1 Details of Adjoint Method

Given an objective function \( \phi(q, f) \) with a state vector \( q \) and a control vector \( f \), the goal of the adjoint method is to efficiently compute the gradient of the objective function with respect to the control vector:

\[
\frac{d\phi}{df} = \frac{\partial \phi}{\partial q} \frac{dq}{df} + \frac{\partial \phi}{\partial f},
\]

with the constraint due to the forward simulation:

\[
q = F(q, f).
\]

This constraint can be linearized by differentiating (2) with respect to \( f \) to obtain

\[
\frac{\partial q}{\partial f} = \frac{\partial F}{\partial q} \frac{dq}{df} + \frac{\partial F}{\partial f},
\]

which can be rearranged as

\[
\left( I - \frac{\partial F}{\partial q} \right) \frac{\partial q}{\partial f} = \frac{\partial F}{\partial f}.
\]

In the gradient formulation (1), direct computation of \( \frac{dq}{df} \) is known as extremely expensive since this term requires computing the gradient for each state with respect to each control. The adjoint method avoids this expensive computation by computing \( \frac{\partial \phi}{\partial q} \frac{dq}{df} \) without explicitly forming \( \frac{dq}{df} \) as follows.

First, for clarity, we introduce a vector \( s = \left( \frac{\partial \phi}{\partial q} \right)^T \) and a matrix \( Y = \frac{dq}{df} \) such that \( \frac{\partial \phi}{\partial q} \frac{dq}{df} = s^T Y \). If we rewrite (4) as \( XYZ \) with \( X = \left( I - \frac{\partial F}{\partial q} \right) \) and \( Z = \frac{\partial F}{\partial f} \), and introduce the adjoint vector \( r \) such that \( X^T r = s \), we obtain \( s^T Y = r^T \frac{\partial F}{\partial f} \), i.e.,

\[
\frac{\partial \phi}{\partial q} \frac{dq}{df} = r^T \frac{\partial F}{\partial f},
\]

with the constraint \( (X^T r = s) \):

\[
\left( I - \frac{\partial F}{\partial q} \right)^T r = \left( \frac{\partial \phi}{\partial q} \right)^T .
\]

which can be reformulated as

\[
r = \left( \frac{\partial F}{\partial q} \right)^T r + \left( \frac{\partial \phi}{\partial q} \right)^T .
\]

The key for the efficiency of the adjoint method comes from the sparse structure of \( \frac{\partial F}{\partial f} \) and \( \frac{\partial F}{\partial q} \). Since the forward simulation typically involves control at simulation step \( i \) (\( f_i \), where \( i \) denotes simulation step index), and consecutive states \( (q_i, q_{i+1}) \) only, we can efficiently compute \( \frac{\partial F_i}{\partial f_i} \), \( \frac{\partial F_i}{\partial q_i} \), and adjoint states with the recursive relation:

\[
r_i = \left( \frac{\partial F_i}{\partial q_i} \right)^T r_{i+1} + \left( \frac{\partial \phi}{\partial q_i} \right)^T ,
\]

where \( r_n = \left( \frac{\partial \phi}{\partial q_n} \right)^T \). These reformulations finally allow for efficient computations of \( r^T \frac{\partial F}{\partial f} \) and thus the gradient \( \frac{d\phi}{df} \).