Constrained Optimization

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Motivation

Manufacturing

- Suppose we have *m* different materials; we have *s_i* units of each material *i* in stock.
- We can manufacture k different products; product j gives us profit p_j and uses c_{ij} amount of material i to make.
- To maximize profits, we can solve the following optimization problem for the total amount x_j we should manufacture of each item j:

$$\max_{x \in \mathbb{R}^n} \sum_{j=1}^k p_j x_j$$

such that $x_j \ge 0 \ \forall \ j \in \{1, 2, \dots, k\}$ (1)
$$\sum_{i=1}^k c_{ij} x_j \le s_i, \ \forall \ i \in \{1, 2, \dots, m\}$$

- The first constraint ensures that we do not make negative numbers of any product,
- and the second ensures that we do not use more than our stock of each material.

Constrained Problem

A general formulation of these problems is:

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, & i \in \mathscr{E} \\ c_j(x) \ge 0, & j \in \mathscr{I} \end{cases}$$
(2)

f and c_i are scalar valued functions of the vector of unknowns x and $\mathscr E$ and $\mathscr I$ are set of indices.

- x is a vector of variables, also called unknown or parameters;
- *f* is the objective function, a function of *x* that we want to optimise (minimise or maximise);
- *c* is the vector function of constraints that must be satisfied by the unknowns *x*.
- c_i , $i \in \mathscr{E}$ are the equality constraints.
- c_i , $i \in \mathscr{I}$ are the inequality constraints.

Compact form of Constrained Problem

Definition

Define the feasible set Ω to be the set of points x that satisfy the constraints; that is,

$$\Omega = \{ x \mid c_i(x) = 0, \quad i \in \mathscr{E}; \quad c_i(x) \ge 0, \quad i \in \mathscr{I} \}, \quad (3)$$

Now (2) can be rewritten more compactly as:

Constrained Problem

$$\min_{x\in\Omega}f(x).$$

(4)

Characterizations of the Solutions

- For the unconstrained optimization problems the solution point *x*^{*} was characterised in the following way:
- Necessary conditions: Local minima of unconstrained problems have

$$\nabla f(x^*) = 0$$

and,

 $\nabla^2 f(x^*)$ is positive semidefinite

• Sufficient conditions: Any point x^* at which $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite is a strong local minimiser of f.

- We have seen already that global solutions are difficult to find even when there are no constraints.
- The situation may improve when we add constraints.
- The feasible set might exclude many of the local minima.
- It might be comparatively easy to pick the global minimum from those that remain.

• Consider the problem

$$\min_{x \in \mathbb{R}^n} ||x||_2^2, \quad \text{subject to } ||x||_2^2 \ge 1.$$
 (5)

- Without the constraint, this is a convex quadratic problem with unique minimiser x = 0.
- When the constraint is added, any vector x with ||x|| = 1 solves the problem.
- There are infinitely many such vectors (hence, infinitely many local minima) whenever $n \ge 2$

- Addition of a constraint produces a large number of local solutions that do not form a connected set.
- Consider

$$\min_{x\in\mathbb{R}^2}(x_2+100)^2+0.01x_1^2, \quad ext{subject to } x_2-\cos x_1\geq 0, \quad (6)$$

- Without the constraint, the problem has the unique solution (-100, 0).
- With the constraint there are local solutions near the points

$$(x_1, x_2) = (k\pi, -1), \text{ for } k = \pm 1, \pm 3, \pm 5, \dots$$



Figure Constrained problem with many isolated local solutions.

- Local and global solutions are defined in a very similar fashion as they were for the unconstrained case.
- The new caveat that comes into action in the definitions for the constrained case is the inclusion of constraints leading to a restriction imposed via a feasible set (space).

Definition

A vector x^* is a local solution of the constrained minimisation problem (4) if $x^* \in \Omega$ and there exists a neighbourhood \mathscr{N} of x^* such that

 $f(x^*) \leq f(x)$ for all $x \in \Omega \cap \mathscr{N}$

Definition

A vector x^* is called a strict local solution (also called a strong local solution) if $x^* \in \Omega$ and there is a neighbourhood \mathscr{N} of x^* such that

$$f(x^*) < f(x)$$
 for all $x \in \mathscr{N} \cap \Omega$ with $x \neq x^*$

Definition

A point x^* is an isolated local solution if $x^* \in \Omega$ and there is a neighbourhood \mathcal{N} of x^* such that x^* is the only local minimiser in $N \cap \Omega$.

- Smoothness of objective functions and constraints is an important issue in characterizing solutions.
- Just as in the unconstrained case, it ensures that the objective function and the constraints all behave in a reasonably predictable way.
- Allows algorithms to make good choices for search directions.
- Non-smooth functions contain "kinks" or "jumps" where the smoothness breaks down.
- The feasible region for any given constrained optimization problem usually contains many kinks and sharp edges.

• Does this mean that the constraint functions that describe these regions are non-smooth?



Figure: A feasible region with a non-smooth boundary can be described by smooth constraints.

• The answer is often no, because the non-smooth boundaries can often be described by a collection of smooth constraint functions.

- The figure above shows a diamond-shaped feasible region in \mathbb{R}^2 .
- It could be described by the single non-smooth constraint

$$||x||_1 = |x_1| + |x_2| \le 1.$$

• Or, it could also be brought out as an intersection of four smooth (in fact, linear) constraints:

$$x_1 + x_2 \leq 1$$
, $x_1 - x_2 \leq 1$, $-x_1 + x_2 \leq 1$, $-x_1 - x_2 \leq 1$.

- Each of the four constraints represents one edge of the feasible polytope.
- The constraint functions are chosen so that each one represents a smooth piece of the boundary of Ω.

- In general, the constraint functions are chosen so that each one represents a smooth piece of the boundary of Ω.
- Non-smooth, unconstrained optimization problems can sometimes be reformulated as smooth constrained problems.
- Consider the unconstrained scalar problem of minimizing a non-smooth function f(x) defined by,

$$f(x) = \max(x^2, x)$$

- It has kinks at x = 0 and x = 1.
- The solution at $x^* = 0$.
- A smooth, constrained formulation of this problem can be obtained by adding an artificial variable *t* and writing,

min
$$t$$
, s.t, $t \ge x$, $t \ge x^2$.

- In the examples above we expressed inequality constraints in a slightly different way from the form $c_i(x) \ge 0$.
- However, any collection of inequality constraints with ≥ or ≤ and nonzero right-hand-sides can be expressed in the form c_i(x) ≥ 0 by simple rearrangement of the inequality.

$$t-x\geq 0, \quad t-x^2\geq 0.$$



• To introduce the basic principles behind the characterization of solutions of constrained optimization problems, we work through three simple examples.

Definition

At a feasible point x, the inequality constraint $i \in \mathscr{I}$ is said to be active if $c_i(x) = 0$ and inactive if the strict inequality $c_i > 0$ is satisfied.

Definition

The active set $\mathscr{A}(x)$ at any feasible x consists of the equality constraint indices from \mathscr{E} together with the indices of the inequality constraints *i* for which $c_i(x) = 0$; that is,

$$\mathscr{A}(x) = \mathscr{E} \cup \{i \in \mathscr{I} | c_i(x) = 0\}.$$

Example-1

The first example is a two-variable problem with a single equality constraint:

min
$$x_1 + x_2$$
 $x_1^2 + x_2^2 - 2 = 0$ (7)

•
$$f(x) = x_1 + x_2$$
, $\mathscr{I} = \phi$, $\mathscr{E} = \{1\}$

- $c_1(x) = x_1^2 + x_2^2 2$
- The feasible set for this problem is the circle of radius \sqrt{2} centered at the origin.
- Just the boundary of this circle, not its interior.
- The solution x^* is $(-1, -1)^T$.

Example-1



Figure: showing constraint and function gradients at various feasible points.

- From any other point on the circle, it is easy to find a way to move that stays feasible (that is, remains on the circle) while decreasing *f*.
- From the point $x = (\sqrt{2}, 0)^T$, any move in the clockwise direction around the circle has the desired effect.

- From the figure we see that at the solution x^* , the normal to the constraint $\nabla c_1(x^*)$ is parallel to $\nabla f(x^*)$.
- ullet There is a scalar λ_1^* (in this case $\lambda_1^*=-1/2)$ such that

$$\nabla f(x^*) = \lambda_1^* \nabla c_1(x^*). \tag{8}$$

To retain feasibility with respect to the function c₁(x) = 0, it is require for any small (but nonzero) step s to satisfy that c₁(x + s) = 0; i.e:

$$0 = c_1(x+s) \approx c_1(x) + \nabla c_1(x)^T s = \nabla c_1(x)^T s.$$

• The step *s* retains feasibility with respect to *c*₁, to first order, when it satisfies

$$\nabla c_1(x)^T s = 0. \tag{9}$$

• If we want s to produce a decrease in f;

$$0 > f(x+s) - f(x) \approx \nabla f(x)^T s$$

• or to first order

$$\nabla f(x)^T s < 0 \tag{10}$$

- Existence of a small step s that satisfies both (9) and (10) strongly suggests existence of a direction d where we can get some improvement in the process of minimisation.
- The size of d could be not small; we could have d ≈ s/||s|| to ensure that the norm of d is close to 1 with the same properties, namely

$$\nabla c_1(x)^T d = 0 \quad \nabla f(x)^T d < 0. \tag{11}$$

- If there is no direction d with the properties (11), then is it likely that we cannot find a small step s with the properties (9) and (10).
- In this case, x^* would appear to be a local minimiser.
- The only way that a d satisfying (11) doesn't exist is if ∇f(x) and ∇c₁(x) are parallel.

• Or precisely if the condition

$$\nabla f(x) = \lambda_1 \nabla c_1(x)$$

holds at x for some scalar λ_1 .

• If $\nabla f(x)$ and $\nabla c_1(x)$ are not parallel then we can set:

$$\bar{d} = -\left(\nabla f(x) - \frac{\nabla c_1(x)\nabla f(x)\nabla c_1(x)^{\mathsf{T}}}{||\nabla c_1(x)||^2}\right)$$
(12)

and

$$d = \frac{\bar{d}}{||\bar{d}||} \tag{13}$$

• It can be verified that (13) satisfies (11).

• To write the condition (11) more succinctly we introduce the notion of the *Lagrangian function*.

$$\mathscr{L}(x,\lambda_1) = f(x) - \lambda_1 c_1(x). \tag{14}$$

• The gradient w.r.t x of the Lagrangian is given by

$$\nabla_{x}\mathscr{L}(x,\lambda_{1}) = \nabla f(x) - \lambda_{1}\nabla c_{1}(x)$$
(15)

 With the above introduced notions the condition (11) can now be stated as: At the solution x^{*}, there is a scalar λ₁^{*} such that

$$\nabla_{\mathbf{x}}\mathscr{L}(\mathbf{x}^*,\lambda_1^*) = \mathbf{0}.$$
 (16)

- This observation suggests that we can search for solutions of the equality-constrained problem (7) by seeking stationary points of the Lagrangian function.
- The scalar quantity λ₁ is called a Lagrange multiplier for the constraint c₁(x) = 0.
- Though the condition

$$\nabla f(x^*) = \lambda_1^* \nabla c_1(x^*)$$

appears to be necessary for an optimal solution of the problem, it is clearly not sufficient.

- The condition is satisfied at the point x = (1, 1) with $\lambda_1 = \frac{1}{2}$.
- But, (1,1) is obviously not a solution.
- In fact, it maximizes the function *f* on the circle.

- What may seem a way out from the observation we made in regards to the previous problem is to obtain a sufficient condition for equality-constrained problems is: simply by placing some restriction on the sign of λ₁.
- Consider the constraint

$$x_1^2 + x_2^2 - 2 = 0$$

by its negative i.e.

$$2 - x_1^2 - x_2^2 = 0$$

in the example under consideration.

• The solution of the problem is not affected, but the value of λ_1^* that satisfies the condition (16) changes from $\lambda_1^* = -\frac{1}{2}$ to $\lambda_1^* = \frac{1}{2}$.

- Here we consider a small modification of Example-1.
- Here the equality constraint is replaced by an inequality.

EXAMPLE-2

Consider

$$\min x_1 + x_2 \qquad 2 - x_1^2 - x_2^2 \ge 0 \tag{17}$$

•
$$f(x) = x_1 + x_2$$
, $\mathscr{I} = \{1\}$, $\mathscr{E} = \phi$

•
$$c_1(x) = 2 - x_1^2 - x_2^2$$

- The feasible region for this problem is the circle of radius √2 centered at the origin.
- Just not the boundary of this circle, but its interior as well.

- The solution x^* is still $(-1, -1)^T$.
- And the Lagrange multiplier condition holds at (-1, -1) for the value of $\lambda_1^* = \frac{1}{2}$.
- However, this inequality-constrained problem differs from the equality-constrained problem.
- The sign of the Lagrange multiplier plays a significant role, as we now argue.
- Let us conjecture that a given feasible point x is not optimal if we can find a small step s that both retains feasibility and decreases the objective function f to first order.
- The main difference between problems with inequality constraint and equality constraint comes in the handling of the feasibility condition.

• The step s improves the objective function, to first order, if

$$\nabla f(x)^T s < 0.$$

• s retains feasibility if

$$0 \leq c_1(x+s) \approx c_1(x) + \nabla c_1(x)^T s.$$

• That is to first order, feasibility is retained if

$$c_1(x) + \nabla c_1(x)^T s \ge 0.$$
 (18)

 In determining whether a step s exists that satisfies both the conditions, we consider the following two cases,

In determining whether a step s exists that satisfies both the conditions, we consider the following two cases,



Figure: Improvement directions s from two feasible points x for the problem at which the constraint is active and inactive, respectively

CASE-1

- Consider first the case in which x lies strictly inside the circle.
- the strict inequality $c_1(x) > 0$ holds.
- In this case, any step vector *s* satisfies the condition (18), provided only that its length is sufficiently small.
- In fact, whenever ∇f(x) ≠ 0, we can obtain a step s that satisfies both the conditions (10) and (18).
- Precisely

$$s = -\alpha \nabla f(x),$$

for any positive scalar α sufficiently small.

• This definition does not give a step s with the required properties when

$$\nabla f(x) = 0$$

CASE-2

- Consider now the case in which x lies on the boundary of the circle.
- So that $c_1(x) = 0$.
- The conditions (10) and (18) therefore become:

$$\nabla f(x)^{\mathsf{T}} s < 0, \qquad \nabla c_1(x)^{\mathsf{T}} s \ge 0. \tag{19}$$

- The first of these conditions defines an open half-space.
- While the second defines a closed half-space.



Figure: A direction d that satisfies both conditions (10) and (18) lies in the intersection of a closed half-plane and an open half-plane.

 It is clear from this figure that the intersection of these two regions is empty only when ∇f(x) and ∇c₁(x) point in the same direction.

• That is, when

$$abla f(x) = \lambda_1 \nabla c_1(x), \quad \text{for some } \lambda_1 \ge 0.$$
 (20)

- The sign of the multiplier is significant here.
- If the Lagrange multiplier condition were satisfied with a negative value of λ₁, then ∇f(x) and ∇c₁(x) would point in opposite directions.
- We see from the figure that the set of directions that satisfy both conditions (10) and (18) would make up an entire open half-plane.

- The optimality conditions for both cases I and II can again be summarized neatly with reference to the Lagrangian function £.
- When no first-order feasible descent direction exists at some point *x**, we have

$$abla_x \mathscr{L}(x^*, \lambda_1^*) = 0, \qquad \text{for some } \lambda_1^* \ge 0, \qquad (21)$$

where we also require that

$$\lambda_1^* c_1(x^*) = 0$$
 (22)

• Condition (22) is known as a complementarity condition

- It implies that the Lagrange multiplier λ_1 can be strictly positive only when the corresponding constraint c_1 is active.
- In case I, we have that $c_1(x^*) > 0$.
- So (22) requires that

$$\lambda_1^* = 0$$

• And (21) reduces to

$$\nabla f(x^*) = 0$$

as was required by Case-I.

In case-II, (22) allows λ₁^{*} to take on a non-negative value, so
 (21) becomes equivalent to (20).

Example-3

- Suppose we add an extra constraint to the previous problem.
- Consider

min
$$x_1 + x_2$$
 $2 - x_1^2 - x_2^2 \ge 0$, $x_2 \ge 0$. (23)

•
$$f(x) = x_1 + x_2$$
, $\mathscr{I} = \{1, 2\}$, $\mathscr{E} = \phi$

•
$$c_1(x) = 2 - x_1^2 - x_2^2$$

•
$$c_2(x) = x_2$$

• The feasible region for this problem is the upper half disk of radius $\sqrt{2}$ centered at the origin.



Figure: Feasible region, illustrating the gradients of the active constraints and objective at the solution

- The solution lies at $(-\sqrt{2},0)^T$.
- It is a point at which both constraints are active.

• By repeating the arguments for the previous examples, we would expect a direction d of first-order feasible descent to satisfy

$$abla c_i(x)^T d \ge 0, \qquad i \in \mathscr{I} = \{1, 2\} \qquad
abla f^T d < 0 \qquad (24)$$

- It is clear from the figure that no such direction can exist when $x = (-\sqrt{2}, 0)^T$.
- The conditions $\nabla c_i(x)^T d \ge 0$ i = 1, 2 are both satisfied only if d lies in the quadrant defined by $\nabla c_1(x)$ and $\nabla c_2(x)$.
- But it is clear that all vectors d in this quadrant satisfy $\nabla f^T d \ge 0$.

- Let us see how the Lagrangian and its derivatives behave for this problem and the solution point $x = (-\sqrt{2}, 0)^T$.
- First, for each additional constraint $c_i(x)$ an additional term $\lambda_i c_i(x)$ is added in the Lagrangian function \mathscr{L}

$$\mathscr{L}(x,\lambda) = f(x) - \lambda_1 c_1(x) - \lambda_2 c_2(x), \qquad (25)$$

- $\lambda = (\lambda_1, \lambda_2)^T$ is the vector of Lagrange multipliers.
- The extension of the Lagrangian condition to this case is

$$abla_x \mathscr{L}(x^*,\lambda^*) = 0, \qquad ext{for some }, \lambda^* \geq 0.$$
 (26)

•
$$\lambda \geq 0$$
 means $\lambda_i^* \geq 0, \forall i$.

• Applying the complementarity condition (22) to both inequality constraints gives:

$$\lambda_1^* c_1(x^*) = 0 \qquad \lambda_2^* c_2(x^*) = 0 \tag{27}$$

• Now when
$$x* = (-\sqrt{2}, 0)^T$$
, we have

$$\nabla f(x^*) = \begin{bmatrix} 1\\1 \end{bmatrix}, \quad \nabla c_1(x^*) = \begin{bmatrix} 2\sqrt{2}\\0 \end{bmatrix}, \quad \nabla c_2(x^*) = \begin{bmatrix} 0\\1 \end{bmatrix}$$
(28)

• We have

$$\nabla_{\mathbf{x}}\mathscr{L}(\mathbf{x}^*,\lambda^*) = \nabla f(\mathbf{x}^*) - \lambda_1 \nabla c_1(\mathbf{x}^*) - \lambda_2 \nabla c_2(\mathbf{x}^*)$$

• The Lagrange multiplier for x* can be obtained as the solution of

$$\nabla_{x}\mathscr{L}(x^{*},\lambda^{*})=0$$

• That is λ^* is given as:

$$\lambda^* = \begin{bmatrix} 1/(2\sqrt{2}) \\ 1 \end{bmatrix}$$

- Now let us consider some other feasible points that are not solutions of, and examine the properties of the Lagrangian and its gradient at these points.
- For $x = (\sqrt{2}, 0)^T$, both constraints are active.



Figure: Illustrating the gradients of the active constraints and objective at a non-optimal point.

- From this point it is easy to identify points that satisfy (24)
- $d = (-1, 0)^T$ is one such vector (there are many others).

• For the value $x = (\sqrt{2}, 0)^T$ it is easy to verify that the Lagrange multiplier condition

$$\nabla_{\mathsf{x}}\mathscr{L}(\mathsf{x},\lambda)=\mathsf{0}$$

is satisfied only when $\lambda = (-1/(2\sqrt{2}), 1)^T$.

- The first component $\lambda_1 < 0$.
- So the condition (26) are not satisfied at this point.
- Let us consider the point $(1,0)^T$.
- Here only the second constraint c_2 is active.
- Any small step s away from this point will continue to satisfy $c_1(x+s) > 0$

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TWO INEQUALITY CONSTRAINTS

- We need to consider only the behavior of c_2 and;
- f in determining whether s is indeed a feasible descent step.
- Using similar arguments as made before for the previous example we find that the direction of feasible descent *d* must satisfy

$$\nabla c_2(x)^T d \ge 0, \qquad \nabla f(x)^T d < 0. \tag{29}$$

$$abla f(x) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \qquad
abla c_2(x) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

• The vector $d = (-\frac{1}{2}, \frac{1}{4})^T$ satisfies (29) and is therefore a descent direction.

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TWO INEQUALITY CONSTRAINTS

- The optimality conditions (26) and (27) fail.
- We note first from (27) that since $c_1(x) > 0$, we must have $\lambda_1 = 0$.
- In trying to satisfy ∇_x ℒ(x, λ) = 0, we are left to search for a value λ₂.

$$\nabla f(x) - \lambda_2 \nabla c_2(x) = 0.$$

- It can be shown that no such λ_2 exists.
- This point fails to satisfy the optimality conditions.