Lagrange Multipliers

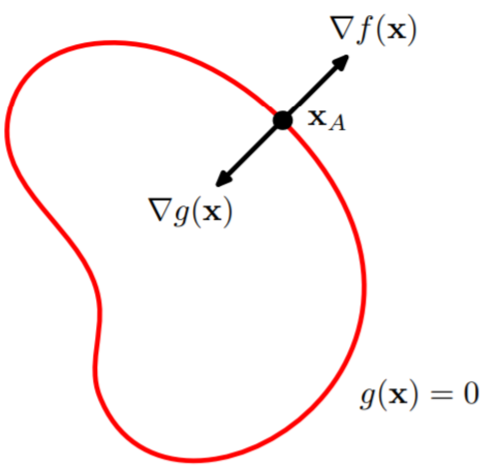
Lagrange multipliers, a.k.a. undetermined multipliers, are used to find **the stationary points** of a function of several variables subject to one or more constraints.

Equality Constraint

Sometime it may be difficult to find a analytic solution of the constraint between variables x_i. We can introduce a parameter λ called Lagrange multiplier. From a geometrical perspective, consider a D-dimensional variable $\mathrm{x} = (x_1, \ldots, x_D)^T$. The constraint equation $g(\mathrm{x}) = 0$ is a $(D-1)$-dimensional surface in x-space.

> *Lemma-1*. At any point on the surface $g(\mathrm{x}) = 0$ the gradient ∇g will be orthogonal to the surface.
>
> *Proof*. Consider a point x on the surface, and consider a nearby point $\mathrm{x} + \epsilon$ that also on the surface. If we make a Taylor expansion around this point, we have:
>
> $$g(\mathrm{x} + \epsilon) \approx g(\mathrm{x}) + \epsilon^T \nabla g(\mathrm{x}) \qquad (1)$$
>
> because $g(\mathrm{x} + \epsilon) = g(\mathrm{x})$, we have $\epsilon^T \nabla g(\mathrm{x}) \approx 0$. And if $\|\epsilon\| \to 0$, we have $\epsilon^T \nabla g(\mathrm{x}) = 0$. And because at this time ϵ is parallel to the surface $g(\mathrm{x}) = 0$, so ∇g is normal to the surface.

A geometrical picture of the technique of Lagrange multipliers in which we seek to maximize a function $f(\mathbf{x})$, subject to the constraint $g(\mathbf{x}) = 0$. If $\mathbf{x}$ is D dimensional, the constraint $g(\mathbf{x}) = 0$ corresponds to a subspace of dimensionality $D-1$, indicated by the red curve. The problem can be solved by optimizing the Lagrangian function $L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$.



> *Lemma-2.* If x^* on $g(\mathrm{x}) = 0$ and $\forall \mathrm{x}$ on $g(\mathrm{x}) = 0$, we have $f(\mathrm{x}^*) \geq f(\mathrm{x})$, then $\nabla f(\mathrm{x}^*)$ is orthogonal to the surface $g(\mathrm{x}) = 0$.
>
> *Proof*. Otherwise we could increase the value of $f(\mathrm{x})$ by moving a short distance along the surface.

From *Lemma-1* and *Lemma-2* we have:

$$\nabla f + \lambda \nabla g = 0 \qquad (2)$$

where $\lambda \neq 0$ is the Lagrange multiplier.

Then we can define the *Lagrangian* function

$$L(\mathrm{x}, \lambda) := f(\mathrm{x}) + \lambda g(\mathrm{x}) \qquad (3)$$

And

$$\begin{aligned} \nabla_{\mathrm{x}} L = 0 &\Rightarrow \nabla f + \lambda \nabla g = 0 \\ \frac{\partial L}{\partial \lambda} = 0 &\Rightarrow g(\mathrm{x}) = 0 \end{aligned}$$

Thus to find the maximum of f s.t. $g(\mathrm{x}) = 0$, we solve the equation

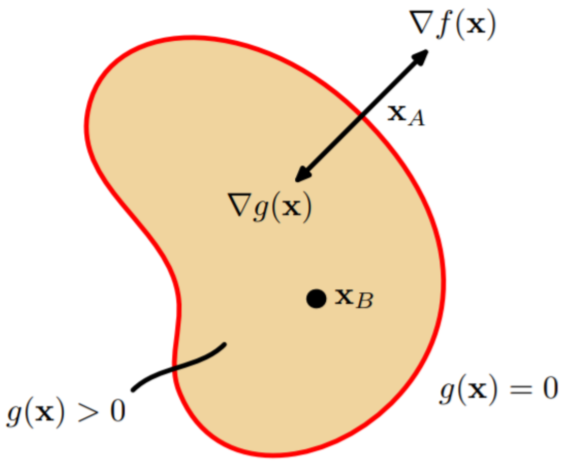
$$\begin{cases} \nabla_{\mathrm{x}} L = 0 & \Rightarrow & \nabla f + \lambda \nabla g = 0 \\ \frac{\partial L}{\partial \lambda} = 0 & \Rightarrow & g(\mathrm{x}) = 0 \end{cases} \qquad (4)$$

and get a $(D+1)$-dimension equations to get stationary points.

Inequality Constraint

The problem of maximizing f with inequality constraint of the form $g(\mathrm{x}) \geq 0$.

Illustration of the problem of maximizing $f(\mathbf{x})$ subject to the inequality constraint $g(\mathbf{x}) \geqslant 0$.



There are two kinds of solution possible.

- *inactive* constraint: The stationary point lies in the region $g(\mathrm{x}) > 0$. The function $g(\mathrm{x})$ is useless, $\lambda = 0$.
- *active* constraint: The stationary point lies in the surface $g(\mathrm{x}) = 0$. This is analogous to the equality constraint case, $\lambda \neq 0$.

Note that now the sign of λ is crucial, because f only be at a maximum if its gradient is oriented away from the region $g(\mathrm{x}) > 0$. Therefore $\lambda > 0$ (if we want a minimum, we set $\lambda < 0$).

For either cases, we have $\lambda g(\mathrm{x}) = 0$. Then we can define:

> **KKT(Karush-Kuhn-Tucker) conditions**
>
> $$\begin{aligned} g(\mathrm{x}) &\geq 0 \\ \lambda &\geq 0 \\ \lambda g(\mathrm{x}) &= 0 \end{aligned}$$

And the solution is also straightforward.