



Nonlinear Programming (NLP) for Stable, Robust and High Performance NMPC

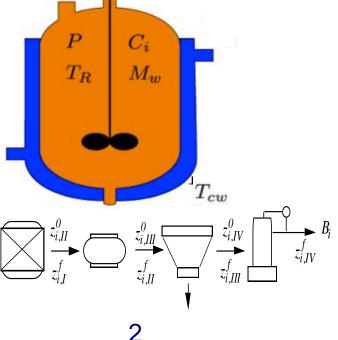
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Model Predictive Control and Dynamic Optimization in Chemical Processes

- Model Predictive Control
 - MIMO with many states and constraints
 - Detailed nonlinear dynamic models
 - Slower dynamics (seconds, minutes)
 - Optimal reference trajectories
- Dynamic Real-time Optimization (eNMPC)
 - Moving Horizon Framework
 - Extensions of MPC
 - Stage costs may not be dissipative
- Can NLPs with first principle dynamics be solved on-line with stability and robustness guarantees?







NMPC Nominal Stability with Terminal Cost (Rawlings and Mayne, 2009)

,

$$\begin{split} V(x(k)) &= \min_{u} \quad \sum_{l=0}^{N} \psi(z_{l}, v_{l}) + \Psi(z_{N}) \\ s.t. &\quad z_{l+1} = f(z_{l}, v_{l})) \\ z_{0} &= x(k), \ z_{l} \in X, \ v_{l} \in U, z_{N} \in X_{f} \\ &= > u(k) = v_{0}, \ Set \ k = k+1 \end{split}$$

Assumptions:

• *f*(*x*, *u*) is Lipschitz continuous (*will assume smooth*)

λT

- There exists a local control law $u = \kappa_f(x)$ for all $x \in \mathcal{X}_{\phi}$ such that $\Psi(f(x, \kappa_f(x))) - \Psi(x) \leq -\psi(x, \kappa_f(x))$
- $\psi(x, u), \Psi(x)$ satisfy $\alpha_p(|x|) \le \psi(x, u), \alpha_q(|x|) \le \Psi(x)$ where $\alpha_p(\bullet), \alpha_q(\bullet)$ are \mathcal{K} functions.
- N sufficiently long, $\Psi(x)$ sufficiently large (Pannocchia, Rawlings, 2011) \rightarrow no terminal constraints needed
- Stability Properties: Lyapunov Function based on Stage Costs



MFCQ for Reformulated NLP

$$V(x(k)) := \min_{v_l, z_l} \Psi(z_N) + \sum_{l=0}^{N-1} \psi(z_l, v_l) + \sum_{l=0}^{N} \rho \xi_l$$

s.t.
$$z_{l+1} = f(z_l, v_l)$$

$$z_0 = x(k)$$

$$v_l \in U, l = 0, ..., N - 1$$

$$g(z_l) \le \xi_l, \xi_l \ge 0, l = 0, ..., N$$

$$e = [1, 1, 1, 1...1]^T$$

- Choose ρ and a sufficiently large N to determine nominal stability
- Softened state constraints with exact penalties are enough to satisfy:
 - MFCQ: equalities have full rank Jacobian, ξ can always be increased
 - to satisfy: $\nabla g(z)^T d_z d_\xi < \theta$
 - CRCQ: inequalities are linear
 - GSSOSC: assume weights on quadratic stage costs are chosen sufficiently large
- The solution and V(x(k)) are uniformly continuous



KKT Properties and Constraint Qualifications for Sensitivity

For $s^*(p) = (x^*, \lambda^*, v^*)$

- <u>MFCQ, GSSOSC</u> uniform continuity of objective function and x* with respect to p. (Kojima, 1985)
- <u>MFCQ, GSSOSC, CRCQ</u> \rightarrow ($D_{\Delta p} x^*$) directional derivatives calculated with additional LP and QP steps (Ralph and Dempe, 1995)
- LICQ, SOSC, SC → (ds*/dp) derivatives can be calculated (Fiacco, 1983) → KKT matrix is nonsingular



NLP Sensitivity

Parametric Program

$$\begin{array}{ccc} \min & f(x,p) \\ \text{s.t.} & c(x,p) = 0 \\ & x \ge 0 \end{array} \end{array} \begin{array}{c} \mathbf{P}(p) \\ \end{array}$$

Solution Triplet

 $s^*(p)^T = [x^{*T} \ \lambda^{*T} \ \nu^{*T}]$

Optimality Conditions P(p)

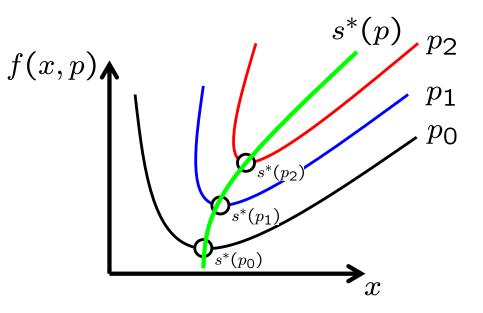
$$\nabla_x f(x,p) + \nabla_x c(x,p) \lambda - \nu = 0$$

$$c(x,p) = 0$$

$$XVe = 0$$

NLP Sensitivity \rightarrow Rely upon Existence and Differentiability of $s^*(p)$

→ Main Idea: Obtain
$$\frac{\partial s}{\partial p}\Big|_{p_0}$$
 and find $\hat{s}^*(p_1)$ by Taylor Series Expansion $\hat{s}^*(p_1)$
 $\hat{s}^*(p_1) \approx s^*(p_0) + \frac{\partial s}{\partial p}^T\Big|_{p_0} (p_1 - p_0)$
 $s^*(p_0)$





NLP Sensitivity with IPOPT (Pirnay, Lopez Negrete, B., 2011)

Obtaining

 ∂s

 $\overline{\partial p}$

Optimality Conditions of *P*(*p*)**: Solved with Newton's Method in IPOPT**

$$\nabla_{x}\mathcal{L} = \nabla_{x}f(x,p) + \nabla_{x}c(x,p)\lambda - \nu = 0$$

$$c(x,p) = 0$$

$$XVe = 0$$

$$Q(s,p) = 0$$

Apply Implicit Function Theorem to Q(s,p) = 0 around $(p_0, s^*(p_0))$

$$\frac{\partial \mathbf{Q}(s^*(p_0), p_0)}{\partial s} \left. \frac{\partial s}{\partial p} \right|_{p_0} + \frac{\partial \mathbf{Q}(s^*(p_0), p_0)}{\partial p} = 0$$

$$\begin{bmatrix} W(s^*(p_0)) & A(x^*(p_0)) & -I \\ A(x^*(p_0))^T & 0 & 0 \\ V^*(p_0) & 0 & X^*(p_0) \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial p} \\ \frac{\partial \lambda}{\partial p} \\ \frac{\partial \nu}{\partial p} \end{bmatrix} + \begin{bmatrix} \nabla_{x,p} \mathcal{L}(s^*(p_0)) \\ \nabla_p c(x^*(p_0)) \\ 0 \end{bmatrix} = 0$$

KKT Matrix IPOPT

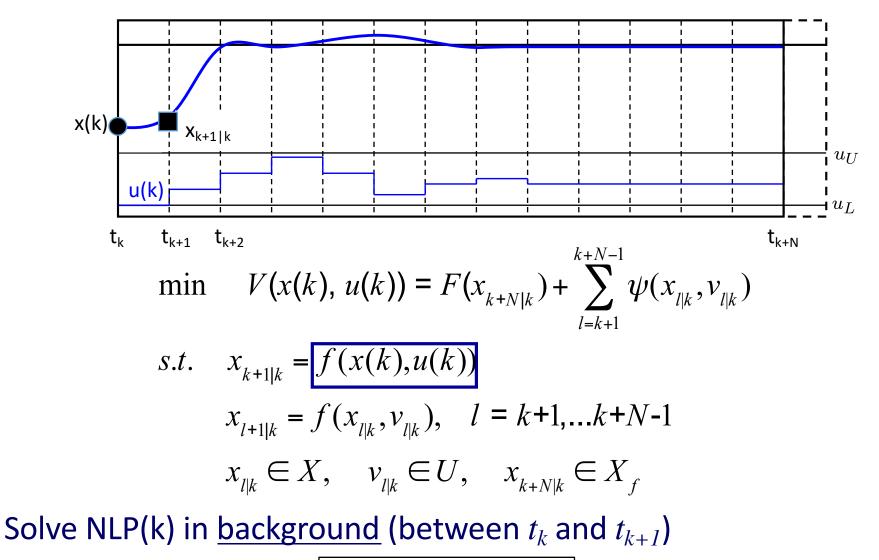
$\int W(x_k,\lambda_k)$	$A(x_k)$	-I
$A(x_k)^T$	0	0
V_k	0	X_k

→ Already Factored from Newton Step in IPOPT
→ Sensitivity Calculation from Single Backsolve
→ Approximate Solution Retains Active Set



Advanced Step Nonlinear MPC (Zavala, B., 2009)

Solve NLP in background (between steps, not on-line) Update using sensitivity on-line

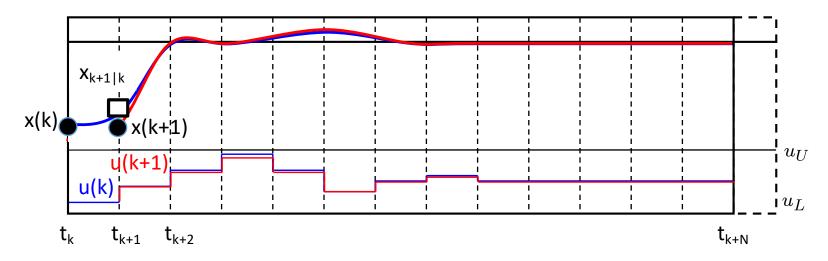


Offline Predictor



Advanced Step Nonlinear MPC (Zavala, B., 2009)

Solve NLP in background (between steps, not on-line) Update using sensitivity on-line



$$\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta \mathbf{x} \\ \Delta \lambda \\ \Delta z \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ x_{k+1|k} - x(k+1) \\ 0 \end{bmatrix}$$

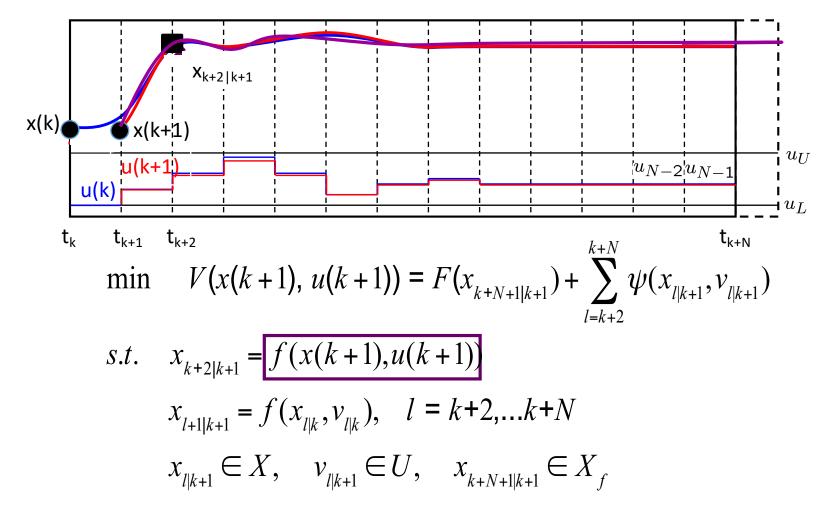
Solve NLP(k) in <u>background</u> (between t_k and t_{k+1}) Sensitivity to update problem <u>on-line</u> to get (u(k+1))

Online Corrector



Advanced Step Nonlinear MPC (Zavala, B., 2009)

Solve NLP in background (between steps, not on-line) Update using sensitivity on-line



Solve NLP(k) in <u>background</u> (between t_k and t_{k+1}) Sensitivity to update problem <u>on-line</u> to get (u(k+1)) Solve NLP(k+1) in <u>background</u> (between t_{k+1} and t_{k+2})



asNMPC: Concepts and Properties

- <u>Interpretation</u>: Fast linear MPC controller using *linearization* of nonlinear model at previous step.
- NLP solved between samples, "instantaneous" sensitivity update at sampling time
- On-line computation <u>2-3 orders of magnitude faster</u>;

Computational delay virtually eliminated

• Second order errors compared to ideal NMPC

→ Nominal and ISS stability (Zavala, B., 2009)

• ISpS stability when coupled with embedded state estimators (Huang, Patwardhan, B., 2009a,b, 2010a-c, 2012)



Nonrobust NMPC Problem

Dynamic system: $f_{1}(x, u, w) = \frac{-(x_{1}^{2} + x_{2}^{2})u + x_{1}}{1 + (x_{1}^{2} + x_{2}^{2})u^{2} - 2x_{1}u} + w_{1}$ $f_{2}(x, u, w) = \frac{x_{2}}{1 + (x_{1}^{2} + x_{2}^{2})u^{2} - 2x_{1}u} + w_{2}$ Inequality Constraints: $\mathbb{X} = \{x : x \in \mathbb{R}^{2}, x_{1} \leq .25\}$ $\mathbb{U} = [-1, 1]$ $\mathbb{X}_{f} = .1\mathcal{B}_{2}$ $\mathbb{X}_{f} = .1\mathcal{B}_{2}$

Cost functions:

$$\Psi(x) = |x| \cos^{-1}\delta \frac{(x_2 - |x|)(-|x|)}{|x|\sqrt{x_1^2 + (x_2 - |x|)^2}}$$

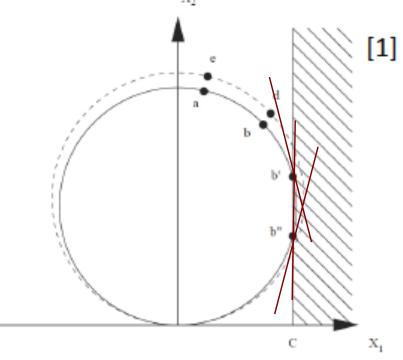
$$\psi(x, u) = |x| \cos^{-1}\delta \frac{x_1 f_1(x, -1) + (x_2 - |x|)(f_2(x, -1) - |x|)}{\sqrt{x_1^2 + (x_2 - |x|)^2}\sqrt{f_1(x, -1)^2 + (f_2(x, -1) - |x|)^2}}$$

Grimm, G., Messina, M. J., Tuna, S. and Teel, A. [2004], 'Examples when nonlinear model predictive control is nonrobust', *Automatica* **40**, **523–533**.



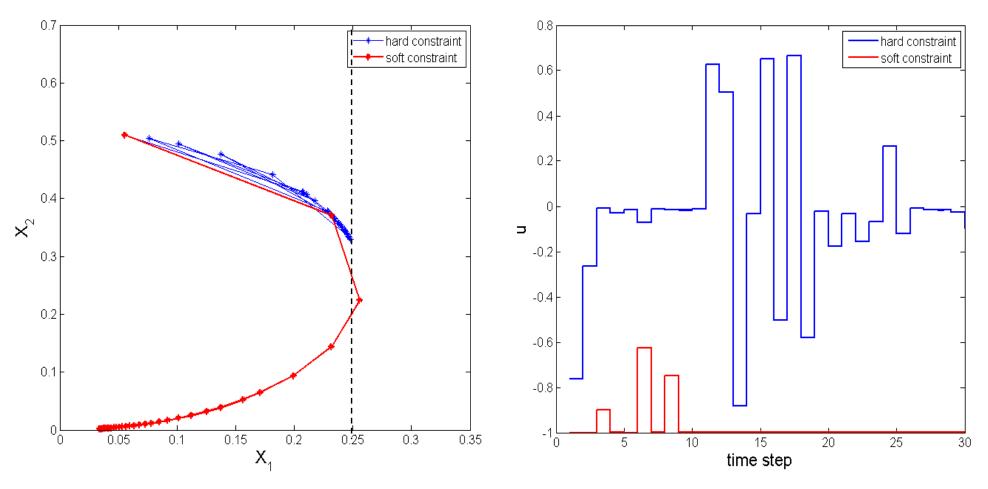
Source of Nonrobustness

- Nonrobustness is caused by the hard state constraint
- There exists a critical circle with radius $r_c = c/\sqrt{1-c^2}$ outside of which there exists no feasible c.w. solution
- Thus the value function of the NLP is discontinuous at this circle





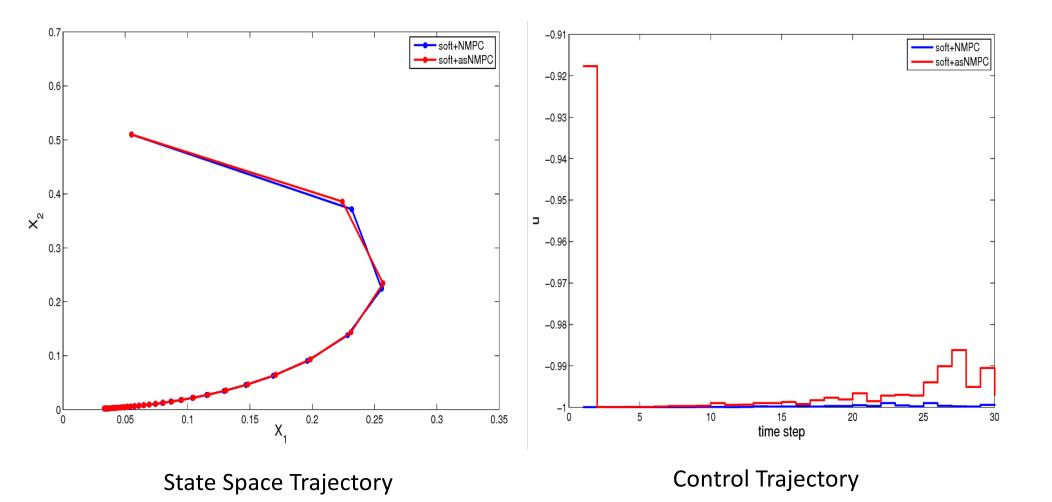
Impact of Reformulation (ℓ_1 penalties and/or larger N)



- Hard constraint $x_1 \le c$ prevents trajectory from going beyond $x_1=c$
- Soft constraint allows the trajectory to exceed x₁=c and converge
- MFCQ and GSSOSC satisfied



Ideal NMPC vs. asNMPC Results (small amount of noise, $\sigma = 0.05$)





Terminal Conditions

$$\begin{split} V(x(k)) &= \min_{u} \quad \sum_{l=0}^{N} \psi(z_{l}, v_{l}) + \Psi(z_{N}) \\ s.t. \\ z_{l+1} &= f(z_{l}, v_{l})) \\ z_{0} &= x(k), \ z_{l} \in X, \ v_{l} \in U, z_{N} \in X_{f}, \end{split}$$

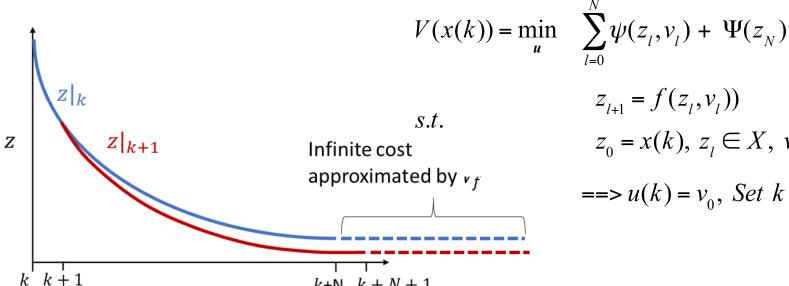
• Assume large, $N \rightarrow \infty$?

$$==> u(k) = v_0, Set \ k = k+1$$

- Hard to check, Can result in large NLPs
- Typically ignored in real applications
- Endpoint constraint $z_N = 0$
 - Requires N controllability.
 - What is *N*? Potential difficulty in finding feasible solutions
- Terminal region $z_N \in \mathcal{X}_f$ and/or terminal cost $\Psi(z_N)$
 - Avoids problems of previous two methods
 - Selection of region or cost not obvious
 - Recursive feasibility requires $\Psi(x_{k+1}) \Psi(x_k) \le -\psi(x_k, u_k) \forall x_k \in \mathcal{X}_f$

hemical

Quasi-Infinite Horizon NMPC



 $z_{l+1} = f(z_l, v_l)$ $z_0 = x(k), z_1 \in X, v_1 \in U, z_N \in X_f,$

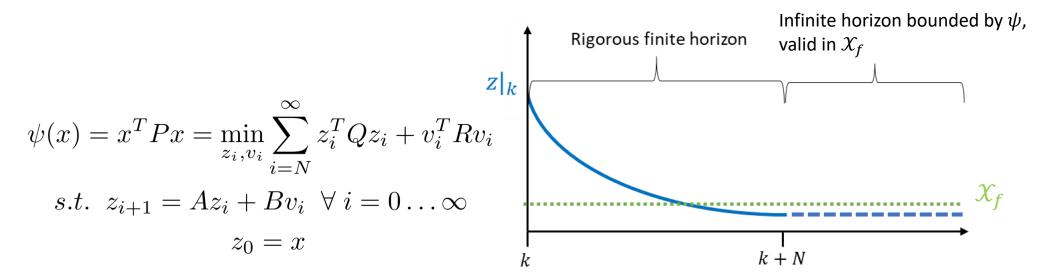
 $==> u(k) = v_0$, Set k = k + 1

Framework for terminal conditions that bound infinite horizon problem

- Accounts for what happens after predictive horizon
- Robustness maintained as time proceeds
- Terminal cost Ψ represents infinite horizon controller stabilizing in \mathcal{X}_f
- Choose LQR (linear quadratic regulator) to bound V_{∞} in the terminal region
- H. Chen and F. Allgöwer. A quasi-infinite horizon nonlinear model predictive control scheme with guaranteed stability. Automatica, 34:1205-1218, 1998.
- C. Rajhans, S. Patwardhan, and H. Pillai. Two Alternate Approaches for Characterization of the Terminal Region for Continuous Time Quasi-Infinite Horizon NMPC. Proceedings of the 12th IEEE International Conference on Control and Automation, 98-103, 2016.
- M. Lazar, M. Tetteroo, IFAC Papers Online 51(20) (2018), pp. 141-146 ٠
- S. Lucia, P. Rumschinski, A. J. Krener, R. Findeisen, IFAC Papers Online 48(23) (2015), pp. 254-259 ٠



Terminal Cost Based on LQR



- Terminal cost ψ becomes infinite horizon cost for linearized system
 - *P* found from Ricatti equation $P = A^T P A A^T P B (R + B^T P B)^{-1} B^T P A + Q$
- Computing terminal region \mathcal{X}_f is equivalent to finding region where LQR stabilizes nonlinear system
- Terminal region can be derived from Lyapunov function descent ==> provides bound on system nonlinearities
- To bound nonlinearities, method <u>must scale to many states</u>

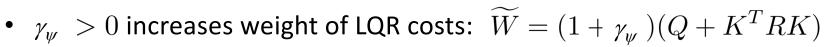


Bounding nonlinearities

• <u>Apply scalable method (off-line)</u>

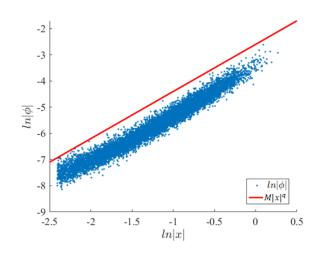
 $|f(x, -Kx) - Ax + BKx| = |\phi(x)| \le M|x|^q$

- Sample one-step CL-LQR simulations
- Apply Taylor's Theorem
- Simple and effective for large systems
- $\underline{X_f}$ computed from *M* and *q*:



- Cost to go P and gain K satisfy the Lyapunov equation for the LQR
- Terminal region given by $\mathcal{X}_{f} = \{x \mid |x| \leq c_{f}\}$ $c_{f} := \left(\frac{-\hat{\sigma}\Lambda_{P} + \sqrt{(\hat{\sigma}\Lambda_{P})^{2} + \lambda_{\Delta W}^{min}\Lambda_{P}}}{\Lambda_{P}M}\right)^{\frac{1}{q-1}}$
- $\hat{\sigma}$ is the maximum singular value of $A_K = A BK$ and $\Lambda_P = \frac{\lambda_{\widetilde{W}}^{max}}{1 \hat{\sigma}^2}$
- Satisfies assumptions on terminal region/cost formulation for asymptotic stability

Example of nonlinearity bound





Robust QIH-NMPC Reformulation

$$V_{N}^{r}(x_{k}) = \min_{z_{i},v_{i}} \sum_{i=0}^{N-1} \left(z_{i}^{T}Qz_{i} + v_{i}^{T}Rv_{i} + \rho\xi_{i}^{T}e \right) + z_{N}^{T}Pz_{N} + \rho\xi_{N}^{T}e$$

$$s.t. \ z_{i+1} = f(z_{i},v_{i}) \ \forall \ i = 0 \dots N - 1$$

$$z_{0} = x_{k}$$

$$h(z_{i}) \leq \xi_{i},\xi_{i} \geq 0 \ \forall \ 0 = 1 \dots N - 1$$

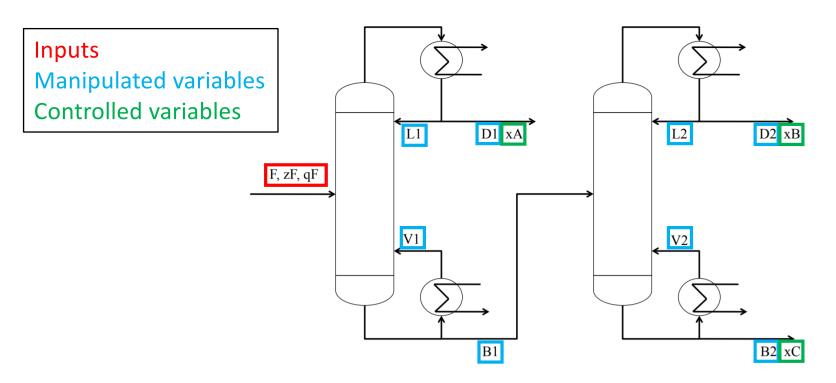
$$v_{i} \in \mathbb{U} \ \forall \ i = 0 \dots N - 1$$

$$|z_{N}| \leq c_{f} + \xi_{N}, \xi_{N} \geq 0$$

- Penalty weight ho chosen sufficiently large to inherit nominal stability
- Formulation satisfies MFCQ (feasible search direction exists)
- GSSOSC holds if Q, R large enough
- Thus V_N^r is uniformly continuous ==> Input-to-state stability (ISS) holds



Distillation Example



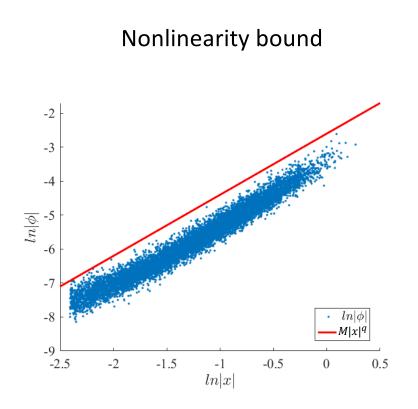
- Separation of three component mixture A,B,C maintain product purities
- 246 States tray holdups and compositions at 41 trays in each column
- 8 Controls reflux, boilup, distillate flow, bottoms flow
- ~ 10000 variables, 200 dofs

R.B. Leer. Self-optimizing control structures for active constraint regions of a sequence of distillation columns. Master's thesis, Norwegian University of Science and Technology, 2012.



Terminal Regions for Distillation

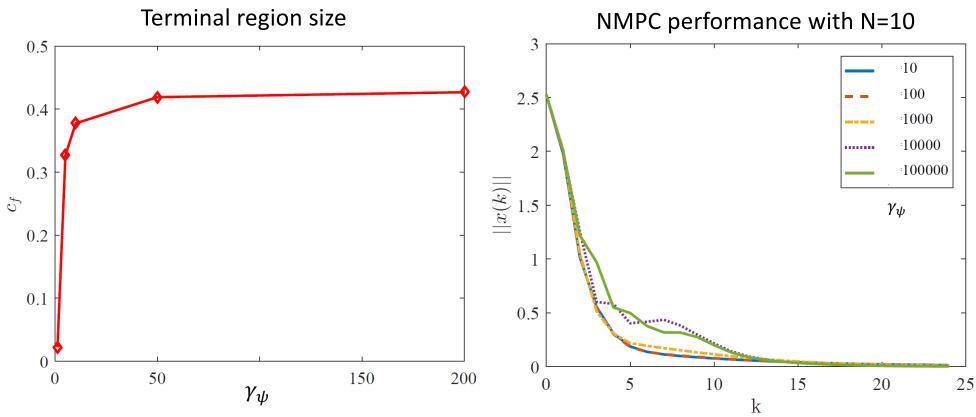
- Nonlinearity bound set with q= 1.8 and M = 0.0743
- 10,000 one-step simulations under LQR (10 CPU min done offline)
- State and control constraints imposed independently
- Terminal region size and NMPC performance compared as function of terminal cost weight γ_{ψ}



 $|f(x, -Kx) - Ax + BKx| = |\phi(x)| \le M|x|^q$



Distillation Results



- Terminal region given by $\mathcal{X}_f = \{z_N \mid |z_N| \le c_f\}$
- LQR cost given by $(1 + \gamma_{\psi})(Q + K^T R K)$
- Terminal region size increases with terminal cost weight, but plateaus
- Tracking performance degrades with large terminal cost weight
- ==> choose moderate weights



Adaptive Horizon NMPC: How long is N?

$$V_N(x_k) = \min_{z_i, v_i} \sum_{i=0}^{N-1} \left(z_i^T Q z_i + v_i^T R v_i \right) + z_N^T P z_N$$

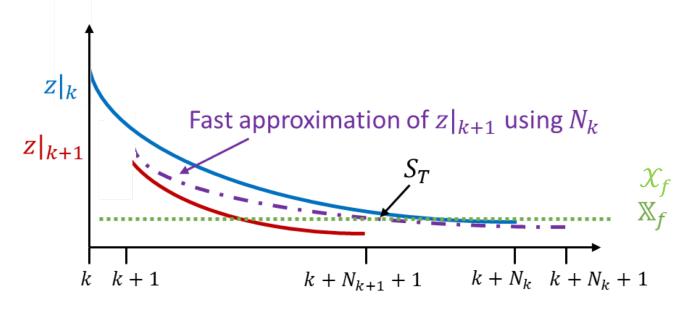
s.t. $z_{i+1} = f(z_i, v_i) \quad \forall i = 0 \dots N - 1$
 $z_0 = x_k$
 $z_i \in \mathbb{X} \quad \forall i = 0 \dots N - 1$
 $v_i \in \mathbb{U} \quad \forall i = 0 \dots N - 1$
 $|z_N| \le c_f$

- Horizon length *N* balances computation and robustness
 - N too long: long solve times \Rightarrow delayed control actions
 - N too short: limited robustness \Rightarrow unstable or infeasible
 - Practical applications must use conservatively long horizon lengths
- Magnitude of trade-off changes with system state
 - Longer horizon necessary further from steady state
- Adaptively choose N in real time
- D. W. Griffith, S. C. Patwardhan and LTB, Journal of Process Control, 70, pp. 109{122 (2018)
- A. J. Krener, ArXiv:1062.08619 (2016)



Horizon Length Selection

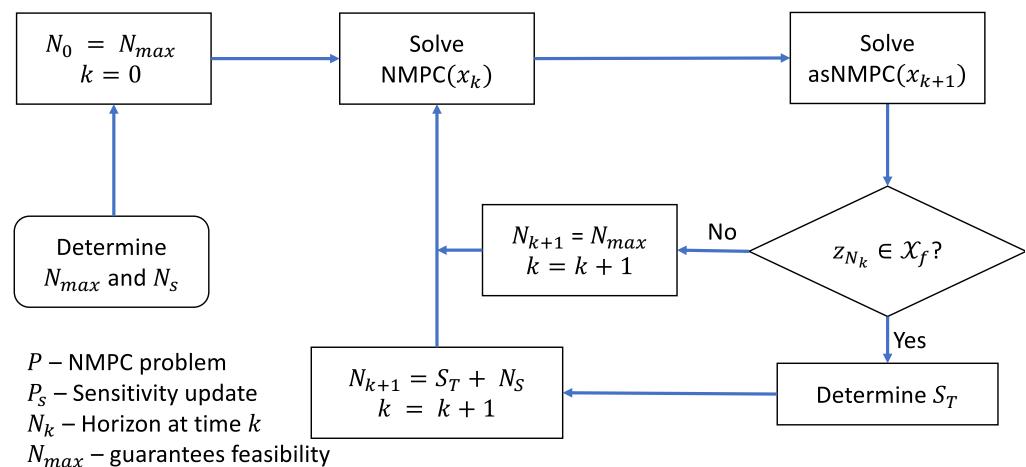
- NLP Sensitivity provides fast updates for perturbations to parametric NLPs
- Fast (~1 sec) estimates to NMPC problems obtained online by treating initial condition as parameter, <u>as in asNMPC</u>
- Approach: use slpopt to predict the time step S_T at which the NMPC solution will reach \mathcal{X}_f



- Pirnay, H., Lopez-Negrete, R., LTB. (2012). Optimal sensitivity based on Ipopt. Math. Prog. Comp., 4, 307-331.
- Zavala, V.M., LTB. (2009). The advanced-step NMPC controller: Optimality, stability, and robustness. Automatica, 45, 86-93.



Adaptive Horizon Algorithm



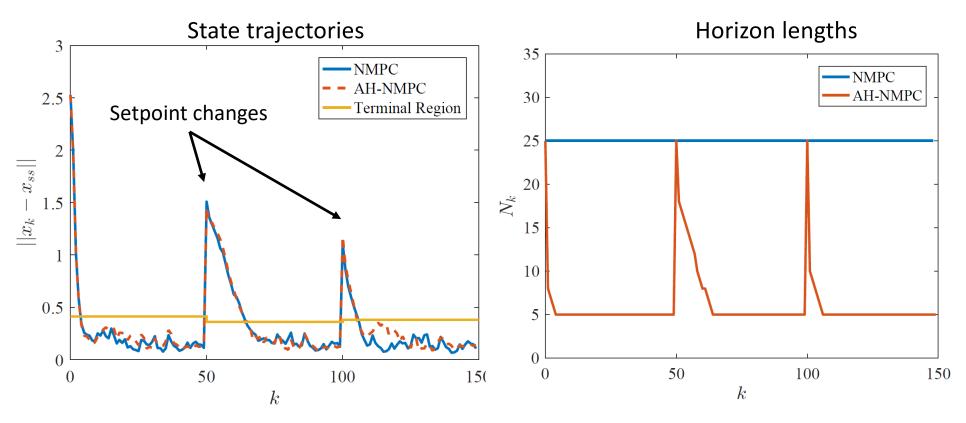
- N_{max} guarantees reasi
- N_S safety factor

$\boldsymbol{S_T}$ – Time step at which the solution reaches the terminal region

- x_k system state at time k
- z_{N_k} sensitivity prediction of terminal state at time k



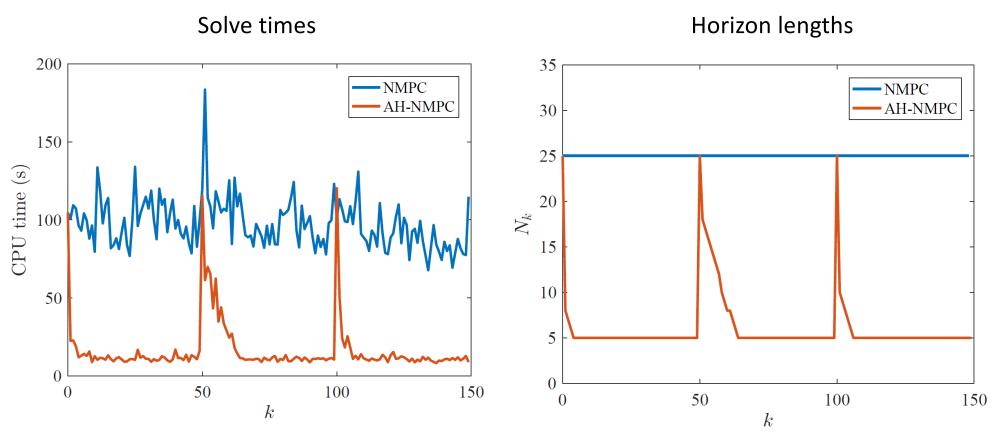
Distillation Example with Noise



- Noise: 10% variance in feed flow and composition
- Horizon selection is robust, all problems are feasible
- Tracking performances similar to noise-free case
- AH-NMPC contracts horizon as the setpoint is approach, similar performance as with N = 25
- Feasible horizons chosen despite noise



Solve Times with Noise



(Off-line) Solve Times

- NMPC average solve time <u>97 CPU s</u>
- AH-NMPC, average <u>17 CPU s</u>
- Application of asNMPC --> additional on-line computational savings

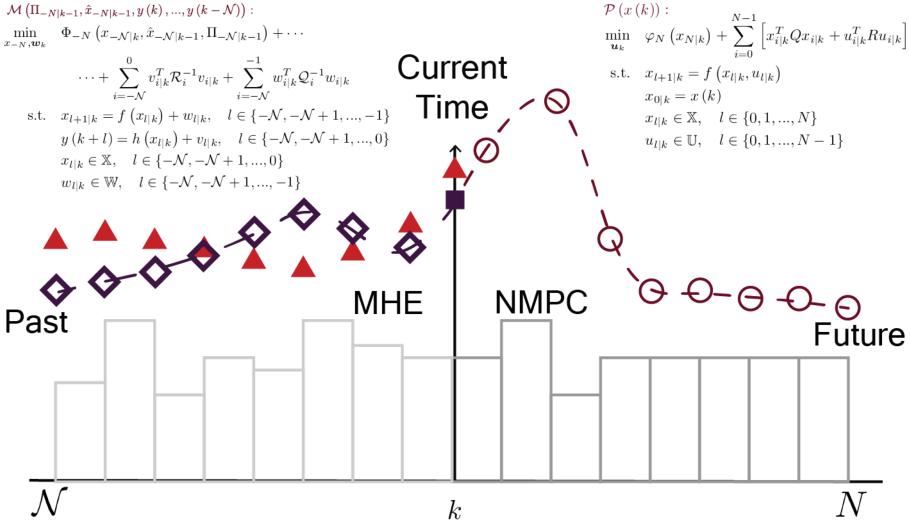


Conclusions

- Robust NLP reformulations
 - Uniform continuity/sensitivity of NLP guaranteed by KKT conditions and CQs (SSOSC, MFCQ, LICQ)
 - Soft output constraints lead to robustly stable NMPC
- Advanced Step NMPC
 - Fast off-line solutions
 - Virtually no on-line computation
 - Leads to ISS Stability
- Terminal conditions for large scale systems
 - Allows for reachability analysis and ultimately shorter horizons
 - Based on LQR control in $\mathcal{X}_{\mathrm{fr}}$ and applying Taylor expansions
 - Easily embedded in NMPC formulation
- Adaptive Horizon NMPC
 - Faster solve times via horizon length adaption utilizing sIPOPT
 - Robustness stability properties retained



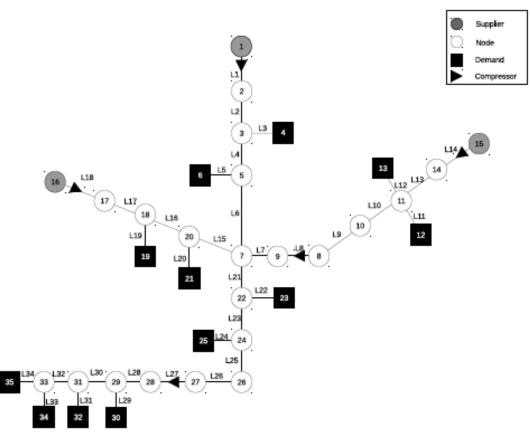
Advanced Step Moving Horizon State Estimation



V. M. Zavala, and LTB, "Optimization-Based Strategies for the Operation of Low-Density Polyethylene Tubular Reactors: Moving Horizon Estimation," Computers and Chemical Engineering, 33, pp. 379-390 (2009)



- Advanced Step Moving Horizon State Estimation
- Embedded discrete decisions for nonsmooth dynamics

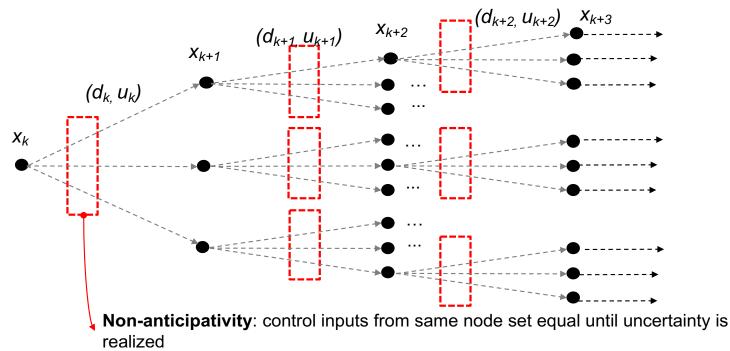


- A. Gopalakrishnan, LTB, "Economic Nonlinear Model Predictive Control for the Periodic Optimal Operation of Gas Pipeline Networks," Computers and Chemical Engineering , 52, pp. 90-99, (2013)
- Kai Liu, Saif R. Kazi, LTB, Bingjian Zhang,, Qinglin Chen, "Dynamic optimization for gas blending in pipeline networks with gas interchangeability control," submitted for publication (2019)



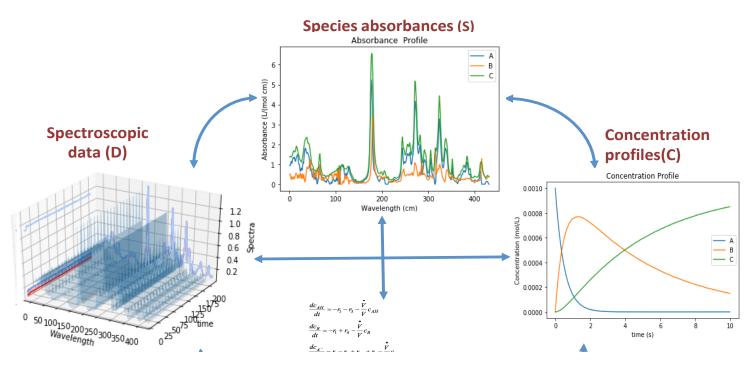
- Advanced Step Moving Horizon State Estimation
- Embedded discrete decisions for nonsmooth dynamics
- Multi-stage Stochastic formulations for NMPC with uncertainties and recourse variables

Scenario branching: effect of uncertainty while optimizing control input



F. Holtorf, A. Mitsos, LTB, "Multistage NMPC with on-line generated scenario trees: Application to a semi-batch polymerization process," Journal of Process Control , 80, pp. 167-179 (2019)

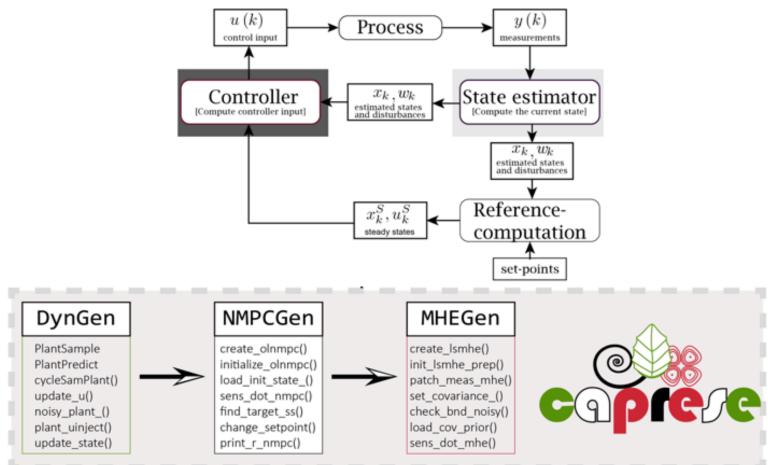




- Larger, more challenging applications
 - Big data in MHE (spectral measurements)
 - PDEs as process models
 - Exploit multiple time scales (ODEs --> DAEs)

M. Short, C. Schenk, D. Thierry, J. S. Rodriguez, LTB, S. Garcia-Munoz, "KIPET, An Open Source Kinetic Parameter Estimation Toolkit," Proc. 9 Intl Conference on Foundations of Computer-Aided Process Design, 293-302, (2019)





 <u>CAPRESE</u>: Python/Pyomo framework for asNMPC/asMHE and Sufficient horizon lengths found via sIPOPT

D. M. Thierry, LTB, "Dynamic Real-time Optimization for a CO2 Capture Process," AIChE J., 65, 7, pp. 1-11 (2019)



- Advanced Step Moving Horizon State Estimation
- Embedded discrete decisions for nonsmooth dynamics
- Multi-stage Stochastic formulations for NMPC with uncertainties and recourse variables
- Structured Dynamic Decompositions for Newton Steps in IPOPT
- Larger, more challenging applications
 - Big data in MHE (spectral measurements)
 - PDEs as process models
 - Exploit multiple time scales
- <u>CAPRESE:</u> Python/Pyomo framework for asNMPC/asMHE and Sufficient horizon lengths found via sIPOPT