**Am Fachbereich Informatik
der Technischen Universität Darmstadt
eingereichte Dissertation zur Erlangung des
akademischen Grades eines Doktor-Ingenieur (Dr.-Ing.)**

Derivative Free Surrogate Optimization for Mixed-Integer Nonlinear Black Box Problems in Engineering

Dipl.-Math. Thomas Hemker

(geboren in Steinfurt, Westfalen)

Referenten der Arbeit:	Prof. Dr. Oskar von Stryk
	Prof. Dr. ir. Dick den Hertog, Tilburg University
Tag der Einreichung:	17. November 2008
Tag der mündlichen Prüfung:	19. Dezember 2008

Darmstädter Dissertation

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Abstract

Optimization problems arise in many disciplines when trying to guarantee the best possible utilization of restricted resources and optimization denotes the determination of the best possible solution for defined problems.
Optimization problems based on black boxes as they often arise in engineering applications are the focus of this thesis. Such black boxes typically represent the simulated or experimentally obtained behavior of systems for which almost no internal, structural or analytical knowledge can be provided on a relevant level for the optimization's objective. Furthermore, the black boxes may produce noise which results in a disturbed response with low accuracy by only a small number of digits. Typically, no appropriate alternatives to these black boxes exist which would have a competitive accuracy and the ability to be coupled closely with special adapted optimization methods. Thus, the direct incorporation of the black box responses into the optimization problem formulation is required.
The price to overcome this lack of profound knowledge are the computational or experimental costs for evaluations of the black box to aggregate information from its response. A fitting expression for this situation is that: *There's no such thing as a free lunch!*
The optimization variables are defined on continuous and integer-valued domains and describe system internal parameters or even possible system topologies. The variables are explicitly included in the optimization problem's objective and constraints. They also affect the problem implicitly because changes in the optimization variables result in different black box responses.
Such non-relaxable mixed-integer nonlinear black box-based optimization problems cannot be carried out efficiently by today's optimization methods. Thus, there is a need for general and robust optimization methods to solve these optimization problems.
In this thesis, a new derivative free optimization approach is presented and surrogate functions will provide the main basics. The performance of this method will be demonstrated for several benchmark and real world problems from electrical engineering, environmental sciences, and robotics. It will be shown that huge improvements of the optimization's objectives can be achieved for all applications, simply by applying a reasonable number of black box evaluations.

Zusammenfassung

Optimierungsprobleme spielen in vielen wissenschaftlichen Disziplinen eine immer wichtigere Rolle, z.B. zur optimalen Nutzung begrenzter Ressourcen oder zur Auswahl optimaler Lösungen aus einer großen, endlichen oder unendlichen Menge von Alternativen. Die existierenden Methoden und Werkzeuge für die rechnergestützte Optimierung werden zur Lösung der unterschiedlichsten Probleme angewandt. Optimierung soll problemspezifisch die bezüglich eines definierten Gütekriteriums bestmögliche Ausnutzung vorhandener Ressourcen garantieren. In den Ingenieurwissenschaften ergibt sich allerdings häufig die Situation, dass die Standardoptimierungsverfahren nicht geeignet sind, um die sich ergebenden Problemstellungen effizient zu lösen. Im Rahmen dieser Arbeit werden speziell Fragestellungen betrachtet, in die neben einer expliziten analytischen Formulierung auch das Verhalten von nicht einsehbaren abgeschlossenen Systemen („Black Box") wie komplexen ingenieurwissenschaftlichen Simulationsprogrammen oder reale Roboter (z.B. Roboter) eingeht.
Häufig sind Ergebnisse komplexer numerischer Simulationen bei der Optimierung zu berücksichtigen, welche zusätzlich meist hohe Rechenzeiten einfordern. Komplexe Simulationssoftware ist in den Ingenieurwissenschaften über Jahre und Jahrzehnte entstanden und ermöglicht nun in vielen Anwendungen eine realitätsnahe Simulation. Es ist daher wünschenswert, diese auch für eine systematische, iterative Optimierung von Systemparametern und Systemverhalten einzusetzen. Ein entscheidender Faktor für den praktische Einsatz ist die Anzahl verfügbarer Auswertungen aufgrund nur beschränkt verfügbarer Ressourcen an Entwicklungs- und Rechenzeit.
Die innerhalb von komplexer numerischer Simulationssoftware verwendeten Methoden, unterlagerte und miteinander gekoppelte iterative Berechnungsverfahren, Approximationen tabellarischer Daten, führen zu Optimierungsproblemstellungen, die häufig vordergründig deterministisch sind, jedoch gewissen Störungen und sehr niedrigen Differenzierbarkeitsordnungen (z.B. Unstetigkeiten in Funktion oder Ableitungen) bezüglich der Optimierungsvariablen unterliegen. Neben den reinen Ausgabewerten der Simulationssoftware stehen meist keine weiteren Systeminformationen zur Verfügung, und können auch mit größerem Aufwand nicht explizit generiert werden. Insbesondere können gradienten- oder modellbasierte Optimierungsverfahren nicht oder nur mit sehr begrenzten Erfolg eingesetzt werden. Weiterhin muss angenommen werden, dass die Optimierungsvariablen sowohl kontinuierlich als auch rein diskret sein können. Für die entstehenden gemischt ganzzahligen, Black Box basierten, nichtlinearen Optimierungsprobleme existieren noch sehr wenige allgemein anwendbare und effiziente Optimierungsverfahren. Auf diese Problemklasse zielt die vorliegende Arbeit ab.
Zunächst ist die Einführung einer neuen Problemformulierung nötig, die zwischen explizit analytischen und implizit nur durch Black Box Auswertungen gegebenen Problemkomponenten unterscheidet. Dies ermöglicht die Anwendung eines neuen, auf Ersatzfunktionen basierenden Optimierungsverfahrens. Etwaige explizit gegebene Teile der Optimierungsproblemformulierung bleiben damit komplett erhalten und können durch

dieses Optimierungsverfahrens vorteilhaft ausgenützt werden. Die impliziten, Black Box basierten Komponenten werden durch geeignete stochastische Approximationsfunktionen ersetzt, und führen so zu einem Ersatzproblem für dessen Auswertung im Rahmen des Optimierungsverfahrens die impliziten Komponenten nicht mehr nötig sind. Durch geeignete Wahl der Ersatzfunktionen ergibt sich ein glattes (d.h. mehrfach differenzierbares), relaxierbares, sowie numerisch hoch effizient auswertbares Optimierungsproblem.
Zur Berechnung von Lösungskandidaten für das Originalproblem werden effiziente gradientenbasierte Verfahren der gemischt ganzzahligen nichtlinearen Optimierung auf den Ersatzproblemen angewendet. Mit Hilfe von Fehlerschätzern der Approximationsfunktionen wird gewährleistet, dass der Raum der zulässigen Optimierungsvariablen dabei weiträumig exploriert wird. Die eigentliche Qualität der Kandidaten wird anhand der Gütefunktion des Originalproblems durch Auswertung der Black Box Komponenten bestimmt. Die Ergebnisse jeder dieser Auswertungen fügen weitere Approximationsinformationen für die Ersatzfunktionen hinzu. Eingebunden in einen iterativen Prozess werden so immer neue Kandidaten zur Auswertung auf schrittweise verfeinerten Ersatzproblemen bestimmt. Das entwickelte Verfahren reduziert die zur Optimierung benötigte Anzahl von Black Box Auswertungen erheblich, so dass im Rahmen dieser Arbeit erstmals eine effizient rechnergestützte Optimierung für eine Reihe schwieriger gemischt ganzzahlige Black Box basierte Anwendungsprobleme möglich wird.
Für die Designoptimierung von Magnetlagern und supraleitenden Synchrotronmagneten können die theoretisch erreichbaren Zielkriterien in nur einem Bruchteil des Aufwands, verglichen mit früheren verwendeten Ansätzen, erfüllt werden. Die bisherige Lösung ohne Berücksichtung und damit ohne Anpassung der ganzzahligen Variablen erforderte bei der Optimierung des Synchrotronmagneten vergleichbar viele numerische Simulationen wie die Lösung des Gesamtproblems mit dem in dieser Arbeit hergeleiteten Optimierungsverfahren.
Für eine aktuelle Sammlung von Benchmarkproblemen aus dem Bereich des Grundwassermanagements, die auf komplexen Strömungsdynamiksimulationen beruhen, können neue kostenminimale Systemauslegungen berechnet werden. Dabei ist eine erhebliche Reduktion der benötigten Simulationsauswertungen und damit der benötigten Rechenzeit verglichen mit publizierten Lösungen zu verzeichnen.
Mit dem Ziel die Laufgeschwindigkeit eines humanoider Roboterprototyps zu maximieren, werden Messungen am realen technischen System direkt mit dem entwickelten Optimierungsverfahren gekoppelt. Auch bei dieser Anwendung stellt sich eine erhebliche Verbesserung der Laufstabilität und eine Geschwindigkeitssteigerung von zu Beginn unter 10 cm/s auf über 40 cm/s am Ende der Optimierung ein.
Die direkte Kopplung des hergeleiteten Optimierungsansatzes mit Black Box basierten Problemen ermöglicht es nun auch Problemstellungen erfolgreich zu behandeln, die bisher entweder nur mit sehr viel höheren Rechenaufwand, oder gar nicht lösbar waren. Auf diese Weise kann das in die Entwicklung der Black Box Komponenten über Jahre und Jahrzehnte eingeflossene Expertenwissen für eine systematische Optimierung von Systemparametern und Systemverhalten nutzbar gemacht werden.

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