# Notes on Binary Classification

DSBA Mathematics Refresher 2025

**Abstract**

This session will explore different methods for constrained optimization, with a particular focus on the Lagrange multiplier technique.

## 1 Unconstrained Optimization

Unconstrained optimization refers to the problem of optimizing a function without any restrictions or constraints on the variables. Mathematically, this can be expressed as:

$$\text{Find } \mathbf{x}^* \text{ such that } f(\mathbf{x}^*) = \min_{\mathbf{x}} f(\mathbf{x})$$

where $f(\mathbf{x})$ is the objective function.

The necessary condition for $\mathbf{x}^*$ to be an extremum is that the gradient of $f$ at $\mathbf{x}^*$ is zero:

$$\nabla f(\mathbf{x}^*) = \mathbf{0}$$

### 1.1 Direct Calculation Method

The direct method involves taking the derivative of the function with respect to each variable, setting these derivatives equal to zero, and solving the resulting system of equations.

**Example:**
Consider the function $f(x, y) = x^2 + y^2$. To find the minimum, we calculate:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial f}{\partial y} = 2y$$

Setting these equal to zero, we get:

$$2x = 0 \quad \text{and} \quad 2y = 0$$

This gives $x = 0$ and $y = 0$, which is the minimum point.

### 1.2 Iterative Process

In a previous session, we explored iterative process to find the extremum of a function. This is often used when solving $\nabla f(\mathbf{x}^*) = \mathbf{0}$ can not be done in reasonable time.

# 2 Constrained Optimization

In many practical problems, the optimization process is subject to certain constraints. These constraints can be either equality or inequality constraints.

## 2.1 Equality Constrained Optimization

Equality constrained optimization problems can be expressed as:

$$\text{Minimize } f(\mathbf{x}) \quad \text{subject to} \quad g_i(\mathbf{x}) = 0 \quad \text{for } i = 1, \ldots, m$$

### 2.1.1 Direct Calculation Method

For some simple problems, we can solve the constraint explicitly and substitute it back into the objective function to reduce the problem to an unconstrained optimization problem.

**Example:** Minimize $f(x, y) = x^2 + y^2$ subject to the constraint $x + y = 1$. Solve the constraint for $y = 1 - x$, and substitute into $f(x, y)$:

$$f(x, 1 - x) = x^2 + (1 - x)^2 = 2x^2 - 2x + 1$$

Minimize the resulting function by finding the derivative and setting it to zero:

$$\frac{d}{dx}(2x^2 - 2x + 1) = 4x - 2 = 0$$

This gives $x = \frac{1}{2}$, and hence $y = \frac{1}{2}$.

### 2.1.2 Lagrange Multiplier Method

The Lagrange multiplier method introduces an auxiliary variable (the Lagrange multiplier) to incorporate the constraints into the objective function.

**Lagrange Function:**

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x})$$

To find the stationary points, we solve the system:

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \lambda) = \mathbf{0}$$

**Example:** Minimize $f(x, y) = x^2 + y^2$ subject to $x + y = 1$.

**Step 1: Construct the Lagrange Function**

The Lagrangian is:

$$\mathcal{L}(x, y, \lambda) = x^2 + y^2 + \lambda(x + y - 1)$$

**Step 2: Compute the Partial Derivatives**

The partial derivatives of the Lagrangian are:

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + \lambda = 0, \quad \frac{\partial \mathcal{L}}{\partial y} = 2y + \lambda = 0, \quad \frac{\partial \mathcal{L}}{\partial \lambda} = x + y - 1 = 0$$

**Step 3: Solve the System of Equations**
Solving this system gives $x = y = \frac{1}{2}$, $\lambda = -1$, which matches our previous result.

**Step 4: Determine the Optimal Point**
Substitute $x = \frac{1}{2}$, $y = \frac{1}{2}$ into the original function:

$$f\left(\frac{1}{2}, \frac{1}{2}\right) = \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$$

Thus, the minimum value of $f(x, y) = x^2 + y^2$ subject to $x + y = 1$ is $\frac{1}{2}$ at the point $\left(\frac{1}{2}, \frac{1}{2}\right)$.

## 2.2 Inequality Constrained Optimization

Equality constrained optimization problems can be expressed as:

$$\text{Minimize } f(\mathbf{x}) \quad \text{subject to} \quad g_i(\mathbf{x}) \geq 0 \quad \text{for } i = 1, \ldots, m$$

### 2.2.1 Direct Method

When the constraint is active (i.e., it holds as an equality), it can be treated similarly to the equality-constrained case. If inactive, it is ignored.

**Example:** Minimizing a Quadratic Function with an Inequality Constraint
Minimize $f(x, y) = x^2 + y^2$ subject to $x \geq 0$ and $y \geq 0$.
This can be approached by checking the boundary and interior points. The minimum will be at $(0, 0)$ given the non-negative constraints.
Note that if the constraint was $x + y \geq 1$, showing that the minimum is at $(0.5, 0.5)$ is much harder via direct calculations.

### 2.2.2 Lagrange Multiplier Method with Slack Variables

We note that:

$$g_i(\mathbf{x}) \geq 0 \iff g_i(\mathbf{x}) - s^2 = 0 \quad \text{for some } s \in \mathbb{R}$$

Here, $s$ is called a "slack variable". It is then possible to use the Lagrange trick as before.
The Lagrange multiplier method introduces now multiple auxiliary variables: the Lagrange multiplier and some slack variables to incorporate the inequality constraints into the objective function.

**Lagrange Function:**

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i \left(g_i(\mathbf{x}) - s_i^2\right)$$

To find the stationary points, we solve the system:

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \lambda) = \mathbf{0}$$

**Example:** Minimizing a Quadratic Function with an Inequality Constraint
Consider the problem of minimizing the function $f(x, y) = x^2 + y^2$ subject to the inequality constraint $x + y \geq 1$.

**Step 1: Introduce the Slack Variable**
The constraint can be written as:

$$x + y - s^2 = 1 \quad \text{as } s^2 \geq 0 \quad \forall s \in \mathbb{R}$$

where $s$ is the slack variable. The constraint is now an equality constraint.

**Step 2: Construct the Lagrange Function**
The Lagrange function incorporating the constraint is:

$$\mathcal{L}(x, y, s, \lambda) = x^2 + y^2 + \lambda\left((x + y) - s^2 - 1\right)$$

where $\lambda$ is the Lagrange multiplier.

**Step 3: Compute the Partial Derivatives**
To find the stationary points, take the partial derivatives of $\mathcal{L}$ with respect to $x$, $y$, $s$, and $\lambda$, and set them to zero:

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + \lambda = 0$$

$$\frac{\partial \mathcal{L}}{\partial y} = 2y + \lambda = 0$$

$$\frac{\partial \mathcal{L}}{\partial s} = -2\lambda s = 0$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = x + y - s^2 - 1 = 0$$

**Step 4: Solve the System of Equations**
From $\frac{\partial \mathcal{L}}{\partial x} = 0$ and $\frac{\partial \mathcal{L}}{\partial y} = 0$, we have:

$$2x + \lambda = 0 \quad \text{and} \quad 2y + \lambda = 0$$

This implies $x = y$.
From $\frac{\partial \mathcal{L}}{\partial s} = 0$, we have:

$$-2\lambda s = 0$$

This implies $\lambda = 0$ or $s = 0$.

1. If $\lambda = 0$, then $x = 0$ and $y = 0$, but this would violate the constraint $x + y \geq 1$. Hence, this case is not valid.
2. If $s = 0$, the constraint simplifies to $x + y = 1$. Since $x = y$, we have $2x = 1$, so $x = \frac{1}{2}$ and $y = \frac{1}{2}$.

**Step 5: Determine the Optimal Point**
Substitute $x = \frac{1}{2}$, $y = \frac{1}{2}$ into the original function: $f\left(\frac{1}{2}, \frac{1}{2}\right) = \frac{1}{2}$. Thus, the minimum value of $f(x, y) = x^2 + y^2$ subject to $x + y \geq 1$ is $\frac{1}{2}$ at the point $\left(\frac{1}{2}, \frac{1}{2}\right)$.