

MAE 546 Notes

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Introduction

Chapter 1

Finite Dimensional Conditions

1.1 Motivations

We denote by \mathcal{A} the standard problem

$$\inf_{u \in \mathcal{U}} \left\{ J(u; t_0, t_f, X_0) = K(t_f, X_f) + \int_{t_0}^{t_f} L(s, X_s, u_s) \, ds \right\}$$

where J is the objective function which we want to minimize, u is our control state from the admissible control \mathcal{U} , K is the terminal cost, L is the running cost, and the system is driven by a vector field f with

$$dX_t = f(t, X_t, u_t) \, dt$$

We may also need to satisfy equality constraints (like boundary conditions) and inequality constraints (like path constraints or bounds). If we impose regularity demands on any of the cost functions, solutions, or constraints, which will in turn change the conditions for solutions. We will also focus on finding local minima, though conditions like convexity can elevate these to global minima.

Example 1.1: Double Integrator Problem

Consider the minimum time problem where the cost function is given by

$$J(u; t_0, X_0) = \int_{t_0}^{t_f(u)} ds = t_f(u) - t_0$$

where the dynamics are

$$\ddot{X}(t) = u(t)$$

and the system ends at time $t_f(u)$ when it is stopped, in other words

$$X_f = 0$$

$$\dot{X}_f = 0$$

In essence the goal is merely to stop at the origin as quickly as possible, within the admissible control set. Here we'll use $\mathcal{U} = \text{PC}([t_0, \infty] \rightarrow [-1, 1])$, where PC denotes

the set of piecewise continuous functions.

The solutions satisfy the “**bang bang principle**”, where the optimal solution u^* takes values only on the vertices of the range; that is, its range is in $\{\pm 1\}$. It will be governed by a switching function φ and a **costate** or **adjoint** p^* , under

$$u^* = \begin{cases} 1, & \varphi(t; p^*) > 0 \\ -1, & \varphi(t; p^*) < 0 \\ \pm 1, & \varphi(t; p^*) = 0 \end{cases}$$

Solutions to this problem are known as **closed loop solutions**, meaning that the solution can be built over time by measuring the feedback output, as opposed to solving for the entire solution at once.

Example 1.2: Linear Quadratic Regulator

Consider the case of a lunar lander attempting to following a trajectory γ , but which has some error in its position (i.e. off course). We can compute a retargeting flight path $\delta\gamma$ using the linearization

$$\dot{\delta\gamma} \approx \nabla_{\gamma} f \delta\gamma + \nabla_u g \delta u$$

Here the cost function is given quadratically as

$$J(u; t_0, t_f, X_0) = \frac{1}{2} \int_{t_0}^{t_f} \langle X_s, Q(s) X_s \rangle + \langle u_s, R(s) u_s \rangle ds$$

where Q, R are symmetric, Q is positive semidefinite, and R is positive definite. and the dynamics are

$$dX_t = A(t)X_t dt + B(t)u_t dt$$

$A \in \mathbb{R}^{m \times m}, B \in \mathbb{R}^{m \times n}$, and the admissible control set is $C^1([t_0, t_f] \rightarrow \mathbb{R}^n)$. This is solved by

$$u_t^* = -R^{-1}(t)B^T(t)P(t)X_t^*$$

with P satisfying the **Riccati differential equation**

$$\dot{P}(t) = -P(t)A(t) - A^T(t)P(t) - Q(t) + P(t)B(t)R^{-1}(t)B^T(t)P(t)$$

and $P(t_f) = 0$.

In practice, control problems may be difficult or impossible to solve directly, so we may require transcription of the problem into a form amenable to numerical methods. This may be done directly, or first by deriving the necessary conditions through the costates.

There are a few methods for transcribing problems into a discretized form. **Shooting methods** involve transcription of only the control state, but the state process is still solved using the ODE involving f . For instance, if the admissible control states are $C^1([t_0, t_f] \rightarrow \mathbb{R})$,

we might discretize \mathcal{U} into four dimensions by replacing it with functions that take constant values on each of the four subintervals in $[t_0, t_f]$.

On the other hand, **collocation methods** transcribe both the control and state process at the same time.

1.2 Definitions and Conventions

We will denote a metric space by (M, d) , and a topology by T . We assume all metric spaces are given the induced topology. For $x \in M$ a metric space, we denote the open ε -ball about x by $B(x, \varepsilon)$, and the closed ball by $\bar{B}(x, \varepsilon)$. The closure of a set A is denoted \bar{A} , its interior A° , and its boundary ∂A .

Definition 1.1

If (X, T) is a topological space, then $x^* \in X$ is a local minimum for $f : X \rightarrow \mathbb{R}$ if there exists a neighborhood $A \in T$ of x^* where x^* minimizes f on A .

Definition 1.2

$C^k(\Omega, \mathbb{R})$ denotes the space of k times continuously differentiable functions from $\Omega \rightarrow \mathbb{R}$. $C_b(\Omega, \mathbb{R})$ is the space of such functions where all derivatives and the function are bounded.

1.3 Unconstrained Optimization

In this section we develop necessary and sufficient conditions for minima and strict minima on open sets in \mathbb{R}^n .

Proposition 1.1

If $x^* \in \Omega^\circ \subseteq \mathbb{R}^n$ is a local minimum for $f \in C^1(\Omega \rightarrow \mathbb{R})$, then

$$\nabla f(x^*) = 0$$

Theorem 1.2: Taylor's Formula with Remainder, Lagrange Form

Let $f \in C^{k+1}(\mathbb{R}, \mathbb{R})$. Let $x, x^* \in \mathbb{R}$, $\delta x = x - x^*$. Then there exists a point y strictly between x, x^* such that

$$f(x) = f(x^*) + f'(x^*)\delta x + \frac{1}{2!}f''(x^*)\delta x^2 + \dots + \frac{1}{k!}f^{(k)}(x^*)\delta x^k + \frac{1}{(k+1)!}f^{(k+1)}(y)\delta x^{k+1}$$

Proposition 1.3

If $x^* \in \Omega^o \subseteq \mathbb{R}^n$ is a local minimum for $f \in C^2(\overline{\Omega}, \mathbb{R})$, then

$$\frac{\partial^2 f}{\partial x^2}|_{x^*} \geq 0$$

Definition 1.3

The **Hessian** of a function $f \in C^2(\Omega, \mathbb{R})$ at a point $x^* \in \Omega^o$ is

$$(\nabla_x^{\otimes 2} f|_{x^*})_{ij} = \partial_i \partial_j f$$

In particular the Hessian is symmetric.

Proposition 1.4

For $f \in C^2(\overline{\Omega}, \mathbb{R})$ and $\Omega \subseteq \mathbb{R}^n$, a sufficient condition for $x^* \in \Omega^o$ to be a strict local minimum of f is for

$$\begin{aligned} \nabla_x f|_{x^*} &= 0 \\ \nabla_x^{\otimes 2} f|_{x^*} &> 0 \end{aligned}$$

(where the second line says the Hessian is positive definite.)

Proof. Since all the eigenvalues are positive, and the Hessian is symmetric, we write

$$\nabla_x^{\otimes 2} f|_{x^*} = Q \Lambda Q^T$$

such that

$$\langle \hat{q}_i, Q \Lambda Q^T \hat{q}_j \rangle = \delta_{ij} \lambda_i > 0$$

Then take $B(x^*, \varepsilon) \subseteq \Omega^o$ and define $g(\alpha, q) : [0, \varepsilon] \times S^{n-1} \rightarrow \mathbb{R}$ by $\alpha \times q \mapsto f(x^* + \alpha q)$. This gives the trace of f in the direction of q . Pick $q = \hat{q}_1$ and pick $\alpha \in (0, \varepsilon)$. By Taylor's theorem with remainder in α for $0 < \beta < \alpha$

$$g(\alpha, \hat{q}_1) = f(x^* + \alpha \hat{q}_1) = g|_0 + \partial_\alpha g|_0 \alpha + \frac{1}{2} \partial_\alpha^2 g(\hat{q}_1)|_\beta \alpha^2$$

By assumption, $\partial_\alpha g|_0 = \nabla_x f|_{x^*} \cdot \hat{q}_1 = 0$. So we see that

$$g(\alpha, \hat{q}_1) - g(0, \hat{q}_1) = \frac{1}{2} \partial_\alpha^2 g(\hat{q}_1)|_\beta \alpha^2$$

Assume $\alpha \ll 1$, so that

$$\text{sign}(\partial_\alpha^2 g(\hat{q}_1)|_\beta) = \text{sign}(\partial_\alpha^2 g(\hat{q}_1)|_0)$$

(possible since f is C^2). This shows that $f(x^* + \alpha \hat{q}_1) > f(x^*)$ for $0 < \alpha < \alpha_1^+$. We can repeat this work to show the same for $-\alpha_1^- < \alpha < 0$. We can also repeat this for the other eigenvalues. Finally set $\alpha^* = \min\{\alpha_i^+, \alpha_i^-\}$. It follows that

$$f(x^*) < f(y)$$

for any $y \in B(x^*, \alpha)$. □

Theorem 1.5: Taylor's Formula with Remainder, Peano Form

Let $f \in C^K(\mathbb{R}, \mathbb{R})$ and $x, x^* \in \mathbb{R}$, with $\delta x := x - x^*$. Then there exists $R_K : \mathbb{R} \rightarrow \mathbb{R}$ such that

$$f(x) = \sum_{i=0}^K \frac{1}{i!} \partial_x^i f|_{x^*} \delta x^i + R_K(x) \delta x^K$$

such that $\lim_{x \rightarrow x^*} R_K(x) = 0$. For convenience we use asymptotic notation

$$f(x) = \sum_{i=0}^K \frac{1}{i!} \partial_x^i f|_{x^*} \delta x^i + o(\delta x^K)$$

Alternate Proof of 1.4. Use the Peano form to write

$$f(x^* + \alpha q) = f(x^*) + \frac{1}{2} \langle q, \nabla^{\otimes 2} f|_{x^*}, q \rangle \alpha^2 + o(\alpha^2, q)$$

For $q \in S^{n-1}$, define

$$h(q) = \sup \left\{ \varepsilon > 0 : \alpha \in B(0, \varepsilon) \setminus \{0\} \implies |o(\alpha^2, q)| < \frac{1}{2} \langle q, \nabla_x^{\otimes 2} f|_{x^*} q \rangle \alpha^2 \right\}$$

By compactness, h attains a minimum on S^{n-1} , so there exists ε^* such that the inequality is true on $B(0, \varepsilon^*) \setminus \{0\}$. □

1.4 Equality Constrained Optimization

Now we introduce equality constraints to study more interesting sets over which we may optimize. For $m \leq n$, define a set of constraints

$$\{h_i \in C^1(\mathbb{R}^n, \mathbb{R})\}_{i=1}^m$$

and define the collective zero locus

$$M = \bigcap_i \{h_i = 0\}$$

We will always assume that our constraints are nondegenerate, so that $M \neq \emptyset$.

Definition 1.4

A **regular point** is an element $q \in M$ such that the gradients

$$\{\nabla_x h_i|_q\}_i$$

are linearly independent. Note that if any gradient is zero, then q is not regular.

Definition 1.5

Let $h \in C^1(\Omega, \mathbb{R}^m)$, $\Omega \subseteq \mathbb{R}^n$. Then the **Jacobian** of h at $q \in \Omega^\circ$ is

$$(\nabla_x h|_q)_{ij} = \frac{\partial h_i}{\partial x_j}|_q = \begin{bmatrix} \nabla h_1^T \\ \vdots \\ \nabla h_m^T \end{bmatrix}$$

If the Jacobian is full rank, that is $\text{rank}(\nabla_x h|_q) = \min(m, n)$, then q is a regular point. We define the tangent space in two equivalent ways:

Definition 1.6: Tangent Space, Geometric

Let $q \in M = M_k$ be a point on a k -dimensional surface. The **tangent space** to M at q , denoted $T_q M$, is the vector space isomorphic to \mathbb{R}^k defined by

$$T_q M := \{(q, y) \in M \times \mathbb{R}^k : \langle \nabla_x h_i, y \rangle = 0 \quad \forall i\}$$

Definition 1.7: Tangent Space, Curves

Consider the family of curves $\{\psi_\lambda \in C^1((-1, 1), M_K)\}_{\lambda \in \Lambda}$ such that $\psi_\alpha(0) = q$. Let $f \in C^1(M_K, \mathbb{R})$. Then by the chain rule,

$$\partial_\alpha(f \circ \psi_\lambda)|_0 = \langle \nabla_x f|_q, \partial_\alpha \psi_\lambda|_0 \rangle$$

In particular for $f = h_i$, $h_i(\psi_\lambda(\alpha)) \equiv 0$, so

$$\langle \nabla_x h_i|_q, \partial_\alpha \psi_\lambda(0) \rangle = 0$$

This is the same inner product condition as the geometric definition, so we can just define the tangent space to be the collection of $\partial_\alpha \psi_\lambda(0)$, endowed with vector space structure and equivalence via curve equivalence.

Now we give necessary conditions on optimization on equality hypersurfaces.

Proposition 1.6

Let $M = M_k \subseteq \mathbb{R}^n$ and $k = n - m$, with M defined by $(h_i)_{i=1}^m$. If $x^* \in M$ is a minimum of $f \in C^1(M, \mathbb{R})$ and x^* is a regular point, then there exists $\lambda \in \mathbb{R}^m$ such that

$$0 = \nabla_x f|_{x^*} + \nabla_x h|_{x^*} \lambda$$

In other words, f is linearly dependent with the gradients of the constraints.

Proof. Since x^* is a regular point, we can form a basis of \mathbb{R}^n given by the m gradients $(\nabla_x h_i|_{x^*})_{i=1}^m$ and a basis of $T_{x^*}M$ (say, $(\partial_\alpha \psi_j(0))_{j=1}^k$ for some ψ_j). Thus we can write $\nabla_x f|_{x^*}$ as

$$\nabla_x f|_{x^*} = \sum_{i=1}^m \langle \nabla_x f|_{x^*}, \nabla_x h_i|_{x^*} \rangle \nabla_x h_i|_{x^*} + \sum_{j=1}^k \langle \nabla_x f|_{x^*}, \partial_\alpha \psi_j(0) \rangle \partial_\alpha \psi_j(0)$$

For any ψ_j , write $g_j = f \circ \psi_j$. Then $g \equiv 0$ since $f = 0$ on M_k , so

$$0 = \partial_\alpha|_0 = \langle \nabla_x f|_{x^*}, \partial_\alpha \psi|_0 \rangle$$

So $\nabla_x f|_{x^*}$ is a linear combination of the $\nabla_x h_i|_{x^*}$. □

The above proof is essentially a statement that the method of **Lagrange multipliers** works.

Analytic Proof. This proof works for $m = 1$. Let $d_1, d_2 \in \mathbb{R}^n$ and define $F : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ by

$$F(\alpha_1, \alpha_2) = (f(x^* + \alpha_1 d_1 + \alpha_2 d_2), h(x^* + \alpha_1 d_1 + \alpha_2 d_2))$$

In particular $F(0, 0) = (f(x^*), 0)$. Now consider the matrix

$$\nabla F|_{(0,0)} = \begin{bmatrix} \langle \nabla f, d_1 \rangle & \langle \nabla f, d_2 \rangle \\ \langle \nabla h, d_1 \rangle & \langle \nabla h, d_2 \rangle \end{bmatrix}$$

Suppose the rank of this matrix is 2. Then F is locally invertible at x^* . So there is an open neighborhood around $(f(x^*), 0)$ where F is invertible, and by passing through the inverse map, there is (α_1, α_2) such that

$$\begin{aligned} \pi_1 \circ F(\alpha_1, \alpha_2) &= f(x^* + \alpha_1 d_1 + \alpha_2 d_2) < f(x^*) \\ \pi_2 \circ F(\alpha_1, \alpha_2) &= 0 \end{aligned}$$

But this is a contradiction. So ∇F is not full rank. Since x^* is a regular point, we can choose d_1 such that $\langle \nabla h, d_1 \rangle \neq 0$. Let d_2 be arbitrary, and define

$$\lambda^* = -\frac{\langle \nabla f, d_1 \rangle}{\langle \nabla h, d_1 \rangle}$$

Now, ∇F has rank exactly 1, so the columns are proportional. This means there is β such that

$$\begin{aligned}\langle \nabla h, d_1 \rangle &= \frac{1}{\beta} \langle \nabla h, d_2 \rangle \\ \langle \nabla f, d_1 \rangle &= \frac{1}{\beta} \langle \nabla f, d_2 \rangle\end{aligned}$$

Then

$$\langle \nabla f, d_2 \rangle = \beta \langle \nabla f, d_1 \rangle = \beta (-\lambda \langle \nabla h, d_1 \rangle) = -\lambda \langle \nabla h, d_2 \rangle \implies \langle \nabla f + \lambda \nabla h, d_2 \rangle = 0$$

Since d_2 is arbitrary,

$$\nabla f + \lambda \nabla h = 0$$

□

Definition 1.8

Let $h : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and define the **augmented Lagrangian cost function** $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ by

$$\mathcal{L}(x, \lambda) = f(x) + \langle \lambda, h(x) \rangle$$

Corollary 1.7

In the same setup as the previous theorem, there is $\lambda^* \in \mathbb{R}^m$ such that

$$\nabla_x \mathcal{L}|_{(x^*, \lambda^*)} = \nabla_x f|_{x^*} + \nabla h_{x^*}^T \lambda^* = 0$$

and

$$\nabla_\lambda \mathcal{L}|_{(x^*, \lambda^*)} = h(x^*) = 0$$

Essentially, the Lagrangian extends our constrained optimization to a higher dimension space, on which we may perform unconstrained optimization (so long as the minimum is regular). Thus the necessary and sufficient conditions look very similar to the unconstrained case.

Theorem 1.8: Second Order Necessary Condition

Let M be the zero locus of $h : \mathbb{R}^n \rightarrow \mathbb{R}^m$, with $h_i \in C^2(\mathbb{R}^n, \mathbb{R})$, $f \in C^2(M, \mathbb{R})$, and let \mathcal{L} be the augmented Lagrangian. Then the Hessian of the augmented Lagrangian with respect to x is

$$\nabla_x^{\otimes 2} \mathcal{L}|_{(x, \lambda)} = \nabla_x^{\otimes 2} f|_{(x, \lambda)} + \sum_i \lambda_i \nabla_x^{\otimes 2} h_i|_{(x, \lambda)}$$

Moreover, if x^* is a minimum of f and a regular point of M , then there exists $\lambda^* \in \mathbb{R}^m$ such that $\nabla_x^{\otimes 2} \mathcal{L}|_{(x^*, \lambda^*)}$ is positive semidefinite on TM_{x^*} .

Theorem 1.9: Second Order Sufficient Condition

If

$$\nabla_x \mathcal{L}|_{(x^*, \lambda^*)} = 0 \in \mathbb{R}^n$$

$$\nabla_\lambda \mathcal{L}|_{(x^*, \lambda^*)} = 0 \in \mathbb{R}^M$$

and $\nabla_x^{\otimes 2} \mathcal{L}|_{(x^*, \lambda^*)}$ is positive definite on TM_{x^*} , and moreover x^* is regular, then x^* is a strict local minimum of f .

1.5 Mixed Constraint Mathematical Programs

Definition 1.9

A **mixed constraint mathematical program** is a problem of the form of finding

$$\inf_{\mathbb{R}^n} f$$

subject to the constraints

$$h_e(x) = 0, \quad e \in E$$

$$c_i(x) \leq 0, \quad i \in I$$

with $|E| = m < n$ and $|I| \in \mathbb{N}$. When f, h, c are all linear functions, this is called a **linear program** (LP); when f is quadratic and h, c are linear, this is a **quadratic program** (QP). If f, h, c are all convex, then it is called a **convex program** (CVP). Most generally, this can be called a **nonlinear program** (NLP).

While solving NLPs, it is often helpful to break it into sequential programs of simpler type, like QPs or CVPs. For instance, **sequential quadratic programs** (SQP) involve a method similar to gradient descent, but by solving a QP at every step, since we know f locally looks like a QP at a minimum.

Definition 1.10

Let $A \subseteq \mathbb{R}^m$ be convex, and let $f : A \rightarrow \mathbb{R}$. Define the **epigraph** of f by

$$B = \{(x, y) : x \in A, y \geq f(x)\} \subseteq A \times \mathbb{R}$$

f is said to be **convex** if B is convex in \mathbb{R}^{m+1} . Equivalently, f is said to be convex if it is continuous and for $x, y \in A, t \in [0, 1]$,

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y)$$

Definition 1.11

A set $\mathcal{C} \subseteq \mathbb{R}^n$ is called a **cone** if for all $x \in \mathcal{C}$, $t > 0$, $tx \in \mathcal{C}$.

Definition 1.12

For a mixed constraint program with equality constraints $h_e, e \in E$ and inequality constraints $c_i, i \in I$, the **feasible set** is the set

$$\Omega = \{x \in \mathbb{R}^n : c_i(x) = 0, h_e(x) = 0\}$$

The **active set** at a point $x \in \Omega$ is the set of indices for which x achieves equality; that is,

$$A(x) = \{i \in I : c_i(x) = 0\} \sqcup E$$

Example 1.3

Suppose $f \in C^1(\mathbb{R}^n, \mathbb{R})$ and let $c \in C^1$ be the only inequality constraint. Let $x \in \Omega$ be a point in the feasible set. Let us try to find $q \in S^{n-1}, \alpha > 0$ such that $x + \alpha q \in \Omega$ and $f(x + \alpha q) < f(x)$.

If $c(x) < 0$ then $A(x) = \emptyset$, otherwise if $c(x) = 0$ then $A(x) = \{1\}$. In the first case this locally just looks like unconstrained optimization and we are done by our previous work, setting $q = -\nabla_x f|_x$.

Otherwise, we want to have $\langle \nabla f|_x, q \rangle < 0$ and $c(x + \alpha q) \leq 0$. Suppose such q, α exist. Applying the mean value theorem to c , there is $0 < \beta < \alpha$ such that

$$c(x + \alpha q) = c(x) + \alpha \langle \nabla c|_{x+\beta q}, q \rangle = \alpha \langle \nabla c|_{x+\beta q}, q \rangle \leq 0$$

Let α be small enough such that for all $\beta < \alpha$,

$$\text{sign}(\langle \nabla c|_x, q \rangle) = \text{sign}(\langle \nabla c|_{x+\beta q}, q \rangle)$$

So in particular we have

$$\langle \nabla f|_x, q \rangle < 0, \quad \langle \nabla c|_x, q \rangle \leq 0$$

As a result, this cannot happen (which occurs at minima) if

$$\langle \nabla f|_x, q \rangle = -\lambda \langle \nabla c|_x, q \rangle$$

for some $\lambda \geq 0$. A concise way to express conditions for this under both cases of $c(x)$ is that there exists $\lambda \geq 0$ such that

$$\begin{aligned} \nabla_x \mathcal{L}|_{(x, \lambda)} &= 0 \\ \lambda c(x) &= 0 \end{aligned}$$

The second of these conditions is called the **complementarity condition**.

Definition 1.13

We say that the **linear independence constraint qualification** (LICQ) holds at a point $a \in \Omega$ if

$$\text{span} \{ \nabla c_i : i \in A(x) \} = \mathbb{R}^{|A(x)|}$$

Proposition 1.10

Suppose x^* is a minimum of f and the LICQ holds at x^* . Then there exists $\lambda^* \in \mathbb{R}^{|E \sqcup I|}$ such that

$$\nabla_x \mathcal{L}|_{(x^*, \lambda^*)} = 0$$

and $\lambda_i^* \geq 0$ for all $i \in I$ with

$$\lambda_i^* c_i(x) = 0, \quad i \in I$$

Chapter 2

Infinite Dimensional Conditions

2.1 Calculus of Variations

Here we use the results from the calculus of variations to consider the infinite dimensional and continuous time cases.

Definition 2.1

Let $I \in \mathbb{R}^{n \times m}$, $E \in \mathbb{R}^{n \times p}$. Then the **closed convex cone** generated by them is

$$K := \{Iy + Ew : y \in \mathbb{R}_{\geq 0}^m, w \in \mathbb{R}^p\}$$

Lemma 2.1: Farkas

If $I \in \mathbb{R}^{n \times m}$, $E \in \mathbb{R}^{n \times p}$, then for any $g \in \mathbb{R}^n$, only one of the following can be true:

- $g \in K$,
- There exists $d \in \mathbb{R}^n$ with $\langle d, g \rangle < 0$ and $I^T d \geq 0$, $Ed = 0$.

Definition 2.2

On the space $C^k(\mathbb{R}^n, \mathbb{R})$, for any $j \leq k$ there is an associated supremum norm

$$\|f\|_{j,\infty} = \sum_{|\alpha| \leq j} \sup_{\mathbb{R}^n} |D^\alpha f|$$

We denote $\mathfrak{X}_{j,k} = (C^k(\mathbb{R}^n, \mathbb{R}), \|\cdot\|_{j,\infty})$.

Definition 2.3

A functional on a normed vector space V over \mathbb{F} is a map $F : V \rightarrow \mathbb{F}$.

We need to extend the notion of differentiability to infinite dimensional spaces. In \mathbb{R}^n , directional derivatives and total derivatives are essentially equivalent, but in infinite dimensions this is not generally true and interpolation cannot necessarily be made. So instead we have two notions of derivatives, but we will show that they are ultimately equivalent under certain conditions.

Definition 2.4

If $\mathfrak{X}, \mathfrak{Y}$ are two normed vector spaces, then the space of **linear continuous operators** $\psi : \mathfrak{X} \rightarrow \mathfrak{Y}$ is denoted $L_C(\mathfrak{X}, \mathfrak{Y})$. The operator norm on this space is

$$\|\psi\|_{L_C(\mathfrak{X}, \mathfrak{Y})} = \|\psi\|_{L_C} = \sup_{\|x\|_{\mathfrak{X}} \leq 1} \|\psi(x)\|_{\mathfrak{Y}}$$

Definition 2.5

Let $\mathfrak{X}, \mathfrak{Y}$ be two normed vector spaces, and let $F : \mathfrak{X} \rightarrow \mathfrak{Y}$. For $x \in \mathfrak{X}$, if there exists a continuous linear operator ψ such that

$$\lim_{u \rightarrow x} \frac{\|F(u) - F(x) - \psi(u - x)\|_{\mathfrak{Y}}}{\|u - x\|_{\mathfrak{X}}} = 0$$

then ψ is called the **Frechet derivative** of F at x , denoted $dF|_x$. F is said to be **continuously differentiable** at x if it is differentiable on a neighborhood of x and dF is continuous in the L_C norm.

Theorem 2.2: Taylor's Formula for Frechet Derivatives

Let $F : \mathfrak{X} \rightarrow \mathfrak{Y}$ be differentiable at $x \in \mathfrak{X}$. Then

$$F(x + q) = F(x) + dF|_x(q) + o(\|q\|_{\mathfrak{X}})$$

Define $\Delta F : \mathfrak{X} \otimes \mathfrak{X} \rightarrow \mathfrak{Y}$ by

$$\Delta F(x, q) = F(x + q) - F(x)$$

Then this is equivalent to

$$\Delta F(x, q) = dF_x(q) + o(\|q\|_{\mathfrak{X}})$$

Theorem 2.3

If $dF|_x$ exists then it is unique.

Definition 2.6

Let $F : \mathfrak{X} \rightarrow \mathfrak{Y}$. The **Gateaux derivative** or directional derivative at x in the direction $q \in \mathfrak{X}$ is defined by

$$\partial F|_x(q) = \lim_{\alpha \rightarrow 0} \frac{F(x + \alpha q) - F(x)}{\alpha}$$

if this limit exists. $\partial F|_x(q)$ is said to be continuous (for some fixed q) if it is continuous with respect to x .

Note that the Gateaux derivative in general may not be linear, but it is homogeneous

$$\partial F|_x(\alpha q) = \alpha \partial F|_x(q)$$

If \mathfrak{X} is infinite dimensional then it may not be continuous.

Definition 2.7

If $F : \mathfrak{X} \rightarrow \mathfrak{Y}$ has a Gateaux derivative in each direction $q \in \mathfrak{X}$ for some $x \in X$, and there is a map $\delta F|_x \in L_C(\mathfrak{X}, \mathfrak{Y})$ such that

$$\delta F|_x(q) = \partial F|_x(q)$$

for all q , then F is said to be **Gateaux differentiable** at x with differential $\delta F|_x$.

As we previously mentioned, these two notions of differentiability are effectively equivalent in Euclidean space.

Theorem 2.4

Let $\mathfrak{X}, \mathfrak{Y}$ be finite dimensional normed vector spaces and $F : \mathfrak{X} \rightarrow \mathfrak{Y}$. If $dF|_x$ exists for some x , then for all q , $\partial F|_x(q)$ exists and

$$dF|_x(q) = \partial F|_x(q)$$

Conversely, if $\partial F|_x(q)$ exists for all q and each derivative is continuous at x , then $dF|_x$ exists and the same is true.

In general Frechet differentiability is stronger than Gateaux differentiability.

Theorem 2.5

Let $F : \mathfrak{X} \rightarrow \mathfrak{Y}$ with $\mathfrak{X}, \mathfrak{Y}$ arbitrary normed vector spaces, and let $dF|_x$ exist for some x . Then for any $q \in \mathfrak{X}$, $\partial F|_x(q)$ exists and

$$dF|_x(q) = \partial F|_x(q)$$

Theorem 2.6: Taylor's Formula for Gateaux Derivatives

Let $F : \mathfrak{X} \rightarrow \mathfrak{Y}$ and let $x \in \mathfrak{X}$ be such that $\delta F|_x$ exists. Then for $q \in \mathfrak{X}, \alpha \in \mathbb{R}$,

$$F(x + \alpha q) = F(x) + \delta F|_x(q)\alpha + o(\alpha)$$

as $\alpha \rightarrow 0$. If F is a functional and x is a local minimum for F , then

$$\delta F|_x \equiv 0$$

Definition 2.8

Let J be a functional on a real normed vector space \mathfrak{X} . Suppose that $x \in \mathfrak{X}$ is such that each Gateaux derivative $\partial J|_x(q)$ exists. If there exists $\delta J|_x \in L(\mathfrak{X}, \mathbb{R})$ such that

$$J(x + \alpha q) = J(x) + \delta J|_x(q)\alpha + o_q(\alpha)$$

then δJ is called the **first variation** of J .

When J is sufficiently regular, $dF|_x(q) = \delta F|_x(q)$ are both equal to the first variation.

Theorem 2.7

If J is minimized at $y^* \in \mathfrak{X}$, and the first variation exists at y^* , then it is zero.

Definition 2.9

Let $\mathcal{L} \in C^2([a, b] \times \mathbb{R}^2 \rightarrow \mathbb{R})$ be a Lagrangian denoted by

$$(x, u, v) \mapsto \mathcal{L}(x, u, v)$$

We define the associated **cost functional** $J : \mathfrak{X}_{j,k} \rightarrow \mathbb{R}$ by

$$J(y) = \int_a^b \mathcal{L}(x, y(x), \partial_x y(x)) \, dx$$

In particular, for the CoV problem we are interested in minimizing the case $k = 2$ with fixed boundary conditions

$$y^* = \operatorname{argmin} \{ J(y) : y \in \mathfrak{X}_{j,2}, y(a) = y_1, y(b) = y_2 \}$$

Definition 2.10

Let y^* be a minimum of J for the CoV problem. Then if y^* is a minimum on $\mathfrak{X}_{1,2}$ under the $\|\cdot\|_{1,\infty}$ norm, y^* is called a **weak extremum**. If it is a minimum on $\mathfrak{X}_{0,2}$ under $\|\cdot\|_{0,\infty} = \|\cdot\|_\infty$, it is called a **strong extremum**.

If y^* is a strong extremum it is also a weak extremum.

Theorem 2.8: Euler-Lagrange

If y is a weak extremum for a cost functional J , then

$$\frac{d}{dx} \left(\frac{\partial}{\partial v} \mathcal{L}|_{(x, y(x), \partial_x y(x))} \right) = \frac{\partial}{\partial u} \mathcal{L}|_{(x, y(x), \partial_x y(x))}$$

for all $x \in [a, b]$. We call this condition the **Euler-Lagrange equation**.

Proof. We know that $\delta J|_y(\eta) \equiv 0$. Let $\eta \in \mathfrak{X}$ be some variation such that $\eta(a) = \eta(b) = 0$. Then

$$J(y + \alpha\eta) = \int_a^b \mathcal{L}(x, y + \alpha\eta, \partial_x y + \alpha\partial_x \eta) dx$$

Applying Taylor's theorem, this is

$$\int_a^b [\mathcal{L}(x, y, \partial_x y) + \partial_u \mathcal{L}(x, y, \partial_y) \alpha\eta + \partial_v \mathcal{L}(x, y, \partial_y) \alpha\partial_x \eta] dx + o(\alpha)$$

So by linearity, the first variation is

$$\begin{aligned} \delta J|_y(\eta) &= \int_a^b [\partial_u \mathcal{L}(x, y, \partial_y) \alpha\eta + \partial_v \mathcal{L}(x, y, \partial_y) \alpha\partial_x \eta] dx \\ &= \underbrace{\partial_v \mathcal{L}(x, y, \partial_x y) \eta|_a^b}_{=0} + \int_a^b [\partial_u \mathcal{L}(x, y, \partial_y) - \partial_x \partial_v \mathcal{L}(x, y, \partial_y)] \eta dx = 0 \end{aligned}$$

Since this is true for all η , the result follows. \square

Theorem 2.9: Transversality

Suppose y^* is a minimum for the CoV problem under the half-free boundary conditions

$$y^* = \operatorname{argmin} \{ J(y) : y \in \mathfrak{X}_{j,2}, y(a) = y_1 \}$$

Then the Euler-Lagrange equation holds, and also the **transversality condition** holds:

$$\partial_v \mathcal{L}|_{b, y(b), \partial_y(b)} = 0$$

The point of this theorem is that the departing flow of y^* must be perpendicular to the boundary. This holds more generally when considering flows departing from manifolds.

Proof. Using the same strategy as in the previous theorem, we have

$$0 = \delta J_y(\eta) = \int_a^b [\partial_u \mathcal{L}(x, y, \partial_y) - \partial_x \partial_v \mathcal{L}(x, y, \partial_y) \eta] dx + \partial_v \mathcal{L}|_{b, y(b), \partial_y(b)} \eta(b)$$

For η such that $\eta(b) = 0$, the integral is zero, which proves that Euler-Lagrange holds. From there, it follows that the second term is also always zero, which proves transversality. \square

Definition 2.11

Let (q, p) be the canonical position and momentum which are the solutions of an ODE for some dynamical system. The system is said to be a **Hamiltonian dynamical system** if there is $H : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}$ given by

$$H(t, q, p)$$

such that

$$\begin{aligned}\dot{q}(t) &= \nabla_p H \\ \dot{p}(t) &= -\nabla_q H\end{aligned}$$

If \mathbb{J} is the symplectic block matrix

$$\mathbb{J} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

Then we can equivalently write

$$\frac{d}{dt} \begin{bmatrix} q \\ p \end{bmatrix} = \mathbb{J} \nabla H$$

Suppose we are given some system under a Lagrangian \mathcal{L} , and define

$$p_y(x) = \partial_v \mathcal{L}(x, y(x), \partial y(x))$$

Define

$$H(x, y, v, p) = \langle p, v \rangle - \mathcal{L}(x, y(x), v)$$

2.2 Variational Constraints

In this section we proceed as follows: first, we consider how the CoV problem extends to equality constrained variation. We apply this to the equality constraints given by system dynamics, producing a *costate* function p which arises as the analogue of Lagrange multipliers. Then, we identify the first variation of the cost function with respect to perturbations in the control. Expressed in terms of the *control Hamiltonian*, we derive the canonical equations for the Hamiltonian and find that the Hamiltonian is stationary at optimal controls.

Theorem 2.10: Isoperimetric Problem

Consider the CoV problem of minimizing J_L while constrained by an integral

$$J_G(y) = \int_a^b G(x, y(x), \partial y(x)) dx = 0$$

Given a weak local minimizer y , there are $\lambda_L, \lambda \in \mathbb{R}$ not both zero such that y is also a weak extremal of

$$\lambda_L J_L + \lambda J_G$$

Proof. The admissible perturbations are those satisfying $\delta J_G(\eta) = 0$, since $y + \alpha\eta$ is admissible when

$$J_G(y + \alpha\eta) = \delta J_G(\eta)\alpha + o(\alpha)$$

So

□

It follows that for nonintegral constraints, we can view these as an infinite collection of time-parameterized integral constraints, and therefore we get

Theorem 2.11

Given the basic CoV problem of minimizing J subject to a single non-integral equality constraint $G(x, y(x), \partial y(x)) = 0$, for any weak local minimizer y^* there is $\lambda_L \in \{0, 1\}$ and $\lambda : [a, b] \rightarrow \mathbb{R}$ measurable such that Euler-Lagrange holds for

$$\lambda_L L(x, y(x), \partial y(x)) + \lambda(x) G(x, y(x), \partial y(x))$$

Now, let us consider a basic optimal control problem in the general Bolza form, with fixed final time and initial state, but free final state. The state is governed by system dynamics as

$$X_s = X_0 + \int_{t_0}^{t_f} f(t, X_t, u_t) dt$$

If we make a linear perturbation $u \mapsto u + \alpha\xi$, ξ fixed, then we obtain a perturbation in X_s as well, but this is generally nonlinear so we have to write

$$X_s \mapsto X_s(\alpha; \xi) := X_s + \alpha\eta(s; \xi) + o(\alpha; \xi)$$

where η here is the first variation of X at s . We can compute η :

Lemma 2.12

Fix a control u and let X be the associated state. Let α, ξ be a perturbation as above, and let $\eta(s; \xi)$ be the first variation of X at s as above. Then

$$\eta_s = \int_{t_0}^s [\nabla_x f|_t \eta(t; \xi) + \nabla_u f|_t \xi(t)] dt$$

where $f|_t = f(t, X_t, u_t)$.

Proof. We have by definition

$$\eta(t; \xi) = \partial_\alpha X_t(\alpha; \xi)$$

Let $u^* = u + \alpha\xi$, and let X^* be the associated state. Then

$$\begin{aligned} \dot{\eta}_t &= \partial_\alpha \partial_{t'} \left(X_0 + \int_{t_0}^{t'} f(s, X_s^*, u_s^*) ds \right) \Big|_{\alpha=0, t'=t} = \partial_\alpha f(t, X_t^*, u_t^*) \Big|_{\alpha=0} \\ &= \partial_\alpha (f(t, X_t + \alpha\eta(t; \xi) + o(\alpha; \xi), u_t + \alpha\xi(t))) \Big|_{\alpha=0} = \nabla_x f|_t \eta(t; \xi) + \nabla_u f|_t \xi(t) \end{aligned}$$

Integrate and conclude using the fact that $\eta_0 = 0$. □

Noting that $\nabla_x f, \nabla_u f$ are matrices, we are led to consider the linearized ODE.

Definition 2.12

Given the system

$$dX_t = A(t)X_t dt + B(t)u_t dt$$

where A is square and $B \in \mathbb{R}^{m \times n}$, the solution is

$$X_t = \Phi(0 \rightarrow t)X_0 + \Phi(0 \rightarrow t) \int_0^t \Phi(0 \rightarrow s)B(s)u_s ds$$

where $\Phi(t \rightarrow s)$ is defined to be the **state transition matrix**.

The collection $\Phi(t \rightarrow s)$ forms a group, with $\Phi(0, 0) = \text{id}$, $\Phi(t \rightarrow s)\Phi(r \rightarrow s) = \Phi(r \rightarrow t)$ and $\Phi(t \rightarrow s)^{-1} = \Phi(s \rightarrow t)$.

Definition 2.13

If X_t, Y_t are governed by the equations

$$\dot{X}_t = A(t)X_t$$

$$\dot{Y}_t = A^\dagger(t)Y_t$$

then X, Y are **adjoint**. In this case it is the case that $\langle X_t, Y_t \rangle$ is constant.

With the first variation of the state computed, it is now possible to compute the first variation of the cost function. We rewrite J in terms of the Hamiltonian:

$$J(u) = K(X_f) + \int_{t_0}^{t_f} \langle p, \dot{X} \rangle - H(t, X, u, p)$$

Definition 2.14

The **control Hamiltonian** is defined as

$$H(t, X_t, u_t, p_t) = \langle p_t, \dot{X}_t \rangle - \mathcal{L}(t, X_t, \dot{X}_t)$$

where $\dot{X}_t = f(t, X_t, u_t)$.

Here the costate p is defined to be the measurable function so that Euler-Lagrange holds. Then we have

$$\begin{aligned} J(u + \alpha\xi) - J(u) &= \\ &= K(X_f^*) - K(X_f) + \int_{t_0}^{t_f} \langle p_s, \dot{X}_s^* - \dot{X}_s \rangle ds \\ &\quad - \int_{t_0}^{t_f} H(s, X_s^*, u_s + \alpha\xi_s, p_s) - H(s, X_s, u_s, p_s) ds \end{aligned}$$

The terminal costs expand in α as

$$K(X_f^*) - K(X_f) = \alpha \langle \nabla_x K(X_f), \eta(t_f; \xi) \rangle + o(\alpha; \xi)$$

For the first integral term we compute

$$\begin{aligned} \int_{t_0}^{t_f} \langle p_s, \dot{X}_s^* - \dot{X}_s \rangle ds &= \langle p_s, X_s^* - X_s \rangle \Big|_{s=t_0}^{t_f} - \int_{t_0}^{t_f} \langle \dot{p}_s, X_s^* - X_s \rangle ds \\ &= \langle p_{t_f}, \alpha\eta(t_f; \xi) \rangle - \alpha \int_{t_0}^{t_f} \langle \dot{p}_s, \eta(t_f; \xi) \rangle ds + o(\alpha) \end{aligned}$$

and for the second,

$$H(s, X_s^*, u_s + \alpha\xi_s, p_s) - H(s, X_s, u_s, p_s) = \alpha \langle \nabla_x H(X_s), \eta(s; \xi) \rangle + \alpha \langle \nabla_u H(X_s), \xi_s \rangle + o(\alpha)$$

so

Theorem 2.13

In the basic optimal control problem as above, the first variation of the cost functional is

$$\delta J(\xi) = \langle \dot{p}_{t_f} + \nabla_x K(X_f), \eta(t_f; \xi) \rangle - \int_{t_0}^{t_f} \langle \dot{p}_s + \nabla_x H|_s, \eta(s; \xi) \rangle + \langle \nabla_u H|_s, \xi_s \rangle ds$$

The application of first order necessary conditions $\delta J = 0$ gives

Theorem 2.14

If u^* optimizes J and X^* is the associated state, then there is a costate function p^* such that

$$\begin{aligned}\dot{X}_s^* &= \nabla_p H \\ \dot{p}_s^* &= -\nabla_x H\end{aligned}$$

with boundary

$$\begin{aligned}\dot{X}_{t_0}^* &= X_0 \\ \dot{p}_{t_f}^* &= -\nabla_x K(X_{t_f})\end{aligned}$$

and such that

$$\nabla_u H(s, X_s^*, u_s^*, p_s^*) = 0$$

for all s .

2.3 Optimality Conditions

We recall that the general optimal control problem is formulated as finding the **control** $u(t) \in \mathbb{R}^m$ which minimizes the objective

$$J(u) = J(u, x, t_f) = \mathcal{M}(u, x, t_f) + \int_{t_0}^{t_f} \mathcal{L}(t, u(t), x(t)) dt$$

where \mathcal{M} is the fixed **terminal cost**, \mathcal{L} is the fixed **running cost**, and x is uniquely specified as

$$\dot{x} = f(t, u(t), x(t))$$

Also, the constraints

$$g(t, u(t), x(t)) \leq 0$$

are enforced. If $\mathcal{M} = 0$ the problem is said to be in **Lagrange form**, if $\mathcal{L} = 0$ the problem is in **Mayer form**, and if both are nonzero the problem is in **Bolza form**. Here we are optimizing u over the admissible control set \mathcal{U} , where \mathcal{U} consists of some subset of functions into a compact set in \mathbb{R}^m , and $x(t_0) \in \mathcal{X}_0, x(t_f) \in \mathcal{X}_f$, with $\mathcal{X}_0, \mathcal{X}_f$ closed. Also, the constraint set

$$\mathcal{Z}_t = \{(x, u) : g(t, u, x)\} \subseteq \mathbb{R}^{n+m}$$

is closed for all t . Equivalently, g is continuous.

Theorem 2.15

Suppose the dynamics f is a measurable function on $[t_0, t_f]$, f, g are continuous functions of u, x for each t . Suppose f is Lipschitz in x , uniformly for all t, u . Suppose \mathcal{L} is bounded below on the admissible set $\{(t, u, x) : g(t, u, x) \leq 0\}$, and \mathcal{M} is bounded below on $[t_0, t_f], \mathcal{X}_f$.

Also assume that there is a compact set containing all feasible constraints, or that there exist proper, radially unbounded functions $\alpha_x, \alpha_u : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}$ such that

$$\begin{aligned}\mathcal{L}(t, u, x) &\geq \alpha_x(\|x\|) + \alpha_u(\|u\|) - c(t) \\ \mathcal{M}(t_f, x_{t_f}) &\geq \alpha(\|x_{t_f}\|) - C\end{aligned}$$

for some constant C . This implies that if a minimizing sequence takes $\|u\|$ or $\|x\|$ to infinity, then the cost is also unbounded.

Lastly, for each t, x , define the collection of admissible derivatives and upper bounds on the Lagrangian:

$$\mathcal{V}_{t,x} := \{(v, l) : \exists u \in \mathcal{U}, v = f(t, u, x), l \geq \mathcal{L}(t, u, x), g(t, u, x) \leq 0\}$$

If $\mathcal{V}_{t,x}$ is nonempty, closed, and convex for all (t, x) , and set of bounded function $u : [t_0, t_f] \rightarrow \mathcal{U}$ which satisfy the constraints is nonempty, there is at least one optimal solution (t_f^*, u^*, x^*) , with x^* absolutely continuous and u^* measurable.

Chapter 3

Direct Methods

In direct methods, we first transcribe the problem into finite dimensions using an approximation in terms of basis functions. This parameterization may be done only for the control, or for both control and state. Then the problem is optimized using a nonlinear programming solver, or a lower order solver when possible.

3.1 Single Shooting

We discretize time into $t_0 = \tau_0 < \dots < t_N = t_f$. We define some basis set of functions $\psi_1, \dots, \psi_{n_p}$, and approximate the control as

$$u^p(t) = \sum_{j=1}^{n_p} p_j \psi_j(t)$$

Define the dynamic flow operator

$$\phi_{s \rightarrow t}(x_s, u) = x_t$$

Then the single shooting optimization problem is

$$\min_{t_f, p} \mathcal{M}(t_f, x(t_f)) + \sum_{l=0}^{N_q} w_l \mathcal{L}(\hat{t}_l, u^p(\hat{t}_l), x(\hat{t}_l))$$

where the state is computed as

$$x(\tau_{i+1}) = \phi_{\tau_i \rightarrow \tau_{i+1}}(x(\tau_i), u^p), x_{\tau_0} = x_0$$

and we optimize only over t_f, p such that

$$g(\tau_i, u^p(\tau_i), x(\tau_i)) \leq 0$$

The weights w_l and quadrature points \hat{t}_l define a particular choice of quadrature rule.

3.2 Multiple Shooting

In multiple shooting, rather than propagate forward from time t_0 , each subinterval on the time mesh performs single shooting independently, with independent start point. Continuity is added as an additional equality constraint. This allows instabilities to be more localized rather than propagating in time, and allows for parallelization, but is more expensive computationally. However, due to localization, the Jacobian of the objective is sparse, which makes solving easier.

3.3 Collocation

In **trapezoidal collocation**, we approximate integrals using the trapezoidal rule:

$$\int_{t_0}^{t_f} w(\tau) d\tau \approx \sum_{k=0}^{N-1} \frac{h_k}{2} (w_k + w_{k+1})$$

$$\int_{t_k}^{t_{k+1}} f(\tau, x_\tau, u_\tau) d\tau \approx \sum_{k=0}^{N-1} \frac{h_k}{2} (f_k + f_{k+1})$$

This rule gives us a linear interpolation scheme between the control variable, and quadratic interpolation in state (which implies continuous gradient).

We can get higher order accuracy on the state and control by imposing better integral approximations. In **Hermite-Simpson collocation**, we use Simpson's rule:

$$\int_{t_0}^{t_f} w(\tau) d\tau = \sum_{k=0}^{N-1} \frac{h_k}{6} \left(w_k + 4w_{k+\frac{1}{2}} + w_{k+1} \right)$$

This adds an additional node in the middle of each interval. On the other hand, we get quadratic approximations in control and cubic approximations in state.

The methods described above suggest a general scheme by which we may increase accuracy by refining the discretization, or by applying higher order approximations. The first are known as **H methods**, which are roughly defined as low order methods that achieve convergence by increasing the number of segments. On the other hands, **P methods** are higher order methods which achieve convergence by increasing the order of the method (like polynomial approximation).

Collocations improve on multiple shooting by providing higher accuracy, promoting sparse matrices to help with scalability, and allowing computations over intervals to be parallelized. However, the mesh must be computed effectively, and the dimensionality of the problem is inherently higher. Also, it is harder to enforced path constraints between nodes.

Chapter 4

Higher Order Variational Conditions

Just as we derived second and higher order necessary and sufficient conditions for extrema in finite dimensions, we can derive analogous conditions for infinite dimensional optimization.

4.1 Second Order Necessary Conditions

Definition 4.1

Let $J : \mathfrak{X} \rightarrow \mathbb{R}$ be a functional and let $x \in \mathfrak{X}$. If $\delta^2 J : \mathfrak{X} \rightarrow \mathbb{R}$ is a quadratic functional (meaning there is a bilinear functional $F : \mathfrak{X} \times \mathfrak{X} \rightarrow \mathbb{R}$ such that $\delta^2 J(q) = F(q, q)$), and

$$J(x_\alpha q) = J(x) + \delta J|_x(q)\alpha + \delta^2 J(q)\alpha^2 + o(\alpha^2; q)$$

then $\delta^2 J$ is called the **second variation** of J at x and it is denoted $\delta^2 J|_x$.

Theorem 4.1: Second Order Necessary Condition

If $x^* \in \mathfrak{X}$ is a local minimum of J and $\delta J|_x, \delta^2 J|_x$ both exist, then for any $q \in \mathfrak{X}$,

$$\delta J|_x(q) = 0$$

$$\delta^2 J|_x(q) \geq 0$$

Theorem 4.2: Legendre's Condition

Let $J = \int_a^b \mathcal{L} \, dx$ for some Lagrangian $\mathcal{L} = \mathcal{L}(x, u, v) \in C^3$, and let $y \in \mathfrak{X}_{1,2}$. If

$$y^* = \operatorname{argmin} \{J(y) : y \in \mathfrak{X}_{1,2}, y(a) = y_0, y(b) = y_1\}$$

is a weak local minima, then

$$0 \leq \frac{\partial^2}{\partial v^2} \mathcal{L}|_{(x, y^*, \partial y^*)}$$

for all $x \in [a, b]$.

Define the **control Hamiltonian**

$$H(x, y, v, p) = \langle p, v \rangle - \mathcal{L}(x, y, v)$$

and define the marginal Hamiltonian

$$\tilde{H}(\alpha; x, y(x), p(x)) = H(x, y(x), \alpha, p(x))$$

We know that for all x ,

$$\partial_\alpha \tilde{H}|_{\partial_x y} = 0$$

when

$$p(x, y, \partial y) = \partial_v \mathcal{L}|_{(x, y, \partial y)}$$

Applying Legendre's condition gives the following:

Theorem 4.3

Let \mathcal{L} be a Lagrangian, \tilde{H} the associated marginal Hamiltonian, and $p(x, y, \partial y) = \partial_v \mathcal{L}|_{(x, y, \partial y)}$. If y^* is a weak minima of $J = \int \mathcal{L}$, then

$$0 \leq -\frac{\partial^2}{\partial \alpha^2} \tilde{H}|_{\partial_x y^*}$$

So in particular H is maximized along optimal controls with respect to the control variable.

In addition, we have the following:

Theorem 4.4: Legendre-Clebsch

If u^* is a minimizing control then

$$\nabla_{uu}^{\otimes 2} H|_{t, X^*, u^*, p^*}$$

is negative semidefinite for all t .

Proof. The general idea is to explicitly write out the second variation ζ for the cost in the control as we did for the first variation. The entire Hessian

$$\nabla^{\otimes^2} H = \begin{bmatrix} \nabla_{xx}^{\otimes^2} H & \nabla_{ux}^{\otimes^2} H \\ \nabla_{xu}^{\otimes^2} H & \nabla_{uu}^{\otimes^2} H \end{bmatrix}$$

appears but only the uu term depends on the ε perturbation. □

4.2 Second Order Sufficient Conditions

We now explore sufficient conditions. The general form is

Theorem 4.5

Let J be a functional on \mathfrak{X} a normed vector space. If $x^* \in \mathfrak{X}$ is such that the first and second variations exist, and also $\gamma > 0$ is such that

$$\delta J|_{x^*}(q) = 0, \quad \delta^2 J|_{x^*}(q) \geq \gamma \|q\|_{1,\infty}^2$$

for all q , then x^* is a strict local minima.

Note that when deriving the second order necessary condition, we expanded the cost function in the input for CoV and obtained a remainder term $o(\alpha^2; \eta)$. This remainder term can be explicitly written as

$$\alpha^2 \int_a^b [Q\eta^2 + P(\partial\eta)^2] ds$$

where Q, P are functions of $(x, \eta, \partial\eta, \alpha)$ and as $\alpha \rightarrow 0$, Q, P converge uniformly to 0 in $\|\cdot\|_{1,\infty}$.

Definition 4.2

A point $c \in (a, b]$ is called a **conjugate point to the Jacobi equation** relative to a if $v(c) = v(a)$, where v solves the differential equation

$$Q(x; y, L)v(x) = \frac{d}{dx} \left(P(x; y, L) \frac{d}{dx} v(x) \right)$$

Generally speaking, conjugate points are convergence points of geodesics; in our case they are a degeneracy condition that can prevent optimality of a solution. This allows us to convert our necessary condition into a sufficient one, removing this degeneracy condition.

Theorem 4.6

If y^* is a weak extremal such that

$$0 < \frac{\partial^2}{\partial v^2} \mathcal{L}|_{(x, y^*(x), \partial y^*(x))}, \quad x \in [a, b]$$

and there are no conjugate points to the Jacobi equation on $[a, b]$, then y^* is a strict (weak) local minimum.

4.3 Corner Conditions

Definition 4.3

A function ψ on $[a, b]$ is in the piecewise continuous space of order k , denoted $\psi \in \text{PC}^k$, if it is C^{k-1} and is C^k on each of a finite number of intervals partitioning $[a, b]$. A **corner point** is one of the boundaries between these intervals.

For $\psi \in \text{PC}^1$, for each $t^* \in [a, b]$ we denote

$$\begin{aligned} \partial\psi^-(t^*) &= \lim_{t \rightarrow t^{*-}} \frac{\psi(t) - \psi(t^*)}{t - t^*} \\ \partial\psi^+(t^*) &= \lim_{t \rightarrow t^{*+}} \frac{\psi(t) - \psi(t^*)}{t - t^*} \end{aligned}$$

Theorem 4.7

Let $J = \int_a^b \mathcal{L} dx$ for a C^3 Lagrangian, and suppose we seek to optimize over

$$y^* = \operatorname{argmin} \left\{ J(y) : y \in (\text{PC}^1, \|\cdot\|_{0,\infty}), y(a) = y_0, y(b) = y_1 \right\}$$

Define the auxiliary Lagrangian

$$\tilde{\mathcal{L}}(x, u, v) = \langle v, \partial_v \mathcal{L}(x, u, v) \rangle - \mathcal{L}(x, u, v)$$

If y^* is a strong local extremum and (c_i) is the collection of corner points for y^* , then y^* satisfies Euler-Lagrange between the corner points, and for any corner point c_i ,

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0^+} \partial_v \mathcal{L}|_{c_i + \varepsilon} - \partial_v \mathcal{L}|_{c_i - \varepsilon} &= 0 \\ \lim_{\varepsilon \rightarrow 0^+} \tilde{\mathcal{L}}|_{c_i + \varepsilon} - \tilde{\mathcal{L}}|_{c_i - \varepsilon} &= 0 \end{aligned}$$

Proof. Without loss of generality assume there is only one corner point $c \in (a, b)$. Let y denote the strong extremum.

Now we work to define the class of admissible perturbations. Because the corner point is

able to move, define $c(\alpha) = c + \alpha\Delta x$, where $\delta x \in \mathbb{R}$ is fixed. We will define y_1 to be the linear extrapolation of the left hand side of y :

$$y_1(x) = \begin{cases} y(x), & x \in [a, c] \\ y(c) + \partial y^-|_c(x - c), & x \in (c, b] \end{cases}$$

and similarly we extrapolate the right hand side as y_2 . Similarly, let η be a function which is C^1 on $[a, c)$ and $(c, b]$ (though not necessarily continuous at c), which satisfies $\eta(a) = \eta(b) = 0$. Extend η at c similarly:

$$\eta_1(x) = \begin{cases} \eta(x), & x \in [a, c] \\ \eta(c) + \partial \eta^-|_c(x - c), & x \in (c, b] \end{cases} \quad (4.1)$$

Finally, for small $\alpha\Delta x$, we define

$$y(x; \alpha) = \begin{cases} y_1(x) + \alpha\eta_1(x), & x \in [a, c(\alpha)] \\ y_2(x) + \alpha\eta_2(x), & x \in (c(\alpha), b] \end{cases}$$

and although η is not required to be continuous, y is, so the continuity requirement on η is

$$y_1(c(\alpha)) + \alpha\eta_1(c(\alpha)) = y_2(c(\alpha)) + \alpha\eta_2(c(\alpha))$$

Define J_1, J_2 such that

$$J(y) = \int_a^b \mathcal{L} dx = \int_a^c \mathcal{L}|_{y_1} dx + \int_c^b \mathcal{L}|_{y_2} dx = J_1(y_1) + J_2(y_2)$$

Then $\delta J|_y = \delta J_1|_{y_1} = \delta J_2|_{y_2}$. Taking the first variation and applying Leibniz's rule and integrating by parts,

$$\begin{aligned} J_1(y_1 + \alpha\eta_1, \alpha\Delta x) &= \int_a^{c+\alpha\Delta x} \mathcal{L}(x, y_1 + \alpha\eta_1, \partial y_1 + \alpha\eta_1) dx \\ \implies 0 = \delta J_1|_{y_1}(\eta_1) &= \frac{d}{d\alpha}|_{\alpha \rightarrow 0^+} \int_a^{c+\alpha\Delta x} \mathcal{L}(x, y_1 + \alpha\eta_1, \partial y_1 + \alpha\eta_1) dx \\ &= \int_a^c \partial_u \mathcal{L}(x, y_1, \partial y_1) \eta_1 + \partial_v \mathcal{L}(x, y_1, \partial y_1) \partial \eta_1 dx + \mathcal{L}(c, y_1(c), \partial y_1(c)) \Delta x \\ &= \int_a^c (\partial_u - \partial_x \partial_v) \mathcal{L}(x, y_1, \partial y_1) \eta_1 dx + \partial_v \mathcal{L}(x, y_1, \partial y_1) \eta_1|_a^c + \mathcal{L}(c, y_1(c), \partial y_1(c)) \\ &= \int_a^c (\partial_u - \partial_x \partial_v) \mathcal{L}(x, y_1, \partial y_1) \eta_1 dx + \partial_v \mathcal{L}(x, y_1(c), \partial y_1(c)) \eta_1(c) + \mathcal{L}(c, y_1(c), \partial y_1(c)) \end{aligned}$$

In particular we can specialize to the case where $\Delta x = \eta_1(c) = \eta_2(c)$. Applying the extremum condition on y gives Euler-Lagrange on $[a, c]$. So the first term drops out. The same is true for y_2 , with signs flipped:

$$\begin{aligned} \delta J_1|_{y_1} &= \partial_v \mathcal{L}(x, y_1(c), \partial y_1(c)) \eta_1(c) + \mathcal{L}(c, y_1(c), \partial y_1(c)) \\ \delta J_2|_{y_2} &= -\partial_v \mathcal{L}(x, y_2(c), \partial y_2(c)) \eta_2(c) - \mathcal{L}(c, y_2(c), \partial y_2(c)) \end{aligned}$$

We differentiate □

We observe that the auxiliary Lagrangian as defined here is the Hamiltonian of the system, and $\partial_v \mathcal{L} = p$ is the costate. So this result tells us that both the Hamiltonian and the costate must be continuous at the corner points.

Definition 4.4

Let \mathcal{L} be the Lagrangian to a system. The **Weierstrass excess function** is $E : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ defined by

$$(t, y, z, w) \mapsto \mathcal{L}(t, y, w) - \mathcal{L}(t, y, z) - \langle \partial_z \mathcal{L}(t, y, z), w - z \rangle$$

Theorem 4.8: Weierstrass Strong Necessary Condition

Let y^* be a strong local minimum over $\mathfrak{Z}_{0,1}$ of a Lagrangian problem. If $(c_i)_{i=0}^l$ are the corner points of y^* in $[a, b]$ with $c_0 = a, c_l = b$, then

$$E(x, y(x), \partial_x y(x), w) \geq 0 \quad \forall x \in [a, b] \setminus \{c_i\}, w \in \mathbb{R}$$

Proof. The result is local so let x^* be in a small interval $[x^*, d]$ which contains no corner points. Let $w \in \mathbb{R}$ and define

$$y_\varepsilon(x) = \begin{cases} y(x), & x \leq x^*, x \geq d \\ y(x^*) + w(x - x^*), & x \in [x^*, x^* + \varepsilon] \\ y(x) + \frac{d-x}{d-(x^*+\varepsilon)}(y(x^*) + w\varepsilon - y(x^* + \varepsilon)), & x \in [x^* + \varepsilon, d] \end{cases}$$

Then $\|y_\varepsilon - y\|_{0,\infty} \leq w\varepsilon$, so $\|y_\varepsilon - y\|_{0,\infty} \rightarrow 0$. We evaluate J :

$$\begin{aligned} J(y_\varepsilon) &= \int_a^{x^*} \mathcal{L}(x, y, \partial y) dx + \int_{x^*}^{x^*+\varepsilon} \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) dx \\ &\quad + \int_{x^*+\varepsilon}^d \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) dx + \int_d^b \mathcal{L}(x, y, \partial y) dx \end{aligned}$$

We differentiate with respect to ε to isolate the middle terms. The second term is

$$\begin{aligned} \frac{d}{d\varepsilon} \int_{x^*}^{x^*+\varepsilon} \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) dx &= \mathcal{L}(x^* + \varepsilon, y_\varepsilon(x^* + \varepsilon), \partial y_\varepsilon(x^* + \varepsilon)) \\ &= \mathcal{L}(x^* + \varepsilon, y(x^*) + w\varepsilon, w) \end{aligned}$$

The third term is

$$\begin{aligned} \frac{d}{d\varepsilon} \int_{x^*+\varepsilon}^d \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) dx &= -\mathcal{L}(x^* + \varepsilon, y_\varepsilon(x^* + \varepsilon), \partial y_\varepsilon(x^* + \varepsilon)) \\ &\quad + \int_{x^*+\varepsilon}^d [\partial_u \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) \partial_\varepsilon y_\varepsilon + \partial_v \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) \partial_\varepsilon \partial_x y_\varepsilon] dx \end{aligned}$$

We integrate by parts the second term of the integral

$$\int_{x^*+\varepsilon}^d \partial_v \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) \partial_x \partial_\varepsilon y_\varepsilon = \partial_\varepsilon y_\varepsilon \partial_v \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) \Big|_{x^*+\varepsilon}^d - \int_{x^*+\varepsilon}^d \partial_x \partial_v \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) \partial_\varepsilon y_\varepsilon \, dx$$

To evaluate the boundary term, we have

$$\begin{aligned} \partial_\varepsilon y_\varepsilon(x) &= (w - \partial y(x^* + \varepsilon)) \frac{d - x}{d - (x^* + \varepsilon)} + \frac{d - x}{(d - (x^* + \varepsilon))^2} (y(x^*) + w\varepsilon - y(x^* + \varepsilon)) \\ &\implies \partial_\varepsilon y_\varepsilon(x^* + \varepsilon) \xrightarrow{\varepsilon \rightarrow 0} (w - \partial y(x^*)) \\ &\quad \partial_\varepsilon y_\varepsilon(d) = 0 \\ y_\varepsilon(x^* + \varepsilon) &= y(x^*) + w\varepsilon \xrightarrow{\varepsilon \rightarrow 0} y(x^*) \\ \partial_x^+ y_\varepsilon(x^* + \varepsilon) &= \partial_x y(x^* + \varepsilon) - \frac{y(x^*) + w\varepsilon - y(x^* + \varepsilon)}{d - (x^* + \varepsilon)} \xrightarrow{\varepsilon \rightarrow 0} \partial_x y(x^*) \end{aligned}$$

so

$$\lim_{\varepsilon \rightarrow 0^+} \partial_\varepsilon y_\varepsilon \partial_v \mathcal{L}(x, y_\varepsilon, \partial y_\varepsilon) \Big|_{x^*+\varepsilon}^d = -(w - \partial y(x^*)) \partial_v \mathcal{L}(x^*, y(x^*), \partial_x y(x^*))$$

As $\varepsilon \rightarrow 0$, second term in the original integral becomes

$$\mathcal{L}(x^*, y(x^*), w)$$

and the third is

$$\begin{aligned} & -\mathcal{L}(x^*, y(x^*), \partial_x y(x^*)) - (w - \partial y(x^*)) \partial_v \mathcal{L}(x^*, y(x^*), \partial y(x^*)) \\ & \quad + \int_{x^*}^d [\partial_u \mathcal{L}(x, y, \partial y) - \partial_x \partial_v \mathcal{L}(x, y, \partial y)] \partial_\varepsilon x \, dx \end{aligned}$$

Since y is a strong local minimum the integral vanishes by Euler-Lagrange. Also, since it is a minimum and $y_\varepsilon \rightarrow y$ in $\mathfrak{Z}_{0,1}$,

$$\begin{aligned} 0 &\leq \frac{d}{d\varepsilon} J(y_\varepsilon) = \mathcal{L}(x^*, y(x^*), w) - \mathcal{L}(x^*, y(x^*), \partial_x y(x^*)) \\ &\quad - \langle \partial_v \mathcal{L}(x^*, y(x^*), \partial_x y(x^*)), (w - \partial_x y(x^*)) \rangle = E(x^*, y(x^*), \partial_x y(x^*), w) \end{aligned} \quad \square$$

In the Hamiltonian formulation, with the definition $p(x; y) = \partial_v \mathcal{L}(x, y(x), \partial_x y(x))$, then

$$E(x, y(x), \partial_x y(x), w) = H(x, y(x), \partial_x y(x), p(x)) - H(x, y(x), w, p(x)) \geq 0$$

so a strong local minima maximizes H as $\partial_x y(x)$ ranges over fixed y, p for all non-corner points x , together with the corner conditions this implies it is true for all x . This is Pontryagin's maximum principle for the class of PC^1 curves.

Chapter 5

Pontryagin's Maximum Principle

The Pontryagin Maximum Principle extends the results on Hamiltonian extrema that we have derived to classes of functions with less regularity than PC^1 , as well as by allowing us to work with functions with bounded codomains. Moreover, working in the Hamiltonian formulation gives global conditions in $x \in U$, rather than local conditions at the extrema.

The setting of the Principle is the following: we seek to maximize an objective in autonomous Lagrangian form:

$$\inf J(u, t_f; t_0, X_0, X_f) = \int_{t_0}^{t_f} \mathcal{L}(X_s, u_s) ds$$

with admissible control set

$$u \in \mathcal{U} = PC([t_0, \infty) \rightarrow U \subseteq \mathbb{R}^n)$$

dynamics

$$dX_t = f(X_t, u_t) dt$$

and regularity

$$\begin{aligned} \mathcal{L} &\in C^{1,0}(\mathbb{R}^m, \mathbb{R}^n \rightarrow \mathbb{R}) \\ f &\in C^{1,0}(\mathbb{R}^m, \mathbb{R}^n \rightarrow \mathbb{R}^m) \end{aligned}$$

($C^{1,0}$ means that these functions are C^1 in the state but only continuous in the control).

Definition 5.1

A control u^* is optimal in the L^1 sense if there exists $\varepsilon > 0$ such that $J(u^*) \leq J(u)$ for any $u \in \bar{\mathcal{U}}$ with

$$\int_{t_0}^{t_f^*} |u_s^* - u_s| ds < \varepsilon$$

Theorem 5.1: Pontryagin's Maximum Principle

If u^* is an optimal control in the L^1 sense, and X^* is the state generated by it, then there exists $P^* \in C^1([t_0, t_f^*] \rightarrow \mathbb{R}^m)$ and a number $p_0^* \leq 0$ such that

$$(p_t^*, p_0^*) \neq (0, 0) \quad \forall t \in [t_0, t_f^*]$$

and the Hamiltonian canonical equation holds:

$$\begin{aligned} \dot{X}_t^* &= \nabla_p \mathcal{H}|_* \\ \dot{p}_t^* &= -\nabla_x \mathcal{H}|_* \end{aligned}$$

which is a $2m$ -dimensional ODE, possibly with $2m$ boundary conditions given by X_0, X_f . Recall the control Hamiltonian is given by

$$\mathcal{H}(x, u; p, p_0) = \langle p, f(x, u) \rangle + p_0 \mathcal{L}(x, u)$$

If u^* is an optimal control and X^*, p^* are the associated state and costate, then for any $t \in [t, t_f^*]$ and any $u \in \mathcal{U}$,

$$\mathcal{H}(X_t^*, u, p_t^*, p_0^*) \leq \mathcal{H}(X_t^*, u_t^*, p_t^*, p_0^*) = 0$$

5.1 Proof of Pontryagin's Maximum Principle

We begin by converting the Lagrange form problem to a Mayer form problem, by adding a state variable to track the running cost:

$$Y_t = \begin{bmatrix} X_t \\ X_t^0 \end{bmatrix}$$

where $X_t^0 \in \mathbb{R}$, $X_0^0 = 0$, and the new dynamics are

$$dY_t = \begin{bmatrix} f(X_t, u_t) \\ \mathcal{L}(X_t, u_t) \end{bmatrix} dt = g(Y_t, u_t) dt$$

and the Mayer cost is

$$K(Y_{t_f}) = X_{t_f}^0$$

Now we consider time perturbations to the optimal control. Define

$$t_f(\tau; \varepsilon) = t_f^* + \tau \varepsilon$$

Then we consider time perturbations of the form

$$u(t; \tau, \varepsilon) = u^*(\min\{t, t_f^*\}), \quad t \in [0, t_f(\tau; \varepsilon)]$$

Then the final state under the perturbation is

$$Y_{t_f(\tau; \varepsilon)} = Y_{t_f^*}^* + \frac{d}{dt} Y^*|_{t_f^*} \varepsilon \tau + o(\varepsilon) = Y_{t_f^*}^* + g(Y_{t_f^*}^*, u_{t_f^*}^*) \varepsilon \tau + o(\varepsilon) = Y_{t_f^*}^* + \varepsilon \delta(\tau) + o(\varepsilon)$$

which means that to first order, the reachable final states lie in the convex cone

$$\mathcal{C}_t = \left\{ Y_{t_f}^* + \delta(\tau), \tau \in \mathbb{R} \right\}$$

(which is 1-dimensional since δ is linear in τ).

Now we consider spatial control perturbations. If b is a point of continuity of u^* , then define

$$u(t; b, \varepsilon, a, w) = \begin{cases} u(t) : t \notin I(b, \varepsilon, a) := (b - \varepsilon a, b] \\ w \in U : t \in I(b, \varepsilon, a) \end{cases}$$

Essentially this overrides the control for a small period in time. The parameters w, b control where this perturbation happens (corresponding to a direction in \mathcal{U} -space), and ε, a control the size of this perturbation. To evaluate the resulting state perturbation, we have

$$Y_{b-\varepsilon a}^* = Y_b^* - g(Y_b^*, u_b^*)\varepsilon a + o(\varepsilon)$$

On the other hand, under the perturbation we have

$$Y_b = Y_{b-\varepsilon a} + \partial_t^+ Y_{b-\varepsilon a} \varepsilon a + o(\varepsilon) = Y_{b-\varepsilon a}^* + g(Y_{b-\varepsilon a}^*, w)\varepsilon a + o(\varepsilon)$$

since the state up to $b - \varepsilon a$ is unchanged. Expanding g , we have

$$\begin{aligned} g(Y_{b-\varepsilon a}^*, w) &= g(Y_b^*, w) + \partial_y g(y_b^*, w)(Y_{b-\varepsilon a}^* - Y_b^*) + o(\varepsilon) \\ &= g(Y_b^*, w) - \partial_y g(Y_b^*, w)g(Y_b^*, u_b^*)\varepsilon a + o(\varepsilon) \end{aligned}$$

so

$$Y_b = Y_{b-\varepsilon a}^* + g(Y_b^*, w)\varepsilon a + \varepsilon^2 a^2 g(Y_b^*, u_b^*)\partial_y g(Y_b^*, w) + o(\varepsilon) = Y_{b-\varepsilon a}^* + g(Y_b^*, w)\varepsilon a + o(\varepsilon)$$

meaning

$$Y_b - Y_b^* = \varepsilon a(g(Y_b^*, w) - g(Y_b^*, u_b^*)) + o(\varepsilon) = \varepsilon a \nu_b(w) + o(\varepsilon) = \varepsilon \eta_b + o(\varepsilon)$$

Now, we analyze this variation using the calculus of variations. We have

$$\begin{aligned} \dot{\eta}_s &= \nabla_y g|_{Y_s^*, u_s^*} \eta_s \\ \nabla_y g &= \begin{bmatrix} \nabla_x f & 0 \\ \nabla_x \mathcal{L} & 0 \end{bmatrix} \end{aligned}$$

and we can wrap this in a single formula for the final first order variation as

$$\eta_{t_f^*} = \phi(t_f^*, b)\eta_b$$

where ϕ is the state transition matrix taking the state at time b to the state at time t_f^* . So

$$Y_{t^*} = Y_{t^*}^* + \varepsilon \eta_{t_f^*} + o(\varepsilon) = Y_{t^*}^* + \varepsilon \delta(w, b, a) + o(\varepsilon)$$

So for each a , there is a first order one-dimensional reachable cone in ε .

Now we work out how to handle the combination of multiple needle perturbations.

Lemma 5.2

Let $I_1 = I(b_1, \varepsilon, a_1)$, $I_2 = I(b_2, \varepsilon, a_2)$ be disjoint, with $b_1 < b_2$, and $w_1, w_2 \in U$. Let Y_t be the path defined by perturbing the control at both I_1, I_2 . Then

$$Y_{t_f^*} - Y_{t_f^*}^* = \varepsilon \delta(w_1, b_1, a_1) + \varepsilon \delta(w_2, b_2, a_2) + o(\varepsilon)$$

Proof. We use the state transition matrix approach:

$$Y_{b_2} = Y_{b_2}^* + \varepsilon (\phi(b_2, b_1) \eta_{b_1}(I_1) + \eta_{b_2}(I_2)) + o(\varepsilon)$$

and

$$\begin{aligned} Y_{t_f^*} &= Y_{t_f^*}^* + \varepsilon \phi(t_f^*, b_2) (\phi(b_2, b_1) \eta_{b_1} + \eta_{b_2}) + o(\varepsilon) \\ &= Y_{t_f^*}^* + \varepsilon \phi_{t_f^*, b_1} \eta_{b_1} + \varepsilon \phi(t_f^*, b_2) \eta_{b_2} + o(\varepsilon) = \varepsilon \delta(w_1, b_1, a_1) + \varepsilon \delta(w_2, b_2, a_2) + o(\varepsilon) \quad \square \end{aligned}$$

When the needle perturbations are allowed to overlap, we instead get a convex combination of the perturbations:

$$Y_{t_f^*} - Y_{t_f^*}^* = \varepsilon \sum_{i=1}^k \gamma_i \delta(w_i, b_i, a_i) + o(\varepsilon), \quad \sum_i \gamma_i = 1$$

So our first order spatial reachable set is indeed the convex hull of the cones that we derived for the individual perturbations, and we define the entire first order reachable set C by the convex combination of the spatially and temporally reachable set.

Lemma 5.3

Define $\mu = (0, \dots, 0, -1) \in \mathbb{R}^{m+1}$, and define $C_\mu = \{Y_{t_f^*}^* + \beta \mu : \beta \geq 0\}$. Then $C_\mu \cap C^o = \emptyset$.

Proof. Assume not. Let $Y \in C_\mu \cap C^o$, and pick a ball $\overline{B}(Y, \varepsilon) \subseteq C^o$, and let β be such that $Y = Y_{t_f^*}^* + \varepsilon \beta \mu$. By definition, Y is the linear variation of some spatial and temporal perturbations. The actual realization of those is first order accurate but not exactly Y , so we write

$$Y_\varepsilon = Y_{t_f^*}^* + \varepsilon \beta \mu + o(\varepsilon)$$

Similarly for any $q \in \overline{B}(Y, \varepsilon)$, we can write $q = Y_{t_f^*}^* + \varepsilon v_q$, and then it follows that

$$q_\varepsilon = Y_{t_f^*}^* + \varepsilon v_q + o(\varepsilon)$$

The map $\psi_\varepsilon : q \mapsto q_\varepsilon$ is a continuous deformation of $\overline{B}(Y, \varepsilon)$ because of our dynamics.

Consider what happens as we take $\varepsilon \rightarrow 0$. Y approaches $Y_{t_f^*}^*$, and since C is a cone, $\overline{B}(Y, \varepsilon) \subseteq C^o$ for all ε . Also because C_μ is a cone, $\overline{B}(Y, \varepsilon) \cap C_\mu \neq \emptyset$ for all ε . We want to show that $\psi_\varepsilon(B(Y, \varepsilon)) = \tilde{B}(Y, \varepsilon)$ intersects C_μ for all sufficiently small ε . This implies that $Y_{t_f^*}^*$ is not optimal.

To show this, we know that for any $\alpha > 0$ there is $\delta > 0$ such that for $\delta' < \delta$,

$$d(\overline{B}(Y, \delta'), \psi_{\delta'}(\overline{B}(Y, \delta'))) = o(\delta') \leq \alpha\delta'$$

Fix $\alpha < 1$ and let $\eta = \alpha\delta'$. Then for $y \in \overline{B}(Y, \delta')$,

$$d(y, \psi_{\delta'}(y)) \leq \eta$$

Define

$$\begin{aligned} \overline{\psi}_{\delta'}(y; z) : \overline{B}(Y, \delta') \times \overline{B}(Y, \delta' - \eta) &\rightarrow \mathbb{R}^{m+1} \\ (y; z) &\mapsto y - \psi_{\delta'}(y) + z \end{aligned}$$

Then

$$|\overline{\psi}_{\delta'}(y; z)| \leq \eta + |z| \leq \delta'$$

So for any fixed z , $\overline{\psi}_{\delta'}(\cdot; z)$ is a continuous map from $\overline{B}(Y, \delta')$ into itself. By Brouwer's fixed point theorem, it has a fixed point y such that

$$y = \tilde{\psi}_{\delta'}(y; z) \implies \psi_{\delta'}(y) = z$$

In particular, taking $z = Y \in C_\mu$, we have that $\tilde{B}(Y, \varepsilon) \cap C_\mu \neq \emptyset$ for all ε , contradicting optimality. \square

Theorem 5.4: Separating Hyperplanes

Let $C, D \in \mathbb{R}^k$ be disjoint, nonempty, and convex. Then there is $a \in \mathbb{R}^k$ nonzero, $\alpha \in \mathbb{R}$ such that for any $x \in C, y \in D$,

$$\langle a, x \rangle \leq \alpha \leq \langle a, y \rangle$$

Theorem 5.5: Supporting Hyperplanes

If C is convex with nonempty interior and $z \in \partial C$, then there is $a \in \mathbb{R}^k$ nonzero, $\alpha \in \mathbb{R}$, such that for any $x \in C$,

$$\langle a, x \rangle \leq \alpha = \langle a, z \rangle$$

Given a, α from one of the two theorems, a hyperplane is determined by

$$G(a, \alpha) = \{x \in \mathbb{R}^k : \langle a, x \rangle = \alpha\}$$

In the case of Pontryagin, the sets C^o, C_μ satisfy the assumptions of one of the two theorems. So we are given

$$a = \overline{p}_{t_f^*} = (p_{t_f^*}^*, p_0^*) \in \mathbb{R}^{m+1}$$

We know the hyperplane must pass through the cone vertex $Y_{t_f^*}^*$, so the hyperplane is

$$G_{t_f^*} = \left\{ y : \langle \overline{p}_{t_f^*}^*, y \rangle = \langle \overline{p}_{t_f^*}^*, Y_{t_f^*}^* \rangle \right\}$$

So $\langle \bar{p}_{t_f}^*, \mu \rangle \leq 0$, which implies that $p_0^* \leq 0$. In the separating case we can choose $p_0^* < 0$. In the nonseparating case we must have $p_0^* = 0$, so there must be a choice of $p_{t_f}^*$ nonzero by the supporting hyperplane theorem. In either case

$$\bar{p}_{t_f}^* \neq 0 \in \mathbb{R}^{m+1}$$

Let Y^* be an optimal process to reach $X_{t_f}^*$. The principle of optimality says that for any $s < t_f^*$, the optimal path to X_s^* is also $Y_{t_f}^*$ (otherwise, there is a more efficient path to X_s^* , and then one takes the same path to $X_{t_f}^*$). We can ask whether there is some relationship between the costates at each point. To show that the Hamiltonian is maximized, we consider points of continuity and discontinuity separately. Let $s \in [t_0, t_f^*]$ be a point of continuity for $u^* \in \text{PC}$. The costates are chosen so that for any w , the hyperplanes give

$$\begin{aligned} 0 &\geq \langle p_{t_f}^*, \eta_{t^*} \rangle = \langle p_{t_f}^*, \Phi(s \rightarrow t_f^*) \eta_s \rangle = \langle \Phi(t_f^* \rightarrow s) p_{t_f}^*, \eta_s \rangle = \langle p_s^*, \eta_s \rangle \\ &= \langle p_s^*, \nu_s(w) a \rangle = a [H(X_s^*, w, p_s^*, p_0^*) - H(X_s^*, u_s^*, p_s^*, p_0^*)] \end{aligned}$$

For points of discontinuity, we can at least choose u to be continuous from one direction, and then take the limit, since H, f, \mathcal{L}, X, p are all continuous.

We have made the stronger claim that $H(u^*) = 0$. To see this at the final time, first recall that the first order reachable states are given by the convex cone C which is the convex combination of C_t, C_u , the temporal and spatial reachable cones. Moreover, we know that $\langle p_{t_f}^*, \eta \rangle \leq 0$ for any $\eta \in C - Y_{t_f}^*$. In particular this is true for temporally reachable perturbations. Recall that $\eta(\tau) = g(Y_{t_f}^*, u_{t_f}^*) \tau$ for $\tau \in \mathbb{R}$. In particular since this is true for τ both positive and negative, we must have that this inner product is zero, so

$$H(X_{t_f}^*, u_{t_f}^*, p_{t_f}^*, p_0^*) = 0$$

We argued earlier that H_* might be only left- or right-continuous where u^* is discontinuous. But actually the continuity of X^*, p^* combined with the maximum principle gives a stronger result.

Lemma 5.6

$H_*(s)$ is continuous.

Proof. As argued above this is true where u^* is continuous. Let s be a point of discontinuity for u^* . $u^* \in \text{PC}$ has isolated points of discontinuity, so there is an interval $(s - \varepsilon, s + \varepsilon)$ with no other points of discontinuity. Then by the maximum principle,:

$$\begin{aligned} \lim_{t \rightarrow s^-} H(X_t^*, u_{s+}^*, p_t^*, p_0^*) &= H(X_{s-}^*, u_{s+}^*, p_{s-}^*, p_0^*) \leq H(X_{s-}^*, u_{s-}^*, p_{s-}^*, p_0^*) \\ \lim_{t \rightarrow s^+} H(X_t^*, u_{s-}^*, p_t^*, p_0^*) &= H(X_{s+}^*, u_{s-}^*, p_{s+}^*, p_0^*) \leq H(X_{s+}^*, u_{s+}^*, p_{s+}^*, p_0^*) \end{aligned}$$

By continuity of X, p , we have

$$H(X_s^*, u_{s+}^*, p_s^*, p_0^*) \leq H(X_s^*, u_{s-}^*, p_s^*, p_0^*) \leq H(X_s^*, u_{s+}^*, p_s^*, p_0^*)$$

so H_* is continuous. □

We also want to show that $H|_*(u^*) = 0$ at all times. Define

$$M(x, p) = \sup_{u \in U} H(x, u, p, p_0^*)$$

When x, p are taken to be X_t^*, p_t^* , M is continuous in time. By the maximum principle,

$$\begin{aligned} H(X_s^*, u_t^*, p_s^*, p_0^*) - H(X_t^*, u_t^*, p_t^*, p_0^*) &\leq M(X_s^*, p_s^*) - M(X_t^*, p_t^*) = H|_*(s) - M(X_t^*, p_t^*) \\ &\leq H|_*(s) - H(X_t^*, u_s^*, p_t^*, p_0^*) \end{aligned}$$

We expand the time derivative of H :

$$\begin{aligned} \left. \frac{d}{dt} H(X_t^*, w, p_t^*, p_0^*) \right|_s &= \langle p_s^*, f(X_s^*, w) \rangle + \langle p_s^*, \nabla_x f(X_s^*, w) \dot{X}_s^* \rangle + \langle p_0^*, \nabla_x \mathcal{L}(X_s^*, w) \dot{X}_s^* \rangle \\ &= \langle \nabla_x f^T|_* p_s^*, f(X_s^*, w) \rangle - p_0^* \langle \nabla_x \mathcal{L}(X_s^*, u_s^*), f(X_s^*, w) \rangle \\ &\quad + \langle p_s^*, \nabla_x f(X_s, w) f|_* \rangle + p_0^* \langle \nabla_x \mathcal{L}(X_s^*, w), f|_* \rangle \end{aligned}$$

f, \mathcal{L} are C^1 in time, p^*, X^* are continuous in time, and u^* is PC in time, so all the terms are uniformly bounded in $s \in [t_0, t_f^*]$, $w = u^*(\tau)$. So

$$|M(X_s^*, p_s^*) - M(X_t^*, p_t^*)| \leq L_H |t - s|$$

So M is Lipschitz, hence absolutely continuous, and $\dot{M}_t = 0$ almost everywhere. So $H|_* \equiv 0$.

5.2 Generalizations

The maximum principle admits many changes to the assumptions, with slight modifications to the conclusions. For instance, suppose that the right endpo condition is no longer fixed but simply that $X_{t_f} \in M_f$ for some manifold

$$M_f = \{h_i(x) = 0, 1 \leq i \leq k\}$$

Then the existence of nontrivial costates for the canonical Hamiltonian equations still holds. Moreover, if X_{t_f} is a regular point of M_f , then there is an additional transversality condition:

$$\langle p_{t_f}^*, d \rangle = 0$$

for any $d \in T_{X_{t_f}^*} M_f$.

This arises the the topological lemmas. The cone C_μ represented the linearly feasible space of final states with lower cost. Since $X_{t_f}^*$ is now linearly free up to the tangent space, the new cone is

$$C_{\mu, M} = \left\{ Y_{t_f}^* + \beta \mu + (d, 0) : \beta \geq 0, d \in T_{X_{t_f}^*} M_f \right\}$$

Then the lemma that $C_{\mu, M}^o \cap C^o = \emptyset$ is proved the same way, except that we have to require that ε is small enough that $T_{X_{t_f}^*} M_f$ approximates M_f to order $o(\varepsilon)$. The proofs of

the separating and supporting hyperplanes proceeds identically. In particular, the tangent space is now represented in our cone, so

$$\langle p_{t_f^*}^*, d \rangle \leq 0$$

for any d in the tangent space. (Recall that using the same inequality for $d = \mu$ gave $p_0^* \leq 0$). Since $-d$ is also in the tangent space, we see that $p_{t_f^*}^*$ is precisely orthogonal to M_f .

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