



MAY 4 LECTURE

TEXTBOOK REFERENCE:

- *Vector Calculus*, Colley, 4th Edition: §4.3, 4.4

LAGRANGE MULTIPLIERS; LINEAR REGRESSION

KEYWORDS: the method of Lagrange multipliers, linear regression, polynomial regression

Let $f(x, y)$, $g(x, y)$ be differentiable functions. We are interested in the constrained optimisation problem

$$\begin{array}{l} \text{maximise/minimise } f(x, y) \\ \text{subject to } g(x, y) = 0 \end{array}$$

Remark: An equation $h(x, y) = c$, c constant, is called a **constraint**. Note that any constraint $h(x, y) = c$ can be rearranged to a constraint of the form $g(x, y) = 0$ by letting $g(x, y) = h(x, y) - c$.

In the last lecture we saw that the solutions to this problem - the **constrained extrema** - came in two flavours:

- (I) the points (x, y) satisfying $\nabla f(x, y) = 0$ and $g(x, y) = 0$;
- (II) the points (x, y) satisfying $\nabla f(x, y) = \lambda \nabla g(x, y)$ and $g(x, y) = 0$, for some nonzero λ , called a **Lagrange multiplier**.

Note that type (I) points can be considered to be type (II) points for the case $\lambda = 0$.

We generalise to the setting of several variables:

Method of Lagrange multipliers: single constraint

Let $f(\underline{x})$, $g(\underline{x})$ be differentiable functions of n variables. If \underline{x} is a solution to the constrained optimisation problem

$$\begin{array}{l} \text{maximise/minimise } f(\underline{x}) \\ \text{subject to } g(\underline{x}) = 0 \end{array}$$

then there exists some λ such that (\underline{x}, λ) is a solution to the equation

$$\nabla f(\underline{x}) = \lambda \nabla g(\underline{x})$$

Remark: The method of Lagrange multipliers can be extended to the case of multiple constraints $g_1(\underline{x}) = \dots = g_k(\underline{x}) = 0$. In this case there are two flavours of constrained extrema:

- (I) the points \underline{x} satisfying $\nabla f(\underline{x}) = 0$ and $g_1(\underline{x}) = \dots = g_k(\underline{x}) = 0$;
- (II) the points \underline{x} satisfying $\nabla f(\underline{x}) = \sum_{i=1}^k \lambda_i \nabla g_i(\underline{x})$ and $g_1(\underline{x}) = \dots = g_k(\underline{x}) = 0$, for some $\lambda_1, \dots, \lambda_k$ (not all equal to zero).

The gradient condition states that $\nabla f(\underline{x})$ is orthogonal to the tangent space of the space defined by $g_1 = \dots = g_k = 0$. For details see p.284 of the textbook.

Example: Model the surface of the Earth by the unit sphere $x^2 + y^2 + z^2 = 1$. A satellite is orbiting the earth at a fixed height - in our model the satellite's orbit is constrained to lie in the sphere $x^2 + y^2 + z^2 = 9$. Assume we are standing at $(1, 0, 0)$ on the surface of the Earth. Let's use Lagrange multipliers to confirm the obvious(?) geometric fact: the satellite is closest to our position when the satellite is at $(3, 0, 0)$.

We model this problem as a constrained optimisation problem:

$$\begin{aligned} &\text{minimise} && d(x, y, z) = (x-1)^2 + y^2 + z^2 \\ &\text{subject to} && g(x, y, z) = x^2 + y^2 + z^2 - 9 = 0 \end{aligned}$$

Solution:

$$\nabla d = [2(x-1) \quad 2y \quad 2z]$$

$$\nabla g = [2x \quad 2y \quad 2z]$$

Solve:

$$2(x-1) = 2\lambda x \quad (1)$$

$$2y = 2\lambda y \quad (2)$$

$$2z = 2\lambda z \quad (3)$$

$$x^2 + y^2 + z^2 = 9 \quad (4)$$

$$z \neq 0: (3) \Rightarrow \lambda = 1$$

$$(1) \Rightarrow 2x - 2 = 2x \quad \downarrow$$

$$\Rightarrow \boxed{z=0}$$

$$y \neq 0: (2) \Rightarrow \lambda = 1$$

$$(1) \Rightarrow 2x - 2 = 2x \quad \downarrow$$

$$\Rightarrow \boxed{y=0}$$

$$(4) \Rightarrow z^2 = 9 \Rightarrow x = \pm 3.$$

Applications of Extrema

Linear regression A set S of k points in the plane

$$S = \{(x_1, y_1), \dots, (x_k, y_k)\}$$

Then $(\pm 3, 0, 0)$ are constrained extrema

$$d(3, 0, 0) = 4 < d(-3, 0, 0)$$

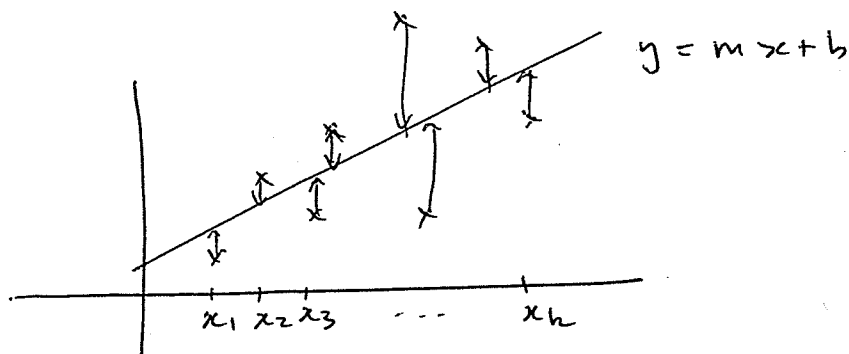
$\Rightarrow (3, 0, 0)$ is minimum.

can be interpreted as a data set relating two quantities x and y . For example, x could represent SAT scores and y could represent college grades.

We want to understand what the general linear correlation is between the quantities x and y i.e. we want to find the **line of best fit** $y = mx + b$. Mathematically, we want to solve the optimisation problem:

$$\text{minimise} \quad D(m, b) = (y_1 - (mx_1 + b))^2 + \dots + (y_k - (mx_k + b))^2$$

Diagram:



We need to find the extrema of the function D . We compute ∇D :

$$\frac{\partial D}{\partial m} = \frac{\sum_{i=1}^k 2(y_i - (mx_i + b)) \cdot (-x_i)}{1} = -2 \sum_{i=1}^k x_i y_i + 2m(\sum x_i^2) + 2b(\sum x_i)$$

$$\frac{\partial D}{\partial b} = \frac{\sum 2(y_i - (mx_i + b))(-1)}{1} = -2 \sum y_i + 2m(\sum x_i) + 2kb$$

Setting both partial derivatives equal to zero gives the equations

$$(\sum x_i^2)m + (\sum x_i)b = \sum x_i y_i$$

$$(\sum x_i)m + kb = \sum y_i$$

This is a system of linear equations in the two variables m and b . We solve to obtain the single solution:

$$m = \frac{k(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{k(\sum x_i^2) - (\sum x_i)^2}$$

$$b = \frac{(\sum x_i^2)(\sum y_i) - (\sum x_i)(\sum x_i y_i)}{k(\sum x_i^2) - (\sum x_i)^2}$$

This approach can be used to solve more general polynomial regression. For example, we could try to determine a parabola of best fit $y = ax^2 + bx + c$. Then, we aim to minimise

$$D(a, b, c) = \sum_{i=1}^k (y_i - (ax_i^2 + bx_i + c))^2$$