4

Equality Constrained Minimization

We shall now be interested in the development of efficient algorithms for

$$\min_{\mathbf{x}\in\Omega_E} f(\mathbf{x}), \tag{4.1}$$

where $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathsf{A}\mathbf{x} - \mathbf{x}^T\mathbf{b}$, $\mathbf{b}$ is a given column n-vector, A is an $n \times n$ symmetric positive definite matrix, $\Omega_E = \{\mathbf{x} \in \mathbb{R}^n : \mathsf{B}\mathbf{x} = \mathbf{c}\}$, $\mathsf{B} \in \mathbb{R}^{m\times n}$, and $\mathbf{c} \in \mathrm{Im}\mathsf{B}$. We assume that $\mathsf{B} \neq \mathsf{O}$ is not a full column rank matrix, so that $\mathrm{Ker}\mathsf{B} \neq \{\mathbf{o}\}$, but we allow dependent rows of B. Using a simple observation of Sect. 4.6.7, we can extend our results to the solution of problems with A positive definite on $\mathrm{Ker}\mathsf{B}$.

There are several reasons why we consider the constraint matrix B with dependent rows. First, for large problems, it may be expensive to identify the dependent rows, as this can often be done only by an expensive rank revealing decomposition. Second, the removal of the dependent constraints may complicate the precision control of the removed equations when we accept approximate solutions. For example, if we carry out the minimization subject to $x_1 = x_2 = x_3$, but control only that $|x_1 - x_2| \leq \varepsilon$ and $|x_2 - x_3| \leq \varepsilon$, then it can easily happen that $|x_1 - x_3| > \varepsilon$. Finally, the whole concept of the dependence assumes that all computations are carried out in exact arithmetics, so that it is better to avoid such assumption whenever we assume our algorithms to be implemented in computer arithmetics.

Here we are interested in large sparse problems with a well-conditioned A, and in algorithms that can be used also for the solution of equality and inequality constrained problems. Our choice is the class of inexact augmented Lagrangian algorithms which enforce the feasibility condition by the Lagrange multipliers generated in the outer loop, while unconstrained minimization is carried out by the conjugate gradient algorithm in the inner loop. A new feature of our approach is that the algorithm is viewed as a repeated implementation of the penalty method. We combine this approach with an adaptive precision control of the inner loop to get the convergence results which are independent of the representation of Ω_E.

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Overview of Algorithms

If we add the penalization function, which is zero on the feasible domain and which achieves large values outside the feasible region, to the original cost function, we can approximate a solution of the original equality constrained problem by the solution of the unconstrained minimization problem with the modified (penalized) cost function. The resulting *penalty method* presented in Sect. 4.2 is probably the most simple way to reduce the equality constrained problem to the unconstrained one. If the penalized problem is solved by an iterative method, the Hessian of the penalized problem can be preconditioned by a special *preconditioner* of Sect. 4.2.6 which preserves the gap in the spectrum.

A prototype of the method studied in this chapter is the *exact augmented Lagrangian method* and its specialization called the *Uzawa algorithm*. See Algorithm 4.2 for their formal description. These methods reduce the original bound constrained problem to a sequence of the unconstrained, optionally moderately penalized problems that are solved exactly, typically by the direct methods of Sect. 1.5.

The auxiliary problems of the augmented Lagrangian method need not be solved exactly. An extreme case is Algorithm 4.1, known as the *Arrows–Hurwitz algorithm*, which carries out only one gradient iteration with the fixed steplength to approximate the solution of the auxiliary problem.

The *asymptotically exact augmented Lagrangian method*, which is described in Sect. 4.4 as Algorithm 4.3, controls the precision of the solution of the auxiliary unconstrained problems by a forcing sequence decreasing to zero. The forcing sequence should be defined by the user.

The precision of the solution of the auxiliary unconstrained problems can also be controlled by the current feasibility error. To achieve convergence, the *adaptive augmented Lagrangian method* modifies also the regularization parameter by means of the forcing sequence generated in the process of solution. The method is described in Sect. 4.5 as Algorithm 4.4.

The most sophisticated method presented in this chapter is the *semimonotonic augmented Lagrangian method for equality constraints* referred to as SMALE. The algorithm is described in Sect. 4.6 as Algorithm 4.5. Similarly to the adaptive augmented Lagrangian method, SMALE controls the precision of the solution of the auxiliary unconstrained problems by the feasibility error, but the penalty parameter is adapted in order to guarantee a sufficient increase of the augmented Lagrangians. The unique theoretical results concerning SMALE include a small explicit bound on the penalty parameter which guarantees that the number of iterations that are necessary to find an approximate solution can be bounded by a number independent of the constraints. The preconditioning preserving the bound on the rate of convergence of Sect. 4.2.6 can be applied also to SMALE.

4.1 Review of Alternative Methods

Before we embark on the study of inexact augmented Lagrangians, let us briefly review alternative methods for the solution of the equality constrained problem (4.1).

Using Proposition 2.8, it follows that (4.1) is equivalent to the solution of the *saddle point system of linear equations*

$$\begin{bmatrix} \mathsf{A} & \mathsf{B}^T \\ \mathsf{B} & \mathsf{O} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}. \tag{4.2}$$

If B is a full row rank matrix, we can solve (4.2) effectively by the *Gauss elimination* with a suitable pivoting strategy, or by a *symmetric factorization* which takes into account that (4.2) is indefinite. Alternatively, we can also use *MINRES*, a Krylov space method which generates the iterates minimizing the Euclidean norm of the residual in the Krylov space. The performance of MINRES depends on the distribution of the spectrum of the KKT system (4.2) similarly as the performance of the CG method. A recent comprehensive review of the methods for the solution of saddle point systems with many references is in Benzi, Golub, and Liesen [10]; see also Elman, Sylvester, and Wathen [81].

We can also reduce (4.2) to a symmetric positive definite case. If B is a full row rank matrix, and if we are able to evaluate the action of A^{-1} effectively, we can multiply the first block row in (4.2) by $\mathsf{B}\mathsf{A}^{-1}$, subtract the second row from the result, and change the signs to obtain the symmetric positive definite *Schur complement system*

$$\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T\boldsymbol{\lambda} = \mathsf{B}\mathsf{A}^{-1}\mathbf{b} - \mathbf{c}, \tag{4.3}$$

which can be solved by the methods described in Chap. 3. The method is also known as the *range-space method*. Let us point out that if we solve (4.3) by the CG method, then it is not necessary to evaluate $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T$ explicitly. Using the CG method and the left generalized inverse of Sect. 1.4, the method can be extended to A positive semidefinite and B with dependent rows. We shall see that the range-space method is closely related to the Uzawa-type methods that we shall study later in this chapter.

Alternatively, we can use the *null-space* method, provided we have a basis Z of $\mathrm{Ker}\mathsf{B}$ and a feasible $\mathbf{x}_0$,

$$\mathsf{B}\mathbf{x}_0 = \mathbf{c}.$$

Observing that $\Omega_E = \{\mathbf{x}_0 + \mathsf{Z}\mathbf{y} : \ \mathbf{y} \in \mathbb{R}^d\}$, we can substitute into (4.1) to get

$$\min_{\mathbf{x}\in\Omega_E} f(\mathbf{x}) = \min_{\mathbf{y}\in\mathbb{R}^d} f(\mathbf{x}_0 + \mathsf{Z}\mathbf{y}) = \frac{1}{2}\mathbf{y}^T\mathsf{Z}^T\mathsf{A}\mathsf{Z}\mathbf{y} - (\mathbf{b} - \mathsf{A}\mathbf{x}_0)^T\mathsf{Z}\mathbf{y} + \frac{1}{2}\mathbf{x}_0^T\mathsf{A}\mathbf{x}_0,$$

so that we can evaluate $\mathbf{y}$ by solving the gradient equation

$$\mathsf{Z}^T\mathsf{A}\mathsf{Z}\mathbf{y} = \mathsf{Z}^T(\mathbf{b} - \mathsf{A}\mathbf{x}_0).$$

If the resulting system is solved by the CG method, then the method can be directly applied to the problems with A positive semidefinite and B with dependent rows.

Results concerning application of domain decomposition methods can be found in the monograph by Toselli and Widlund [175].

A class of algorithms which is important for our exposition is based on the mixed formulation

$$L_0(\widehat{\mathbf{x}}, \widehat{\boldsymbol{\lambda}}) = \max_{\boldsymbol{\lambda} \in \mathbb{R}^m} \min_{\mathbf{x} \in \mathbb{R}^n} L_0(\mathbf{x}, \boldsymbol{\lambda})$$

for the problems with full row rank B. As an example let us recall the *Arrow–Hurwitz algorithm* 4.1, which exploits the first-order approximation of L_0 given by

$$L_0(\mathbf{x} + \alpha\mathbf{d}, \boldsymbol{\lambda} + r\boldsymbol{\delta}) \approx L_0(\mathbf{x}, \boldsymbol{\lambda}) + \alpha \nabla_{\mathbf{x}} L_0(\mathbf{x}, \boldsymbol{\lambda})\mathbf{d} + r \nabla_{\boldsymbol{\lambda}} L_0(\mathbf{x}, \boldsymbol{\lambda})\boldsymbol{\delta}$$

to improve the approximations of the solution $\widehat{\mathbf{x}}$ by taking small steps in the direction opposite to the gradient

$$\nabla_{\mathbf{x}} L_0(\mathbf{x}, \boldsymbol{\lambda}) = \mathsf{A}\mathbf{x} - \mathbf{b} + \mathsf{B}^T \boldsymbol{\lambda},$$

and to improve the approximations of the Lagrange multipliers $\widehat{\boldsymbol{\lambda}}$ by taking small steps in the direction

$$\nabla_{\boldsymbol{\lambda}} L_0(\mathbf{x}, \boldsymbol{\lambda}) = \mathsf{B}\mathbf{x} - \mathbf{c}.$$

Algorithm 4.1. Arrow–Hurwitz algorithm.

Given a symmetric positive definite matrix $\mathsf{A} \in \mathbb{R}^{n \times n}$, *a matrix* $\mathsf{B} \in \mathbb{R}^{m \times n}$ *with the nonempty kernel,* $\mathbf{b} \in \mathbb{R}^n$, *and* $\mathbf{c} \in \mathrm{Im}\mathsf{B}$.

Step 0. {*Initialization.*}
Choose $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, $\mathbf{x}^{-1} \in \mathbb{R}^n$, $\alpha > 0$, $r > 0$

for *k=0,1,2,...*
Step 1. {*Reducing the value of* L_0 *in* $\mathbf{x}$ *direction.*}
$\mathbf{x}^k = \mathbf{x}^{k-1} - \alpha \nabla_{\mathbf{x}} L_0(\mathbf{x}^{k-1}, \boldsymbol{\lambda}^k) = \mathbf{x}^{k-1} - \alpha(\mathsf{A}\mathbf{x} - \mathbf{b} + \mathsf{B}^T\boldsymbol{\lambda})$

Step 2. {*Increasing the value of* L_0 *in* $\boldsymbol{\lambda}$ *direction.*}
$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + r\nabla_{\boldsymbol{\lambda}} L_0(\mathbf{x}^k, \boldsymbol{\lambda}^k) = \boldsymbol{\lambda}^k + r(\mathsf{B}\mathbf{x}^k - \mathbf{c})$
end for

The Arrow–Hurwitz algorithm is known to converge for sufficiently small steplengths α and r. Even though its convergence is known to be slow, the algorithm has found its applications due to the low cost of the iterations and minimal memory requirements. It can be considered as an extreme case of the inexact Uzawa-type algorithms, the main topic of this chapter.

4.2 Penalty Method

Probably the most simple way to reduce the equality constrained quadratic programming problem (4.1) to the unconstrained one is to enhance the constraints into the objective function by adding a suitable term which penalizes the violation of the constraints. In this section we consider the *quadratic penalty method* which approximates the solution $\widehat{\mathbf{x}}$ of (4.1) by the solution $\widehat{\mathbf{x}}_\varrho$ of

$$\min_{\mathbf{x}\in\mathbb{R}^n} f_\varrho(\mathbf{x}), \quad f_\varrho(\mathbf{x}) = f(\mathbf{x}) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2, \tag{4.4}$$

where $\varrho \geq 0$ is the *penalty parameter* and $\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2$ is the *penalty function*.

Intuitively, if the penalty parameter ϱ is large, then the solution $\widehat{\mathbf{x}}_\varrho$ of (4.4) can hardly be far from the solution of (4.1). Indeed, if ϱ were infinite, then the minimizer of f_ϱ would solve the equality constrained problem (4.1). Thus it is natural to expect that if ϱ is sufficiently large, then the penalty approximation $\widehat{\mathbf{x}}_\varrho$ is a suitable approximation to the solution $\widehat{\mathbf{x}}$ of (4.1). The effect of the penalty term is illustrated in Fig. 4.1. Notice that the penalty approximation is typically near the feasible set, but does not belong to it. That is why our penalty method is also called the *exterior penalty method*.

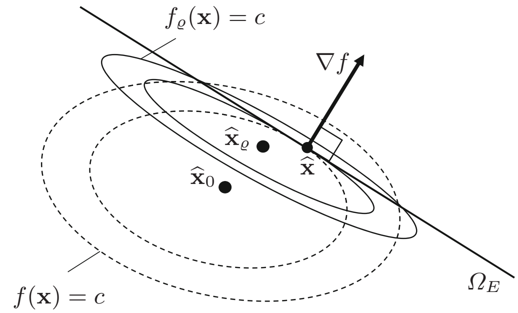

Fig. 4.1. The effect of the quadratic penalty

In the following sections, we shall often use the more general *augmented Lagrangian* penalty function $L : \mathbb{R}^{n+m+1} \to \mathbb{R}$ which is defined by

$$L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) = f(\mathbf{x}) + (\mathsf{B}\mathbf{x} - \mathbf{c})^T\boldsymbol{\lambda} + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 = L_0(\mathbf{x}, \lambda) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2, \tag{4.5}$$

where $\boldsymbol{\lambda} \in \mathbb{R}^m$ is arbitrary and $L_0(\mathbf{x}, \boldsymbol{\lambda}) = L(\mathbf{x}, \boldsymbol{\lambda}, 0)$ is the Lagrangian function (2.20). Notice that $f_\varrho(\mathbf{x}) = L(\mathbf{x}, \mathbf{o}, \varrho)$. Since $\varrho\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2$ and $(\mathsf{B}\mathbf{x} - \mathbf{c})^T\boldsymbol{\lambda}$ vanish when $\mathsf{B}\mathbf{x} = \mathbf{c}$, it follows that

$$f(\mathbf{x}) = f_\varrho(\mathbf{x}) = L(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$$

for any $\mathbf{x} \in \Omega_E$, $\boldsymbol{\lambda} \in \mathbb{R}^m$, and $\varrho \geq 0$.

4.2.1 Minimization of Augmented Lagrangian

Let us start with the modified problem

$$\min_{\mathbf{x}\in\Omega_E} L(\mathbf{x},\boldsymbol{\lambda},\varrho). \tag{4.6}$$

Since the gradient of the augmented Lagrangian is given by

$$\nabla_{\mathbf{x}} L(\mathbf{x},\boldsymbol{\lambda},\varrho) = \mathsf{A}\mathbf{x} - \mathbf{b} + \mathsf{B}^T\big(\boldsymbol{\lambda} + \varrho(\mathsf{B}\mathbf{x}-\mathbf{c})\big), \tag{4.7}$$

it follows that the KKT system for (4.6) reads

$$\begin{bmatrix} \mathsf{A}_\varrho & \mathsf{B}^T \\ \mathsf{B} & \mathsf{O} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{b} + \varrho\mathsf{B}^T\mathbf{c} \\ \mathbf{c} \end{bmatrix}, \tag{4.8}$$

where $\mathsf{A}_\varrho = \mathsf{A} + \varrho\mathsf{B}^T\mathsf{B}$. Eliminating $\mathbf{x}$, we get that any multiplier $\overline{\lambda}$ satisfies

$$\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T\overline{\boldsymbol{\lambda}} = \mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{b} + \varrho\mathsf{B}^T\mathbf{c}) - \mathbf{c}. \tag{4.9}$$

Moreover, if we substitute $\mathsf{B}\mathbf{x} = \mathbf{c}$ into the first block equation, we get that (4.8) is equivalent to the KKT system (2.31), so the saddle points of L_0 are exactly the saddle points of L. This result is not surprising as

$$L(\mathbf{x},\boldsymbol{\lambda},\varrho) = f_\varrho(\mathbf{x}) + (\mathsf{B}\mathbf{x}-\mathbf{c})^T\boldsymbol{\lambda}$$

is the Lagrangian for the penalized equality constrained problem

$$\min_{\mathbf{x}\in\Omega_E} f_\varrho(\mathbf{x}).$$

To see how the penalty method enforces the feasibility, let us assume that $\boldsymbol{\lambda}\in\mathbb{R}^m$ is fixed, and let us denote by $\widehat{\mathbf{x}}_0$ and $\widehat{\mathbf{x}}_\varrho$ the minimizers of $L_0(\mathbf{x},\boldsymbol{\lambda})$ and $L(\mathbf{x},\boldsymbol{\lambda},\varrho)$, respectively. Then the solution $\widehat{\mathbf{x}}$ satisfies

$$L_0(\widehat{\mathbf{x}}_\varrho,\boldsymbol{\lambda}) + \frac{\varrho}{2}\|\mathsf{B}\widehat{\mathbf{x}}_\varrho - \mathbf{c}\|^2 = L(\widehat{\mathbf{x}}_\varrho,\boldsymbol{\lambda},\varrho) \le L(\widehat{\mathbf{x}},\boldsymbol{\lambda},\varrho) = f(\widehat{\mathbf{x}}),$$

so that, using $L_0(\widehat{\mathbf{x}}_0,\boldsymbol{\lambda}) \le L_0(\widehat{\mathbf{x}}_\varrho,\boldsymbol{\lambda})$, we get

$$\|\mathsf{B}\widehat{\mathbf{x}}_\varrho - \mathbf{c}\|^2 \le \frac{2}{\varrho}\big(f(\widehat{\mathbf{x}}) - L_0(\widehat{\mathbf{x}}_\varrho,\boldsymbol{\lambda})\big) \le \frac{2}{\varrho}\big(f(\widehat{\mathbf{x}}) - L_0(\widehat{\mathbf{x}}_0,\boldsymbol{\lambda})\big).$$

It follows that the feasibility error $\|\mathsf{B}\widehat{\mathbf{x}}_\varrho - \mathbf{c}\|$, which corresponds to the second block equation of the KKT system (2.31), can be made arbitrarily small. We shall give stronger or easier computable bounds later in this section.

To see how $\widehat{\mathbf{x}}_\varrho$ satisfies the first block equation of the KKT conditions (4.2), let us recall that the gradient of the augmented Lagrangian is given by (4.7) and denote

$$\widetilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda} + \varrho(\mathsf{B}\widehat{\mathbf{x}}_\varrho - \mathbf{c}). \tag{4.10}$$

Then

$$\mathsf{A}\widehat{\mathbf{x}}_\varrho - \mathbf{b} + \mathsf{B}^T\widetilde{\boldsymbol{\lambda}} = \nabla_{\mathbf{x}} L_0(\widehat{\mathbf{x}}_\varrho, \widetilde{\boldsymbol{\lambda}}) = \nabla_{\mathbf{x}} L(\widehat{\mathbf{x}}_\varrho, \boldsymbol{\lambda}, \varrho) = \mathbf{o},$$

so that $(\widehat{\mathbf{x}}_\varrho, \widetilde{\boldsymbol{\lambda}})$ satisfies the first block equation of the KKT conditions exactly. Moreover, if $\boldsymbol{\lambda}$ is considered as an approximation of a vector of Lagrange multipliers of the solution of (4.1), then our observations indicate that $\widetilde{\boldsymbol{\lambda}}$ is a better approximation. Using Proposition 2.12, we conclude that $(\widehat{\mathbf{x}}_\varrho, \widetilde{\boldsymbol{\lambda}})$ can approximate the KKT pair of (4.1) with arbitrarily small error.

4.2.2 An Optimal Feasibility Error Estimate for Homogeneous Constraints

Let us first examine the feasibility error of an approximate solution $\mathbf{x}$ of the problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} f_\varrho(\mathbf{x}), \quad f_\varrho(\mathbf{x}) = f(\mathbf{x}) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2, \tag{4.11}$$

where f and B are from the definition of problem (4.1) and $\varrho > 0$. We assume that $\mathbf{x}$ satisfies

$$\|\nabla f_\varrho(\mathbf{x})\| \le \varepsilon\|\mathbf{b}\|, \tag{4.12}$$

where $\varepsilon > 0$ is a small number.

Notice that our $\mathbf{x}$ can be considered as an approximation to the solution $\widehat{\mathbf{x}}$ of the equality constrained problem (4.1) in case that the equality constraints are homogeneous, i.e., $\mathbf{c} = \mathbf{o}$. To check that $\mathbf{x}$ satisfies approximately the first part of the KKT conditions (4.2), observe that

$$\nabla f_\varrho(\mathbf{x}) = (\mathsf{A} + \varrho\mathsf{B}^T\mathsf{B})\mathbf{x} - \mathbf{b}.$$

After denoting $\boldsymbol{\lambda} = \varrho\mathsf{B}\mathbf{x}$ and $\mathbf{g} = \nabla f_\varrho(\mathbf{x})$, we get

$$\mathsf{A}\mathbf{x} - \mathbf{b} + \mathsf{B}^T\boldsymbol{\lambda} = \mathbf{g}, \tag{4.13}$$

which can be considered as an approximation of the first block equation of the KKT conditions (4.2).

The feasibility error is considered in the next theorem.

Theorem 4.1. *Let* A, B, *and* $\mathbf{b}$ *be those of the definition of problem (4.1) with* B *not necessarily a full rank matrix, let* $\lambda_{\min} = \lambda_{\min}(\mathsf{A}) > 0$ *denote the smallest eigenvalue of* A, *and let* $\varepsilon \ge 0$ *and* $\varrho > 0$.

If $\mathbf{x}$ *is an approximate solution of (4.11) such that*

$$\|\nabla f_\varrho(\mathbf{x})\| \le \varepsilon\|\mathbf{b}\|,$$

then

$$\|\mathsf{B}\mathbf{x}\| \le \frac{1+\varepsilon}{\sqrt{\lambda_{\min}\varrho}}\|\mathbf{b}\|. \tag{4.14}$$

Proof. Let us denote

$$\mathsf{A}_\varrho = \mathsf{A} + \varrho \mathsf{B}^T\mathsf{B}$$

and notice that for any $\mathbf{x}, \mathbf{d} \in \mathbb{R}^n$

$$f_\varrho(\mathbf{x}+\mathbf{d}) = f_\varrho(\mathbf{x}) + \mathbf{g}^T\mathbf{d} + \frac{1}{2}\mathbf{d}^T\mathsf{A}_\varrho\mathbf{d} \geq f_\varrho(\mathbf{x}) - \|\mathbf{g}\|\|\mathbf{d}\| + \frac{1}{2}\lambda_{\min}\|\mathbf{d}\|^2$$
$$\geq \min_{\xi\in\mathbb{R}}\left(f_\varrho(\mathbf{x}) - \|\mathbf{g}\|\xi + \frac{1}{2}\lambda_{\min}\xi^2\right) \geq f_\varrho(\mathbf{x}) - \frac{1}{2\lambda_{\min}}\|\mathbf{g}\|^2,$$

where $\mathbf{g} = \nabla f_\varrho(\mathbf{x})$. Recalling that by (2.11)

$$\min_{\mathbf{d}\in\mathbb{R}^n} f_\varrho(\mathbf{x}+\mathbf{d}) = \min_{\mathbf{y}\in\mathbb{R}^n} f_\varrho(\mathbf{y}) = -\frac{1}{2}\mathbf{b}^T\mathsf{A}_\varrho^{-1}\mathbf{b},$$

we get

$$0 \geq -\frac{1}{2}\mathbf{b}^T\mathsf{A}_\varrho^{-1}\mathbf{b} \geq f(\mathbf{x}) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2 - \frac{1}{2\lambda_{\min}}\|\mathbf{g}\|^2.$$

Let us now assume that $\mathbf{x}$ satisfies $\|\mathbf{g}\| \leq \varepsilon\|\mathbf{b}\|$. After substituting into the last inequality and using (2.11), (1.24), and the properties of the Euclidean norm, we get

$$0 \geq f(\mathbf{x}) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2 - \frac{1}{2\lambda_{\min}}\|\mathbf{g}\|^2 \geq \min_{\mathbf{y}\in\mathbb{R}^n} f(\mathbf{y}) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2 - \frac{\varepsilon^2}{2\lambda_{\min}}\|\mathbf{b}\|^2$$
$$= -\frac{1}{2}\mathbf{b}^T\mathsf{A}^{-1}\mathbf{b} + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2 - \frac{\varepsilon^2}{2\lambda_{\min}}\|\mathbf{b}\|^2$$
$$\geq -\frac{1}{2\lambda_{\min}}\|\mathbf{b}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2 - \frac{\varepsilon^2}{2\lambda_{\min}}\|\mathbf{b}\|^2 \geq \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2 - \frac{1+\varepsilon^2}{2\lambda_{\min}}\|\mathbf{b}\|^2.$$

Equation (4.14) can be obtained by simple manipulations with application of $1+\varepsilon^2 \leq (1+\varepsilon)^2$. □

An interesting feature of Theorem 4.1 is that *the estimate is independent of the constraint matrix* B. In particular, the estimate (4.14) is valid even if B has dependent rows. The assumption that the constraints are homogeneous was used to get that the unconstrained minimum of f_ϱ is not positive.

Theorem 4.1 implies a simple optimality result concerning the approximation by the penalty method. To formulate it, let $\mathcal{T}$ denote any set of indices and assume that for any $t \in \mathcal{T}$, there is defined a problem

$$\min_{\mathbf{x}\in\Omega_E^t} f_t(\mathbf{x}), \tag{4.15}$$

where $f_t(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathsf{A}_t\mathbf{x} - \mathbf{b}_t^T\mathbf{x}$, $\mathsf{A}_t \in \mathbb{R}^{n_t\times n_t}$ is SPD with the eigenvalues in the interval $[a_{\min}, a_{\max}]$, $0 < a_{\min} < a_{\max}$, $\mathbf{b}_t, \mathbf{x} \in \mathbb{R}^{n_t}$, $\mathsf{B}_t \in \mathbb{R}^{m_t\times n_t}$, and $\Omega_E^t = \{\mathbf{x} \in \mathbb{R}^{n_t} : \mathsf{B}_t\mathbf{x} = \mathbf{o}\}$.

Corollary 4.2. *For each* $\varepsilon > 0$*, there is* $\varrho > 0$ *such that if approximate solutions* $\mathbf{x}_{t,\varrho}$ *of* (4.15) *satisfy*

$$\nabla f_{t,\varrho}(\mathbf{x}_{t,\varrho}) \leq \varepsilon \|\mathbf{b}_t\|, \quad t \in \mathcal{T},$$

then

$$\|\mathsf{B}_t \mathbf{x}_{t,\varrho}\| \leq \varepsilon \|\mathbf{b}_t\|, \quad t \in \mathcal{T}.$$

Proof. Notice that by Theorem 4.1

$$\|\mathsf{B}_t \widehat{\mathbf{x}}_{t,\varrho}\| \leq \frac{1}{\sqrt{a_{\min}\varrho}} \|\mathbf{b}_t\|$$

for any $\varrho > 0$. It is enough to set $\varrho = 1/(a_{\min}\varepsilon^2)$. □

We conclude that the *prescribed bound on the relative feasibility error for all problems (4.15) can be achieved with one value of the penalty parameter* $\varrho_t = \varrho$. Numerical experiments which illustrate the optimal feasibility estimates in the framework of FETI methods can be found in Dostál and Horák [65, 66].

4.2.3 Approximation Error and Convergence

Using the feasibility estimate (4.14) of the previous subsection and an error bound on the violation of the first block equation of the KKT conditions (2.46), we can bound the approximation error of the penalty method for homogeneous constraints.

Theorem 4.3. *Let problem (4.1) be defined by* $\mathsf{A}, \mathsf{B}, \mathbf{b}$*, and* $\mathbf{c} = \mathbf{o}$*, with* $\mathsf{B} \neq \mathsf{O}$ *not necessarily a full rank matrix, let* $(\widehat{\mathbf{x}}, \boldsymbol{\lambda}_{\mathrm{LS}})$ *denote the least square KKT pair for (4.1) with* $\mathbf{c} = \mathbf{o}$*, let* $\lambda_{\min}$ *denote the least eigenvalue of* A*, let* $\overline{\sigma}_{\min}$ *denote the least nonzero singular value of* B*, let* $\varepsilon > 0$*,* $\varrho > 0$*, and let*

$$\boldsymbol{\lambda} = \varrho \mathsf{B} \mathbf{x}. \tag{4.16}$$

If $\mathbf{x}$ *is such that*

$$\|\nabla f_{\varrho}(\mathbf{x})\| \leq \varepsilon \|\mathbf{b}\|,$$

then

$$\|\mathbf{x} - \widehat{\mathbf{x}}\| \leq \varepsilon \frac{\kappa(\mathsf{A}) + 1}{\lambda_{\min}} \|\mathbf{b}\| + \frac{1 + \varepsilon}{\sqrt{\varrho}} \frac{\kappa(\mathsf{A})}{\overline{\sigma}_{\min}\sqrt{\lambda_{\min}}} \|\mathbf{b}\| \tag{4.17}$$

and

$$\|\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}\| \leq \frac{1}{\overline{\sigma}_{\min}} \Big(\varepsilon \kappa(\mathsf{A}) \|\mathbf{b}\| + \frac{1 + \varepsilon}{\sqrt{\varrho}} \frac{\|\mathsf{A}\|}{\overline{\sigma}_{\min}\sqrt{\lambda_{\min}}} \|\mathbf{b}\| \Big). \tag{4.18}$$

Proof. Let us denote $\mathbf{g} = \nabla f_\varrho(\mathbf{x})$ and $\mathbf{e} = \mathsf{B}\mathbf{x}$, so that

$$\mathsf{A}\mathbf{x} + \mathsf{B}^T\boldsymbol{\lambda} = \mathbf{b} + \mathbf{g} \quad \text{and} \quad \mathsf{B}\mathbf{x} = \mathbf{e}, \tag{4.19}$$

and notice that by the assumptions $\boldsymbol{\lambda} \in \mathrm{Im}\mathsf{B}$. Assuming that

$$\|\mathbf{g}\| = \|\nabla f_\varrho(\mathbf{x})\| \le \varepsilon\|\mathbf{b}\|,$$

it follows by Theorem 4.1 that

$$\|\mathsf{B}\mathbf{x}\| \le \frac{1+\varepsilon}{\sqrt{\lambda_{\min}\varrho}}\|\mathbf{b}\|.$$

Substituting into the estimates (2.48) and (2.49) of Proposition 2.12, we get (4.17) and (4.18). □

Notice that the error bounds (4.17) and (4.18) depend on the representation of Ω_E, namely, on the constraint matrix B.

The performance of the penalty method can also be described in terms of convergence. Let $\varepsilon_k > 0$ denote a sequence converging to zero, let $\varrho_k > 0$ denote an increasing unbounded sequence, let $\mathbf{g}^k = \nabla f_{\varrho_k}(\mathbf{x}^k)$, and let $\mathbf{x}^k$ satisfy

$$\|\mathbf{g}^k\| = \|\nabla f_{\varrho_k}(\mathbf{x}^k)\| \le \varepsilon_k\|\mathbf{b}\|.$$

Let us denote

$$\boldsymbol{\lambda}^k = \varrho_k\mathsf{B}\mathbf{x}^k.$$

Then by (4.17) there is a constant C_1 dependent on A and C_2 dependent on A, B such that

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\| \le \varepsilon_k C_1\|\mathbf{b}\| + \frac{1+\varepsilon_k}{\sqrt{\varrho_k}}C_2\|\mathbf{b}\|,$$

and by (4.18) there are constants C_3 and C_4 dependent on A, B such that

$$\|\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}}\| \le \varepsilon_k C_3\|\mathbf{b}\| + \frac{1+\varepsilon_k}{\sqrt{\varrho_k}}C_4\|\mathbf{b}\|. \tag{4.20}$$

It follows that $\boldsymbol{\lambda}^k$ converges to $\boldsymbol{\lambda}_{\mathrm{LS}}$ and $\mathbf{x}^k$ converges to $\widehat{\mathbf{x}}$.

4.2.4 Improved Feasibility Error Estimate

We shall now give a feasibility error estimate for the penalty approximation of (4.1) which is valid for nonhomogeneous constraints with $\mathbf{c} \ne \mathbf{o}$. Our new bound on the error is proportional to ϱ^{-1}, but *dependent on* B and $\mathbf{c}$.

Theorem 4.4. *Let* $\mathsf{A}, \mathsf{B}, \mathbf{b}$, *and* $\mathbf{c}$ *be those of the definition of problem (4.1) with* $\mathsf{B} \ne \mathsf{O}$ *not necessarily a full rank matrix, let* $\overline{\beta}_{\min} > 0$ *denote the smallest nonzero eigenvalue of* $\mathsf{B}^T\mathsf{A}^{-1}\mathsf{B}$, *let* ε *denote a given positive number, and let* $\varrho > 0$.

If $\mathbf{x}$ *is such that*

$$\|\nabla f_\varrho(\mathbf{x})\| \le \varepsilon \|\mathbf{b}\|,$$

then the feasibility error satisfies

$$\|\mathsf{B}\mathbf{x} - \mathbf{c}\| \le \left(1 + \overline{\beta}_{\min}\varrho\right)^{-1} \left((1+\varepsilon)\|\mathsf{B}\mathsf{A}^{-1}\|\|\mathbf{b}\| + \|\mathbf{c}\|\right). \tag{4.21}$$

Proof. Let us recall that for any vector $\mathbf{x}$

$$\nabla f_\varrho(\mathbf{x}) = (\mathsf{A} + \varrho \mathsf{B}^T\mathsf{B})\mathbf{x} - \mathbf{b} - \varrho \mathsf{B}^T\mathbf{c},$$

so that, after denoting $\mathbf{g} = \nabla f_\varrho(\mathbf{x})$ and $\mathsf{A}_\varrho = \mathsf{A} + \varrho \mathsf{B}^T\mathsf{B}$,

$$\mathbf{x} = \mathsf{A}_\varrho^{-1}(\mathbf{g} + \mathbf{b} + \varrho \mathsf{B}^T\mathbf{c}).$$

It follows that

$$\mathsf{B}\mathbf{x} = \mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{g} + \mathbf{b}) + \varrho \mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T\mathbf{c}.$$

Using equation (1.41) of Lemma 1.4 and simple manipulations, we get

$$\begin{aligned}
\mathsf{B}\mathbf{x} - \mathbf{c} &= \mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{g} + \mathbf{b}) + \varrho(\mathsf{I} + \varrho \mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T)^{-1}\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T\mathbf{c} - \mathbf{c} \\
&= \mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{g} + \mathbf{b}) + (\mathsf{I} + \varrho \mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T)^{-1}\left((\mathsf{I} + \varrho \mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T) - \mathsf{I}\right)\mathbf{c} - \mathbf{c} \\
&= \mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{g} + \mathbf{b}) - (\mathsf{I} + \varrho \mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T)^{-1}\mathbf{c}.
\end{aligned}$$

To finish the proof, use the assumptions that $\mathbf{c} \in \mathrm{Im}\mathsf{B}$ and $\|\mathbf{g}\| \le \varepsilon\|\mathbf{b}\|$, Lemma 1.6, and the properties of norms. □

Numerical experiments which illustrate (4.21) can be found in Dostál and Horák [65, 66].

4.2.5 Improved Approximation Error Estimate

Using the improved feasibility estimate (4.21) of the previous section, we can improve the bounds on the approximation error of the penalty method given in Sect. 4.2.3.

Theorem 4.5. *Let* $\mathsf{A}, \mathsf{B}, \mathbf{b}$*, and* $\mathbf{c}$ *be those of the definition of problem (4.1) with* B *not necessarily a full rank matrix, let* $\lambda_{\min}$ *denote the least eigenvalue of* A*, let* $\overline{\sigma}_{\min}$ *denote the least nonzero singular value of* B*, let* $(\widehat{\mathbf{x}}, \boldsymbol{\lambda}_{\mathrm{LS}})$ *denote the least square KKT pair for (4.1), let* $\overline{\beta}_{\min} > 0$ *denote the least nonzero eigenvalue of the matrix* $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T$*, let* $\varepsilon > 0$*,* $\varrho > 0$*, and*

$$\boldsymbol{\lambda} = \varrho(\mathsf{B}\mathbf{x} - \mathbf{c}). \tag{4.22}$$

If $\mathbf{x}$ *is such that*

$$\|\nabla f_\varrho(\mathbf{x})\| \le \varepsilon \|\mathbf{b}\|,$$

then

$$\|\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}\| \le \varepsilon \frac{\kappa(\mathsf{A})\|\mathbf{b}\|}{\overline{\sigma}_{\min}} + \frac{\|\mathsf{A}\| \left((1+\varepsilon)\|\mathsf{BA}^{-1}\|\|\mathbf{b}\| + \|\mathbf{c}\|\right)}{\overline{\sigma}_{\min}^2 (1 + \varrho \overline{\beta}_{\min})} \tag{4.23}$$

and

$$\|\mathbf{x} - \widehat{\mathbf{x}}\| \le \varepsilon \frac{\kappa(\mathsf{A}) + 1}{\lambda_{\min}} \|\mathbf{b}\| + \frac{\kappa(\mathsf{A}) \left((1+\varepsilon)\|\mathsf{BA}^{-1}\|\|\mathbf{b}\| + \|\mathbf{c}\|\right)}{\overline{\sigma}_{\min} (1 + \varrho \overline{\beta}_{\min})}. \tag{4.24}$$

Proof. Let us denote $\mathbf{g} = \nabla f_\varrho(\mathbf{x})$ and $\mathbf{e} = \mathsf{B}\mathbf{x} - \mathbf{c}$, so that

$$\mathsf{A}\mathbf{x} + \mathsf{B}^T \boldsymbol{\lambda} = \mathbf{b} + \mathbf{g} \quad \text{and} \quad \mathsf{B}\mathbf{x} = \mathbf{c} + \mathbf{e}.$$

If

$$\|\mathbf{g}\| = \|\nabla f_\varrho(\mathbf{x})\| \le \varepsilon \|\mathbf{b}\|,$$

then by Theorem 4.4

$$\|\mathsf{B}\mathbf{x} - \mathbf{c}\| \le \frac{1}{1 + \varrho \overline{\beta}_{\min}} \left((1+\varepsilon)\|\mathsf{BA}^{-1}\|\|\mathbf{b}\| + \|\mathbf{c}\|\right).$$

Substituting into the estimates (2.47) and (2.48) of Proposition 2.12, we get

$$\|\mathsf{B}^T(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}})\| \le \varepsilon \kappa(\mathsf{A}) \|\mathbf{b}\| + \frac{\|\mathsf{A}\| \left((1+\varepsilon)\|\mathsf{BA}^{-1}\|\|\mathbf{b}\| + \|\mathbf{c}\|\right)}{\overline{\sigma}_{\min} (1 + \varrho \overline{\beta}_{\min})} \tag{4.25}$$

and (4.24). To finish the proof, notice that $\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}} \in \mathrm{Im}\mathsf{B}$, so that by (1.34)

$$\overline{\sigma}_{\min} \|\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}\| \le \|\mathsf{B}^T(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}})\|,$$

apply the latter estimate to the left-hand side of (4.25), and divide the resulting chain of inequalities by $\overline{\sigma}_{\min}$. □

We can also get the improved rates of convergence compared with those of Sect. 4.2.3. Let $\varepsilon_k \ge 0$ denote again a sequence converging to zero, let $\varrho_k > 0$ denote an increasing unbounded sequence, let $\mathbf{x}^k$ satisfy

$$\|\mathbf{g}^k\| = \|\nabla f_{\varrho_k}(\mathbf{x}^k)\| \le \varepsilon_k \|\mathbf{b}\|,$$

and let us denote

$$\boldsymbol{\lambda}^k = \varrho_k (\mathsf{B}\mathbf{x}^k - \mathbf{c}).$$

Then by (4.23) there are constants C_1, C_2, and C_3 dependent on A, B such that

$$\|\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}}\| \le \varepsilon_k C_1 \|\mathbf{b}\| + \frac{1+\varepsilon_k}{\varrho_k} C_2 \|\mathbf{b}\| + \frac{C_3}{\varrho_k} \|\mathbf{c}\|,$$

and by (4.24) there is a constant C_4 dependent on A and constants C_5, C_6 dependent on A, B such that

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\| \le \varepsilon_k C_4 \|\mathbf{b}\| + \frac{1+\varepsilon_k}{\varrho_k} C_5 \|\mathbf{b}\| + \frac{C_6}{\varrho_k} \|\mathbf{c}\|.$$

Thus $\boldsymbol{\lambda}^k$ converges to $\boldsymbol{\lambda}_{\mathrm{LS}}$ and $\mathbf{x}^k$ converges to $\widehat{\mathbf{x}}$.

4.2.6 Preconditioning Preserving Gap in the Spectrum

We have seen that the penalty method reduces the solution of the equality constrained minimization problem (4.1) to the unconstrained penalized problem (4.4). The resulting problem may be solved either by a suitable direct method such as the Cholesky decomposition, or by an iterative method such as the conjugate gradient method. If the penalty parameter ϱ is large, then the Hessian matrix

$$\mathsf{A}_\varrho = \mathsf{A} + \varrho \mathsf{B}^T \mathsf{B}$$

of the cost function f_ϱ of the penalized problem (4.4) is obviously ill-conditioned. Thus the estimates based on the condition number do not guarantee fast convergence of the conjugate gradient method, and a natural idea is to reduce the condition number of A_ϱ by a suitable preconditioning. This is indeed possible as has been shown, e.g., by Hager [111, 113].

Here we consider an alternative approach which exploits the fast convergence of the conjugate gradient method for the problems with a gap in the spectrum. The method is based on two results: the bounds on the rate of convergence independent of ϱ given by (3.23) and (3.24) and Lemma 1.7 on the distribution of the spectrum of A_ϱ. The method presented here is applicable for large ϱ provided we have an effective preconditioner M for A that can be used by the preconditioned conjugate gradient algorithm of Sect. 3.6. To simplify our exposition, we assume that $\mathsf{M} = \mathsf{L}\mathsf{L}^T$, where L is a sparse lower triangular matrix.

To express briefly the effects of the preconditioning strategies presented in this section, let $k(\mathsf{W}, \varepsilon)$ denote the number of the conjugate gradient iterations that are necessary to reduce the residual of any system with the symmetric positive definite matrix W by ε, and let

$$\overline{k}(\mathsf{W}, \varepsilon) = \mathrm{int}\left(\frac{1}{2}\sqrt{\kappa(\mathsf{W})}\ln(2/\varepsilon) + 1\right) \tag{4.26}$$

denote the upper bound on $k(\mathsf{W}, \varepsilon)$ which may be easily obtained from (3.23).

Let us first assume that the rank m of the constraint matrix $\mathsf{B} \in \mathbb{R}^{p \times n}$ in the original problem (4.1) is small. Then it is possible to use L to redistribute the spectrum of the penalized matrix A_ϱ directly. In this case (1.51) and the estimate (3.23) of the rate of the conjugate gradient method for the case that the Hessian of the cost function has m isolated eigenvalues give the bound

$$k(L^{-1}\mathsf{A}_\varrho \mathsf{L}^{-T}, \varepsilon) \le \overline{k}(\mathsf{L}^{-1}\mathsf{A}\mathsf{L}^{-T}, \varepsilon) + m. \tag{4.27}$$

Such preconditioning can be implemented even without the factorization of the preconditioner $\mathsf{M} = \mathsf{L}\mathsf{L}^T$ as in Algorithm 3.3, provided we can solve efficiently the linear systems with the matrix M.

If m dominates in the expression on the right-hand side of (4.27), then the bound (4.27) can be improved at the cost of increased computational complexity. In particular, this may be useful when we have several problems (4.4) with the same matrix B. Noticing that for any nonsingular matrix Q

$$\Omega_E = \{\mathbf{x} \in \mathbb{R}^n : \ \mathsf{QB}\mathbf{x} = \mathsf{Q}\mathbf{c}\},$$

choosing the matrix Q in such a way that the rows of QBL^{-T} are orthonormal, and denoting $\overline{\mathsf{B}} = \mathsf{QB}$, we can observe that minimizer of the penalized function with the Hessian

$$\overline{\mathsf{A}}_\varrho = \mathsf{A} + \varrho \overline{\mathsf{B}}^T \overline{\mathsf{B}}$$

also approximates the solution of (4.1), but the spectrum $\sigma(\mathsf{L}^{-1}\overline{\mathsf{A}}_\varrho \mathsf{L}^{-T})$ of the preconditioned Hessian $\mathsf{L}^{-1}\overline{\mathsf{A}}_\varrho \mathsf{L}^{-T}$ satisfies by (1.50) and (1.51)

$$\sigma(\mathsf{L}^{-1}\overline{\mathsf{A}}_\varrho \mathsf{L}^{-T}) \subseteq [a_{\min}, a_{\max}] \cup [a_{\min} + \varrho, a_{\max} + \varrho],$$

where $a_{\min} = \lambda_1(\mathsf{L}^{-1}\mathsf{A}\mathsf{L}^{-T})$ and $a_{\max} = \lambda_n(\mathsf{L}^{-1}\mathsf{A}\mathsf{L}^{-T})$. Since the spectrum is located in two intervals of the same length, we can use (3.24) to get the bound

$$k(\mathsf{L}^{-1}\overline{\mathsf{A}}_\varrho \mathsf{L}^{-T}, \varepsilon) \leq \min\{\overline{k}(\mathsf{L}^{-1}\mathsf{A}\mathsf{L}^{-T}, \varepsilon) + m, 2\overline{k}(\mathsf{L}^{-1}\mathsf{A}\mathsf{L}^{-T}, \varepsilon)\}, \tag{4.28}$$

which is optimal with respect to both ϱ and m. Results of some numerical experiments with this strategy can be found in [44].

Observe that $\mathsf{Q}^T\mathsf{Q}$ represents a scalar product on $\mathbb{R}^m$. The method can be efficient also in the case that the rows of QBL^{-T} are orthonormal only approximately [144]. If $\mathsf{A} = \mathsf{LL}^T$ and QBL^{-T} are orthonormal, then $\sigma(\mathsf{L}^{-1}\overline{\mathsf{A}}_\varrho \mathsf{L}^{-T}) = \{1, \varrho\}$ and the CG algorithm finds the solution in just two steps.

4.3 Exact Augmented Lagrangian Method

Because of its simplicity and intuitive appeal, the penalty method is often used in computations. However, a good approximation of the solution may require a very large penalty parameter, which can cause serious problems in computer implementation. The remedy can be based on the observation that having a solution $\mathbf{x}_\varrho$ of the penalized problem (4.4), we can modify the linear term of f in such a way that the unconstrained minimum of the modified cost function $\overline{f}$ *without the penalization term* is achieved again at $\mathbf{x}_\varrho$. Then we can hopefully find a better approximation by adding the penalization term to the modified cost function $\overline{f}$, possibly with the same value of the penalty parameter, and look for the minimizer of $\overline{f}_\varrho$ as in Fig. 4.2. The result is the well-known classical *augmented Lagrangian algorithm*, also named the *method of multipliers*, which was proposed by Hestenes [116] and Powell [160].

In this section, we present as the augmented Lagrangian algorithm a little more general algorithm; its special cases are the classical Uzawa algorithm [1] and the original algorithm by Hestenes and Powell. We review and slightly extend the well-known arguments presented, e.g., in the classical monographs by Bertsekas [11] and Glowinski and Le Tallec [100].

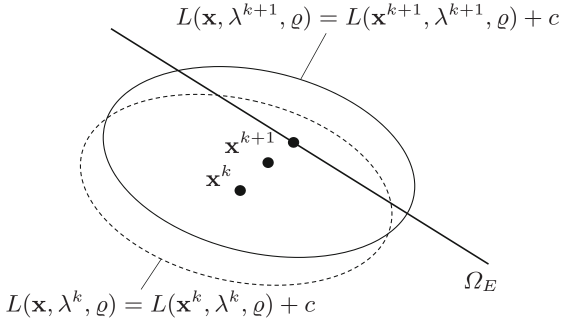

Fig. 4.2. Augmented Lagrangian iteration

4.3.1 Algorithm

The augmented Lagrangian algorithm is based, similarly as the Arrow–Hurwitz algorithm 4.1, on the mixed formulation (2.38) of the equality constrained problem (4.1). However, the augmented Lagrangian algorithm differs from the Arrow–Hurwitz algorithm applied to the penalized problem (4.4) in Step 1, where the former algorithm assigns $\mathbf{x}^k$ the minimizer of $L(\mathbf{x}, \lambda^k, \varrho_k)$ with respect to $\mathbf{x} \in \mathbb{R}^n$. Both algorithms use the same update rule for the Lagrange multipliers in Step 2. Here we present a variant of the augmented Lagrangian algorithm whose special cases are the original *Uzawa algorithm* [1], which corresponds to $\varrho_k = 0,\ k = 0, 1, \ldots$, and the original *method of multipliers*, which corresponds to $r_k = \varrho_k$. Our augmented Lagrangian algorithm reads as follows.

Algorithm 4.2. Exact augmented Lagrangian algorithm.

Given a symmetric positive definite matrix $\mathsf{A} \in \mathbb{R}^{n \times n}$, $\mathsf{B} \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^n$, *and* $\mathbf{c} \in \mathrm{Im}\mathsf{B}$.

Step 0. {*Initialization.*}
Choose $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, $r > 0$, $r_k \geq r$, $\varrho_k \geq 0$
for *k=0,1,2,...*
Step 1. {*Minimization with respect to* $\mathbf{x}$.}
$\mathbf{x}^k = \arg\ \min\{L(\mathbf{x}, \boldsymbol{\lambda}^k, \varrho_k) :\ \mathbf{x} \in \mathbb{R}^n\}$
Step 2. {*Updating the Lagrange multipliers.*}
$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + r_k(\mathsf{B}\mathbf{x}^k - \mathbf{c})$
end for

Since $\mathbf{x}^k$ is the unconstrained minimizer of the Lagrangian L with respect to its first variable, it follows that

$$\nabla_{\mathbf{x}} L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) = (\mathsf{A} + \varrho_k \mathsf{B}^T\mathsf{B})\mathbf{x}^k - \mathbf{b} - \varrho_k \mathsf{B}^T\mathbf{c} + \mathsf{B}^T\boldsymbol{\lambda}^k = \mathbf{o},$$

so that Step 1 of Algorithm 4.2 can be implemented by solving the system

$$(\mathsf{A} + \varrho_k \mathsf{B}^T\mathsf{B})\mathbf{x}^k = \mathbf{b} + \varrho_k \mathsf{B}^T\mathbf{c} - \mathsf{B}^T\boldsymbol{\lambda}^k. \tag{4.29}$$

To understand better the algorithm, we shall examine its alternative formulation which we obtain after eliminating $\mathbf{x}^k$ or $\boldsymbol{\lambda}^k$ from Algorithm 4.2. Thus denoting for any $\varrho \in \mathbb{R}$

$$\mathsf{A}_\varrho = \mathsf{A} + \varrho \mathsf{B}^T\mathsf{B},$$

we can use (4.29) to get

$$\mathbf{x}^k = \mathsf{A}_{\varrho_k}^{-1}(\mathbf{b} + \varrho_k \mathsf{B}^T\mathbf{c} - \mathsf{B}^T\boldsymbol{\lambda}^k).$$

After substituting for $\mathbf{x}^k$ into Step 2 of Algorithm 4.2 and simple manipulations, we can rewrite our augmented Lagrangian algorithm as

$$\text{Choose } \boldsymbol{\lambda}^0 \in \mathbb{R}^{\mathrm{m}}, \tag{4.30}$$
$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k - r_k \left(\mathsf{B}\mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T\boldsymbol{\lambda}^k - \mathsf{B}\mathsf{A}_{\varrho_k}^{-1}(\mathbf{b} + \varrho_k \mathsf{B}^T\mathbf{c}) + \mathbf{c}\right). \tag{4.31}$$

To understand the formula (4.31), notice that

$$f_\varrho(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathsf{A}_\varrho\mathbf{x} - (\mathbf{b} + \varrho \mathsf{B}^T\mathbf{c})^T\mathbf{x} + \frac{\varrho}{2}\|\mathbf{c}\|^2.$$

Using the formula (2.36) for the dual function Θ for problem (4.1), we can check that the explicit expression for the dual function Θ_ϱ for the minimum of $f_\varrho(\mathbf{x})$ subject to $\mathbf{x} \in \Omega_E$ reads

$$\begin{aligned}\Theta_\varrho(\boldsymbol{\lambda}) = &-\frac{1}{2}\boldsymbol{\lambda}^T\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T\boldsymbol{\lambda} + \left(\mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{b} + \varrho\mathsf{B}^T\mathbf{c}) - \mathbf{c}\right)\boldsymbol{\lambda} \\ &-\frac{1}{2}(\mathbf{b} + \varrho\mathsf{B}^T\mathbf{c})^T\mathsf{A}^{-1}(\mathbf{b} + \varrho\mathsf{B}^T) + \frac{\varrho}{2}\|\mathbf{c}\|^2.\end{aligned}$$

It follows that

$$\nabla\Theta_{\varrho_k}(\boldsymbol{\lambda}^k) = -\mathsf{B}\mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T\boldsymbol{\lambda}^k + \mathsf{B}\mathsf{A}_{\varrho_k}^{-1}(\mathbf{b} + \varrho_k\mathsf{B}^T\mathbf{c}) - \mathbf{c}. \tag{4.32}$$

Comparing the latter formula with (4.31), we conclude that

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + r_k\nabla\Theta_{\varrho_k}(\boldsymbol{\lambda}^k).$$

Thus the augmented Lagrangian algorithm may be interpreted as the gradient method for maximization of the dual function Θ_ϱ for the penalized problem (4.4) with the steplength r_k.

Alternatively, we can eliminate $\boldsymbol{\lambda}^k$ from Algorithm 4.2 to get

$$\mathbf{x}^0 = \mathsf{A}_{\varrho_0}^{-1}(\mathbf{b} + \varrho_k\mathsf{B}^T\mathbf{c} - \mathsf{B}^T\boldsymbol{\lambda}^0), \tag{4.33}$$
$$\mathbf{x}^{k+1} = \mathbf{x}^k - r_k\mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T(\mathsf{B}\mathbf{x}^k - \mathbf{c}). \tag{4.34}$$

4.3.2 Convergence of Lagrange Multipliers

Let us first recall that, by Proposition 2.10(iii) and the discussion at the end of Sect. 2.4.2, any Lagrange multiplier $\overline{\boldsymbol{\lambda}}$ of the equality constrained problem (4.1) can be expressed as

$$\overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} + \boldsymbol{\delta}, \qquad \boldsymbol{\lambda}_{\mathrm{LS}} \in \mathrm{Im}\mathsf{B}, \qquad \boldsymbol{\delta} \in \mathrm{Ker}\mathsf{B}^T,$$

where $\boldsymbol{\lambda}_{\mathrm{LS}}$ is the Lagrange multiplier with the minimal Euclidean norm. If we denote by P and $\mathsf{Q} = \mathsf{I} - \mathsf{P}$ the orthogonal projectors on $\mathrm{Im}\mathsf{B}$ and $\mathrm{Ker}\mathsf{B}^T$, respectively, then the components of $\overline{\boldsymbol{\lambda}}$ are given by

$$\boldsymbol{\lambda}_{\mathrm{LS}} = \mathsf{P}\overline{\boldsymbol{\lambda}}, \qquad \boldsymbol{\nu} = \mathsf{Q}\overline{\boldsymbol{\lambda}}.$$

To simplify the notations, we shall assume that $\varrho_k = \varrho$ and $r_k = r$.

To study the convergence of $\boldsymbol{\lambda}^k$ generated by Algorithm 4.2, let $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, let us denote

$$\overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} + \mathsf{Q}\boldsymbol{\lambda}^0,$$

and observe that

$$\begin{aligned}
\boldsymbol{\lambda}^0 - \overline{\boldsymbol{\lambda}} &= \mathsf{P}\boldsymbol{\lambda}^0 + \mathsf{Q}\boldsymbol{\lambda}^0 - \boldsymbol{\lambda}_{\mathrm{LS}} - \mathsf{Q}\boldsymbol{\lambda}^0 = \mathsf{P}(\boldsymbol{\lambda}^0 - \boldsymbol{\lambda}_{\mathrm{LS}}) \in \mathrm{Im}\mathsf{B},\\
\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}} &= (\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}) - r(\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T\boldsymbol{\lambda}^k - \mathsf{B}\mathsf{A}_\varrho^{-1}(\mathbf{b} + \varrho\mathsf{B}^T\mathbf{c}) + \mathbf{c})\\
&= (\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}) - r\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T(\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}),
\end{aligned}$$

where we used $\mathsf{P}\boldsymbol{\lambda}_{\mathrm{LS}} = \boldsymbol{\lambda}_{\mathrm{LS}}$ and (4.9). It follows that

$$\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}} = (\mathsf{I} - r\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T)(\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}) \tag{4.35}$$

and

$$\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}} \in \mathrm{Im}\mathsf{B}, \quad k = 0, 1, \ldots.$$

Therefore the analysis of convergence of $\boldsymbol{\lambda}^k$ reduces to the analysis of the spectrum of the restriction of the iteration matrix $\mathsf{I} - r\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T$ to its invariant subspace $\mathrm{Im}\mathsf{B}$.

Using (1.26) and Lemma 1.5, we get that the eigenvalues μ_i of the iteration matrix are related to the eigenvalues $\overline{\beta}_i$ of $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T|\mathrm{Im}\mathsf{B}$ by

$$\mu_i = 1 - \frac{r\overline{\beta}_i}{1 + \varrho\overline{\beta}_i} = \frac{1 + (\varrho - r)\overline{\beta}_i}{1 + \varrho\overline{\beta}_i},$$

so that

$$\|(\mathsf{I} - r\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T)|\mathrm{Im}\mathsf{B}\| = \max_{\substack{i\in\{1,\ldots,m\}\\ \beta_i>0}} \frac{|1 + (\varrho - r)\beta_i|}{1 + \varrho\beta_i}.$$

Denoting

$$R(\varrho, r) = \max_{\substack{i\in\{1,\ldots,m\}\\ \beta_i>0}} \frac{|1 + (\varrho - r)\beta_i|}{1 + \varrho\beta_i} \tag{4.36}$$

and using that the norm is submultiplicative, we get for $R(\varrho, r) < 1$ the linear rate of convergence

$$\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| \le R(\varrho, r)\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|. \tag{4.37}$$

We have thus reduced the study of convergence of Algorithm 4.2 to the analysis of $R(\varrho, r)$. We shall formulate the result on the convergence of the Lagrange multipliers in the following theorem.

Theorem 4.6. *Let $\boldsymbol{\lambda}^k,\ k = 0, 1, \dots,$ denote the sequence of vectors generated by Algorithm 4.2 for problem (4.1) with a given ϱ_k and r_k starting from a given vector $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$. Let $\boldsymbol{\lambda}_{\mathrm{LS}}$ denote the least square Lagrange multiplier, let P denote the orthogonal projector on* $\mathrm{Im}\mathsf{B}$, *let $\beta_{\max}$ denote the largest eigenvalue of $\mathsf{BA}^{-1}\mathsf{B}^T$, and denote*

$$\overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0.$$

If there are $\varepsilon > 0$ and $M > 0$ such that

$$\varepsilon \le r_k \le \frac{2}{\beta_{\max}} + 2\varrho_k - \varepsilon \le M, \tag{4.38}$$

then $\boldsymbol{\lambda}^k$ converge to $\overline{\boldsymbol{\lambda}}$ and the rate of convergence is at least linear, i.e., there is $R < 1$ such that

$$\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| \le R\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|.$$

Proof. Elementary, but a bit laborious analysis of $R(\varrho_k, r_k)$, where R is defined by (4.36), reveals that if ϱ_k, r_k satisfy (4.38), then

$$\sup_{k=0,1,\dots} R(\varrho_k, r_k) = R < 1.$$

To finish the proof, it is enough to substitute this result into (4.37). □

Using different arguments, it is possible to prove convergence of Algorithm 4.2 under more relaxed conditions. For example, Glowinski and Le Tallec [100] give the condition

$$0 < \varepsilon \le r_k \le 2\varrho_k.$$

4.3.3 Effect of the Steplength

Let us now examine possible options of the steplength $r = r(\varrho)$ as a function of ϱ, including their effect on $R(\varrho, r)$. We shall denote by $\overline{\beta}_{\min}$ the smallest nonzero eigenvalues of $\mathsf{BA}^{-1}\mathsf{B}^T$, i.e., the smallest eigenvalue of $\mathsf{BA}^{-1}\mathsf{B}^T|\mathrm{Im}\mathsf{B}$. Our examples are from Glowinski and Le Tallec [100].

Optimal choice of r *with* $\varrho = 0$.

In this case, which corresponds to the original Uzawa algorithm,

$$R(\varrho, r) = R(0, r) = \max_{\substack{i\in\{1,\dots,m\}\\ \beta_i>0}} |1 - r\beta_i|, \tag{4.39}$$

so that the best choice of r is given by

$$\begin{aligned} R(0, r_{\text{opt}}) &= \min_r \max_{\substack{i\in\{1,\dots,m\}\\ \beta_i>0}} |1 - r\beta_i| = \min_r \max_{\substack{i\in\{1,\dots,m\}\\ \beta_i>0}} \{1 - r\beta_i, r\beta_i - 1\} \\ &= \min_r \max\{1 - r\overline{\beta}_{\min}, r\beta_{\max} - 1\}. \end{aligned}$$

A simple analysis reveals that r_{opt} satisfies

$$1 - r\overline{\beta}_{\min} = r\beta_{\max} - 1.$$

Solving the last equation with respect to r, we get

$$r_{\text{opt}} = \frac{2}{\overline{\beta}_{\min} + \beta_{\max}}$$

and

$$R(0, r_{\text{opt}}) = 1 - r_{\text{opt}}\overline{\beta}_{\min} = \frac{\beta_{\max} - \overline{\beta}_{\min}}{\beta_{\max} + \overline{\beta}_{\min}} = \frac{\beta_{\max}/\overline{\beta}_{\min} - 1}{\beta_{\max}/\overline{\beta}_{\min} + 1}.$$

This is of course the optimal rate of convergence of the gradient method of Sect. 3.4 applied to the dual function. Inspection of (4.39) reveals that $R(0, r) < 1$ requires that $1 - r\beta_{\max} > -1$, i.e.,

$$r < 2/\beta_{\max},$$

so that r_{opt} is typically near the bound which guarantees the convergence.

Choice $r = \varrho$.

In this case, which is natural from the point of view of our analysis of the penalty method,

$$R(\varrho, \varrho) = \max_{\substack{i\in\{1,\dots,m\}\\ \beta_i>0}} \frac{1}{1 + \varrho\beta_i} = \frac{1}{1 + \varrho\beta_{\min}}. \tag{4.40}$$

An interesting feature of this choice is that

$$\lim_{\varrho\to\infty} R(\varrho, \varrho) = 0,$$

so that by increasing ϱ, it is possible to achieve arbitrary preconditioning effect.

Choice $r = (1 + \delta)\varrho$.

Let us now consider the choice $r = (1 + \delta)\varrho$ with $\delta > -1$. In this case

$$R\big(\varrho, (1+\delta)\varrho\big) = \max_{\substack{i \in \{1,\ldots,m\} \\ \beta_i > 0}} \frac{|1 - \delta\varrho\beta_i|}{1 + \varrho\beta_i},$$

so that $r > 0$ and $R\big(\varrho, (1+\delta)\varrho\big) < 1$ if and only if $-1 < \delta < 1 + 2/(\varrho\beta_{\max})$. Moreover

$$\lim_{\varrho \to \infty} R(\varrho, (1+\delta)\varrho) = |\delta|.$$

It follows that the preconditioning effect which can be achieved by increasing the penalty parameter is limited when $\delta \neq 0$.

Optimal steplength for a given ϱ.

If ϱ is given, then the optimal steplength $r_{\mathrm{opt}}(\varrho)$ is given by

$$r_{\mathrm{opt}} = \arg\min_{r \geq 0} \left(\max_{\substack{i \in \{1,\ldots,m\} \\ \beta_i > 0}} \frac{|1 + (\varrho - r)\beta_i|}{1 + \varrho\beta_i} \right).$$

To find it, let us denote

$$\varphi_i(r) = \frac{1 + (\varrho - r)\beta_i}{1 + \varrho\beta_i} = \frac{(1 + \varrho\beta_i) - r\beta_i}{1 + \varrho\beta_i},$$

and observe that if $\beta_i > 0$, then $\varphi_i(r)$ is decreasing. Since $\varphi_i(0) = 1$, it follows that for $r \geq 0$

$$\max_{\substack{i \in \{1,\ldots,m\} \\ \beta_i > 0}} \varphi_i(r) = \max_{\substack{i \in \{1,\ldots,m\} \\ \beta_i > 0}} \frac{1 + (\varrho - r)\beta_i}{1 + \varrho\beta_i} = \frac{1 + (\varrho - r)\overline{\beta}_{\min}}{1 + \varrho\overline{\beta}_{\min}}.$$

Similarly $-\varphi_i(0) = -1$, and if $\beta_i > 0$, then $-\varphi_i(r)$ is increasing. Therefore

$$\max_{\substack{i \in \{1,\ldots,m\} \\ \beta_i > 0}} -\varphi_i(r) = \max_{\substack{i \in \{1,\ldots,m\} \\ \beta_i > 0}} -\frac{1 + (\varrho - r)\beta_i}{1 + \varrho\beta_i} = -\frac{1 + (\varrho - r)\overline{\beta}_{\max}}{1 + \varrho\overline{\beta}_{\max}}$$

for nonnegative r. Since the both maxima are nonnegative on the positive interval $[\varrho + 1/\beta_{\max}, \varrho + 1/\beta_{\min}]$, it follows that the optimal choice $r_{\mathrm{opt}}(\varrho)$ is a nonnegative solution of

$$\frac{1 + (\varrho - r)\overline{\beta}_{\min}}{1 + \varrho\overline{\beta}_{\min}} = -\frac{1 + (\varrho - r)\beta_{\max}}{1 + \varrho\beta_{\max}}.$$

Carrying out the computations, we get that

$$r_{\mathrm{opt}}(\varrho) = \varrho + \frac{2 + \varrho(\overline{\beta}_{\min} + \beta_{\max})}{2\varrho\overline{\beta}_{\min}\beta_{\max} + \overline{\beta}_{\min} + \beta_{\max}}.$$

We conclude that the optimal steplength $r_{\text{opt}}(\varrho)$ based on the estimate (4.37) is *longer* than the penalization parameter ϱ, but $r_{\text{opt}}(\varrho)$ approaches ϱ for large values of ϱ as

$$\lim_{\varrho \to \infty} r_{\text{opt}}(\varrho)/\varrho = 1.$$

This is in agreement with the above discussion and our analysis of the penalty method in Sect. 4.2.1, which suggests that a suitable steplength for large ϱ is given by $r = \varrho$.

Given $\mathbf{x}^k$ which minimizes $L(\mathbf{x}, \boldsymbol{\lambda}^k, \varrho)$ with respect to $\mathbf{x} \in \mathbb{R}^n$, then $\mathbf{x}^k$ satisfies

$$\mathsf{A}\mathbf{x}^k + \mathsf{B}^T \left(\boldsymbol{\lambda}^k + \varrho(\mathsf{B}\mathbf{x}^k - \mathbf{c})\right) - \mathbf{b} = \mathbf{o}.$$

Thus the choice $r = \varrho$ results in

$$\nabla L_0(\mathbf{x}^k, \boldsymbol{\lambda}^{k+1}) = \mathbf{o},$$

so that it is optimal also in the sense that

$$\varrho = \arg\min_{r \geq 0} \|\mathsf{A}\mathbf{x}^k + \mathsf{B}^T \left(\boldsymbol{\lambda}^k + r(\mathsf{B}\mathbf{x}^k - \mathbf{c})\right) - \mathbf{b}\|.$$

Maximizing the Gradient Ascent.

In Sect. 4.3.1, we have shown that Algorithm 4.2 may be interpreted as a gradient algorithm applied to the maximization of the dual function Θ_ϱ. Thus it seems natural to define r_k by maximizing the quadratic function

$$\phi(r) = \Theta_{\varrho_k}(\boldsymbol{\lambda}^k + r\mathbf{g}^k),$$

where $\mathbf{g}^k = \nabla\Theta_{\varrho_k}(\boldsymbol{\lambda}^k)$, with respect to r. Denoting $\mathsf{A}_{\varrho_k} = \mathsf{A} + \varrho_k \mathsf{B}^T\mathsf{B}$,

$$\mathsf{F}_{\varrho_k} = \mathsf{B}\mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T, \qquad \text{and} \qquad \mathbf{d} = \mathbf{d}_{\varrho_k} = \mathsf{B}\mathsf{A}_{\varrho_k}^{-1}(\mathbf{b} + \varrho_k \mathsf{B}^T\mathbf{c}) - \mathbf{c},$$

we can write

$$\phi(r) = -\frac{1}{2}(\boldsymbol{\lambda}^k + r\mathbf{g}^k)^T \mathsf{F}_{\varrho_k}(\boldsymbol{\lambda}^k + r\mathbf{g}^k) + (\boldsymbol{\lambda}^k + r\mathbf{g}^k)^T\mathbf{d},$$

so that the maximizer satisfies

$$\frac{d}{dr}\phi(r) = -r(\mathbf{g}^k)^T\mathsf{F}_{\varrho_k}\mathbf{g}^k - (\mathbf{g}^k)^T(\mathsf{F}_{\varrho_k}\boldsymbol{\lambda}^k - \mathbf{d}) = -r(\mathbf{g}^k)^T\mathsf{F}_{\varrho_k}\mathbf{g}^k + (\mathbf{g}^k)^T\mathbf{g}^k = 0.$$

Thus we can use the steepest ascent formula

$$r_k = \frac{\|\mathbf{g}^k\|^2}{(\mathbf{g}^k)^T\mathsf{F}_{\varrho_k}\mathbf{g}^k}, \tag{4.41}$$

which may be applied to obtain the largest increase of Θ_{ϱ_k} in step k. For large ϱ_k, we get by (1.47) and (1.48) that r_k is close to ϱ_k in agreement with the optimal choice of the steplength based on the estimate (4.37). Notice that the steplength based on (4.41) depends on the current iteration.

4.3.4 Convergence of the Feasibility Error

To estimate the feasibility error $\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|$, let us multiply equation (4.34) by B and then subtract $\mathbf{c}$ from both sides of the result to get

$$\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c} = \mathsf{B}\mathbf{x}^k - \mathbf{c} - r_k \mathsf{B}\mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T(\mathsf{B}\mathbf{x}^k - \mathbf{c}),$$

where $\mathsf{A}_{\varrho_k} = \mathsf{A} + \varrho_k \mathsf{B}^T\mathsf{B}$. It follows that

$$\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\| \le \|(\mathsf{I} - r_k \mathsf{B}\mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T)|\mathrm{Im}\mathsf{B}\|\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|, \tag{4.42}$$

so that, under the assumptions of Theorem 4.6, we can use the same arguments to prove the linear convergence of the feasibility error. We can thus state the following theorem.

Theorem 4.7. *Let* $\mathbf{x}^k,\ k = 0, 1, \ldots,$ *be generated by Algorithm 4.2 for problem (4.1) with given* ϱ_k, r_k, *and* $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$. *Let* $\beta_{\max}$ *denote the largest eigenvalue of* $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T$.

If there are $\varepsilon > 0$ *and* $M > 0$ *such that*

$$\varepsilon \le r_k \le \frac{2}{\beta_{\max}} + 2\varrho_k - \varepsilon \le M, \tag{4.43}$$

then the feasibility error $\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|$ *converges to zero and the rate of convergence is at least linear, i.e., there is* $R < 1$ *such that*

$$\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\| \le R\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|. \tag{4.44}$$

We have thus obtained exactly the same rate of convergence of the feasibility error as that for the Lagrange multipliers.

4.3.5 Convergence of Primal Variables

Having the proofs of convergence of the Lagrange multipliers and of the feasibility error, we may use Proposition 2.12 to prove the convergence of the primal variables.

Theorem 4.8. *Let* $\mathbf{x}^k,\ k = 0, 1, \ldots,$ *be generated by Algorithm 4.2 for problem (4.1) with given* ϱ_k, r_k, *and* $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, *let* $\widehat{\mathbf{x}}$ *denote the unique solution of (4.1), let* $\overline{\sigma}_{\min}$ *denote the least nonzero singular value of* B, *and let* $\beta_{\max}$ *denote the largest eigenvalue of* $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T$.

If there are $\varepsilon > 0$ *and* $M > 0$ *such that*

$$\varepsilon \le r_k \le \frac{2}{\beta_{\max}} + 2\varrho_k - \varepsilon \le M, \tag{4.45}$$

then $\|\mathbf{x}^k - \widehat{\mathbf{x}}\|$ *converges to zero and the rate of convergence is at least R-linear, i.e., there is* $R < 1$ *such that*

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\| \le R^k \frac{\kappa(\mathsf{A})\|B\|}{\overline{\sigma}_{\min}}\|\mathbf{x}^0 - \widehat{\mathbf{x}}\|. \tag{4.46}$$

Proof. First recall that by the assumptions and (4.44),

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le R^k \|\mathsf{B}\mathbf{x}^0 - \mathbf{c}\| = R^k \|\mathsf{B}(\mathbf{x}^0 - \widehat{\mathbf{x}})\| \le R^k \|\mathsf{B}\| \|\mathbf{x}^0 - \widehat{\mathbf{x}}\|,$$

where $R < 1$. Using (2.48), we get that

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\| \le \frac{\kappa(\mathsf{A})}{\overline{\sigma}_{\min}} \|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le R^k \frac{\kappa(\mathsf{A})\|\mathsf{B}\|}{\overline{\sigma}_{\min}} \|\mathbf{x}^0 - \widehat{\mathbf{x}}\|.$$

We have used the fact that $\nabla_{\mathbf{x}} L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho) = \mathbf{o}$. □

4.3.6 Implementation

Since it is possible to approximate the solution of (4.1) with a single step of the penalty method, the above discussion suggests to take $r_k = \varrho_k = \varrho$ as large as possible.

The auxiliary problems in Step 1 can be effectively solved by the Cholesky factorization

$$\mathsf{L}\mathsf{L}^T = \mathsf{A}_\varrho,$$

which should be carried out after each update of ϱ, and the multiplication of a vector $\boldsymbol{\lambda}$ by $\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T$ should be carried out as

$$\mathsf{B}\mathsf{A}_\varrho^{-1}\mathsf{B}^T\boldsymbol{\lambda} = \mathsf{B}\big(\mathsf{L}^{-T}\left(\mathsf{L}^{-1}(\mathsf{B}^T\boldsymbol{\lambda})\right)\big).$$

The multiplication by the inverse factors should be implemented as the solution of the related triangular systems. Since the sensitivity to round-off errors is greater when ϱ is large, the algorithm should be implemented in double precision.

Application of iterative solvers can hardly be efficient for implementation of Step 1 of Algorithm 4.2, where an exact solution is required, but it can be very efficient for the implementation of inexact augmented Lagrangian algorithms discussed in the rest of this chapter.

On Application of the Conjugate Gradient Method

Since the augmented Lagrangian algorithm maximizes the dual function, we can alternatively forget it and apply the CG algorithm of Sect. 3.3 to maximize the dual function Θ. This strategy may be very efficient as indicated by the success of the FETI methods introduced by Farhat and Roux [86, 87]. The large penalty parameters result in efficient preconditioning of the Hessian of Θ (1.48), so that, due to the optimal properties of the conjugate gradient method, the latter is a natural choice provided we can solve exactly the auxiliary linear problems. The picture changes when inexact solutions of the auxiliary problems are considered, as a perturbed conjugate gradient need not be even a decrease direction as indicated in Fig. 3.2. Thus it is mainly the *capability to accept the inexact solutions and treat separately the constraints and minimization* that makes the augmented Lagrangian algorithm an attractive alternative for the solution of equality constrained QP problems.

4.4 Asymptotically Exact Augmented Lagrangian Method

The augmented Lagrangian method considered in the previous section assumed that the minimization in Step 1 is carried out exactly. Since such iterations are expensive, there is a good chance to reduce the cost of the outer iterates without a large increase of the number of iterations due to the approximate minimization, especially when we recall that the gradient is a robust ascent direction.

In this section we carry out the analysis of convergence of the augmented Lagrangian algorithm when the precisions of the solutions of the auxiliary problems in Step 1 are determined by the bounds on the norm of the gradient. We assume that the bounds are prescribed by the *forcing sequence* $\{\varepsilon_k\}$, where $\varepsilon^k > 0$ and $\lim_{k\to\infty} \varepsilon_k = 0$. The latter condition implies that the stopping criterion becomes more stringent with the increasing index of the outer iterations so that the minimization is asymptotically exact. Taking into account the discussion of Sect. 4.3.3, we consider the steplength $r_k = \varrho_k$.

4.4.1 Algorithm

The augmented Lagrangian algorithm with asymptotically exact solution of auxiliary unconstrained problems differs from the exact algorithm only in Step 1. We restrict our attention to the inexact version of the original augmented Lagrangian method which reads as follows.

Algorithm 4.3. Asymptotically Exact Augmented Lagrangians.

Given a symmetric positive definite matrix $\mathsf{A} \in \mathbb{R}^{n\times n}$, $\mathsf{B} \in \mathbb{R}^{m\times n}$, $\mathbf{b} \in \mathbb{R}^n$, *and* $\mathbf{c} \in \mathrm{Im}\mathsf{B}$.

Step 0. {*Initialization.*}
Choose $\varepsilon_i > 0$ *so that* $\lim_{i\to\infty} \varepsilon_i = 0$, $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, $\varrho_i \geq \varrho > 0$
for *k=0,1,2,...*
Step 1. {*Minimization with respect to* $\mathbf{x}$.}
Choose $\mathbf{x}^k \in \mathbb{R}^n$ *so that* $\|\nabla_{\mathbf{x}} L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k)\| \leq \varepsilon_k$
Step 2. {*Updating the Lagrange multipliers.*}
$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \varrho_k(\mathsf{B}\mathbf{x}^k - \mathbf{c})$
end for

We assume that the inexact solution of the auxiliary problems in Step 1 of Algorithm 4.3 is implemented by a suitable iterative method such as the conjugate gradient method introduced in Chap. 3. Thus the algorithm solves approximately the auxiliary unconstrained problems in the inner loop while it generates the approximations of the Lagrange multipliers in the outer loop. Let us recall that effective application of the conjugate gradient method assumes that the iterations are carried out with the matrix which has a favorable distribution of the spectrum. This can be achieved by a problem-dependent preconditioning discussed in Sect. 3.6 in combination with the gap-preserving strategy of Sect. 4.7.

4.4.2 Auxiliary Estimates

Our analysis of the augmented Lagrangian algorithm is based on the following lemma.

Lemma 4.9. *Let* $\mathsf{A}, \mathsf{B}, \mathbf{b}$, *and* $\mathbf{c}$ *be those of the definition of problem (4.1) with* $\mathsf{B} \neq \mathsf{O}$ *not necessarily a full rank matrix. For any vectors* $\mathbf{x} \in \mathbb{R}^n$ *and* $\boldsymbol{\lambda} \in \mathbb{R}^m$, *let us denote*

$$\widetilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda} + \varrho(\mathsf{B}\mathbf{x} - \mathbf{c}),$$
$$\mathbf{g} = \nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) = \mathsf{A}_\varrho \mathbf{x} - \mathbf{b} + \mathsf{B}^T \boldsymbol{\lambda} - \varrho \mathsf{B}^T \mathbf{c}.$$

Let $\boldsymbol{\lambda}_{\mathrm{LS}}$ *denote the vector of the least square Lagrange multipliers for problem (4.1), and let* $\overline{\beta}_{\min}$ *denote the least nonzero eigenvalue of* $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}$.

Then for any $\boldsymbol{\lambda} \in \mathrm{Im}\mathsf{B}$

$$\|\widetilde{\boldsymbol{\lambda}} - \boldsymbol{\lambda}_{\mathrm{LS}}\| \leq \frac{\|\mathsf{B}\mathsf{A}^{-1}\|}{\overline{\beta}_{\min} + \varrho^{-1}} \|\mathbf{g}\| + \frac{\varrho^{-1}}{\overline{\beta}_{\min} + \varrho^{-1}} \|\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}\|. \tag{4.47}$$

Proof. The definitions of $\widetilde{\boldsymbol{\lambda}}$ and $\mathbf{g}$ imply that

$$\begin{aligned} \mathsf{A}\mathbf{x} + \mathsf{B}^T \widetilde{\boldsymbol{\lambda}} &= \mathbf{b} + \mathbf{g}, \\ \mathsf{B}\mathbf{x} - \varrho^{-1} \widetilde{\boldsymbol{\lambda}} &= -\varrho^{-1}(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}) - \varrho^{-1}\boldsymbol{\lambda}_{\mathrm{LS}} + \mathbf{c}, \end{aligned} \tag{4.48}$$

and the solution $\widehat{\mathbf{x}}$ and $\boldsymbol{\lambda}_{\mathrm{LS}}$ satisfy by the assumptions

$$\begin{aligned} \mathsf{A}\widehat{\mathbf{x}} + \mathsf{B}^T \boldsymbol{\lambda}_{\mathrm{LS}} &= \mathbf{b}, \\ \mathsf{B}\widehat{\mathbf{x}} - \varrho^{-1} \boldsymbol{\lambda}_{\mathrm{LS}} &= -\varrho^{-1}\boldsymbol{\lambda}_{\mathrm{LS}} + \mathbf{c}. \end{aligned} \tag{4.49}$$

Subtracting (4.49) from (4.48) and switching to the matrix notation, we get

$$\begin{bmatrix} \mathsf{A} & \mathsf{B}^T \\ \mathsf{B} & -\varrho^{-1}\mathsf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} - \widehat{\mathbf{x}} \\ \widetilde{\boldsymbol{\lambda}} - \boldsymbol{\lambda}_{\mathrm{LS}} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ -\varrho^{-1}(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}) \end{bmatrix}. \tag{4.50}$$

After multiplying the first block row of (4.50) by $-\mathsf{B}\mathsf{A}^{-1}$, adding the result to the second block row, and simple manipulations, we get

$$\widetilde{\boldsymbol{\lambda}} - \boldsymbol{\lambda}_{\mathrm{LS}} = \mathsf{S}_\varrho^{-1}\mathsf{B}\mathsf{A}^{-1}\mathbf{g} + \varrho^{-1}\mathsf{S}_\varrho^{-1}(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\mathrm{LS}}), \tag{4.51}$$

where $\mathsf{S}_\varrho = \mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T + \varrho^{-1}\mathsf{I}$.

Noticing that $\boldsymbol{\lambda}_{\mathrm{LS}} - \boldsymbol{\lambda} \in \mathrm{Im}\mathsf{B}$ and taking norms, we get

$$\|\widetilde{\boldsymbol{\lambda}} - \boldsymbol{\lambda}\| \leq \|\mathsf{S}_{\varrho}^{-1}|\mathrm{Im}\mathsf{B}\| \left(\|\mathsf{BA}^{-1}\|\|\mathbf{g}\| + \varrho^{-1}\|\boldsymbol{\lambda}_{\mathrm{LS}} - \boldsymbol{\lambda}\|\right). \tag{4.52}$$

To estimate the first factor on the right-hand side, notice that by (1.43) our task reduces to finding an upper bound for

$$\|(\varrho^{-1}\mathsf{I} + \mathsf{BA}^{-1}\mathsf{B}^{T})^{-1}|\mathrm{Im}\mathsf{BA}^{-1}\mathsf{B}^{\mathrm{T}}\|.$$

Since $\mathrm{Im}\mathsf{B}^{\mathrm{T}}\mathsf{A}^{-1}\mathsf{B}$ is an invariant subspace of any matrix function of $\mathsf{B}^{T}\mathsf{A}^{-1}\mathsf{B}$, and the eigenvectors of $\mathsf{BA}^{-1}\mathsf{B}^{T}|\mathrm{Im}\mathsf{BA}^{-1}\mathsf{B}^{\mathrm{T}}$ are just the eigenvectors of $\mathsf{BA}^{-1}\mathsf{B}^{T}$ which correspond to the nonzero eigenvalues, it follows by (1.24) and (1.26) that

$$\|\mathsf{S}_{\varrho}^{-1}|\mathrm{Im}\mathsf{B}\| = \|(\varrho^{-1}\mathsf{I} + \mathsf{BA}^{-1}\mathsf{B}^{\mathrm{T}})^{-1}|\mathrm{Im}\mathsf{B}\| = 1/(\varrho^{-1} + \overline{\beta}_{\min}).$$

After substituting into (4.52), we get (4.47). □

To simplify applications of Lemma 4.9 for $\boldsymbol{\lambda}^0 \notin \mathrm{Im}\mathsf{B}$, let us formulate the following easy lemma.

Lemma 4.10. *Let* $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, *let*

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \mathbf{u}^k, \quad \mathbf{u}^k \in \mathrm{Im}\mathsf{B}, \quad k = 0, 1, \dots,$$

let $\boldsymbol{\lambda}_{\mathrm{LS}}$ *denote the vector of the least square Lagrange multipliers for problem (4.1), so that* $\boldsymbol{\lambda}_{\mathrm{LS}} \in \mathrm{Im}\mathsf{B}$, *let* P *denote the orthogonal projector onto* $\mathrm{Im}\mathsf{B}$, *and let*

$$\overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0. \tag{4.53}$$

Then

$$\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}} = \mathsf{P}\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}}, \quad k = 0, 1, \dots. \tag{4.54}$$

Proof. Since for $k = 0, 1, \dots$

$$(\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^{k+1} = (\mathsf{I} - \mathsf{P})(\boldsymbol{\lambda}^k + \mathbf{u}^k) = (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^k = \cdots = (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0,$$

we have

$$\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}} = \mathsf{P}\boldsymbol{\lambda}^k + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}} - (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0 = \mathsf{P}\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}}.$$

□

4.4.3 Convergence Analysis

Now we are ready to use Lemma 4.9 in the proof of convergence of Algorithm 4.3.

Theorem 4.11. *Let* $\mathbf{x}^k$, $\boldsymbol{\lambda}^k$, $k = 0, 1, \ldots,$ *be generated by Algorithm 4.3 for the solution of* (4.1) *with given* $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, $\varrho > 0$, $\varrho_k \geq \varrho$, *and* $\varepsilon_k > 0$ *such that* $\lim_{k\to\infty} \varepsilon_k = 0$. *Let* $(\widehat{\mathbf{x}}, \ \boldsymbol{\lambda}_{\mathrm{LS}})$ *denote the least square KKT pair for (4.1). Let* P *denote the orthogonal projector on* $\mathrm{Im}\mathsf{B}$, *let* $\overline{\beta}_{\min}$ *denote the least nonzero eigenvalue of* $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T$, *let* $\lambda_{\min}$ *denote the least eigenvalue of* A, *and denote*

$$\overline{\boldsymbol{\lambda}} = \mathsf{P}\boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0 = \boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0.$$

Then

$$\lim_{i\to\infty} \mathbf{x}^k = \widehat{\mathbf{x}}, \qquad \lim_{i\to\infty} \boldsymbol{\lambda}^k = \overline{\boldsymbol{\lambda}},$$

and for any positive integers $k, s, \ k + s = i$,

$$\|\boldsymbol{\lambda}^{k+s} - \overline{\boldsymbol{\lambda}}\| \leq C\overline{\varepsilon}_k \frac{1}{1-\nu} + \nu^s C\overline{\varepsilon}_0 \frac{1}{1-\nu} + \nu^{k+s}\|\boldsymbol{\lambda}^0 - \overline{\boldsymbol{\lambda}}\|, \tag{4.55}$$

$$\|\mathbf{x}^i - \widehat{\mathbf{x}}\| \leq \lambda_{\min}^{-1}\|\mathsf{B}\| \left(\|\boldsymbol{\lambda}^i - \overline{\boldsymbol{\lambda}}\| + \varepsilon_i\right), \tag{4.56}$$

where $\overline{\varepsilon}_k = \max\{\varepsilon_k, \varepsilon_{k+1}, \ldots\}$,

$$C = \frac{\|\mathsf{B}\mathsf{A}^{-1}\|}{\overline{\beta}_{\min} + \varrho^{-1}}, \quad \textit{and} \quad \nu = \frac{\varrho^{-1}}{\overline{\beta}_{\min} + \varrho^{-1}} < 1. \tag{4.57}$$

Proof. First notice that by the assumptions

$$(\mathsf{A} + \varrho_k \mathsf{B}^T\mathsf{B})\mathbf{x}^k = \mathbf{b} + \varrho_k \mathsf{B}^T\mathbf{c} - \mathsf{B}^T\boldsymbol{\lambda}^k + \mathbf{g}^k, \quad \|\mathbf{g}^k\| \leq \varepsilon_k, \tag{4.58}$$

where $\mathbf{g}^k = \nabla_{\mathbf{x}} L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k)$, and observe that the update rule in Step 2 of Algorithm 4.3 and Lemma 4.10 with $\mathbf{u}^k = \varrho_k(\mathsf{B}\mathbf{x}^k - \mathbf{c})$ imply that

$$\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}} = \mathsf{P}\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}}, \ k = 0, 1, \ldots.$$

Since

$$\mathsf{P}\boldsymbol{\lambda}^{k+1} = \mathsf{P}\boldsymbol{\lambda}^k + \varrho_k(\mathsf{B}\mathbf{x}^k - \mathbf{c})$$

and $\mathsf{P}\boldsymbol{\lambda}^k \in \mathrm{Im}\mathsf{B}$, we can apply Lemma 4.9 with

$$\boldsymbol{\lambda} = \mathsf{P}\boldsymbol{\lambda}^k \quad \text{and} \quad \widetilde{\boldsymbol{\lambda}} = \mathsf{P}\boldsymbol{\lambda}^k + \varrho_k(\mathsf{B}\mathbf{x}^k - \mathbf{c}) = \mathsf{P}\boldsymbol{\lambda}^{k+1}$$

and use the assumptions to get

$$\begin{aligned} \|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| = \|\mathsf{P}\boldsymbol{\lambda}^{k+1} - \boldsymbol{\lambda}_{\mathrm{LS}}\| &\leq \frac{\|\mathsf{B}\mathsf{A}^{-1}\|}{\overline{\beta}_{\min} + \varrho_k^{-1}}\|\mathbf{g}^k\| + \frac{\varrho_k^{-1}}{\overline{\beta}_{\min} + \varrho_k^{-1}}\|\mathsf{P}\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}}\| \\ &\leq C\varepsilon_k + \nu\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|, \end{aligned}$$

where C and ν are defined by (4.57).

It follows that for any positive integer s and $k = 0, 1, \ldots,$ we have

$$\begin{aligned}\|\boldsymbol{\lambda}^{k+s} - \overline{\boldsymbol{\lambda}}\| &\le C\varepsilon_{k+s-1} + \nu\|\boldsymbol{\lambda}^{k+s-1} - \overline{\boldsymbol{\lambda}}\| \\ &\le C(\varepsilon_{k+s-1} + \nu\varepsilon_{k+s-2} + \cdots + \nu^{s-1}\varepsilon_k) + \nu^s\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| \\ &\le C\overline{\varepsilon}_k(1 + \nu + \nu^2 + \cdots + \nu^{s-1}) + \nu^s\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| \\ &\le C\overline{\varepsilon}_k\frac{1}{1-\nu} + \nu^s\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|.\end{aligned}$$

To prove (4.55), it is enough to use the above inequalities to bound the last term by

$$\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| = \|\boldsymbol{\lambda}^{0+k} - \overline{\boldsymbol{\lambda}}\| \le C\overline{\varepsilon}_0\frac{1}{1-\nu} + \nu^k\|\boldsymbol{\lambda}^0 - \overline{\boldsymbol{\lambda}}\|.$$

Observing that any large integer may be expressed as a sum of two large integers, and that $\overline{\varepsilon}_k$ converges to zero, we conclude that $\boldsymbol{\lambda}^k$ converges to $\overline{\boldsymbol{\lambda}}$.

To prove the convergence of the primal variables, denote $\mathsf{A}_{\varrho_k} = \mathsf{A} + \varrho_k\mathsf{B}^T\mathsf{B}$ and observe that

$$\mathsf{A}_{\varrho_k}\widehat{\mathbf{x}} = \mathbf{b} + \varrho_k\mathsf{B}^T\mathbf{c} - \mathsf{B}^T\overline{\boldsymbol{\lambda}}.$$

After subtracting the last equation from (4.58) and simple manipulations, we get

$$\mathbf{x}^k - \widehat{\mathbf{x}} = \mathsf{A}_{\varrho_k}^{-1}\mathsf{B}^T\left(\overline{\boldsymbol{\lambda}} - \boldsymbol{\lambda}^k + \mathbf{g}^k\right).$$

Taking norms, using the properties of norms, the assumptions, and

$$\|\mathsf{A}_{\varrho_k}^{-1}\| \le \lambda_{\min}^{-1},$$

we get (4.56). It follows by assumptions that $\mathbf{x}^k$ converges to $\widehat{\mathbf{x}}$. □

The analysis of the asymptotically exact augmented Lagrangian algorithm for more general equality constrained problems may be found in Chap. 2 of Bertsekas [11].

4.5 Adaptive Augmented Lagrangian Method

The analysis of the previous section reveals that it is possible to use an inexact solution of the auxiliary problems in Step 1 of the augmented Lagrangian algorithm. However, the terms related to the precision in the inequalities (4.55) and (4.56) indicate that the convergence can be considerably slowed down if the precision control is relaxed. The price paid for the inexact minimization is an additional term in the estimate of the rate of convergence.

Here we present a different approach which arises from the intuitive argument that the precision of the solution $\mathbf{x}^k$ of the auxiliary problems should be related to the feasibility of $\mathbf{x}^k$, i.e., $\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|$, since it does not seem reasonable to solve the auxiliary problems to high precision at the early stage of computations with $\boldsymbol{\lambda}^k$ far from the Lagrange multiplier of the solution. Our approach is based on the observation of Sect. 4.3 that the rate of convergence of the augmented Lagrangian algorithm with the steplength $r_k = \varrho_k$ can be controlled by the penalty parameter (4.40).

4.5.1 Algorithm

The new features of the algorithm that we present here are the precision control in Step 1 and the update rule for the penalty parameter.

Algorithm 4.4. Augmented Lagrangians with Adaptive Precision Control.

Given a symmetric positive definite matrix $\mathsf{A} \in \mathbb{R}^{n\times n}$, $\mathsf{B} \in \mathbb{R}^{m\times n}$, $\mathbf{b} \in \mathbb{R}^n$, *and* $\mathbf{c} \in \mathrm{Im}\mathsf{B}$.

Step 0. {*Initialization.*}
Choose $\eta_0 > 0,\ 0 < \alpha < 1,\ \beta > 1,\ M > 0,\ \varrho_0 > 0,\ \boldsymbol{\lambda}^0 \in \mathbb{R}^m$

for *k=0,1,2,...*

Step 1. {*Approximate minimization with respect to* $\mathbf{x}$.}
Choose $\mathbf{x}^k \in \mathbb{R}^n$ *so that*

$$\|\nabla_{\mathbf{x}} L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k)\| \le M\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \tag{4.59}$$

Step 2. {*Updating the Lagrange multipliers.*}
$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \varrho_k(\mathsf{B}\mathbf{x}^k - \mathbf{c})$

Step 3. {*Updating* $\varrho_k,\ \eta_k$.}
if $\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le \eta_k$

$$\varrho_{k+1} = \varrho_k,\ \ \eta_{k+1} = \alpha\eta_k \tag{4.60}$$

else

$$\varrho_{k+1} = \beta\varrho_k,\ \ \eta_{k+1} = \eta_k \tag{4.61}$$

end *if*
end *for*

The next lemma shows that Algorithm 4.4 is well defined, that is, any convergent algorithm for the solution of the auxiliary problems required in Step 1 generates either $\mathbf{x}^k$ that satisfies (4.59) in a finite number of steps, or a sequence of approximations that converge to the solution of (4.1). Thus there is no hidden enforcement of exact solution in (4.59) and consequently typically inexact solutions of the auxiliary unconstrained problems are obtained in Step 1.

Lemma 4.12. *Let* $M > 0$, $\boldsymbol{\lambda} \in \mathbb{R}^m$, *and* $\varrho \ge 0$ *be given and let* $\{\mathbf{y}^k\}$ *denote any sequence that converges to the unique solution* $\widehat{\mathbf{y}}$ *of the problem*

$$\min_{\mathbf{y}\in\mathbb{R}^n} L(\mathbf{y}, \boldsymbol{\lambda}, \varrho). \tag{4.62}$$

Then $\{\mathbf{y}^k\}$ *either converges to the solution* $\widehat{\mathbf{x}}$ *of problem (4.1), or there is an index* k *such that*

$$\|\nabla L(\mathbf{y}^k, \boldsymbol{\lambda}, \varrho)\| \le M\|\mathsf{B}\mathbf{y}^k - \mathbf{c}\|. \tag{4.63}$$

Proof. First observe that $\nabla L(\mathbf{y}^k, \boldsymbol{\lambda}, \varrho)$ converges to zero by the assumptions. Thus if (4.63) does not hold for any k, then we must have $\mathsf{B}\widehat{\mathbf{y}} = \mathbf{c}$. In this case, since $\widehat{\mathbf{y}}$ is the solution of (4.62), it follows that

$$\mathsf{A}\widehat{\mathbf{y}} - \mathbf{b} + \mathsf{B}^T\boldsymbol{\lambda} + \varrho\mathsf{B}^T(\mathsf{B}\widehat{\mathbf{y}} - \mathbf{c}) = \mathbf{o}. \tag{4.64}$$

After substituting $\mathsf{B}\widehat{\mathbf{y}} = \mathbf{c}$ into (4.64), we get

$$\mathsf{B}\widehat{\mathbf{y}} - \mathbf{b} + \mathsf{B}^T\boldsymbol{\lambda} = \mathbf{o}. \tag{4.65}$$

However, since (4.65) and $\mathsf{B}\widehat{\mathbf{y}} = \mathbf{c}$ are sufficient conditions for $\widehat{\mathbf{y}}$ to be the unique solution of (4.1), we have $\widehat{\mathbf{y}} = \widehat{\mathbf{x}}$. □

4.5.2 Convergence of Lagrange Multipliers for Large ϱ

The convergence analysis of Algorithm 4.4 is based on the following lemma.

Lemma 4.13. *Let* $\mathsf{A}, \mathsf{B}, \mathbf{b}$, *and* $\mathbf{c}$ *be those of the definition of problem (4.1) with* $\mathsf{B} \neq \mathsf{O}$ *not necessarily a full rank matrix, let* $M > 0$, *and let*

$$\overline{\varrho} = \|\mathsf{B}\mathsf{A}^{-1}\| M / \overline{\beta}_{\min}, \tag{4.66}$$

where $\overline{\beta}_{\min}$ *denotes the least nonzero eigenvalue of* $\mathsf{B}\mathsf{A}^{-1}\mathsf{B}^T$. *Let* $\boldsymbol{\lambda}_{\mathrm{LS}}$ *denote the vector of the least square Lagrange multipliers for problem (4.1), let* P *denote the orthogonal projector onto* $\mathrm{Im}\mathsf{B}$, *and let for any* $\boldsymbol{\lambda} \in \mathbb{R}^m$

$$\overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda} \quad \textit{and} \quad \widetilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda} + \varrho(\mathsf{B}\mathbf{x} - \mathbf{c}). \tag{4.67}$$

If $\varrho \geq 2\overline{\varrho}$, $\mathbf{x} \in \mathbb{R}^n, \boldsymbol{\lambda} \in \mathbb{R}^m$, *and*

$$\|\nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \varrho)\| \leq M\|\mathsf{B}\mathbf{x} - \mathbf{c}\|, \tag{4.68}$$

then

$$\|\widetilde{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}\| \leq \frac{2}{\varrho}(\overline{\varrho} + \overline{\beta}_{\min}^{-1})\|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\|. \tag{4.69}$$

Proof. Let us first denote $\boldsymbol{\mu} = \mathsf{P}\boldsymbol{\lambda}$ and $\widetilde{\boldsymbol{\mu}} = \mathsf{P}\widetilde{\boldsymbol{\lambda}}$, so that $\boldsymbol{\mu} \in \mathrm{Im}\mathsf{B}$ and $\widetilde{\boldsymbol{\mu}} \in \mathrm{Im}\mathsf{B}$, and observe that by the definition of $\overline{\boldsymbol{\lambda}}$

$$\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda} - (\boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}) = \boldsymbol{\mu} - \boldsymbol{\lambda}_{\mathrm{LS}}, \tag{4.70}$$

$$\widetilde{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda} + \varrho(\mathsf{B}\mathbf{x} - \mathbf{c}) - \big(\boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}\big) = \widetilde{\boldsymbol{\mu}} - \boldsymbol{\lambda}_{\mathrm{LS}}. \tag{4.71}$$

Since $\mathsf{P}\mathsf{B} = \mathsf{B}$, we have

$$\mathsf{B}^T\boldsymbol{\lambda} = (\mathsf{P}\mathsf{B})^T\boldsymbol{\lambda} = \mathsf{B}^T\mathsf{P}\boldsymbol{\lambda} = \mathsf{B}^T\boldsymbol{\mu},$$
$$\nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) = \mathsf{A}_\varrho\mathbf{x} - \mathbf{b} + \mathsf{B}^T\boldsymbol{\lambda} - \varrho\mathsf{B}^T\mathbf{c} = \mathsf{A}_\varrho\mathbf{x} - \mathbf{b} + \mathsf{B}^T\boldsymbol{\mu} - \varrho\mathsf{B}^T\mathbf{c},$$

where $\mathsf{A}_\varrho = \mathsf{A} + \varrho \mathsf{B}^T\mathsf{B}$. Thus the assumption (4.68) is equivalent to

$$\|\nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\mu}, \varrho)\| = \|\nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \varrho)\| \leq M\|\mathsf{B}\mathbf{x} - \mathbf{c}\|. \tag{4.72}$$

Finally, notice that by the definition of $\widetilde{\boldsymbol{\lambda}}$ in (4.67), we have

$$\mathsf{B}\mathbf{x} - \mathbf{c} = \varrho^{-1}(\widetilde{\boldsymbol{\lambda}} - \boldsymbol{\lambda}). \tag{4.73}$$

Let us now denote

$$\mathbf{g} = \nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\mu}, \varrho)$$

and assume that $\mathbf{x}$, $\boldsymbol{\lambda}$, and ϱ satisfy the assumptions including (4.68), so that by (4.72)

$$\|\mathbf{g}\| \leq M\|\mathsf{B}\mathbf{x} - \mathbf{c}\|. \tag{4.74}$$

Using (4.71), Lemma 4.9, (4.70), (4.74), (4.73), and notation (4.66), we get

$$\begin{aligned}
\|\widetilde{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}\| &= \|\widetilde{\boldsymbol{\mu}} - \boldsymbol{\lambda}_{\mathrm{LS}}\| \\
&\leq \frac{\|\mathsf{B}\mathsf{A}^{-1}\|}{\overline{\beta}_{\min} + \varrho^{-1}}\|\mathbf{g}\| + \frac{\varrho^{-1}}{\overline{\beta}_{\min} + \varrho^{-1}}\|\boldsymbol{\mu} - \boldsymbol{\lambda}_{\mathrm{LS}}\| \\
&\leq \frac{\|\mathsf{B}\mathsf{A}^{-1}\|}{\overline{\beta}_{\min} + \varrho^{-1}} M\|\mathsf{B}\mathbf{x} - \mathbf{c}\| + \frac{\varrho^{-1}}{\overline{\beta}_{\min} + \varrho^{-1}}\|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\| \\
&= \frac{\|\mathsf{B}\mathsf{A}^{-1}\|}{\overline{\beta}_{\min} + \varrho^{-1}} \frac{M}{\varrho}\|\widetilde{\boldsymbol{\lambda}} - \boldsymbol{\lambda}\| + \frac{\varrho^{-1}}{\overline{\beta}_{\min} + \varrho^{-1}}\|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\| \\
&\leq \frac{\overline{\varrho}}{\varrho}\left(\|\widetilde{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}\| + \|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\|\right) + \frac{1}{\overline{\beta}_{\min}\varrho}\|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\|.
\end{aligned}$$

Thus, since $\varrho \geq 2\overline{\varrho}$, it follows that

$$\|\widetilde{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}\| \leq \left(\frac{\overline{\varrho}}{\varrho} + \frac{1}{\overline{\beta}_{\min}\varrho}\right)\|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\| / \left(1 - \frac{\overline{\varrho}}{\varrho}\right) \leq \frac{2}{\varrho}(\overline{\varrho} + \overline{\beta}_{\min}^{-1})\|\boldsymbol{\lambda} - \overline{\boldsymbol{\lambda}}\|.$$

□

Lemma 4.13 suggests that the Lagrange multipliers generated by Algorithm 4.4 converge to the solution $\overline{\boldsymbol{\lambda}}$ linearly when the penalty parameter is sufficiently large. We shall formulate this result explicitly.

Corollary 4.14. *Let $\{\boldsymbol{\lambda}^k\}$,$\{\mathbf{x}^k\}$, and $\{\varrho_k\}$ be generated by Algorithm 4.4 for problem (4.1) with the initialization defined in Step 0. Using the notation of Lemma 4.13, let for any index $k \geq 0$*

$$\varrho_k \geq 2\alpha_0^{-1}(\overline{\varrho} + \overline{\beta}_{\min}^{-1}), \tag{4.75}$$

where $\alpha_0 < 1$ is a positive constant.

Then

$$\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| \leq \alpha_0\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|. \tag{4.76}$$

Proof. Let k satisfy (4.75). Comparing (4.59) with (4.68), we can check that all the assumptions of Lemma 4.13 are satisfied for $\mathbf{x} = \mathbf{x}^k$, $\boldsymbol{\lambda} = \boldsymbol{\lambda}^k$, and $\varrho = \varrho_k$. Substituting into (4.69) and using $\boldsymbol{\lambda}^{k+1} = \widetilde{\boldsymbol{\lambda}}$, we get

$$\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| \le 2\varrho_k{}^{-1}(\overline{\varrho} + \overline{\beta}_{\min}^{-1})\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| \le \alpha_0\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|.$$

□

Notice that in (4.76), there is no term which accounts for inexact solutions of auxiliary problems. This compares favorably with (4.55).

4.5.3 R-Linear Convergence for Any Initialization of ϱ

The following lemma gives us a simple key to the proof of R-Linear convergence of Algorithm 4.4 for any initial regularization parameter $\varrho_0 \ge 0$.

Lemma 4.15. *Let $\{\boldsymbol{\lambda}^k\}$, $\{\mathbf{x}^k\}$, and $\{\varrho_k\}$ be generated by Algorithm 4.4 for problem (4.1) with the assumptions of Lemma 4.13 and the initialization defined in Step 0.*

Then ϱ_k is bounded and there is a constant C such that

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le C\alpha^k, \tag{4.77}$$

where $\alpha < 1$ is a positive constant defined in Step 0 of Algorithm 4.4.

Proof. Using the notation of Lemma 4.13, let us first assume that for any index k, $\varrho_k < 2(\overline{\varrho} + \overline{\beta}_{\min}^{-1})/\alpha$, so that there is k_0 such that for $k \ge k_0$ the values of ϱ_k and η_k are updated by the rule (4.60) in Step 3 of Algorithm 4.4. It follows that for any $k \ge k_0$,

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le \eta_k = \alpha^{k-k_0}\eta_{k_0} = C\alpha^k,$$

where $\alpha < 1$ is defined in Step 0 of Algorithm 4.4.

If there is k_0 such that $\varrho_{k_0} \ge 2(\overline{\varrho} + \overline{\beta}_{\min}^{-1})/\alpha$, then, since $\{\varrho_k\}$ is nondecreasing, we can use Corollary 4.14 to get that for $k > k_0$

$$\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| \le \alpha^{k-k_0}\|\boldsymbol{\lambda}^{k_0} - \overline{\boldsymbol{\lambda}}\|. \tag{4.78}$$

Using the update rule of Step 2 of Algorithm 4.4, we get

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| = \varrho_k^{-1}\|\boldsymbol{\lambda}^{k+1} - \boldsymbol{\lambda}^k\| \le \varrho_k^{-1}(\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| + \|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|).$$

Combining the last inequality with (4.78), we get

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le \varrho_k^{-1}(\alpha^{k-k_0+1} + \alpha^{k-k_0})\|\boldsymbol{\lambda}^{k_0} - \overline{\boldsymbol{\lambda}}\| \le 2\alpha^{k-k_0}\varrho_{k_0}^{-1}\|\boldsymbol{\lambda}^{k_0} - \overline{\boldsymbol{\lambda}}\| = C\alpha^k.$$

This proves (4.77).

To prove that $\{\varrho_k\}$ is bounded, notice that we can express each $k \ge 0$ as a sum $k = k_1 + k_2$, where $\eta_k = \alpha^{k_1}\eta_0$ and $\varrho_k = \beta^{k_2}\varrho_0$. Hence given k, k_1 and k_2 denote the numbers of preceding steps that invoked the updates (4.60) and (4.61), respectively. Moreover, $\varrho_{k+1} = \beta\varrho_k > \varrho_k$ if and only if $\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| > \eta^k$, and for such k

$$\alpha^{k_1}\eta_0 = \eta_k < \|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le C\alpha^k = C\alpha^{k_1+k_2}.$$

Since $\alpha < 1$, it follows that k_2 is finite and ϱ_k is bounded. □

Using that ϱ_k is uniformly bounded, it is now easy to show that $\{\boldsymbol{\lambda}^k\}$ and $\{\mathbf{x}^k\}$ converge R-linearly.

Corollary 4.16. *Let* $\{\boldsymbol{\lambda}^k\}$,$\{\mathbf{x}^k\}$, *and* $\{\varrho_k\}$ *be generated by Algorithm 4.4 for problem (4.1) with the initialization defined in Step 0. Then there are constants* C_1 *and* C_2 *such that*

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\| \le C_1\alpha^k \quad \textit{and} \quad \|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| \le C_2\alpha^k, \tag{4.79}$$

where $\overline{\boldsymbol{\lambda}}$ *is defined by (4.67),* $\widehat{\mathbf{x}}$ *is a unique solution of (4.1), and* $\alpha < 1$ *is a parameter of Algorithm 4.4.*

Proof. Observe that Lemma 4.15 and the condition (4.59) in the definition of Step 1 imply that there is a constant C such that

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le C\alpha^k \quad \text{and} \quad \|\mathbf{g}^k\| \le C\alpha^k.$$

To finish the proof, it is enough to use Proposition 2.12 and simple manipulations. □

4.6 Semimonotonic Augmented Lagrangians (SMALE)

In the previous section, we have shown that Algorithm 4.4 always achieves the R-linear rate of convergence given by the constant α which controls the decrease of the feasibility error. This looks like not a bad result, its only drawback being that such a rate of convergence is achieved *only with the penalty parameter* ϱ_k *which exceeds a threshold which depends on the constraint matrix* B. Is it possible to propose an inexact algorithm with any reasonable kind of convergence *independent of the constraint matrix* B? A key to getting a positive answer is to return to the augmented Lagrangian algorithm viewed as an alternative implementation of the penalty method with the adaptive precision control used by Algorithm 4.4. We shall also see that the convergence can be achieved with a rather small threshold on the penalty parameter independent of the singular values of the constraint matrix B.

4.6.1 SMALE Algorithm

The algorithm presented here is based on the observation that, having for a sufficiently large ϱ an *approximate* minimizer $\mathbf{x}_\varrho$ of the augmented Lagrangian $L(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$ with respect to $\mathbf{x}$, we can modify $\boldsymbol{\lambda}$ in such a way that $\mathbf{x}_\varrho$ is also an *approximate* unconstrained minimizer of $L(\mathbf{x}, \widetilde{\boldsymbol{\lambda}}, 0)$. Thus we can hopefully find a better approximation by minimizing $L(\mathbf{x}, \widetilde{\boldsymbol{\lambda}}, \varrho)$. Since the better penalty approximation results in an increased value of the Lagrangian, it is natural to increase the penalty parameter until increasing values of the Lagrangian are generated. We shall show that the threshold value for the penalty parameter is rather small and independent of the constraint matrix B. The algorithm that we consider here reads as follows.

Algorithm 4.5. Semimonotonic augmented Lagrangians (SMALE).

Given a symmetric positive definite matrix $\mathsf{A} \in \mathbb{R}^{n\times n}$, $\mathsf{B} \in \mathbb{R}^{m\times n}$, $\mathbf{b} \in \mathbb{R}^n$, *and* $\mathbf{c} \in \mathrm{Im}\mathsf{B}$.

Step 0. {*Initialization.*}
Choose $\eta > 0,\ \beta > 1,\ M > 0,\ \varrho_0 > 0,\ \boldsymbol{\lambda}^0 \in \mathbb{R}^m$

for *k=0,1,2,. . .*

Step 1. {*Inner iteration with adaptive precision control.*}
Find $\mathbf{x}^k$ *such that*

$$\|\mathbf{g}(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k)\| \le \min\{M\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|, \eta\}. \tag{4.80}$$

Step 2. {*Updating the Lagrange multipliers.*}

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \varrho_k(\mathsf{B}\mathbf{x}^k - \mathbf{c}) \tag{4.81}$$

Step 3. {*Update* ϱ *provided the increase of the Lagrangian is not sufficient.*}
if $k > 0$ *and*

$$L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) < L(\mathbf{x}^{k-1}, \boldsymbol{\lambda}^{k-1}, \varrho_{k-1}) + \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \tag{4.82}$$

$\varrho_{k+1} = \beta\varrho_k$

else

$\varrho_{k+1} = \varrho_k.$

end if

end for

In Step 1 we can use any convergent algorithm for the minimization of the strictly convex quadratic function such as the preconditioned conjugate gradient method of Sect. 3.3. Let us point out that Algorithm 4.5 differs from Algorithm 4.4 by the condition (4.82) on the update of the penalization parameter in Step 3.

To see that Algorithm 4.5 is well defined, let $\{\mathbf{y}^k\}$ be a sequence generated by any convergent algorithm for the solution of the auxiliary problem

$$\text{minimize } \{L(\mathbf{y}, \boldsymbol{\lambda}, \varrho) : \mathbf{y} \in \mathbb{R}^n\}.$$

Then there is an integer k_0 such that for $k \geq k_0$

$$\|\mathbf{g}(\mathbf{y}^k, \boldsymbol{\lambda}, \varrho)\| \leq \eta$$

and we can use Lemma 4.12 to show that either $\{\mathbf{y}^k\}$ converges to the solution $\widehat{\mathbf{x}}$ of (4.1) or there is k such that (4.80) holds. Thus there is no hidden enforcement of the exact solution in (4.80) and consequently typically inexact solutions of the auxiliary unconstrained problems are obtained in Step 1.

4.6.2 Relations for Augmented Lagrangians

In this section we establish the basic inequalities that relate the bound on the norm of the gradient $\mathbf{g}$ of the augmented Lagrangian L to the values of the augmented Lagrangian L. These inequalities are the key ingredients in the proof of convergence of Algorithm 4.5.

Lemma 4.17. *Let* A, B, $\mathbf{b}$, *and* $\mathbf{c}$ *be those of problem (4.1),* $\mathbf{x} \in \mathbb{R}^n$, $\boldsymbol{\lambda} \in \mathbb{R}^m$, $\varrho > 0$, $\eta > 0$, *and* $M > 0$. *Let* $\lambda_{\min}$ *denote the least eigenvalue of* A *and* $\widetilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda} + \varrho(\mathsf{B}\mathbf{x} - \mathbf{c})$.
(i) If

$$\|\mathbf{g}(\mathbf{x}, \boldsymbol{\lambda}, \varrho)\| \leq M\|\mathsf{B}\mathbf{x} - \mathbf{c}\|, \tag{4.83}$$

then for any $\mathbf{y} \in \mathbb{R}^n$

$$L(\mathbf{y}, \widetilde{\boldsymbol{\lambda}}, \varrho) \geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \frac{1}{2}\left(\varrho - \frac{M^2}{\lambda_{\min}}\right)\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2. \tag{4.84}$$

(ii) If

$$\|\mathbf{g}(\mathbf{x}, \boldsymbol{\lambda}, \varrho)\| \leq \eta, \tag{4.85}$$

then for any $\mathbf{y} \in \mathbb{R}^n$

$$L(\mathbf{y}, \widetilde{\boldsymbol{\lambda}}, \varrho) \geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2 - \frac{\eta^2}{2\lambda_{\min}}. \tag{4.86}$$

(iii) If (4.85) holds and $\mathbf{z}_0$ *is any vector such that* $\mathsf{B}\mathbf{z}_0 = \mathbf{c}$, *then*

$$L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) \leq f(\mathbf{z}_0) + \frac{\eta^2}{2\lambda_{\min}}. \tag{4.87}$$

Proof. Let us denote $\boldsymbol{\delta} = \mathbf{y} - \mathbf{x}$, $\mathsf{A}_\varrho = \mathsf{A} + \varrho\mathsf{B}^T\mathsf{B}$, $\mathbf{g} = \mathbf{g}(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$, and $\widetilde{\mathbf{g}} = \mathbf{g}(\mathbf{x}, \widetilde{\boldsymbol{\lambda}}, \varrho)$. Using

$$L(\mathbf{x}, \widetilde{\boldsymbol{\lambda}}, \varrho) = L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \varrho\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 \text{ and } \mathbf{g}(\mathbf{x}, \widetilde{\boldsymbol{\lambda}}, \varrho) = \mathbf{g}(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \varrho\mathsf{B}^T(\mathsf{B}\mathbf{x} - \mathbf{c}),$$

we get

$$
\begin{aligned}
L(\mathbf{y}, \widetilde{\boldsymbol{\lambda}}, \varrho) &= L(\mathbf{x}, \widetilde{\boldsymbol{\lambda}}, \varrho) + \boldsymbol{\delta}^T \widetilde{\mathbf{g}} + \frac{1}{2}\boldsymbol{\delta}^T \mathsf{A}_\varrho \boldsymbol{\delta} \\
&= L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \boldsymbol{\delta}^T \mathbf{g} + \frac{1}{2}\boldsymbol{\delta}^T \mathsf{A}_\varrho \boldsymbol{\delta} + \varrho \boldsymbol{\delta}^T \mathsf{B}^T(\mathsf{B}\mathbf{x} - \mathbf{c}) + \varrho\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 \\
&\geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \boldsymbol{\delta}^T \mathbf{g} + \frac{\lambda_{\min}}{2}\|\boldsymbol{\delta}\|^2 + \varrho \boldsymbol{\delta}^T \mathsf{B}^T(\mathsf{B}\mathbf{x} - \mathbf{c}) + \frac{\varrho}{2}\|\mathsf{B}\boldsymbol{\delta}\|^2 \\
&\quad + \varrho\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2.
\end{aligned}
$$

Noticing that

$$
\frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2 = \frac{\varrho}{2}\|\mathsf{B}\boldsymbol{\delta} + (\mathsf{B}\mathbf{x} - \mathbf{c})\|^2 = \varrho \boldsymbol{\delta}^T \mathsf{B}^T(\mathsf{B}\mathbf{x} - \mathbf{c}) + \frac{\varrho}{2}\|\mathsf{B}\boldsymbol{\delta}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2,
$$

we get

$$
L(\mathbf{y}, \widetilde{\boldsymbol{\lambda}}, \varrho) \geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \boldsymbol{\delta}^T \mathbf{g} + \frac{\lambda_{\min}}{2}\|\boldsymbol{\delta}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2. \quad (4.88)
$$

Assuming (4.83) and using simple manipulations, we get

$$
\begin{aligned}
L(\mathbf{y}, \widetilde{\boldsymbol{\lambda}}, \varrho) &\geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) - M\|\boldsymbol{\delta}\|\|\mathsf{B}\mathbf{x} - \mathbf{c}\| + \frac{\lambda_{\min}}{2}\|\boldsymbol{\delta}\|^2 \\
&\qquad + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2 \\
&= L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \left(\frac{\lambda_{\min}}{2}\|\boldsymbol{\delta}\|^2 - M\|\boldsymbol{\delta}\|\|\mathsf{B}\mathbf{x} - \mathbf{c}\| + \frac{M^2\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2}{2\lambda_{\min}}\right) \\
&\quad - \frac{M^2\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2}{2\lambda_{\min}} + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2 \\
&\geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \frac{1}{2}\left(\varrho - \frac{M^2}{\lambda_{\min}}\right)\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2,
\end{aligned}
$$

which proves (i).

If we assume that (4.85) holds, then by (4.88) and similar manipulations as above

$$
\begin{aligned}
L(\mathbf{y}, \widetilde{\boldsymbol{\lambda}}, \varrho) &\geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) - \|\boldsymbol{\delta}\|\eta + \frac{\lambda_{\min}}{2}\|\boldsymbol{\delta}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2 \\
&\geq L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x} - \mathbf{c}\|^2 + \frac{\varrho}{2}\|\mathsf{B}\mathbf{y} - \mathbf{c}\|^2 \ - \frac{\eta^2}{2\lambda_{\min}},
\end{aligned}
$$

which proves (ii).

Finally, let $\widehat{\mathbf{y}}$ denote the solution of the auxiliary problem

$$
\text{minimize} \quad L(\mathbf{y}, \boldsymbol{\lambda}, \varrho) \quad \text{s.t.} \quad \mathbf{y} \in \mathbb{R}^n, \quad (4.89)
$$

$\mathsf{B}\mathbf{z}_0 = \mathbf{c}$, and $\widehat{\boldsymbol{\delta}} = \widehat{\mathbf{y}} - \mathbf{x}$. If (4.85) holds, then

$$0 \ge L(\widehat{\mathbf{y}}, \boldsymbol{\lambda}, \varrho) - L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) = \widehat{\boldsymbol{\delta}}^T \mathbf{g} + \frac{1}{2}\widehat{\boldsymbol{\delta}}^T \mathsf{A}_\varrho \widehat{\boldsymbol{\delta}} \ge -\|\widehat{\boldsymbol{\delta}}\|\eta + \frac{1}{2}\lambda_{\min}\|\widehat{\boldsymbol{\delta}}\|^2 \ge -\frac{\eta^2}{2\lambda_{\min}}.$$

Since $L(\widehat{\mathbf{y}}, \boldsymbol{\lambda}, \varrho) \le L(\mathbf{z}_0, \boldsymbol{\lambda}, \varrho) = f(\mathbf{z}_0)$, we conclude that

$$L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) \le L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) - L(\widehat{\mathbf{y}}, \boldsymbol{\lambda}, \varrho) + f(\mathbf{z}_0) \le f(\mathbf{z}_0) + \frac{\eta^2}{2\lambda_{\min}}.$$

□

4.6.3 Convergence and Monotonicity

The analysis of SMALE is based on the following lemma.

Lemma 4.18. *Let $\{\mathbf{x}^k\}$, $\{\boldsymbol{\lambda}^k\}$, and $\{\varrho_k\}$ be generated by Algorithm 4.5 for the solution of problem (4.1) with $\eta > 0$, $\beta > 1$, $M > 0$, $\varrho_0 > 0$, and $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$. Let $\lambda_{\min}$ denote the least eigenvalue of the Hessian A of f.*
(i) If $k \ge 0$ and

$$\varrho_k \ge M^2/\lambda_{\min}, \tag{4.90}$$

then

$$L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) \ge L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) + \frac{\varrho_{k+1}}{2}\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\|^2. \tag{4.91}$$

(ii) For any $k \ge 0$

$$\begin{aligned} L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) \ge L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) &+ \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \\ &+ \frac{\varrho_{k+1}}{2}\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\|^2 - \frac{\eta^2}{2\lambda_{\min}}. \end{aligned} \tag{4.92}$$

(iii) For any $k \ge 0$ and $\mathbf{z}_0$ such that $\mathsf{B}\mathbf{z}_0 = \mathbf{c}$

$$L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) \le f(\mathbf{z}_0) + \frac{\eta^2}{2\lambda_{\min}}. \tag{4.93}$$

Proof. In Lemma 4.17, let us substitute $\mathbf{x} = \mathbf{x}^k$, $\boldsymbol{\lambda} = \boldsymbol{\lambda}^k$, $\varrho = \varrho_k$, and $\mathbf{y} = \mathbf{x}^{k+1}$, so that inequality (4.83) holds by (4.80), and by (4.81) $\widetilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda}^{k+1}$.

If (4.90) holds, we get by (4.84)

$$L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_k) \ge L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) + \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\|^2. \tag{4.94}$$

To prove (4.91), it is enough to add

$$\frac{\varrho_{k+1} - \varrho_k}{2}\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\|^2 \tag{4.95}$$

to both sides of (4.94) and to notice that

$$L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) = L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_k) + \frac{\varrho_{k+1} - \varrho_k}{2}\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\|^2. \quad (4.96)$$

If we notice that by the definition of Step 1 of Algorithm 4.5

$$\|\mathbf{g}(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k)\| \leq \eta,$$

we can apply the same substitution as above to Lemma 4.17(ii) to get

$$\begin{aligned} L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_k) \geq \quad & L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) \\ & + \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 + \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^{k+1} - \mathbf{c}\|^2 - \frac{\eta^2}{2\lambda_{\min}}. \quad (4.97) \end{aligned}$$

After adding the nonnegative expression (4.95) to both sides of (4.97) and using (4.96), we get (4.92). Similarly, inequality (4.93) results from application of the substitution to Lemma 4.17(iii). □

Theorem 4.19. *Let $\{\mathbf{x}^k\}$, $\{\boldsymbol{\lambda}^k\}$, and $\{\varrho_k\}$ be generated by Algorithm 4.5 for the solution of problem (4.1) with $\eta > 0$, $\beta > 1$, $M > 0$, $\varrho_0 > 0$, and $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$. Let $\lambda_{\min}$ denote the least eigenvalue of the Hessian A of f and let $s \geq 0$ denote the smallest integer such that*

$$\beta^s \varrho_0 \geq M^2/\lambda_{\min}.$$

(i) The sequence $\{\varrho_k\}$ is bounded and

$$\varrho_k \leq \beta^s \varrho_0. \quad (4.98)$$

(ii) If $\mathbf{z}_0$ denotes any vector such that $\mathsf{B}\mathbf{z}_0 = \mathbf{c}$, then

$$\sum_{k=1}^{\infty} \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \leq f(\mathbf{z}_0) - L(\mathbf{x}^0, \boldsymbol{\lambda}^0, \varrho_0) + (1+s)\frac{\eta^2}{2\lambda_{\min}}. \quad (4.99)$$

(iii) The sequence $\{\mathbf{x}^k\}$ converges to the solution $\widehat{\mathbf{x}}$ of (4.1).
(iv) The sequence $\{\boldsymbol{\lambda}^k\}$ converges to the vector

$$\overline{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} + (\mathsf{I} - \mathsf{P})\boldsymbol{\lambda}^0,$$

where P is the orthogonal projector onto $\mathrm{Im}\mathsf{B}$, and $\boldsymbol{\lambda}_{\mathrm{LS}}$ is the least square Lagrange multiplier of (4.1).

Proof. Let $s \geq 0$ denote the smallest integer such that $\beta^s \varrho_0 \geq M^2/\lambda_{\min}$ and let $\mathcal{I}$ denote the set of all indices k_i such that $\{\varrho_{k_i} > \varrho_{k_{i-1}}\}$. Using Lemma 4.18(i), $\varrho_{k_i} = \beta\varrho_{k_{i-1}} = \beta^i \varrho_0$ for $k_i \in \mathcal{I}$, and $\beta^s \varrho_0 \geq M^2/\lambda_{\min}$, we conclude that there is no k such that $\varrho_k > \beta^s \varrho_0$. Thus $\mathcal{I}$ has at most s elements and (4.98) holds.

By the definition of Step 3, for $k > 0$ either $k+1 \notin \mathcal{I}$ and

$$\frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \le L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) - L(\mathbf{x}^{k-1}, \boldsymbol{\lambda}^{k-1}, \varrho_{k-1}),$$

or $k+1 \in \mathcal{I}$ and by (4.92)

$$\begin{aligned}\frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 &\le \frac{\varrho_{k-1}}{2}\|\mathsf{B}\mathbf{x}^{k-1} - \mathbf{c}\|^2 + \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \\ &\le L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) - L(\mathbf{x}^{k-1}, \boldsymbol{\lambda}^{k-1}, \varrho_{k-1}) + \frac{\eta^2}{2\lambda_{\min}}.\end{aligned}$$

Summing up the appropriate cases of the last two inequalities for $k = 1, \dots, n$ and taking into account that $\mathcal{I}$ has at most s elements, we get

$$\sum_{k=1}^{n} \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \le L(\mathbf{x}^n, \boldsymbol{\lambda}^n, \varrho_n) - L(\mathbf{x}^0, \boldsymbol{\lambda}^0, \varrho_0) + s\frac{\eta^2}{2\lambda_{\min}}. \tag{4.100}$$

To get (4.99), it is enough to replace $L(\mathbf{x}^n, \boldsymbol{\lambda}^n, \varrho_n)$ by the upper bound (4.93).

To prove (iii) and (iv), let us denote

$$\mathbf{g}^k = \mathbf{g}(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) = \mathsf{A}_{\varrho_k}\mathbf{x}^k + \mathsf{B}^T\boldsymbol{\lambda}^k - \mathbf{b} - \varrho_k\mathsf{B}^T\mathbf{c}, \quad \mathsf{A}_{\varrho_k} = \mathsf{A} + \varrho_k\mathsf{B}^T\mathsf{B},$$

and let us assume that B is a full row rank matrix. Since the unique KKT pair $(\widehat{\mathbf{x}}, \widehat{\boldsymbol{\lambda}})$ is fully determined by

$$\begin{aligned}\mathsf{A}\widehat{\mathbf{x}} + \mathsf{B}^T\widehat{\boldsymbol{\lambda}} &= \mathbf{b},\\ \mathsf{B}\widehat{\mathbf{x}} \qquad\quad &= \mathbf{c},\end{aligned}$$

we can rewrite $\mathbf{g}^k$ as

$$\mathbf{g}^k = \mathsf{A}_{\varrho_k}(\mathbf{x}^k - \widehat{\mathbf{x}}) + \mathsf{B}^T(\boldsymbol{\lambda}^k - \widehat{\boldsymbol{\lambda}}). \tag{4.101}$$

The last equation together with

$$\mathsf{B}(\mathbf{x}^k - \widehat{\mathbf{x}}) = \mathsf{B}\mathbf{x}^k - \mathbf{c} \tag{4.102}$$

may be written in the matrix form as

$$\begin{pmatrix} \mathsf{A}_{\varrho_k} & \mathsf{B}^T \\ \mathsf{B} & 0 \end{pmatrix}\begin{pmatrix} \mathbf{x}^k - \widehat{\mathbf{x}} \\ \boldsymbol{\lambda}^k - \widehat{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \mathbf{g}^k \\ \mathsf{B}\mathbf{x}^k - \mathbf{c} \end{pmatrix}. \tag{4.103}$$

Since $\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|$ converges to zero due to (4.99), $\|\mathbf{g}^k\| \le M\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|$, and the matrix of the system (4.103) is regular, we conclude, using Proposition 2.12, that $\mathbf{x}^k$ converges to $\widehat{\mathbf{x}}$ and $\boldsymbol{\lambda}^k$ converges to $\widehat{\boldsymbol{\lambda}}$. Since B is a full rank matrix, it follows that $\widehat{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_{\mathrm{LS}} = \overline{\boldsymbol{\lambda}}$.

If B is not a full rank matrix, then the augmented matrix on the left-hand side of (4.103) is singular, but the solution $\widehat{\mathbf{x}}$ is still uniquely determined, as $\mathrm{Ker}\mathsf{A} \cap \mathrm{Ker}\mathsf{B} \subseteq \mathrm{Ker}\mathsf{A} = \{\mathbf{o}\}$ by the assumptions. Since any KKT pair $(\widehat{\mathbf{x}}, \overline{\boldsymbol{\lambda}})$ satisfies

$$\begin{pmatrix} \mathsf{A}_{\varrho_k} & \mathsf{B}^T \\ \mathsf{B} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{x}^k - \widehat{\mathbf{x}} \\ \boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \mathbf{g}^k \\ \mathsf{B}\mathbf{x}^k - \mathbf{c} \end{pmatrix}, \tag{4.104}$$

we can use the same arguments as above and Proposition 2.12 to find out again that $\mathbf{x}^k$ converges to $\widehat{\mathbf{x}}$, but now we shall get only that $\mathsf{B}^T\boldsymbol{\lambda}^k$ converges to $\mathsf{B}^T\overline{\lambda}$. However, using Lemma 4.10, we get

$$\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}} = \mathsf{P}\boldsymbol{\lambda}^k - \boldsymbol{\lambda}_{\mathrm{LS}},$$

so that in particular $\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}} \in \mathrm{Im}\mathsf{B}$. It follows by (1.34) that

$$\|\mathsf{B}^T(\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}})\| \geq \overline{\sigma}_{\min}\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|.$$

Since the right-hand side converges to zero, we conclude that $\boldsymbol{\lambda}^k$ converges to $\overline{\boldsymbol{\lambda}}$, which completes the proof of (iii) and (iv). □

4.6.4 Linear Convergence for Large ϱ_0

Using the estimates of the previous section, we can prove that Algorithm 4.5 converges to the solution $\overline{\boldsymbol{\lambda}}$ linearly provided ϱ_0 is sufficiently large. We shall formulate this result explicitly.

Proposition 4.20. *Let $\{\boldsymbol{\lambda}^k\}$,$\{\mathbf{x}^k\}$, and $\{\varrho_k\}$ be generated by Algorithm 4.5 for problem (4.1) with the initialization defined in Step 0 and*

$$\varrho_0 \geq 2\alpha^{-1}(\overline{\varrho} + \overline{\beta}_{\min}^{-1}), \tag{4.105}$$

where we use the notation of Lemma 4.13 and α is an arbitrary constant such that $0 < \alpha < 1$.

(i) For any index $k \geq 0$

$$\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| \leq \alpha\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|. \tag{4.106}$$

(ii) There is a constant C_1 such that for any index $k \geq 0$

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \leq C_1\alpha^k. \tag{4.107}$$

(iii) There is a constant C_2 such that for any index $k \geq 0$

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\| \leq C_2\alpha^k. \tag{4.108}$$

Proof. (i) Let ϱ_0 satisfy (4.105). Comparing (4.80) with (4.68) and taking into account that $\varrho_k \geq \varrho_0$, we can check that all the assumptions of Lemma 4.13 are satisfied for $\mathbf{x} = \mathbf{x}^k$, $\boldsymbol{\lambda} = \boldsymbol{\lambda}^k$, and $\varrho = \varrho_k$. Substituting into (4.69) and using $\boldsymbol{\lambda}^{k+1} = \widetilde{\boldsymbol{\lambda}}$, we get

$$\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| \leq 2{\varrho_k}^{-1}(\overline{\varrho} + \overline{\beta}_{\min}^{-1})\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\| \leq \alpha\|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|.$$

This proves (4.106).
(ii) Using the update rule of Step 2 of Algorithm 4.5, we get

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| = \varrho_k^{-1}\|\boldsymbol{\lambda}^{k+1} - \boldsymbol{\lambda}^k\| \leq \varrho_k^{-1}(\|\boldsymbol{\lambda}^{k+1} - \overline{\boldsymbol{\lambda}}\| + \|\boldsymbol{\lambda}^k - \overline{\boldsymbol{\lambda}}\|),$$

and by (4.106), we get

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \leq \varrho_k^{-1}(\alpha^{k+1} + \alpha^k)\|\boldsymbol{\lambda}^0 - \overline{\boldsymbol{\lambda}}\| \leq 2\alpha^k\varrho_0^{-1}\|\boldsymbol{\lambda}^0 - \overline{\boldsymbol{\lambda}}\| = C_1\alpha^k.$$

This proves (4.107).
(iii) Observe that (4.107) and the condition (4.80) in the definition of Step 1 of Algorithm 4.5 imply that there is a constant C_1 such that

$$\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \leq C_1\alpha^k \quad \text{and} \quad \|\mathbf{g}^k\| \leq C_1\alpha^k.$$

To finish the proof, it is enough to use Proposition 2.12 and simple manipulations. □

4.6.5 Optimality of the Outer Loop

Theorem 4.19 suggests that for homogeneous constraints, it is possible to give a rate of convergence of the feasibility error that does not depend on the constraint matrix B. To present explicitly this qualitatively new feature of Algorithm 4.5, at least as compared to the related Algorithm 4.4, let $\mathcal{T}$ denote any set of indices and assume that for any $t \in \mathcal{T}$ there is defined a problem

$$\text{minimize} \quad f_t(\mathbf{x}) \quad \text{s.t.} \quad \mathbf{x} \in \Omega_t \tag{4.109}$$

with $\Omega_t = \{\mathbf{x} \in \mathbb{R}^{n_t} : \mathsf{B}_t\mathbf{x} = \mathbf{o}\}$, $f_t(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathsf{A}_t\mathbf{x} - \mathbf{b}_t^T\mathbf{x}$, $\mathsf{A}_t \in \mathbb{R}^{n_t \times n_t}$ symmetric positive definite, $\mathsf{B}_t \in \mathbb{R}^{m_t \times n_t}$, and $\mathbf{b}_t, \mathbf{x} \in \mathbb{R}^{n_t}$. Our optimality result then reads as follows.

Theorem 4.21. *Let $\{\mathbf{x}_t^k\}, \{\boldsymbol{\lambda}_t^k\}$, and $\{\varrho_{t,k}\}$ be generated by Algorithm 4.5 for (4.109) with $\|\mathbf{b}_t\| \geq \eta_t > 0$, $\beta > 1$, $M > 0$, $\varrho_{t,0} = \varrho_0 > 0$, $\boldsymbol{\lambda}_t^0 = \mathbf{o}$. Let $0 < a_{\min}$ be a given constant. Finally, let the class of problems (4.109) satisfy*

$$a_{\min} \leq \lambda_{\min}(\mathsf{A}_t),$$

where $\lambda_{\min}(\mathsf{A}_t)$ denotes the smallest eigenvalue of A_t, and denote

$$a = (2 + s)/(a_{\min}\varrho_0),$$

where $s \geq 0$ is the smallest integer such that $\beta^s\varrho_0 \geq M^2/a_{\min}$. Then for each $\varepsilon > 0$ there are the indices k_t, $t \in \mathcal{T}$, such that

$$k_t \le a/\varepsilon^2 + 1$$

and $\mathbf{x}_t^{k_t}$ *is an approximate solution of (4.109) satisfying*

$$\|\mathbf{g}_t(\mathbf{x}_t^{k_t}, \boldsymbol{\lambda}_t^{k_t}, \varrho_{t,k_t})\| \le M\varepsilon\|\mathbf{b}_t\| \quad \textit{and} \quad \|\mathsf{B}_t\mathbf{x}_t^{k_t}\| \le \varepsilon\|\mathbf{b}_t\|. \tag{4.110}$$

Proof. First notice that for any index j

$$\frac{j\varrho_0}{2} \min_{i\in\{1,\dots,j\}} \|\mathsf{B}_t\mathbf{x}_t^i\|^2 \le \sum_{i=1}^{j} \frac{\varrho_{t,i}}{2}\|\mathsf{B}_t\mathbf{x}_t^i\|^2 \le \sum_{i=1}^{\infty} \frac{\varrho_{t,i}}{2}\|\mathsf{B}_t\mathbf{x}_t^i\|^2. \tag{4.111}$$

Denoting by $L_t(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$ the Lagrangian for problem (4.109), we get for any $\mathbf{x} \in \mathbb{R}^{n_t}$ and $\varrho \ge 0$

$$L_t(\mathbf{x}, \mathbf{o}, \varrho) = \frac{1}{2}\mathbf{x}^T(\mathsf{A}_t + \varrho\mathsf{B}_t^T\mathsf{B}_t)\mathbf{x} - \mathbf{b}_t^T\mathbf{x} \ge \frac{1}{2}a_{\min}\|\mathbf{x}\|^2 - \|\mathbf{b}_t\|\|\mathbf{x}\| \ge -\frac{\|\mathbf{b}_t\|^2}{2a_{\min}}.$$

If we substitute this inequality and $\mathbf{z} = \mathbf{z}_0^t = \mathbf{o}$ into (4.99) and use $\|\mathbf{b}_t\| \ge \eta_t$, we get for any $t \in \mathcal{T}$

$$\sum_{i=1}^{\infty} \frac{\varrho_{t,i}}{2}\|\mathsf{B}_t\mathbf{x}_t^i\|^2 \le \frac{\|\mathbf{b}_t\|^2}{2a_{\min}} + \frac{(1+s)\eta_t^2}{2a_{\min}} \le \frac{2+s}{2a_{\min}}\|\mathbf{b}_t\|^2 = \frac{a\varrho_0}{2}\|\mathbf{b}_t\|^2. \tag{4.112}$$

Combining the latter inequality with (4.111), we get

$$\min\{\|\mathsf{B}_t\mathbf{x}_t^i\|^2 : i = 1, \dots, k\} \le a\|\mathbf{b}_t\|^2/j. \tag{4.113}$$

Taking for j the smallest integer that satisfies $a/j \le \varepsilon^2$, so that

$$a/\varepsilon^2 \le j \le a/\varepsilon^2 + 1,$$

and denoting for any $t \in \mathcal{T}$ by $k_t \in \{1, \dots, j\}$ the index which minimizes $\{\|\mathsf{B}_t\mathbf{x}_t^i\| : i = 1, \dots, j\}$, we can use (4.113) to obtain

$$\|\mathsf{B}_t\mathbf{x}_t^{k_t}\|^2 = \min\{\|\mathsf{B}_t\mathbf{x}_t^i\|^2 : i = 1, \dots, j\} \le a\|\mathbf{b}_t\|^2/j \le \varepsilon^2\|\mathbf{b}_t\|^2.$$

Thus

$$\|\mathsf{B}_t\mathbf{x}_t^{k_t}\|^2 \le \varepsilon^2\|\mathbf{b}_t\|^2,$$

and, using the definition of Step 1 of Algorithm 4.5, we get also the inequality

$$\|\mathbf{g}_t(\mathbf{x}_t^{k_t}, \boldsymbol{\lambda}_t^{k_t}, \varrho_{t,k_t})\| \le M\|\mathsf{B}_t\mathbf{x}_t^{k_t}\| \le M\varepsilon\|\mathbf{b}_t\|.$$

□

Let us recall that

$$\|\mathbf{g}_t(\mathbf{x}_t^{k_t}, \boldsymbol{\lambda}_t^{k_t+1}, 0)\| = \|\mathbf{g}_t(\mathbf{x}_t^{k_t}, \boldsymbol{\lambda}_t^{k_t}, \varrho_{t,k_t})\|,$$

so that $(\mathbf{x}_t^{k_t}, \boldsymbol{\lambda}_t^{k_t+1})$ is an approximate KKT pair of problem (4.109). The assumption on homogeneity of the constraints was used to find $\mathbf{z}_0^t$ such that $f(\mathbf{z}_0^t)$ is uniformly bounded, in this case by zero.

4.6.6 Optimality of SMALE with Conjugate Gradients

We shall need the following simple lemma to prove optimality of the inner loop.

Lemma 4.22. *Let* $\{\mathbf{x}^k\}, \{\boldsymbol{\lambda}^k\}$, *and* $\{\varrho_k\}$ *be generated by Algorithm 4.5 for problem* (4.1) *with* $\eta > 0$, $\beta > 1$, $M > 0$, $\varrho_0 > 0$, *and* $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$. *Let* $\lambda_{\min}$ *denote the least eigenvalue of* A.

Then for any $k \geq 0$

$$L(\mathbf{x}^k, \boldsymbol{\mu}^{k+1}, \varrho_{k+1}) - L(\mathbf{x}^{k+1}, \boldsymbol{\mu}^{k+1}, \varrho_{k+1}) \leq \frac{\eta^2}{2\lambda_{\min}} + \frac{\beta\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2. \quad (4.114)$$

Proof. Notice that by definition of the Lagrangian function and by the update rule (4.81)

$$\begin{aligned} L(\mathbf{x}^k, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) &= L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) + \varrho_k\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 + \frac{\varrho_{k+1} - \varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2 \\ &= L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) + \frac{\varrho_{k+1} + \varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2. \end{aligned}$$

After subtracting $L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1})$ from both sides and observing that by (4.92)

$$L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k) - L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) \leq \frac{\eta^2}{2\lambda_{\min}} - \frac{\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2,$$

we get

$$L(\mathbf{x}^k, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) - L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho_{k+1}) \leq \frac{\eta^2}{2\lambda_{\min}} + \frac{\beta\varrho_k}{2}\|\mathsf{B}\mathbf{x}^k - \mathbf{c}\|^2.$$

□

Now we are ready to prove our main result concerning the inner loop.

Theorem 4.23. *Let* $\{\mathbf{x}_t^k\}, \{\boldsymbol{\lambda}_t^k\}$, *and* $\{\varrho_{t,k}\}$ *be generated by Algorithm 4.5 for (4.109) with* $\|\mathbf{b}_t\| \geq \eta_t > 0$, $\beta > 1$, $M > 0$, $\varrho_{t,0} = \varrho_0 > 0$, $\boldsymbol{\lambda}_t^0 = \mathbf{o}$. *Let* $0 < a_{\min} < a_{\max}$ *and* $0 < B_{\max}$ *be given constants. Let Step 1 be implemented by the conjugate gradient method which generates the iterates* $\mathbf{x}_t^{k,0}, \mathbf{x}_t^{k,1}, \ldots, \mathbf{x}_t^{k,l} = \mathbf{x}_t^k$ *starting from* $\mathbf{x}_t^{k,0} = \mathbf{x}_t^{k-1}$ *with* $\mathbf{x}_t^{-1} = \mathbf{o}$, *where* $l = l(k,t)$ *is the first index satisfying either*

$$\|g(\mathbf{x}_t^{k,l}, \boldsymbol{\lambda}_t^k, \varrho_k)\| \leq M\|\mathsf{B}_t\mathbf{x}_t^{k,l}\| \quad (4.115)$$

or

$$\|g(\mathbf{x}_t^{k,l}, \boldsymbol{\lambda}_t^k, \varrho_k)\| \leq \varepsilon M\|\mathbf{b}_t\|. \quad (4.116)$$

Finally, let the class of problems (4.109) satisfy

$$a_{\min} \le \lambda_{\min}(\mathsf{A}_t) \le \lambda_{\max}(\mathsf{A}_t) = \|\mathsf{A}_t\| \le a_{\max} \quad \textit{and} \quad \|\mathsf{B}_t\| \le B_{\max}. \tag{4.117}$$

Then Algorithm 4.5 generates an approximate solution $\mathbf{x}_t^{k_t}$ *of any problem (4.109) which satisfies (4.110) at* $O(1)$ *matrix–vector multiplications by the Hessian of the augmented Lagrangian* L_t *for (4.109).*

Proof. Let $t \in \mathcal{T}$ be fixed and let us denote by $L_t(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$ the augmented Lagrangian for problem (4.109), so that for any $\mathbf{x} \in \mathbb{R}^p$ and $\varrho \ge 0$

$$L_t(\mathbf{x}, \mathbf{o}, \varrho) = \frac{1}{2}\mathbf{x}^T(\mathsf{A}_t + \varrho \mathsf{B}_t^T \mathsf{B}_t)\mathbf{x} - \mathbf{b}_t^T\mathbf{x} \ge \frac{1}{2} a_{\min}\|\mathbf{x}\|^2 - \|\mathbf{b}_t\|\|\mathbf{x}\| \ge -\frac{\|\mathbf{b}_t\|^2}{2a_{\min}}.$$

Applying the latter inequality to (4.99) with $\mathbf{z}_0 = \mathbf{o}$ and $\boldsymbol{\lambda}_t^0 = \mathbf{o}$, we get, using the assumption $\|\mathbf{b}_t\| \ge \eta_t$, that for any $k \ge 0$

$$\begin{aligned} \frac{\varrho_{t,k}}{2}\|\mathsf{B}_t\mathbf{x}_t^k\|^2 &\le \sum_{i=1}^{\infty} \frac{\varrho_{t,i}}{2}\|\mathsf{B}_t\mathbf{x}_t^i\|^2 \le f(\mathbf{z}_0) - L(\mathbf{x}_t^0, \boldsymbol{\lambda}_t^0, \varrho_{t,0}) + (1+s)\frac{\eta_t^2}{2a_{\min}} \\ &\le (2+s)\|\mathbf{b}_t\|^2/(2a_{\min}), \end{aligned}$$

where $s \ge 0$ denotes the smallest integer such that $\beta^s \varrho_0 \ge M^2/a_{\min}$. Thus by (4.114)

$$\begin{aligned} L_t(\mathbf{x}_t^{k-1}, \boldsymbol{\lambda}_t^k, \varrho_{t,k}) - L_t(\mathbf{x}_t^k, \boldsymbol{\lambda}_t^k, \varrho_{t,k}) &\le \frac{\eta_t^2}{2a_{\min}} + \frac{\beta\varrho_{t,k-1}}{2}\|\mathsf{B}_t\mathbf{x}_t^{k-1}\|^2 \\ &\le (3+s)\beta\|\mathbf{b}_t\|^2/(2a_{\min}), \end{aligned} \tag{4.118}$$

and, since the minimizer $\overline{\mathbf{x}}_t^k$ of $L_t(\,.\,, \boldsymbol{\lambda}_t^k, \varrho_{t,k})$ satisfies (4.115) and is a possible choice for $\mathbf{x}_t^k$, also

$$L_t(\mathbf{x}_t^{k-1}, \boldsymbol{\lambda}_t^k, \varrho_{t,k}) - L_t(\overline{\mathbf{x}}_t^k, \boldsymbol{\lambda}_t^k, \varrho_{t,k}) \le (3+s)\beta\|\mathbf{b}_t\|^2/(2a_{\min}). \tag{4.119}$$

Denoting

$$a_1 = (3+s)\beta/a_{\min},$$

we can estimate the energy norm of the gradient by

$$\|\mathbf{g}_t(\mathbf{x}_t^{k,0}, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\|^2_{\mathsf{A}_{t,k}^{-1}} = 2\big(L_t(\mathbf{x}_t^{k-1}, \boldsymbol{\lambda}_t^k, \varrho_{t,k}) - L_t(\overline{\mathbf{x}}_t^k, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\big) \le a_1\|\mathbf{b}_t\|^2,$$

where

$$\mathsf{A}_{t,k} = \mathsf{A}_t + \frac{\varrho_{t,k}}{2}\mathsf{B}_t^T\mathsf{B}_t.$$

Since

$$a_{\min} \le \lambda_{\min}(\mathsf{A}_{t,k}) \le \|\mathsf{A}_{t,k}\| \le \|\mathsf{A}_t\| + \varrho_{t,k}\|\mathsf{B}_t\|^2 \le a_{\max} + \beta^s\varrho_0 B_{\max}^2,$$

we can also bound the spectral condition number $\kappa(\mathsf{A}_{t,k})$ of $\mathsf{A}_{t,k}$ by

$$K = \left(a_{\max} + \beta^s\varrho_0 B_{\max}^2\right)/a_{\min}.$$

Combining this bound with the estimate (3.21) which reads in our case

$$\|\mathbf{g}_t(\mathbf{x}_t^{k,l}, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\|^2_{\mathsf{A}_{t,k}^{-1}} \le 4 \left(\frac{\sqrt{\kappa(\mathsf{A}_{t,k})} - 1}{\sqrt{\kappa(\mathsf{A}_{t,k})} + 1} \right)^{2l} \|\mathbf{g}_t(\mathbf{x}_t^{k,0}, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\|^2_{\mathsf{A}_{t,k}^{-1}},$$

we get

$$\begin{aligned}\|\mathbf{g}_t(\mathbf{x}_t^{k,l}, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\|^2 &\le \frac{1}{a_{\min}} \|\mathbf{g}_t(\mathbf{x}_t^{k,l}, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\|^2_{\mathsf{A}_{t,k}^{-1}} \le \frac{4\sigma^{2l}}{a_{\min}} \|\mathbf{g}_t(\mathbf{x}_t^{k,0}, \boldsymbol{\lambda}_t^k, \varrho_{t,k})\|^2_{\mathsf{A}_{t,k}^{-1}} \\ &\le \frac{4a_1}{a_{\min}} \sigma^{2l} \|\mathbf{b}_t\|^2,\end{aligned}$$

where

$$\sigma = \frac{\sqrt{K} - 1}{\sqrt{K} + 1} < 1.$$

It simply follows by the inner stop rule (4.116) that the number of the inner iterations is uniformly bounded by any index $l = l_{\max}$ which satisfies

$$\frac{4a_1}{a_{\min}} \sigma^{2l} \|\mathbf{b}_t\|^2 \le \varepsilon^2 \|\mathbf{b}_t\|^2 M^2.$$

To finish the proof, it is enough to combine this result with Theorem 4.21. □

We can observe optimality in the solution of more general classes of problems than those considered in Theorem 4.23 provided we can bound the number of iterations in the inner loop. For an example of optimality when $\|\mathsf{B}_t\|$ is not bounded see Sect. 4.8.2.

4.6.7 Solution of More General Problems

If A is positive definite only on the kernel of B, then we can use a suitable penalization to reduce such problem to the convex one. Using Lemma 1.3, it follows that there is $\overline{\varrho} > 0$ such that $\mathsf{A} + \overline{\varrho}\mathsf{B}^T\mathsf{B}$ is positive definite, so that we can apply our SMALE algorithm to the equivalent penalized problem

$$\min_{\mathbf{x} \in \Omega_E} f_{\overline{\varrho}}(\mathbf{x}), \tag{4.120}$$

where

$$f_{\overline{\varrho}}(\mathbf{x}) = \mathbf{x}^T(\mathsf{A} + \overline{\varrho}\mathsf{B}^T\mathsf{B})\mathbf{x} - \mathbf{b}^T\mathbf{x}.$$

Alternatively, we can modify the inner loop of SMALE so that it leaves the inner loop and increases the penalty parameter whenever the negative curvature is recognized. Let us point out that such modification does not guarantee optimality of the modified algorithm.

4.7 Implementation of Inexact Augmented Lagrangians

We shall complete the discussion of inexact augmented Lagrangian algorithms by a few hints concerning their implementation.

4.7.1 Stopping, Modification of Constraints, and Preconditioning

While implementing the inexact augmented Lagrangian algorithms of Sects. 4.4 and 4.6, a stopping criterion should be added not only after Step 1, but also into the procedure which generates $\mathbf{x}^k$ in Step 1. We use in our experiments the stopping criterion

$$\|\nabla L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho_k)\| \le \varepsilon_g \|\mathbf{b}\| \text{ and } \|\mathsf{B}\mathbf{x}^k - \mathbf{c}\| \le \varepsilon_f \|\mathbf{b}\|.$$

The relative precisions ε_f and ε_g should be judiciously determined. Our stopping criterion in the inner conjugate gradient loop of SMALE reads

$$\|\mathbf{g}(\mathbf{y}^i, \boldsymbol{\lambda}^i, \varrho_i)\| \le \min\{M\|\mathsf{B}\mathbf{y}^i - \mathbf{c}\|, \eta\} \text{ or } \|\mathbf{g}(\mathbf{y}^i, \boldsymbol{\lambda}^i, \varrho_i)\| \le \min\{\varepsilon_g, M\varepsilon_f\}\|\mathbf{b}\|,$$

so that the inner loop is interrupted when either the solution or a new iterate $\mathbf{x}^k = \mathbf{y}^i$ is found.

Before applying the algorithms presented to problems with a well-conditioned Hessian A, we strongly recommend to rescale the equality constraints so that $\|\mathsf{A}\| \approx \|\mathsf{B}\|$. Taking into account the estimate of the rate of convergence like (4.69), it is also useful to orthonormalize or at least normalize the constraints. This approach has been successfully applied, e.g., in the FETI-DP-based solver for analysis of layered composites [137].

If the Hessian A is ill-conditioned and there is an approximation M of A that can be used as preconditioner, then we can use the preconditioning strategies introduced in the discussion on implementation of the penalty method in Sect. 4.2.6. The construction of the matrix M is typically problem dependent. We refer interested readers to the books by Axelsson [4], Saad [163], van der Vorst [178], or Chen [21].

Sometimes it is possible to exploit the structure of the problem for very efficient implementation of preconditioning. For example, it has been shown that it is possible to find multigrid preconditioners to the discretized Stokes problem so that the latter can be solved by SMALE with asymptotically linear complexity [144].

4.7.2 Initialization of Constants

Though all the inexact algorithms converge with $0 < \alpha < 1$, $\beta > 1$, $\eta > 0$, $\eta_0 > 0$, $\varrho_0 > 0$, $M > 0$, and $\boldsymbol{\lambda}^0 \in \mathbb{R}^m$, their choice affects the performance of the algorithms and should exploit available information. Here we give a few hints and heuristics that can be useful for their efficient implementation.

The parameter α is used only in the adaptive augmented Lagrangian algorithm 4.4. This parameter determines the final rate of convergence of approximations of the Lagrange multipliers in the outer loop; however, its small value can slow down the convergence in the inner loop via increasing the penalty parameter. We use $\alpha = 0.1$.

The parameter β is used by SMALE algorithm 4.5 and the adaptive augmented Lagrangian algorithm 4.4 to increase the penalty parameter. Our experience indicates that $\beta = 10$ is a reasonable choice.

The parameter η is used only by SMALE algorithm 4.5. It helps to avoid outer iterations that do not invoke the inner CG iterations; we use $\eta = 0.1\|\mathbf{b}\|$.

The parameter η_0 is used by Algorithm 4.4 to define the initial bound on the feasibility error which is used to control the update of the penalty parameter. The algorithm does not seem to be sensitive with respect to η_0; we use $\eta_0 = 0.1\|\mathbf{b}\|$.

The estimate (4.99) shows that a large value of the initial penalty parameter ϱ_0 guarantees fast convergence of the outer loop. By analysis of the penalty method in Sect. 4.2, it is even possible to find the solution in one outer iteration. At the same time, the large value of the penalty parameter slows down the rate of convergence of the conjugate gradient method in the inner loop, but the analysis of the conjugate gradient method in Sect. 4.2.6 based on the effective condition number of $\mathsf{A}_\varrho = \mathsf{A} + \varrho \mathsf{B}^T\mathsf{B}$ indicates that the slowdown need not be severe when the number of constraints is small, or when the constraints are close to orthogonal. If neither is the case and at least crude estimates of $\|\mathsf{A}\|$ and $\|\mathsf{B}\|$ are available, a simple strategy can be based on the observation that

$$\lambda_{\min}(\mathsf{A}) \le \lambda_{\min}(\mathsf{A}_\varrho) \quad \text{and} \quad \|\mathsf{A}_\varrho\| \le \|\mathsf{A}\| + \varrho\|\mathsf{B}\|^2,$$

so that

$$\varrho\|\mathsf{B}\|^2 \le C\|\mathsf{A}\| \Rightarrow \kappa(\mathsf{A} + \varrho\mathsf{B}^T\mathsf{B}) \le (C+1)\kappa(\mathsf{A}).$$

For example, choosing $\varrho_0 = 8\times\|\mathsf{A}\|/\|\mathsf{B}\|^2$ seems to be a reasonable guess which results in $\kappa(\mathsf{A}_\varrho) \le 9\kappa(\mathsf{A})$. Let us stress that the update of the penalty parameter should be considered as a safeguard that guarantees the convergence; we should always try to avoid invoking increase of the penalty parameter as the iterates with too small penalty parameters are inefficient.

The parameter M balances the weight of the cost function and the constraints. In our implementations we use

$$M = \varepsilon_g/\varepsilon_f.$$

Notice that by Lemma 4.18 small M can prevent the penalty parameter from increasing. We can even replace the update of the penalty parameter in Step 3 by the reduction of the parameter M using $M_{k+1} = M_k/\beta$ and obvious modifications of the rest of Algorithm 4.5. See also Sect. 6.11.

If there is no better guess of the initial approximation of $\boldsymbol{\lambda}^0$, we use $\boldsymbol{\lambda}^0 = \mathbf{o}$. Recall that using $\boldsymbol{\lambda}^0 \in \mathrm{Im}\mathsf{B}$ results in $\boldsymbol{\lambda}^k$ converging to the least square Lagrange multiplier $\boldsymbol{\lambda}_{\mathrm{LS}}$.

4.8 Numerical Experiments

Here we illustrate the performance of the exact Uzawa algorithm, the exact augmented Lagrangian algorithm, and SMALE Algorithm 4.5 on minimization of the cost functions $f_{\mathrm{L},h}$ and $f_{\mathrm{LW},h}$ introduced in Sect. 3.10 subject to ill-conditioned multipoint constraints. Let us recall that we refer to Algorithm 4.2 as the Uzawa algorithm when $\varrho = 0$, and as the augmented Lagrangian algorithm when $\varrho > 0$.

4.8.1 Uzawa, Exact Augmented Lagrangians, and SMALE

Let us start with minimization of the quadratic function $f_{\mathrm{L},h}$ defined by the discretization parameter h (see page 98) subject to the multipoint constraints which join the displacements of the node with the coordinates $(0, 1/3)$ with all the other nodes in the square $[h, 1/3] \times [1/3, 2/3]$. Let us recall that the Hessian $\mathsf{A}_{\mathrm{L},h}$ of $f_{\mathrm{L},h}$ is ill-conditioned with the spectral condition number $\kappa(\mathsf{A}_{\mathrm{L},h}) \approx h^{-2}$.

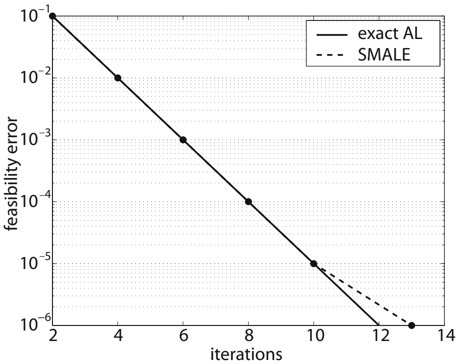

Fig. 4.3. Outer iterations of exact AL and SMALE algorithms

The graph of the relative feasibility error (vertical axis) against the numbers of outer iterations (horizontal axis) for exact augmented Lagrangians (exact AL) with $r_k = \varrho_k = 10$ and SMALE algorithm with $\varrho_0 = 10$ is in Fig. 4.3. The results were obtained with $h = 1/33$, which corresponds to $n = 1156$ unknowns and 131 multipliers. The inexact solution of auxiliary problems by SMALE has a small effect on the number of outer iterations. The SMALE algorithm required 964 CG iterations to reach the final precision. The same result was achieved by the original Uzawa algorithm with the optimal steplength after 3840 (!!!) iterations, each of them comprising direct solves of auxiliary linear problems. We conclude that even moderate regularization improves the convergence of the outer loop and the rate of convergence need not be slowed down by the inexact solution of auxiliary problems.

4.8.2 Numerical Demonstration of Optimality

To illustrate the optimality of SMALE for the solution of (4.1), let us consider the class of problems to minimize the quadratic function $f_{\mathrm{LW},h}$ (see page 99) subject to the multipoint constraints defined above. The class of problems can be given a mechanical interpretation associated to the expanding and partly stiff spring systems on Winkler's foundation. The spectrum of the Hessian $\mathsf{A}_{\mathrm{LW},h}$ of $f_{\mathrm{LW},h}$ is located in the interval $[2, 10]$. Thus the assumptions of Theorem 4.21 are satisfied and the number of outer iterations is bounded. Moreover, the rows of $\mathsf{B} \in \mathbb{R}^{m \times n}$ have a simple pattern given by

$$\mathsf{B}_{i*} = [0, \ldots, 0, 1, 0, \ldots, 0, -1, 0, \ldots, 0], \quad i = 1, \ldots, m.$$

It can be checked that $\mathsf{B}^T\mathsf{B}$ can be expressed as the sum of a matrix with the norm not exceeding four and a matrix of rank two. Using the reasoning of Sect. 4.2.6, we get that also the number of inner iterations is bounded.

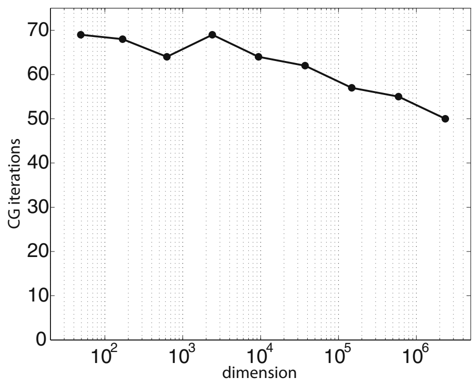

Fig. 4.4. Optimality of SMALE

In Fig. 4.4, on the vertical axis, we can see the numbers of the CG iterations k_n required to reduce the norm of the gradient and of the feasibility error to $10^{-6}\|\nabla f_{\mathrm{LW},h}(\mathbf{o})\|$ for the problems with the dimension n ranging from $n = 49$ to $n = 2362369$. The dimension n on the horizontal axis is in the logarithmic scale. We can see that k_n varies mildly with varying n, in agreement with Theorem 4.23 and the optimal property of CG. Moreover, since the cost of the matrix–vector multiplications is in our case proportional to the dimension n of the matrix $\mathsf{A}_{\mathrm{LW},h}$, it follows that the cost of the solution is also proportional to n. The number of outer iterations ranged from seven to ten.

The purpose of the above numerical experiment was just to illustrate the concept of optimality. For practical applications, it is necessary to combine SMALE with a suitable preconditioning. Application of SMALE with the multigrid preconditioning to development of in a sense optimal algorithm for the solution of the discretized Stokes problem is in Lukáš and Dostál [144].

4.9 Comments and References

The penalty method was exploited by a number of researchers to the solution of contact problems of elasticity [9, 108, 123, 125]. Theoretical results concerning the penalty method (e.g., Dostál [40], or Sect. 3.5 of Kikuchi and Oden [127]) yield that the norm of the approximation error depends on the condition number of the Hessian of the cost function. The analysis presented here generalizes the results of Dostál and Horák [65, 66]. The optimal feasibility estimate for the penalty methods (4.14) was used in development of a scalable algorithm for variational inequalities [65, 66]. The preconditioning preserving the gap in the spectrum was proposed in Dostál [44]. Reducing the spectrum of the penalized term to the one point, this preconditioning seems to be related to the constraint preconditioning for the saddle point systems introduced in nonlinear programming by Lukšan and Vlček [145]; see also Keller, Gould, and Wathen [126].

Augmented Lagrangian method was proposed independently by Powell [160] and Hestenes [116] for problems with a general cost function subject to general equality constraints. Comprehensive analysis of the augmented Lagrangian method (called the Lagrange multiplier method) including the asymptotically exact minimization of auxiliary problems was presented in the monograph by Bertsekas [11]. Applications to the solution of boundary value problems are discussed in Glowinski and Fortin [91] and Glowinski and Le Tallec [100]. Hager in [111, 113] obtained global convergence results for an algorithm of this type using inexact minimization in the solution of the auxiliary problems. In both papers the size of the optimality error was compared with the size of the feasibility error of the solution of the auxiliary problems trying to balance these quantities throughout the whole process. In [111] this comparison was used to decide whether the penalty parameter will be increased or not. In [113] it was used as a stopping criterion for the minimization of the auxiliary problems. The rate of convergence was free of any term due to inexact minimization when the least squares estimate of the Lagrange multipliers is used. Similar results for the linear update combined with the update of the penalty parameter that enforces a priori prescribed reduction of feasibility error were obtained by Dostál, Friedlander, and Santos [56] and Dostál, Friedlander, Santos, and Alesawi [58]. The same strategy was used by Conn, Gould, and Toint [26] for the solution of more general bound and equality constrained problems.

The SMALE algorithm was proposed by Dostál [46, 50]. The most attractive feature of this algorithm is a bound on the number of iterations which is independent of the constraint data. The bound has been obtained by a kind of global analysis; the result can hardly be obtained by analysis of one step of the algorithm. The algorithm has been combined with a multigrid preconditioning to develop in a sense optimal solver for the solution of a class of equality constrained problems arising from discretization of the Stokes problem; see Lukáš and Dostál [144].

Let us point out that our optimality results for the SMALE algorithm refer to the type of convergence which is known from the classical analysis of infinite series, but which is seldom exploited in numerical analysis. We shall call it the *sum bounding convergence of the second order* as it exploits the bound on the sum of the squares of errors. Though our sum bounding convergence does not guarantee even the linear rate of convergence, it is in our opinion rather a different characteristic of convergence than only a weaker one. For example, it does guarantee that the error bound for the following iterations is essentially reduced after any "bad" (here far from feasible) iteration, which is the property not guaranteed by more standard types of convergence. In our case, since we can control the upper bound by the penalty parameter, the sum bounding convergence offers an explanation to the fast convergence of the outer loop of SMALE which was observed in our numerical experiments [144].