CH 12 - P1

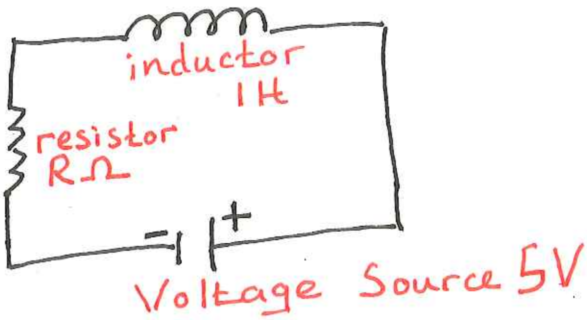
Initial Value Problems for ODEs

$$\text{(IVP)}\quad \begin{cases} y' = f(x, y) \\ y(x_0) = y_0 \quad \text{(initial condition)} \end{cases}$$

$f : \Omega \to \mathbb{R}$ (where $\Omega \subseteq \mathbb{R}^2$)

$y(x) : [x_0, X_M] \to \mathbb{R}$

Ex



initially
$i(0) = 0$

$$5 = 1 \cdot i'(t) + R\, i(t)$$

Assume $R = (1 + i^2)\,\Omega$

$$i'(t) = 5 - i(t) - i^3(t)$$

$$i(0) = 0$$

Assumption: (IVP) has a unique solution.

THM (Uniqueness)

Let

$$S := \{(x,y) \mid x \in [x_0, x_0+a],\ y \in [y_0-b, y_0+b]\}.$$

$(\subseteq \Omega)$

Suppose f is continuous on S, indeed $\exists \gamma > 0$ such that

$$|f(x,y) - f(x,\tilde{y})| \leqslant \gamma |y - \tilde{y}| \quad \forall (x,y), (x,\tilde{y}) \in S.$$

Then (IVP) has a unique solution in $[x_0, x_0+\alpha]$ where

$$\alpha := \min\left\{a, \frac{b}{M}\right\} \quad \text{with } M := \max_{(x,y)\in S} |f(x,y)|.$$

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e.g.

$$\begin{aligned} i'(t) &= \underbrace{5 - i(t) - i^3(t)}_{f(t,i)} \\ i(0) &= 0 \end{aligned}$$

$f(t,i)$ is continuous, indeed Lipschitz continuous on any $[0,a] \times [-b,b]$; $i(t)$ the solution is unique on any $[0,\alpha]$

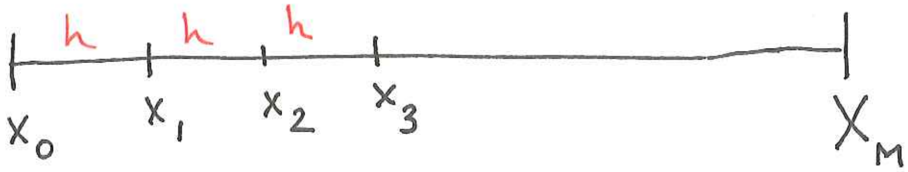
For simplicity for the rest, assume

f is continuous on $\mathbb{R}^2$, and

$\exists \gamma > 0 \quad |f(x,y) - f(x,\tilde{y})| \leqslant \gamma |y - \tilde{y}| \quad \forall (x,y), (x,\tilde{y}) \in \mathbb{R}^2$

(IVP) has a unique soln $y(x) : [x_0, X_M] \to \mathbb{R}$

General Numerical Approach



let $x_j = x_0 + jh \qquad j = 0, 1, \ldots, N$

where $h = \dfrac{X_M - x_0}{N}$

step size

$$y_j \approx y(x_j)$$

Numerical (approximate) solution

exact solution

Euler's Method

$$y(x_{n+1}) = y(x_n) + y'(x_n)\,h + O(h^2)$$

$$= y(x_n) + f(x_n, y(x_n))\,h + \underbrace{O(h^2)}_{\text{2nd order terms}}$$

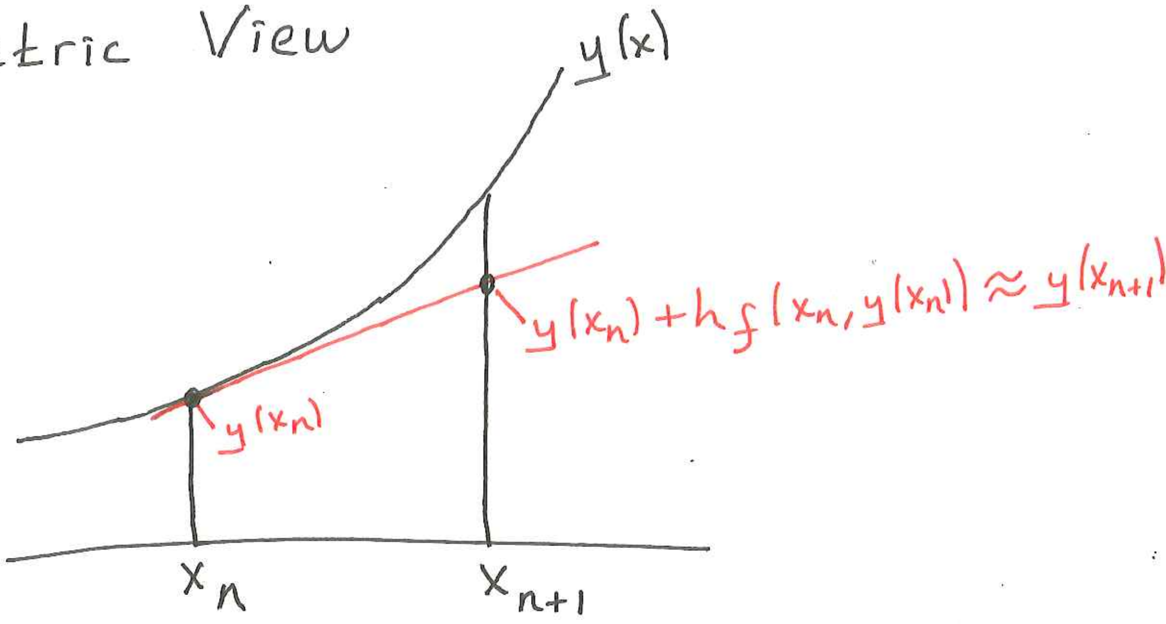
by Taylor's thm assuming y is at least twice differentiable

Discarding 2nd order terms

$$\boxed{\begin{array}{l} y_{n+1} = y_n + f(x_n, y_n)\,h \\ n = 0, 1, \ldots, N-1 \end{array}}$$

Euler update rule

Geometric View



One-step Methods

$$(+) \quad y_{n+1} = y_n + h\,\phi(x_n, y_n; h)$$

Global Error

$$e_n := y(x_n) - y_n \qquad n = 0, 1, 2, \dots, N$$

Truncation Error

$$T_n := \frac{y(x_{n+1}) - y(x_n)}{h} - \phi(x_n, y(x_n); h)$$

$$n = 0, 1, 2, \dots, N-1.$$

THM

Suppose ϕ in (+) is such that for some $\tilde{\gamma} > 0$

$$|\phi(x, u; h) - \phi(x, v; h)| \leq \tilde{\gamma}\,|u - v| \quad \forall (x,u), (x,v) \in \mathbb{R}^2$$

and for all h sufficiently small. Then

$$(\times) \quad |e_n| \leq \frac{T}{\tilde{\gamma}}\left(e^{\tilde{\gamma}(x_n - x_0)} - 1\right) \quad \text{for } n = 0, 1, 2, \dots, N$$

where $T := \max\{|T_j| \mid j = 0, 1, \dots, N-1\}$.

Proof

We have

$$y(x_{n+1}) = y(x_n) + h\,\phi(x_n, y(x_n); h) + hT_n,$$

$$y_{n+1} = y_n + h\,\cancel{f(x_n,y_n)}\,\phi(x_n, y_n; h)$$

Subtracting 2nd eqn from 1st yields

$$e_{n+1} = e_n + h\,\{\phi(x_n, y(x_n); h) - \phi(x_n, y_n; h)\} + hT_n.$$

Due to Lipschitz continuity of ϕ, we have

$$|e_{n+1}| \leqslant |e_n| + h\tilde{\gamma}\underbrace{|y(x_n) - y_n|}_{|e_n|} + hT$$

(where we assumed h is small enough), that is

$$(*)\quad |e_{n+1}| \leqslant (1 + h\tilde{\gamma})\,|e_n| + hT.$$

Next we show $(*)$ implies

$$(**)\quad |e_n| \leqslant \frac{T}{\tilde{\gamma}}\{(1+h\tilde{\gamma})^n - 1\} \qquad n = 0, 1, \ldots, N.$$

by induction. As the base case with $n = 0$

$$e_0 = 0 = \frac{T}{\tilde{\gamma}}\{(1+h\tilde{\gamma})^0 - 1\}.$$

As for the inductive case, suppose $(**)$ holds. Plugging this in $(*)$,

$$|e_{n+1}| \leqslant (1+h\tilde{\gamma})\frac{T}{\tilde{\gamma}}\{(1+h\tilde{\gamma})^n - 1\} + hT$$

$$= \frac{T}{\tilde{\gamma}}\{(1+h\tilde{\gamma})^{n+1} - 1\}$$

proving $(**)$. Now (x) follows from $(**)$ by observing $(1+h\tilde{\gamma}) \leqslant e^{h\tilde{\gamma}}$ (as $e^{h\tilde{\gamma}} = 1 + h\tilde{\gamma} + \frac{(h\tilde{\gamma})^2}{2} + \cdots$). $\square$

Global Error of Euler's method

For Euler's method

$$\phi(x_n, y_n; h) = f(x_n, y_n)$$

with the Lipschitz constant Υ (w.r.t 2nd parameter).

By Taylor's thm with 2nd order remainder (assuming now y'' is continuous on $[x_0, X_M]$)

$$y(x_{n+1}) = y(x_n) + y'(x_n)h + \frac{y''(\xi_n)h^2}{2}$$

$$\Longrightarrow \frac{y(x_{n+1}) - y(x_n)}{h} - \underbrace{y'(x_n)}_{f(x_n, y(x_n))}\cancel{h} = \frac{y''(\xi_n)}{2} h$$

$$\Longrightarrow T_n = \frac{y''(\xi_n)}{2} h$$

$$\Longrightarrow T \leqslant \frac{M_2}{2} h$$

for some $\xi_n \in (x_0, X_M)$, and where $M_2 := \max_{x \in [x_0, X_M]} |y''(x)|$.

Inequality (x) on page 4 implies

$$|e_n| \leqslant \frac{M_2}{2} \left\{ \frac{e^{\Upsilon(x_n - x_0)} - 1}{\Upsilon} \right\} h$$

$$\leqslant \frac{M_2}{2} \left\{ \frac{e^{\Upsilon(X_M - x_0)} - 1}{\Upsilon} \right\} h \qquad n = 0, 1, \dots, N$$

Ex

$$\underline{y}' = \underbrace{\cos \underline{y}}_{f(x,y)}$$

$$\underline{y}(0) = 0$$

Apply Euler's method on $[0,2]$.

(i) Lipschitz constant γ

$$\left| \frac{\partial f(x,\underline{y})}{\partial \underline{y}} \right| = |\sin \underline{y}| \leqslant 1 \quad \forall \underline{y}$$

$\Longrightarrow \gamma = 1$ a Lipschitz constant

for $f(x,\underline{y}) = \cos \underline{y}$ w.r.t. $\underline{y}$

(ii) M_2 (bound on $|\underline{y}''(x)|$ over $[0,2]$)

$$\underline{y}''(x) = -\sin \underline{y} \quad \Longrightarrow \quad |\underline{y}''(x)| \leqslant M_2 = 1 \quad \forall x \in [0,2]$$

Global error

$$|e_n| \leqslant \frac{1}{2}\{e^{\overbrace{hn}^{\in [0,2]}} - 1\}\, h$$

$$\leqslant \frac{1}{2}\{e^2 - 1\}\, h$$

$n = 0, 1, \ldots, N.$

Terminology Regarding One-Step Methods

A one-step method is called consistent if for every $\varepsilon > 0$ there exists $h(\varepsilon) > 0$ s.t.

$$|T_n| < \varepsilon \quad \forall n \quad \forall h \in (0, h(\varepsilon)).$$

consistency

Now suppose

$h \to 0$ whereas $n \to \infty$,

moreover

$x_n \longrightarrow x \in [x_0, X_M]$.

Consistency implies

$$0 = \lim_{n \to \infty} T_n = y'(x) - \phi(x, y(x); 0)$$
$$= f(x, y(x)) - \phi(x, y(x); 0)$$

for all x. Indeed $y(x)$ can also be chosen as any continuously differentiable function. Consistency implies (actually equivalent to)

$$f(x, y) \equiv \phi(x, y; 0).$$

e.g. Euler's method is consistent.

A one-step method has order of accuracy p if there exist constants K and h_0 s.t.

$$|T_n| \leqslant K h^p \qquad \forall n \ \forall h \in (0, h_0],$$

and p is the largest integer satisfying this.

order

Order of Euler's Method

$$T_n = \frac{y''(\xi_n)}{2} h \qquad \left(\text{see page ⑥ in CH 12-P1} \right)$$

Hence, for Euler's method order of accuracy is 1.

An implicit one-step method

$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} y'(x)\,dx$$

By using the Trapezoidal rule for the integral on the right

$$y(x_{n+1}) - y(x_n) = h \left\{ \frac{y'(x_{n+1}) + y'(x_n)}{2} \right\}$$

$$= h \left\{ \frac{f(x_{n+1}, y(x_{n+1})) + f(x_n, y(x_n))}{2} \right\}$$

Trapezoidal Method

$$y_{n+1} = y_n + \frac{h}{2} \left\{ f(x_n, y_n) + f(x_{n+1}, y_{n+1}) \right\}$$

$n = 0, 1, \ldots, N-1$

called an implicit method, i.e., determination of y_{n+1} requires solution of a nonlinear eq

Truncation error

$$T_n = \frac{y(x_{n+1}) - y(x_n)}{h} - \left\{\frac{f(x_n, y(x_n)) + f(x_{n+1}, y(x_{n+1}))}{2}\right\}$$

$$= \frac{y(x_{n+1}) - y(x_n)}{h} - \left\{\frac{y'(x_n) + y'(x_{n+1})}{2}\right\}$$

By the error bound for the trapezoidal rule for integration

$$(+) \quad |T_n| \leqslant \frac{M_3}{12} h^2$$

where $M_3 := \max_{x \in [x_0, X_M]} \left| [y'(x)]'' \right| = \max_{x \in [x_0, X_M]} |y'''(x)|$.

The order of accuracy is 2 (as the inequality in (+) can be made an equality for certain $y(x)$, e.g. $y(x) = \frac{M_3}{6} x^3$)

Global error of Trapezoidal Method

Find $\tilde{\gamma}$ Lipschitz constant for $\phi(x, y; h)$

$$h\,\phi(x_n, y_n; h) = \frac{h}{2}\{f(x_n, y_n) + f(x_{n+1}, y_{n+1})\}$$

$$= \frac{h}{2}\{f(x_n, y_n) + f(x_{n+1}, y_n + h\phi(x_n, y_n; h))\}$$

Now

$$\{\phi(x_n, u; h) - \phi(x_n, v; h)\}$$

$$= \frac{1}{2}\Big\{\big[f(x_n, u) + f(x_{n+1}, u + h\,\phi(x_n, u; h))\big] - \big[f(x_n, v) + f(x_{n+1}, v + h\,\phi(x_n, v; h))\big]\Big\}$$

implying (recall Υ, Lipschitz constant for f)

$$|\phi(x_n, u; h) - \phi(x_n, v; h)|$$

$$\leq \frac{\Upsilon}{2}|u - v| + \frac{h\Upsilon}{2}\{\phi(x_n, u; h) - \phi(x_n, v; h)\}$$

$$\Longrightarrow$$

$$|\phi(x_n, u; h) - \phi(x_n, v; h)|$$

$$\leqslant \frac{(\Upsilon/2)}{(1 - h\Upsilon/2)}|u - v|$$

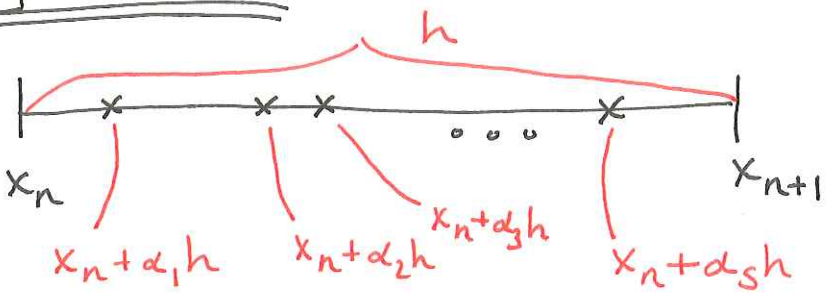
that is $\widetilde{\Upsilon} = \Upsilon/(2 - h\Upsilon)$.

It follows from (x) on page 4 of CH 2 - P1

$$|e_n| \leqslant \frac{M_3 h^2}{12\widetilde{\Upsilon}}\left(e^{\widetilde{\Upsilon}(x_n - x_0)} - 1\right)$$

$$\leqslant \frac{M_3 h^2}{12\widetilde{\Upsilon}}\left(e^{\widetilde{\Upsilon}(x_M - x_0)} - 1\right) \quad \forall n.$$

Runge-Kutta Methods



Use intermediate points;
An s-step method $x_n+\alpha_1 h, \ldots, x_n+\alpha_s h$
$\exists\, \alpha_1, \ldots, \alpha_s \in (0,1)$.

Explicit 2-step methods with order of accuracy 2.

$$y_{n+1} = y_n + h\{a k_1 + b k_2\}$$

with

$$k_1 = f(x_n, y_n)$$

$$k_2 = f(x_n + \alpha_1 h, y_n + \beta_1 \cancel{k}) \quad \to f(x_n, y_n) h$$

To be determined: a, b, α_1, β_1

Consistency requirement

$$\phi(x_n, y_n; h) = a f(x_n, y_n) + b f(x_n + \alpha_1 h, y_n + \beta_1 h \overset{f(x_n,y_n)}{})$$

As $h \to 0$ and $n \to \infty$, as well as $x_n \to x$
we must have (true $\forall x, y$)

$$\phi(x, y; 0) = a f(x, y) + b f(x, y) \quad \left(\begin{smallmatrix}\text{i.e.}\\ y = y(x)\end{smallmatrix}\right)$$

$$\Longrightarrow \quad a + b = 1$$

Order of accuracy requirement ($\geqslant 2$)

$$T_n = \frac{y(x_{n+1}) - y(x_n)}{h} - \phi(x_n, y(x_n); h)$$

Notation $\left\{ \begin{array}{l} \text{Let } y := y(x_n),\ f := f(x_n, y(x_n)),\ y' := y'(x_n) \\ f_x := \partial f(x_n, y(x_n))/\partial x,\ f_y := \partial f(x_n, y(x_n))/\partial y \\ \text{similarly for higher order derivatives of } f, y. \end{array} \right.$

By Taylor's thm with 4th order remainder

$$y(x_{n+1}) = y + y'h + y''\frac{h^2}{2} + y'''\frac{h^3}{6} + O(h^4)$$

$$= y + fh + \{f_x + f_y y'\}\frac{h^2}{2} + \{f_{xx} + 2f_{xy}y' + f_{yy}(y')^2 + f_y y''\}\frac{h^3}{6} + O(h^4)$$

$$\Rightarrow \frac{y(x_{n+1}) - y(x_n)}{h} = f + \{f_x + f_y y'\}\frac{h}{2} + \{f_{xx} + 2f_{xy}y' + f_{yy}(y')^2 + f_y y''\}\frac{h^2}{6} + O(h^3)$$

By Taylor's thm (for functions of two variables) with 3rd order remainder $\left(\begin{array}{l}\text{stated and proved}\\ \text{formally on page 10}\end{array}\right)$

$$\phi(x_n, y(x_n); h) = af + b\{f + f_x(\alpha h) + f_y(\beta h f)$$
$$+ f_{xx}(\alpha h)^2 + 2f_{xy}(\alpha h)(\beta h f) + f_{yy}(\beta h f)^2\} + O(h^3)$$

Putting these together (and exploiting $a+b=1$)

(x) $$T_n = h\left\{ f_x\left[\tfrac{1}{2}-\alpha_1 b\right] + f_y y'\left[\tfrac{1}{2}-\beta_1 b\right]\right\}$$
$$+ h^2\left\{ f_{xx}\left[\tfrac{1}{6}-\alpha_1^2 b\right] + 2 f_{xy} y'\left[\tfrac{1}{6}-\alpha_1\beta_1 b\right] + f_{yy}(y')^2\left[\tfrac{1}{6}-\beta_1^2 b\right] + f_y y''/6\right\} + O(h^3)$$

For order of accuracy ≥ 2

(+) $\alpha_1 b = \beta_1 b = 1/2$ (in addition to $a+b=2$)

Procedure

① Choose $\alpha_1 \in (0, 1]$

② Choose $\beta_1 = \alpha_1$, $b = 1/2\alpha_1$, $a = 1 - 1/2\alpha_1$

Ex

① Choose $\alpha_1 = 1$, $\beta_1 = 1$, $b = 1/2$, $a = 1/2$

(improved Euler method) $$y_{n+1} = y_n + \frac{h}{2}\left\{ f(x_n, y_n) + f(x_n+h, y_n + hf(x_n, y_n))\right\}$$

② Choose $\alpha_1 = 1/2$, $\beta_1 = 1/2$, $b = 1$, $a = 0$

(modified Euler method) $$y_{n+1} = y_n + h f(x_n + h/2, y_n + (h/2) f(x_n, y_n))$$

3rd order accuracy is not possible with 2-stages

e.g. Consider $y' = y$

From (x) and choosing α, β, a, b as in (+)

$$T_n = h^2/6 + O(h^3)$$

General Runge-Kutta Framework

$$(*)\quad \begin{cases} y_{n+1} = y_n + h \sum_{j=1}^{s} b_j f(x_n + \alpha_j h, \varepsilon_j) \\ \text{where} \\ \varepsilon_j = y_n + h \sum_{k=1}^{s} c_{jk} f(x_n + \alpha_k h, \varepsilon_k) \end{cases}$$

To be determined

$\alpha_1, \ldots, \alpha_s \in [0, 1]$ - Runge-Kutta nodes

$b_1, \ldots, b_s$ - Runge-Kutta weights

$\begin{bmatrix} c_{11} & \cdots & c_{1s} \\ \vdots & & \vdots \\ c_{s1} & & c_{ss} \end{bmatrix}$ - Runge-Kutta matrix

Collocation Methods (Runge-Kutta methods with high order of accuracy)

Use Gaussian quadratures for the integrals below

$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} f(x, y(x))\, dx$$

$$y(x_n + \alpha_k h) - y(x_n) = \int_{x_n}^{x_n + \alpha_k h} f(x, y(x))\, dx \quad (k = 1, 2, \ldots, s)$$

equivalently (letting $x = x_n + \alpha h$)

$$y(x_{n+1}) - y(x_n) = h \int_0^1 f(x_n + \alpha h, y(x_n + \alpha h))\, d\alpha$$

$$y(x_n + \alpha_k h) - y(x_n) = h \int_0^{\alpha_k} f(x_n + \alpha h, y(x_n + \alpha h))\, d\alpha$$

$k = 1, \ldots, s$

Choose $\alpha_1, \ldots, \alpha_n$ as the roots of φ_n w.r.t. inner product

$$\langle f, g \rangle = \int_0^1 f(x) g(x) \, dx,$$

compute b_j, c_{kj} based on Lagrange intepolation.

Letting y_{n+1}, y_n, ξ_k numerical solutions for $y(x_{n+1})$, $y(x_n)$, $y(x_n + \alpha_k h)$, we obtain formulas of the form $(*)$ on page 8.

Order of accuracy of the resulting method is $2s$.

Taylor's thm for functions of two variables with 3rd order remainder

Let $f := f(x,y) : \mathbb{R}^2 \to \mathbb{R}$ be three times differentiable.

Then

$$f(a+hp,\, b+hq) = f(a,b) + f_x(a,b)(hp) + f_y(a,b)(hq)$$

$$+ \frac{1}{2} f_{xx}(a,b)(hp)^2 + f_{xy}(a,b)(hp)(hq) + \frac{1}{2} f_{yy}(a,b)(hq)^2$$

$$+\, O(h^3).$$

<u>Proof</u>

Let $F(t) := f(a+thp,\, b+thq)$, and apply the usual Taylor's thm to F.

$$F(1) = F(0) + F'(0) + F''(0)/2 + F'''(\varepsilon)/6 \quad \exists\, \varepsilon \in (0,1)$$

$$\Longrightarrow$$

$$f(a+hp,\, b+hq) =$$

$$f(a,b) + \underbrace{\{f_x(a,b)(hp) + f_y(a,b)(hq)\}}_{F'(0)\ \text{(Using chain-rule)}}$$

$$+ \underbrace{\{f_{xx}(a,b)(hp)^2 + 2 f_{xy}(a,b)(hp)(hq) + f_{yy}(a,b)(hq)\}}_{F''(0)} / 2$$

$$+ \underbrace{O(h^3)}_{f'''(\varepsilon)/6}$$