We present a new full space exact Hessian SQP algorithm for large scale dynamic optimization that makes mainly use of two ingredients:

- We start by a process simulator (the adaptive DAE solver DAESOL-II [1]) that is able to generate adjoint sensitivities by the principle of internal numerical differentiation. Thus, a gradient computation is available at the cost of about five process simulations.
- Second, we work in the framework of Bock and Plitt’s direct multiple shooting method [2] by introducing intermediate but constrained ”node” variables into the optimization problem. It is a well known technique for reducing nonlinearity and increasing robustness of the optimization procedure, in particular for boundary value problems e.g. with end point quality constraints.

By a combination of both ingredients, we are able to derive a full space exact hessian SQP method that iterates in the very large space of all node variables, yet needs to evaluate only the same amount of derivatives as would be needed in a single shooting approach. This is similar to Schloeder’s trick [4] which was however only applicable to least squares cost functions and not yet combined with adjoint techniques.

By a smart programming trick, the algorithm can easily be derived by “lifting” a standard single shooting SQP method, thus avoiding the tedious programming work usually avoided with new variants of direct multiple shooting.

We consider here the following type of nonlinear optimization problem

$$\min_u F(u) = 0$$

s.t. \( H(u) \geq 0 \).  

This problem is then lifted by introducing intermediate node values \( x \) and corresponding constraints \( G \) to a problem of type

$$\min_{u,x} F(u, x) = 0$$

s.t. \( G(u, x) = 0 \)

\( H(u, x) \geq 0 \),

We can then efficiently calculate the quantities needed for the SQP method by evaluating directional derivatives only with respect to the original degrees of freedom \( u \), and after solving a quadratic problem in \( \Delta u \) we need just another directional derivative to expand this QP solution to a step in the full variable space.

The algorithm is advantageous in case of large process models with few degrees of freedom. We present also an extension to online optimization in nonlinear model predictive control. Here we use the ideas of real-time iterations and initial value embedding as presented in [3]. We extend the latter idea to a more general parameter embedding. We consider the lifted online optimal control problem as dependent on some process parameters \( p \)

$$\min_{u,x} F(u, p, x) = 0$$

s.t. \( G(u, p, x) = 0 \)

\( H(u, p, x) \geq 0 \),
which could include the current process state. Then we embed these parameters in our problem by adding new nodes $\bar{p}$ and the trivial constraint $\bar{G} = \bar{p} - p$ to the optimization problem. We end up with

\[
\begin{align*}
\min_{u, \tilde{x}} & \quad F(u, p, \tilde{x}) = 0 \\
\text{s.t.} & \quad \bar{G}(u, p, \tilde{x}) = 0 \\
& \quad H(u, p, \tilde{x}) \geq 0,
\end{align*}
\]

where $\tilde{x} = (x, \bar{p})$ and $\bar{G} = (G, \bar{G})$. This allows us a smoother transition between two successive optimization problems, while the linearity of the constraints ensure that they are fulfilled after one SQP iteration.

Finally we demonstrate the performance of our approach at examples from chemical engineering.

REFERENCES


