A Newton-Picard Inexact SQP Method for Time-Periodic PDE Constrained Optimization

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Outline

Application: Simulated Moving Bed Process (SMB)

Constrained Optimization Problem Formulation

Newton-Picard Inexact SQP

Theoretical Convergence and Complexity Analysis

Numerical Convergence Results
Simulated Moving Bed Processes (SMB)

- Goal: Separation of two chemical species in a solution
  - Distillation not possible
  - Eg. Glucose/fructose separation, enantiomere separation
- Used in: Soft drinks, pharmacy
- Preparative chromatography:
  Separation by different adsorption properties
- Simple batch form:

![Diagram of SMB process](image)

- Mixture
- Column
- Adsorbent fixed bed
- Separated Peaks
Simulated Moving Bed Principle I

- Control: Port flows, switching period
- Fixed controls: Process attains cyclic/periodic steady state
Simulated Moving Bed II

Advantages:

▶ Chemical: Better separation properties
▶ Economical: Continuous process
  ⇒ Continuous production

Goal:

▶ Optimize cyclic steady state (CSS)
SMB Model

- General Rate Model (1D) [Gu, 1990, 1995]
- System of diffusion-advection-adsorption equations
- Main difficulty: Highly nonlinear coupling via algebraic isotherm equations
- E.g. Bi-Langmuir isotherm equation

\[
q_i = \frac{H_i^1 c_{p,i}}{1 + \sum_{m=1}^{2} k_m^1 c_{p,m}} + \frac{H_i^2 c_{p,i}}{1 + \sum_{m=1}^{2} k_m^2 c_{p,m}}
\]
Constrained Optimization Problem

- Optimize cyclic steady state (CSS)

\[
\begin{align*}
\min_{y,u,T} & \quad f(y(T), u) \\
\text{s.t.} & \quad \partial_t y = L(y, u) \quad \text{in } [0, T] \times \Omega, \quad \text{plus BC on } \partial \Omega, \\
& \quad y(0) - Py(T) = 0, \\
& \quad h_1(y(T)) \geq 0, \quad \text{(range}(h_i) \subset \mathbb{R}^m), \\
& \quad h_2(u(t), T) \geq 0, \quad t \in [0, T]
\end{align*}
\]

- Main difficulty: Boundary value constraint on \( y \)
Discretize then Optimize

- Discretize states in space and controls in time
- Parametrize states in time by Shooting technique
  \[ \Rightarrow \text{Large scale NLP} \]
- Solved by Inexact SQP
- Generation of forward and adjoint directional derivatives via Internal Numerical Differentiation/Automatic Differentiation
- \( q \): Discretized controls plus parameters and switch period
- \( s \): Discretized initial state
- \( \hat{s}(t; s, q) \): Parametrized state
Inexact SQP (a.k.a. adjoint-based SQP)


- SQP: Sequentially solve Quadratic Programs with approximated Hessians
- Inexact SQP: Also approximate constraint Jacobians
- Solve QP-KKT systems in each iteration:

\[
\begin{pmatrix}
H_{ss} & H_{sq} & A_s^T & B_s^T \\
H_{qs} & H_{qq} & A_q^T & B_q^T \\
A_s & A_q & 0 & 0 \\
B_s & B_q & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\Delta s \\
\Delta q \\
-\Delta \lambda \\
-\Delta \mu_{\text{active}}
\end{pmatrix}
= -
\begin{pmatrix}
\nabla_s L \\
\nabla_q L \\
s - P\hat{s}(T; s, q) \\
h_{\text{active}}(s, q)
\end{pmatrix}
\]

- Calculation of $\nabla L$ by adjoint solve
- Quasi Newton Hessian approximation $H$ (BFGS)
- Newton-Picard projective approximation for $A_s$
  (data-sparse)
Elimination of states from QP

- Use data-sparse $A_s$ to directly eliminate $\Delta s$ and periodicity constraint from QP: $\Delta s = C\Delta q + r$

- Solve small QP with standard active set QP solver
- Recover $\Delta s$
- Recover $\Delta \lambda$ by KKT transformation rules (requires one additional adjoint solve)
Consider discretized periodicity constraint for $s$ with fixed $q$:

$$s - P\hat{s}(T; s, q) = 0$$

Use Newton-type method:

$$A^k_s \Delta s^k = - (s^k - P\hat{s}(T; s^k, q)) , \quad s^{k+1} = s^k + \Delta s^k$$

Full Newton: $A^k_s = \mathbb{I} - M^k$, where

$$M^k = P \frac{d\hat{s}}{ds}(T; s^k, q)$$

is the so called monodromy matrix
Typical Spectrum of the SMB $M$

- Cluster of EV around 0
- Few large EV
- Idea: Calculate $M$ only for “slow” EV
- Picard for fast EV
- Philosophy: High-dimensional discretization but low-dimensional dynamics
Newton-Picard [Lust et al. 1998]

- Use expensive Newton method on “slow” modes
- Use inexpensive functional (Picard) iteration on “fast” modes
- Let orthonormal $V_p \in \mathbb{R}^{ns \times p}$ span the “slow” invariant subspace, i.e. the $p$-dimensional dominant subspace of $M$
- Approximation of $\mathbb{I} - M$:

$$A_s = \mathbb{I} - MV_pV_p^T,$$

- For $A_s$ and $A_s^{-1}$, only the action $MV_p$ is needed
- Can be evaluated by $p$ directional forward derivatives of DE
- Algorithmically, $V_p$ is only approximated with a piggy-back Subspace Iteration simultaneously with the Newton-type method
- Picard contraction can be improved by introduction of a shift [Potschka et al. 2008]
Local Convergence I

- By increasing $p$, $A_s$ can be ameliorated
- Algorithmically, an estimate for the inexactness is available from the Subspace Iteration for $V_p$

$$\sigma_r(A_s - (I - M)) < \lambda_p$$
Local Convergence II [Wirsching et al., 2006]

Assumptions:

- \( w^* = (s^*, q^*, \lambda^*, \mu^*) \) KKT-point
- LICQ and strict complementarity holds in \( w^* \)
- \( H_k \) positive definite, bounded
- Exact KKT matrix \( \hat{K}(w_k) \), approximate \( K_k \)
- \( K_k^{-1} \) uniformly bounded for all \( k \)
- There exists \( \kappa < 1 \) such that
  \[
  \left\| K_{k+1}^{-1} \left( K_k - \hat{K}(w_k + \alpha \Delta w_k) \right) \Delta w_k \right\| \leq \kappa \left\| \Delta w_k \right\| , \quad \forall \alpha \in [0, 1]
  \]

- Full steps

Then:

- Stationary active set and q-linear convergence in a neighborhood of \( w^* \) with convergence rate \( \kappa \)
## Complexity Analysis

<table>
<thead>
<tr>
<th>Per Iteration</th>
<th>Newton-Picard iSQP</th>
<th>SQP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forward solves</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Forward dir. der.</td>
<td>$n_u \frac{3M+1}{2} + S \cdot p + 1$</td>
<td>$n_u \frac{M+1}{2} + n_s$</td>
</tr>
<tr>
<td>Adjoint solves</td>
<td>$3 \ (2)$</td>
<td>0</td>
</tr>
</tbody>
</table>

- $M$ control intervals (typically $\leq 20$)
- $p$ dimension of subspace (typically 1–20)
- $S$ subspace iterations (typically 1–5)
- Effort for linear algebra negligible
- Number of solves per Newton-Picard iSQP iteration independent of $n_s$
Numerical Convergence of Newton-Picard iSQP

Andreas Potschka

Newton-Picard iSQP for time-periodic PDE Opt

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Summary

- Newton-Picard Inexact SQP Method: Simultaneous approach for solution of time-periodic PDE optimization problems
- Exploitation of low-dimensional dynamics of a high-dimensional discretization
- Used to solve SMB application