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Principles of Optimal Design

Modeling and Computation, third edition

Design optimization is a standard concept in engineering design, and in other disciplines which utilize mathematical decision-making methods. This textbook focuses on the close relationship between a design problem's mathematical model and the solution-driven methods which optimize it. Along with extensive material on modeling problems, this book also features useful techniques for checking whether a model is suitable for computational treatment. Throughout, key concepts are discussed in the context of why and when a particular algorithm may be successful, and a large number of examples demonstrate the theory or method right after it is presented. This book also contains step-by-step instructions for executing a design optimization project – from building the problem statement to interpreting the computer results. All chapters contain exercises from which instructors can easily build quizzes, and a chapter on "principles and practice" offers the reader tips and guidance based on the authors' vast research and instruction experience.

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Douglass J. Wilde is Professor Emeritus of Mechanical Engineering at Stanford University. He conducted research in optimization, computational geometry, and control theory. On retirement he began exploring student team building in design contests. In addition to previous editions of *Principles of Optimal Design*, he has written two books, *Teamology* (2009) and *Jung's Personality Theory Quantified* (2011).

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Principles of Optimal Design

Modeling and Computation

THIRD EDITION

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To our families

And thus both here and in that journey of a thousand years,
whereof I have told you, we shall fare well.

Plato (*The Republic*, *Book X*)

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Preface to the Third Edition

It is almost three decades since this book was first written. Much has changed since then. Perhaps the change most relevant to our readers is the central role that design has taken in society's interests, and in education and research, but also in how it impacts our lives. Design of products and systems is recognized as an important element of a vibrant economy and an innovative society. More importantly, there is increased awareness that the many big problems we face today, such as environmental sustainability, can be addressed through thoughtful design and up-front assessment of the trade-offs involved, rather than as remedial efforts made after the fact.

Understanding and quantifying such trade-offs to support our collective decision making means that design optimization is now more important than ever. Optimal design is the goal not only of engineering, but also of every other social effort to shape our world. Many of our problems usually grow from our inability to agree on what is "optimal."

The book was born out of our own desire to address explicitly what we mean by "optimal" and to put the concept of optimal design on a firm, rigorous foundation. There is an intimate relationship between the mathematical model that describes a design and the solution methods that optimize it. A basic premise from the start was that a good model can make optimization almost trivial, whereas a bad one can make correct optimization difficult or impossible. Software tools today provide capabilities for intricate analysis of many difficult performance aspects of a system. These analysis models, often referred to also as simulations, can be coupled with numerical optimization software to generate better designs iteratively. This virtual prototyping ability has grown dramatically and is an important contributor to reducing product development time and increasing robustness of systems.

The success of such attempts depends strongly on how well the design problem has been formulated for an optimization study, and on how familiar the designer is with the workings and pitfalls of mathematical optimization techniques. As our computing capability increases, so does the complexity of our design problems. Hence, the basic premise of this book remains a modern one: there is need for a more than

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casual understanding of the interactions between modeling and solution strategies in optimal design.

The book grew out of graduate engineering design courses developed and taught at Michigan and Stanford for more than four decades. Definitions of new concepts and rigorous proofs of principles are followed by immediate application to simple examples. In our courses a term design project has been an integral part of the experience, and so the book attempts to support that goal, namely to offer an integrated procedure of design optimization where global analysis and local iterative methods complement each other in a natural way.

In this third edition, the chapters on model analysis, particularly with respect to boundedness and monotonicity, have been consolidated into a new Chapter 3. The discussion on metamodels using neural nets and kriging has been updated. A completely new chapter on nongradient methods has been added, recognizing that these methods are now mature and part of our toolkit. A new chapter on systems design optimization has also been added to address the reality that most design problems today must be viewed as system problems. The final chapter on optimization practice has been expanded to include a short discussion on global optimization and when it may be worthwhile investing in this most elusive optimization goal.

The book contains much more material than would be necessary for three lecture hours a week for one semester. Any course that requires an optimal design project should include Chapters 1, 2, and 9. Placing emphasis on problem formulation should include Chapter 3. A strong theme on gradient-based solution methods would include material from Chapters 4, 5, and 6. A selection from the nongradient approaches in Chapter 7 would round out the basic ideas for all algorithms in use today. Chapter 8 on systems optimization would be the basis for a course that emphasizes what has become known as multidisciplinary design optimization strategies. Linear programming for problems with purely linear functions is included in Chapter 5 on boundary optima, as a special case of boundary-tracking, active set strategy algorithms, thus avoiding the overhead of the specialized terminology traditionally associated with the subject. Problems with discrete variables first encountered in Chapter 3 can be addressed with the methods described in Chapter 7.

An effort has been expended to maintain consistency in terminology and symbols whilst bringing together concepts from a diversity of narrower disciplines and topics. We try to avoid using the same symbol with different meanings. The list of notation at the beginning of the book should help in this respect. For design examples and applications, we have maintained the symbols used locally for the particular problem and have not included them in the notation.

Some instructors may wish to have their students code basic optimization algorithms. This is a very useful experience for students who are well versed in coding. We have occasionally required such coding as homework, but in a tight teaching term we have typically chosen to let students use existing optimization codes and concentrate on the mathematical model, while studying the theory behind the algorithms. Such decisions depend often on the availability and content of other optimization courses

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at a given institution, which may augment the course offered using this book as a text. Increased student familiarity with high-level, general purpose, computational tools and symbolic mathematics will continue to affect instructional strategies.

Specialized design optimization topics, such as structural optimization and optimal control, are beyond the scope of this book. However, the ideas developed here are useful in understanding the specialized approaches needed for the solution of these problems. We have made notes throughout the text pointing to such directions.

The book was also designed with self study in mind. A design engineer would require a brush up of introductory calculus and linear algebra before making good use of this book. Then, starting with the first two chapters and the checklist in Chapter 9, one can model a problem and proceed toward numerical solution using commercial optimization software. After getting (or *not* getting) some initial results, one can go to Chapter 9 and start reading about what may go wrong. Understanding the material in Chapter 9 would require selective backtracking to the main chapters on modeling (Chapter 3), the foundations of gradient-based algorithms (Chapters 4, 5, and 6), and the concepts behind nongradient algorithms (Chapter 7). In a way, the book aims to give a stronger sense of control to the design engineers that use optimization tools.

The book's engineering flavor should not discourage its study by operations analysts, business analysts, economists, and other optimization practitioners. Monotonicity and boundedness analysis in particular may be applied to all optimization problems, not just to the design examples developed here for engineers. We offer our approach to design as a paradigm for studying and solving *any* decision problem.

Many colleagues and students have reviewed or studied parts of the manuscript and offered valuable comments. We are particularly grateful to all of the students at Michigan and other institutions who found various errors in the first two editions and also pointed to desired improvements in the manuscript. For this third edition, we especially acknowledge Alparslan Emrah Bayrak, Alex Burnap, Namwoo Kang, and Max Yi Ren, who provided extensive help in editing the new parts of the book and using them for teaching the design optimization course at Michigan. Comments and feedback by James Allison, Harrison Kim, Michael Kokkolaras, Jeremy Michalek, and Steven Hoffenson were most valuable in improving clarity and catching errors.

The material on neural nets and kriging was based on guest lectures prepared for the Michigan course by Sigurd Nelson and updated by Max Yi Ren and Alex Burnap. The material on trust regions was also a contribution by Sigurd Nelson based on his dissertation. Chapter 3 was carefully edited by Alparslan Emrah Bayrak. The new Chapter 7 uses materials from the masters theses of Ryan Fellini and John Whitefoot, further expanded by Alex Burnap and Max Yi Ren during their teaching of the Michigan course. The new Chapter 8 uses materials from the dissertations of James Allison, Hossam Fathy, Namwoo Kang, Ramprasad Krishnamachari, Harrison Kim, Diane Peters, and Terry Wagner. Allison's design examples in that chapter were originally developed for his dissertation. Special thanks go to Michael Kokkolaras for sustained advice on how to improve the textbook from his own experiences teaching the design optimization course both at Michigan and at McGill.

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The third edition is largely due to the insistence and patience of the editor, Peter Gordon (now retired), who never lost faith in the value of another edition. Starting with David Tranah, who recruited me (PYP) for the first edition, Cambridge University Press has been a faithful and pleasant partner. Finishing this third edition has once again required the indulgence of my family, for which I am always grateful. I remain particularly grateful to my co-author and long-time mentor Douglass Wilde for encouraging me into this venture while he continues to study how design teams work most effectively. Doug taught me to think in optimization terms about almost everything, a practice I have followed ever since.

P.Y.P.
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Notation

Integrating different approaches with different traditions brings typical notation difficulties. While one wishes for a uniform and consistent notation throughout, tradition and practice force us to use the same symbol with different meanings, or different symbols with the same meanings, depending on the subject treated. This is particularly important in an introductory book that encourages excursions to other specialized texts. In this book we have tried to use the notation that most commonly appears for the subject matter in each chapter – particularly for those chapters that lead to further study from other texts. Recognizing this additional burden on comprehension, we list symbols that are typically used in more than one section. The meanings given are those most commonly used in the text, but are not exclusive. The engineering examples throughout may employ many of these symbols in the specialized way of the particular discipline of the example. These symbols are not included in the list; they are given in the section containing the relevant examples. All symbols are defined the first time they occur.

A general notation practice used in this text for mathematical theory and examples is as follows. Lowercase bold letters indicate vectors; uppercase bold letters (usually Latin) indicate matrices; and uppercase script letters represent sets. Lowercase italic letters from the beginning of the alphabet (e.g., a, b, c) are often used for parameters, whereas those from the end of the alphabet (e.g., u, v, x, y, z) frequently indicate variables. Lowercase italic letters from the middle of the alphabet (e.g., i, j, k, l, m, n, p, q) are typically used as indices, subscripts, or superscripts. Lowercase Greek letters from the beginning of the alphabet (e.g., α, β, γ) are often used as exponents. In engineering examples, when convenient, uppercase italic (but not bold) letters represent parameters, and lowercase letters stand for design variables.

Symbols

$\mathbf{A}$	coefficient matrix of linear constraints
$\mathcal{A}$	working set (in active set strategies)

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a_i	ith analysis function
$\mathbf{b}$	right-hand-side coefficient vector of linear constraints
$\mathbf{B}$	(1) quasi-Newton approximation to the inverse of the Hessian; (2) "bordered" Hessian of the Lagrangian
$B(x)$	barrier function (in penalty transformations)
$\mathbf{c}$	vector of consistency constraints
$\mathbf{c}^k$	vector of consistency constraints at kth iteration
C_g	number of linking inequality constraints
C_h	number of linking equality constraints
$\mathbf{d}$	decision variables
$\mathbf{D}$	(1) diagonal matrix; (2) inverse of coefficient matrix $\mathbf{A}$ (in linear programming)
$\mathcal{D}_i$	feasible domain of all inequality constraints except the ith
$\mathcal{D}_s$	set of indices of analysis functions that depend on shared variable
$\det(\mathbf{A})$	determinant of $\mathbf{A}$
$\mathbf{e}$	(1) unit vector; (2) error vector
$\mathbb{E}$	expected value of
$f(\mathbf{x})$	objective function to be minimized with respect to (wrt) $\mathbf{x}$
$f_a(\mathbf{x})$	artifact design objective function to be minimized
$f_c(\mathbf{x})$	controller design objective function to be minimized
$f(x^+)$	function increasing wrt x
$f(x^-)$	function decreasing wrt x
$f^n(x)$	nth derivative of $f(x)$
$\partial f/\partial x_i$	first partial derivative of $f(\mathbf{x})$ wrt x_i
$\partial^2 f/\partial \mathbf{x}^2$, $f_{\mathbf{xx}}$, $\nabla^2 f$	Hessian matrix of $f(\mathbf{x})$; its element $\partial^2 f/\partial x_i \partial x_j$ is the ith row and jth column (other symbol: $\mathbf{H}$)
$\partial f/\partial \mathbf{x}$, $f_{\mathbf{x}}$, ∇f	gradient vector of $f(x)$ – a row vector (other symbol: $\mathbf{g}^T$)
$\partial \mathbf{f}/\partial \mathbf{x}$, $\nabla \mathbf{f}$	Jacobian matrix of $\mathbf{f}$ wrt $\mathbf{x}$; it is $m \times m$ if $\mathbf{f}$ is an m-vector and $\mathbf{x}$ is an n-vector (other symbol: $\mathbf{J}$)
$\mathcal{F}$	feasible set (other symbol: $\mathcal{X}$)
g_j, $g_j(\mathbf{x})$	jth inequality constraint function usually written in negative null form
$\mathbf{g}(\mathbf{x})$	(1) vector of inequality constraint functions; (2) the transpose of the gradient of the objective function: $\mathbf{g} = \nabla f^T$, a column vector
$\mathbf{g}_a(\mathbf{x})$	vector of inequality constraint functions for artifact design
$\mathbf{g}_c(\mathbf{x})$	vector of inequality constraint functions for controller design
g	greatest lower bound of $f(x)$
$\partial \mathbf{g}/\partial \mathbf{x}$, $\nabla \mathbf{g}$	Jacobian matrix of inequality constraints $\mathbf{g}(\mathbf{x})$
$\partial^2 \mathbf{g}/\partial \mathbf{x}^2$	column vector of Hessians of $\mathbf{g}(\mathbf{x})$; *see* $\partial^2 \mathbf{y}/\partial \mathbf{x}^2$
h	step size in finite differencing

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h_j, $h_j(\mathbf{x})$	jth equality constraint function
$\mathbf{h}(\mathbf{x})$	vector of equality constraint functions
$\mathbf{h}_a(\mathbf{x})$	vector of equality constraint functions for artifact design
$\mathbf{h}_c(\mathbf{x})$	vector of equality constraint functions for controller design
$\partial\mathbf{h}/\partial\mathbf{x}$, $\nabla\mathbf{h}$	Jacobian of equality constraints $\mathbf{h}(\mathbf{x})$
$\partial^2\mathbf{h}/\partial\mathbf{x}^2$, $\mathbf{h}_{\mathbf{xx}}$	column vector of Hessians of $\mathbf{h}(\mathbf{x})$; see $\partial^2\mathbf{y}/\partial\mathbf{x}^2$
$\mathbf{H}$	Hessian matrix of the objective function f
$\mathbf{h}_{aux}$	auxiliary constraints
$\mathbf{I}$	identity matrix
$\mathbf{J}$	Jacobian matrix
k	(subscript only) denotes values at kth iteration
$\mathcal{K}_i$	constraint set defined by ith constraint
l	lower bound of $f(x)$
$l(x)$	lower bounding function
L	Lagrangian function
$L_{\mathbf{xx}}$	Hessian of the Lagrangian wrt $\mathbf{x}$
$\mathbf{L}$	lower triangular matrix
$\mathbf{LDL}^T$	Cholesky factorization of a matrix
$\mathcal{L}_i$	index set of conditionally critical constraints bounding x_i from below
$\mathbf{M}$, $\mathbf{M}_k$	a "metric" matrix, i.e., a symmetric positive-definite replacement of the Hessian in local iterations
μ_k	parameter in modification of $\mathbf{H}_k$ in $\mathbf{M}_k$
n	number of design variables
$N(0, \sigma^2)$	normal distribution with standard deviation σ
$\mathcal{N}(x)$	normal subspace (hyperplane) of constraint surface defined by equalities and/or inequalities
$\mathcal{N}$	set of nonnegative real numbers including infinity
$o(x)$	order higher than x; it implies terms negligible compared to x
$\mathbf{P}$	projection matrix
P_i	ith subproblem
P_{ij}	jth subproblem at the ith level
$P(x)$	penalty function (in penalty transformation)
$\mathcal{P}$	set of positive finite real numbers
$q(\mathbf{x})$	quadratic function of $\mathbf{x}$
r, $\mathbf{r}$	(1) controlling parameters in penalty transformations; (2) lower bound on the condition number
r_i	response quantity computed by ith analysis function
$\mathbf{r}_{ji}$	responses from subproblem P_i to subproblem P_j
R	(1) rank of Jacobian of tight constraints in a case; (2) condition number of a matrix
$\mathcal{R}_j$	set of neighbors for which subproblem j computes responses

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$\Re^n$	n-dimensional Euclidean (real) space
$\mathbf{s}$	(1) state or solution variables; (2) search direction vectors (s_k at kth iteration)
$\mathbf{S}$	Boolean matrix selecting components of analysis functions that correspond to coupling variables
$\mathbf{t}_{ij}$	targets from subproblem P_j to subproblem P_i
$\mathcal{T}(\mathbf{x})$	tangent subspace (hyperplane) of the constraint surface defined by equalities and/or inequalities
$\mathcal{T}_j$	set of neighbors for which subproblem j sets targets
$T(\mathbf{x}, \mathbf{r})$	penalty transformation
$T(\mathbf{x}, \lambda, \mathbf{r})$	augmented Lagrangian function (a penalty transformation)
$\mathbf{v}$	penalty weights for linear terms of augmented Lagrangian penalty function
$\mathbf{w}$	penalty weights for quadratic terms of augmented Lagrangian penalty function
$\mathcal{U}_i$	index set of conditionally critical constraints bounding x_i from above
$x\,(x_i)$	(ith) design variable
x_L	lower bound on x
x_U	upper bound on x
$\mathbf{x}$	vector of design variables, a point in $\mathcal{R}^n$; $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$
$\mathbf{x}_a$	vector of design variables for artifact design
$\mathbf{x}_c$	vector of design variables for controller design
$\mathbf{x}_0, \mathbf{x}_1, \ldots$	vectors corresponding to points 0, 1, . . .; not to be confused with the components $x_0, x_1, \ldots$
$x_i^{(j)}$	ith component of vector $\mathbf{x}_j$; not used very often
$x_{i,k}$	ith component of vector $\mathbf{x}_k$(k is iteration number)
x_{li}	local variable of ith analysis function
x_{si}	shared variable of ith analysis function
∂x_i	ith element of $\partial\mathbf{x}$, equals $x_i - x_i^{(0)}$
$\partial\mathbf{x}$	perturbation vector about point $\mathbf{x_0}$, equals $\mathbf{x} - \mathbf{x_0}$; subscript 0 is dropped for simplicity
$\partial\mathbf{x}_k$	perturbation vector about $\mathbf{x}_k$, equals $\mathbf{x}_{k+1} - \mathbf{x}_k$
$\underline{x}\,(\overline{x})$	argument of the infinum (supremum) of the problem over $\mathcal{P}$
$\underline{x}_i$	argument of the partial minumum (i.e., the minimizer) of the objective wrt x_i
$\mathbf{X}_i$	an $n - 1$ vector made from $\mathbf{x} = (x_1, \ldots, x_n)^T$ with all components fixed except x_i; we write $\mathbf{x} = (x_i; \mathbf{X}_i)$
$\underline{\mathbf{x}}$	minimizer to a relaxed problem
$\mathcal{X}$	a subset of $\mathcal{R}^n$ to which $\mathbf{x}$ belongs; the feasible domain; the set constraint

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$\underline{\mathcal{X}}$	set of $\underline{\mathbf{x}}$
$\mathcal{X}_i$	set of minimizers to a problem with the ith constraint relaxed
$\mathcal{X}_*$	set of all minimizers in a problem
y_{ij}	coupling variable computed by the jth analysis function and required as input to ith analysis function
$\mathbf{y}_p(\mathbf{x})$	solution to the system analysis equations for a given design
$\partial^2\mathbf{y}/\partial\mathbf{x}^2$	a vector of Hessians $\partial^2 y_i/\partial\mathbf{x}^2$, $i = 1, \dots, m$, of a vector function $\mathbf{y} = (y_1, \dots, y_m)^T$; it equals $(\partial^2 y_1/\partial\mathbf{x}^2, \partial^2 y_2/\partial\mathbf{x}^2, \dots, \partial^2 y_m/\partial\mathbf{x}^2)$
$\mathbf{z}_i$	set of linking variables of subproblem i including shared and coupling variables
$z(\mathbf{d})$	reduced objective function, equals f as a function of $\mathbf{d}$ only
$\partial z/\partial\mathbf{d}$	reduced gradient of f
$\partial^2 z/\partial\mathbf{d}^2$	reduced Hessian of f
$(\partial z/\partial\mathbf{h})_*$	sensitivity coefficient wrt equality constraints at the optimum
α, α_k	step length in line search, kth iteration
$\mathbf{\Gamma}_v$	coupling vector
$\mathbf{\Gamma}_m$	coupling matrix
Δ	step length used in coordinate search
δ	a small positive quantity
ε	a small positive quantity – often used in termination criteria
$\boldsymbol{\lambda}$	Lagrange multiplier vector associated with equality constraints
$\lambda_{\min}, \lambda_{\max}$	smallest and largest eigenvalues of the Hessian of f at x_*
$\boldsymbol{\mu}$	Lagrange multiplier vector associated with inequality constraints
ϕ	(approximate) penalty function
φ	line search function, including merit function in sequential quadratic programming
Φ	exact penalty function
ω_i	weights of entity i

Special Symbols

$\leq, \geq$	inequality (active or inactive)
$=$	equality (active or inactive)
$<, >$	inactive inequality
$\leqq, \geqq$	active or critical inequality
$\not\leq, \not\geq$	uncritical inequality constraint
$\equiv$	active equality constraint
$\equiv<, \equiv>$	active directed equality
$\lVert\cdot\rVert$	norm; a Euclidean norm is assumed unless otherwise stated

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∂x	perturbation in the quantity x; a small (differential) change in x
∇f	gradient of f (a row vector)
$\nabla^2 f$	Hessian of f (a symmetric matrix)
$\sum_{i=1}^{n} x_i$	sum over i; $i = 1, 2, \ldots, n$ $(= x_1 + x_2 + \cdots + x_n)$
$\prod_{i=1}^{n} x_i$	product over i; $i = 1, 2, \ldots, n$ $(= x_1 x_2 \ldots x_n)$
$\arg\min f(x)$	the value of x (argument) that minimizes f
$\dagger$	(subscript only) denotes values of quantities at stationary points
$*$	(subscript only) denotes values of quantities at minimizing point(s)
T	(superscript only) transpose of a vector or matrix
$\triangleq$	definition
$\subset, \subseteq$	subset of
$\in$	belongs
$\circ$	Hadamard product, element-by-element vector multiplication
$(\cdot)^U$	upper-level variables
$(\cdot)^L$	lower-level variables

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