

APPLICATION OF OPTIMIZATION ALGORITHMS TO NONLINEAR MPC

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Abstract: This paper investigates application of SQP optimization algorithms to nonlinear model predictive control. It considers feasible vs. infeasible path methods, sequential vs. simultaneous methods and reduced vs. full space methods. The suitable choices between these various strategies are assessed informally through a case study.

Keywords: model predictive control, optimization

1. INTRODUCTION

Nonlinear model predictive control (NMPC) is a control strategy where application of nonlinear optimization methods is essential. This paper is application oriented, and contributes to the practical knowledge of implementation of NMPC. The paper focuses on application of SQP optimization algorithms in NMPC, but emphasizes that appropriate model discretization is essential for the performance. A rule of thumb is that if it is impossible to integrate a model with a certain method, the method cannot be used in NMPC. The paper addresses the differences and similarities between feasible and infeasible path methods, sequential and simultaneous methods and reduced and full space methods. The suitable choices between these various strategies are informally assessed by applying them to a case; a CSTR with first order reaction.

The theory of optimization algorithms is not dependent on how the equality constraints are formed. For instance in optimal control, and in particular in the special case of NMPC, much concern is put into discretization schemes for the nonlinear equality constraints. These equality constraints result from a continuous-time nonlinear dynamical system repeated over a time horizon P . Three major variants are usually considered to handle unstable modes; orthogonal collocation, multiple shooting and single shooting (possibly with a variable grid). Ascher *et al.* (1995) discuss the general benefits of these approaches, and Barclay *et al.* (1998) discusses this in conjunction with SQP algorithms. Vassiliadis (1993) addresses the dynamic optimization of general DAE systems. These approaches seek to find formulations of the equality constraints that are less hard to satisfy, while simultaneously reducing the discretization error.

Nonlinear inequality constraints may be introduced for stability purposes in NMPC (Scokaert *et al.* (1999), Chen and Allgöwer (1998b), Chen and Allgöwer

(1998a)). These references extend earlier work (Li *et al.* (1990), de Oliveira and Biegler (1995)), which are concerned with nominal stability. Hence, termination prior to convergence of the optimizer cannot guarantee stability unless the equality constraints are satisfied.

The immediate answer to the need for early termination is single shooting, i.e., solve the model at each iteration with an initial value solver. Single shooting algorithms progress towards a solution by iterating between solving the model and solving a reduced size optimization problem. Due to this, single shooting is said to be a sequential method. Single shooting produces a reduced gradient problem in the free variables to be solved at each NMPC iteration. Maintaining feasibility of nonlinear inequalities involving dependent variables can then be obtained by use of FSQP' (Lawrence and Tits 2000). Single shooting may be costly if evaluation of the problem functions is costly, e.g. if an implicit discretization scheme must be applied. In addition single shooting lacks robustness when applied to unstable systems (Ascher *et al.* 1995), section 4.1 and 4.6.2.

To solve optimization problems with stabilizing end-point constraints simultaneous methods must be applied. End-point constraints make the problem a two-point boundary value problem (TPBVP) which in general cannot be resolved with single shooting. Simultaneous methods do not solve the model at each iteration. Instead a simultaneous search for a model solution and optimal point is carried out. Multiple-shooting and orthogonal collocation, possibly on finite elements (Finlayson 1980), are the most widely used simultaneous methods. Since simultaneous methods do not solve the model at each iteration, they cannot guarantee stability in the nominal stability setting of dual-mode or quasi-infinite horizon NMPC if terminated prior to convergence. Note that the results reported in (Bock *et al.* 2000) show that termination prior to convergence in multiple shooting may be

viable for some applications. Decomposition strategies for orthogonal collocation on finite elements have been considered by (Cervantes and Biegler 2000) and (Biegler *et al.* 2001).

For convenience, define the superscript notation $z^k = \{z_k\}_{k \in \mathbb{N}}$ for an entity z indexed by k . The nonlinear MPC problem with $\dim(u_k) = n_u$ and $\dim(x_k) = n_x$

$$\begin{aligned} \min_{x, u; k} \quad & \frac{1}{2} \left(\sum_{k=0}^{P-1} \|x_{k+1}\|_Q^2 + \sum_{k=0}^M \|u_k\|_R^2 \right) \\ \text{s.t.} \quad & c_{\mathcal{E},k} = c_{\mathcal{E}}(x^k, u^k) = 0 \\ & x^k \in \mathbb{X} \times \cdots \times \mathbb{X} \\ & u^k \in \mathbb{U} \times \cdots \times \mathbb{U} \end{aligned} \quad (1)$$

with $M < P$ is considered in this paper. The equality constraints in (1) are formed by assuming an appropriate discretization scheme of the continuous time model constraint $f(x, u; t) = 0$ repeated over the horizon P along with a suitable parametrization of the control profile. Endpoint constraints or augmentation of the objective may be included to guarantee nominal stability of the MPC algorithm, see (Mayne *et al.* 2000). Observe that reference tracking and non-zero set-points can be handled in this framework with minor modifications. It is assumed that sufficiently smooth 1st principles state-space models with measured states, analytic 1st order derivatives are used and that

$$(\mathcal{X}, \mathcal{U}) = (\mathbb{X} \times \cdots \times \mathbb{X}, \mathbb{U} \times \cdots \times \mathbb{U})$$

can be described by bounds.

The paper continues with a conceptual comparison between single shooting and reduced Hessian methods in section 2. Simulation results follow in section 3. Discussion and conclusions to the paper follow in sections 4 and 5.

2. OPTIMIZATION METHODS

First SQP methods in general are considered. The MPC problem (1) can be restated as a general nonlinear programming (NLP) problem:

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & c_{\mathcal{E}}(x) = 0 \\ & c_{\mathcal{I}}(x) \leq 0 \end{aligned} \quad (2)$$

where $f : n \rightarrow p$, $c_{\mathcal{E}} : n \rightarrow m$ and $c_{\mathcal{I}} : n \rightarrow p$ where $n = n_x P + n_u M$, $m = n_x (P + 1)$ and $p = 2n$ (assuming upper and lower bounds on (x_k, u_k) over the horizons P and M). The Jacobian matrix of the equality constraints is denoted $A_k^T = A(x_k)^T = [\nabla c_{\mathcal{E}}^1(x_k), \nabla c_{\mathcal{E}}^2(x_k), \dots, \nabla c_{\mathcal{E}}^m(x_k)]$ where $c_{\mathcal{E}}^i(x_k)$ is the i -th component of the vector $c(x_k)$. The matrix $G(x_k)$ made up of A_k^T and the gradients of the active inequality constraints is assumed to have full column rank. The null-space of $G(x_k)^T$ defines the tangent space to the equality and active inequality constraints at x_k . Denote $H\mathcal{L}_k$ the Hessian of the Lagrangian function $\mathcal{L}(x_k, \lambda_{\mathcal{E},k}, \lambda_{\mathcal{I},k}) = f(x_k) + \lambda_{\mathcal{E},k}^T c_{\mathcal{E}}(x_k) + \lambda_{\mathcal{I},k}^T c_{\mathcal{I}}(x_k)$ where $\lambda_{\mathcal{E},k}$ and $\lambda_{\mathcal{I},k}$ are the multiplier vectors. We assume strong second order sufficient

conditions, i.e. that x^* is an isolated minimum of the NLP (2) and that $\lambda_{\mathcal{E}}^*$ and $\lambda_{\mathcal{I}}^*$ are unique.

In SQP, a sequence of subproblems are solved, where the model is linearized and a quadratic model of the Hessian of the Lagrangian is formed. This gives a quadratic programming problem to be solved at each iteration of the SQP algorithm:

$$\begin{aligned} \min_{d_k} \quad & \nabla f(x_k)^T d_k + \frac{1}{2} d_k^T B_k d_k \\ \text{s.t.} \quad & \nabla c_{\mathcal{E}}(x_k)^T d_k + c_{\mathcal{E}}(x_k) = 0 \\ & \nabla c_{\mathcal{I}}(x_k)^T d_k + c_{\mathcal{I}}(x_k) \leq 0 \end{aligned} \quad (3)$$

where $B_k \succ 0$ usually is an approximation to $H\mathcal{L}_k$. The solution d_k to (3) is a search direction. The SQP algorithm searches along d_k for a new iterate x_{k+1} that gives a reduction in a merit function. The merit function ϕ_ν is needed to give convergence to a point satisfying the strong 2nd order assumptions from any starting point under certain additional assumptions.

2.1 Reduced gradient methods

The qp (3) can be resolved in the full space of free and independent variables, or in the reduced space of free variables by a suitable elimination of variables. Elimination of variables exploits that if $n_x P - n_u M \gg n_u M$ and that $n_u M$ is small, the reduced subproblem for the null-space step will be small (but dense). In the full space the sparsity of both the Hessian (which commonly requires analytic Hessians) and the Jacobian can be exploited to yield fast solutions (Rao *et al.* 1998). This section shows that a reduced gradient approach can be derived by following two different strategies. The first uses a sequential approach, see e.g. (de Oliveira and Biegler 1995), while the second follows the simultaneous null-space approach (Nocedal and Wright 1999), (Biegler *et al.* 1995).

2.1.1. Sequential approach (sSQP) By iterating the model over the horizon P , the transformation $x^k = \Psi(x_0, u^k)$ allows the equivalent form which is essentially a projection onto the subspace \mathcal{U} . The sequential approach solves the model at each iteration, i.e. the qp-subproblem is solved following a feasible path strategy. The algorithm evolves the model to get $x^k = \Psi(x_0, u^k)$. Then the algorithm solves the a qp for a direction d_k^u , giving u^{k+1} by a line search, which again is used to evolve the model giving x^{k+1} and so on.

In sSQP the second order derivatives of the model are neglected. This sacrifices the quadratic convergence of Newtons method, but it gives a positive definite Hessian. This is also known as the Gauss-Newton method, which will deteriorate to linear convergence if the projected contributions of the model are significant (Biegler 2000). Since the Hessian $H\mathcal{L}^*$ is positive definite, linear convergence results. Otherwise, near the solution quadratic convergence of sSQP may occur, if no state variable bounds are active at the solution.

2.1.2. *Reduced Hessian approach (rSQP)* In the null-space method a decomposition is applied to the KKT conditions to eliminate variables. It can be shown that the sSQP approach coincide with the rSQP approach for the choice $B_k = \text{diag}(\nabla_{xx}^2 f_k, \nabla_{uu}^2 f_k)$ and by decomposing A_k into range and null space according to the natural partitioning given by the states and controls.

In comparing the two approaches observe that the sequential approach maintains feasibility of all iterates, while rSQP searches for feasibility and optimality simultaneously. In addition the sequential method solves the model at each iteration, while rSQP solves the model only at the solution x^* . Also note that the sequential approach only handles initial value problems (IVP), i.e. $x_P \in \Omega_x$ cannot be guaranteed since it implements a shooting strategy in evolving the model over the horizon. The endpoint constraint changes the problem into a boundary value problem (BVP) which must be handled by simultaneous strategies. Therefore the sequential approach is limited to open-loop stable and non-stiff systems. In fact, the stability of the algorithm requires an infinite prediction horizon which is intractable unless the step length can be increased to infinity, see (de Oliveira 1994) and (Chen and Allgöwer 1998a) for details.

There are a number of commercial routines available for both dense and sparse algebra that can be applied. Decomposition strategies for sparse matrices are implemented in the Harwell subroutine libraries MA28 and MA48 (Harwell Laboratory 1995). Alternatives to computing the Jacobian by analytic partial derivatives is by perturbation or by forward differences. This will have a significant impact on the computational demands, see the results in section 3.2.

3. SIMULATIONS

NMPC was implemented on a simple case with three different optimization methods. The first is a basic full space SQP method. The second is the reduced Hessian method rSQP, and the third is the sequential method sSQP. The case is a CSTR with first order reaction. The CSTR example was thoroughly explored by application of various discretization methods and finite difference approximations to the Jacobian.

3.1 Implementation issues

The basic SQP full-space method and rSQP were implemented with the common l_1 -penalty function. sSQP implemented an l_1 -penalty function without penalization of equality constraints, since sSQP always remain feasible with respect to equalities. The line search for all methods is backtracking line search.

The relaxed convergence criteria from (Gill *et al.* 1981), section 8.2.3, were implemented with tolerance 10^{-5} for the basic SQP method and sSQP. In rSQP the algorithm stops whenever a certain KKT measure

is decreased below the tolerance 10^{-5} . The implementation of rSQP is generally more carefully performed than the basic SQP and sSQP methods. Hence, the relaxed termination criteria used in basic SQP and sSQP partly compensates for a rudimentary implementation. However, as the discussion in section 2 indicates, the sSQP method may show linear convergence in certain circumstances, and relaxed termination criteria can therefore be of crucial importance in production codes as well.

For the CSTR case the model was discretized with explicit and implicit Euler, Lobatto IIIC and ordinary Runge-Kutta 4. The Jacobian matrices with associated almost block-diagonal (ABD) structure for the selected discretization methods. The CSTR case was implemented with both analytic Jacobian and finite difference approximations of the Jacobian. Finite differences were considered for both the full Jacobian (a dense matrix) and the elements along the block diagonal (a sparse matrix). In sSQP analytic and finite difference Jacobians were implemented. I.e. the sensitivity matrix \mathcal{S} was approximated directly by finite difference perturbations of the simulator. The CSTR case was investigated with different sampling rates and prediction and move horizons.

The sSQP method was implemented as a Gauss-Newton method with analytic 2nd derivatives of the objective, while rSQP was implemented with BFGS updates.

3.2 Case: CSTR

The case is the following isothermal CSTR with 1st order reaction from (Matsuura and Kato 1967) also investigated by (de Oliveira 1994)

$$\begin{aligned} \frac{dx_1}{dt} &= u_1 + u_2 - k_1 \sqrt{x_1} \\ \frac{dx_2}{dt} &= (C_{B_1} - x_2) \frac{u_1}{x_1} + (C_{B_2} - x_2) \frac{u_2}{x_1} - \frac{k_2 x_2}{(1+x_2)^2} \end{aligned} \quad (4)$$

with parameter values $k_1 = 0.2$, $k_2 = 1$, $C_{B_1} = 24.9$ and $C_{B_2} = 0.1$. For $(u_1, u_2) = (1, 1)$ the CSTR has three equilibrium points at $x_1 = 100$, $x_2 \in (0.633, 2.72, 7.07)$, with the middle equilibrium point being unstable, and the others stable. The system (4) was discretized with a time step h , prediction horizon P , move horizon M and simulated for N_{MPC} samples, i.e. the NMPC problem is repeatedly solved N_{MPC} times. At time step 10 the process experiences a +50% step in C_{B_1} which is seen by the NMPC algorithm through the feedback only. The weights are $Q = 10I_{n_x}$ and $R = I_{n_u}$ in equation (1) and deviation from stationary values is penalized. Here the control objective is to keep the states and controls at their initial values $x = (100, 0.633)$ and $u = (1, 1)$.

The physical bounds $(x_i, u_i) \geq 0$ are imposed over the horizons. The SQP-algorithms were initialized with the output from the previous call for each NMPC iteration. Note that integral action is not implemented. This is justified by that only a comparison of the optimization methods is investigated, and it is ex-

pected that introducing integral action will not influence this comparison. A representative simulation result is shown in Figure 1. The process was simulated by MATLAB's `ode45` in all cases.

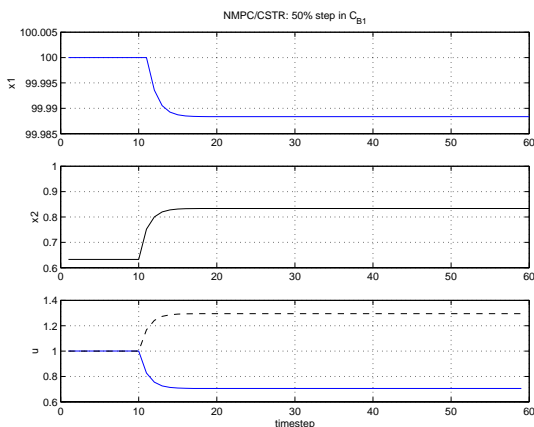


Fig. 1. *NMPC of CSTR*. The figure shows typical results for NMPC of the CSTR case with $h = 1$. The various discretization methods produced nearly identical results. In the lower subfigure the solid curve is for u_1 and the dashed curve is for u_2 . The step in C_{B_1} enters at time step 10, and this drives the state x_2 away from the equilibrium. If the control inputs are kept at the equilibrium input $[1, 1]$, the system will settle at an equilibrium point at $x = (100, 15.94)$.

Note that with the given initial conditions and the given disturbance, this case is pathological with respect to inequality constraints, i.e. the active set is empty and unaltered throughout the horizon P .

The computations were implemented in MATLAB with the `qp`-routines available as `mex/dll`-files on a Compaq Deskpro EN / Pentium II / 450MHz / 128Mb RAM running Windows NT4.0. Computational results are shown in Tables 1-3. The results in Tables 1-3 are summarized in the following conclusions:

- $sSQP$ is sensitive to the choice between implicit and explicit integration methods, while both basic SQP and $rSQP$ is insensitive to this.
- Finite difference approximations of the full Jacobian in basic SQP and $rSQP$ should be avoided.
- Reduced gradient methods are superior for a large number of variables with few degrees of freedom.

Note that a consequence of the first item is that simultaneous SQP methods can have fewer variables when implemented with implicit discretization methods. Here the step length h can be increased beyond the stability limit of explicit methods (but not beyond reasonable accuracy). Since the basic SQP and $sSQP$ methods are approximately similar in implementation complexity, $sSQP$ should be chosen when explicit discretization schemes suffice. In the face of more challenging processes reduced Hessian methods are superior provided that the assumption that there are few degrees of freedom continue to hold. This assumption commonly holds in NMPC.

4. DISCUSSION

In this paper different MPC strategies were implemented on a case and the computational load and quality of the results were investigated. From tables 1-3 it is observed that among the different NMPC methods, the $rSQP$ method are preferable in view of computational time if implicit discretization methods are required. In NMPC computational time is limited, and feasibility of intermediate iterates is essential for stability (Mayne *et al.* 2000), (Scokaert *et al.* 1999). Generally, SQP involves an adaptive subproblem, i.e. its computational time is not deterministic. Consequently, in NMPC feasible path SQP methods are preferred since they allow termination prior to convergence (Mayne 1997). Such methods must solve the model constraints at each SQP iteration, which may be time consuming if the model is represented with an implicit discretization scheme. Hence, $sSQP$ becomes computationally demanding if implicit discretization methods are applied, whereas simultaneous SQP methods perform equally well regardless of whether implicit or explicit discretization scheme are applied. Both methods require that the selected discretization scheme is appropriate, i.e. if the model cannot be simulated with a given method, it cannot be expected that the optimization algorithms perform well either.

Feasibility with respect to inequality constraints is easier to achieve. $FSQP'$ (Lawrence and Tits 2000) and $rFSQP$ (Martinsen and Foss 2001) maintain feasibility with respect to inequality constraints, and *asymptotic* feasibility with respect to nonlinear equality constraints by combining these with an exact penalty function and an arc search. The feasible path $sSQP$ method is expected not to perform well in the presence of strong nonlinearities (Ascher *et al.* 1995). This is contradictory to the needs for NMPC; e.g. problems with strong nonlinearities and trajectory tracking (Qin and Badgwell 2000).

5. CONCLUSION

The practical considerations discussed in this paper explore the choices an engineer must take if he wants to implement NMPC at a given process. The interplay between discretization methods and optimization algorithms has been investigated through a case study.

First the engineer must select an appropriate discretization scheme. If he chooses an explicit discretization scheme, he can choose between sequential or simultaneous optimization methods. Sequential methods are easy to implement, while simultaneous methods are harder to implement. This applies in particular to reduced Hessian methods which may be quite sophisticated. If implicit discretization methods must be applied, the performance of $sSQP$ deteriorates while simultaneous SQP does not degrade.

Discretization method	Horizons $h/P/M$	# vars. tot/dep/free	Jacobian analytic/fd1/fd2	Results	
				Obj	CPU time
Explicit Euler	2/6/5	22/12/10	analytic	33.55	5.9s
Explicit Euler	1/12/10	44/24/20	analytic	28.33	19s
Implicit Euler	2/6/5	22/12/10	analytic	31.41	9.5s
Implicit Euler	1/12/10	44/24/20	analytic	27.85	45s
Lobatto IIIC	2/6/5	34/24/10	analytic	32.37	7.3s
Lobatto IIIC	2/6/5	34/24/10	fd1	32.35	22s
Lobatto IIIC	2/6/5	34/24/10	fd2	32.35	25s
Lobatto IIIC	1/12/10	68/48/20	analytic	28.07	35s
Lobatto IIIC	1/12/10	68/48/20	fd1	28.06	96s
Lobatto IIIC	1/12/10	68/48/20	fd2	28.06	222s
RK4	2/6/5	70/60/10	analytic	32.40	14.1s
RK4	2/6/5	70/60/10	fd1	32.39	30s
RK4	2/6/5	70/60/10	fd2	32.40	117s
RK4	1/12/10	140/120/20	analytic	28.05	119s
RK4	1/12/10	140/120/20	fd1	28.04	338s
RK4	1/12/10	140/120/20	fd2	28.05	1136s

Table 1. *Nonlinear MPC on a CSTR: Basic SQP*. The table shows results for the basic SQP method. $h/P/M$ are the sampling time, prediction and move horizons. The # vars. tot/dep/free are the total, dependent and free number of variables. Note that there are no active inequality constraints in this case. The Jacobian is either analytic or approximated by finite differences. In mode fd1 only elements along the block diagonal were approximated, while in mode fd2 the full (dense) Jacobian was approximated. Obj is the objective value measured by summing the actual process outputs and implemented control actions over the NMPC horizon N_{MPC} . CPU time is the time measured by MATLAB's `cpu time` command from start to end of the main NMPC loop.

Discretization method	Horizons $h/P/M$	# vars. tot/dep/free	Jacobian analytic/fd	Results	
				Obj	CPU time
Explicit Euler	2/6/5	22/12/10	analytic	33.18	4.4s
Explicit Euler	2/6/5	22/12/10	fd	33.54	5.7s
Explicit Euler	1/12/10	44/24/20	analytic	28.15	13.1s
Explicit Euler	1/12/10	44/24/20	fd	28.33	19.4s
Implicit Euler	2/6/5	22/12/10	analytic	31.41	33s
Implicit Euler	2/6/5	22/12/10	fd	31.41	131s
Implicit Euler	1/12/10	44/24/20	analytic	27.85	94s
Implicit Euler	1/12/10	44/24/20	fd	27.83	745s
Lobatto IIIC	2/6/5	34/24/10	analytic	32.37	49s
Lobatto IIIC	2/6/5	34/24/10	fd	32.36	192s
Lobatto IIIC	1/12/10	68/48/20	analytic	28.07	118s
Lobatto IIIC	1/12/10	68/48/20	fd	28.07	1121s
RK4	2/6/5	70/60/10	analytic	32.40	4.3s
RK4	2/6/5	70/60/10	fd	32.40	10.0s
RK4	1/12/10	140/120/20	analytic	28.05	12.2s
RK4	1/12/10	140/120/20	fd	28.05	58s
ode45	2/6/5	22/12/10	fd	23.03	36s
ode45	1/12/10	44/24/20	fd	28.49	149s

Table 2. *Nonlinear MPC on a CSTR: sSQP*. The table shows results for the sSQP method. The results for ode45 with $h = 2$ showed some ripple that were caused by the relaxed termination criteria. See table 1 for explanation of symbols.

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Discretization method	Horizons $h/P/M$	# vars. tot/dep/free	Jacobian analytic/fd1/fd2	Results	
				Obj	CPU time
Explicit Euler	2/6/5	22/12/10	analytic	33.57	6.1s
Explicit Euler	1/12/10	44/24/10	analytic	28.27	13.4s
Implicit Euler	2/6/5	22/12/10	analytic	31.43	6.2s
Implicit Euler	1/12/10	44/24/10	analytic	27.99	12.8s
Lobatto IIIC	2/6/5	34/24/10	analytic	32.37	7.1s
Lobatto IIIC	2/6/5	34/24/10	fd1	32.35	11.5s
Lobatto IIIC	2/6/5	34/24/10	fd2	32.35	17.3s
Lobatto IIIC	1/12/10	68/48/20	analytic	28.07	17.2s
Lobatto IIIC	1/12/10	68/48/20	fd1	28.05	39s
Lobatto IIIC	1/12/10	68/48/20	fd2	28.06	95s
RK4	2/6/5	70/60/10	analytic	32.40	9.1s
RK4	2/6/5	70/60/10	fd1	32.39	19s
RK4	2/6/5	70/60/10	fd2	32.40	71s
RK4	1/12/10	140/120/20	analytic	28.05	23s
RK4	1/12/10	140/120/20	fd1	28.04	58s
RK4	1/12/10	140/120/20	fd2	28.05	781s

Table 3. *Nonlinear MPC on a CSTR: rFSQP*. The table shows results for the rFSQP method. See table 1 for explanation of symbols.

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