Preface

The objective of this monograph is the treatment of a general class of nonlinear variational problems of the form

$$\begin{aligned} &\min_{y\in Y,\, u\in U} \quad f(y,u) \\ &\text{subject to} \;\; e(y,u)=0, \quad g(y,u)\in K, \end{aligned} \tag{0.0.1}$$

where $f: Y\times U \to \mathbb{R}$ denotes the cost functional, and $e: Y\times U \to W$ and $g: Y\times U \to Z$ are functionals used to describe equality and inequality constraints. Here Y, U, W, and Z are Banach spaces and K is a closed convex set in Z. A special choice for K is simple box constraints

$$K = \{z \in Z : \phi \le z \le \psi\}, \tag{0.0.2}$$

where Z is a lattice with ordering $\le$, and ϕ, ψ are elements in Z. Theoretical issues which will be treated include the existence of minimizers, optimality conditions, Lagrange multiplier theory, sufficient optimality considerations, and sensitivity analysis of the solutions to (0.0.1) with respect to perturbations in the problem data. These topics will be covered mainly in the first part of this monograph. The second part focuses on selected computational methods for solving the constrained minimization problem (0.0.1). The final chapter is devoted to the characterization of shape gradients for optimization problems constrained by partial differential equations.

Problems which fit into the framework of (0.0.1) are quite general and arise in application areas that were intensively investigated during the last half century. They include optimal control problems, structural optimization, inverse and parameter estimation problems, contact and friction problems, problems in image reconstruction and mathematical finance, and others. The variable y is often referred to as the state variable and u as the control or design parameter. The relationship between the variables y and u is described by e. It typically represents a differential or a functional equation. If e can be used to express the variable y as a function of u, i.e., $y = \Phi(u)$, then (0.0.1) reduces to

$$\min_{u\in U} J(u) = f(\Phi(u),u) \quad \text{subject to} \quad g(\Phi(u),u)\in K. \tag{0.0.3}$$

This is referred to as the reduced formulation of (0.0.1). In the more general case when y and u are both independent variables linked by the equation constraint $e(y,u)=0$ it will be convenient at times to introduce $x=(y,u)$ in $X = Y\times U$ and to express (0.0.1) as

$$\min_{x\in X} f(x) \quad \text{subject to} \quad e(x)=0, \quad g(x)\in K. \tag{0.0.4}$$

From a computational perspective it can be advantageous to treat y and u as independent variables even though a representation of y in terms of u is available.

As an example consider the inverse problem of determining the diffusion parameter a in

$$-\nabla \cdot (a\, \nabla y) = f \text{ in } \Omega, \quad y|_{\partial\Omega} = 0 \tag{0.0.5}$$

from the measurement y_{obs}, where Ω is a bounded open set in $\mathbb{R}^2$ and $f \in H^{-1}(\Omega)$. A nonlinear least squares approach to this problem can be formulated as (0.0.1) by choosing $y \in Y = H_0^1(\Omega)$, $a \in U = H^1(\Omega) \cap L^\infty(\Omega)$, $W = H^{-1}(\Omega)$, $Z = L^2(\Omega)$ and considering

$$\begin{aligned} &\min \int_\Omega (|y - y_{obs}|^2 + \beta\, |\nabla a|^2)\, dx \\ &\text{subject to (0.0.5) and } \underline{a} \le a \le \bar{a}, \end{aligned} \tag{0.0.6}$$

where $0 < \underline{a} < \bar{a} < \infty$ are lower and upper bounds for the "control" variable a. In this example, given $a \in U$, the state $y \in Y$ can be uniquely determined by solving the elliptic boundary value problem (0.0.5) for y, and we obtain a problem of type (0.0.3).

The general approach that we follow in this monograph for the analytical as well as the numerical treatment of (0.0.1) is based on Lagrange multiplier theory. Let us subsequently suppose that Y, U, and W are Hilbert spaces and discuss the case $Z = U$ and $g(y, u) = u$, i.e., the constraint $u \in K$. We assume that f and e are C^1 and denote by f_y, f_u the Fréchet derivatives of f with respect to y and u, respectively. Let W^* be the dual space of W and let the duality product be denoted by $\langle \cdot, \cdot \rangle_{W^*,W}$. The analogous notation is used for Z and Z^*. We form the Lagrange functional

$$L(y, u, \lambda) = f(y, u) + \langle e(y, u), \lambda \rangle_{W,W^*}, \tag{0.0.7}$$

where $\lambda \in W^*$ is the Lagrange multiplier associated with the equality constraint $e(y, u) = 0$ which, for the present discussion, is supposed to exist. It will be shown that a minimizing pair (y, u) satisfies

$$\begin{aligned} &L_y(y, u) = f_y(y, u) + e_y(y, u)^*\lambda = 0, \\ &\langle f_u(y, u) + e_u(y, u)^*\lambda\, ,\, v - u \rangle_{Z^*,Z} \ge 0 \text{ for all } v \in K, \\ &e(y, u) = 0 \text{ and } u \in K. \end{aligned} \tag{0.0.8}$$

In the case $K = Z$ the second equation of (0.0.8) results in the equality $f_y(y, u) + e_u(y, u) = 0$. In this case a first possibility for solving the system (0.0.8) for the unknowns (y, u, λ) is the use of a direct equation solver of Newton type, for example. Here the Lagrange multiplier λ is treated as an independent variable just like y and u. Alternatively, for (y, u) satisfying $e(y, u) = 0$ and λ satisfying $f_y(y, u) + e_u(y, u)^*\lambda = 0$ the gradient of $J(u)$ of (0.0.4) can be evaluated as

$$J_u = f_u(y, u) + e_u(y, u)^*\lambda. \tag{0.0.9}$$

Thus the combined step of determining $y \in Y$ for given $u \in K$ such that $e(y, u) = 0$ and finding $\lambda \in W^*$ satisfying $f_y(y, u) + e_u(y, u)^*\lambda = 0$ for $(y, u) \in Y \times U$ provides a possibility for evaluating the gradient of J at u. If in addition u has to satisfy a constraint of the form $u \in K$, the projected gradient is obtained by projecting $f_u(y,u) + e_u(y,u)^*\lambda$ onto K, and (projected) gradient-based iterative methods can be employed to solve (0.0.1).

In optimal control of differential equations, the multiplier λ is called the adjoint state and the second equation in (0.0.8) is called the optimality condition. Further the system (0.0.8) coincides with the celebrated Pontryagin maximum principle. The steps in the procedure explained above for obtaining the gradient are referred to as the forward equation step for the state equation (the third equation in (0.0.8)) and the backward equation step for the adjoint equation (the first equation). This terminology is motivated by time-dependent problems, where the third equation is an initial value problem and the first one is a problem with terminal time boundary condition. Lastly, if K is of type (0.0.2), then the second equation of (0.0.8) can be written as the complementarity condition

$$\begin{aligned} &f_u(y,u) + e_u(y,u)^*\lambda + \eta = 0, \\ &\eta = \max(0, \eta + (u-\psi)) + \min(0, \eta + (u-\phi)). \end{aligned} \tag{0.0.10}$$

Due to the nondifferentiability of the max and min operations classical Newton methods are not directly applicable to system (0.0.10). Active set methods provide a very efficient alternative. They turn out to be equivalent to semismooth Newton methods in function spaces. If appropriate structural conditions are met, including that f be quadratic and e affine, then such techniques are globally convergent. Moreover, under more general conditions they exhibit local superlinear convergence. Due to the practical relevance of problems with box constraints, a significant part of this monograph is devoted to the analysis of these methods.

A frequently employed alternative to the multiplier approach is given by the penalty method. To explain the procedure consider the sequence of minimization problems

$$\min_{y\in Y, u\in K} f(y,u) + \frac{c_k}{2}\,|\,e(y,u)|_W^2 \tag{0.0.11}$$

for an increasing sequence of penalty parameter c_k. That is, the equality constraint is eliminated through the quadratic penalty function. This requires to solve the unconstrained minimization problem (0.0.11) over $Y \times K$ for a sequence of $\{c_k\}$ tending to infinity. Under mild assumptions it can be shown that the sequence of minimizers (y_k, u_k) determined by (0.0.11) converges to a minimizer of (0.0.1) as $c_k \to \infty$. Moreover, (y_k, u_k) satisfies

$$\begin{aligned} &f_y(y_k,u_k) + e_y(y_k,u_k)^*(c_k\, e(y_k,u_k)) = 0, \\ &\langle f_u(y_k,u_k) + e_u(y_k,u_k)^*(c_k\, e(y_k,u_k)),\, v - u_k\rangle_{Z^*,Z} \geq 0. \end{aligned} \tag{0.0.12}$$

Comparing (0.0.12) with (0.0.8) it is natural to ask whether $c_k\, e(y_k,u_k)$ tends to a Lagrange multiplier associated to $e(y,u) = 0$ as $c_k \to \infty$. Indeed this can be shown under suitable conditions. Despite disadvantages due to slow convergence and possible ill-conditioning for solving (0.0.12) with large values of c_k, the penalty method is widely accepted in practice. This is due, in part, to the simplicity of the approach and the availability of powerful algorithms for solving (0.0.12) if $K = Z$, when the inequality in (0.0.12) becomes an equality.

A third methodology is given by duality techniques. They are based on the introduction of the dual functional

$$d(\lambda) = \inf_{y\in Y,\, u\in K} L(y,u,\lambda) \tag{0.0.13}$$

and the duality property

$$\sup_{\lambda \in Y} d(\lambda) = \inf_{y \in Y,\, u \in K} f(y,u) \quad \text{subject to } e(y,u) = 0. \tag{0.0.14}$$

The duality method for solving (0.0.1) requires minimizing $L(y, u, \lambda_k)$ over $(y, u) \in Y \times K$ and updating λ by means of

$$\lambda_{k+1} = \lambda_k + \alpha_k \mathcal{J} e(y_k, u_k), \tag{0.0.15}$$

where

$$(y_k, u_k) = \underset{y \in Y,\, u \in K}{\operatorname{argmin}} \; L(y, u, \lambda_k),$$

$\alpha_k > 0$ is an appropriately chosen step size and $\mathcal{J}$ denotes the Riesz mapping from W onto W^*. It can be argued that $e(y_k, u_k)$ is the gradient of $d(\lambda)$ at λ_k and (0.0.15) is in turn a steepest ascent method for the maximization of $d(\lambda)$ under appropriate conditions. Such methods are called primal-dual methods. Despite the fact that the method can be justified only under fairly restrictive convexity assumptions on $L(y, u, \lambda)$ with respect to (y, u), it provides an elegant use of Lagrange multipliers and is a basis for so-called augmented Lagrangian methods.

Augmented Lagrangian methods with $K = Z$ are based on the following problem which is equivalent to (0.0.1):

$$\begin{aligned} &\min_{y \in Y, u \in K} \; f(y,u) + \frac{c}{2} |e(y,u)|_W^2 \\ &\text{subject to} \quad e(y,u) = 0. \end{aligned} \tag{0.0.16}$$

Under rather mild conditions the quadratic term enhances the local convexity of $L(y, u, \lambda)$ in the variables (y, u) for sufficiently large $c > 0$. It helps the convergence of direct solvers based on the necessary optimality conditions (0.0.8). To carry this a step further we introduce the augmented Lagrangian functional

$$L_c(y, u, \lambda) = f(x, u) + \langle e(y,u), \lambda \rangle + \frac{c}{2} |e(y,u)|_W^2. \tag{0.0.17}$$

The first order augmented Lagrangian method is the primal-dual method applied to (0.0.17), i.e.,

$$\begin{aligned} (y_k, u_k) &= \underset{y \in Y,\, u \in K}{\operatorname{argmin}} \; L_c(y, u, \lambda_k), \\ \lambda_{k+1} &= \lambda_k + c\, \mathcal{J}\, e(y_k, u_k). \end{aligned} \tag{0.0.18}$$

Its advantage over the penalty method is attributed to the fact that local convergence of (y_k, u_k) to a minimizer (y, u) of (0.0.1) holds for all sufficiently large and fixed $c > 0$, without requiring that $c \to \infty$. As we noted, $L_c(y, u, \lambda)$ has local convexity properties under well-studied assumptions, and the primal-dual viewpoint is applicable to the multiplier update. The iterates (y_k, u_k, λ_k) converge linearly to the triple (y, u, λ) satisfying the first order necessary optimality conditions, and convergence can improve as $c > 0$ increases. Due to these attractive characteristics and properties, the method of multipliers and its subsequent Newton-like variants have been recognized as a powerful method for minimization problems with equality constraints. They constitute an important part of this book.

In (0.0.16) and (0.0.18) the constraint $u \in K$ remained as explicit constraint and was not augmented. To describe a possibility for augmenting inequalities we return to the general form $g(y,u) \in K$ and consider inequality constraints with finite rank, i.e., $Z = \mathbb{R}^p$ and $K = \{z \in \mathbb{R}^p : z_i \le 0,\ 1 \le i \le p\}$. Then under appropriate conditions the formulation

$$\begin{aligned} &\min_{y\in Y,\ u\in U,\ q\in\mathbb{R}^p} L_c(y,u,\lambda) + (\mu, g(y,u)-q) + \frac{c}{2}\,|g(y,u)-q|^2_{\mathbb{R}^p} \\ &\text{subject to } q \le 0 \end{aligned} \tag{0.0.19}$$

is equivalent to (0.0.1). Here $\mu \in \mathbb{R}^p$ is the Lagrange variable associated with the inequality constraint $g(y,u) \le 0$. Minimizing the functional in (0.0.19) over $q \le 0$ results in the augmented Lagrangian functional

$$L_c(y,u,\lambda,\mu) = L_c(y,u,\lambda) + \frac{1}{2}\,|\max(0, \mu + c\, g(y,u))|^2_{\mathbb{R}^p} - \frac{c}{2}|\mu|^2_{\mathbb{R}^p}, \tag{0.0.20}$$

where equality and finite rank inequality constraints are augmented. The corresponding augmented Lagrangian method is

$$\begin{aligned} (y_k, u_k) &= \operatorname*{argmin}_{y\in Y,\ u\in K}\ L_c(y,u,\lambda_k,\mu_k), \\ \lambda_{k+1} &= \lambda_k + c\,\mathcal{J}\, e(y_k,u_k), \\ \mu_{k+1} &= \max(0, \mu_k + c\, g(y_k,u_k)). \end{aligned} \tag{0.0.21}$$

In the discussion of box-constrained problems we already pointed out the relevance of numerical methods for nonsmooth problems; see (0.0.10). In many applied variational problems, for example in mechanics, fluid flow, or image analysis, nonsmooth cost functionals arise. Consider as a special case the simplified friction problem

$$\min\ f(y) = \int_\Omega \frac{1}{2}\,(|\nabla y|^2 + |y|^2) - \tilde{f}\, y\, dx + g\int_\Gamma |y|\, ds \quad \text{over } y \in H^1(\Omega), \tag{0.0.22}$$

where Ω is a bounded domain with boundary Γ. This is an unconstrained minimization problem with $X = H^1(\Omega)$ and no control variables. Since the functional is not continuously differentiable, the necessary optimality condition $f_y(y) = 0$ is not applicable. However, with the aid of a generalized Lagrange multiplier theory a necessary optimality condition can be written as

$$\begin{aligned} &-\Delta y + y = \tilde{f}, \quad \frac{\partial y}{\partial \nu} = g\,\lambda \quad \text{on } \Gamma, \\ &|\lambda(x)| \le 1 \text{ and } \lambda(x) y(x) = |\,y(x)| \quad \text{a.e. in } \Gamma. \end{aligned} \tag{0.0.23}$$

From a Lagrange multiplier perspective, problems with L^1-type cost functionals as in (0.0.22) and box-constrained problems are dual to each other. So it comes as no surprise that again semismooth Newton methods provide an efficient technique for solving (0.0.22) or (0.0.23). We shall analyze them and provide a theoretical basis for their numerical efficiency.

This monograph also contains the analysis of optimization problems constrained by partial differential equations which are singular in the sense that the state variable cannot be differentiated with respect to the control. This, however, does not preclude that the cost functional is differentiable with respect to the control and that an optimality principle can be derived. In terms of shape optimization problems this means that the cost functional is shape differentiable while the state is not differentiable with respect to the shape.

In summary, Lagrange multiplier theory provides a tool for the analysis of general constrained optimization problems with cost functionals which are not necessarily C^1 and with state equations which are in some sense singular. It also leads to a theoretical basis for developing efficient and powerful iterative methods for solving such problems. The purpose of this monograph is to provide a rather thorough analysis of Lagrange multiplier theory and to show its impact on the development of numerical algorithms for problems which are posed in a function space setting.

Let us give a short description of the book for those readers who do not intend to read it by consecutive chapters. Chapter 1 provides a variety of tools to establish existence of Lagrange multipliers and is called upon in all the following chapters. Here, as in other chapters, we do not attempt to give the most general results, nor do we strive for covering the complete literature. Chapter 2 is devoted to the sensitivity analysis of abstract constrained nonlinear programming problems and it essentially stands for itself. This chapter is of great importance, addressing continuity, Lipschitz continuity, and differentiability of the solutions to optimization and optimal control problems with respect to parameters that appear in the problem formulation. Such results are not only of theoretical but also of practical importance. The sensitivity equations have been a starting point for the development of algorithmic concepts for decades. Nevertheless, readers who are not interested in this topic at first may skip this chapter without missing technical results which might be needed for later chapters.

Chapters 3, 5, and 6 form a unit which is devoted to smooth optimization problems. Chapter 3 covers first order augmented Lagrangian methods for optimization problems with equality and inequality constraints. Here as in the remainder of the book, the inequality constraints that we have in mind typically represent partial differential equations. In fact, during the period in which this monograph was written, the terminology "PDE-constrained optimization" emerged. Inverse problems formulated as regularized least squares problems and optimal control problems for (partial) differential equations are primary examples for the theories that are discussed here. Chapters 5 and 6 are devoted to second order iterative solution methods for equality-constrained problems. Again the equality constraints represent partial differential equations. This naturally gives rise to the following situation: The variables with respect to which the optimization is carried out can be classified into two groups. One group contains the state variables of the differential equations and the other group consists of variables which represent the control or input variables for optimal control problems, or coefficients in parameter estimation problems. If the state variables are considered as functions of the independent controls, inputs, or coefficients, and the cost functional in the optimization problem is only considered as a functional of the latter, then this is referred to as the *reduced* formulation. Applying a second order method to the reduced functional we arrive at the Newton method for optimization problems with partial differential equations as constraints. If both state and control variables are kept as independent variables and the optimality system involving primal and adjoint variables, which are the Lagrange multipliers corresponding to the PDE-constraints, is derived, we arrive at the sequential quadratic programming (SQP) technique: It essentially consists of applying a Newton algorithm to the first order necessary optimality conditions. The Newton method for the reduced formulation and the SQP technique are the focus of Chapter 5. Chapter 6 is devoted to second order augmented Lagrangian techniques which are closely related, as we shall see, to SQP methods. Here the equation constraint is augmented in a penalty term, which has the effect of locally convexifying the optimization problem. Since augmented Lagrangians also involve Lagrange multipliers, there is, however, no necessity to let the penalty parameter tend to infinity and, in fact, we do not suggest doing so.

A second larger unit is formed by Chapters 4, 7, 8, and 9. Nonsmoothness, primal-dual active set strategy, and semismooth Newton methods are the keywords which characterize the contents of these chapters. Chapter 4 is essentially a recapture of concepts from convex analysis in a format that is used in the remaining chapters. A key result is the formulation of differential inclusions which arise in optimality systems by means of nondifferentiable equations which are derived from Yosida–Moreau approximations and which will serve as the basis for the primal-dual active set strategy. Chapter 7 is devoted to the primal-dual active set strategy and its global convergence properties for unilaterally and bilaterally constrained problems. The local analysis of the primal-dual active set strategy is achieved in the framework of semismooth Newton methods in Chapter 8. It contains the notion of Newton derivative and establishes local superlinear convergence of the Newton method for problems which do not satisfy the classical sufficient conditions for local quadratic convergence. Two important classes of applications of semismooth Newton methods are considered in Chapter 9: image restoration and deconvolution problems regularized by the bounded variation (BV) functional and friction and contact problems in elasticity.

Chapter 10 is devoted to a Lagrangian treatment of parabolic variational inequalities in unbounded domains as they arise in the Black–Scholes equation, for example. It contains the use of monotone techniques for analyzing parabolic systems without relying on compactness assumptions in a Gelfand-triple framework. In Chapter 11 we provide a calculus for obtaining the shape derivative of the cost functional in shape optimization problems which bypasses the need for using the shape derivative of the state variables of the partial differential equations. It makes use of the expansion technique that is proposed in Chapters 1 and 5 for weakly singular optimal control problems, and of the assumption that an appropriately defined adjoint equation admits a solution. This provides a versatile technique for evaluating the shape derivative of the cost functional using Lagrange multiplier techniques.

There are many additional topics which would fit under the title of this monograph which, however, we chose not to include. In particular, issues of discretization, convergence, and rate of convergence are not discussed. Here the issue of proper discretization of adjoint equations consistent with the discretization of the primal equation and the consistent time integration of the adjoint equations must be mentioned. We do not enter into the discussion of whether to discretize an infinite-dimensional nonlinear programming problem first and then to decide on an iterative algorithm to solve the finite-dimensional problems, or the other way around, consisting of devising an optimization algorithm for the infinite-dimensional problem which is subsequently discretized. It is desirable to choose a discretization and an iterative optimization strategy in such a manner that these two approaches commute. Discontinuous Galerkin methods are well suited for this purpose; see, e.g., [BeMeVe]. Another important area which is not in the focus of this monograph is the efficient solution of those large scale linear systems which arise in optimization algorithms. We refer the reader to, e.g., [BGHW, BGHKW], and the literature cited there. The solution of large scale time-dependent optimal control problems involving the coupled system of primal and adjoint equations, which need to be solved in opposite directions with respect to time, still offers a significant challenge, despite the advances that were made with multiple shooting, receding horizon, and time-domain decomposition techniques. From the point of view of optimization theory there are several topics as well into which one could expand. These include globalization strategies, like trust region methods, exact penalty methods, quasi-Newton methods, and a more abstract Lagrange multiplier theory than that presented in Chapter 1.

As a final comment we stress that for a full treatment of a variational problem in function spaces, both its infinite-dimensional analysis as well as its proper discretization and the relation between the two are indispensable. Proceeding from an infinite-dimensional problem directly to its disretization without such a treatment, important issues can be missed. For instance discretization without a well-posed analysis may result in the use of inappropriate inner products, which may lead to unnecessary ill-conditioning, which entails unnecessary preconditioning. Inconsiderate discretization may also result in the loss of structural properties, as for instance symmetry properties.