

Chapter 13: Penalty and Augmented Lagrangian Methods

Outline

- 1 The Quadratic Penalty Method
- 2 Nonsmooth Penalty Functions
- 3 Augmented Lagrangian Method: Equality Constraints
- 4 Practical Augmented Lagrangian Methods
- 5 Perspective and Software

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Motivation

Consider the equality-constrained problem

$$\min_x f(x) \quad \text{s.t.} \quad c_i(x) = 0, \quad i \in \mathcal{E}. \quad (1.1)$$

The quadratic penalty function $Q(x; \mu)$ for this formulation is

$$Q(x; \mu) \equiv f(x) + \frac{\mu}{2} \sum_{i \in \mathcal{E}} c_i^2(x), \quad (1.2)$$

where $\mu > 0$ is the *penalty parameter*. By driving $\mu \rightarrow \infty$, we penalize the constraint violations with increasing severity. It makes good intuitive sense to consider a sequence of values $\{\mu_k\}$ with $\mu_k \uparrow \infty$ as $k \rightarrow \infty$, and to seek the approximate minimizer x_k of $Q(x; \mu_k)$ for each k .

Example

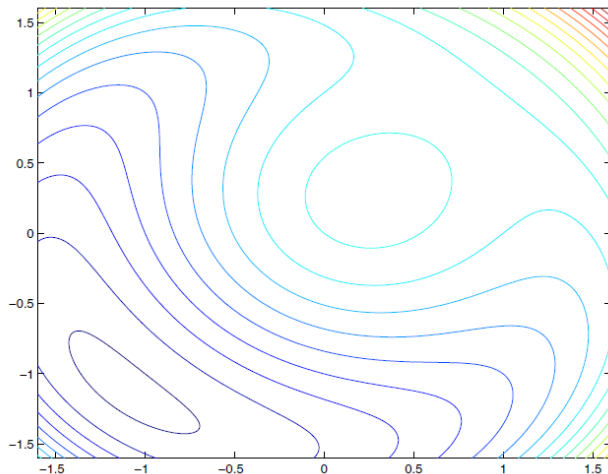
Consider the problem

$$\min_x x_1 + x_2 \quad \text{s.t.} \quad x_1^2 + x_2^2 - 2 = 0,$$

for which the solution is $(-1, -1)^T$ and the quadratic function is

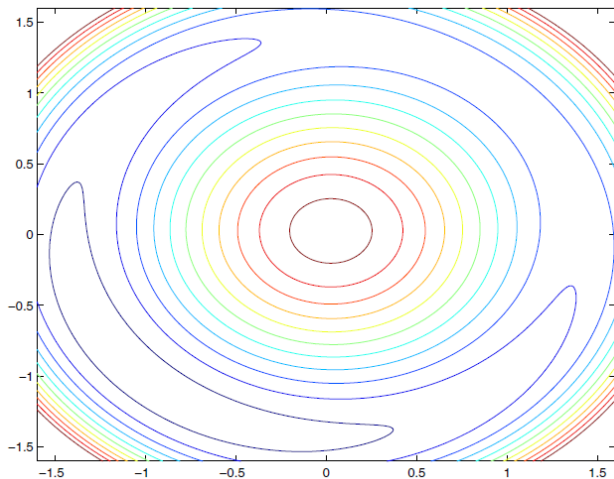
$$Q(x; \mu) = x_1 + x_2 + \frac{\mu}{2}(x_1^2 + x_2^2 - 2)^2.$$

Demo



Contours of $Q(x; \mu)$ for $\mu = 1$, contour spacing 0.5. It has a minimizer near $(-1.1, -1.1)^T$ and a local maximizer near $(0.3, 0.3)^T$.

Demo



Contours of $Q(x; \mu)$ for $\mu = 10$, contour spacing 2. It has a minimizer near $(-1, -1)^T$ and a local maximizer near $(0, 0)^T$.

One Deficiency

For a given value of the penalty parameter μ , the penalty function may be unbounded below even if the original constrained problem has a unique solution. Consider for example

$$\min -5x_1^2 + x_2^2 \quad s.t. \quad x_1 = 1,$$

whose solution is $(1, 0)^T$. The penalty function is unbounded for any $\mu < 10$. For such values of μ , the iterates generated by an unconstrained minimization method would usually diverge. This deficiency is, unfortunately, common to all the penalty functions discussed in this chapter.

Properties: Equality-case

Let $x(\mu)$ be the minimizer of $f(x) + \frac{\mu}{2} \|c(x)\|^2$.

Lemma 1

If $\mu_2 > \mu_1 \geq 0$, then $\|c(x(\mu_2))\| \leq \|c(x(\mu_1))\|$, $f(x(\mu_2)) \geq f(x(\mu_1))$.

Lemma 2

For any given $\mu > 0$, $x(\mu)$ solves

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & \|c(x)\| \leq \delta, \quad \text{where } \delta = \|c(x(\mu))\|. \end{array}$$

Lemma 3

If $f(x) + \frac{\mu}{2} \|c(x)\|^2$ is bounded below for some $\bar{\mu} > 0$. Then

$$\lim_{\mu \rightarrow \infty} \|c(x(\mu))\| = \min_{x \in \mathbb{R}^n} \|c(x)\|, \quad \lim_{\mu \rightarrow \infty} f(x(\mu)) = \min_{x \in \hat{X}} f(x)$$

where $\hat{X} := \{x : \|c(x)\| = \min_{x \in \mathbb{R}^n} \|c(x)\|\}$.

The Quadratic Penalty Function: General Case

Consider the general constrained problem

$$\min_x f(x) \quad \text{s.t. } c_i(x) = 0, \quad i \in \mathcal{E}; \quad c_i(x) \geq 0, \quad i \in \mathcal{I}. \quad (1.4)$$

The quadratic penalty functions are defined as

$$Q(x; \mu) \equiv f(x) + \frac{\mu}{2} \sum_{i \in \mathcal{E}} c_i^2(x) + \frac{\mu}{2} \sum_{i \in \mathcal{I}} ([c_i(x)]^-)^2, \quad (1.5)$$

where $[y]^-$ denotes $\max(-y, 0)$. In this case, Q may be less smooth than the objective and constraint functions.

Algorithm 1: Algorithmic Framework for Quadratic Penalty Method-Equality Case

Given $\mu_0 > 0$, a nonnegative sequence $\{\tau_k\}$ with $\tau_k \rightarrow 0$, and a starting point x_0^s ;
for $k = 0, 1, 2, \dots$
 Find an approximate minimizer x_k of $Q(\cdot; \mu_k)$, starting at x_k^s , and
 terminating when $\|\nabla_x Q(x; \mu_k)\| \leq \tau_k$;
 if final convergence test satisfied
 stop with approximate solution x_k ;
 end(if)
 Choose new penalty parameter $\mu_{k+1} > \mu_k$;
 Choose new starting point x_{k+1}^s ;
end(for)

Convergence of the Quadratic Penalty Method

Theorem 4

Suppose that each x_k is the exact global minimizer of $Q(x; \mu_k)$ in above algorithm, and that $\mu_k \uparrow \infty$. Then every limit point x^ of the sequence $\{x_k\}$ is a global solution of the problem (1.1).*

Theorem 5

Suppose that the tolerances and penalty parameters in above algorithm framework satisfy $\tau_k \rightarrow 0$ and $\mu_k \uparrow \infty$. Then

- if a limit point x^* of the sequence $\{x_k\}$ is infeasible, it is a stationary point of the function $\|c(x)\|^2$;*
- if a limit point x^* is feasible and the constraint gradients $\nabla c_i(x^*)$ are linearly independent, then x^* is a KKT point for the problem (1.1). For such points, we have for any infinite subsequence \mathcal{K} such that $\lim_{k \in \mathcal{K}} x_k = x^*$ that*

$$\lim_{k \in \mathcal{K}} -\mu_k c_i(x_k) = \lambda_i^*, \quad \forall i \in \mathcal{E},$$

where λ^ is the multiplier vector that satisfies the KKT conditions.*

ILL Conditioning and Reformulations

- The Hessian is given by the formula

$$\nabla_{xx}^2 Q(x; \mu_k) = \nabla^2 f(x) + \sum_{i \in \mathcal{E}} \mu_k c_i(x) \nabla^2 c_i(x) + \mu_k A(x)^T A(x), \quad (1.6)$$

where $A(x)^T = [\nabla c_i(x)]_{i \in \mathcal{E}}$.

- Suppose that x is close to the minimizer of $Q(\cdot; \mu_k)$ and the conditions of the above theorem is satisfied, then

$$\nabla_{xx}^2 Q(x; \mu_k) \approx \nabla_{xx}^2 \mathcal{L}(x, \lambda^*) + \mu_k A(x)^T A(x). \quad (1.7)$$

We see from this expression that $\nabla_{xx}^2 Q(x; \mu_k)$ is approximately equal to the sum of

- ▶ a matrix whose elements are independent of μ_k (the Lagrangian term), and
- ▶ a matrix of rank $|\mathcal{E}|$ whose nonzero eigenvalues are of order μ_k (the summation term in (1.7)).

ILL Conditioning and Reformulations

- Since the number of constraints $|\mathcal{E}|$ is usually fewer than n , the summation term is singular, and the overall matrix has some of its eigenvalues approaching a constant, while others are of order μ_k . Since $\mu_k \uparrow \infty$, the increasing ill conditioning of $Q(x; \mu_k)$ is apparent.
- One consequence of the ill conditioning is possible inaccuracy in the calculation of the Newton step for $Q(x; \mu_k)$, which is obtained by solving:

$$\nabla_{xx}^2 Q(x; \mu_k) p = -\nabla_x Q(x; \mu_k). \quad (1.8)$$

Significant roundoff errors will appear in p regardless of the solution technique used, and algorithms will break down as the matrix becomes numerically singular. For the same reason, iterative methods can be expected to perform poorly unless accompanied by a preconditioning strategy that removes the systematic ill conditioning. The presence of roundoff error may not disqualify p from being a good direction of progress for Newton's method.

ILL Conditioning and Reformulations

- By introducing a new variables ζ defined by $\zeta = \mu A(x)p$, we see that the vector p that solves (1.8) also satisfies the following system:

$$\begin{bmatrix} \nabla^2 f(x) + \sum_{i \in \mathcal{E}} \mu_k c_i(x) \nabla^2 c_i(x) & A(x)^T \\ A(x) & -(1/\mu_k)I \end{bmatrix} \begin{bmatrix} p \\ \zeta \end{bmatrix} = \begin{bmatrix} -\nabla_x Q(x; \mu_k) \\ 0 \end{bmatrix}. \quad (1.9)$$

- When x is not too far from the solution x^* , the coefficient matrix in (1.9) does not have large values (of order μ_k), so the system (1.9) can be viewed as a well conditioned reformulation of (1.8).
- (1.9) allows us to view the quadratic penalty method either as the application of unconstrained minimization to the penalty function $Q(\cdot, \mu_k)$ or as a variation on the SQP methods.

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Exact Penalty Functions

- Some penalty functions are *exact*, which means that, for certain choices of their penalty parameters, a single minimization with respect to x can yield the exact solution of the nonlinear programming problem.
- This property is desirable because it makes the performance of penalty methods less dependent on the strategy for updating the penalty parameter.
- A popular nonsmooth penalty function for the general nonlinear programming problem (1.4) is the ℓ_1 *penalty function* defined by

$$\phi_1(x; \mu) = f(x) + \mu \sum_{i \in \mathcal{E}} |c_i(x)| + \mu \sum_{i \in \mathcal{I}} [c_i(x)]^-, \quad (2.1)$$

where $[y]^- = \max\{0, -y\}$. Note that $\phi_1(x; \mu)$ is not differentiable at some x , because of the presence of the absolute value and $[\cdot]^-$ functions.

ℓ_1 Penalty Function

Theorem 6

Suppose that x^* is a strict local solution of the nonlinear programming problem (1.4) at which the first-order necessary conditions are satisfied with Lagrangian multiplier λ_i^* , $i \in \mathcal{E} \cup \mathcal{I}$. Then x^* is a local minimizer of $\phi_1(x; \mu)$ for all $\mu > \mu^*$, where

$$\mu^* = \|\lambda^*\|_\infty = \max_{i \in \mathcal{E} \cup \mathcal{I}} |\lambda_i^*|. \quad (2.2)$$

If, in addition, the second-order sufficient conditions hold and $\mu > \mu^*$, then x^* is a strict local minimizer of $\phi_1(x; \mu)$.

Theorem 7

Suppose that \hat{x} is stationary point of the penalty function $\phi_1(x; \mu)$ for all μ greater than a certain threshold $\hat{\mu} > 0$. Then, if \hat{x} is feasible for the nonlinear program (1.4), it satisfies the KKT conditions. If \hat{x} is not feasible for (1.4), it is a stationary point of the measure of infeasibility.

Example I

Consider the following problem in one variable:

$$\min x \quad \text{s.t. } x \geq 1.$$

whose solution is $x^* = 1$. We have that

$$\phi_1(x, \mu) = x + \mu[x - 1]^- = \begin{cases} (1 - \mu)x + \mu & \text{if } x \leq 1, \\ x & \text{if } x > 1. \end{cases} \quad (2.3)$$

The penalty function has a minimizer at x^* when $\mu > |\lambda^*| = 1$, but is a monotone increasing function when $\mu < 1$.

Demo

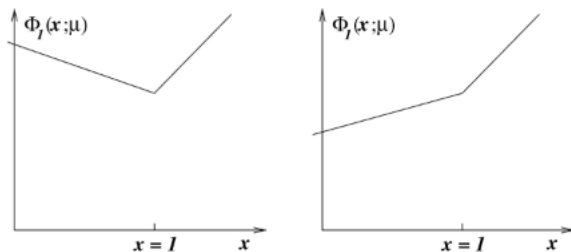


Figure 1: Penalty function (2.3) with $\mu > 1$ (left) and $\mu < 1$ (right)

Example II

Consider again the problem

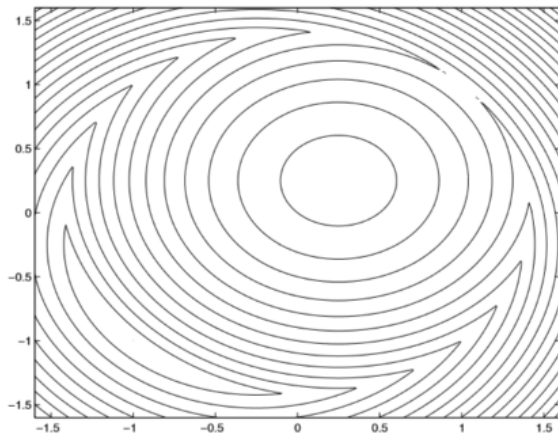
$$\min_x x_1 + x_2 \quad \text{s.t.} \quad x_1^2 + x_2^2 - 2 = 0,$$

for which ℓ_1 penalty function is

$$\phi_1(x; \mu) = x_1 + x_2 + \mu |x_1^2 + x_2^2 - 2|.$$

We find that for all $\mu > |\lambda^*| = 0.5$, the minimizer of $\phi_1(x; \mu)$ coincides with $x^* = (-1, -1)^T$.

Demo



Contours of $\phi_1(x; \mu)$ for $\mu = 2$, contour spacing 0.5. The sharp corners on the contours indicate nonsmoothness along the boundary of the circle defined by $x_1^2 + x_2^2 = 2$.

Algorithm 2: Classical ℓ_1 Penalty Method

Given $\mu_0 > 0$, tolerance $\tau > 0$, starting point x_0^s ;
for $k = 0, 1, 2, \dots$
 Find an approximate minimizer x_k of $\phi_1(x; \mu_k)$, starting at x_k^s ;
 if the constraint violation satisfies $h(x_k) \leq \tau$
 stop with a approximate solution x_k ;
 end(if)
 Choose new penalty parameter $\mu_{k+1} > \mu_k$;
 Choose new starting point x_{k+1}^s ;
end(for)

A General Class of Nonsmooth Penalty Methods

Exact nonsmooth penalty functions can be defined in terms of norms other than the ℓ_1 norm. We can write

$$\phi(x; \mu) = f(x) + \mu \|c_{\mathcal{E}}(x)\| + \mu \|[c_{\mathcal{I}}(x)]^-\|. \quad (2.4)$$

where $\|\cdot\|$ is any vector norm, and all the equality and inequality constraints have been grouped in the vector functions $c_{\mathcal{E}}$ and $c_{\mathcal{I}}$, respectively. The most common norms used in practice are the ℓ_1 , ℓ_∞ and ℓ_2 (not squared).

- The algorithm framework for ℓ_1 penalty function applies to any of these penalty functions; we simply redefine the measure of infeasibility as $h(x) = \|c_{\mathcal{E}}(x)\| + \|[c_{\mathcal{I}}(x)]^-\|$.
- The theoretical properties described for the ℓ_1 function extend to the general class (2.4) without modification, except that (2.2) is replaced by $\mu^* = \|\lambda^*\|_D$, where $\|\cdot\|_D$ is the dual norm of $\|\cdot\|$.

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Motivation

- Consider equality-case.
- In quadratic penalty method, Theorem 5 shows that

$$c_i(x_k) \approx -\lambda_i^*/\mu_k, \forall i \in \mathcal{E}. \quad (3.1)$$

To be sure, this perturbation vanishes as $c_i(x_k) \rightarrow 0$ as $\mu_k \uparrow \infty$.

- But one may ask whether we can alter the quadratic penalty function $Q(x; \mu_k)$ to avoid this systematic perturbation - that is, to make the approximate minimizers more nearly satisfy the equality constraints $c_i(x) = 0$, even for moderate values of μ_k .
- By doing so, we may avoid the need to increase μ to infinity, and thereby avoid the ill conditioning and numerical problems associated with $Q(x; \mu)$ for large values of this penalty parameter.

Motivation

The augmented Lagrangian function $\mathcal{L}_A(x, \lambda; \mu)$ achieves these goals by including an explicit estimate of the Lagrange multipliers λ , based on the formula (3.1), in the objective. From the definition

$$\mathcal{L}_A(x, \lambda; \mu) \equiv f(x) - \sum_{i \in \mathcal{E}} \lambda_i c_i(x) + \frac{\mu}{2} \sum_{i \in \mathcal{E}} c_i^2(x), \quad (3.2)$$

we see that the augmented Lagrangian differs from the (standard) Lagrangian for (1.1) by the presence of the squared terms, while it differs from the quadratic penalty function (1.2) in the presence of the summation term involving the λ . In this sense, it is a combination of the Lagrangian and quadratic penalty functions.

Motivation

Fix μ_k and λ^k at k th iteration. Using x_k to denote the approximate minimizer of $\mathcal{L}_A(x, \lambda^k; \mu_k)$, we have

$$0 \approx \nabla_x \mathcal{L}_A(x_k, \lambda^k; \mu_k) = \nabla f(x_k) - \sum_{i \in \mathcal{E}} [\lambda_i^k - \mu_k c_i(x_k)] \nabla c_i(x_k). \quad (3.3)$$

By comparing with the optimality condition for (1.1), we can deduce that

$$\lambda_i^* \approx \lambda_i^k - \mu_k c_i(x_k), \quad \forall i \in \mathcal{E}. \quad (3.4)$$

By rearranging this expression, we have that

$$c_i(x_k) \approx -\frac{1}{\mu_k} (\lambda_i^* - \lambda_i^k), \quad \forall i \in \mathcal{E},$$

so if λ_k is close to the optimal multiplier vector λ^* , the infeasibility in x_k will be much smaller than $(1/\mu_k)$, rather than being proportional to $(1/\mu_k)$ as in (3.1).

Motivation

How can we update the multiplier estimates λ^k from iteration to iteration, so that they approximate λ^* more and more accurately, based on current information? Equation (3.4) immediately suggests the formula

$$\lambda_i^{k+1} = \lambda_i^k - \mu_k c_i(x_k), \quad \forall i \in \mathcal{E}. \quad (3.5)$$

Algorithm 3: Augmented Lagrangian Method

Given $\mu_0 > 0$, tolerance $\tau_0 > 0$, starting point x_0^s and λ^0 ;

for $k = 0, 1, 2, \dots$

Find an approximate minimizer x_k of $\mathcal{L}_A(\cdot, \lambda^k; \mu_k)$, starting at x_k^s ;

and terminating when $\|\nabla_x \mathcal{L}_A(x_k, \lambda^k; \mu_k)\| \leq \tau_k$;

if a convergence test for (1.1) is satisfied

stop with approximate solution x_k ;

end(if)

Update Lagrange multipliers using (3.5) to obtain λ^{k+1} ;

Choose new penalty parameter $\mu_{k+1} > \mu_k$;

Choose new starting point x_{k+1}^s ;

Select tolerance τ_{k+1} ;

end(for)

Comments on the Algorithm

- We show below that convergence of this method can be assured without increasing μ indefinitely.
- Ill conditioning is therefore less of a problem than in the framework of quadratic function, so the choice of starting point x_{k+1}^s in the above framework is less critical. (In fact, we simply start the search at iteration $k+1$ from the previous approximate minimizer x_k .)
- The tolerance τ_k could be chosen to depend on the infeasibility $\sum_{i \in \mathcal{E}} |c(x_k)|$.
- The penalty parameter μ may be increased if the reduction in this infeasibility measure is insufficient at the present iteration.

Example

Consider again the problem

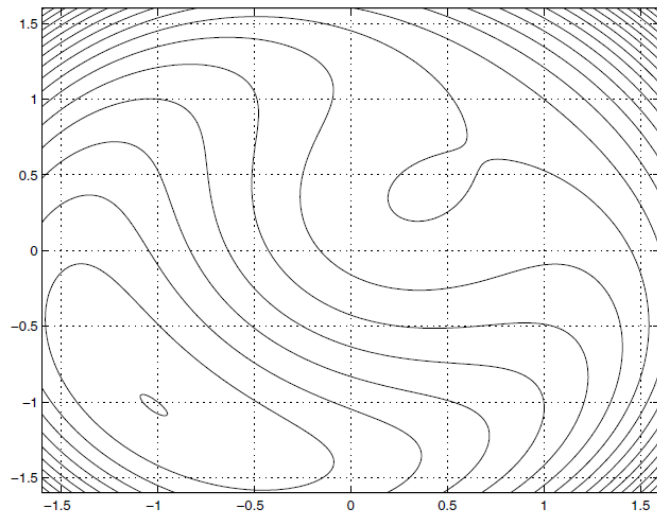
$$\min_x x_1 + x_2 \text{ s.t. } x_1^2 + x_2^2 - 2 = 0,$$

for which the solution is $x^* = (-1, -1)^T$ and the optimal Lagrangian multiplier is $\lambda^* = -0.5$. Consider the augmented Lagrangian

$$\mathcal{L}_A(x, \lambda; \mu) = x_1 + x_2 - \lambda(x_1^2 + x_2^2 - 2) + \frac{\mu}{2}(x_1^2 + x_2^2 - 2)^2.$$

Suppose that at iterate k we have $\mu_k = 1$, while the current multiplier estimate is $\lambda^k = -0.4$.

Demo



Contours of $\mathcal{L}_A(x, -0.4; 1)$, contour spacing 0.5.

Example

Note that the spacing of the contours indicates that the conditioning of this problem is similar to that of the quadratic penalty function $Q(x; 1)$. However, the minimizing value of $x_k \approx (-1.02, -1.02)$ is much closer to the solution $x^* = (-1, -1)^T$ than is the minimizing value of $Q(x; 1)$, which is approximately $(-1.1, -1.1)$. This example shows that the inclusion of the Lagrange multiplier term in the function $\mathcal{L}_A(x, \lambda; \mu)$ can result in a substantial improvement over the quadratic penalty method, as a way to reformulate the constrained optimization problem (1.4).

Properties of the Augmented Lagrangian

Theorem 8

Let x^ be a local solution of (1.1) at which the LICQ is satisfied (that is, the gradients $\nabla c_i(x^*)$, $i \in \mathcal{E}$, are linearly independent vectors), and the second-order sufficient conditions are satisfied for $\lambda = \lambda^*$. Then there is a threshold value $\bar{\mu}$ such that for all $\mu \geq \bar{\mu}$, x^* is a strict local minimizer of $\mathcal{L}_A(x, \lambda^*; \mu)$.*

This result validates the approach of algorithm 3 by showing that when we have knowledge of the exact Lagrange multiplier vector λ^* , the solution x^* of (1.1) is a strict minimizer of $\mathcal{L}_A(x, \lambda^*; \mu)$ for all μ sufficiently large. Although we do not know λ^* exactly in practice, the result and its proof strongly suggest that we can obtain a good estimate of x^* by minimizing $\mathcal{L}_A(x, \lambda; \mu)$ even when μ is not particularly large, provided that λ is a reasonable estimate of λ^* .

Properties of the Augmented Lagrangian

The second result, given by Bertsekas, describes the more realistic situation of $\lambda \neq \lambda^*$. It gives conditions under which there is a minimizer of $\mathcal{L}_A(x, \lambda; \mu)$ that lies close to x^* and gives error bounds on both x_k and the updated multiplier estimate λ^{k+1} obtained from solving the subproblem at iteration k .

Theorem 9

Suppose that the assumptions of above theorem are satisfied at x^ and λ^* , and let $\bar{\mu}$ be chosen as in that theorem. Then there exist positive scalars δ , ϵ , and M such that the following claims hold:*

(a) For all λ_k and μ_k satisfying

$$\|\lambda^k - \lambda^*\| \leq \mu_k \delta, \quad \mu_k \geq \bar{\mu}, \quad (3.6)$$

the problem

$$\min_x \mathcal{L}_A(x, \lambda_k; \mu_k) \text{ s.t. } \|x - x^*\| \leq \epsilon$$

has a unique solution x_k . Moreover, we have

$$\|x_k - x^*\| \leq M \|\lambda^k - \lambda^*\| / \mu_k. \quad (3.7)$$

Properties of the Augmented Lagrangian

Theorem 10

(b) For all λ_k and μ_k that satisfy (3.6), we have

$$\|\lambda^{k+1} - \lambda^*\| \leq M\|\lambda^k - \lambda^*\|/\mu_k, \quad (3.8)$$

where λ^{k+1} is given by the formula (3.5).

(c) For all λ^k and μ_k that satisfy (3.6), the matrix $\nabla_{xx}^2 \mathcal{L}_A(x_k, \lambda^k; \mu_k)$ is positive definite and the constraint gradients $\nabla c_i(x_k)$, $i \in \mathcal{E}$, are linearly independent.

Properties of the Augmented Lagrangian

This theorem illustrates some salient properties of the augmented Lagrangian approach.

- The bound (3.7) shows that x_k will be close to x^* if λ_k is accurate *or* if the penalty parameter μ_k is large. Hence, this approach gives us two ways of improving the accuracy of x_k , whereas the quadratic penalty approach gives us only one option: increasing μ_k .
- The bound (3.8) states that, locally, we can ensure an improvement in the accuracy of the multiplier by choosing a sufficient large value of μ_k .
- The final observation of the theorem shows that second-order sufficient conditions for unconstrained minimization are also satisfied for the k th subproblem under the given conditions, so one can expect good performance by applying standard unconstrained minimization techniques.

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Bound-Constrained Formulation

Given the general nonlinear program (1.4), we can convert it to a problem with equality constraints and bound constraints by introducing slack variables s_i and replacing the general inequalities $c_i(x) \geq 0$, $i \in \mathcal{I}$, by

$$c_i(x) - s_i = 0, \quad s_i \geq 0, \quad \forall i \in \mathcal{I}. \quad (4.1)$$

Bound constraints, $l \leq x \leq u$, need not be transformed. By reformulating in this way, we can write the nonlinear program as follows:

$$\min_{x \in \mathbb{R}^n} \quad f(x) \quad (4.2a)$$

$$\text{s.t.} \quad c_i(x) = 0, \quad i = 1, 2, \dots, m, \quad (4.2b)$$

$$l \leq x \leq u. \quad (4.2c)$$

Some of the components of the lower bound vector l may be set to $-\infty$, signifying that there is no lower bound on the components of x in question; similarly for u .

Bound-Constrained Lagrangian

The bound-constrained Lagrangian (BLC) approach incorporates only the equality constraints from (4.2) into the augmented Lagrangian, that is,

$$\mathcal{L}_A(x, \lambda; \mu) = f(x) - \sum_{i=1}^m \lambda_i c_i(x) + \frac{\mu}{2} \sum_{i=1}^m c_i^2(x). \quad (4.3)$$

The bound constraints are enforced explicitly in the subproblem, which has the form

$$\min_x \quad \mathcal{L}_A(x, \lambda; \mu) \quad (4.4a)$$

$$\text{s.t} \quad l \leq x \leq u. \quad (4.4b)$$

After this problem has been solved approximately, the multipliers λ and the penalty parameter μ are updated and the process is repeated.

Subproblem Solution by Gradient Projection Method

By specializing the KKT conditions to the problem (4.4), we find that the first-order necessary condition for x to be a solution of (4.4) is that

$$x - P(x - \nabla_x \mathcal{L}_A(x, \lambda, \mu), l; u) = 0, \quad (4.5)$$

where $P(g, l, u)$ is the projection of the vector $g \in \mathbb{R}^n$ onto the rectangular box $[l, u]$ defined as follows

$$P(g, l, u) = \begin{cases} l_i & \text{if } g_i \leq l_i, \\ g_i & \text{if } g_i \in (l_i, u_i), \\ u_i & \text{if } g_i \geq u_i. \end{cases} \quad \forall i = 1, 2, \dots, n. \quad (4.6)$$

Algorithm 4: Bound-Constrained Lagrangian Method

Given an initial point x_0 and initial multiplier λ^0 ;

Choose convergence tolerances η_* and ω_* ; Set $\mu_0 = 10$, $\omega_0 = 1/\mu_0$, and $\eta_0 = 1/\mu_0^{0.1}$;

for $k = 0, 1, 2, \dots$

Find an approximate minimizer x_k of the subproblem (4.4) such that

$$\|x_k - P(x_k - \nabla_x \mathcal{L}_A(x_k, \lambda^k, \mu_k), l, u)\| \leq \omega$$

if $\|c(x_k)\| \leq \eta_k$

(* test for convergence *)

if $\|c(x_k)\| \leq \eta_*$ and $\|x_k - P(x_k - \nabla_x \mathcal{L}_A(x_k, \lambda^k, \mu_k), l, u)\| \leq \omega_k$

stop with approximate solution x_k ;

end(if)

(* Update Lagrange multipliers, tighten tolerances *)

$$\lambda^{k+1} = \lambda^k - \mu_k c(x_k); \mu_{k+1} = \mu_k; \eta_{k+1} = \eta_k / \mu_{k+1}^{0.9}; \omega_{k+1} = \omega_k / \mu_{k+1};$$

else

(* increase penalty parameter, tighten tolerances *)

$$\lambda^{k+1} = \lambda^k; \mu_{k+1} = 100\mu_k; \eta_{k+1} = 1/\mu_{k+1}^{0.1}; \omega_{k+1} = 1/\mu_{k+1};$$

end(if)

end(for)

Linearly Constrained Lagrangian

If we use the formulation (4.2) of the nonlinear programming problem, the subproblem used in the LCL approach takes the form

$$\min_x F_k(x) \quad (4.7a)$$

$$s.t. \quad c(x_k) + A_k(x - x_k) = 0, \quad l \leq x \leq u. \quad (4.7b)$$

There are several possible choices for $F_k(x)$. Current LCL methods define F_k to be the augmented Lagrangian function

$$F_k(x) = f(x) - \sum_{i=1}^m \lambda_i^k \bar{c}_i^k(x) + \frac{\mu}{2} \sum_{i=1}^m [\bar{c}_i^k(x)]^2. \quad (4.8)$$

where $\bar{c}_i^k(x)$ is the difference between $c_i(x)$ and its linearization at x_k , that is,

$$\bar{c}_i^k(x) = c_i(x) - (c_i(x_k) + \nabla c_i(x_k)^T(x - x_k)). \quad (4.9)$$

Unconstrained Formulation

We can obtain an unconstrained form of the augmented Lagrangian subproblem for inequality-constrained problems by using a derivation based on the proximal point approach. Suppose for simplicity that the problem has no equality constraints ($\mathcal{E} = \emptyset$), we can write the problem (1.4) equivalently as an unconstrained optimization problem:

$$\min_{x \in \mathbb{R}^n} F(x), \quad (4.10)$$

where

$$F(x) = \max_{\lambda \geq 0} \left\{ f(x) - \sum_{i \in \mathcal{I}} \lambda_i c_i(x) \right\} = \begin{cases} f(x) & \text{if } x \text{ is feasible} \\ \infty & \text{otherwise.} \end{cases} \quad (4.11)$$

By combining (4.10) and (4.11), we have

$$\min_{x \in \mathbb{R}^n} F(x) = \min_{x \text{ feasible}} f(x), \quad (4.12)$$

which is simply the original inequality-constrained problem.

Unconstrained Formulation

We can make this approach more practical by replacing F by a smooth approximation $\hat{F}(x; \lambda^k, \mu_k)$ which depends on the penalty parameter μ_k and Lagrange multiplier estimate λ^k . This approximation is defined as follows:

$$\hat{F}(x; \lambda^k, \mu_k) = \max_{\lambda \geq 0} \{f(x) - \sum_{i \in \mathcal{I}} \lambda_i c_i(x) - \frac{1}{2\mu_k} \sum_{i \in \mathcal{I}} (\lambda_i - \lambda_i^k)^2\}. \quad (4.13)$$

The final term in this expression applies a penalty for any move of λ away from the previous estimate λ^k ; it encourages the new maximizer λ to stay *proximal* to the previous estimate λ^k . Since (4.13) represents a bound-constrained quadratic problem in λ , separable in the individual components λ_i , we can perform the maximization explicitly, to obtain

$$\lambda_i = \begin{cases} 0 & \text{if } -c_i(x) + \lambda_i^k/\mu_k \leq 0; \\ \lambda_i^k - \mu_k c_i(x) & \text{otherwise.} \end{cases} \quad (4.14)$$

Unconstrained Formulation

By substituting these values in (4.13), we find that

$$\hat{F}(x; \lambda^k, \mu_k) = f(x) + \sum_{i \in \mathcal{I}} \psi(c_i(x), \lambda_i^k; \mu_k), \quad (4.15)$$

where the function ψ of three scalar arguments is defined as follows:

$$\psi(t, \sigma; \mu) \equiv \begin{cases} -\sigma t + \frac{\mu}{2} t^2 & \text{if } t - \sigma/\mu \leq 0, \\ -\frac{1}{2\mu} \sigma^2 & \text{otherwise,} \end{cases} \quad (4.16)$$

Hence, we can obtain the new iterate x_k by minimizing $\hat{F}(x; \lambda^k, \mu_k)$ with respect to x , and use the formula (4.14) to obtain the updated Lagrange multiplier estimate λ^{k+1} .

Outline

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Perspective and Software

Augmented Lagrangian methods have been popular for many years because, in part, of their simplicity. The MINOS and LANCELOT packages rank among the best implementation of augmented Lagrangian methods. Both are suitable for large-scale nonlinear programming problems. At a general level, the linearly constrained Lagrangian of MINOS and the bound-constrained Lagrangian method of LANCELOT have important features in common. They differ significantly, however, in the formulation of the step computation subproblems and in the techniques used to solve these subproblems.

- MINOS follows a reduced-space approach to handle linearized constraints and employs a (dense) quasi-Newton approximation to the Hessian of the Lagrangian. As a result, Minos is most successful for problems with relatively few degrees of freedom.
- LANCELOT, on the other hand, is more effective when there are relatively few constraints. LANCELOT does not require a factorization of the constraint Jacobian matrix A , again enhancing its suitability for very large problems, and provides a variety of Hessian approximation options and preconditioners.

Thanks for your attention!