Note for NODE Approach to the MQCD Phase Diagram via Holography

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1 Deduction

Assume a vector field representation of the governing equations:

$$\vec{\Theta}(z) = \begin{bmatrix} \Phi(z) \\ F(z) \\ \Sigma(z) \\ A(z) \\ G(z) \end{bmatrix} \triangleq \begin{bmatrix} u_1(z) \\ u_2(z) \\ u_3(z) \\ u_4(z) \\ u_5(z) \end{bmatrix} \triangleq \vec{u}(z). \tag{1}$$

Further assume the system dynamics are governed by:

$$\begin{aligned} \frac{d\vec{\Theta}(z)}{dz} &= \begin{bmatrix} \frac{d}{dz}\Phi(z) \\ \frac{d}{dz}F(z) \\ \frac{d}{dz}\Sigma(z) \\ \frac{d}{dz}A(z) \\ \frac{d}{dz}G(z) \end{bmatrix} \triangleq \frac{d\vec{u}}{dz} = \begin{bmatrix} \frac{du_1(z)}{dz} \\ \frac{du_2(z)}{dz} \\ \frac{du_3(z)}{dz} \\ \frac{du_4(z)}{dz} \\ \frac{du_5(z)}{dz} \end{bmatrix} = \vec{f}\left(\vec{u}; \widehat{Z}\left(z\Phi\left(z;\vec{\xi}\right)\right), \frac{\partial \widehat{Z}\left(z\Phi\left(z;\vec{\xi}\right)\right)}{\partial z\Phi\left(z;\vec{\xi}\right)}\right) \\ &= \vec{f}\left(\vec{u}; u_6\left(x;\vec{\xi}\right), u_7\left(x;\vec{\xi}\right)\right) = \begin{bmatrix} f_1\left(z; \vec{u}, u_6\left(x;\vec{\xi}\right), \frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x}\right) \\ f_2\left(z; \vec{u}, u_6\left(x;\vec{\xi}\right), \frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x}\right) \\ f_3\left(z; \vec{u}, u_6\left(x;\vec{\xi}\right), \frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x}\right) \\ f_4\left(z; \vec{u}, u_6\left(x;\vec{\xi}\right), \frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x}\right) \\ f_5\left(z; \vec{u}, u_6\left(x;\vec{\xi}\right), \frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x}\right) \end{bmatrix}, \end{aligned} \tag{2}$$

where $u_6\left(x;\vec{\xi}\right) = \widehat{Z}\left(z\Phi(z);\vec{\xi}\right)$ with $x = z\Phi(z)$, under the assumption that $\frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x} = u_7\left(x;\vec{\xi}\right)$.

The constrained optimization problem seeks to minimize:

$$\min_{\vec{\xi}} J\left(\vec{u}(z);\vec{\xi}\right), \quad s.t. \;\; \vec{f}\left(z,\vec{u}(z);u_6\left(x;\vec{\xi}\right),u_7\left(x;\vec{\xi}\right)\right)-\frac{d\vec{u}}{dz}=\vec{0}, \tag{3}$$

with the loss functional defined as:

$$J(\vec{u})=\int_{z_0}^{z_T} g(\vec{u})\,dz+J_1\left(\vec{u}(z_T)\right). \tag{4}$$

The corresponding Lagrangian functional is constructed as:

$$\begin{aligned} L\left(\vec{u},\vec{\lambda}\right)=&J_1\left(\vec{u}(z_T)\right)+\int_{z_0}^{z_T} g(\vec{u})\,dz+\int_{z_0}^{z_T}\vec{\lambda}^T\left(\vec{f}(z;\vec{u},u_6,u_7)-\frac{d\vec{u}}{dz}\right)dz\\ =&J_1\left(\vec{u}(z_T)\right)+\int_{z_0}^{z_T}\left[g(\vec{u})+\vec{\lambda}^T\left(\vec{f}(z;\vec{u},u_6,u_7)-\frac{d\vec{u}}{dz}\right)\right]dz, \end{aligned} \tag{5}$$

Taking the total derivative with respect to the parameter vector $\vec{\xi}$ yields:

$$\frac{dL}{d\vec{\xi}}=\left.\frac{\partial J_1}{\partial\vec{u}}\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T}+\int_{z_0}^{z_T}\left[\frac{\partial g}{\partial\vec{u}}\frac{d\vec{u}}{d\vec{\xi}}+\vec{\lambda}^T\left(\frac{\partial\vec{f}}{\partial\vec{u}}\frac{d\vec{u}}{d\vec{\xi}}+\frac{\partial\vec{f}}{\partial u_6}\frac{du_6}{d\vec{\xi}}+\frac{\partial\vec{f}}{\partial u_7}\frac{du_7}{d\vec{\xi}}-\frac{d}{d\vec{\xi}}\left(\frac{d\vec{u}}{dz}\right)\right)\right]dz, \tag{6}$$

where $\frac{\partial\vec{f}}{\partial\vec{u}}=\begin{bmatrix}\frac{\partial\vec{f}}{\partial u_1} & \frac{\partial\vec{f}}{\partial u_2} & \frac{\partial\vec{f}}{\partial u_3} & \frac{\partial\vec{f}}{\partial u_4} & \frac{\partial\vec{f}}{\partial u_5}\end{bmatrix}$, $\frac{\partial u_6}{\partial\vec{\xi}}=\begin{bmatrix}\frac{\partial u_6}{\partial\xi_1} & \frac{\partial u_6}{\partial\xi_2} & \cdots & \cdots & \frac{\partial u_6}{\partial\xi_p}\end{bmatrix}^T$ and other terms follow analogously.

Applying integration by parts to the term $\frac{d}{d\vec{\xi}}\left(\frac{d\vec{u}}{dz}\right)$:

$$\begin{aligned} &\int_{z_0}^{z_T}-\vec{\lambda}^T\frac{d}{d\vec{\xi}}\left(\frac{d\vec{u}}{dz}\right)dz=\int_{z_0}^{z_T}-\vec{\lambda}^T\frac{d}{dz}\left(\frac{d\vec{u}}{d\vec{\xi}}\right)dz=-\left[\vec{\lambda}^T\frac{d\vec{u}}{d\vec{\xi}}\right]\Bigg|_{z_0}^{z_T}+\int_{z_0}^{z_T}\left(\frac{d\vec{\lambda}}{dz}\right)^T\frac{d\vec{u}}{d\vec{\xi}}dz\\ =&\left(\vec{\lambda}(z_0)\right)^T\left.\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_0}-\left(\vec{\lambda}(z_T)\right)^T\left.\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T}+\int_{z_0}^{z_T}\left(\frac{d\vec{\lambda}}{dz}\right)^T\frac{d\vec{u}}{d\vec{\xi}}dz=-\left(\vec{\lambda}(z_T)\right)^T\left.\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T}+\int_{z_0}^{z_T}\left(\frac{d\vec{\lambda}}{dz}\right)^T\frac{d\vec{u}}{d\vec{\xi}}dz. \end{aligned} \tag{7}$$

where we assume $\left.\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_0}=\vec{0}$ due to initial condition independence.

Substituting equation (7) into (6) yields:

$$
\begin{aligned}
\frac{dL}{d\vec{\xi}} &= \left.\frac{\partial J_1}{\partial \vec{u}}\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T} + \int_{z_0}^{z_T}\left[\frac{\partial g}{\partial \vec{u}}\frac{d\vec{u}}{d\vec{\xi}} + \vec{\lambda}^T\left(\frac{\partial \vec{f}}{\partial \vec{u}}\frac{d\vec{u}}{d\vec{\xi}} + \frac{\partial \vec{f}}{\partial u_6}\frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7}\frac{\partial u_7}{\partial \vec{\xi}}\right) + \left(\frac{d\vec{\lambda}}{dz}\right)^T\frac{d\vec{u}}{d\vec{\xi}}\right]dz - \left.\left(\vec{\lambda}\left(z_T\right)\right)^T\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T} \\
&= \int_{z_0}^{z_T}\left[\left[\frac{\partial g}{\partial \vec{u}} + \vec{\lambda}^T\frac{\partial \vec{f}}{\partial \vec{u}} + \left(\frac{d\vec{\lambda}}{dz}\right)^T\right]\frac{d\vec{u}}{d\vec{\xi}} + \vec{\lambda}^T\left(\frac{\partial \vec{f}}{\partial u_6}\frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7}\frac{\partial u_7}{\partial \vec{\xi}}\right)\right]dz + \left.\left(\frac{\partial J_1}{\partial \vec{u}} - \left(\vec{\lambda}\left(z_T\right)\right)^T\right)\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T},
\end{aligned}
\tag{8}
$$

To address the computational challenges posed by $\frac{d\vec{u}}{d\vec{\xi}}$ and $\left.\frac{d\vec{u}}{d\vec{\xi}}\right|_{z=z_T}$ in (8), we enforce the adjoint system:

$$
\begin{cases}
\frac{\partial g}{\partial \vec{u}} + \vec{\lambda}^T\frac{\partial \vec{f}}{\partial \vec{u}} + \left(\frac{d\vec{\lambda}}{dz}\right)^T = \vec{0}, \\
\vec{\lambda}\left(z_T\right) = \frac{\partial J_1}{\partial \vec{u}}\left(z_T\right).
\end{cases}
\tag{9}
$$

It yields the simplified sensitivity expression through the equivalence $\frac{dL}{d\vec{\xi}} = \frac{dJ}{d\vec{\xi}}$:

$$
\frac{dJ}{d\vec{\xi}} = \int_{z_0}^{z_T}\vec{\lambda}^T\left(\frac{\partial \vec{f}}{\partial u_6}\frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7}\frac{\partial u_7}{\partial \vec{\xi}}\right)dz. \tag{10}
$$

In summary:

1. Initial value problem: Solve forward

$$
\begin{cases}
\frac{d\vec{u}}{dz} = f\left(z;\vec{u},u_6\left(x;\vec{\xi}\right),u_7\left(x;\vec{\xi}\right)\right) \\
\vec{u}\left(z=1\right) = \vec{u}_0
\end{cases}
\tag{11}
$$

This system can be expanded as:

$$
\begin{cases}
\begin{bmatrix} \frac{du_1}{dz} \\ \frac{du_2}{dz} \\ \frac{du_3}{dz} \\ \frac{du_4}{dz} \\ \frac{du_5}{dz} \end{bmatrix} = \begin{bmatrix} f_1\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) \\ f_2\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) \\ f_3\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) \\ f_4\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) \\ f_5\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) \end{bmatrix}, \\
\begin{bmatrix} u_1\left(z=1\right) \\ u_2\left(z=1\right) \\ u_3\left(z=1\right) \\ u_4\left(z=1\right) \\ u_5\left(z=1\right) \end{bmatrix} = \begin{bmatrix} u_{10} \\ u_{20} \\ u_{30} \\ u_{40} \\ u_{50} \end{bmatrix}.
\end{cases}
\tag{12}
$$

This system is solved by determining u_1 through u_5 via NDSolve, with u_6 and u_7 are provided by the neural network.

2. Terminal value problem: Solve backward

$$
\begin{cases}
\frac{\partial g}{\partial \vec{u}} + \vec{\lambda}^T \frac{\partial \vec{f}}{\partial \vec{u}} + \left(\frac{d\vec{\lambda}}{dz}\right)^T = \vec{0}, \\
\vec{\lambda}\left(z = z_T = 0\right) = \frac{\partial J_1}{\partial \vec{u}}\left(z_T\right),
\end{cases}
\tag{13}
$$

for $\vec{\lambda}(z)$.

Now, in detail, we have the following system of equations:

$$
\begin{aligned}
&\begin{bmatrix} \frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \end{bmatrix} + \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5 \end{bmatrix} \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \frac{\partial f_1}{\partial u_3} & \frac{\partial f_1}{\partial u_4} & \frac{\partial f_1}{\partial u_5} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} & \frac{\partial f_2}{\partial u_3} & \frac{\partial f_2}{\partial u_4} & \frac{\partial f_2}{\partial u_5} \\ \frac{\partial f_3}{\partial u_1} & \frac{\partial f_3}{\partial u_2} & \frac{\partial f_3}{\partial u_3} & \frac{\partial f_3}{\partial u_4} & \frac{\partial f_3}{\partial u_5} \\ \frac{\partial f_4}{\partial u_1} & \frac{\partial f_4}{\partial u_2} & \frac{\partial f_4}{\partial u_3} & \frac{\partial f_4}{\partial u_4} & \frac{\partial f_4}{\partial u_5} \\ \frac{\partial f_5}{\partial u_1} & \frac{\partial f_5}{\partial u_2} & \frac{\partial f_5}{\partial u_3} & \frac{\partial f_5}{\partial u_4} & \frac{\partial f_5}{\partial u_5} \end{bmatrix} + \cdots \\
&\cdots + \begin{bmatrix} \frac{\partial \lambda_1}{\partial z} & \frac{\partial \lambda_2}{\partial z} & \frac{\partial \lambda_3}{\partial z} & \frac{\partial \lambda_4}{\partial z} & \frac{\partial \lambda_5}{\partial z} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \end{bmatrix}
\end{aligned}
\tag{14}
$$

That is,

$$
\begin{aligned}
&\frac{\partial g}{\partial u_1} + \left[\lambda_1 \frac{\partial f_1}{\partial u_1} + \lambda_2 \frac{\partial f_2}{\partial u_1} + \cdots + \lambda_5 \frac{\partial f_5}{\partial u_1}\right] + \frac{\partial \lambda_1}{\partial z} = 0,\\
&\frac{\partial g}{\partial u_2} + \left[\lambda_1 \frac{\partial f_1}{\partial u_2} + \lambda_2 \frac{\partial f_2}{\partial u_2} + \cdots + \lambda_5 \frac{\partial f_5}{\partial u_2}\right] + \frac{\partial \lambda_2}{\partial z} = 0,\\
&\vdots\\
&\frac{\partial g}{\partial u_7} + \left[\lambda_1 \frac{\partial f_1}{\partial u_5} + \lambda_2 \frac{\partial f_2}{\partial u_5} + \cdots + \lambda_7 \frac{\partial f_7}{\partial u_5}\right] + \frac{\partial \lambda_5}{\partial z} = 0.
\end{aligned}
\tag{15}
$$

In other words, we can express the system as:

$$
\frac{\partial g}{\partial u_i} + \sum_{j=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_i} + \frac{\partial \lambda_i}{\partial z} = 0, \quad i \in [1, 5]\,. \tag{16}
$$

Finally, the system in (13) becomes:

$$
\begin{cases}
\dfrac{\partial g}{\partial u_i} + \displaystyle\sum_{j=1}^{7} \lambda_j \frac{\partial f_j}{\partial u_i} + \frac{\partial \lambda_i}{\partial z} = 0, \\
\lambda_i \left(z = 0\right) = \dfrac{\partial J_1}{\partial u_i},
\end{cases}
\qquad i \in [1, 7]\,. \tag{17}
$$

3. Evaluate

$$
\begin{aligned}
\frac{dJ}{d\vec{\xi}} &= \int_{z_0}^{z_T} \vec{\lambda}^T \left(\frac{\partial \vec{f}}{\partial u_6} \frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7} \frac{\partial u_7}{\partial \vec{\xi}} \right) dz \\
&= \int_1^0 \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5 \end{bmatrix} \left(\begin{bmatrix} \frac{\partial f_1}{\partial u_6} \\ \frac{\partial f_2}{\partial u_6} \\ \frac{\partial f_3}{\partial u_6} \\ \frac{\partial f_4}{\partial u_6} \\ \frac{\partial f_5}{\partial u_6} \end{bmatrix} \frac{\partial u_6}{\partial \vec{\xi}} + \begin{bmatrix} \frac{\partial f_1}{\partial u_7\left(x;\vec{\xi}\right)} \\ \frac{\partial f_2}{\partial u_7\left(x;\vec{\xi}\right)} \\ \frac{\partial f_3}{\partial u_7\left(x;\vec{\xi}\right)} \\ \frac{\partial f_4}{\partial u_7\left(x;\vec{\xi}\right)} \\ \frac{\partial f_5}{\partial u_7\left(x;\vec{\xi}\right)} \end{bmatrix} \frac{\partial u_7\left(x;\vec{\xi}\right)}{\partial \vec{\xi}} \right) dz \\
&= \int_1^0 \left[\left(\sum_{i=1}^{5} \lambda_i \frac{\partial f_i}{\partial u_6} \right) \frac{\partial u_6}{\partial \vec{\xi}} + \left(\sum_{i=1}^{5} \lambda_i \frac{\partial f_i}{\partial u_7\left(x;\vec{\xi}\right)} \right) \frac{\partial u_7\left(x;\vec{\xi}\right)}{\partial \vec{\xi}} \right] dz \\
&= \int_1^0 \left[\left(\sum_{j=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_6} \right) \frac{\partial u_6}{\partial \vec{\xi}} + \left(\sum_{j=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_7\left(x;\vec{\xi}\right)} \right) \frac{\partial u_7\left(x;\vec{\xi}\right)}{\partial \vec{\xi}} \right] dz.
\end{aligned}
\tag{18}
$$

2 Implement

To solve this problem using a system of first-order differential equations, we introduce auxiliary variables $\Phi_2(z)$ and $G_2(z)$, defined as $\Phi_2(z) = \Phi'(z)$ and $G_2(z) = G'(z)$, respectively. Consequently, $\vec{\Theta}(z)$ can be expressed as:

$$\vec{\Theta}(z) = \begin{bmatrix} \Phi_2(z) \\ G_2(z) \\ \Phi(z) \\ G(z) \\ \Sigma(z) \\ F(z) \end{bmatrix} = \begin{bmatrix} u_1(z) \\ u_2(z) \\ u_3(z) \\ u_4(z) \\ u_5(z) \\ u_6(z) \end{bmatrix} = \vec{u}(z), \tag{19}$$

with the system dynamics:

$$\frac{d\vec{\Theta}(z)}{dz} = \begin{bmatrix} \frac{d}{dz}\Phi_2(z) \\ \frac{d}{dz}G_2(z) \\ \frac{d}{dz}\Phi(z) \\ \frac{d}{dz}G(z) \\ \frac{d}{dz}\Sigma(z) \\ \frac{d}{dz}F(z) \end{bmatrix} = \begin{bmatrix} \frac{du_1(z)}{dz} \\ \frac{du_2(z)}{dz} \\ \frac{du_3(z)}{dz} \\ \frac{du_4(z)}{dz} \\ \frac{du_5(z)}{dz} \\ \frac{du_6(z)}{dz} \end{bmatrix} = \vec{f}\left(\vec{u}; u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) = \begin{bmatrix} f_1\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_2\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_3\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_4\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_5\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_6\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \end{bmatrix}, \tag{20}$$

where $u_7\left(x;\vec{\xi}\right) = \widehat{Z}\left(z\Phi(z);\vec{\xi}\right)$ with $x = z\Phi(z)$, and assume that $\frac{\partial u_7\left(x;\vec{\xi}\right)}{\partial x} = u_8\left(x;\vec{\xi}\right)$.

1. Solve forward

$$\begin{bmatrix} \frac{du_1}{dz} \\ \frac{du_2}{dz} \\ \frac{du_3}{dz} \\ \frac{du_4}{dz} \\ \frac{du_5}{dz} \\ \frac{du_6}{dz} \end{bmatrix} = \begin{bmatrix} f_1\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_2\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_3\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_4\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_5\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \\ f_6\left(z;\vec{u}, u_7\left(x;\vec{\xi}\right), u_8\left(x;\vec{\xi}\right)\right) \end{bmatrix}, \tag{21}$$

with the initial values:

$$\begin{bmatrix} u_1\left(z=1\right) \\ u_2\left(z=1\right) \\ u_3\left(z=1\right) \\ u_4\left(z=1\right) \\ u_5\left(z=1\right) \\ u_6\left(z=1\right) \end{bmatrix} = \begin{bmatrix} u_{10} \\ u_{20} \\ u_{30} \\ u_{40} \\ u_{50} \\ u_{60} \end{bmatrix}. \tag{22}$$

The system will be solved using NDSolve, with u_7 and u_8 are provided by the neural network.

2. Solve backward

$$\begin{cases} \dfrac{\partial \lambda_i}{\partial z} + \displaystyle\sum_{j=1}^{6} \lambda_j \dfrac{\partial f_j}{\partial u_i} + \dfrac{\partial g}{\partial u_i} = 0, \\ \lambda_i\left(z=0\right) = \dfrac{\partial J_1}{\partial u_i}, \end{cases} \qquad i \in [1,6]\,. \tag{23}$$

for λ_i, $i \in [1,6]$.

3. Evaluate

$$\frac{dJ}{d\vec{\xi}} = \int_1^0 \left[\left(\sum_{j=1}^{6} \lambda_j \frac{\partial f_j}{\partial u_7\left(x;\vec{\xi}\right)} \right) \frac{\partial u_7\left(x;\vec{\xi}\right)}{\partial \vec{\xi}} + \left(\sum_{j=1}^{6} \lambda_j \frac{\partial f_j}{\partial u_8\left(x;\vec{\xi}\right)} \right) \frac{\partial u_8\left(x;\vec{\xi}\right)}{\partial \vec{\xi}} \right] dz. \tag{24}$$

```
NDSolve[{(class["Φ2eom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["G2eom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &,
   (class["Φeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Geom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &,
   (class["Σeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Feom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &,
   Φ[1 - IRcutoff] == class["Φ_IR"] // SetAccuracy[#, 100] &, Φ2[1 - IRcutoff] == class["Φ'_IR"] // SetAccuracy[#, 100] &,
   F[1 - IRcutoff] == class["F_IR"] // SetAccuracy[#, 100] &, Σ[1 - IRcutoff] == class["Σ_IR"] // SetAccuracy[#, 100] &,
   G[1 - IRcutoff] == class["G_IR"] // SetAccuracy[#, 100] &, G2[1 - IRcutoff] == class["G'_IR"] // SetAccuracy[#, 100] &},
  {Φ, F, Σ, G, Φ2, G2}, {z, 1 - IRcutoff, UVcutoff}, WorkingPrecision → 30, MaxSteps → 20000, AccuracyGoal → 15][[1]]
```

Fig. 1: Incomplete codes for (21).

```
class["backfun"] = NDSolve[{(backequ["back"]["hΦ2"] /. {B → class["B"]} // SetAccuracy[#, 100] &) == 0,
    (backequ["back"]["hG2"] /. {B → class["B"]} // SetAccuracy[#, 100] &) == 0,
    (backequ["back"]["hΦ"] /. {B → class["B"]} // SetAccuracy[#, 100] &) == 0,
    (backequ["back"]["hG"] /. {B → class["B"]} // SetAccuracy[#, 100] &) == 0,
    (backequ["back"]["hΣ"] /. {B → class["B"]} // SetAccuracy[#, 100] &) == 0,
    (backequ["back"]["hF"] /. {B → class["B"]} // SetAccuracy[#, 100] &) == 0,
    hΦ2[20 UVcutoff] == (hΦ2[z] /. class["normal pduv"] // SetAccuracy[#, 100] &),
    hG2[20 UVcutoff] == (hG2[z] /. class["normal pduv"] // SetAccuracy[#, 100] &),
    hΦ[20 UVcutoff] == (hΦ[z] /. class["normal pduv"] // SetAccuracy[#, 100] &),
    hG[20 UVcutoff] == (hG[z] /. class["normal pduv"] // SetAccuracy[#, 100] &),
    hΣ[20 UVcutoff] == (hΣ[z] /. class["normal pduv"] // SetAccuracy[#, 100] &),
    hF[20 UVcutoff] == (hF[z] /. class["normal pduv"] // SetAccuracy[#, 100] &)
   }, {hΦ2, hG2, hΦ, hG, hΣ, hF}, {z, 20 UVcutoff, 1 - IRcutoff}, WorkingPrecision → 20, MaxSteps → 10000][[1]];
```

Fig. 2: Incomplete codes for (23).

```
class["zlist"] = Table[i, {i, 1 / 100, 99 / 100, 1 / 1000}];
class["dz"] = 1 / 1000;
(*实际上Z函数及其导数里面的参数总是z Φ[z]，所以做出z Φ[z]的表格以供神经网络使用*)
class["nn_zlist"] = Table[class["zlist"][[i]] × Φ[class["zlist"][[i]]] /. class["date_IRtoUV"], {i, 1, Length[class["zlist"]]}];
class["zint_pd_list"] = Table[backequ["zint'"] /. z → class["zlist"][[i]] /. class["backfun"] /. class["date_IRtoUV"] /. B → class["B"],
  {i, 1, Length[class["zlist"]]}];
class["zint_pd_2_list"] = Table[backequ["zint''"] /. z → class["zlist"][[i]] /. class["backfun"] /. class["date_IRtoUV"] /. B → class["B"],
  {i, 1, Length[class["zlist"]]}];
class["nn_B"] = class["dz"] × Sum[backequ["B"] /. z → class["zlist"][[i]] /. class["backfun"] /. class["date_IRtoUV"] /. B → class["B"],
   {i, 1, Length[class["zlist"]]}];
(*反向传播到神经网络*)
Module[{nni}, For[nni = 1, nni ≤ Length[class["zlist"]], nni++,
  (*这里将z的导数导数通过1/10000的步长拆分成z函数进行反向传播*)
  zintforward1[class["nn_zlist"][[nni]]];
  class["g"] = class["zint_pd_list"][[nni]] - 1000 class["zint_pd_2_list"][[nni]];

  class["g"] = class["dz"] × class["g"];
  Gnet["back"][class["g"]];
  addGnet["func"];

  zintforward1[class["nn_zlist"][[nni]] + 1 / 1000];
  class["g"] = 1000 class["zint_pd_2_list"][[nni]];

  class["g"] = class["dz"] × class["g"];
  Gnet["back"][class["g"]];
```

Fig. 3: Incomplete codes for (24).