QuantumCollocation.jl Implementation Notes

Aaron Trowbridge

Contents

0 Introduction

The goal of QOC is to generate a *pulse* $\mathbf{a}(t)$ that minimizes some cost between

$$|\psi(T)\rangle = U(T,0)\,|\psi\rangle_{\text{init}} \tag{1}$$

where

$$U(T,0) = \mathcal{T}\exp\left(\frac{-i}{\hbar}\int_0^T dt\ H(\mathbf{a}(t),t)\right) \tag{2}$$

and $|\psi\rangle_{\text{goal}}$. This cost is typically defined to be the infidelity:

$$\ell(|\psi(T)\rangle) = 1 - \left|\langle\psi(T)|\psi\rangle_{\text{goal}}\right|^2 \tag{3}$$

The QOC optimization problem can then be defined as finding the pulse that minimizes the infidelity; this is accomplished by discretizing the trajectory of $|\psi(t)\rangle$ and $\mathbf{a}(t)$, with a time step Δt and solving the following optimization problem:

$$\begin{aligned}
\hat{\mathbf{a}}_{1:T-1} = \arg\min_{\mathbf{a}_{1:T-1}} \quad & \ell(|\psi(T)\rangle) \\
\text{s.t.} \quad & |\psi(T)\rangle = \prod_{t=1}^{T-1}\exp\left(\frac{-i}{\hbar}\ H(\mathbf{a}_t,t)\ \Delta t\right)|\psi\rangle_{\text{init}}
\end{aligned}$$

1 Problem Formulation

Given a quantum system with a Hamiltonian of the form

$$H(\mathbf{a}(t),t) = H_{\text{drift}} + \sum_{j=1}^{c} a^j(t) H^j_{\text{drive}}$$

we solve the constrained optimization problem

$$\begin{aligned}
\underset{\mathbf{x}_{1:T},\ \mathbf{u}_{1:T-1}}{\text{minimize}} \quad & \frac{1}{2}\sum_{t=1}^{T-1}\left(\mathbf{a}_t^\top R_{\mathbf{a}}\mathbf{a}_t + \dot{\mathbf{a}}_t^\top R_{\dot{\mathbf{a}}}\dot{\mathbf{a}}_t + \mathbf{u}_t^\top R_{\mathbf{u}}\mathbf{u}_t\right) + Q\cdot\ell(\tilde{\psi}^i_T) \\
\text{subject to} \quad & \mathbf{f}(\mathbf{x}_{t+1},\mathbf{x}_t,\mathbf{u}_t) = \mathbf{0} \\
& \tilde{\psi}^i_1 = \tilde{\psi}^i_{\text{init}} \\
& \tilde{\psi}^1_T = \tilde{\psi}^1_{\text{goal}} \quad \text{if} \ \ \mathsf{pin_first_qstate} = \mathsf{true} \\
& \textstyle\int \mathbf{a}_1 = \mathbf{a}_1 = \mathrm{d}_t\mathbf{a}_1 = \mathbf{0} \\
& \textstyle\int \mathbf{a}_T = \mathbf{a}_T = \mathrm{d}_t\mathbf{a}_T = \mathbf{0} \\
& \left|a^j_t\right| \le a^j_{\text{bound}}
\end{aligned}$$

The *state* vector $\mathbf{x}_t$ contains both the n ($\mathsf{nqstates}$) quantum isomorphism states $\tilde{\psi}^i_t$ (each of dimension $\mathsf{isodim} = 2{*}\mathsf{ketdim}$) and the augmented control states $\int\mathbf{a}_t$, $\mathbf{a}_t$, and $\mathrm{d}_t\mathbf{a}_t$ (the number of augmented state vector is augdim). The *action* vector $\mathbf{u}_t$ contains the second derivative of the *control* vector $\mathbf{a}_t$, which has dimension $\mathsf{ncontrols}$. Thus, we have:

$$\mathbf{x}_t = \begin{pmatrix} \tilde{\psi}^1_t \\ \vdots \\ \tilde{\psi}^n_t \\ \int\mathbf{a}_t \\ \mathbf{a}_t \\ \mathrm{d}_t\mathbf{a}_t \end{pmatrix} \quad \text{and} \quad \mathbf{u}_t = \left(\mathrm{d}_t^2\mathbf{a}_t\right) \tag{4}$$

In summary,

$$\begin{aligned}\dim(\mathbf{x}_t) &= \mathsf{nstates} = \mathsf{nqstates} \text{ * } \mathsf{isodim} + \mathsf{ncontrols} \text{ * } \mathsf{augdim} \\ \dim(\mathbf{u}_t) &= \mathsf{ncontrols}\end{aligned}$$

Additionally the cost function ℓ can be chosen somewhat liberally, the default is currently

$$\ell(\tilde{\psi}, \tilde{\psi}_{\text{goal}}) = 1 - |\langle\psi|\psi_{\text{goal}}\rangle|^2$$

2 Dynamics

Finally, $\mathbf{f}(\mathbf{x}_{t+1}, \mathbf{x}_t, \mathbf{u}_t)$ describes the dynamics of all the variables in the system, where the controls' dynamics are trivial and formally $\tilde{\psi}_t^i$ satisfies a discretized version of the isomorphic Schröedinger equation:

$$\frac{\mathrm{d}\tilde{\psi}^i}{\mathrm{d}t} = \widetilde{(-iH)}(\mathbf{a}(t), t)\tilde{\psi}^i$$

I will the use the notation $G(H)(\mathbf{a}(t), t) = \widetilde{(-iH)}(\mathbf{a}(t), t)$, to describe this operator (the Generator of time translation), which acts on the isomorphic quantum state vectors

$$\tilde{\psi} = \begin{pmatrix} \psi^{\mathrm{Re}} \\ \psi^{\mathrm{Im}} \end{pmatrix}$$

It can be shown that

$$G(H) = -\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes H^{\mathrm{Re}} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes H^{\mathrm{Im}}$$

where $\otimes$ is the Kronecker product. We then have the linear isomorphism dynamics equation:

$$\frac{\mathrm{d}\tilde{\psi}}{\mathrm{d}t} = G(\mathbf{a}(t), t)\tilde{\psi}$$

where

$$G(\mathbf{a}(t), t) = G(H_{\mathrm{drift}}) + \sum_j a^j(t) G(H_{\mathrm{drive}}^j)$$

The implicit dynamics constraint function $\mathbf{f}$ can be decomposed as follows:

$$\mathbf{f}(\mathbf{x}_{t+1}, \mathbf{x}_t, \mathbf{u}_t) = \begin{pmatrix} \mathbf{P}^{(m)}(\tilde{\psi}_{t+1}^1, \tilde{\psi}_t^1, \mathbf{a}_t) \\ \vdots \\ \mathbf{P}^{(m)}(\tilde{\psi}_{t+1}^n, \tilde{\psi}_t^n, \mathbf{a}_t) \\ \int \mathbf{a}_{t+1} - (\int \mathbf{a}_t + \mathbf{a}_t \cdot \Delta t_t) \\ \mathbf{a}_{t+1} - (\mathbf{a}_t + \mathrm{d}_t \mathbf{a}_t \cdot \Delta t_t) \\ \mathrm{d}_t \mathbf{a}_{t+1} - (\mathrm{d}_t \mathbf{a}_t + \mathbf{u}_t \cdot \Delta t_t) \end{pmatrix}$$

2.1 Padé integrators

We define (and implement) just the $m \in \{2, 4\}$ order Padé integrators $\mathbf{P}^{(m)}$:

$$
\begin{aligned}
\mathbf{P}^{(2)}(\tilde{\psi}^i_{t+1}, \tilde{\psi}^i_t, \mathbf{a}_t) &= \left(I - \frac{\Delta t}{2} G(\mathbf{a}_t)\right) \tilde{\psi}^i_{t+1} - \left(I + \frac{\Delta t}{2} G(\mathbf{a}_t)\right) \tilde{\psi}^i_t \\
\mathbf{P}^{(4)}(\tilde{\psi}^i_{t+1}, \tilde{\psi}^i_t, \mathbf{a}_t) &= \left(I - \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2\right) \tilde{\psi}^i_{t+1} \\
&\quad - \left(I + \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2\right) \tilde{\psi}^i_t
\end{aligned}
$$

Where again

$$
G(\mathbf{a}_t) = G_{\text{drift}} + \mathbf{a}_t \cdot \mathbf{G}_{\text{drive}}
$$

with $\mathbf{G}_{\text{drive}} = (G^1_{\text{drive}}, \ldots, G^c_{\text{drive}})^\top$, where $c = \mathsf{ncontrols}$

3 Differentiation

Our problem consists of $Z_{\text{dim}} = (\mathsf{nstates} + \mathsf{ncontrols}) \times \mathsf{T}$ total variables, arranged into a vector

$$\mathbf{Z} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{u}_1 \\ \vdots \\ \mathbf{x}_T \\ \mathbf{u}_T \end{pmatrix} = \begin{pmatrix} \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_T \end{pmatrix} \tag{5}$$

where $\mathbf{z}_t = \begin{pmatrix} \mathbf{x}_t \\ \mathbf{u}_t \end{pmatrix}$ is referred to as a *knot point* and has dimension

$$z_{\text{dim}} = \mathsf{vardim} = \mathsf{nstates} + \mathsf{ncontrols}.$$

Also, as of right now, $\mathbf{u}_T$ is included in $\mathbf{Z}$ but is ignored in calculations.

3.1 Objective Gradient

Given the objective

$$J(\mathbf{Z}) = Q \sum_{i=1}^{n} \ell(\tilde{\psi}_T^i, \tilde{\psi}_{\text{goal}}^i) + \frac{R}{2} \sum_{t=1}^{T-1} \mathbf{u}_t^2 \tag{6}$$

we arrive at the gradient

$$\boldsymbol{\nabla}_{\mathbf{Z}} J(\mathbf{Z}) = \begin{pmatrix} \mathbf{0}_{x_{\text{dim}}} \\ R \cdot \mathbf{u}_1 \\ \vdots \\ \mathbf{0}_{x_{\text{dim}}} \\ R \cdot \mathbf{u}_t \\ \vdots \\ \mathbf{0}_{x_{\text{dim}}} \\ R \cdot \mathbf{u}_{T-1} \\ Q \cdot \boldsymbol{\nabla}_{\tilde{\psi}^1} \ell^1 \\ \vdots \\ Q \cdot \boldsymbol{\nabla}_{\tilde{\psi}^n} \ell^n \\ \mathbf{0} \end{pmatrix} \tag{7}$$

where $\ell^i = \ell(\tilde{\psi}_T^i, \tilde{\psi}_{\text{goal}}^i)$. $\boldsymbol{\nabla}_{\tilde{\psi}^i} \ell^i$ is currently not calculated by hand, but at compile time via Symbolics.jl.

3.2 Dynamics Jacobian

Writing, $\mathbf{f}(\mathbf{z}_t, \mathbf{z}_{t+1}) = \mathbf{f}(\tilde{\psi}_{t+1}^i, \tilde{\psi}_t^i, \mathbf{a}_t)$, we can arrange the dynamics constraints into a vector

$$\mathbf{F} = \begin{pmatrix} \mathbf{f}(\mathbf{z}_1, \mathbf{z}_2) \\ \vdots \\ \mathbf{f}(\mathbf{z}_{T-1}, \mathbf{z}_T) \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \vdots \\ \mathbf{f}_{T-1} \end{pmatrix} \tag{8}$$

where we have defined $\mathbf{f}_t = \mathbf{f}(\mathbf{z}_t, \mathbf{z}_{t+1})$.

The dynamics Jacobian matrix $\frac{\partial \mathbf{F}}{\partial \mathbf{Z}}$ then has dimensions

$$F_{\text{dim}} \times Z_{\text{dim}} = (f_{\text{dim}} \cdot (T-1)) \times (z_{\text{dim}} \cdot T)$$

This matrix has a block diagonal structure:

$$
\frac{\partial \mathbf{F}}{\partial \mathbf{Z}} = \begin{pmatrix}
\frac{\partial \mathbf{f}_1}{\partial \mathbf{z}_1} & \frac{\partial \mathbf{f}_1}{\partial \mathbf{z}_2} & & & & \\
& \ddots & \ddots & & & \\
& & \frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_t} & \frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_{t+1}} & & \\
& & & \ddots & \ddots & \\
& & & & \frac{\partial \mathbf{f}_T}{\partial \mathbf{z}_{T-1}} & \frac{\partial \mathbf{f}_T}{\partial \mathbf{z}_T}
\end{pmatrix} \tag{9}
$$

We just need the $f_{\dim} \times z_{\dim}$ Jacobian matrices $\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_t}$ and $\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_{t+1}}$.

$\mathbf{f}_t$ Jacobian expressions

With $\mathbf{P}_t^{(m),i} = \mathbf{P}^{(m)}(\tilde{\psi}_{t+1}^i, \tilde{\psi}_t^i, \mathbf{a}_t)$, we first have

$$
\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_t} = \begin{pmatrix}
\ddots & & & \vdots & & & \\
& \frac{\partial \mathbf{P}_t^{(m),i}}{\partial \tilde{\psi}_t^i} & & \frac{\partial \mathbf{P}_t^{(m),i}}{\partial \mathbf{a}_t} & & & \\
& & \ddots & \vdots & & & \\
& & & -I_c^{\int \mathbf{a}_t} \quad -\Delta t I_c^{\mathbf{a}_t} & & & \\
& & & -I_c^{\mathbf{a}_t} & -\Delta t I_c^{\mathrm{d}_t \mathbf{a}_t} & & \\
& & & & \ddots & \ddots & \\
& & & & & -I_c^{\mathrm{d}_t^{c-1} \mathbf{a}_t} & -\Delta t I_c^{\mathbf{u}_t}
\end{pmatrix} \tag{10}
$$

where, $c =$ ncontrols, and the diagonal dots in the bottom right indicate that the number of $-I_c$ blocks on the diagonal should equal augdim, which is set to 3 by default.

Lastly,

$$\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_{t+1}} = \begin{pmatrix} \frac{\partial \mathbf{P}_t^{(m),1}}{\partial \tilde{\psi}_{t+1}^1} & & & \\ & \ddots & & \\ & & \frac{\partial \mathbf{P}_t^{(m),n}}{\partial \tilde{\psi}_{t+1}^n} & \\ & & & I_{c \cdot \mathsf{augdim}} \end{pmatrix} \tag{11}$$

$\mathbf{P}_t^{(m),i}$ Jacobian expressions

For the $\tilde{\psi}^i$ components, we have, for $m = 2$,

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_t^i} = -\left(I + \frac{\Delta t}{2} G(\mathbf{a}_t)\right) \tag{12}$$

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_{t+1}^i} = I - \frac{\Delta t}{2} G(\mathbf{a}_t) \tag{13}$$

and, for $m = 4$,

$$\frac{\partial \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_t^i} = -\left(I + \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2\right) \tag{14}$$

$$\frac{\partial \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_{t+1}^i} = I - \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2. \tag{15}$$

Now, for the $\mathbf{a}_t$ components, we have, for $m = 2$,

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial a_t^j} = \frac{-\Delta t}{2} G_{\text{drive}}^j \left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) \tag{16}$$

and, for $m = 4$,

$$\frac{\partial \mathbf{P}_t^{(4),i}}{\partial a_t^j} = \frac{-\Delta t}{2} G_{\text{drive}}^j \left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) + \frac{(\Delta t)^2}{9} \left\{G_{\text{drive}}^j, G(\mathbf{a}_t)\right\} \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i\right) \tag{17}$$

where $\{A, B\} = AB + BA$ is the anticommutator.

3.3 Hessian of the Lagrangian

The Lagrangian function is defined to be

$$\mathscr{L}(\mathbf{Z};\sigma,\boldsymbol{\mu}) = \sigma \cdot J(\mathbf{Z}) + \boldsymbol{\mu} \cdot \mathbf{F}(\mathbf{Z}) \tag{18}$$

where $\boldsymbol{\mu}$ is a Z_{dim}-dimensional vector provided by the solver.

For the Hessian we have

$$\nabla^2 \mathscr{L} = \sigma \cdot \nabla^2 J + \boldsymbol{\mu} \cdot \nabla^2 \mathbf{F}. \tag{19}$$

We will look at $\nabla^2 J$ and $\boldsymbol{\mu} \cdot \nabla^2 \mathbf{F}$ separately.

Objective Hessian

With $\ell^i = \ell(\tilde{\psi}^i_T, \tilde{\psi}^i_{\text{goal}})$, we have

$$\nabla^2 J(\mathbf{Z}) = \begin{pmatrix} \ddots & & & & & & & \\ & \mathbf{0} & & & & & & \\ & & R_t I_c & & & & & \\ & & & \ddots & & & & \\ & & & & \ddots & & & \\ & & & & & Q \cdot \nabla^2 \ell^i & & \\ & & & & & & \ddots & \\ & & & & & & & \mathbf{0} \end{pmatrix} \tag{20}$$

where $\nabla^2 \ell^i$ is again calculated using Symbolics.jl.

Dynamics Hessian

With $\boldsymbol{\mu} = (\vec{\mu}_1, \ldots, \vec{\mu}_T)$, $\vec{\mu}_t = \left(\mu_t^1, \ldots, \mu_t^{z_{\text{dim}}}\right)$, and using

$$\vec{\mu}_t^{\tilde{\psi}^i} = \left(\mu_t^{(i-1)\cdot\tilde{\psi}_{\text{dim}}+1}, \ldots, \mu_t^{i\cdot\tilde{\psi}_{\text{dim}}}\right)$$

we have

$$\boldsymbol{\mu} \cdot \nabla^2 \mathbf{F} = \begin{pmatrix} & \vdots & & & & \\ & \left(\frac{\partial^2 \mathbf{P}_t^{(m),i}}{\partial \tilde{\psi}_t^i \partial a_t^j}\right)^\top \vec{\mu}_t^{\tilde{\psi}^i} & & & & \\ & \vdots & & & & \\ \ddots & \mathbf{0} & & & & \\ & \sum_{i=1}^n \vec{\mu}_t^{\tilde{\psi}^i} \cdot \frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial a_t^k \partial a_t^j} & \mathbf{0} & \ldots & \left(\vec{\mu}_t^{\tilde{\psi}^i}\right)^\top \frac{\partial^2 \mathbf{P}_t^{(m),i}}{\partial a_t^k \partial \tilde{\psi}_{t+1}^i} & \ldots \\ & & \ddots & & & \end{pmatrix} \tag{21}$$

with

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial a_t^k \partial a_t^j} = \frac{(\Delta t)^2}{9} \left\{G_{\text{drive}}^j, G_{\text{drive}}^k\right\} \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i\right) \tag{22}$$

with, again, $\{A, B\} = AB + BA$, being the anticommutator.

since

$$x \cdot (Ay) = x^\top Ay = (A^\top x)^\top y$$

For the mixed partials we have:

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_t^i \partial a_t^j} = \frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_{t+1}^i \partial a_t^j} = -\frac{\Delta t}{2} G_{\text{drive}}^j \tag{23}$$

and

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_t^i \partial a_t^j} = -\frac{\Delta t}{2} G_{\text{drive}}^j - \frac{(\Delta t)^2}{9} \left(\left\{G_{\text{drive}}^j, G_{\text{drift}}\right\} + \mathbf{a}_t \cdot \left\{G_{\text{drive}}^j, \mathbf{G}_{\text{drive}}\right\}\right) \tag{24}$$

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_{t+1}^i \partial a_t^j} = -\frac{\Delta t}{2} G_{\text{drive}}^j + \frac{(\Delta t)^2}{9} \left(\left\{G_{\text{drive}}^j, G_{\text{drift}}\right\} + \mathbf{a}_t \cdot \left\{G_{\text{drive}}^j, \mathbf{G}_{\text{drive}}\right\}\right) \tag{25}$$

4 Minimum Time Problem

Once a solution has been found for a given *time horizon*, we can solve the time minimization problem below, initialized with the given solution.

$$\begin{aligned} \underset{\substack{\mathbf{x}_{1:T},\ \mathbf{u}_{1:T-1} \\ \Delta t_{1:T-1}}}{\text{minimize}} \quad & \sum_t \Delta t_t + \frac{1}{2} \sum_t \mathbf{u}_t^\top R_u \mathbf{u}_t + \frac{R_s}{2} \sum_t (\mathbf{u}_{t+1} - \mathbf{u}_t)^2 \\ \text{subject to} \quad & \mathbf{f}(\mathbf{x}_{t+1}, \mathbf{x}_t, \mathbf{u}_t, \Delta t_t) = \mathbf{0} \\ & \mathbf{x}_T = \mathbf{x}_T^{\text{nominal}} \end{aligned}$$

For this problem we will define, with $\mathbf{Z}$ as defined before

$$\mathbf{\Delta t} = \begin{pmatrix} \Delta t_1 \\ \vdots \\ \Delta t_{T-1} \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{Z}} = \begin{pmatrix} \mathbf{Z} \\ \mathbf{\Delta t} \end{pmatrix}$$

4.1 Objective Gradient

Let's write the objective function as

$$J = J_{\Delta t} + J_u + J_s \tag{26}$$

then

$$\nabla_{\bar{\mathbf{Z}}} J = \begin{pmatrix} \nabla_{\mathbf{Z}} J \\ \nabla_{\mathbf{\Delta t}} J \end{pmatrix} = \begin{pmatrix} \nabla_{\mathbf{Z}} J_u + \nabla_{\mathbf{Z}} J_s \\ \nabla_{\mathbf{\Delta t}} J_{\Delta t} \end{pmatrix} \tag{27}$$

where

$$\nabla_{\mathbf{Z}} J_u = \begin{pmatrix} \vdots \\ \mathbf{0} \\ R_u \mathbf{u}_t \\ \vdots \end{pmatrix}, \qquad \nabla_{\mathbf{Z}} J_s = \begin{pmatrix} \mathbf{0} \\ R_s(\mathbf{u}_1 - \mathbf{u}_2) \\ \vdots \\ \mathbf{0} \\ R_s(-\mathbf{u}_{t-1} + 2\mathbf{u}_t - \mathbf{u}_{t+1}) \\ \vdots \\ \mathbf{0} \\ R_s(-\mathbf{u}_{T-2} + \mathbf{u}_{T-1}) \end{pmatrix}, \tag{28}$$

and

$$\nabla_{\mathbf{\Delta t}} J_{\Delta t} = \mathbf{1}_{T-1} \tag{29}$$

4.2 Dynamics Jacobian

We then have, with $\mathbf{F}$ defined as before (but taking the corresponding Δt_t):

$$\frac{\partial \mathbf{F}}{\partial \bar{\mathbf{Z}}} = \begin{pmatrix} \frac{\partial \mathbf{F}}{\partial \mathbf{Z}} & \frac{\partial \mathbf{F}}{\partial \mathbf{\Delta t}} \end{pmatrix} \tag{30}$$

where

$$\frac{\partial \mathbf{F}}{\partial \mathbf{\Delta t}} = \begin{pmatrix} \frac{\partial \mathbf{f}_1}{\partial \Delta t_1} & & \\ & \ddots & \\ & & \frac{\partial \mathbf{f}_{T-1}}{\partial \Delta t_{T-1}} \end{pmatrix} \tag{31}$$

with

$$\frac{\partial \mathbf{f}_t}{\partial \Delta t_t} = \begin{pmatrix} \vdots \\ \frac{\partial \mathbf{P}_t^{(n),i}}{\partial \Delta t_t} \\ \vdots \\ -\mathbf{a}_t \\ -\dot{\mathbf{a}}_t \\ -\mathbf{u}_t \end{pmatrix} \tag{32}$$

and

$$\begin{aligned} \frac{\partial \mathbf{P}_t^{(4),i}}{\partial \Delta t_t} &= \left(-\frac{1}{2}G(\mathbf{a}_t) + \frac{2\Delta t_t}{9}G(\mathbf{a}_t)^2\right)\tilde{\psi}_{t+1}^i - \left(\frac{1}{2}G(\mathbf{a}_t) + \frac{2\Delta t_t}{9}G(\mathbf{a}_t)^2\right)\tilde{\psi}_t^i \\ &= -\frac{1}{2}G(\mathbf{a}_t)\left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) + \frac{2\Delta t_t}{9}G(\mathbf{a}_t)^2\left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i\right) \end{aligned} \tag{33}$$

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial \Delta t_t} = -\frac{1}{2}G(\mathbf{a}_t)\left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) \tag{34}$$

4.3 Hessian of the Lagrangian

As before we will first define the objective Hessian and then the dynamics Lagrangian Hessian

Objective Hessian

Decomposing as before, we have

$$\nabla^2_{\bar{\mathbf{Z}}} J = \begin{pmatrix} \nabla^2_{\mathbf{Z}} J_u + \nabla^2_{\mathbf{Z}} J_s & \\ & \nabla^2_{\mathbf{\Delta t}} J_{\Delta t} \end{pmatrix} = \begin{pmatrix} \nabla^2_{\mathbf{Z}} J_u + \nabla^2_{\mathbf{Z}} J_s & \\ & \mathbf{0}_{T-1 \times T-1} \end{pmatrix}$$

where

$$\nabla^2_{\mathbf{Z}} J_u = \begin{pmatrix} \ddots & & & \\ & \mathbf{0} & & \\ & & R_u I & \\ & & & \ddots \end{pmatrix} \tag{35}$$

and, showing the upper triangular structure of the Hessian,

$$\nabla^2_{\mathbf{Z}} J_s = \begin{pmatrix} \mathbf{0} & & \mathbf{0} & & & & & \\ & R_s I & & -R_s I & & & & \\ & & \mathbf{0} & & \mathbf{0} & & & \\ & & & 2R_s I & & -R_s I & & \\ & & & & \mathbf{0} & & \ddots & \\ & & & & & 2R_s I & & -R_s I \\ & & & & & & \ddots & \\ & & & & & & & R_s I \end{pmatrix} \tag{36}$$

Hessian of the Dynamics Lagrangian

Defining

$$\mathcal{L}_f = \boldsymbol{\mu} \cdot \mathbf{F}$$

we want to compute

$$\nabla^2_{\bar{\mathbf{Z}}} \mathcal{L}_f = \begin{pmatrix} \nabla^2_{\mathbf{Z}} \mathcal{L}_f & \nabla^\top_{\mathbf{\Delta t}} \nabla_{\mathbf{Z}} \mathcal{L}_f \\ \nabla^\top_{\mathbf{Z}} \nabla_{\mathbf{\Delta t}} \mathcal{L}_f & \nabla^2_{\mathbf{\Delta t}} \mathcal{L}_f \end{pmatrix}$$

we have already computed $\nabla^2_{\mathbf{Z}} \mathcal{L}_f$ above, so we then have

$$\nabla^2_{\mathbf{\Delta t}} \mathcal{L}_f = \begin{pmatrix} \ddots & & \\ & \vec{\mu}_t \cdot \dfrac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t^2} & \\ & & \ddots \end{pmatrix} \tag{37}$$

where

$$\vec{\mu}_t \cdot \frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t^2} = \vec{\mu}_t \cdot \begin{pmatrix} \vdots \\ \dfrac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t^2} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} = \sum_i \vec{\mu}_t^{\tilde{\psi}_i} \cdot \frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t^2} \tag{38}$$

with

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t^2} = \frac{2}{9} G(\mathbf{a}_t)^2 \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i \right) \tag{39}$$

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t^2} = \mathbf{0} \tag{40}$$

We also have

$$\nabla_{\Delta \mathbf{t}}^\top \nabla_{\mathbf{z}} \mathcal{L}_f = \begin{pmatrix} \ddots & & & \\ & \left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_t} \right)^\top \vec{\mu}_t & & \\ & \left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_{t+1}} \right)^\top \vec{\mu}_t & \left(\frac{\partial^2 \mathbf{f}_{t+1}}{\partial \Delta t_{t+1} \partial \mathbf{z}_{t+1}} \right)^\top \vec{\mu}_{t+1} & \\ & & \left(\frac{\partial^2 \mathbf{f}_{t+1}}{\partial \Delta t_{t+1} \partial \mathbf{z}_{t+2}} \right)^\top \vec{\mu}_{t+1} & \\ & & & \ddots \end{pmatrix} \tag{41}$$

where

$$\left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_t} \right)^\top \vec{\mu}_t = \begin{pmatrix} \vdots \\ \left(\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \tilde{\psi}_t^i} \right)^\top \vec{\mu}_t^{\tilde{\psi}^i} \\ \vdots \\ \mathbf{0} \\ -\vec{\mu}_t^{\int \mathbf{a}} + \sum_i \left(\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \mathbf{a}_t} \right)^\top \vec{\mu}_t^{\tilde{\psi}^i} \\ -\vec{\mu}_t^{\mathbf{a}} \\ -\vec{\mu}_t^{\dot{\mathbf{a}}} \end{pmatrix} \tag{42}$$

and

$$\left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_{t+1}} \right)^\top \vec{\mu}_t = \begin{pmatrix} \vdots \\ \left(\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \tilde{\psi}_{t+1}^i} \right)^\top \vec{\mu}_t^{\tilde{\psi}^i} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \tag{43}$$

with

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t \partial \tilde{\psi}_t^i} = -\left(\frac{1}{2} G(\mathbf{a}_t) + \frac{2\Delta t_t}{9} G(\mathbf{a}_t)^2 \right) \tag{44}$$

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t \partial \tilde{\psi}_{t+1}^i} = -\frac{1}{2} G(\mathbf{a}_t) + \frac{2\Delta t_t}{9} G(\mathbf{a}_t)^2 \tag{45}$$

and

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t \partial \tilde{\psi}_t^i} = \frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t \partial \tilde{\psi}_{t+1}^i} = -\frac{1}{2} G(\mathbf{a}_t) \tag{46}$$

and for the jth column of $\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \mathbf{a}_t}$ we have

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t \partial a_t^j} = -\frac{1}{2} G_{\text{drive}}^j \Big(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i \Big) + \frac{2\Delta t_t}{9} \Big\{ G_{\text{drive}}^j, G(\mathbf{a}_t) \Big\} \Big(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i \Big) \tag{47}$$

and

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t \partial a_t^j} = -\frac{1}{2} G_{\text{drive}}^j \Big(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i \Big) \tag{48}$$

5 Unitary Implementation

5.1 Vectorized Isomorphic Unitary Padé Dynamics

We show later on that we can efficiently vectorize the Padé dynamics for the isomorphic representation of the unitary, i.e. retain information about only the real and imaginary parts of the unitary. The resulting dynamics expression is given by

$$\hat{\mathbf{P}}(\vec{\tilde{U}}_{t+1}, \vec{\tilde{U}}_t, \mathbf{a}_t, h_t) = \hat{B}(\mathbf{a}_t, h_t)\vec{\tilde{U}}_{t+1} - \hat{F}(\mathbf{a}_t, h_t)\vec{\tilde{U}}_t.$$

Here

$$\begin{aligned}
\hat{B}(\mathbf{a}_t, h_t) &= (I_2 \otimes I_N) \otimes B^{\mathrm{R}}(\mathbf{a}_t, h_t) + (\mathrm{Im} \otimes I_N) \otimes B^{\mathrm{I}}(\mathbf{a}_t, h_t) \\
\hat{F}(\mathbf{a}_t, h_t) &= (I_2 \otimes I_N) \otimes F^{\mathrm{R}}(\mathbf{a}_t, h_t) - (\mathrm{Im} \otimes I_N) \otimes F^{\mathrm{I}}(\mathbf{a}_t, h_t),
\end{aligned}$$

along with

$$\begin{aligned}
B^{\mathrm{R}}(\mathbf{a}_t, h_t) &= I - \frac{h_t}{2} H^{\mathrm{I}}(\mathbf{a}_t) + \frac{h_t^2}{9}\Big(\big(H^{\mathrm{I}}(\mathbf{a}_t)\big)^2 - \big(H^{\mathrm{R}}(\mathbf{a}_t)\big)^2\Big) \\
B^{\mathrm{I}}(\mathbf{a}_t, h_t) &= \frac{h_t}{2} H^{\mathrm{R}}(\mathbf{a}_t) - \frac{h_t^2}{9}\big\{H^{\mathrm{R}}(\mathbf{a}_t), H^{\mathrm{I}}(\mathbf{a}_t)\big\},
\end{aligned}$$

and

$$\begin{aligned}
F^{\mathrm{R}}(\mathbf{a}_t, h_t) &= I + \frac{h_t}{2} H^{\mathrm{I}}(\mathbf{a}_t) + \frac{h_t^2}{9}\Big(\big(H^{\mathrm{I}}(\mathbf{a}_t)\big)^2 - \big(H^{\mathrm{R}}(\mathbf{a}_t)\big)^2\Big) \\
F^{\mathrm{I}}(\mathbf{a}_t, h_t) &= \frac{h_t}{2} H^{\mathrm{R}}(\mathbf{a}_t) + \frac{h_t^2}{9}\big\{H^{\mathrm{R}}(\mathbf{a}_t), H^{\mathrm{I}}(\mathbf{a}_t)\big\}.
\end{aligned}$$

5.2 Derivation of the Dynamics

Isomorphic Vectorization

To store just the real and imaginary parts of complex-valued matrices $A = A^{\mathrm{R}} + iA^{\mathrm{I}} \in \mathbb{C}^{N\times N}$ in a vector, for numerical purposes, we define a projection matrix $\hat{P} \in \mathbb{R}^{2N^2\times 4N^2}$ that will act on the vectorization of the real-valued isomorphic representation $\tilde{A} = \mathrm{iso}(A) = I_2 \otimes A^{\mathrm{R}} + \mathrm{Im} \otimes A^{\mathrm{I}} \in \mathbb{R}^{2N\times 2N}$ as follows:

$$\begin{aligned}
\mathrm{isovec}\big(\tilde{A}\big) &= \hat{P}\ \mathrm{vec}(\tilde{A}) \\
&= \hat{P}\ \mathrm{vec}\big(I_2 \otimes A^{\mathrm{R}} + \mathrm{Im} \otimes A^{\mathrm{I}}\big) \\
&= \begin{pmatrix} \mathrm{vec}(A^{\mathrm{R}}) \\ \mathrm{vec}(A^{\mathrm{I}}) \end{pmatrix}.
\end{aligned}$$

Given projection matrices $P_{\mathrm{Re}} = \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{N\times 2N}$ and $P_{\mathrm{Im}} = \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} \in \mathbb{R}^{N\times 2N}$ we can write the projection matrix $\hat{P}$ as

$$\hat{P}_1 = (P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}) \otimes P_{\mathrm{Re}},$$

or equivalently as

$$\hat{P}_2 = \big(P_{\mathrm{Im}}^\top P_{\mathrm{Re}} + P_{\mathrm{Re}}^\top P_{\mathrm{Im}}\big) \otimes P_{\mathrm{Im}}.$$

Both of these projectors produce identically correct results, i.e. $\hat{P}_1 \mathrm{vec}(\tilde{A}) = \hat{P}_2 \mathrm{vec}(\tilde{A})$, so we will write $\hat{P}_1 \simeq \hat{P}_2$. This is demonstrated as follows:

$$\begin{aligned}
\hat{P}_1 \mathrm{vec}(\tilde{A}) &= \big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big) \otimes P_{\mathrm{Re}}\big)\ \mathrm{vec}(\tilde{A}) \\
&= \big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} \otimes P_{\mathrm{Re}}\big)\ \mathrm{vec}(\tilde{A}) - \big(P_{\mathrm{Im}}^\top P_{\mathrm{Im}} \otimes P_{\mathrm{Re}}\big)\ \mathrm{vec}(\tilde{A}) \\
&= \mathrm{vec}\Big(P_{\mathrm{Re}} \tilde{A} P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Re}} \tilde{A} P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\Big) \\
&= \mathrm{vec}\left(\begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} \begin{pmatrix} A^{\mathrm{R}} & -A^{\mathrm{I}} \\ A^{\mathrm{I}} & A^{\mathrm{R}} \end{pmatrix} \begin{pmatrix} I_N \\ \mathbf{0} \end{pmatrix} \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} - \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} \begin{pmatrix} A^{\mathrm{R}} & -A^{\mathrm{I}} \\ A^{\mathrm{I}} & A^{\mathrm{R}} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ I_N \end{pmatrix} \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix}\right) \\
&= \mathrm{vec}\left(\begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} \begin{pmatrix} A^{\mathrm{R}} \\ A^{\mathrm{I}} \end{pmatrix} \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} - \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} \begin{pmatrix} -A^{\mathrm{I}} \\ A^{\mathrm{R}} \end{pmatrix} \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix}\right) \\
&= \mathrm{vec}\big(A^{\mathrm{R}} \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix} + A^{\mathrm{I}} \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix}\big) \\
&= \mathrm{vec}\big(\begin{pmatrix} A^{\mathrm{R}} & A^{\mathrm{I}} \end{pmatrix}\big) \\
&= \begin{pmatrix} \mathrm{vec}(A^{\mathrm{R}}) \\ \mathrm{vec}(A^{\mathrm{I}}) \end{pmatrix}.
\end{aligned}$$

And also

$$\begin{aligned}
\hat{P}_2 \mathrm{vec}(\tilde{A}) &= \big(\big(P_{\mathrm{Im}}^\top P_{\mathrm{Re}} + P_{\mathrm{Re}}^\top P_{\mathrm{Im}}\big) \otimes P_{\mathrm{Im}}\big)\ \mathrm{vec}(\tilde{A}) \\
&= \big(P_{\mathrm{Im}}^\top P_{\mathrm{Re}} \otimes P_{\mathrm{Im}}\big)\ \mathrm{vec}(\tilde{A}) + \big(P_{\mathrm{Re}}^\top P_{\mathrm{Im}} \otimes P_{\mathrm{Im}}\big)\ \mathrm{vec}(\tilde{A}) \\
&= \mathrm{vec}\Big(P_{\mathrm{Im}} \tilde{A} P_{\mathrm{Re}}^\top P_{\mathrm{Im}} + P_{\mathrm{Im}} \tilde{A} P_{\mathrm{Im}}^\top P_{\mathrm{Re}}\Big) \\
&= \mathrm{vec}\left(\begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} \begin{pmatrix} A^{\mathrm{R}} & -A^{\mathrm{I}} \\ A^{\mathrm{I}} & A^{\mathrm{R}} \end{pmatrix} \begin{pmatrix} I_N \\ \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} + \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} \begin{pmatrix} A^{\mathrm{R}} & -A^{\mathrm{I}} \\ A^{\mathrm{I}} & A^{\mathrm{R}} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ I_N \end{pmatrix} \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix}\right) \\
&= \mathrm{vec}\left(\begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} \begin{pmatrix} A^{\mathrm{R}} \\ A^{\mathrm{I}} \end{pmatrix} \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} + \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} \begin{pmatrix} -A^{\mathrm{I}} \\ A^{\mathrm{R}} \end{pmatrix} \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix}\right) \\
&= \mathrm{vec}\big(A^{\mathrm{I}} \begin{pmatrix} \mathbf{0} & I_N \end{pmatrix} + A^{\mathrm{R}} \begin{pmatrix} I_N & \mathbf{0} \end{pmatrix}\big) \\
&= \mathrm{vec}\big(\begin{pmatrix} A^{\mathrm{R}} & A^{\mathrm{I}} \end{pmatrix}\big) \\
&= \begin{pmatrix} \mathrm{vec}(A^{\mathrm{R}}) \\ \mathrm{vec}(A^{\mathrm{I}}) \end{pmatrix}.
\end{aligned}$$

For later convenience let's now look at the expression $\hat{P}_1\Big(I_{2N}\otimes\tilde{A}\Big)$

$$\begin{aligned}
\hat{P}_1\Big(I_{2N}\otimes\tilde{A}\Big) &= \big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Re}}\big)\Big(I_{2N}\otimes\tilde{A}\Big)\\
&= \big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes\Big(P_{\mathrm{Re}}\tilde{A}\Big)\\
&= \big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes\big(A^{\mathrm{R}}P_{\mathrm{Re}} - A^{\mathrm{I}}P_{\mathrm{Im}}\big)\\
&= \big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes\big(A^{\mathrm{R}}P_{\mathrm{Re}}\big) - \big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes\big(A^{\mathrm{I}}P_{\mathrm{Im}}\big)\\
&= \big(I_{2N}\otimes A^{\mathrm{R}}\big)\big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Re}}\big) - \big(I_{2N}\otimes A^{\mathrm{I}}\big)\big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Im}}\big)\\
&= \big(I_2\otimes I_N\otimes A^{\mathrm{R}}\big)\hat{P}_1 - \big(I_2\otimes I_N\otimes A^{\mathrm{I}}\big)\big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Im}}\big)\\
&= \big(I_2\otimes I_N\otimes A^{\mathrm{R}}\big)\hat{P}_1 + \big(\mathrm{Im}^2\otimes I_N\otimes A^{\mathrm{I}}\big)\big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Im}}\big)\\
&= \big(I_2\otimes I_N\otimes A^{\mathrm{R}}\big)\hat{P}_1 + \big(\mathrm{Im}\otimes I_N\otimes A^{\mathrm{I}}\big)(\mathrm{Im}\otimes I_N\otimes I_N)\big(\big(P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Im}}\big)\\
&= \big(I_2\otimes I_N\otimes A^{\mathrm{R}}\big)\hat{P}_1 + \big(\mathrm{Im}\otimes I_N\otimes A^{\mathrm{I}}\big)\big(\big((\mathrm{Im}\otimes I_N)P_{\mathrm{Re}}^\top P_{\mathrm{Re}} - (\mathrm{Im}\otimes I_N)P_{\mathrm{Im}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Im}}\big)\\
&= \big(I_2\otimes I_N\otimes A^{\mathrm{R}}\big)\hat{P}_1 + \big(\mathrm{Im}\otimes I_N\otimes A^{\mathrm{I}}\big)\big(\big(P_{\mathrm{Im}}^\top P_{\mathrm{Re}} + P_{\mathrm{Re}}^\top P_{\mathrm{Im}}\big)\otimes P_{\mathrm{Im}}\big)\\
&= \big(I_2\otimes I_N\otimes A^{\mathrm{R}}\big)\hat{P}_1 + \big(\mathrm{Im}\otimes I_N\otimes A^{\mathrm{I}}\big)\hat{P}_2\\
&\simeq \big(I_2\otimes I_N\otimes A^{\mathrm{R}} + \mathrm{Im}\otimes I_N\otimes A^{\mathrm{I}}\big)\hat{P}_1\\
&= \hat{A}\hat{P}_1,
\end{aligned}$$

Where we used

$$\begin{aligned}
P_{\mathrm{Re}}\tilde{A} &= \begin{pmatrix} I_N & \mathbf{0}\end{pmatrix}\begin{pmatrix} A^{\mathrm{R}} & -A^{\mathrm{I}}\\ A^{\mathrm{I}} & A^{\mathrm{R}}\end{pmatrix}\\
&= \begin{pmatrix} A^{\mathrm{R}} & -A^{\mathrm{I}}\end{pmatrix}\\
&= A^{\mathrm{R}}P_{\mathrm{Re}} - A^{\mathrm{I}}P_{\mathrm{Im}},
\end{aligned}$$

and

$$\begin{aligned}
(\mathrm{Im}\otimes I_N)P_{\mathrm{Re}}^\top &= \begin{pmatrix} & -I_N\\ I_N & \end{pmatrix}\begin{pmatrix} I_N\\ \mathbf{0}\end{pmatrix} = \begin{pmatrix}\mathbf{0}\\ I_N\end{pmatrix} = P_{\mathrm{Im}}^\top\\
(\mathrm{Im}\otimes I_N)P_{\mathrm{Im}}^\top &= \begin{pmatrix} & -I_N\\ I_N & \end{pmatrix}\begin{pmatrix}\mathbf{0}\\ I_N\end{pmatrix} = -\begin{pmatrix} I_N\\ \mathbf{0}\end{pmatrix} = -P_{\mathrm{Re}}^\top.
\end{aligned}$$

We can then conclude that

$$\boxed{\hat{P}\Big(I_{2N}\otimes\tilde{A}\Big)\simeq\hat{A}\hat{P}.}$$

Isomorphic Padé Dynamics

Our motivation here is to compute the unitary Padé dynamics on the isomorphic vector representation of the unitary, $\vec{\widetilde{U}} = \text{isovec}(\widetilde{U}) = \hat{P}\ \text{vec}(\widetilde{U}) = \hat{P}\ \text{vec}(\text{iso}(U))$. We can write these dynamics As

$$
\begin{aligned}
f(z_t, z_{t+1}) &= f(\vec{\widetilde{U}}_t, \mathbf{a}_t, h_t, \vec{\widetilde{U}}_{t+1}, \mathbf{a}_{t+1}, h_{t+1}) \\
&= \hat{\mathbf{P}}(\vec{\widetilde{U}}_{t+1}, \vec{\widetilde{U}}_t, \mathbf{a}_t, h_t) \\
&= \text{isovec}\Big(\mathbf{P}(\widetilde{U}_{t+1}, \widetilde{U}_t, \mathbf{a}_t, h_t)\Big) \\
&= \hat{P}\ \text{vec}\Big(\tilde{B}(\mathbf{a}_t, h_t)\widetilde{U}_{t+1} - \tilde{F}(\mathbf{a}_t, h_t)\widetilde{U}_t\Big) \\
&= \hat{P}\Big(I_{2N} \otimes \tilde{B}(\mathbf{a}_t, h_t)\Big)\text{vec}\Big(\widetilde{U}_{t+1}\Big) - \hat{P}\Big(I_{2N} \otimes \tilde{F}(\mathbf{a}_t, h_t)\Big)\text{vec}\Big(\widetilde{U}_t\Big) \\
&= \hat{B}(\mathbf{a}_t, h_t)\hat{P}\ \text{vec}\Big(\widetilde{U}_{t+1}\Big) - \hat{F}(\mathbf{a}_t, h_t)\hat{P}\ \text{vec}\Big(\widetilde{U}_t\Big) \\
&= \hat{B}(\mathbf{a}_t, h_t)\vec{\widetilde{U}}_{t+1} - \hat{F}(\mathbf{a}_t, h_t)\vec{\widetilde{U}}_t
\end{aligned}
$$

where

$$
\begin{aligned}
\tilde{B}(\mathbf{a}_t, h_t) &= I_2 \otimes B^{\mathrm{R}}(\mathbf{a}_t, h_t) + \mathrm{Im} \otimes B^{\mathrm{I}}(\mathbf{a}_t, h_t), \\
\tilde{F}(\mathbf{a}_t, h_t) &= I_2 \otimes F^{\mathrm{R}}(\mathbf{a}_t, h_t) - \mathrm{Im} \otimes F^{\mathrm{I}}(\mathbf{a}_t, h_t)
\end{aligned}
$$

and

$$
\begin{aligned}
\hat{B}(\mathbf{a}_t, h_t) &= (I_2 \otimes I_N) \otimes B^{\mathrm{R}}(\mathbf{a}_t, h_t) + (\mathrm{Im} \otimes I_N) \otimes B^{\mathrm{I}}(\mathbf{a}_t, h_t), \\
\hat{F}(\mathbf{a}_t, h_t) &= (I_2 \otimes I_N) \otimes F^{\mathrm{R}}(\mathbf{a}_t, h_t) - (\mathrm{Im} \otimes I_N) \otimes F^{\mathrm{I}}(\mathbf{a}_t, h_t).
\end{aligned}
$$

5.3 Derivatives

Jacobian

For the states we have

$$\frac{\partial f}{\partial \vec{\tilde{U}}_t} = -\hat{F} \quad \text{and} \quad \frac{\partial f}{\partial \vec{\tilde{U}}_{t+1}} = \hat{B}$$

For the drives we have

$$\begin{aligned}
\frac{\partial f}{\partial a_t^j} &= \frac{\partial \hat{B}}{\partial a_t^j}\vec{\tilde{U}}_{t+1} - \frac{\partial \hat{F}}{\partial a_t^j}\vec{\tilde{U}}_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial a_t^j} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial F^{\mathrm{R}}}{\partial a_t^j} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial F^{\mathrm{I}}}{\partial a_t^j} \right) \vec{\tilde{U}}_t
\end{aligned}$$

where, writing $\partial_{a_t^j} H = H_j$, we have

$$\begin{aligned}
\frac{\partial B^{\mathrm{R}}}{\partial a_t^j} &= -\frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9} \left(\{H^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H^{\mathrm{R}}, H_j^{\mathrm{R}}\} \right) \\
&= -\frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9} \left(\{H_0^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_0^{\mathrm{R}}, H_j^{\mathrm{R}}\} + \sum_{i=0}^{d} a_t^i \left(\{H_i^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_i^{\mathrm{R}}, H_j^{\mathrm{R}}\} \right) \right) \\
\frac{\partial B^{\mathrm{I}}}{\partial a_t^j} &= \frac{h_t}{2} H_j^{\mathrm{R}} - \frac{h_t^2}{9} \left(\{H^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H^{\mathrm{I}}, H_j^{\mathrm{R}}\} \right) \\
&= \frac{h_t}{2} H_j^{\mathrm{R}} - \frac{h_t^2}{9} \left(\{H_0^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_0^{\mathrm{I}}, H_j^{\mathrm{R}}\} + \sum_{i} a_t^i \left(\{H_i^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_i^{\mathrm{I}}, H_j^{\mathrm{R}}\} \right) \right)
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial F^{\mathrm{R}}}{\partial a_t^j} &= \frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9} \left(\{H^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H^{\mathrm{R}}, H_j^{\mathrm{R}}\} \right) \\
&= \frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9} \left(\{H_0^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_0^{\mathrm{R}}, H_j^{\mathrm{R}}\} + \sum_{i} a_t^i \left(\{H_i^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_i^{\mathrm{R}}, H_j^{\mathrm{R}}\} \right) \right) \\
\frac{\partial F^{\mathrm{I}}}{\partial a_t^j} &= \frac{h_t}{2} H_j^{\mathrm{R}} + \frac{h_t^2}{9} \left(\{H^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H^{\mathrm{I}}, H_j^{\mathrm{R}}\} \right) \\
&= \frac{h_t}{2} H_j^{\mathrm{R}} + \frac{h_t^2}{9} \left(\{H_0^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_0^{\mathrm{I}}, H_j^{\mathrm{R}}\} + \sum_{i} a_t^i \left(\{H_i^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_i^{\mathrm{I}}, H_j^{\mathrm{R}}\} \right) \right)
\end{aligned}$$

For the timestep h_t we have

$$\begin{aligned}
\frac{\partial f}{\partial h_t} &= \frac{\partial \hat{B}}{\partial h_t}\vec{\tilde{U}}_{t+1} - \frac{\partial \hat{F}}{\partial h_t}\vec{\tilde{U}}_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial h_t} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial h_t} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial F^{\mathrm{R}}}{\partial h_t} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial F^{\mathrm{I}}}{\partial h_t} \right) \vec{\tilde{U}}_t
\end{aligned}$$

where

$$\begin{aligned}\frac{\partial B^{\mathrm{R}}}{\partial h_t} &= -\frac{1}{2}H^{\mathrm{I}} + \frac{2h_t}{9}\Big(\big(H^{\mathrm{I}}\big)^2 - \big(H^{\mathrm{R}}\big)^2\Big)\\ \frac{\partial B^{\mathrm{I}}}{\partial h_t} &= \frac{1}{2}H^{\mathrm{R}} - \frac{2h_t}{9}\{H^{\mathrm{R}}, H^{\mathrm{I}}\}\end{aligned}$$

and

$$\begin{aligned}\frac{\partial F^{\mathrm{R}}}{\partial h_t} &= \frac{1}{2}H^{\mathrm{I}} + \frac{2h_t}{9}\Big(\big(H^{\mathrm{I}}\big)^2 - \big(H^{\mathrm{R}}\big)^2\Big)\\ \frac{\partial F^{\mathrm{I}}}{\partial h_t} &= \frac{1}{2}H^{\mathrm{R}} + \frac{2h_t}{9}\{H^{\mathrm{R}}, H^{\mathrm{I}}\}.\end{aligned}$$

So we then have, with $z_t = \begin{pmatrix}\vec{\tilde{U}}_t & \mathbf{a}_t & h_t\end{pmatrix}^\top$

$$\partial_{z_t:z_{t+1}} f = \begin{pmatrix}\partial_{z_t} f & \partial_{z_{t+1}} f\end{pmatrix} = \begin{pmatrix}-\hat{F} & \partial_{\mathbf{a}_t} f & \partial_{h_t} f & \hat{B} & \mathbf{0} & \mathbf{0}\end{pmatrix}$$

Hessian of the Lagrangian

$$\mathcal{L} = \boldsymbol{\mu}^\top \mathbf{F}(\mathbf{Z}) = \sum_t \mu_t^\top f(z_t, z_{t+1}) = \sum_t \mathcal{L}_t$$

$$\mathcal{L}_t = \mu_t^\top f(z_t, z_{t+1})$$

$$\partial^2_{z_t:z_{t+1}}\mathcal{L}_t = \begin{pmatrix}\partial^2_{z_t}\mathcal{L}_t & \partial_{z_{t+1}}\partial_{z_t}\mathcal{L}_t\\ \ddots & \mathbf{0}\end{pmatrix}$$

$$\partial^2_{z_t}\mathcal{L}_t = \begin{pmatrix}\mathbf{0} & \partial_{\mathbf{a}_t}\partial_{\vec{\tilde{U}}_t}\mathcal{L}_t & \partial_{h_t}\partial_{\vec{\tilde{U}}_t}\mathcal{L}_t\\ & \partial^2_{\mathbf{a}_t}\mathcal{L}_t & \partial_{h_t}\partial_{\mathbf{a}_t}\mathcal{L}_t\\ & & \partial^2_{h_t}\mathcal{L}_t\end{pmatrix}$$

$$\partial_{z_{t+1}}\partial_{z_t}\mathcal{L}_t = \begin{pmatrix}\mathbf{0} & \partial_{\vec{\tilde{U}}_{t+1}}\partial_{\mathbf{a}_t}\mathcal{L}_t & \partial_{\vec{\tilde{U}}_{t+1}}\partial_{h_t}\mathcal{L}_t\\ & \mathbf{0} & \mathbf{0}\\ & & \mathbf{0}\end{pmatrix}$$

$$\begin{aligned}\frac{\partial^2\mathcal{L}_t}{\partial a_t^j \partial\vec{\tilde{U}}_t} &= \frac{\partial}{\partial a_t^j}\frac{\partial\mathcal{L}_t}{\partial\vec{\tilde{U}}_t}\\ &= \frac{\partial}{\partial a_t^j}\Big(-\hat{F}^\top\mu_t\Big)\\ &= -\left(\frac{\partial\hat{F}}{\partial a_t^j}\right)^\top\mu_t\\ &= -\left((I_2\otimes I_N)\otimes\frac{\partial F^{\mathrm{R}}}{\partial a_t^j} - (\mathrm{Im}\otimes I_N)\otimes\frac{\partial F^{\mathrm{I}}}{\partial a_t^j}\right)^\top\mu_t\end{aligned}$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial a_t^j \partial \vec{\vec{U}}_{t+1}} &= \frac{\partial}{\partial a_t^j} \frac{\partial \mathcal{L}_t}{\partial \vec{\vec{U}}_{t+1}} \\
&= \frac{\partial}{\partial a_t^j} \left(\hat{B}^\top \mu_t \right) \\
&= \left(\frac{\partial \hat{B}}{\partial a_t^j} \right)^\top \mu_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial a_t^j} \right)^\top \mu_t
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial a_t^i \partial a_t^j} &= \mu_t^\top \frac{\partial^2 f_t}{\partial a_t^i \partial a_t^j} \\
&= \mu_t^\top \left(\frac{\partial^2 \hat{B}}{\partial a_t^i \partial a_t^j} \vec{\vec{U}}_{t+1} - \frac{\partial^2 \hat{F}}{\partial a_t^i \partial a_t^j} \vec{\vec{U}}_t \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \hat{B}}{\partial a_t^i \partial a_t^j} &= (I_2 \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{I}}}{\partial a_t^i \partial a_t^j} \\
\frac{\partial^2 \hat{F}}{\partial a_t^i \partial a_t^j} &= (I_2 \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{I}}}{\partial a_t^i \partial a_t^j}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 B^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} &= \frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{I}} \right\} - \left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{R}} \right\} \right) \\
\frac{\partial^2 B^{\mathrm{I}}}{\partial a_t^i \partial a_t^j} &= -\frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{I}} \right\} + \left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{R}} \right\} \right)
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial^2 F^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} &= \frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{I}} \right\} - \left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{R}} \right\} \right) \\
\frac{\partial^2 F^{\mathrm{I}}}{\partial a_t^i \partial a_t^j} &= \frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{I}} \right\} + \left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{R}} \right\} \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t \partial \vec{\vec{U}}_t} &= \frac{\partial}{\partial h_t} \frac{\partial \mathcal{L}_t}{\partial \vec{\vec{U}}_t} \\
&= \frac{\partial}{\partial h_t} \left(-\hat{F}^\top \mu_t \right) \\
&= -\left(\frac{\partial \hat{F}}{\partial h_t} \right)^\top \mu_t \\
&= -\left((I_2 \otimes I_N) \otimes \frac{\partial F^{\mathrm{R}}}{\partial h_t} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial F^{\mathrm{I}}}{\partial h_t} \right)^\top \mu_t
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t \partial \vec{\tilde{U}}_{t+1}} &= \frac{\partial}{\partial h_t} \frac{\partial \mathcal{L}_t}{\partial \vec{\tilde{U}}_{t+1}} \\
&= \frac{\partial}{\partial h_t} \left(\hat{B}^\top \mu_t \right) \\
&= \left(\frac{\partial \hat{B}}{\partial h_t} \right)^\top \mu_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial h_t} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial h_t} \right)^\top \mu_t
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t \partial a_t^j} &= \mu_t^\top \frac{\partial^2 f_t}{\partial h_t \partial a_t^j} \\
&= \mu_t^\top \left(\frac{\partial^2 \hat{B}}{\partial h_t \partial a_t^j} \vec{\tilde{U}}_{t+1} - \frac{\partial^2 \hat{F}}{\partial h_t \partial a_t^j} \vec{\tilde{U}}_t \right) \\
&= \mu_t^\top \Bigg(\left((I_2 \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{R}}}{\partial h_t \partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{I}}}{\partial h_t \partial a_t^j} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{R}}}{\partial h_t \partial a_t^j} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{I}}}{\partial h_t \partial a_t^j} \right) \vec{\tilde{U}}_t \Bigg)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 B^{\mathrm{R}}}{\partial h_t \partial a_t^j} &= -\frac{1}{2} H_j^{\mathrm{I}} + \frac{2h_t}{9} \left(\{H^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H^{\mathrm{R}}, H_j^{\mathrm{R}}\} \right) \\
\frac{\partial^2 B^{\mathrm{I}}}{\partial h_t \partial a_t^j} &= \frac{1}{2} H_j^{\mathrm{R}} - \frac{2h_t}{9} \left(\{H^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H^{\mathrm{I}}, H_j^{\mathrm{R}}\} \right)
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial^2 F^{\mathrm{R}}}{\partial h_t \partial a_t^j} &= \frac{1}{2} H_j^{\mathrm{I}} + \frac{2h_t}{9} \left(\{H^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H^{\mathrm{R}}, H_j^{\mathrm{R}}\} \right) \\
\frac{\partial^2 F^{\mathrm{I}}}{\partial h_t \partial a_t^j} &= \frac{1}{2} H_j^{\mathrm{R}} + \frac{2h_t}{9} \left(\{H^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H^{\mathrm{I}}, H_j^{\mathrm{R}}\} \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t^2} &= \mu_t^\top \frac{\partial^2 f_t}{\partial h_t^2} \\
&= \mu_t^\top \left(\frac{\partial^2 \hat{B}}{\partial h_t^2} \vec{\tilde{U}}_{t+1} - \frac{\partial^2 \hat{F}}{\partial h_t^2} \vec{\tilde{U}}_t \right) \\
&= \mu_t^\top \Bigg(\left((I_2 \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{R}}}{\partial h_t^2} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{I}}}{\partial h_t^2} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{R}}}{\partial h_t^2} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{I}}}{\partial h_t^2} \right) \vec{\tilde{U}}_t \Bigg)
\end{aligned}
$$

where

$$
\begin{aligned}
\frac{\partial^2 B^{\mathrm{R}}}{\partial h_t^2} &= \frac{2}{9}\Big(\big(H^{\mathrm{I}}\big)^2 - \big(H^{\mathrm{R}}\big)^2\Big) \\
\frac{\partial^2 B^{\mathrm{I}}}{\partial h_t^2} &= -\frac{2}{9}\big\{H^{\mathrm{R}}, H^{\mathrm{I}}\big\}
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial^2 F^{\mathrm{R}}}{\partial h_t^2} &= \frac{2}{9}\Big(\big(H^{\mathrm{I}}\big)^2 - \big(H^{\mathrm{R}}\big)^2\Big) \\
\frac{\partial^2 F^{\mathrm{I}}}{\partial h_t^2} &= \frac{2}{9}\big\{H^{\mathrm{R}}, H^{\mathrm{I}}\big\}
\end{aligned}
$$

6 State Transfer

For a isomorphic quantum state $\tilde{\psi}$, we have

$$\mathbf{P}(\tilde{\psi}_{k+1}, \tilde{\psi}_k, \mathbf{a}_k, h_k) = B(\mathbf{a}_k, h_k)\tilde{\psi}_{k+1} - F(\mathbf{a}_k, h_k)\tilde{\psi}_k$$

6.1 Jacobian

$$\frac{\partial \mathbf{P}}{\partial \tilde{\psi}_t} = -F \quad \text{and} \quad \frac{\partial \mathbf{P}}{\partial \tilde{\psi}_{t+1}} = B$$

$$\frac{\partial \mathbf{P}}{\partial a_k^j} = \frac{\partial B}{\partial a_k^j}\tilde{\psi}_{k+1} - \frac{\partial F}{\partial a_k^j}\tilde{\psi}_k$$

$$
\begin{aligned}
\frac{\partial B}{\partial a_k^j} &= I_2 \otimes \frac{\partial B^{\mathrm{R}}}{\partial a_k^j} + \mathrm{Im} \otimes \frac{\partial B^{\mathrm{I}}}{\partial a_k^j} \\
\frac{\partial F}{\partial a_k^j} &= I_2 \otimes \frac{\partial F^{\mathrm{R}}}{\partial a_k^j} - \mathrm{Im} \otimes \frac{\partial F^{\mathrm{I}}}{\partial a_k^j}
\end{aligned}
$$

$$\frac{\partial \mathbf{P}}{\partial h_k} = \frac{\partial B}{\partial h_k}\tilde{\psi}_{k+1} - \frac{\partial F}{\partial h_k}\tilde{\psi}_k$$

$$
\begin{aligned}
\frac{\partial B}{\partial h_k} &= I_2 \otimes \frac{\partial B^{\mathrm{R}}}{\partial h_k} + \mathrm{Im} \otimes \frac{\partial B^{\mathrm{I}}}{\partial h_k} \\
\frac{\partial F}{\partial h_k} &= I_2 \otimes \frac{\partial F^{\mathrm{R}}}{\partial h_k} - \mathrm{Im} \otimes \frac{\partial F^{\mathrm{I}}}{\partial h_k}
\end{aligned}
$$