}{}^t_{\hat{u}}|_{\lambda=\lambda(0)}.$$

and denote Z_0 and Z_1 to be restrictions of $\hat{Z}_t$ to the time intervals $[-1,0]$ and $[1,2]$ correspondingly, so that

$$\hat{Z}_t = \begin{cases} Z_0, & \text{if } t < 0, \\ Z_t, & t \in [0,1], \\ Z_1, & \text{if } t > 1. \end{cases}$$

It is worth noting that Z_0 and Z_1 are constant, since $b^t_{\hat{u}}(\lambda)$ is linear in u_0 and u_1 for $t \in [0,1]^c$. Finally we can define the quadratic form

$$H_t = \left.\frac{\partial^2 \hat{b}^t_{\hat{u}}}{\partial \hat{u}^2}\right|_{\hat{u}=\tilde{u}}.$$

Note that since $b^t_{\hat{u}}$ is linear in the control parameters for $t \in [-1,0] \cup [1,2]$, we have $H_t \equiv 0$ on the two intervals.

Recall that $\Pi := \Pi_{\lambda_0}$ denotes the vertical subspace, namely the tangent space to fibre $T^*_q M$ described in equation (50). With the notation set above, the kernel of the differential of the endpoint mapping and the second variation are:

$$\ker d_{\tilde{u}} E = \left\{ \hat{v} \in \mathbb{R}^{\dim N_0} \oplus L^\infty([0,1], \mathbb{R}^k) \oplus \mathbb{R}^{\dim N_1} : \int_{-1}^{2} \hat{Z}_t \hat{v}(t) dt \in \Pi \right\}, \tag{34}$$

$$Q(\hat{v}, \hat{w}) = \int_{-1}^{2} \big[-H_t(\hat{v}(t), \hat{w}(t)) - \int_{-1}^{t} \sigma(\hat{Z}_\tau \hat{v}(\tau), \hat{Z}_t \hat{w}(t)) d\tau \big] dt, \tag{35}$$

where $\hat{v}, \hat{w} \in \ker d_{\tilde{u}} E$. We can expand the expressions for the first and second variations knowing the particular form of $\hat{Z}_t$. We split the integrals into three integrals over the intervals $[-1,0]$, $[0,1]$ and $[1,2]$ and simplify the integrands using the skew-symmetry of σ:

They read as:

$$\ker d_{\tilde{u}} E = \left\{ v \in L^\infty[0,1], v_i \in \mathbb{R}^{\dim N_i} : \int_0^1 Z_t v(t) dt + Z_0 v_0 + Z_1 v_1 \in \Pi \right\}, \tag{36}$$

$$Q(\hat{v}, \hat{w}) = \int_0^1 \Big[-H_t(v(t), w(t)) - \sigma \left(Z_0 v_0 + \int_0^t Z_\tau v(\tau), Z_t w(t) \right) d\tau \Big] dt - \sigma \left(Z_0 v_0 + \int_0^1 Z_t v(t) dt, Z_1 w_1 \right), \tag{37}$$

where we have used the fact that $\hat{Z}_t$ is constant for $t \in [0,1]^c$ and its image lies in a Lagrangian subspace, and hence $\sigma(\hat{Z}_t \hat{v}(t), \hat{Z}_\tau \hat{w}(\tau)) = 0$ for all $\tau, t \in [-1,0]$, all $\tau, t \in [1,2]$ and any variations $\hat{v}, \hat{w} \in \ker d_{\tilde{u}} E$.

We finish the discussion of the first and second variations with an important observation concerning $Z_i v_i$, $i = 0, 1$.

Lemma 4. *For any $v_0 \in \mathbb{R}^{\dim(N_0)}$ $Z_0 v_0$ is tangent to $A(N_0)$. Similarly, for any $v_1 \in \mathbb{R}^{\dim(N_1)}$, $\Phi_* Z_1 v_1$ is tangent to $A(N_1)$.*

Proof. By PMP the initial (and final) covector annihilates N_0 (resp. N_1).

Recall that f_{0i} generate the tangent space to N_0 close to q_0. We define the Hamiltonians

$$l_i(\lambda) = \langle \lambda, f_{0i} \rangle, \qquad i = 1, \dots, \dim N_0.$$

Then $A(N_0)$ can be equivalently described as the common part of the zero locus of l_i:

$$A(N_0) = \{\lambda \in T^*M : \pi(\lambda) \in N_0,\ l_i(\lambda) = 0,\ i = 1, \dots, \dim N_0\}.$$

But then by the definition of a Hamiltonian vector field

$$d_{\lambda(0)} l_i(Z_0 v_0) = d_{\lambda(0)} l_i(\vec{h}_0 v_0) = \sigma_{\lambda(0)}(\vec{h}_0 v_0, \vec{l}_i) = \langle \lambda(0), [f_0 v_0, f_{0i}] \rangle = 0,$$

where the last equality is due to involutivity of the family $f_0 v_0$.

Similarly, one has that $\Phi_* Z_1 u_1$ is always tangent to the image of $A(N_1)$. $\square$

3.3 Jacobi equation and second variation

Set $\mathcal{V} = \ker d_{\tilde{u}}E$. Inside $\mathcal{V}$ we consider the following subspace

$$\mathcal{V}_0 = \{\hat{v} \in \mathcal{V} : v_0 = 0, v_1 = 0\}. \tag{38}$$

$\mathcal{V}_0$ corresponds to the tangent space of the manifold of variations that fix the end-points q_0 and q_1 of an extremal curve γ. Hence $Q|_{\mathcal{V}_0}$ is the second variation of the optimal control problem with fixed end-points and there exist efficient ways of computing the index of this quadratic forms using generalisations of classical Jacobi fields [11, Section 21]. Our goal is to compute the difference

$$\operatorname{ind} Q - \operatorname{ind} Q|_{\mathcal{V}_0}$$

in terms of geometric objects on the manifold M, which will result in formula (16) when $N = N_0 \times N_1$. The main tool for computing the difference of indices is the following folklore lemma.

Lemma 5. *Suppose that Q is a continuous quadratic form on a Hilbert space $\mathcal{H}$. Then, for any subspace V of finite codimension it holds:*

$$\operatorname{ind} Q = \operatorname{ind} Q|_V + \operatorname{ind} Q|_{V^{\perp_Q}} + \dim\big(V \cap V^{\perp_Q}/(V \cap \ker Q)\big). \tag{39}$$

We will take $\mathcal{V}$ as Hilbert space and the second variation as Q. Thus

$$\mathcal{V}_0^{\perp_Q} = \{\hat{v} \in \mathcal{V} : Q(\hat{v}, \hat{w}) = 0, \forall \hat{w} \in \mathcal{V}_0\},$$

and the kernel of Q on $\mathcal{V}$ is

$$\ker Q = \{\hat{v} \in \mathcal{V} : Q(\hat{v}, \hat{w}) = 0, \forall \hat{w} \in \mathcal{V}\}.$$

Now, we reformulate each term appearing in (39) as a boundary value problem for a differential equation on $T_{\lambda_0}T^*M$. For $t \in [0,1]$, let H_t and Z_t be the matrices appearing in equations (34) and (35). *Jacobi equation* (see [11, Theorem 21.1]) is the following linear system:

$$\dot{\eta}(t) = Z_t H_t^{-1} \sigma(Z_t \cdot, \eta(t)), \quad \eta(t) \in T_{\lambda(0)}T^*M. \tag{40}$$

Proposition 4. *Consider system* (40). *To any solution η satisfying*

$$\pi_*\eta(0) \in T_{q_0}N_0, \quad \pi_*\eta(1) \in (\pi \circ P_{\tilde{u}}^{-1})_*(T_{q_1}A(N_1)),$$

we can associate an element $v \in \mathcal{V}_0^{\perp_Q}$. This correspondence is unique modulo solutions satisfying $\eta(0), \eta(1) \in \Pi$ and $\dot{\eta} = 0$. Moreover:

(i) elements in $\mathcal{V}_0 \cap \mathcal{V}_0^{\perp_Q}$ correspond to solutions of (40) *satisfying the boundary conditions:*

$$\eta(0) \in \Pi, \quad \eta(1) \in \Pi;$$

(ii) elements of $\ker Q \cap \mathcal{V}_0$ correspond to solutions satisfying the boundary conditions:

$$\eta(0) \in \Pi \cap T_{\lambda(0)}A(N_0), \quad \eta(1) \in \Pi \cap T_{\lambda(0)}\Phi_1^{-1}(A(N_1));$$

(iii) elements in $\ker Q$ correspond to solutions of (40) *satisfying the boundary conditions:*

$$\eta(0) \in T_{\lambda(0)}A(N_0), \quad \eta(1) \in T_{\lambda(0)}\Phi_1^{-1}(A(N_1)).$$

Proof. By definition, the subspace $\mathcal{V}_0$ is the set of infinitesimal variations $\hat{v} = (v_0, v, v_1)$ such that $\int_0^1 Z_t v(t)dt \in \Pi$ and $v_0 = 0$, $v_1 = 0$. Moreover, since Π is a Lagrangian subspace

$$\int_0^1 Z_t v(t)dt \in \Pi \iff \sigma\left(\int_0^1 Z_t v(t)dt, \nu\right) = 0, \forall\, \nu \in \Pi$$

and so:

$$\begin{aligned} \hat{v} \in \mathcal{V}_0^{\perp_Q} &\iff Q(\hat{v}, \hat{w}) = 0, \forall\, \hat{w} \in \mathcal{V}_0 \\ &\iff Q(\hat{v}, \hat{w}) = \int_{-1}^{2} \sigma(\nu, \hat{Z}_t \hat{w}(t))dt, \quad \forall \nu \in \Pi, \forall\, \hat{w} \in \mathcal{V}_0. \end{aligned}$$

Using the explicit formula for Q given in (37), we have that $\exists\, \nu \in \Pi$ such that, for almost every $t \in [0,1]$:

$$H_t(v(t), \cdot) + \sigma\left(\int_0^t Z_\tau v(\tau)d\tau + Z_0 v_0, Z_t \cdot\right) = \sigma(Z_t \cdot, \nu).$$

By the strong Legendre condition H_t is invertible. This allows us to solve the equation for the variation v and obtain

$$v(t) = H_t^{-1}\sigma\left(Z_t \cdot, \int_0^t Z_\tau v(\tau)d\tau + Z_0 v_0 + \nu\right). \tag{41}$$

Set

$$\eta(t) = \int_0^t Z_\tau v(\tau)d\tau + Z_0 v_0 + \nu. \tag{42}$$

Differentiating η and plugging in the expression for the variation v above, shows that η satisfies the following equation for almost all $t \in [0,1]$:

$$\dot\eta(t) = Z_t H_t^{-1}\sigma(Z_t \cdot, \eta(t)).$$

Using the definition of Z_0 and Lemma 4 we find that $\eta(t)$ satisfies (40) with $\pi_*\eta(0) \in T_{q_0}N_0$. Boundary conditions at $t = 1$ follow from the fact that $\hat v \in \mathcal{V}$. In fact, equation (36) implies that there exists $\xi \in \Pi$ such that:

$$\eta(1) = \int_0^1 Z_\tau v(\tau)d\tau + Z_0 v_0 + \nu = \xi + \nu - Z_1 v_1.$$

Thus a variation $\hat v \in \mathcal{V}_0^{\perp_Q}$ determines a function $\eta : [0,1] \to T_{\lambda(0)}(T^*M)$ which solves the following boundary value problem

$$\begin{cases} \dot\eta(t) = Z_t H_t^{-1}\sigma(Z_t \cdot, \eta(t)), \\ \pi_*\eta(0) \in T_{q_0}N_0, \quad \pi_*\eta(1) \in \pi_*(T_{\lambda(0)}\Phi_1^{-1}A(N_1)). \end{cases} \tag{43}$$

Notice that the second space appearing as boundary condition is the image of the tangent space of N_1 at q_1 through the differential of flow generated by the optimal control $\tilde u$. From (43) we can compute the dimension of $\mathcal{V}_0 \cap \mathcal{V}_0^{\perp_Q}$. If we substitute $v_i = 0$ in the above equations, we get solutions starting from Π and arriving to Π. Since the Jacobi equation derived above is exactly the same as the Jacobi equation for problem with fixed points, we immediately see that $\dim(\mathcal{V}_0 \cap \mathcal{V}_0^{\perp_Q})$ is the multiplicity of the point q_1 as conjugate point.

In a similar fashion we can compute the dimension of $\ker Q \cap \mathcal{V}_0$ We have

$$\ker Q \cap \mathcal{V}_0 = \{\hat v \in \mathcal{V}_0 : Q(\hat v, \hat w) = 0,\ \forall \hat w \in \mathcal{V}\}.$$

Using the same argument as above we find that for every $\nu \in \Pi$

$$\begin{cases} 0 = \sigma(Z_0 \cdot, \nu) \\ Q(v, \cdot) = \sigma(Z_t \cdot, \nu) \\ \sigma\left(\int_0^1 Z_t v(t)dt, Z_1 \cdot\right) = \sigma(Z_1 \cdot, \nu) \end{cases}$$

The second equation tells us that we are dealing with a solution of equation (43). The first equality gives us a condition on ν and consequently on $\eta(0)$, while the third condition give us a condition for $\eta(1)$. Namely:

$$\eta(0) \in \Pi \cap T_{\lambda(0)}A(N_0), \qquad \eta(1) \in \Pi \cap T_{\lambda(0)}(\Phi_1^{-1}A(N_0)).$$

This settles points (i) and (ii). Point (iii) follows similarly.

Up until now, we have built linear maps from $\mathcal{V}_0^{\perp_Q}, \ker Q, \mathcal{V}_0^{\perp_Q} \cap \mathcal{V}_0$ and $\mathcal{V}_0^{\perp_Q} \cap \ker Q$ to suitable subspaces of solution of (40). Now we have to prove that these correspondences are actually bijections. Let us prove injectivity. Suppose that $\hat v$ is mapped to the zero solution of equation (40). It follows, by the injectivity of Z_0 and Z_1 that v_0 and v_1 are both zero. Moreover $\dot\eta(t) = Z_t v(t) = 0$ and consequently, by definition of $\mathcal{V}_0^{\perp_Q}$,

$$0 = Q(\hat v, \hat w) = \int_0^1 H_t(v(t), w(t))dt, \qquad \forall \hat w \in V.$$

In particular $H_t(v(t), v(t)) = 0$ for almost every $t \in [0,1]$. But then by the strong Legendre condition $v = 0$ and thus $\hat v = 0$.

Now we try to invert the correspondence control-solution. Suppose that $\eta(t)$ is a solution of equation (43). We can define a function $v(t)$ using (41), namely:

$$v(t) := H_t^{-1}\sigma(Z_t \cdot, \eta(t)).$$

The initial and final boundary conditions of equation (43) implies that there are unique v_0 and v_1 such that $\eta(0)-Z_0v_0$ and $\eta(1)-Z_1v_1$. Set $\xi(t)=\int_0^t Z_\tau v_\tau+Z_0u_0+\nu$ for $\nu\in\Pi$. Differentiating the function $\eta(t)-\xi(t)$ yields that ν is determined up to constant solutions starting from the fibre. Hence the correspondence solution-control is injective if and only if there are no constant solutions in the fibre.

□

As before, let Ψ be the differential of the Hamiltonian flow given in equation (15) and $\Gamma(\Psi)$ the graph of Ψ.

Remark 7. It can be shown that (40) is closely related to the linearisation of the extremal flow along the fixed extremal λ we are considering, see for example [12]. It is the linearisation at $\lambda(0)$ of the Hamiltonian flow of $b^t_{\tilde{u}}(\lambda)=(H-h_{\tilde{u}(t)})\circ\Phi_t(\lambda)$ which coincides with the linearisation of $(\Phi_t)^{-1}\circ e^{tH}$. Let us denote by Θ_J the flow of the Jacobi equation (40) at time one and let

$$\Gamma(\Theta_J)=\{(\eta(0),\eta(1)):\eta(0)\in T_{\lambda(0)}(T^*M)\}\subset T_{\lambda(0)}(T^*M)\times T_{\lambda(0)}(T^*M)$$

be its graph. Then in this notation

$$\Gamma(\Psi)=(I\times\Phi_1)_*\Gamma(\Theta_J).$$

We can now compute the restriction of Q to $\mathcal{V}_0^{\perp_Q}$ and prove the following result.

Proposition 5. *Let Q be the quadratic form of second variation for the problem* (29)-(31) *and $\mathcal{V}_0$ be the subspace of variations defined in* (38)*. Then*

$$\operatorname{ind}^- Q=\operatorname{ind}^- Q|_{\mathcal{V}_0}+i\big(\Pi^2_{\underline{\lambda}},\Gamma(\Psi),T_{\underline{\lambda}}A(N)\big)+\dim(\Gamma(\Psi)\cap\Pi^2_{\underline{\lambda}})-\dim(\Gamma(\Psi)\cap\Pi^2_{\underline{\lambda}}\cap T_{\underline{\lambda}}A(N))$$

Moreover, the Maslov index of the triple can be replaced by $i\big((\Pi^2_{\underline{\lambda}})^W,\Gamma(\Psi)^W,T_{\underline{\lambda}}A(N)^W\big)$ where $W=T_{\underline{\lambda}}A(N)\cap\Pi^2_{\underline{\lambda}}$ and the superscript means everything is computed on the space reduced by W.

Proof. In view of Proposition 4 and Remark 7 it only remains to prove that

$$\operatorname{ind}^- Q_{\mathcal{V}_0^{\perp_Q}}=i\big(\Pi^2_{\underline{\lambda}},\Gamma(\Psi),T_{\underline{\lambda}}A(N)\big).$$

Since $(v_0,v,v_1)\in\mathcal{V}_0^{\perp_Q}$, we have that:

$$\int_0^1\left[H_t(v,w)+\sigma\left(Z_0v_0+\int_0^t Z_\tau v(\tau)d\tau,Z_tw(t)\right)\right]dt=\sigma\left(\int_0^1 Z_tw(t)dt,\nu\right),\quad\forall w\in L^2[0,1],\forall\nu\in\Pi,$$
$$Z_0v_0+Z_1v_1+\int_0^1 Z_tv(t)dt=\xi\in\Pi.$$

Combining these expressions with (37) gives us:

$$\begin{aligned}Q(\hat{v})&=-\sigma\left(Z_0v_0+\int_0^1 Z_tv(t)dt,Z_1v_1\right)-\sigma\left(\int_0^1 Z_tv(t)dt,\nu\right)\\&=-\sigma(\xi,Z_1v_1)+\sigma(Z_1v_1+Z_0v_0,\nu)\\&=-\sigma(\nu,Z_0v_0)+\sigma(\xi+\nu,-Z_1v_1)\end{aligned}\tag{44}$$

From (42) follows that:

$$\eta(0)=\nu+Z_0v_0\quad\eta(1)=\nu+Z_0v_0+\int_0^1 Z_tv(t)dt=\nu+\xi-Z_1v_1.$$

Hence the restriction of Q to $\mathcal{V}_0^{\perp Q}$ coincides with the quadratic form

$$m\big(\Pi^2,\Gamma(\Theta_J),T_{\lambda(0)}A(N_0)\times T_{\lambda(0)}(\Phi_1^{-1}A(N_1))\big).$$

Note that Z_0v_0 do not span the whole $T_{\lambda(0)}A(N_0)$ and correspondingly Z_1v_1 does not span $T_{\lambda(0)}(\Phi_t^{-1}A(N_1))$. Nevertheless we obtain the correct Maslov form. In fact, the map $Z_0:\mathbb{R}^k\to T_{\lambda(0)}A(N_0)$ is injective and its image is transversal to $\Pi\cap T_{\lambda(0)}A(N_0)$ (and the same is true for the Z_1). Hence $\operatorname{im}Z_0+\Pi=T_{\lambda(0)}A(N_0)+\Pi$ (and similarly for Z_1). Moreover, we can either reduce by $W=\Pi\cap T_{\lambda(0)}A(N_0)\oplus\Pi\cap T_{\lambda(0)}(\Phi_t^{-1}A(N_1))$ or work on the original space. The index is the same since $W\subseteq\ker m$.

We now apply the map $I\times(\Phi_1)_*$ to each Lagrangian space inside the Maslov index of the triple above. By Remark 7 and invariance with respect to symplectomorphism we get

$$i\big(\Pi^2,\Gamma(\Theta_J),T_{\lambda(0)}A(N_0)\times T_{\lambda(0)}(\Phi_1^{-1}A(N_1))\big)=i\big(\Pi^2_{\underline{\lambda}},\Gamma(\Psi),T_{\underline{\lambda}}A(N)\big).$$

□

3.4 Proof of Theorem 1

Before proving the general formula, we prove a corollary of Proposition 5. Assume that we have an optimal control problem (7)-(8) and two sets of possible boundary conditions:

$$(q(0), q(1)) \in N_0 \times N_1 =: N$$

and

$$(q(0), q(1)) \in \tilde{N}_0 \times \tilde{N}_1 =: \tilde{N}.$$

and assume that a curve $\lambda : [0,1] \to TM$ is an extremal for both problems. This amounts to say that λ is a solution of the Hamiltonian system of PMP and satisfies the transversality conditions for both boundary conditions at the same time, i.e. λ_i annihilates the sum $T_{\lambda_i} N_i + T_{\lambda_i} \tilde{N}_i$. A relevant example to keep in mind is when $N \subset \tilde{N}$. In this case if λ satisfies the transversality conditions for $\tilde{N}$, then it automatically satisfies the transversality conditions for N.

Consider the two second variations Q_N and $Q_{\tilde{N}}$, corresponding to the two optimal control problems with boundary conditions like above. We apply Proposition 5 to express the difference between the Morse indices of those two quadratic forms.

Corollary 1. *Using the notations just introduced, the following formula holds:*

$$\begin{aligned} \operatorname{ind}^- Q_{\tilde{N}} - \operatorname{ind}^- Q_N = {} & i\big(T_{\underline{\lambda}} A(N), \Gamma(\Psi), T_{\underline{\lambda}} A(\tilde{N})\big) + \dim(\Gamma(\Psi) \cap T_{\underline{\lambda}} A(N)) + \\ & - \dim(\Gamma(\Psi) \cap T_{\underline{\lambda}} A(N) \cap T_{\underline{\lambda}} A(\tilde{N})) + \dim(T_{\pi(\underline{\lambda})} N \cap T_{\pi(\underline{\lambda})} \tilde{N}) - \dim T_{\pi(\underline{\lambda})} N. \end{aligned} \tag{45}$$

Proof. Apply Proposition 5 to get an expression for $\operatorname{ind}^- Q_{\tilde{N}}$ and $\operatorname{ind}^- Q_N$. Subtracting them gives

$$\begin{aligned} \operatorname{ind}^- Q_{\tilde{N}} - \operatorname{ind}^- Q_N = {} & i\big(\Pi^2_{\underline{\lambda}}, \Gamma(\Psi), T_{\underline{\lambda}} A(\tilde{N})\big) - i\big(\Pi_{\underline{\lambda}}, \Gamma(\Psi), T_{\underline{\lambda}} A(N)\big) + \\ & + \dim(\Gamma(\Psi) \cap \Pi_{\underline{\lambda}} \cap T_{\underline{\lambda}} A(N)) - \dim(\Gamma(\Psi) \cap \Pi_{\underline{\lambda}} \cap T_{\underline{\lambda}} A(\tilde{N})) \end{aligned}$$

Apply formula (55) with $L_0 = \Pi^2_{\underline{\lambda}}$, $L_1 = \Gamma(\Psi)$, $L_2 = T_{\underline{\lambda}} A(\tilde{N})$ and $L_3 = T_{\underline{\lambda}} A(N)$. After cancellations this results in

$$\begin{aligned} \operatorname{ind}^- Q_{\tilde{N}} - \operatorname{ind}^- Q_N = {} & i\big(\Gamma(\Psi), T_{\underline{\lambda}} A(\tilde{N}), T_{\underline{\lambda}} A(N)\big) - i\big(\Pi^2_{\underline{\lambda}}, T_{\underline{\lambda}} A(\tilde{N}), T_{\underline{\lambda}} A(N)\big) + \\ & + \dim(\Gamma(\Psi) \cap T_{\underline{\lambda}} A(N)) - \dim(\Gamma(\Psi) \cap T_{\underline{\lambda}} A(N) \cap T_{\underline{\lambda}} A(\tilde{N})) - \\ & - \dim(\Pi^2_{\underline{\lambda}} \cap T_{\underline{\lambda}} A(\tilde{N})) + \dim(\Pi^2_{\underline{\lambda}} \cap T_{\underline{\lambda}} A(N) \cap T_{\underline{\lambda}} A(\tilde{N})). \end{aligned}$$

We simplify the terms different to $\dim(\Gamma(\Psi) \cap T_{\underline{\lambda}} A(N))$, $\dim(\Gamma(\Psi) \cap T_{\underline{\lambda}} A(N) \cap T_{\underline{\lambda}} A(\tilde{N}))$, which appear in the formula in the statement.

By formula (56) it follows

$$i\big(\Gamma(\Psi), T_{\underline{\lambda}} A(\tilde{N}), T_{\underline{\lambda}} A(N)\big) = i\big(T_{\underline{\lambda}} A(N), \Gamma(\Psi), T_{\underline{\lambda}} A(\tilde{N})\big).$$

By lemma 7 we have

$$i\big(\Pi^2_{\underline{\lambda}}, T_{\underline{\lambda}} A(\tilde{N}), T_{\underline{\lambda}} A(N)\big) = i\big(T_{\underline{\lambda}} A(N), \Pi^2_{\underline{\lambda}}, T_{\underline{\lambda}} A(\tilde{N})\big) = 0.$$

Finally, straight from the definition of an annihilator, it follows that

$$\dim(\Pi^2_{\underline{\lambda}} \cap T_{\underline{\lambda}} A(\tilde{N})) = 2 \dim M - \dim T_{\pi(\underline{\lambda})} \tilde{N}$$

and

$$\dim(\Pi^2_{\underline{\lambda}} \cap T_{\underline{\lambda}} A(N) \cap T_{\underline{\lambda}} A(\tilde{N})) = 2 \dim M - \dim T_{\pi(\underline{\lambda})} \tilde{N} - \dim T_{\pi(\underline{\lambda})} N + \dim(T_{\pi(\underline{\lambda})} N \cap T_{\pi(\underline{\lambda})} \tilde{N}).$$

Combining all of the above results in formula (45).

□

Remark 8. Notice that if $N = \{q_0\} \times \{q_1\}$ we obtain exactly the formula from Proposition 4, as expected. Another necessary remark is that formula (45) might seem asymmetric at first. We expect, that if we exchange N and $\tilde{N}$, then the resulting right-hand side will change sign. This is not entirely obvious just from the expression itself. However, this is indeed the case. The difference between $i\big(T_{\underline{\lambda}} A(N), \Gamma(\Psi), T_{\underline{\lambda}} A(\tilde{N})\big)$ and $i\big(T_{\underline{\lambda}} A(\tilde{N}), \Gamma(\Psi), T_{\underline{\lambda}} A(N)\big)$ is not zero, but an expression involving dimensions of intersections of various subspaces as can be seen from formula (55).

Now we are ready to prove Theorem 1. We will reduce the case of general boundary conditions $(q_0, q_1) \in N \subseteq M \times M$ to the case with separated boundary conditions by introducing extra dummy variables.

Proof of Theorem 1. Consider optimal control problem (7)-(9). We can lift it to an optimal problem on $M \times M$ by considering a new control system:

$$\begin{cases} \dot{x} = 0, \\ \dot{q} = f^t_{u(t)}(q), \end{cases} \tag{46}$$

with boundary conditions

$$(x(0), q(0), x(1), q(1)) \in \Delta \times N \subset M^4. \tag{47}$$

There is a one-to-one correspondence between admissible curves of (7)-(9) and admissible curves of (46)-(47). For this reason we can consider admissible curves (46)-(47) which minimize the functional (9). The Hamiltonian system of PMP is then given by

$$\begin{cases} \dot{\mu} = 0, \\ \dot{\lambda} = \vec{H}^t(\lambda), \end{cases} \qquad \lambda, \mu \in T^*M$$

and its flow is given by $I \times \Psi_t$.

We can now apply directly Corollary 1 to the boundary conditions $\Delta \times \tilde{N}$ and $\Delta \times N$. In order to see that everything indeed reduces to formula (16), we show how to rewrite each term of (45), without writing explicitly the lengthy formula here. Let us go term by term starting from the ones involving dimensions. Let $\underline{\lambda} = (-\lambda(0), \lambda(0), -\lambda(0), \lambda(1))$, initial and final point of the extremal lift. We have

$$\begin{aligned} &\dim\Big(T_{\pi(\underline{\lambda})}(\Delta \times N) \cap T_{\pi(\underline{\lambda})}(\Delta \times \tilde{N})\Big) - \dim\big(T_{\pi(\underline{\lambda})}(\Delta \times N)\big) = \\ &= \dim T_{\pi(\underline{\lambda})}\Delta + \dim(T_{\pi(\underline{\lambda})}N \cap T_{\pi(\underline{\lambda})}\tilde{N}) - \dim T_{\pi(\underline{\lambda})}\Delta - \dim T_{\pi(\underline{\lambda})}N = \dim(T_{\pi(\underline{\lambda})}N \cap T_{\pi(\underline{\lambda})}\tilde{N}) - \dim T_{\pi(\underline{\lambda})}N. \end{aligned}$$

We wish to work on the same symplectic space $T_{\lambda_0}T^*M$. Thus we perform the following change of coordinates $S : (\lambda, \eta) \mapsto (-\lambda, \eta)$ on T^*M. This changes the sign of the symplectic form: we will work with $(-\sigma) \oplus \sigma$. Moreover, this change of coordinates maps

$$A(N) = \{(\lambda_0, \lambda_1) : \langle \lambda_0, X_0 \rangle + \langle \lambda_1, X_1 \rangle = 0, \forall (X_0, X_1) \in TN\}$$

to the submanifold:

$$SA(N) = \{(\lambda_0, \lambda_1) : \langle \lambda_0, X_0 \rangle = \langle \lambda_1, X_1 \rangle, \forall (X_0, X_1) \in TN\},$$

we will have to use the latter in the formulas.

Let us write down explicitly each individual subspace entering the formula.

$$\begin{aligned} T_{\underline{\lambda}}SA(\Delta \times N) &= \{(\xi, \xi, \nu_1, \nu_2) : \xi \in \Sigma, (\nu_1, \nu_2) \in T_{\underline{\lambda}}SA(N)\}, \\ T_{\underline{\lambda}}SA(\Delta \times \tilde{N}) &= \{(\tilde{\xi}, \tilde{\xi}, \tilde{\nu}_1, \tilde{\nu}_2) : \tilde{\xi} \in \Sigma, (\tilde{\nu}_1, \tilde{\nu}_2) \in T_{\underline{\lambda}}SA(\tilde{N})\}, \\ \Gamma(I \times \Psi) &= \{(\eta_1, \eta_2, \eta_1, \Psi\eta_2) : \eta_1, \eta_2 \in \Sigma\}. \end{aligned} \tag{48}$$

Notice that we used that $\{(S\xi, S\xi) : \xi \in T_{\lambda(0)}T^*M\} = \Gamma(I)$ in the last identification. From the expressions in (48) it follows directly that

$$\begin{aligned} \dim(\Gamma(I \times \Psi) \cap T_{\underline{\lambda}}A(\Delta \times N)) &= \dim(\Gamma(\Psi) \cap T_{\underline{\lambda}}A(N)) \\ \dim(\Gamma(I \times \Psi) \cap T_{\underline{\lambda}}A(\Delta \times N) \cap T_{\underline{\lambda}}A(\Delta \times \tilde{N})) &= \dim(\Gamma(\Psi) \cap T_{\underline{\lambda}}A(N) \cap T_{\underline{\lambda}}A(\tilde{N})). \end{aligned}$$

In order to simplify the Maslov index term, we note that the intersection of annihilators contains the following isotropic subspace

$$W = \{(\xi, \xi, 0, 0) : \xi \in T_{\lambda(0)}T^*M\}.$$

We can thus perform a reduction to the space $W^\perp/W$. We have

$$W^\perp = \{(\zeta, \zeta, \xi, \eta) : \zeta, \xi \in T_{\lambda(0)}T^*M, \eta \in T_{\lambda(1)}T^*M\}.$$

Thus we can identify $W^\perp/W$ with the image of the projection

$$\pi_1 : \big(T_{\lambda(0)}T^*M\big)^3 \oplus T_{\lambda(1)}T^*M \to T_{\lambda(0)}T^*M \oplus T_{\lambda(1)}T^*M$$

to the symplectic space $(T_{\lambda(0)}T^*M \oplus T_{\lambda(1)}T^*M, (-\sigma_{\lambda(0)}) \oplus \sigma_{\lambda(1)})$. Let us consider the space $(W^\perp + W) \cap \Gamma(I \times \Theta)$, it is straightforward to check that it projects to $\{(\eta, \Psi\eta) : \eta \in \Sigma\}$. Hence:

$$i\big(T_{\underline{\lambda}}SA(\Delta \times N), \Gamma(I \times \Psi), T_{\underline{\lambda}}SA(\Delta \times \tilde{N})\big) = i\big(T_{\underline{\lambda}}SA(N), \Gamma(\Psi), T_{\underline{\lambda}}SA(\tilde{N})\big).$$

$\square$

A Appendix

A.1 Symplectic geometry

A *symplectic* vector space is a finite dimensional vector space Σ with a non degenerate skew-symmetric bilinear form σ (the *symplectic form*). A *symplectic* manifold M, is a manifold whose tangent space TM is endowed with a symplectic structure at each point (i.e M together with a closed non degenerate $2-$form).

Cotangent spaces of smooth manifolds are always endowed with a symplectic structure which is given by the so called *tautological* form. Call $\pi : T^*M \to M$ the canonical projection. Take $\lambda \in T^*M$ and define the $1-$form $s_\lambda(X) = \lambda(\pi_* X)$. One can check that ds is non degenerate and thus (T^*M, ds) is a symplectic manifold. The $2-$form $\sigma = ds$ on T^*M is called the *canonical symplectic form.*

A linear map Ψ between symplectic vector spaces $(\Sigma_1, \sigma_1) \to (\Sigma_2, \sigma_2)$ is called a (*linear*) symplectomorphism if $\Psi^*\sigma_2 = \sigma_1$. A diffeomorphism is a symplectomorphism if its differential is a linear symplectomorphism.

A natural way to obtain diffeomorphisms is trough flows. Given a (complete) vector field X one obtains a family of diffeomorphisms Φ_t by solving the ODE system

$$\begin{aligned} \dot{\Phi}_t &= X(\Phi_t), \\ \Phi_0 &= Id. \end{aligned}$$

In a similar way one can produce symplectomorphisms using special classes of vector fields: *Hamiltonian* and *symplectic* fields. A vector field X, is *Hamiltonian* if there is a smooth function H such that $dH(Y) = \sigma(Y, X)$ for all smooth vector fields Y. H is called *Hamiltonian* function and X is often denoted by $\vec{H}$. A vector field for which we can find a Hamiltonian only locally, i.e. in a neighbourhood of every point, is called *symplectic.* The flow of Hamiltonian and symplectic vector fields is always a one parameter group of symplectomorphisms.

Given a subspace W of a symplectic vector space Σ, we can define its skew-orthogonal complement $W^\perp$ using the symplectic form.

$$W^\perp = \{u \in \Sigma : \sigma(u, w) = 0, \, \forall w \in W\}.$$

Since the symplectic form is non degenerate, $\dim(W) + \dim(W^\perp) = \dim(\Sigma)$ and $(V + W)^\perp = V^\perp \cap W^\perp$.

Inside a symplectic vector space we distinguish the following classes of subspaces:

- **Isotropic** V such that $\sigma(v, w) = 0$, $\forall u, v \in V$, i.e. $V \subseteq V^\perp$;
- **Lagrangian** V isotropic and maximal, i.e. $V = V^\perp$;
- **Coisotropic** V such that $V^\perp \subseteq V$.

Lagrange subspaces are extremely important in symplectic geometry, their collection is a compact manifold called Lagrange Grassmannian. It is denoted by

$$Lag(\Sigma) = \{V \subseteq \Sigma : V = V^\perp\}.$$

If $\dim(\Sigma) = 2n$ its dimension is $n(n+1)/2$.

The following examples of Lagrangian subspaces are often considered:

Example 1. If Ψ is a linear symplectomorphism then the graph of Ψ is a subspace of the product space $\Sigma_0 \bigoplus \Sigma_1$. The product space can be endowed with a symplectic structure considering $(-\sigma_0) \oplus \sigma_1$. Graphs of symplectomorphisms are always Lagrangian subspaces with this choice.

Example 2. If $N \subseteq M$ is a submanifold of a smooth manifold then we can always consider the following submanifold of the cotangent bundle T^*M:

$$A(N) := \{\lambda \in T^*M : \pi(\lambda) \in N, \lambda(X) = 0, \, \forall \, X \in T_{\pi(\lambda)}N\}. \tag{49}$$

The tangent space to the annihilator at a point λ is a Lagrangian subspace of $T_\lambda(T^*M)$, which means that $A(N)$ is a Lagrangian submanifold.

If M is a product space i.e. $M = M_0 \times M_1$, the annihilator of a submanifold N is a Lagrangian submanifold only with respect to $\sigma_0 \oplus \sigma_1$, which coincides with the canonical symplectic form on $T^*(M_0 \times M_1)$.

To get a Lagrangian submanifold of $(T^*M_0 \oplus T^*M_1, (-\sigma_0) \oplus \sigma_1)$ one has to change the sign to the first or the second covector and thus consider the submanifold $A(N)$ defined in (11). Notice that this distinction is unnecessary when N itself is a product, i.e. when $N = N_0 \times N_1$.

Example 3. A particular instance of the example above is the vertical fibre i.e. the tangent space to T_q^*M. This space can be characterized as the annihilator of the point q or as the kernel of the natural projection, $\ker \pi_*$:

$$\Pi_\lambda = \{\xi \in T_\lambda(T^*M) : \pi_*(\xi) = 0\}. \tag{50}$$

Example 4. Consider as symplectic space $\mathbb{R}^{2n} = \{x = (p, q) : p, q \in \mathbb{R}^n\}$ with the *canonical* symplectic form $\sigma(x, x') = \langle p, q' \rangle - \langle q, p' \rangle$. Using the Euclidean scalar product we can represent σ as:

$$\sigma(x, x') = \langle Jx, x' \rangle \quad \text{where} \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{51}$$

The two subspaces $B = \{p = 0\}$ and $\Pi = \{q = 0\}$ are Lagrangian and any subspace of the form $V_S = \{(q, Sq)\}$ and $V'_S = \{(Sp, p)\}$ is Lagrangian provided that $S = S^*$.

It turns out that if we take two transversal Lagrangian subspaces L_0 and L_2 there always exists a choice of basis, for which L_0 is B and L_2 is Π, and such that the symplectic form σ has the canonical form as in equation (51) (see [26, Theorem 1.15]). These coordinates are sometimes called *Darboux* or *symplectic*.

Using these coordinates we can build charts for the Lagrange Grassmannian $Lag(\Sigma)$. The map $S \mapsto V_S$ from the space of symmetric matrices to $Lag(\Sigma)$ maps onto the set of planes transversal to Π (see for example [26] for details).

A.2 Intersection index of Lagrangian subspaces

It is well known that the all pairs of transversal Lagrangian subspaces can be mapped to each other with a linear symplectomorphism [26, Theorem 1.15]. This is no longer true for a triple of Lagrangian subspaces.

Definition 1 (Maslov index)**.** Take three Lagrangian subspaces L_0, L_1, L_2. Consider the isotropic subspace $L'_1 := L_1 \cap (L_0 + L_2)$, if $l_1 \in L'_1$ then $l_1 = l_0 + l_2$ with $l_i \in L_i$. The following quadratic form is called the Maslov form of the triple (L_0, L_1, L_2):

$$m(l'_1) = \sigma(l_0, l_2).$$

By a slight abuse of notation we will also write $m(L_0, L_1, L_2)$ instead of just m when we want to be explicit about which Lagrangian subspaces are used.

The numbers $\operatorname{ind}^+ m$, $\operatorname{ind}^- m$ and $sg\, m$ and $\dim\ker m$ are invariants of the triple (L_0, L_1, L_2). The *Kashiwara index* is the signature of the Maslov form:

$$\tau(L_0, L_1, L_2) = sg\, m = \operatorname{ind}^+ m - \operatorname{ind}^- m.$$

The *negative Maslov index* is defined as

$$i\big(L_0, L_1, L_2\big) = \operatorname{ind}^- m.$$

Example 5. Suppose L_0 and L_2 are transversal. We can identify the symplectic space with the standard one $(\mathbb{R}^{2n}, \sigma)$ as given in equation (51). Since any couple of Lagrangian subspaces can be mapped into each other, we can find a symplectomorphism which simultaneously maps L_0 to B and L_2 to Π.

Any L_1 can be represented as $L_1 = \{Aq + Cp = 0, q \in B, p \in \Pi\}$ where $AC^* = CA^*$ and $rank[A, C] = n$. If A or C is invertible then the matrix expression of the Maslov form is given by $-A^{-1}C$ or $C^{-1}A$ respectively, which have the same signature of $\mp AC^*$.

The Kashiwara index and the Maslov index have the following properties:

- **Alternating** $\tau(L_{s(0)}, L_{s(1)}, L_{s(2)}) = (-1)^{sg(s)}\tau(L_0, L_1, L_2)$, where s is a permutation.
- **Cocycle property** [26, Theorem 1.32]

$$\tau(L_0, L_1, L_2) - \tau(L_1, L_2, L_3) + \tau(L_0, L_2, L_3) - \tau(L_0, L_1, L_3) = 0. \tag{52}$$

- **Relation between the negative index** [7, Lemma 5]

$$\begin{aligned} \tau(L_0, L_1, L_2) &= -2\, i(L_0, L_1, L_2) + \dim(L_1 \cap (L_0 + L_2)) - \dim\ker m \\ &= -2\, i(L_0, L_1, L_2) + n - \dim(L_0 \cap L_2) - \dim(L_0 \cap L_1) \\ &\quad - \dim(L_1 \cap L_2) + 2\dim(L_0 \cap L_1 \cap L_2). \end{aligned} \tag{53}$$

- **Symplectic reduction** If $V \subseteq L_0 \cap L_2$ is an isotropic subspace we can consider $L^V := (L \cap V^\perp + V)/V$ which is a Lagrangian subspace of the reduced space. It holds that:

$$i\big(L_0, L_1, L_2\big) = i\big(L_0^V, L_1^V, L_2^V\big) \tag{54}$$

The Maslov index satisfies only a *generic* cocycle property. The next lemma will be used in the proof of Theorem 1 and shows that the defect of being a cocycle is measured by the intersections of the four Lagrangian subspaces one considers.

Lemma 6. *The following formulas hold:*

$$\begin{aligned}\sum_{i=0}^{3}(-1)^{i+1} i\big(L_0,\dots,\hat{L}_i,\dots L_3\big) = \dim(L_1\cap L_3) - \dim(L_0\cap L_2) + \\ + \sum_{i=0}^{3}(-1)^{i+1}\dim(L_0\cap\cdots\cap\hat{L}_i\cap\cdots\cap L_3).\end{aligned} \tag{55}$$

$$i\big(L_0,L_1,L_2\big) = i\big(L_1,L_2,L_0\big) = i\big(L_2,L_0,L_1\big). \tag{56}$$

Proof. The proof is just a computation using equations (52) and (53). First apply (53) to express the index in terms of the signature and the dimensions of some intersections. Then use (52) to cancel the signature part.

The dimensions of the intersections of couple of subspaces, after the summation, give the following contribution:

$$2\Big(\dim(L_1\cap L_3) - \dim(L_0\cap L_2)\Big).$$

The triple intersection do not simplify and thus their coboundary appears. Sometimes it is useful to think of this remainder as the difference of the dimensions of two quotient spaces. $L_1\cap L_3$ in which we factor out the space $L_1\cap L_3\cap L_0 + L_1\cap L_3\cap L_0$ and $L_0\cap L_2$ quotient by $L_0\cap L_2\cap L_1 + L_0\cap L_2\cap L_3$.

Finally (56) follows from (55) choosing $L_3 = L_0$.

□

The following lemma will be used in the sequel.

Lemma 7. *Given the standard symplectic structure $(\Sigma,\sigma) = (T_\lambda(T^*M), ds_\lambda)$ and three submanifolds $N_0,N_1,N_2\subset M$. Assume that $\lambda\in A(N_0)\cap A(N_1)\cap A(N_2)$ and $N_1\subseteq N_0$ (or $N_1\subseteq N_2$) , then the following formula holds*

$$m\big(T_\lambda A(N_0), T_\lambda A(N_1), T_\lambda A(N_2)\big) \equiv 0.$$

Moreover if $M = M'\times M'$, T^*M is endowed with the form $(-\sigma')\oplus\sigma'$ and $A(N_i)$ are defined as in equation (11)*, the same is true.*

Proof. Let $L_0 = T_\lambda A(N_0)$, $L_1 = T_\lambda A(N_1)$ and $L_2 = T_\lambda A(N_2)$. Fix some coordinates in a neighbourhood of λ such that ds_λ is the standard form on $\mathbb{R}^{2n}\simeq T_\lambda(T^*M)$. The subspace L_0+L_2 is the space:

$$\begin{pmatrix}\nu_0\\ X_0\end{pmatrix} + \begin{pmatrix}\nu_2\\ X_2\end{pmatrix}, \qquad X_i\in T_{\pi(\lambda)}N_i, \qquad \nu_i(T_{\pi(\lambda)}N_i) = 0,$$

for $i = 0,2$. Since the sum above should lie in $L_1\cap(L_0+L_2)$, we have that $X_0+X_2 = X_1\in T_{\pi(\lambda)}N_1$ and $\nu_0+\nu_2 = \nu_1$, with ν_1 such that $\nu_1(T_{\pi(\lambda)}N_1) = 0$. If we compute now the Maslov form, we get:

$$\left\langle J\begin{pmatrix}\nu_0\\ X_0\end{pmatrix}, \begin{pmatrix}\nu_2\\ X_2\end{pmatrix}\right\rangle = \langle\nu_0, X_2\rangle - \langle\nu_2, X_0\rangle.$$

Suppose without loss of generality that $N_1\subseteq N_0$. The equation $X_0+X_2 = X_1$ implies that $X_2 = X_1 - X_0\in T_{\pi(\lambda)}N_0$ and thus $\langle\nu_0, X_2\rangle = 0$. Therefore the quadratic form is the zero form since:

$$\langle\nu_2, X_0\rangle = \langle\nu_2, X_0+X_2\rangle = \langle\nu_2+\nu_0, X_0+X_2\rangle = \langle\nu_1, X_1\rangle = 0.$$

For the second part, we work on the cotangent bundle of $M = M'\times M'$ which is isomorphic to $T^*M'\times T^*M'$. Label the coordinates as (λ_0,λ_1), call the standard form on T^*M', σ' and consider the following diffeomorphism:

$$S : (\lambda_0,\lambda_1)\mapsto(-\lambda_0,\lambda_1).$$

It is straightforward to check that $S^*(\sigma'\oplus\sigma') = (-\sigma')\oplus\sigma'$ and S maps $A(N_i)$ as given in equation (49) to the corresponding $A(N_i)$ as given by equation (11). Since Maslov index is invariant with respect to the action of symplectomorphisms, the statement follows.

□

A.3 Hermitian Maslov index

In the proof of Iteration Formulae it will be convenient to introduce complex coefficients and work on $\mathbb{C}^{2n}$. Maslov form extends to this setting in the obvious way. Consider the complex version of the symplectic form:

$$\sigma_{\mathbb{C}}(X,Y) = \sigma(\bar{X},Y), \quad X,Y \in \mathbb{C}^{2n}.$$

If V is Lagrangian as a real vector space, then $V \otimes \mathbb{C}$ is Lagrangian with respect to the new symplectic form. If we take three Lagrangian subspaces the Maslov form is still well defined. Suppose that $\lambda_1 \in L_1 \cap (L_0 + L_2)$:

$$m(\lambda_1) = \sigma_{\mathbb{C}}(\lambda_0,\lambda_2) = \sigma(\bar{\lambda}_0,\lambda_2).$$

Lemma 8. *The Maslov form is a Hermitian form.*

Proof. Notice that $\overline{m(\lambda_1)} = \sigma(\lambda_0,\bar{\lambda}_2) = m(\bar{\lambda}_1)$. We have to show that $m(\lambda_1) = m(\bar{\lambda}_1)$ but this follows from the fact the subspaces are Lagrangian.

$$\begin{aligned} m(\lambda_1) - m(\bar{\lambda}_1) &= \sigma(\bar{\lambda}_0,\lambda_2) - \sigma(\lambda_0,\bar{\lambda}_2) = \sigma(\bar{\lambda}_0+\bar{\lambda}_2,\lambda_2) - \sigma(\lambda_0,\bar{\lambda}_2+\bar{\lambda}_0) \\ &= \sigma(\bar{\lambda}_1,\lambda_2) - \sigma(\lambda_0,\bar{\lambda}_1) = \sigma(\bar{\lambda}_1,\lambda_1) = 0. \end{aligned}$$

This means that the quadratic form is real and thus m is Hermitian. □

Thus the eigenvalues of m are real and the index and the signature is well defined exactly as in the real case. Here we list some of the properties of the $\sigma_{\mathbb{C}}$ and complex Lagrange subspaces:

- **Darboux basis** Since $\sigma_{\mathbb{C}}$ is non degenerate, every time two Lagrangian subspaces L_0, L_1 are considered, there exists a basis in which $\sigma_{\mathbb{C}}$ has the standard form.

- **Grassmannian of Lagrangian subspaces** In the real case the Lagrange Grassmannian is a homogeneous space diffeomorphic to $U(n)/O(n)$. It turns out that the *complex* one is diffeomorphic to $U(n)$ (and thus still real as a manifold). We can diagonalize the symplectic form obtaining:

$$\frac{1}{2}\begin{pmatrix} i & -1 \\ 1 & -i \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} -i & 1 \\ -1 & i \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

  Thus we have two subspaces on which $\sigma_{\mathbb{C}}$ is non degenerate, the eigenspace V_i relative to i and V_{-i}, the one relative to $-i$. It is thus clear that if V is Lagrangian, V must be transversal to both the eigenspaces. So it can always be represented as a graph of an invertible linear operator from $V_i \to V_{-i}$ (or vice versa). It remains to check what kind of linear maps are allowed. Using again the coordinates in which $\sigma_{\mathbb{C}}$ is diagonal we get:

$$\sigma_{\mathbb{C}}\Big(\begin{pmatrix} x \\ Rx \end{pmatrix}, \begin{pmatrix} y \\ Ry \end{pmatrix}\Big) = i\langle \bar{x}, y\rangle - i\langle R^*\bar{R}\bar{x}, y\rangle = i\langle (1-R^*\bar{R})\bar{x}, y\rangle.$$

  Since we need this quantity to be zero for any $x, y \in \mathbb{C}^n$ we get $\bar{R}R^* = 1$ and thus $R \in U(n)$. It follows that the complex Grassmannian is diffeomorphic to $U(n)$.

- **Atlas for the Lagrange Grassmannian** Take two transversal subspaces L_0, L_1. Using Darboux coordinates, we can build an affine chart as in the real case (compare with example 4). This time though we consider Hermitian matrices. The subspaces $V_S = \{(x, Sx) : S = \bar{S}^*, x \in L_0\}$ are Lagrangian subspaces.

- **Properties of Kashiwara index** The proof of the cocycle property given in [26, Theorem 1.32] works in the Hermitian case as well since our quadratic forms are all real by Lemma 8. It suffice to substitute the word *symmetric* with the word *Hermitian*. In particular all the properties listed in the previous section remain true in this setting, with real dimensions replaced by complex ones.

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