Numerical Optimal Control

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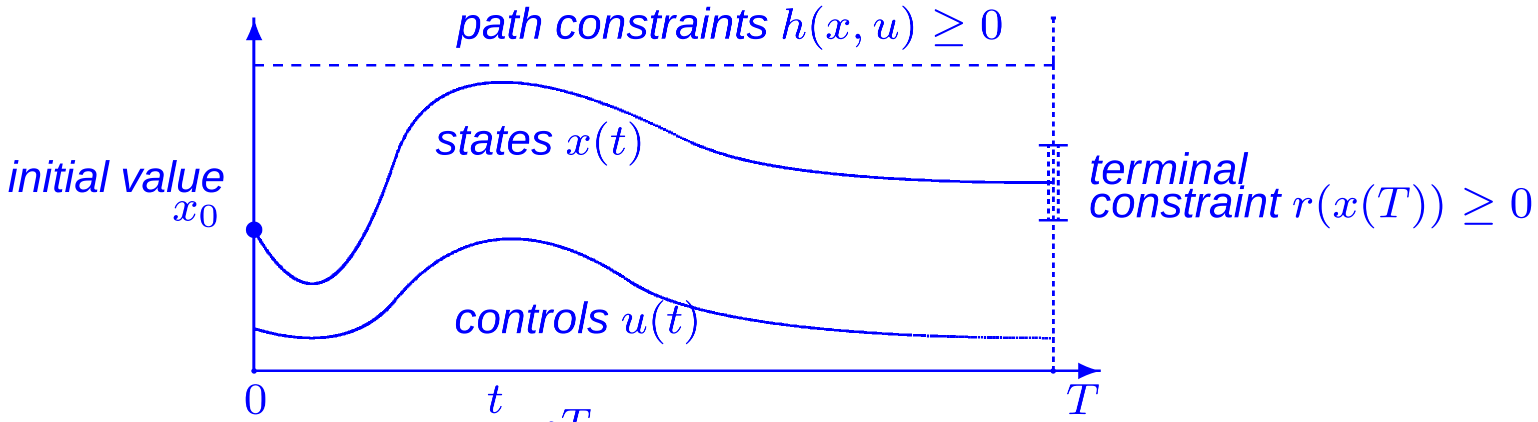
Simplified Optimal Control Problem in ODE



$$\underset{x(\cdot),\,u(\cdot)}{\text{minimize}} \quad \int_0^T L(x(t),u(t))\,dt \; + \; E\,(x(T))$$

subject to

$$\begin{aligned}
x(0) - x_0 &= 0, && && \text{(fixed initial value)} \\
\dot{x}(t) - f(x(t),u(t)) &= 0, && t \in [0,T], && \text{(ODE model)} \\
h(x(t),u(t)) &\geq 0, && t \in [0,T], && \text{(path constraints)} \\
r\,(x(T)) &\geq 0 && && \text{(terminal constraints).}
\end{aligned}$$

More general optimal control problems

Many features left out here for simplicity of presentation:

- multiple dynamic stages
- differential algebraic equations (DAE) instead of ODE
- explicit time dependence
- constant design parameters
- multipoint constraints $r(x(t_0), x(t_1), \ldots, x(t_{\mathrm{end}})) = 0$

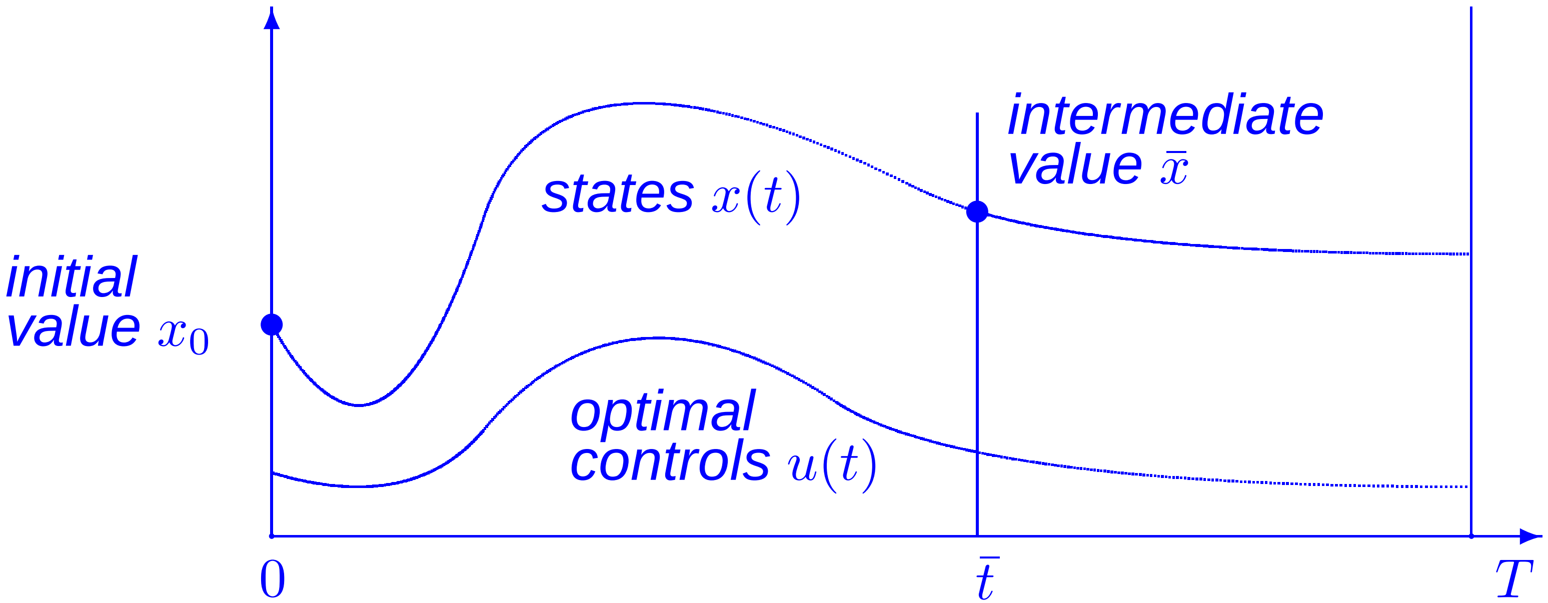
Optimal Control Family Tree

Three basic families:

- Hamilton-Jacobi-Bellmann equation / dynamic programming
- Indirect Methods / calculus of variations / Pontryagin
- Direct Methods (control discretization)

Principle of Optimality

Any subarc of an optimal trajectory is also optimal.



Subarc on $[\bar{t}, T]$ is optimal
solution for initial value $\bar{x}$.

Dynamic Programming Cost-to-go

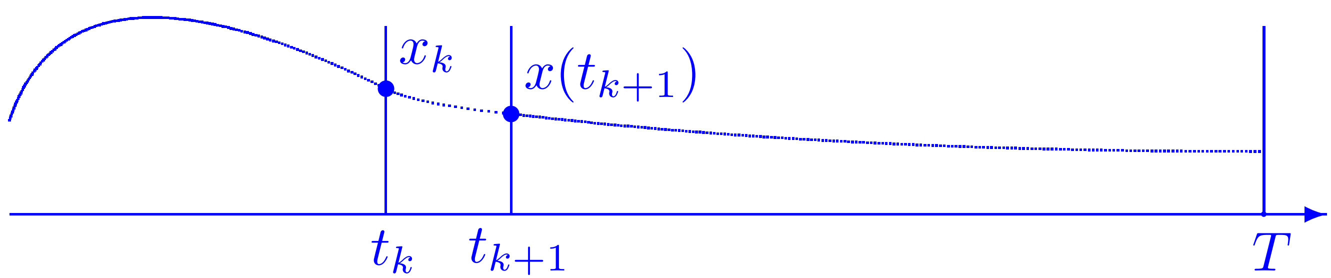
IDEA:

- Introduce **optimal-cost-to-go** function on $[\bar{t}, T]$

$$J(\bar{x}, \bar{t}) := \min_{x,u} \int_{\bar{t}}^{T} L(x,u)dt \ + \ E(x(T)) \ \text{ s.t. } \ x(\bar{t}) = \bar{x}, \ldots$$

- Introduce grid $0 = t_0 < \ldots < t_N = T$.
- Use **principle of optimality** on intervals $[t_k, t_{k+1}]$:

$$J(x_k, t_k) = \min_{x,u} \int_{t_k}^{t_{k+1}} L(x,u)dt + J(x(t_{k+1}), t_{k+1}) \ \text{ s.t. } \ x(t_k) = x_k, \ldots$$



Dynamic Programming Recursion

Starting from $J(x, t_N) = E(x)$, compute recursively backwards, for $k = N-1, \dots, 0$

$$J(x_k, t_k) := \min_{x,u} \int_{t_k}^{t_{k+1}} L(x,u)dt \; + \; J(x(t_{k+1}), t_{k+1}) \;\; \text{s.t.} \;\; x(t_k) = x_k, \dots$$

by solution of short horizon problems for all possible x_k and tabulation in state space.

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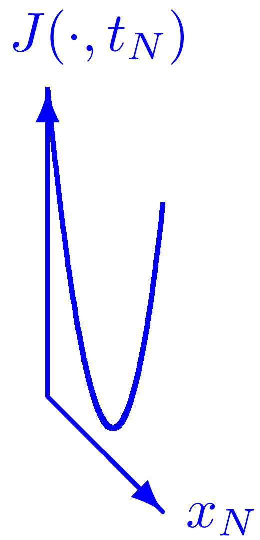

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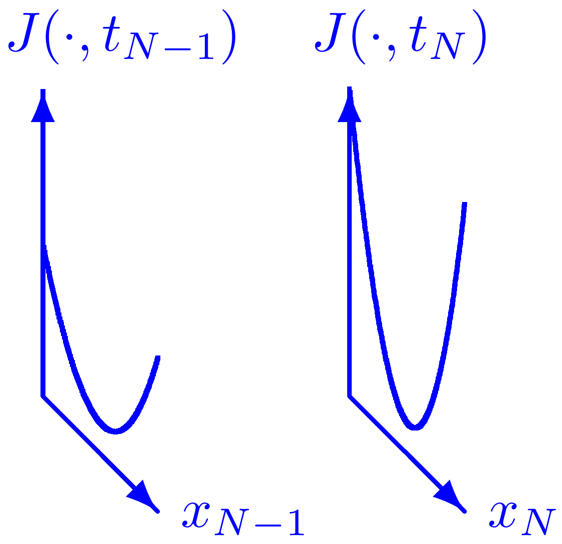

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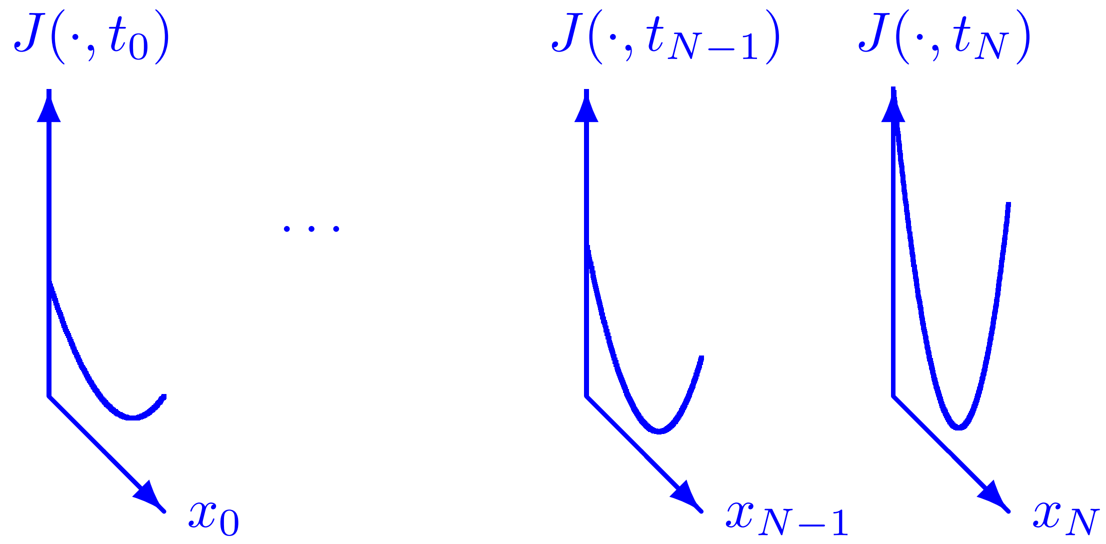
by solution of short horizon problems for all possible x_k and tabulation in state space.



Hamilton-Jacobi-Bellman (HJB) Equation

Dynamic Programming with infinitely small timesteps leads to **Hamilton-Jacobi-Bellman (HJB) Equation**:

$$-\frac{\partial J}{\partial t}(x,t) = \min_u \left(L(x,u) + \frac{\partial J}{\partial x}(x,t) f(x,u) \right) \quad \text{s.t.} \quad h(x,u) \geq 0.$$

Solve this partial differential equation (PDE) backwards for $t \in [0,T]$, starting at the end of the horizon with

$$J(x,T) = E(x).$$

NOTE: Optimal controls for state x at time t are obtained from

$$u^*(x,t) = \arg\min_u \left(L(x,u) + \frac{\partial J}{\partial x}(x,t) f(x,u) \right) \quad \text{s.t.} \quad h(x,u) \geq 0.$$

Dynamic Programming / HJB: Pros and Cons

- “Dynamic Programming” applies to discrete time, “HJB” to continuous time systems.

+ Searches whole state space, finds global optimum.

+ Optimal feedback controls precomputed.

+ Analytic solution to some problems possible (linear systems with quadratic cost $\rightarrow$ Riccati Equation)

- “Viscosity solutions” (Lions et al.) exist for quite general nonlinear problems.

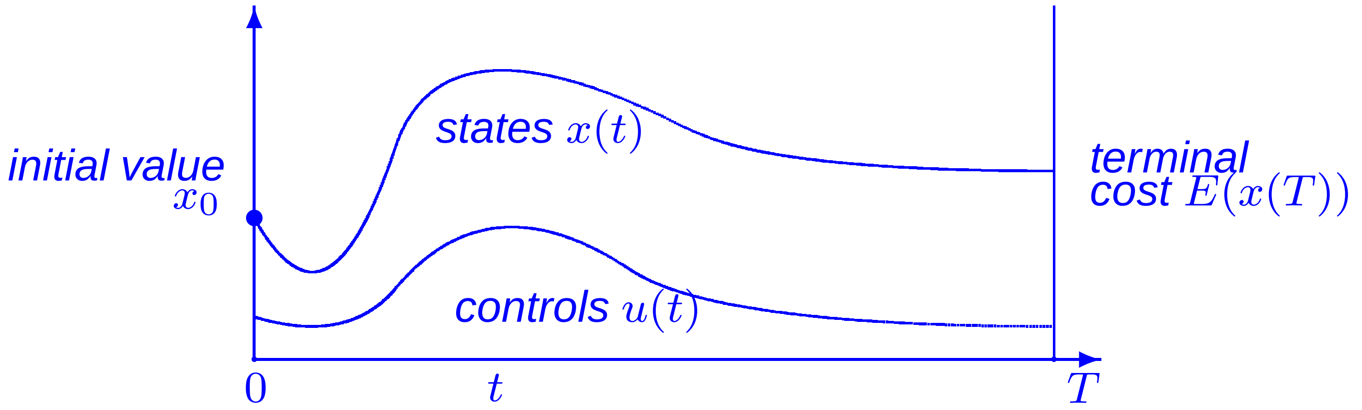
- But: in general intractable, because partial differential equation (PDE) in high dimensional state space: “curse of dimensionality”.

- Possible remedy: Approximate J e.g. in framework of neuro-dynamic programming (Bertsekas and Tsitsiklis, 1996).

- Used for practical optimal control of small scale systems e.g. by Bonnans, Zidani, Lee, Back, ...

Indirect Methods

For simplicity, regard only problem without inequality constraints:



$$\underset{x(\cdot),\,u(\cdot)}{\text{minimize}} \quad \int_0^T L(x(t),u(t))\,dt \;+\; E\left(x(T)\right)$$

subject to

$$\begin{aligned} x(0)-x_0 &= 0, && && \text{(fixed initial value)} \\ \dot{x}(t)-f(x(t),u(t)) &= 0, && t \in [0,T]. && \text{(ODE model)} \end{aligned}$$

Pontryagin's Minimum Principle

OBSERVATION: In HJB, optimal controls

$$u^*(t) = \arg\min_u \left(L(x,u) + \frac{\partial J}{\partial x}(x,t) f(x,u) \right)$$

depend only on derivative $\frac{\partial J}{\partial x}(x,t)$, not on J itself!

IDEA: Introduce **adjoint variables** $\lambda(t) \quad \hat{=} \quad \frac{\partial J}{\partial x}(x(t),t)^T \in \mathbb{R}^{n_x}$ and get controls from **Pontryagin's Minimum Principle**

$$u^*(t,x,\lambda) = \arg\min_u \left(\underbrace{L(x,u) + \lambda^T f(x,u)}_{\textbf{Hamiltonian} =: H(x,u,\lambda)} \right)$$

QUESTION: How to obtain $\lambda(t)$?

Adjoint Differential Equation

- Differentiate HJB Equation

$$-\frac{\partial J}{\partial t}(x,t) = \min_u H(x, u, \frac{\partial J}{\partial x}(x,t)^T)$$

with respect to x and obtain:

$$-\dot{\lambda}^T = \frac{\partial}{\partial x}\left(H(x(t), u^*(t, x, \lambda), \lambda(t))\right).$$

- Likewise, differentiate $J(x, T) = E(x)$
and obtain terminal condition

$$\lambda(T)^T = \frac{\partial E}{\partial x}(x(T)).$$

How to obtain explicit expression for controls?

- In simplest case,

$$u^*(t) = \arg\min_u H(x(t), u, \lambda(t))$$

  is defined by

$$\frac{\partial H}{\partial u}(x(t), u^*(t), \lambda(t)) = 0$$

  (Calculus of Variations, Euler-Lagrange).

- In presence of path constraints, expression for $u^*(t)$ changes whenever active constraints change. This leads to state dependent switches.
- If minimum of Hamiltonian locally not unique, “singular arcs” occur. Treatment needs higher order derivatives of H.

Necessary Optimality Conditions

Summarize optimality conditions as **boundary value problem**:

$$
\begin{array}{rcllr}
x(0) & = & x_0, & & \text{(initial value)} \\
\dot{x}(t) & = & f(x(t), u^*(t)) & t \in [0, T], & \text{(ODE model)} \\
-\dot{\lambda}(t) & = & \frac{\partial H}{\partial x}(x(t), u^*(t), \lambda(t))^T, & t \in [0, T], & \text{(adjoint equations)} \\
u^*(t) & = & \arg\min\limits_{u} H(x(t), u, \lambda(t)), & t \in [0, T], & \text{(minimum principle)} \\
\lambda(T) & = & \frac{\partial E}{\partial x}(x(T))^T. & & \text{(adjoint final value).}
\end{array}
$$

Solve with so called

- gradient methods,
- shooting methods, or
- collocation.

Indirect Methods: Pros and Cons

- “First optimize, then discretize”

+ Boundary value problem with only $2 \times n_x$ ODE.
+ Can treat large scale systems.

- Only necessary conditions for local optimality.
- Need explicit expression for $u^*(t)$, singular arcs difficult to treat.
- ODE strongly nonlinear and unstable.
- Inequalities lead to ODE with state dependent switches.

  (possible remedy: Use interior point method in function space inequalities, e.g. Weiser and Deuflhard, Bonnans and Laurent-Varin)

- Used for optimal control e.g. by Srinivasan and Bonvin, Oberle, ...

Direct Methods

- "First discretize, then optimize"
- Transcribe infinite problem into finite dimensional, **Nonlinear Programming Problem (NLP)**, and solve NLP.

  Pros and Cons:

+ Can use state-of-the-art methods for NLP solution.
+ Can treat inequality constraints and multipoint constraints much easier.
- Obtains only suboptimal/approximate solution.

- Nowadays most commonly used methods due to their easy applicability and robustness.

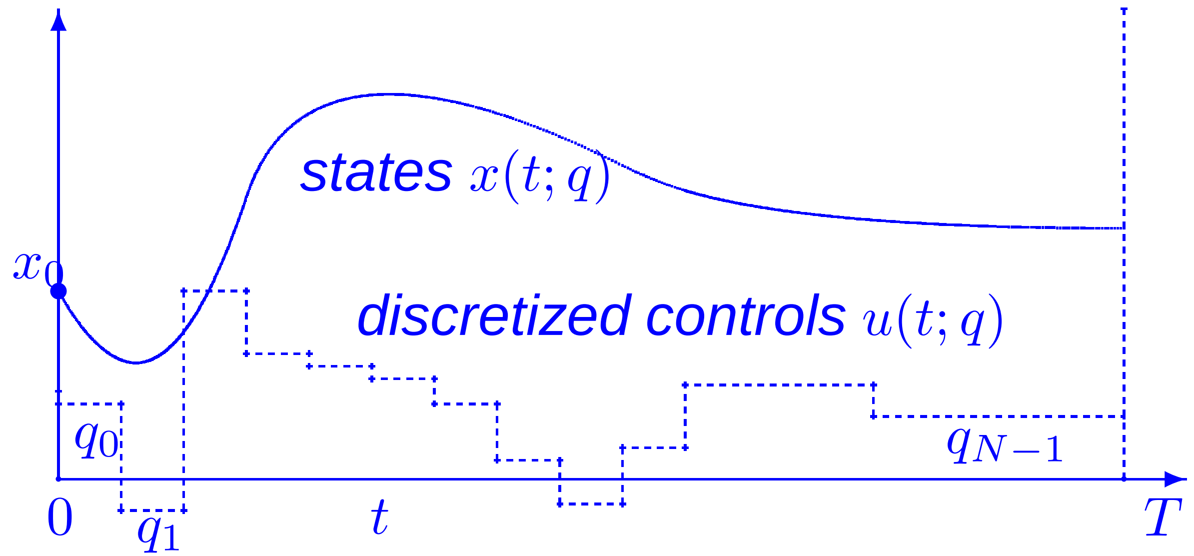
Direct Methods Overview

We treat three direct methods:

- Direct Single Shooting (sequential simulation and optimization)
- Direct Collocation (simultaneous simulation and optimization)
- Direct Multiple Shooting (simultaneous resp. hybrid)

Direct Single Shooting [Hicks, Ray 1971; Sargent, Sullivan 1977]

Discretize controls $u(t)$ on fixed grid $0 = t_0 < t_1 < \ldots < t_N = T$, regard states $x(t)$ on $[0, T]$ as dependent variables.



Use numerical integration to obtain state as function $x(t; q)$ of finitely many control parameters $q = (q_0, q_1, \ldots, q_{N-1})$

NLP in Direct Single Shooting

After control discretization and numerical ODE solution, obtain NLP:

$$\underset{q}{\text{minimize}} \quad \int_0^T L(x(t;q), u(t;q))\, dt \;+\; E\left(x(T;q)\right)$$

subject to

$$\begin{aligned} h(x(t_i;q), u(t_i;q)) &\geq 0, \qquad i = 0, \ldots, N, \quad \text{(discretized path constraints)} \\ r\left(x(T;q)\right) &\geq 0. \qquad \qquad \qquad \qquad \text{(terminal constraints)} \end{aligned}$$

Solve with finite dimensional optimization solver, e.g. Sequential Quadratic Programming (SQP).

Solution by Standard SQP

Summarize problem as

$$\min_q F(q) \;\text{ s.t. }\; H(q) \geq 0.$$

Solve e.g. by Sequential Quadratic Programming (SQP), starting with guess q^0 for controls. $k := 0$

1. Evaluate $F(q^k), H(q^k)$ by ODE solution, and derivatives!

2. Compute correction Δq^k by solution of QP:

$$\min_{\Delta q} \nabla F(q_k)^T \Delta q + \frac{1}{2} \Delta q^T A^k \Delta q \;\text{ s.t. }\; H(q^k) + \nabla H(q^k)^T \Delta q \geq 0.$$

3. Perform step $q^{k+1} = q^k + \alpha_k \Delta q^k$ with step length α_k determined by line search.

ODE Sensitivities

How to compute the sensitivity

$$\frac{\partial x(t;q)}{\partial q}$$

of a numerical ODE solution $x(t;q)$ with respect to the controls q?
Four ways:

1. External Numerical Differentiation (END)
2. Variational Differential Equations
3. Automatic Differentiation
4. Internal Numerical Differentiation (IND)

1 - External Numerical Differentiation (END)

Perturb q and call integrator several times to compute derivatives by finite differences:

$$\frac{x(t; q + \epsilon e_i) - x(t; q)}{\epsilon}$$

Very easy to implement, but several problems:

- Relatively expensive, have overhead of error control for each varied trajectory.
- Due to adaptivity, each call might have different discretization grids: output $x(t; q)$ is not differentiable!
- How to chose perturbation stepsize? Rule of thumb: $\epsilon = \sqrt{\mathrm{TOL}}$ if TOL is integrator tolerance.
- Looses half the digits of accuracy. If integrator accuracy has (typical) value of $\mathrm{TOL} = 10^{-4}$, derivative has only two valid digits!

2 - Variational Differential Equations

Solve additional matrix differential equation

$$\dot{G} = \frac{\partial f}{\partial x}(x,q)G + \frac{\partial f}{\partial q}(x,q), \quad G(0) = 0$$

Very accurate at reasonable costs, but:

- Have to get expressions for $\frac{\partial f}{\partial x}(x,q)$ and $\frac{\partial f}{\partial q}(x,q)$.
- Computed sensitivity is not 100 % identical with derivative of (discretized) integrator result $x(t;q)$.

3- Automatic Differentiation (AD)

Use Automatic Differentiation (AD): differentiate each step of the integration scheme.
Illustration: AD of Euler:

$$G(t_k + h) = G(t_k) + h\frac{\partial f}{\partial x}(x(t_k), q)G(t_k) + h\frac{\partial f}{\partial q}(x(t_k), q)$$

Up to machine precision 100 % identical with derivative of numerical solution $x(t; q)$, but:

- Integrator and right hand side ($f(x, q)$) need be in same or compatible computer languages (e.g. C++ when using ADOL-C)

4 - Internal Numerical Differentiation (IND)

Like END, but evaluate **simultaneously** all perturbed trajectories x_i with **frozen** discretization grid.
Illustration: IND of Euler:

$$x_i(t_k + h_k) = x_i(t_k) + h_k f(x_i(t_k), q + \epsilon e_i)$$

Up to round-off and linearization errors identical with derivative of numerical $x(t; q)$, but:

- How to chose perturbation stepsize? Rule of thumb: $\epsilon = \sqrt{\mathrm{PREC}}$ if PREC is **machine precision**.

Note: adaptivity of nominal trajectory only, reuse of matrix factorization in implicit methods, so not only more accurate, but also cheaper than END.

Numerical Test Problem

$$\underset{x(\cdot),\,u(\cdot)}{\text{minimize}} \qquad \int_0^3 x(t)^2 + u(t)^2 \; dt$$

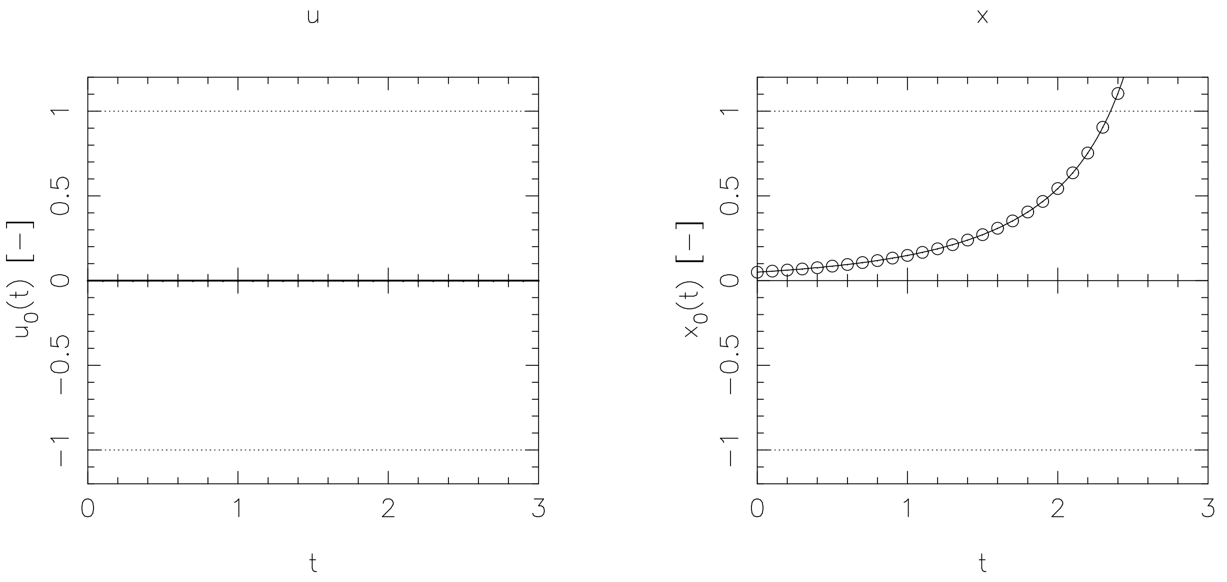
subject to

$$\begin{array}{rcll}
x(0) & = & x_0, & & \text{(initial value)} \\
\dot{x} & = & (1+x)x + u, & t \in [0,3], & \text{(ODE model)} \\
\begin{bmatrix} 1 - x(t) \\ 1 + x(t) \\ 1 - u(t) \\ 1 + u(t) \end{bmatrix} & \geq & \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, & t \in [0,3], & \text{(bounds)} \\
x(3) & = & 0. & & \text{(zero terminal constraint).}
\end{array}$$

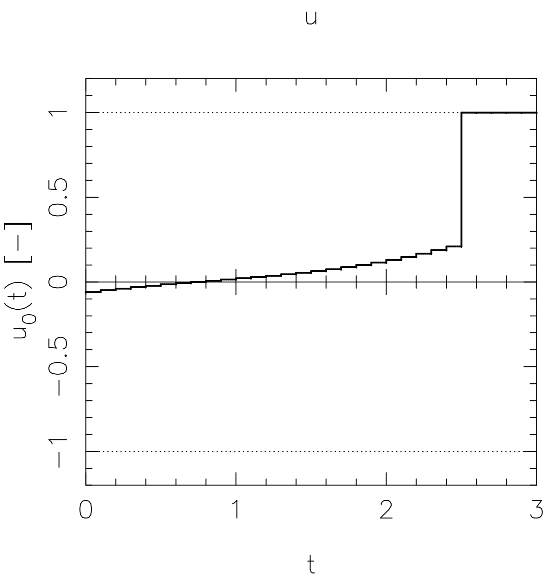
Remark: Uncontrollable growth for $(1+x_0)x_0 - 1 \geq 0 \Leftrightarrow x_0 \geq 0.618$.

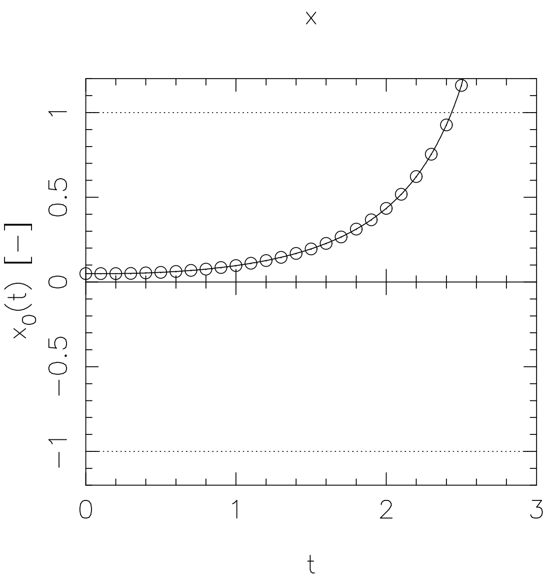
Single Shooting Optimization for $x_0 = 0.05$

- Choose $N = 30$ equal control intervals.
- Initialize with steady state controls $u(t) \equiv 0$.
- Initial value $x_0 = 0.05$ is the maximum possible, because initial trajectory explodes otherwise.

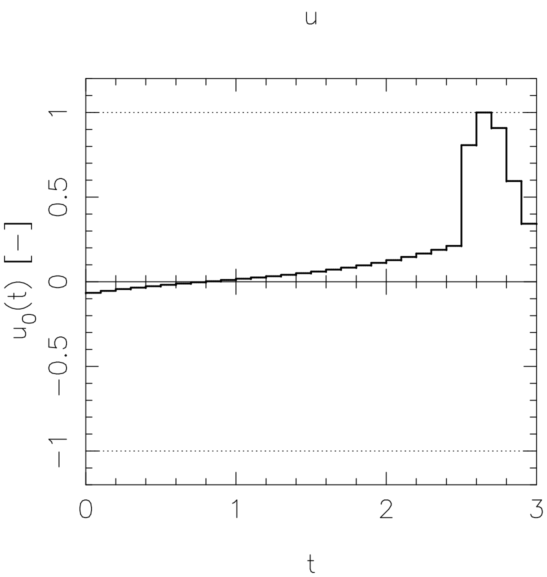


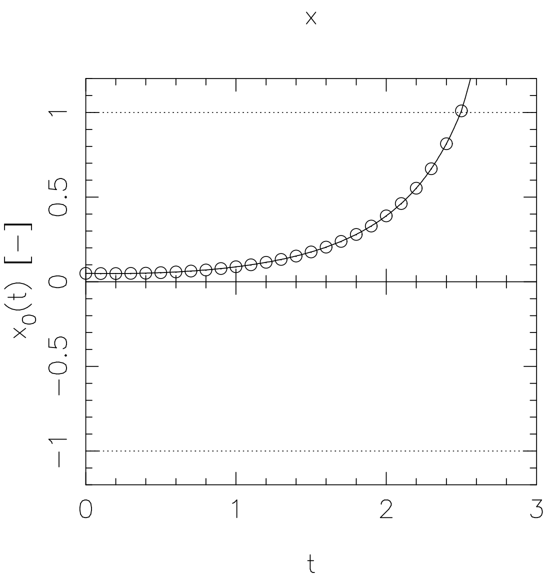
Single Shooting: First Iteration



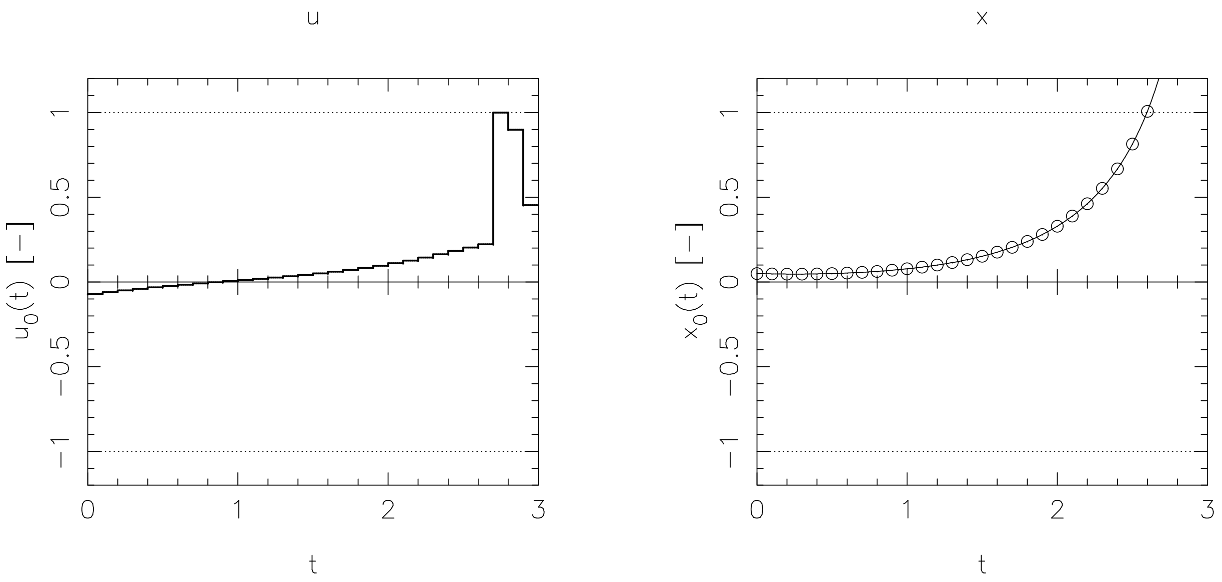


Single Shooting: 2nd Iteration

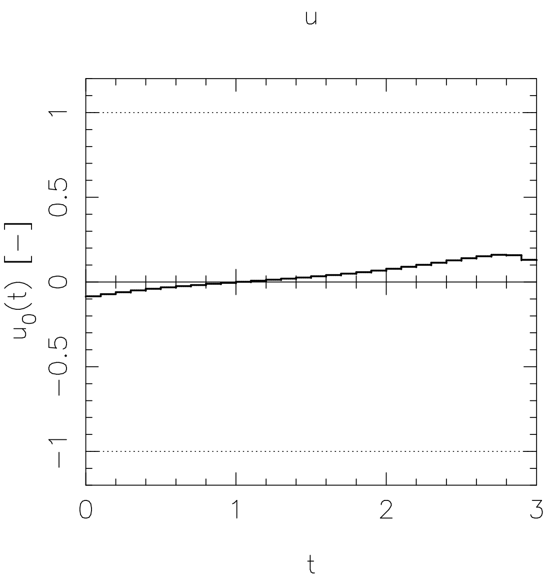


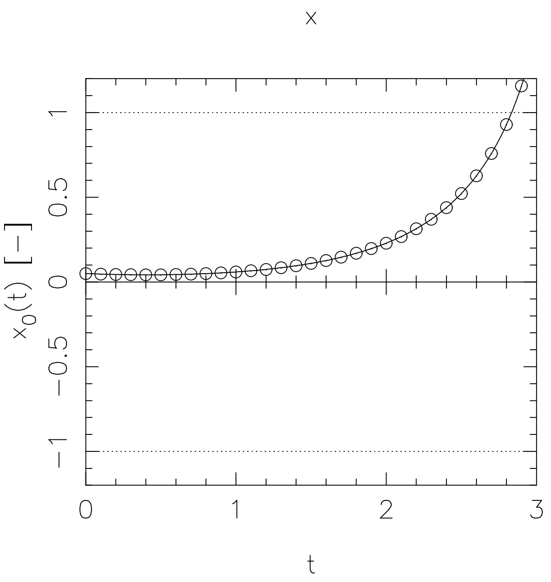


Single Shooting: 3rd Iteration

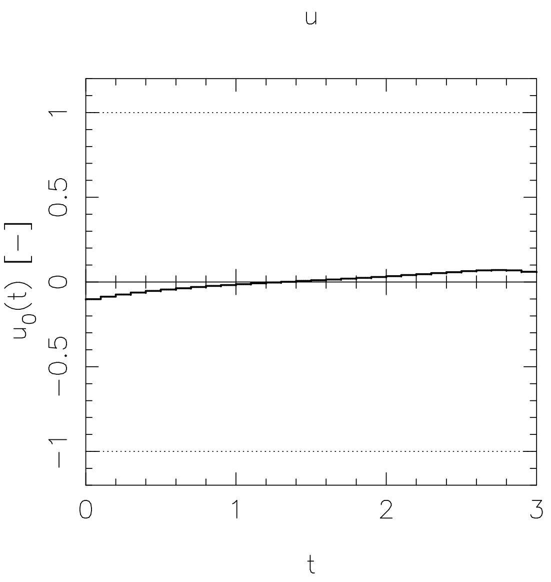


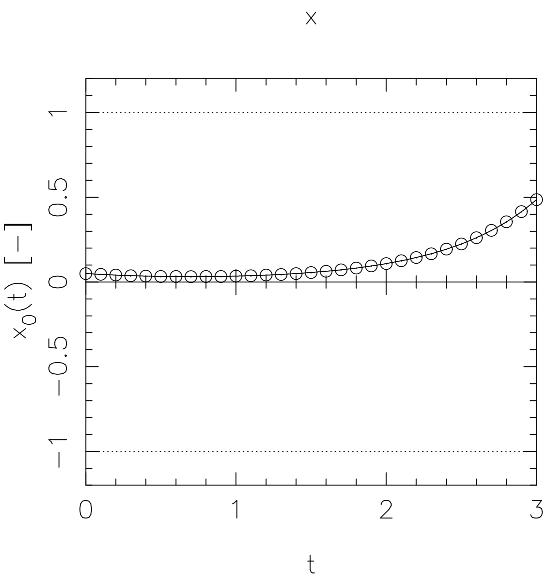
Single Shooting: 4th Iteration



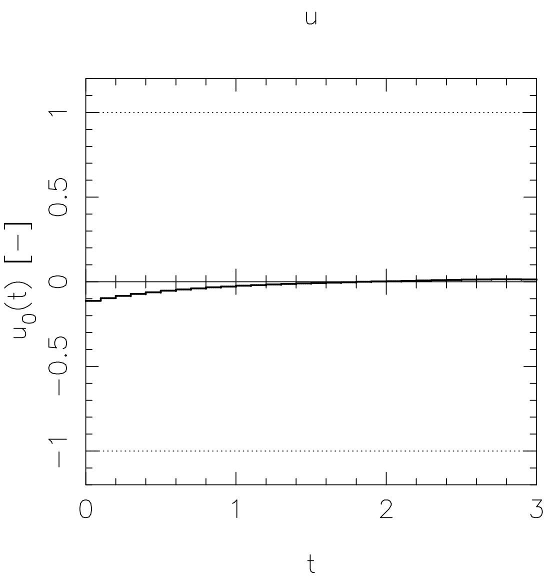


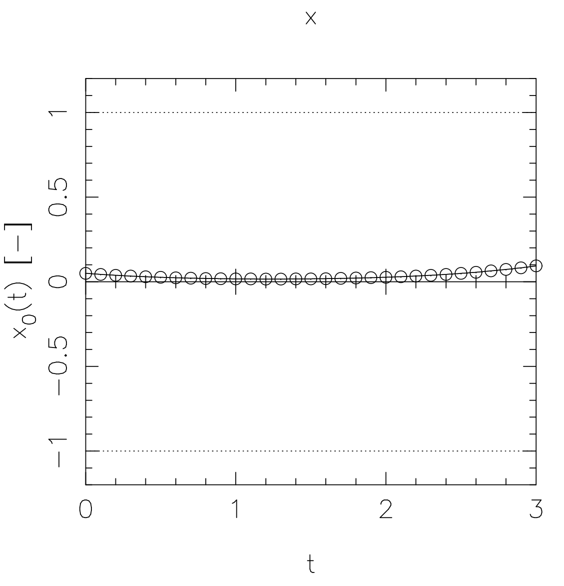
Single Shooting: 5th Iteration



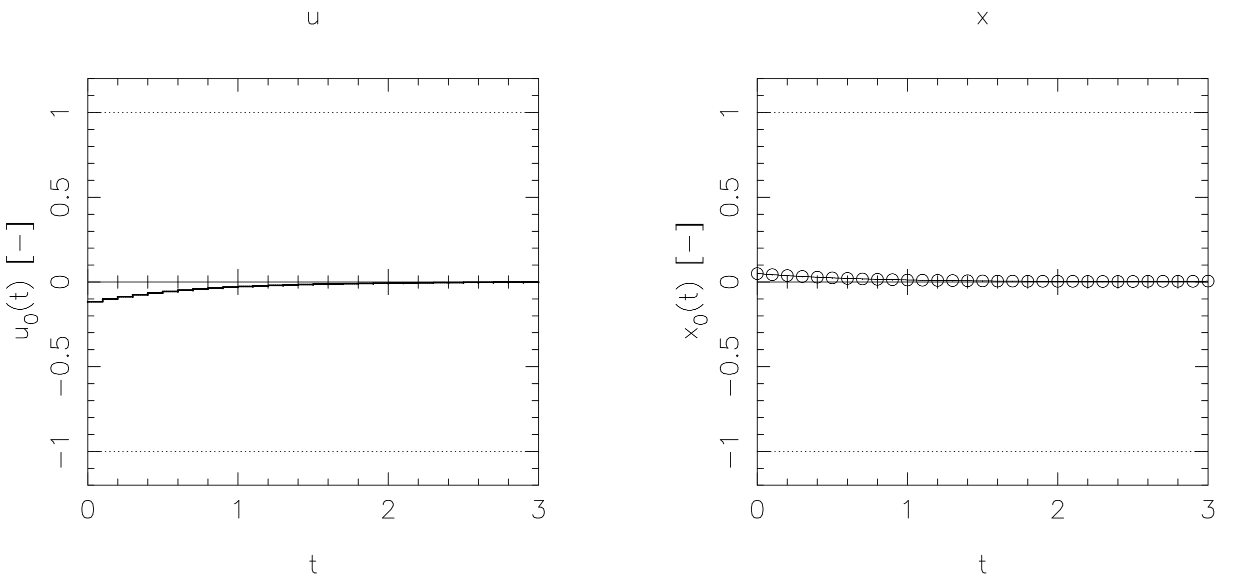


Single Shooting: 6th Iteration





Single Shooting: 7th Iteration and Solution



Direct Single Shooting: Pros and Cons

- **Sequential** simulation and optimization.

+ Can use state-of-the-art ODE/DAE solvers.
+ Few degrees of freedom even for large ODE/DAE systems.
+ Active set changes easily treated.
+ Need only initial guess for controls q.

- Cannot use knowledge of x in initialization (e.g. in tracking problems).
- ODE solution $x(t;q)$ can depend very nonlinearly on q.
- Unstable systems difficult to treat.

- Often used in engineering applications e.g. in packages gOPT (PSE), DYOS (Marquardt), ...

Direct Collocation (Sketch) [Tsang et al. 1975]

- Discretize controls and states on **fine** grid with node values $s_i \approx x(t_i)$.
- Replace infinite ODE

$$0 = \dot{x}(t) - f(x(t), u(t)), \quad t \in [0, T]$$

by finitely many equality constraints

$$\begin{aligned} c_i(q_i, s_i, s_{i+1}) &= 0, \quad i = 0, \ldots, N-1, \\ \text{e.g.} \quad c_i(q_i, s_i, s_{i+1}) &:= \tfrac{s_{i+1} - s_i}{t_{i+1} - t_i} - f\left(\tfrac{s_i + s_{i+1}}{2}, q_i\right) \end{aligned}$$

- Approximate also integrals, e.g.

$$\int_{t_i}^{t_{i+1}} L(x(t), u(t))dt \approx l_i(q_i, s_i, s_{i+1}) := L\left(\frac{s_i + s_{i+1}}{2}, q_i\right)(t_{i+1} - t_i)$$

NLP in Direct Collocation

After discretization obtain large scale, but sparse NLP:

$$\underset{s,\,q}{\text{minimize}} \quad \sum_{i=0}^{N-1} l_i(q_i, s_i, s_{i+1}) \;+\; E\left(s_N\right)$$

subject to

$$\begin{aligned}
s_0 - x_0 &= 0, && && \text{(fixed initial value)}\\
c_i(q_i, s_i, s_{i+1}) &= 0, && i = 0, \ldots, N-1, && \text{(discretized ODE model)}\\
h(s_i, q_i) &\geq 0, && i = 0, \ldots, N, && \text{(discretized path constraints)}\\
r\left(s_N\right) &\geq 0. && && \text{(terminal constraints)}
\end{aligned}$$

Solve e.g. with SQP method for sparse problems.

What is a sparse NLP?

General NLP:

$$\min_{w} F(w) \text{ s.t. } \begin{cases} G(w) & = & 0, \\ H(w) & \geq & 0. \end{cases}$$

is called sparse if the Jacobians (derivative matrices)

$$\nabla_w G^T = \frac{\partial G}{\partial w} = \left(\frac{\partial G}{\partial w_j}\right)_{ij} \quad \text{and} \quad \nabla_w H^T$$

contain many zero elements.

In SQP methods, this makes QP much cheaper to build and to solve.

Direct Collocation: Pros and Cons

- **Simultaneous** simulation and optimization.

+ Large scale, but very sparse NLP.
+ Can use knowledge of x in initialization.
+ Can treat unstable systems well.
+ Robust handling of path and terminal constraints.

\- Adaptivity needs new grid, changes NLP dimensions.

- Successfully used for practical optimal control e.g. by Biegler and Wächter (IPOPT), Betts, Bock/Schulz (OCPRSQP), v. Stryk (DIRCOL), ...

Direct Multiple Shooting [Bock and Plitt, 1981]

- Discretize controls piecewise on a coarse grid

$$u(t) = q_i \quad \text{for} \quad t \in [t_i, t_{i+1}]$$

- Solve ODE on each interval $[t_i, t_{i+1}]$ numerically, starting with artificial initial value s_i:

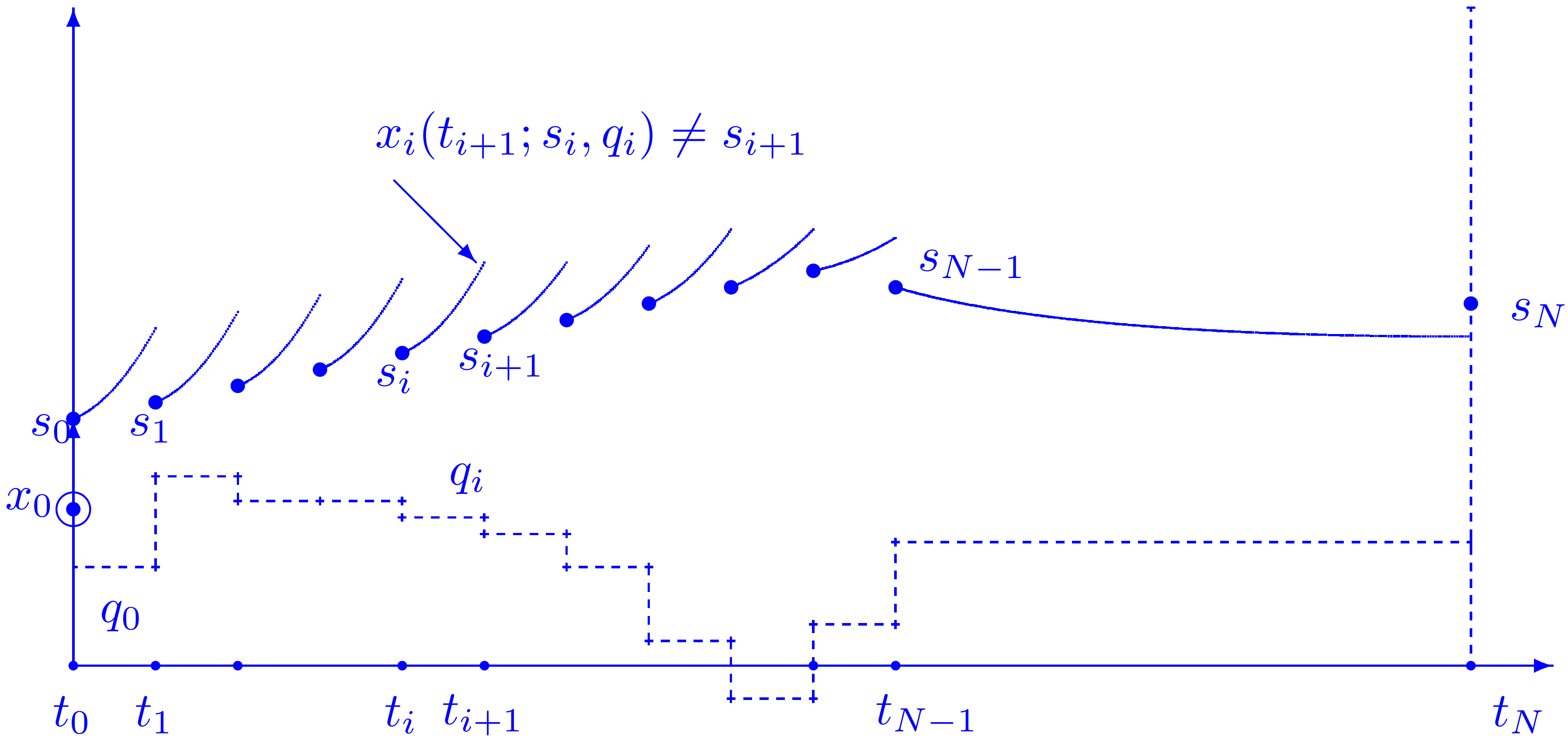
$$\begin{aligned} \dot{x}_i(t; s_i, q_i) &= f(x_i(t; s_i, q_i), q_i), \quad t \in [t_i, t_{i+1}], \\ x_i(t_i; s_i, q_i) &= s_i. \end{aligned}$$

  Obtain trajectory pieces $x_i(t; s_i, q_i)$.

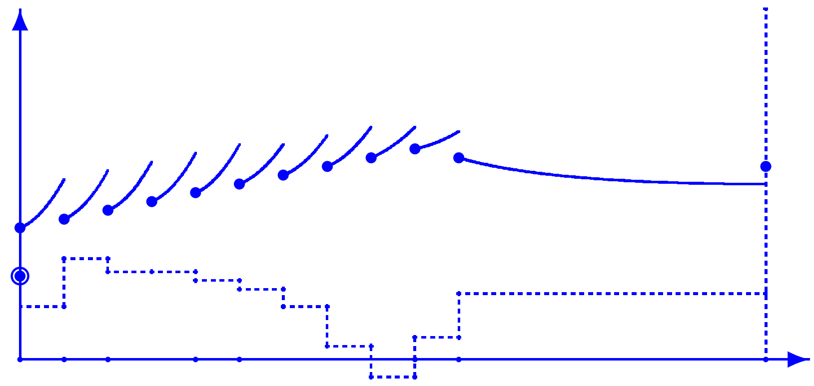
- Also numerically compute integrals

$$l_i(s_i, q_i) := \int_{t_i}^{t_{i+1}} L(x_i(t_i; s_i, q_i), q_i) dt$$

Sketch of Direct Multiple Shooting



NLP in Direct Multiple Shooting



$$\underset{s,\,q}{\text{minimize}} \quad \sum_{i=0}^{N-1} l_i(s_i, q_i) \;+\; E\left(s_N\right)$$

subject to

$$\begin{aligned}
s_0 - x_0 &= 0, && && \text{(initial value)}\\
s_{i+1} - x_i(t_{i+1}; s_i, q_i) &= 0, && i = 0, \ldots, N-1, && \text{(continuity)}\\
h(s_i, q_i) &\geq 0, && i = 0, \ldots, N, && \text{(discretized path constraints)}\\
r\left(s_N\right) &\geq 0. && && \text{(terminal constraints)}
\end{aligned}$$

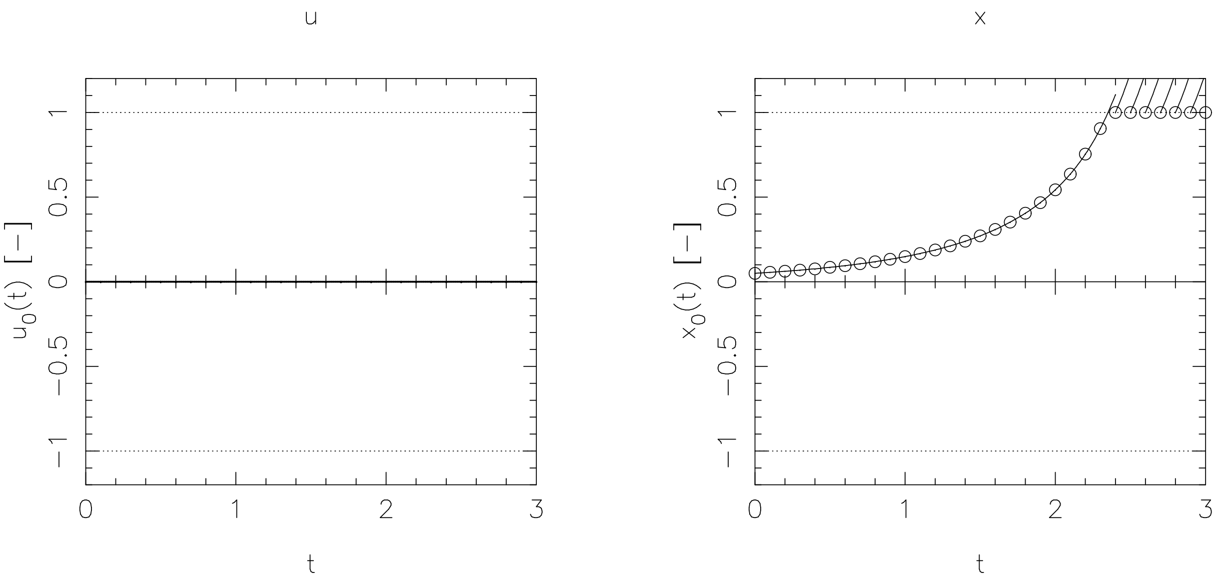
Structured NLP

- Summarize all variables as $w := (s_0, q_0, s_1, q_1, \ldots, s_N)$.
- Obtain structured NLP

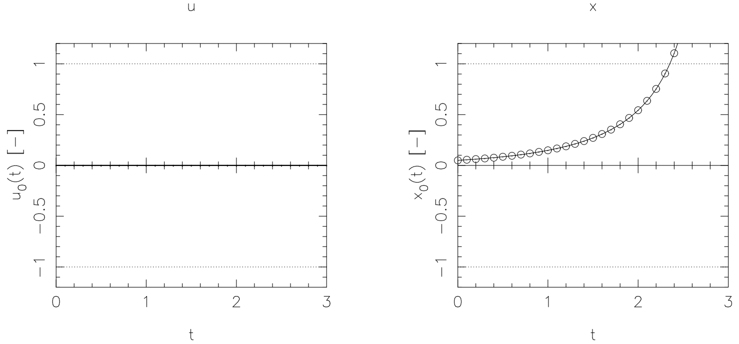
$$\boxed{\min_{w} \; F(w) \quad \text{s.t.} \quad \begin{cases} G(w) & = & 0 \\ H(w) & \geq & 0. \end{cases}}$$

- Jacobian $\nabla G(w^k)^T$ contains dynamic model equations.
- Jacobians and Hessian of NLP are block sparse, can be exploited in numerical solution procedure.

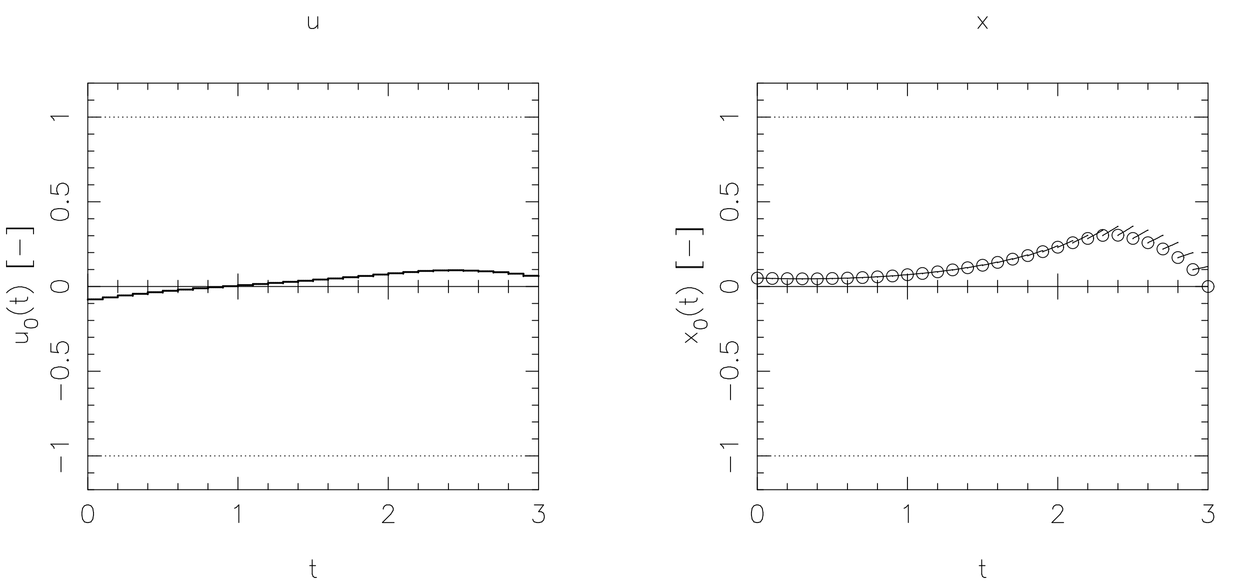
Test Example: Initialization with $u(t) \equiv 0$



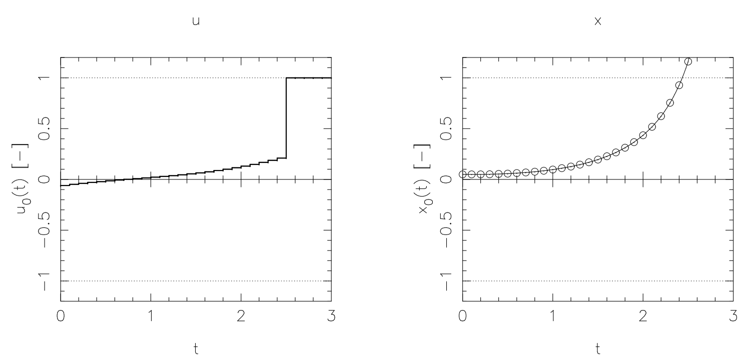
single shooting:



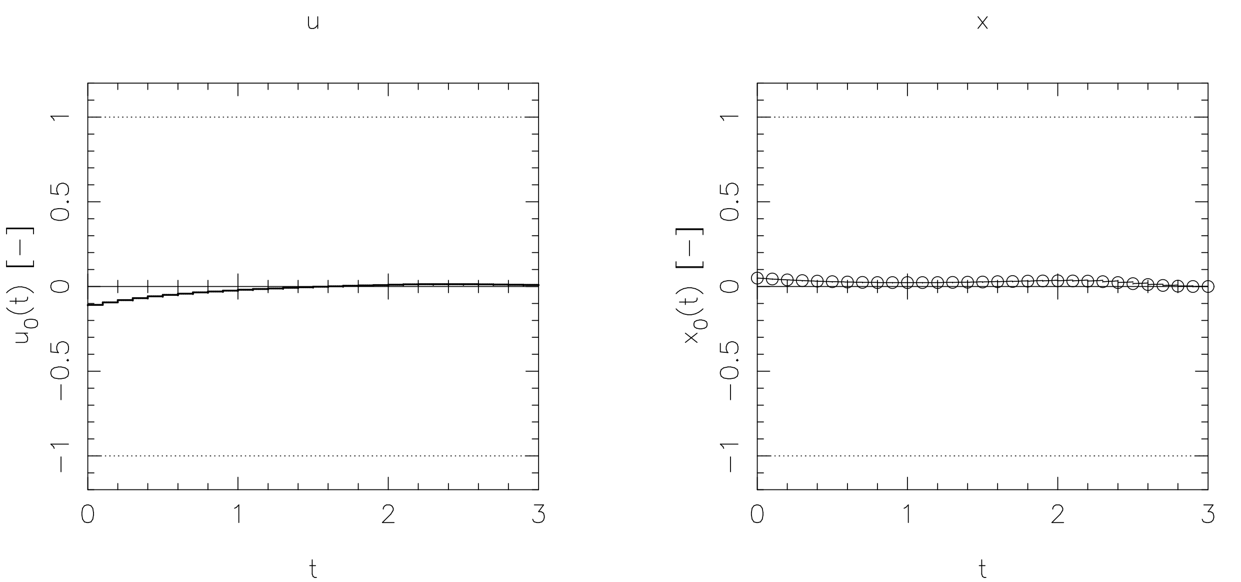
Multiple Shooting: First Iteration



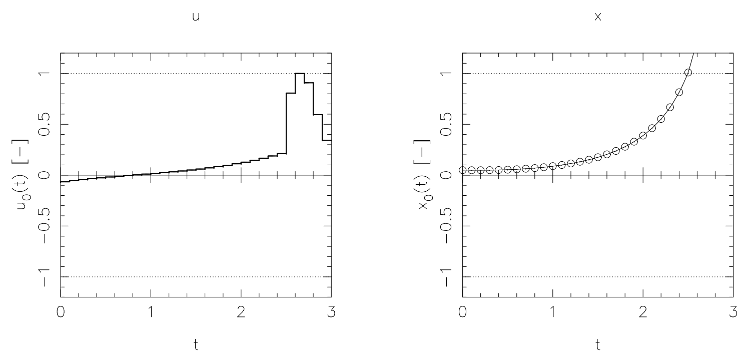
single shooting:



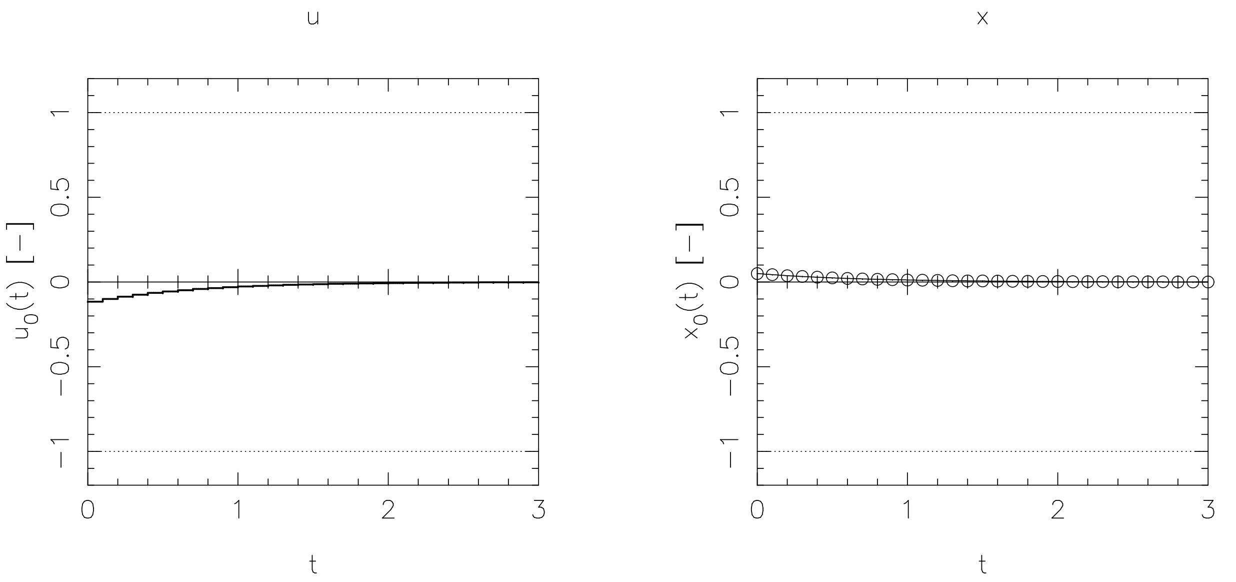
Multiple Shooting: 2nd Iteration



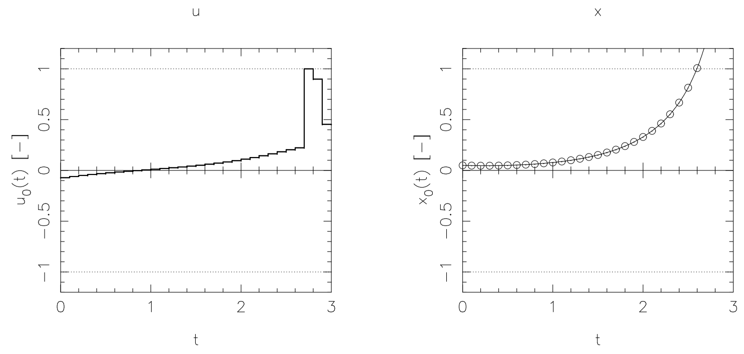
single shooting:



Multiple Shooting: 3rd Iteration and Solution



single shooting:



Direct Multiple Shooting: Pros and Cons

- **Simultaneous** simulation and optimization.

+ uses **adaptive** ODE/DAE solvers
+ but NLP has **fixed dimensions**
+ can use knowledge of x in initialization (here bounds; more important in online context).
+ can treat unstable systems well.
+ robust handling of path and terminal constraints.
+ easy to parallelize.

\- not as sparse as collocation.

- Used for practical optimal control e.g by Franke (“HQP”), Terwen (DaimlerChrysler); Santos and Biegler; Bock et al. (“MUSCOD-II”)

Conclusions: Optimal Control Family Tree

- **Hamilton-Jacobi-Bellman Equation:** *Tabulation in State Space*
- **Indirect Methods, Pontryagin:** *Solve Boundary Value Problem*
- **Direct Methods:** *Transform into Nonlinear Program (NLP)*
  - **Single Shooting:** *Only discretized controls in NLP (sequential)*
  - **Collocation:** *Discretized controls and states in NLP (simultaneous)*
  - **Multiple Shooting:** *Controls and node start values in NLP (simultaneous/hybrid)*

Literature

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