Practical Course: Modeling, Simulation, Optimization

Week 6

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6.B Gradient computation in optimal control problems

Optimal control

We now consider optimization over time dependent functions $\mathbf{u}(t) \in L^2([0,T],\mathbb{R}^M)$.

The prototypical problem:

$$\min_{\mathbf{u}\in L^2([0,T],\mathbb{R}^q)} J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\,\mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R}\mathbf{u}(t)\,\mathrm{d}t,$$

subject to the dynamics

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\mathrm{init}}.$$

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The prototypical problem:

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subject to the dynamics

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\mathrm{init}}.$$

Assumption: $\mathbf{Q}$ and $\mathbf{R}$ are symmetric.
Assumption: the matrix $\mathbf{Q}$ is positive semi-definite and the matrix $\mathbf{R}$ is positive definite, i.e.

$$\mathbf{x}^\top \mathbf{Q}\mathbf{x} \geq 0, \qquad \mathbf{u}^\top \mathbf{R}\mathbf{u} > 0,$$

for all $\mathbf{x} \in \mathbb{R}^N$, $\mathbf{0} \neq \mathbf{u} \in \mathbb{R}^M$.

Theorem

Under this assumption, the minimizer $\mathbf{u}^*(t)$ of $J(\mathbf{u})$ exists and is unique.

This follows because J is α-convex, with $\alpha = \lambda_{\mathrm{min}}(\mathbf{R}) > 0$.

What is the gradient now?

We are now optimizing over the infinite-dimensional space $L^2([0,T],\mathbb{R}^M)$.
We can therefore no longer use that

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \frac{\mathrm{d}J}{\mathrm{d}\mathbf{u}}(\mathbf{u})\tilde{\mathbf{u}},$$

and simply use the chain rule to find $\frac{\mathrm{d}J}{\mathrm{d}\mathbf{u}}(\mathbf{u})$.
(It is not so clear what $\frac{\mathrm{d}J}{\mathrm{d}\mathbf{u}}(\mathbf{u})$ now is supposed to mean!)

We therefore start from the basic definition:

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h\to 0} \frac{J(\mathbf{u}+h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h}.$$

Note: this is the Gateaux derivative of J at point $\mathbf{u}$ in the direction $\tilde{\mathbf{u}}$.

The directional derivative (1/2)

$$J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)) \, \mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R}\mathbf{u}(t) \, \mathrm{d}t,$$

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\text{init}}.$$

$$J(\mathbf{u}+h\tilde{\mathbf{u}}) = \frac{1}{2}\int_0^T (\mathbf{x}^h(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}^h(t) - \mathbf{x}_d(t)) \, \mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t)+h\tilde{\mathbf{u}}(t))^\top \mathbf{R}(\mathbf{u}(t)+h\tilde{\mathbf{u}}(t)) \, \mathrm{d}t$$

$$\mathbf{E}\dot{\mathbf{x}}^h(t) = \mathbf{A}\mathbf{x}^h(t) + \mathbf{B}(\mathbf{u}(t) + h\tilde{\mathbf{u}}(t)), \qquad \mathbf{x}^h(0) = \mathbf{x}_{\text{init}}.$$

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$$J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\, \mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R}\mathbf{u}(t)\, \mathrm{d}t,$$
$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\text{init}}.$$

$$J(\mathbf{u}+h\tilde{\mathbf{u}}) = \frac{1}{2}\int_0^T (\mathbf{x}^h(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}^h(t) - \mathbf{x}_d(t))\, \mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t)+h\tilde{\mathbf{u}}(t))^\top \mathbf{R}(\mathbf{u}(t)+h\tilde{\mathbf{u}}(t))\, \mathrm{d}t$$
$$\mathbf{E}\dot{\mathbf{x}}^h(t) = \mathbf{A}\mathbf{x}^h(t) + \mathbf{B}(\mathbf{u}(t) + h\tilde{\mathbf{u}}(t)), \qquad \mathbf{x}^h(0) = \mathbf{x}_{\text{init}}.$$

Write:

$$\mathbf{x}^h(t) = \mathbf{x}(t) + h\tilde{\mathbf{x}}(t), \qquad \tilde{\mathbf{x}}(t) = \frac{\mathbf{x}^h(t) - \mathbf{x}(t)}{h},$$

Then:

$$\begin{aligned}\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{E}\frac{\dot{\mathbf{x}}^h(t) - \dot{\mathbf{x}}(t)}{h} &= \frac{1}{h}\Big(\mathbf{A}\mathbf{x}^h(t) + \mathbf{B}(\mathbf{u}(t) + h\tilde{\mathbf{u}}(t)) - \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)\Big)\\ &= \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.\end{aligned}$$

The directional derivative (2/2)

$$J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\,\mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R}\mathbf{u}(t)\,\mathrm{d}t,$$

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\mathrm{init}}.$$

$$\begin{aligned} J(\mathbf{u} + h\tilde{\mathbf{u}}) = \frac{1}{2}\int_0^T &(\mathbf{x}(t) + h\tilde{\mathbf{x}}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t) + h\tilde{\mathbf{x}}(t) - \mathbf{x}_d(t))\,\mathrm{d}t \\ &+ \frac{1}{2}\int_0^T (\mathbf{u}(t) + h\tilde{\mathbf{u}}(t))^\top \mathbf{R}(\mathbf{u}(t) + h\tilde{\mathbf{u}}(t))\,\mathrm{d}t, \end{aligned}$$

$$\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.$$

It is now easy to verify that

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h\to 0} \frac{J(\mathbf{u} + h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R}\tilde{\mathbf{u}}(t)\,\mathrm{d}t.$$

But what is the gradient now?

We have found a way to compute the directional derivative:

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h \to 0} \frac{J(\mathbf{u} + h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q} \tilde{\mathbf{x}}(t) \, \mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R} \tilde{\mathbf{u}}(t) \, \mathrm{d}t.$$

$$\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.$$

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We have found a way to compute the directional derivative:

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h \to 0} \frac{J(\mathbf{u} + h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t) \, \mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R}\tilde{\mathbf{u}}(t) \, \mathrm{d}t.$$

$$\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.$$

But how do we find the gradient now?

Not so obvious:
In a finite dimensional space,
we could choose a basis for the space of perturbations $\tilde{\mathbf{u}}(t)$
and evaluate the directional gradient for all basis vectors.

However, in an infinite-dimensional space, this is not possible.
(we never finish evaluating the directional gradient for all basis functions)

The way out: the adjoint state

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h \to 0} \frac{J(\mathbf{u} + h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q} \tilde{\mathbf{x}}(t) \, \mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R} \tilde{\mathbf{u}}(t) \, \mathrm{d}t.$$

$$\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.$$

We define the adjoint state $\varphi(t)$ as the solution of

$$-\mathbf{E}^\top \dot{\varphi}(t) = \mathbf{A}^\top \varphi(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \varphi(T) = \mathbf{0}.$$

Question 1

We have that:

$$\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.$$

$$-\mathbf{E}^\top \dot{\boldsymbol{\varphi}}(t) = \mathbf{A}^\top \boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \boldsymbol{\varphi}(T) = \mathbf{0}.$$

What is

$$\int_0^T \frac{d}{dt}\left((\boldsymbol{\varphi}(t))^\top \mathbf{E}\tilde{\mathbf{x}}(t)\right)\,\mathrm{d}t?$$

A) $(\boldsymbol{\varphi}(0))^\top \mathbf{E}\tilde{\mathbf{x}}(0) - (\boldsymbol{\varphi}(T))^\top \mathbf{E}\tilde{\mathbf{x}}(T)$

B) $(\boldsymbol{\varphi}(T))^\top \mathbf{E}\tilde{\mathbf{x}}(T) - (\boldsymbol{\varphi}(0))^\top \mathbf{E}\tilde{\mathbf{x}}(0)$

C) $(\boldsymbol{\varphi}(T))^\top \mathbf{E}\tilde{\mathbf{x}}(T)$

D) 0

E) None of the above.

Question 2

We have that:

$$\mathbf{E}\dot{\tilde{\mathbf{x}}}(t) = \mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t), \qquad \tilde{\mathbf{x}}(0) = \mathbf{0}.$$
$$-\mathbf{E}^\top\dot{\boldsymbol{\varphi}}(t) = \mathbf{A}^\top\boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \boldsymbol{\varphi}(T) = \mathbf{0}.$$

What is

$$\int_0^T \frac{d}{dt}\left((\boldsymbol{\varphi}(t))^\top\mathbf{E}\tilde{\mathbf{x}}(t)\right)\,\mathrm{d}t = \int_0^T\left(\mathbf{E}^\top\dot{\boldsymbol{\varphi}}(t)\right)^\top\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T(\boldsymbol{\varphi}(t))^\top\mathbf{E}\dot{\tilde{\mathbf{x}}}(t)\,\mathrm{d}t?$$

A) $\int_0^T\left(\mathbf{A}^\top\boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\right)^\top\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T(\boldsymbol{\varphi}(t))^\top\left(\mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t)\right)\,\mathrm{d}t$

B) $-\int_0^T\left(\mathbf{A}^\top\boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\right)^\top\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T(\boldsymbol{\varphi}(t))^\top\left(\mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t)\right)\,\mathrm{d}t$

C) $\int_0^T\left(\mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\right)^\top\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T(\boldsymbol{\varphi}(t))^\top\left(\mathbf{B}\tilde{\mathbf{u}}(t)\right)\,\mathrm{d}t$

D) $-\int_0^T\left(\mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\right)^\top\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T(\boldsymbol{\varphi}(t))^\top\left(\mathbf{B}\tilde{\mathbf{u}}(t)\right)\,\mathrm{d}t$

Answer question 2

$$\int_0^T \frac{d}{dt}\left((\boldsymbol{\varphi}(t))^\top \mathbf{E}\tilde{\mathbf{x}}(t)\right)\,\mathrm{d}t = \int_0^T \left(\mathbf{E}^\top \dot{\boldsymbol{\varphi}}(t)\right)^\top \tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T (\boldsymbol{\varphi}(t))^\top \mathbf{E}\dot{\tilde{\mathbf{x}}}(t)\,\mathrm{d}t$$
$$= -\int_0^T \left(\mathbf{A}^\top \boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t))\right)^\top \tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T (\boldsymbol{\varphi}(t))^\top \left(\mathbf{A}\tilde{\mathbf{x}}(t) + \mathbf{B}\tilde{\mathbf{u}}(t)\right)\,\mathrm{d}t$$
$$= -\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t)\,\mathrm{d}t + \int_0^T (\boldsymbol{\varphi}(t))^\top \mathbf{B}\tilde{\mathbf{u}}(t)\,\mathrm{d}t$$

The gradient

Expression for the directional derivative:

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h\to 0} \frac{J(\mathbf{u}+h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t)\, \mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R}\tilde{\mathbf{u}}(t)\, \mathrm{d}t.$$

Combining the answers from question 1 and 2:

$$-\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t)\, \mathrm{d}t + \int_0^T (\boldsymbol{\varphi}(t))^\top \mathbf{B}\tilde{\mathbf{u}}(t)\, \mathrm{d}t = 0.$$

The gradient

Expression for the directional derivative:

$$\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle = \lim_{h \to 0} \frac{J(\mathbf{u} + h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t)\, \mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R}\tilde{\mathbf{u}}(t)\, \mathrm{d}t.$$

Combining the answers from question 1 and 2:

$$-\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q}\tilde{\mathbf{x}}(t)\, \mathrm{d}t + \int_0^T (\boldsymbol{\varphi}(t))^\top \mathbf{B}\tilde{\mathbf{u}}(t)\, \mathrm{d}t = 0.$$

Therefore also:

$$\begin{aligned}\langle \nabla J(\mathbf{u}), \tilde{\mathbf{u}} \rangle &= \lim_{h \to 0} \frac{J(\mathbf{u} + h\tilde{\mathbf{u}}) - J(\mathbf{u})}{h} = \int_0^T (\boldsymbol{\varphi}(t))^\top \mathbf{B}\tilde{\mathbf{u}}(t)\, \mathrm{d}t + \int_0^T (\mathbf{u}(t))^\top \mathbf{R}\tilde{\mathbf{u}}(t)\, \mathrm{d}t \\ &= \int_0^T \left(\mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t) \right)^\top \tilde{\mathbf{u}}(t)\, \mathrm{d}t = \langle \mathbf{B}^\top \boldsymbol{\varphi} + \mathbf{R}\mathbf{u}, \tilde{\mathbf{u}} \rangle_{L^2}\end{aligned}$$

Resulting gradient (w.r.t. the standard L^2-innerproduct):

$$(\nabla J(\mathbf{u}))\,(t) = \mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t).$$

An algorithm for the computation of the gradient

Computation of $\nabla J(\mathbf{u})$ (gradient in the point $\mathbf{u}(t)$)

- Compute the solution $\mathbf{x}(t)$ (the state) of

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\mathrm{init}}.$$

- Compute the solution of $\boldsymbol{\psi}(t) = \boldsymbol{\varphi}(T-t)$ of

$$\mathbf{E}^\top \dot{\boldsymbol{\psi}}(t) = \mathbf{A}^\top \boldsymbol{\psi}(t) + \mathbf{Q}(\mathbf{x}(T-t) - \mathbf{x}_d(T-t)), \qquad \boldsymbol{\psi}(0) = \mathbf{0}.$$

- The gradient is now given by

$$\left(\nabla J(\mathbf{u})\right)(t) = \mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t) = \mathbf{B}^\top \boldsymbol{\psi}(T-t) + \mathbf{R}\mathbf{u}(t).$$

Step size selection can be done in the same way as explained the previous lecture.

Remaining problem: we still need to discretize time!

6.C Time discretization of optimal control problems

Two main approaches

- Discretize-then-optimize
  Approach: First discretize the cost functional and the forward dynamics,
  then compute the gradient for the discretized problem,
  and use a gradient-based optimization algorithm
  (e.g., conjugate gradients or the one from the previous lecture).

- Optimize-then-discretize
  Approach: first find the equation for the adjoint state,
  then discretize the cost functional, the forward dynamics, and the adjoint equation,
  use the discretized adjoint equation to compute the gradient,
  which can again be used in a gradient-based optimization algorithm.

Two main approaches

- Discretize-then-optimize
  Approach: First discretize the cost functional and the forward dynamics, then compute the gradient for the discretized problem, and use a gradient-based optimization algorithm (e.g., conjugate gradients or the one from the previous lecture).

- Optimize-then-discretize
  Approach: first find the equation for the adjoint state, then discretize the cost functional, the forward dynamics, and the adjoint equation, use the discretized adjoint equation to compute the gradient, which can again be used in a gradient-based optimization algorithm.

Discretize-then-optimize leads to the most accurate solutions of the discretized problem.

In certain cases, solutions of the discretized optimal control contain spurious artefacts, that can be avoided by certain the optimize-then-discretize approaches.
see e.g. Dogin, Morin, Nochetto, Verani, discrete gradient flows for shape optimization and applications, 2007

Ervedoza, Zuazua, Numerical Approximation of Exact Controls for Waves, 2013

In some cases, the result of both approaches coincide.
In this case, we say that the approximation of the gradient is *discretely consistent*.

These ideas will now be demonstrated for a particular example.

Discretization of the forward dynamics

We want to discretize the problem:

$$\min_{\mathbf{u}\in L^2([0,T],\mathbb{R}^q)} J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t)-\mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t)-\mathbf{x}_d(t))\,\mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R}\mathbf{u}(t)\,\mathrm{d}t,$$

subject to the dynamics

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\text{init}}.$$

We consider a uniform grid $t_k = (k-1)\Delta t$ ($k = 1, 2, \dots, N_T$), so $\Delta t = T/(N_T - 1)$.
We denote $\mathbf{x}_k \approx \mathbf{x}(t_k)$ and $\mathbf{u}_k = \mathbf{u}(t_k)$.

We discretize the dynamics with the Crank-Nicolson scheme:

$$\mathbf{E}\frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} = \tfrac{1}{2}\left(\mathbf{A}\mathbf{x}_k + \mathbf{B}u_k\right) + \tfrac{1}{2}\left(\mathbf{A}\mathbf{x}_{k-1} + \mathbf{B}\mathbf{u}_{k-1}\right) = \mathbf{A}\frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B}\frac{\mathbf{u}_k + \mathbf{u}_{k-1}}{2}.$$

Starting from the given initial condition $\mathbf{x}_1 = \mathbf{x}_{\text{init}}$, we compute $\mathbf{x}_k$ from $\mathbf{x}_{k-1}$ by solving

$$\left(\mathbf{E} - \tfrac{\Delta t}{2}\mathbf{A}\right)\mathbf{x}_k = \left(\mathbf{E} + \tfrac{\Delta t}{2}\mathbf{A}\right)\mathbf{x}_{k-1} + \Delta t\mathbf{B}\frac{\mathbf{u}_k + \mathbf{u}_{k-1}}{2}, \qquad k = 2, 3, \dots, N_T.$$

Discretization of the forward dynamics

We want to discretize the problem:

$$\min_{\mathbf{u}\in L^2([0,T],\mathbb{R}^q)} J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t)-\mathbf{x}_d(t))^\top \mathbf{Q}(\mathbf{x}(t)-\mathbf{x}_d(t))\,\mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R}\mathbf{u}(t)\,\mathrm{d}t,$$

subject to the dynamics

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\mathrm{init}}.$$

Observe: We only use

- N_T state variables $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{N_T}$,
- $N_T - 1$ control variables

$$\mathbf{u}_{k-1/2} = \frac{\mathbf{u}_k + \mathbf{u}_{k-1}}{2}, \qquad k = 2, 3, \ldots N_T$$

In these new variables, the discretization of the forward dynamics becomes:

$$\left(\mathbf{E} - \tfrac{\Delta t}{2}\mathbf{A}\right)\mathbf{x}_k = \left(\mathbf{E} + \tfrac{\Delta t}{2}\mathbf{A}\right)\mathbf{x}_{k-1} + \Delta t\mathbf{B}\mathbf{u}_{k-1/2}, \qquad \mathbf{x}_1 = \mathbf{x}_{\mathrm{init}}$$

Discretization of the cost functional

We want to discretize the problem:

$$\min_{\mathbf{u} \in L^2([0,T],\mathbb{R}^q)} J(\mathbf{u}) = \frac{1}{2}\int_0^T (\mathbf{x}(t) - \mathbf{x}_d(t))^\top \mathbf{Q} (\mathbf{x}(t) - \mathbf{x}_d(t)) \, \mathrm{d}t + \frac{1}{2}\int_0^T (\mathbf{u}(t))^\top \mathbf{R} \mathbf{u}(t) \, \mathrm{d}t,$$

subject to the dynamics

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{x}(0) = \mathbf{x}_{\text{init}}.$$

We consider a uniform grid $t_k = (k-1)\Delta t$ ($k = 1, 2, \ldots, N_T$), so $\Delta t = T/(N_T - 1)$.
We denote $\mathbf{x}_k \approx \mathbf{x}(t_k)$ and $\mathbf{u}_k = \mathbf{u}(t_k)$.

We discretize the first part with the trapezoid rule and the second part with the midpoint rule.

$$J = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \Big[(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1}))^\top \mathbf{Q} (\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})) + (\mathbf{x}_k - \mathbf{x}_d(t_k))^\top \mathbf{Q} (\mathbf{x}_k - \mathbf{x}_d(t_k)) \Big]$$

$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2}$$

Discretization of the adjoint state (optimize-then-discretize)

In the continuous time setting, we could compute the gradient from the adjoint state:

$$-\mathbf{E}^\top \dot{\boldsymbol{\varphi}}(t) = \mathbf{A}^\top \boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \boldsymbol{\varphi}(T) = \mathbf{0}.$$

$$\left(\nabla J(\mathbf{u})\right)(t) = \mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t).$$

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$$-\mathbf{E}^\top \dot{\boldsymbol{\varphi}}(t) = \mathbf{A}^\top \boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \boldsymbol{\varphi}(T) = \mathbf{0}.$$

$$(\nabla J(\mathbf{u}))(t) = \mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t).$$

We can now also use the Crank-Nicolson scheme to discretize the adjoint equation. We therefore introduce the adjoint variables in the grid points

$$\boldsymbol{\varphi}_k, \qquad k = 1, 2, \ldots, N_T.$$

We then integrate *backward in time* starting from the final condition $\boldsymbol{\varphi}_{N_T} = \mathbf{0}$

$$-\mathbf{E}^\top \frac{\boldsymbol{\varphi}_k - \boldsymbol{\varphi}_{k-1}}{\Delta t} = \mathbf{A}^\top \frac{\boldsymbol{\varphi}_k + \boldsymbol{\varphi}_{k-1}}{2} + \mathbf{Q}\frac{\mathbf{x}_k + \mathbf{x}_{k-1} - \mathbf{x}_d(t_k) - \mathbf{x}_d(t_{k-1})}{2},$$

$$\left(\mathbf{E}^\top - \tfrac{\Delta t}{2}\mathbf{A}^\top\right)\boldsymbol{\varphi}_{k-1} = \left(\mathbf{E}^\top + \tfrac{\Delta t}{2}\mathbf{A}^\top\right)\boldsymbol{\varphi}_k + \tfrac{\Delta t}{2}\mathbf{Q}\left(\mathbf{x}_k + \mathbf{x}_{k-1} - \mathbf{x}_d(t_k) - \mathbf{x}_d(t_{k-1})\right),$$

which is an equation from which $\boldsymbol{\varphi}_{k-1}$ can be solved from $\boldsymbol{\varphi}_k$.

Discretization of the adjoint state (optimize-then-discretize)

In the continuous time setting, we could compute the gradient from the adjoint state:

$$-\mathbf{E}^\top \dot{\boldsymbol{\varphi}}(t) = \mathbf{A}^\top \boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \boldsymbol{\varphi}(T) = \mathbf{0}.$$

$$\left(\nabla J(\mathbf{u})\right)(t) = \mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t).$$

We can now also use the Crank-Nicolson scheme to discretize the adjoint equation. We therefore introduce the adjoint variables in the grid points

$$\boldsymbol{\varphi}_k, \qquad k = 1, 2, \ldots, N_T.$$

We then integrate *backward in time* starting from the final condition $\boldsymbol{\varphi}_{N_T} = \mathbf{0}$

$$-\mathbf{E}^\top \frac{\boldsymbol{\varphi}_k - \boldsymbol{\varphi}_{k-1}}{\Delta t} = \mathbf{A}^\top \frac{\boldsymbol{\varphi}_k + \boldsymbol{\varphi}_{k-1}}{2} + \mathbf{Q}\frac{\mathbf{x}_k + \mathbf{x}_{k-1} - \mathbf{x}_d(t_k) - \mathbf{x}_d(t_{k-1})}{2},$$

$$\left(\mathbf{E}^\top - \tfrac{\Delta t}{2}\mathbf{A}^\top\right)\boldsymbol{\varphi}_{k-1} = \left(\mathbf{E}^\top + \tfrac{\Delta t}{2}\mathbf{A}^\top\right)\boldsymbol{\varphi}_k + \tfrac{\Delta t}{2}\mathbf{Q}\left(\mathbf{x}_k + \mathbf{x}_{k-1} - \mathbf{x}_d(t_k) - \mathbf{x}_d(t_{k-1})\right),$$

which is an equation from which $\boldsymbol{\varphi}_{k-1}$ can be solved from $\boldsymbol{\varphi}_k$.
Note gradient is (just as the control $\mathbf{u}_{k-1/2}$) defined in the intermediate grid points

$$(\nabla J)_{k-1/2} = \mathbf{B}^\top \frac{\boldsymbol{\varphi}_k + \boldsymbol{\varphi}_{k-1}}{2} + \mathbf{R}\mathbf{u}_{k-1/2}.$$

Discretely consistent gradient (discretize-then-optimize)

In the continuous time setting, we could compute the gradient from the adjoint state:

$$-\mathbf{E}^\top \dot{\boldsymbol{\varphi}}(t) = \mathbf{A}^\top \boldsymbol{\varphi}(t) + \mathbf{Q}(\mathbf{x}(t) - \mathbf{x}_d(t)), \qquad \boldsymbol{\varphi}(T) = \mathbf{0}.$$

$$\left(\nabla J(\mathbf{u})\right)(t) = \mathbf{B}^\top \boldsymbol{\varphi}(t) + \mathbf{R}\mathbf{u}(t).$$

We use the same discretization for the forward dynamics and cost functional as before. We now use adjoint variables defined in the intermediate points (just as the controls):

$$\boldsymbol{\varphi}_{k-1/2}, \qquad k = 2, 3, \dots N_T.$$

We then form the (discretized) Lagrangian

$$\mathcal{L} = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \left[(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1}))^\top \mathbf{Q} \left(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})\right) + (\mathbf{x}_k - \mathbf{x}_d(t_k))^\top \mathbf{Q} \left(\mathbf{x}_k - \mathbf{x}_d(t_k)\right) \right]$$
$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2} + \Delta t \sum_{k=2}^{N_T} \boldsymbol{\varphi}_{k-1/2}^\top \left(\mathbf{A} \frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B}\mathbf{u}_{k-1/2} - \mathbf{E} \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} \right)$$
$$+ \boldsymbol{\varphi}_0^\top (\mathbf{x}_1 - \mathbf{x}_{\text{init}}).$$

Note: the adjoint states are introduced as Lagrange multipliers.
Note: we have also introduced $\boldsymbol{\varphi}_0$ as Lagrange multiplier for the initial condition, but we will see that we do not need $\boldsymbol{\varphi}_0$ to compute the gradient.

Equations for the adjoint state (discretize-then-optimize)

We have defined the (discretized) Lagrangian

$$\mathcal{L} = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \left[(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1}))^\top \mathbf{Q} \, (\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})) + (\mathbf{x}_k - \mathbf{x}_d(t_k))^\top \mathbf{Q} \, (\mathbf{x}_k - \mathbf{x}_d(t_k)) \right]$$
$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2} + \Delta t \sum_{k=2}^{N_T} \varphi_{k-1/2}^\top \left(\mathbf{A} \frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B} \mathbf{u}_{k-1/2} - \mathbf{E} \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} \right)$$
$$+ \varphi_0^\top (\mathbf{x}_1 - \mathbf{x}_{\mathrm{init}}).$$

Equations for the adjoint state (discretize-then-optimize)

We have defined the (discretized) Lagrangian

$$\mathcal{L} = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \left[(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1}))^\top \mathbf{Q} \, (\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})) + (\mathbf{x}_k - \mathbf{x}_d(t_k))^\top \mathbf{Q} \, (\mathbf{x}_k - \mathbf{x}_d(t_k)) \right]$$
$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2} + \Delta t \sum_{k=2}^{N_T} \boldsymbol{\varphi}_{k-1/2}^\top \left(\mathbf{A} \frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B} \mathbf{u}_{k-1/2} - \mathbf{E} \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} \right)$$
$$+ \boldsymbol{\varphi}_0^\top (\mathbf{x}_1 - \mathbf{x}_{\mathrm{init}}).$$

Setting the derivatives of $\mathcal{L}$ w.r.t. the adjoint variables $\boldsymbol{\varphi}_{k-1/2}$ gives the equations for the forward dynamics.

Equations for the adjoint state (discretize-then-optimize)

We have defined the (discretized) Lagrangian

$$\mathcal{L} = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \left[\left(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})\right)^\top \mathbf{Q} \left(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})\right) + \left(\mathbf{x}_k - \mathbf{x}_d(t_k)\right)^\top \mathbf{Q} \left(\mathbf{x}_k - \mathbf{x}_d(t_k)\right) \right]$$
$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2} + \Delta t \sum_{k=2}^{N_T} \boldsymbol{\varphi}_{k-1/2}^\top \left(\mathbf{A} \frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B} \mathbf{u}_{k-1/2} - \mathbf{E} \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} \right)$$
$$+ \boldsymbol{\varphi}_0^\top (\mathbf{x}_1 - \mathbf{x}_{\text{init}}).$$

Setting the derivatives of $\mathcal{L}$ w.r.t. the adjoint variables $\boldsymbol{\varphi}_{k-1/2}$ gives the equations for the forward dynamics.
Requiring that the derivatives of $\mathcal{L}$ w.r.t. the state variables $\mathbf{x}_k$ are zero gives the equations for the adjoint state:

$$0 = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{N_T}} = \frac{\Delta t}{2} \left(\mathbf{x}_{N_T} - \mathbf{x}_d(t_{N_T})\right)^\top \mathbf{Q} + \boldsymbol{\varphi}_{N_T-1/2}^\top \left(\tfrac{\Delta t}{2} \mathbf{A} - \mathbf{E}\right)$$

and, for $k = N_T - 1, N_T - 2, \ldots, 2$ and for $k = 1$

$$0 = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_k} = \Delta t \left(\mathbf{x}_k - \mathbf{x}_d(t_k)\right)^\top \mathbf{Q} + \boldsymbol{\varphi}_{k-1/2}^\top \left(\tfrac{\Delta t}{2} \mathbf{A} - \mathbf{E}\right) + \boldsymbol{\varphi}_{k+1/2}^\top \left(\tfrac{\Delta t}{2} \mathbf{A} + \mathbf{E}\right),$$
$$0 = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_1} = \frac{\Delta t}{2} \left(\mathbf{x}_1 - \mathbf{x}_d(t_1)\right)^\top \mathbf{Q} + \boldsymbol{\varphi}_{1+1/2}^\top \left(\tfrac{\Delta t}{2} \mathbf{A} + \mathbf{E}\right) + \boldsymbol{\varphi}_0^\top.$$

Equations for the adjoint state (discretize-then-optimize)

We have defined the (discretized) Lagrangian

$$\mathcal{L} = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \left[(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1}))^\top \mathbf{Q} (\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})) + (\mathbf{x}_k - \mathbf{x}_d(t_k))^\top \mathbf{Q} (\mathbf{x}_k - \mathbf{x}_d(t_k)) \right]$$
$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2} + \Delta t \sum_{k=2}^{N_T} \boldsymbol{\varphi}_{k-1/2}^\top \left(\mathbf{A} \frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B}\mathbf{u}_{k-1/2} - \mathbf{E} \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} \right)$$
$$+ \boldsymbol{\varphi}_0^\top (\mathbf{x}_1 - \mathbf{x}_{\text{init}}).$$

Requiring that the derivatives of $\mathcal{L}$ w.r.t. the state variables $\mathbf{x}_k$ are zero gives the equations for the adjoint state.
We can now compute the adjoint states as follows: Start by solving $\boldsymbol{\varphi}_{N_T-1/2}$ from

$$\left(\mathbf{E}^\top - \frac{\Delta t}{2} \mathbf{A}^\top \right) \boldsymbol{\varphi}_{N_T-1/2} = \frac{\Delta t}{2} \mathbf{Q} (\mathbf{x}_{N_T} - \mathbf{x}_d(t_{N_T})),$$

and then iteratively compute $\boldsymbol{\varphi}_{k-1/2}$ from

$$\left(\mathbf{E}^\top - \frac{\Delta t}{2} \mathbf{A}^\top \right) \boldsymbol{\varphi}_{k-1/2} = \left(\mathbf{E}^\top + \frac{\Delta t}{2} \mathbf{A}^\top \right) \boldsymbol{\varphi}_{k+1/2} + \Delta t \mathbf{Q} (\mathbf{x}_k - \mathbf{x}_d(t_k)),$$

for $k = N_T - 1, N_T - 2, \ldots, 2$ using the previously obtained $\boldsymbol{\varphi}_{k+1/2}$.

Gradient computation (discretize-then-optimize)

We have defined the (discretized) Lagrangian

$$\mathcal{L} = \frac{\Delta t}{4} \sum_{k=2}^{N_T} \Big[(\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1}))^\top \mathbf{Q} (\mathbf{x}_{k-1} - \mathbf{x}_d(t_{k-1})) + (\mathbf{x}_k - \mathbf{x}_d(t_k))^\top \mathbf{Q} (\mathbf{x}_k - \mathbf{x}_d(t_k)) \Big]$$
$$+ \frac{\Delta t}{2} \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{R} \mathbf{u}_{k-1/2} + \Delta t \sum_{k=2}^{N_T} \boldsymbol{\varphi}_{k-1/2}^\top \left(\mathbf{A} \frac{\mathbf{x}_k + \mathbf{x}_{k-1}}{2} + \mathbf{B} \mathbf{u}_{k-1/2} - \mathbf{E} \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\Delta t} \right)$$
$$+ \boldsymbol{\varphi}_0^\top (\mathbf{x}_1 - \mathbf{x}_{\mathrm{init}}).$$

Taking the partial derivative of $\mathcal{L}$ w.r.t. $\mathbf{u}_{k-1/2}$ gives the (total) derivative

$$\left(\frac{\mathrm{d}J}{\mathrm{d}\mathbf{u}_{k-1/2}} \right)_{k-1/2} = \Delta t \boldsymbol{\varphi}_{k-1/2}^\top \mathbf{B} + \Delta t \mathbf{u}_{k-1/2}^\top \mathbf{R}.$$

The gradient then follows after defining an inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle = \Delta t \sum_{k=2}^{N_T} \mathbf{u}_{k-1/2}^\top \mathbf{v}_{k-1/2}, \qquad (\nabla J)_{k-1/2} = \mathbf{B}^\top \boldsymbol{\varphi}_{k-1/2} + \mathbf{R} \mathbf{u}_{k-1/2}.$$

Remark: The resulting equations have a similar structure as the equations for the optimize-then-discretize approach, but the schemes are different.

(this example was inspired by Apel and Flaig, Crank-Nicolson Schemes for Optimal Control Problems with Evolution Equations)

Step size selection

The step size can again be selected based on a quadratic expansion:

$$J(\mathbf{u} - \beta \nabla J) = J(\mathbf{u}) - \beta G + \frac{\beta^2}{2} H, \qquad \beta_{\text{opt}} = G/H.$$

Linear term:

$$G = \Delta t \sum_{k=2}^{N_T} (\nabla J)_{k-1/2}^\top (\nabla J)_{k-1/2}.$$

Step size selection

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$$J(\mathbf{u} - \beta \nabla J) = J(\mathbf{u}) - \beta G + \tfrac{\beta^2}{2} H, \qquad \beta_{\text{opt}} = G/H.$$

Linear term:

$$G = \Delta t \sum_{k=2}^{N_T} (\nabla J)_{k-1/2}^\top (\nabla J)_{k-1/2}.$$

For the quadratic term, we need the solution of

$$\mathbf{E}\dot{\mathbf{x}}^\nabla(t) = \mathbf{A}\mathbf{x}^\nabla(t) + \mathbf{B}(\nabla J)(t), \qquad \mathbf{x}^\nabla(0) = \mathbf{0}.$$

In discretized form:

$$\left(\mathbf{E} - \tfrac{\Delta t}{2}\mathbf{A}\right)\mathbf{x}_k^\nabla = \left(\mathbf{E} + \tfrac{\Delta t}{2}\mathbf{A}\right)\mathbf{x}_{k-1}^\nabla + \Delta t \mathbf{B}(\nabla J)_{k-1/2}, \qquad \mathbf{x}_1^\nabla = \mathbf{0}.$$

The quadratic term H is then given by

$$H = \frac{\Delta t}{2} \sum_{k=2}^{N_T} \left[\left(\mathbf{x}_k^\nabla\right)^\top \mathbf{Q}\mathbf{x}_k^\nabla + \left(\mathbf{x}_{k-1}^\nabla\right)^\top \mathbf{Q}\mathbf{x}_{k-1}^\nabla \right] + \Delta t \sum_{k=2}^{N_T} (\nabla J)_{k-1/2}^\top \mathbf{R} (\nabla J)_{k-1/2}.$$

Note: we do not need a line search because the considered cost functional is quadratic.