### Robust optimization of discrete time systems and periodic operation with guaranteed stability

Dissertation zur Erlangung des Grades Doktor-Ingenieurin

der Fakultät für Maschinenbau der Ruhr-Universität Bochum

von

Darya Kastsian aus Bobruisk

Bochum 2012

Dissertation eingereicht am: 13.03.2012 Tag der mündlichen Prüfung: 12.07.2012 Erster Referent: Prof. Dr.-Ing. Martin Mönnigmann Zweiter Referent: Prof. Dr.-Ing. Achim Kienle Schriftenreihe des Lehrstuhls für Regelungstechnik und Systemtheorie

Darya Kastsian

Robust optimization of discrete time systems and periodic operation with guaranteed stability

> Shaker Verlag Aachen 2012

#### Bibliographic information published by the Deutsche Nationalbibliothek

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de.

Zugl.: Bochum, Univ., Diss., 2012

Copyright Shaker Verlag 2012 All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior permission of the publishers.

Printed in Germany.

ISBN 978-3-8440-1305-4 ISSN 2195-0113

Shaker Verlag GmbH • P.O. BOX 101818 • D-52018 Aachen Phone: 0049/2407/9596-0 • Telefax: 0049/2407/9596-9 Internet: www.shaker.de • e-mail: info@shaker.de

## Acknowledgments

This thesis has been prepared in the contest of a project supported by the Deutsche Forschungsgemeinschaft (DFG) under grant MO 1086/4. The financial support by DFG is gratefully acknowledged. The first part of the project was accomplished at the Institute for Heat and Fuel Technology at the Technische Universität Braunschweig. The second part was completed at the department of Automatic Control and Systems Theory at the Ruhr-Universität Bochum. I especially thank my advisor Prof. Dr.-Ing. Martin Mönnigmann for his great supervision during the work at these both universities. I am grateful to Prof. Dr.-Ing. Achim Kienle for reviewing this thesis.

In addition, I want to express my gratitude to Prof. Dr. techn. Reinhard Leithner who was the head of the Institute for Heat and Fuel Technology during my work in Braunschweig. I also acknowledge the opportunity to be able to participate in the project funded by the energy company E.ON as part of the E.ON International Research Initiative. In particular, I am thankful to Dr.-Ing. Radgen and Dr.-Ing. Drew for their supervision.

I owe many thanks to my colleges and students. I enjoyed sharing the office in Braunschweig with Shaofei Chen and Christian Wesemeyer. Also many thanks go to my former colleges from Braunschweig Dr.-Ing. Horst Müller, Yevgeniya Heierle, Gulzhan Tleukenova, Sohail Ahmed, Lasse Nielsen, and Christian Schlitzberger. I was very pleased to work on the E.ON project together with Dr.-Ing. Wolfgang Grote. My colleges from Bochum Dr.-Ing. Günter Gehre, Michael Jost, Moritz Schulze Darup, Sebastian Leonow, Tom Quaiser, Annegret Mannhardt-Bürger and Rainer Baese are especially acknowledged for creating a friendly atmosphere and helpful discussions.

The greatest thank goes to my husband and college Martin Kastsian. I am grateful for his constant support during the work on this thesis. Finally, I want to thank my parents.

## Abstract

In this thesis an optimization method for nonlinear discrete time systems and periodic operation is presented. The method is particularly suited for engineering problems, as it can obtain an optimal operation point with desired dynamical properties for models with uncertain parameters. In typical applications of the method, technical systems are optimized with respect to economic objectives with nonlinear programming methods, while the desired dynamical properties are ensured with the so-called normal vector constraints. The desired dynamical properties are guaranteed for all operation points in a robustness region around the optimal point.

The normal vector constraints, which are incorporated in the optimization problem, impose the lower bound on the distance between the optimal point and any critical boundary. Typical critical boundaries of interest are stability and feasibility boundaries. The first ones consist of bifurcation points. The second ones involve points at which constraints on output or input variables are violated. Once the locations of the critical points of a system are known, normal vectors on the critical manifolds can be used to measure the distance from the nominal point of operation to stability and feasibility boundaries in the space of the system design parameters. By staying sufficiently far away from all critical manifolds we can guarantee robust stability and feasibility of the system.

Previously the normal vector constraints were applied to the optimization of steady states of continuous-time systems that are modeled by sets of parametrically uncertain differential-algebraic equations. In this thesis the normal vector constraints are developed for fixed points of nonlinear discrete time systems. Such systems frequently arise in engineering applications, either because the model is intrinsically discrete in time, or because the model is the result of a time discretization. Attention is paid to both of these cases. Since stability properties of discrete time systems and periodically operated systems are closely related, the normal vector constraints are considered for the optimization of oscillating models. Note that besides processes, where only oscillating states occur, there exist models that can be operated periodically or at a steady state. The situation where the normal vector constraints for periodic operation are combined with the case of operation at a steady state is discussed.

The concept of the normal vector constraints is successfully applied to the optimization procedures of supply chains which are modeled as discrete time systems, a fermentation process that results from sampling the continuous time model, and examples of oscillating chemical reactions.

# Contents

Notation				vii	
1	Intr	Introduction		1	
2	Robust optimization of dynamical systems			5	
	2.1	Overv	iew of existing optimization methods	6	
		2.1.1	Optimization methods for stationary operated systems	6	
		2.1.2	Optimization methods for periodically operated systems	8	
	2.2	Norma	al vector method	9	
3	Nor	mal ve	ctor method for fixed points of discrete time systems	14	
	3.1	Syster	n and problem classes of interest	14	
	3.2	Stabil	ity and bifurcations of fixed points of discrete time systems	16	
	3.3			19	
		3.3.1	Necessary conditions for bifurcation points of discrete time sys-		
			tems with algebraic equations	20	
		3.3.2	Augmented systems for Neimark-Sacker bifurcations	25	
		3.3.3	Augmented systems for flip and fold bifurcations	27	
		3.3.4	Augmented systems for degenerate bifurcations	28	
	3.4	Critica	al manifolds of modified bifurcation points	28	
		3.4.1	Augmented systems for modified bifurcation points	29	
	3.5	Norma	al vector systems	30	
3.6 Optimization problem statement with the normal vector co		ization problem statement with the normal vector constraints	33		
		3.6.1	Optimization problem statement with the normal vector con-		
			straints for ellipsoidal robustness region	34	
		3.6.2	Normal vector constraints for generalization of ellipsoidal robust-		
			ness region	35	

		3.6.3	Optimization problem statement with the normal vector con-	
			straints for generalization of ellipsoidal robustness region $\ . \ . \ .$	37
	3.7	Soluti	on strategy of the optimization problem with the normal vector	
		$\operatorname{constr}$	aints	38
4	Арр	licatior	ns of the method for fixed points of discrete time systems	43
	4.1	Vendo	r managed inventory supply chain	43
		4.1.1	Model description and optimization objective	43
		4.1.2	Optimization results	47
	4.2	Three	echelon supply chain	57
		4.2.1	Model description and optimization objective	57
		4.2.2	Optimization results	61
	4.3	Discre	tized continuously stirred-tank reactor	66
		4.3.1	Model description and optimization objective	67
		4.3.2	Optimization results	70
5	Nor	mal ve	ctor method for ODE systems with periodic solutions	73
	5.1	Syster	n and problem class of interest	73
	5.2	Stabil	ity and bifurcations of ODE systems solutions	75
		5.2.1	Stability and bifurcations of equilibria of ODEs	75
		5.2.2	Stability and bifurcations of periodic solutions of ODEs	77
	5.3	3 Critical manifolds of bifurcation points		82
	5.4	Normal vector systems		83
	5.5	Optimization problem statement with the normal vector constraints		86
6	Арр	licatio	ns of the method for ODE systems with periodic solutions	90
	6.1	Non-is	sothermal chemical reaction	90
		6.1.1	Model description and optimization objective	90
		6.1.2	Optimization results	94
	6.2	Peroxi	idase-oxidase reaction	98
		6.2.1	Model description and optimization objective $\ldots \ldots \ldots$	99
		6.2.2	Optimization results	102
7	Conclusion and outlook 10			
	7.1	Concl	usion	106

	7.2	Outloo	ok	108	
		7.2.1	Extension to systems of delay differential equations $\ldots \ldots \ldots$	108	
		7.2.2	Extension to non-smooth dynamical systems	109	
Α	Der	ivation	of the normal vector systems for critical manifolds of fixed point	s	
	of d	iscrete	time systems	111	
	A.1	Norma	al vectors for manifolds of modified Neimark-Sacker bifurcation		
		points		111	
	A.2	Norma	al vectors for manifolds of modified flip and fold bifurcation points	113	
в	Der	Derivation of the normal vector systems for critical manifolds of periodic			
	solu	tions o	f ODE systems	115	
	B.1	Norma	al vectors for manifolds of Neimark-Sacker bifurcation points of		
		cycles		115	
	B.2	Norma	al vectors for manifolds of flip bifurcation points of cycles	117	
	B.3	Norma	al vectors for manifolds of fold bifurcation points of cycles $\ . \ . \ .$	118	
Ρι	ıblica	tions r	elated to the thesis	121	
Bi	bliog	raphy		122	
Cι	ırricu	lum vit	ae	137	

## Notation

The symbols used for particular model descriptions from Chapters 4 and 6 are omitted here. The meaning of these symbols is explained in the corresponding sections together with the model equations.

#### **Roman letters**

- B matrix of normal space basis vectors in columns
- C mass matrix of dynamical system with algebraic equations
- D open neighborhood of a point in  $\mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_\alpha}$
- d distance between critical manifold and candidate optimal point
- F dynamical and algebraic system equations
- $f, \tilde{f}$  dynamical system equations
- G normal vector system equations
- g algebraic system equations
- $\hat{g}$  equation defining robustness manifold
- h system constraints
- I identity matrix
- i square root of -1
- L first Lyapunov coefficient
- M has different meaning through the text. If it is used with superscript, than it means a manifold. If it is used with dependency on t, than it is a fundamental matrix solution of differential equation. The special case of it M(T)is called a monodromy matrix.
- m rate of uncertainty hypersquare approximation
- $n_h$  number of system constraints
- $n_x$  number of dynamic state variables
- $n_y$  number of algebraic state variables

- $n_z$  number of dynamic and algebraic state variables
- $n_{\alpha}$  number of uncertain parameters
- P Poincaré map
- p vector of initial conditions, period, and parameters for periodic orbits
- Q open neighborhood of a point in  $\mathbb{R}^{n_x} \times \mathbb{R}^{n_\alpha}$
- q vector of state variables and parameters for equilibria
- R radius of circle in complex plane
- r normal vector
- s phase condition
- T period
- t time
- U open neighborhood of a point in  $\mathbb{R}^{n_x}$
- u auxiliary variable in normal vector systems
- V open neighborhood of a point in  $\mathbb{R}^{n_y}$
- v eigenvector
- $\hat{v}$  generalized eigenvector
- W open neighborhood of a point in  $\mathbb{R}^{n_{\alpha}}$
- w eigenvector
- $\hat{w}$  generalized eigenvector
- x vector of dynamic state variables
- $\overline{x}$  vector of auxiliary variables in normal vector systems
- y vector of algebraic state variables
- z vector of dynamic and algebraic state variables
- $\overline{z}$  vector of auxiliary variables in normal vector systems

#### **Greek letters**

- $\alpha$  vector of uncertain parameters
- $\gamma$  auxiliary variable in normal vector systems
- $\Delta \alpha_i$  uncertainty of parameter  $\alpha_i$
- $\Delta t$  discretization step-size
- $\zeta$  <br/> ~~ local coordinates on Poincaré section
- $\eta$  number of continuous derivatives
- $\theta$  argument of complex number

- $\kappa$  linear combination of normal space basis vectors
- $\varkappa$  auxiliary variable in normal vector systems
- $\lambda$  eigenvalue
- $\overline{\lambda}$  complex conjugate of  $\lambda$
- $\hat{\lambda}$  generalized eigenvalue
- $\xi$  local solution for algebraic variables
- $\Sigma$  Poincaré section
- au time delay
- $\Phi_0$  periodic orbit
- $\phi$  objective function
- $\varphi, \, \widetilde{\varphi} \quad \text{flow of differential equation}$
- $\omega \qquad {\rm imaginary \ part \ of \ complex \ number}$

#### **Calligraphic letters**

- $\mathcal{I}$  set of normal vector constraints to critical equilibria and fixed points
- ${\mathcal J}_{-}$  set of normal vector constraints to critical periodic solutions
- $\mathcal{L}$  set of close critical points

### Mathematical notation

$\mathbb{C}$	complex numbers
dist	Euclidean distance
inf	infimum
$\mathbb{N}$	natural numbers
$\nabla$	gradient
$\mathbb{R}$	real numbers
$\mathbb{R}^+$	positive real numbers
Range	range of a matrix (column space)
Rank	rank of a matrix
Re	real part of a complex number
$\ \cdot\ $	Euclidean norm
$\langle \cdot, \cdot \rangle$	scalar product
$\forall$	for all

- $\subset$  subset of
- $\cup$  union of sets

### Subscript

i,j,k	index variable
$\max$	maximum value
$\min$	minimum value
0	initial value

### Superscript

С	critical point
end	resulting point of optimization procedure
$i,\hat{i},j,k$	index variable
flip	flip bifurcation point
flip	modified flip point
fold	fold bifurcation point
$\widetilde{\mathrm{fold}}$	modified fold point
Hopf	Hopf bifurcation point
NS	Neimark-Sacker bifurcation point
$\widetilde{\mathrm{NS}}$	modified Neimark-Sacker point
rob	robustness
$\operatorname{sn}$	saddle-node bifurcation point
start	initial point of optimization procedure
T	transposition
0	nominal point

### Abbreviations

APIOBPCS	automatic pipeline, inventory and order based production control
	system
CSTR	continuously stirred-tank reactor
DDE	delay differential equation
NLP	nonlinear program

- ODE ordinary differential equation
- SQP sequential quadratic programming
- VMI vendor managed inventory

#### Derivatives

We assume that subscripts  $\mu$  and  $\nu$  enumerate rows and columns, respectively. Note that, for example, in  $x_{\mu}$ ,  $\mu$  runs from 1 to  $n_x$ , whereas in  $\alpha_{\mu}$ ,  $\mu = 1, \ldots, n_{\alpha}$ . In the thesis the following notations for derivatives are used

$$\begin{split} (F_{z})_{\mu\nu} &= \frac{\partial F_{\mu}}{\partial z_{\nu}}, & (F_{\alpha})_{\mu\nu} &= \frac{\partial F_{\mu}}{\partial \alpha_{\nu}}, \\ (F_{zz}\hat{w})_{\mu\nu} &= \sum_{\rho=1}^{n_{z}} \frac{\partial^{2} F_{\mu}}{\partial z_{\nu} \partial z_{\rho}} \hat{w}_{\rho}, & (F_{z\alpha}\hat{w})_{\mu\nu} &= \sum_{\rho=1}^{n_{z}} \frac{\partial^{2} F_{\mu}}{\partial \alpha_{\nu} \partial z_{\rho}} \hat{w}_{\rho}, \\ (\hat{v}^{T} F_{zz}\hat{w})_{\mu} &= \sum_{\rho,\sigma=1}^{n_{z}} \hat{v}_{\rho} \frac{\partial^{2} F_{\rho}}{\partial z_{\mu} \partial z_{\sigma}} \hat{w}_{\sigma}, & (\hat{v}^{T} F_{z\alpha}\hat{w})_{\mu} &= \sum_{\rho,\sigma=1}^{n_{z}} \hat{v}_{\rho} \frac{\partial^{2} F_{\rho}}{\partial \alpha_{\mu} \partial z_{\sigma}} \hat{w}_{\sigma}, \\ (\varphi_{x_{0}})_{\mu\nu} &= \frac{\partial \varphi_{\mu}}{\partial x_{0\nu}}, & (\varphi_{\alpha})_{\mu\nu} &= \frac{\partial \varphi_{\mu}}{\partial \alpha_{\nu}}, \\ (\varphi_{T})_{\mu} &= \frac{\partial \varphi_{\mu}}{\partial T}, & (\varphi_{x_{0}x_{0}}w)_{\mu\nu} &= \sum_{\rho=1}^{n_{x}} \frac{\partial^{2} \varphi_{\mu}}{\partial x_{0\rho} \omega_{\rho}} w_{\rho}, \\ (\varphi_{x_{0}\alpha}w)_{\mu\nu} &= \sum_{\rho,\sigma=1}^{n_{x}} \frac{\partial^{2} \varphi_{\mu}}{\partial \alpha_{\nu} \partial x_{0\rho}} w_{\rho}, & (v^{T} \varphi_{x_{0}\alpha}w)_{\mu} &= \sum_{\rho,\sigma=1}^{n_{x}} v_{\rho} \frac{\partial^{2} \varphi_{\rho}}{\partial \alpha_{\mu} \partial x_{0\sigma}} w_{\sigma}, \\ v^{T} \varphi_{x_{0}T}w &= \sum_{\rho,\sigma=1}^{n_{x}} v_{\rho} \frac{\partial^{2} \varphi_{\rho}}{\partial T \partial x_{0\sigma}} w_{\sigma}. \end{split}$$