In Situ Adaptive Tabulation for Nonlinear MPC

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22 Sept. 2003
Outline

• Introduction to ISAT
• ISAT Theory
• NMPC with ISAT
• ISAT vs. Neural Nets
• Future Directions
In Situ Adaptive Tabulation (ISAT)

- Developed by Pope\textsuperscript{1} in 1997 for turbulent combustion simulations.
- ASCI C-SAFE application\textsuperscript{2} at the University of Utah in 2002.
- Integrated with FLUENT\textsuperscript{3}, popular computational fluid dynamics software.
In reacting flow simulations, the integration of the chemistry model can occur $>10^8$ times. ISAT is a storage and retrieval method for the integrations.
ISAT Search

• Binary Tree Architecture
  – Search times are $O(\log_2(N))$ compared with $O(N)$ for a sequential search

\[
v = \phi_2 - \phi_1
\]
\[
\alpha = v^T \left( \frac{\phi_2 + \phi_1}{2} \right)
\]
ISAT Integration

- Scenario #1: Inside the region of accuracy

\[
(\phi - \phi_1)^T M (\phi - \phi_1) \leq \epsilon_{tol}
\]
ISAT Integration

- Scenario #2: Outside the region of accuracy but within the error tolerance

\[ (\phi - \phi_1)^T M (\phi - \phi_1) > \epsilon_{tol} \]

Compute \( M_{\text{new}} \) so that the new region is a symmetric, minimum volume ellipsoid that includes \( \phi \).
ISAT Integration

- Scenario #3: Outside the region of accuracy and outside the error tolerance

Define cutting plane

\[ v = \phi - \phi_1 \]

\[ \alpha = v^T \left( \frac{\phi + \phi_1}{2} \right) \]

Find a conservative estimate for the region of accuracy around \( \phi \)
Nonlinear MPC

Dynamic Data Reconciliation\(^4\)

\[
\min_{x, \eta, y} \Phi(x, \eta, y) \overset{\text{def}}{=} \sum_{k=-N}^{-1} [C(x_k, y_k) + \Xi(\eta_k)] + C(x_0, y_0) + \Xi(\eta_0) \quad \text{s.t.}
\]

\[
y \text{ given, } u \text{ given, } x_{k+1} = F(x_k, u_k), Gx_k - \eta_k \leq g, \eta_k \geq 0
\]

Dynamic Optimization\(^5\)

\[
\min_{x, u, \eta} \Phi(x, u, \eta) \quad \text{s.t.}
\]

\[
x_0 \text{ given, } x_{k+1} = F(x_k, u_k), Du_k \leq d, Gx_k - \eta_k \leq g, \eta_k \geq 0
\]
Nonlinear MPC

Given: Continuous DAE model

\[ \dot{x} = f_1(x, u) \]
\[ 0 = f_2(x, u) \]

Need: Discrete DAE model

Dynamic Data Reconciliation

\[ \min_{x, \eta} \Phi(x, \eta, y) = \sum_{k=-N}^{-1} [C(x_k, y_k) + E(\eta_k)] + C(x_0, y_0) + E(\eta_0) \quad \text{s.t.} \]

\[ y \text{ given, } u \text{ given, } x_{k+1} = F(x_k, u_k), Gx_k - \eta_k \leq g, \eta_k \geq 0 \]

Dynamic Optimization

\[ \min_{x, u, \eta} \Phi(x, u, \eta) \quad \text{s.t.} \]

\[ x_0 \text{ given, } x_{k+1} = F(x_k, u_k), Du_k \leq d, Gx_k - \eta_k \leq g, \eta_k \geq 0 \]
ISAT with NMPC

- ISAT replaces the DAE integrator and sensitivity calculator
NMPC Example with ISAT

32 state binary distillation column model
MV: reflux ratio
CV: distillate composition
Simplex optimizer
Soft constraint on the MV
Control Horizon = 10 min
Prediction Horizon = 15 min
Closed Loop Response

- Distillate Composition ($x_A$) vs. Time (min):
  - Set point
  - 32 states/ISAT
  - 32 states
  - 32 states/Linear

- Speed-up Factor vs. Optimization #:
  - 32 states/ISAT
  - 32 states
  - 32 states/Linear

- Average times:
  - 0.28 sec average
  - 0.84 sec average
  - 12.6 sec average
ISAT Performance

- Successful with ODE and DAE models
- Computational speedup 20 – 500 times
- Storage <100MB for 96 state DAE model with $\varepsilon_{\text{tol}} = 10^{-3}$
ISAT vs. Neural Nets

6 state dual CSTR model
MV: cooling rate of CSTR 1
CV: product temperature
ISAT and Neural Net used the same training data
Compared in open loop and closed loop simulations
Control Horizon = 0.4 min
Prediction Horizon = 0.6 min
Open Loop (ISAT vs. Neural Net)

The chart illustrates the comparison between Actual, Neural Net, ISAT Retrieval, ISAT Growth, and ISAT Addition over time. The y-axis represents the temperature in Kelvin (K), while the x-axis represents time in minutes. The lines and markers show the progression of each system over the 10-minute period.
Closed Loop (ISAT vs. Neural Net)

![Graph showing Reactor #2 Temperature (K) vs. Time (min) with set point, 6 states/ISAT, 6 states, and 6 states/Neural Net lines.](image-url)
Future Directions

• Develop ISAT in C++/Fortran (currently in MATLAB)
• Integrate ISAT with NMPC toolbox for Octave
• Control of Reactive Distillation
• Other applications?
• Questions?
References


