UNIVERSIDAD COMPLUTENSE DE MADRID
FACULTAD DE CIENCIAS FISICAS

10 de Febrero de 2017

Examen de Física Computacional - 2016/2017

Nombre y Apellidos:

DNI y Firma:

Advertencias: La calculadora en modo de **radianes**. Sus cuentas deben justificar las respuestas que usted escriba.

1. [2.25 puntos] a) Encontrar los coeficientes a, b tal que la regla de cuadratura

$$\int_0^\infty f(t)\, e^{-t}\, dt \approx af\left(2-\sqrt{2}\right)+bf\left(2+\sqrt{2}\right)$$

sea exacta para polinomios del mayor grado posible.

b) Decir claramente (justificado con cuentas) cuál es el grado máximo del polinomio.

c) Escribir el error de la fórmula anterior.

d) Calcular con dicha regla la integral

$$\int_0^\infty \frac{e^{-t}}{1+t}\, dt$$

cuyo valor exacto es 0.596347.

2. [2.25 puntos]

a) Calcular el período del generador de Fibonacci de números aleatorios

$$x_n = (x_{n-1} + x_{n-2}) \mod 12,$$

con $x_{-1} = 0, x_0 = 1$.

b) Utilizando dos teoremas vistos en clase determinar la longitud del período de los generadores $x_{n+1} = (ax_n + c) \mod m$, siendo 1) $a = 3141592621, c = 2718281829, m = 10000000000$, 2) $a = 5, c = 0, m = 29$.

c) Deducir las condiciones que tienen que cumplir a, b, c para que el número de cuatro cifras $aabc$ sea divisible entre 13. Escribir tres ejemplos.

3. [2.5 puntos] Sean los esquemas iterativos $x_{n+1} = F(x_n)$ y $x_{n+1} = G(x_n)$ donde

$$F(x) = \frac{x^3+33x}{3x^2+11}, \qquad G(x) = \frac{x^2+11}{2x}.$$

1) ¿Qué calcula cada esquema? 2) Si alguno de ellos es un *método de Newton* diga cuál es. 3) Utilizando en ambos el input $x_0 = 2$, calcular $x_1, x_2, x_3, \ldots$ hasta que una iteración y la siguiente difieran en menos de 10^{-6} o sea, seis cifras decimales coincidentes. Trabaje con 10 digitos o tendrá problemas. 4) A la vista del resultado del apartado anterior diga qué método es más rápido. 5) Calcule el orden de convergencia de cada método.

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(1) Gauss-Laguerre cuadratura. Nombre obvio.

$$\int_0^\infty dt\, f(t)\, e^{-t} = a f(2-\sqrt{2}) + b f(2+\sqrt{2}) \quad (*)$$

a) The integrals needed are on the bottom of the page.

$f(t)=1$, $\boxed{1 = a+b}$

$f(t)=t$, $\boxed{1 = a(2-\sqrt{2}) + b(2+\sqrt{2})}$

$= 2(a+b) + \sqrt{2}(-a+b) = 2+\sqrt{2}(-a+b)$

$a+b=1$

or

$\boxed{-\frac{1}{\sqrt{2}} = -a+b}$

solving for a, b we have,

$\boxed{a = \frac{1}{2} + \frac{\sqrt{2}}{4}}$, $\boxed{b = \frac{1}{2} - \frac{\sqrt{2}}{4}}$

Take now $f(t)=t^2$ in (*). The formula is exact for $f=t^2$ if $2 = a(2-\sqrt{2})^2 + b(2+\sqrt{2})^2$, what it is true.

$$a(2-\sqrt{2})^2 + b(2+\sqrt{2})^2 = a(4+2-4\sqrt{2}) + b(4+2+4\sqrt{2})$$
$$= 6\underbrace{(a+b)}_{\to 1} + 4\sqrt{2}\underbrace{(-a+b)}_{\to -\frac{1}{\sqrt{2}}} = 6-4 = 2$$

Since $\int_0^\infty dx\, e^{-ax} = -\frac{1}{a}\left[e^{-ax}\right]_0^\infty = \frac{1}{a}$, just deriving wrt a is obtained that

$$\int_0^\infty dx\, x\, e^{-ax} = \frac{1}{a^2}$$

$$\int_0^\infty dx\, x^2 e^{-ax} = \frac{2}{a^3}$$

$$\int_0^\infty dx\, x^3 e^{-ax} = \frac{6}{a^4}, \quad 6=3!$$

$$\int_0^\infty dx\, x^4 e^{-ax} = \frac{24}{a^5}, \quad 24=4!$$

And it is exact for $f(t)=t^3$ because

$$a(2-\sqrt{2})^3+b(2+\sqrt{2})^3=6$$

but ~~not~~ for $f(t)=t^4$ because now

$$a(2-\sqrt{2})^4+b(2+\sqrt{2})^4\neq 24$$

but

$$a(2-\sqrt{2})^4+b(2+\sqrt{2})^4=20$$

instead.

We check (**) and (***) with a shortcut.
Notice that

$$x\equiv 2-\sqrt{2},\quad y\equiv 2+\sqrt{2},$$

and consequently

$$x+y=4,\quad x\cdot y=2$$

x, y are solutions of the 2-order polynomial

$$x^2-4x+2=0$$

[el famoso $L_2(x)$, poli de Laguerre]

as you can check.

...Léase ... autofunción del hidrógeno...

$$(**)\quad ax^3+by^3=a(14x-8)+b(14y-8)=14(\overset{1}{ax+by})-8(\underset{1}{a+b})=6$$

$$ax^3=ax(4x-2)=a(4x^2-2x)=a(16x-8-2x)=a(14x-8)$$

&

$$by^3=\dots=b(14y-8)$$

or

$$(***)\quad ax^4+by^4=a(4x-2)^2+b(4y-2)^2$$
$$=a(16x^2+4-16x)+b(16y^2+4-16y)$$
$$=16(\underbrace{ax^2+by^2}_{2})+4(\underbrace{a+b}_{1})-16(\underbrace{ax+by}_{1})$$
$$=16\cdot 2+4-16$$
$$=20 \text{ and not } 24$$

$a+b=1 \rightsquigarrow$ exact $f(t)=1$
$ax+by=1 \rightsquigarrow$ exact $f(t)=t$
$ax^2+by^2=2 \rightsquigarrow$ exact $f(t)=t^2$
$ax^3+by^3=6 \rightsquigarrow$ exact $f(t)=t^3$

The difference

$$\int_0^\infty dt\, t^4 e^{-t} = 24$$

$$a f(2-\sqrt{2}) + b f(2+\sqrt{2}) = \underset{\nearrow\, f = t^4}{20}$$

$24 = 20 + \underset{\nwarrow\, \text{error}}{4}$,

that is

$$24 = 20 + 4$$ ← accounts for the error

To finish:

$$\boxed{\int_0^\infty dt\, f(t) e^{-t} = \left(\frac{1}{2}+\frac{\sqrt{2}}{4}\right) f(2-\sqrt{2}) + \left(\frac{1}{2}-\frac{\sqrt{2}}{4}\right) f(2+\sqrt{2}) + \frac{4}{4!} f''''(\xi) \text{ ,}\quad \xi \text{ a number in } [0,\infty)}$$

$\frac{1}{6} = \frac{4}{4!}$

$\frac{4}{4!} = \frac{1}{3!} = \frac{1}{6}$

The precision of the formula is 3 because it is exact for polynomials up to third degree but not fourth.

$$\int_0^\infty dt\, \frac{1}{t+1} e^{-t} \simeq \frac{\frac{1}{2}+\frac{\sqrt{2}}{4}}{3-\sqrt{2}} + \frac{\frac{1}{2}-\frac{\sqrt{2}}{4}}{3+\sqrt{2}} = \frac{4}{7} \simeq 0.5714285\ldots$$

with our formula: $f(t) = \frac{1}{t+1}$

$$\begin{array}{l} \frac{3}{2} + \cancel{\frac{3}{4}\sqrt{2}} + \cancel{\frac{\sqrt{2}}{2}} + \frac{2}{4} \\ + \frac{3}{2} - \cancel{\frac{3\sqrt{2}}{4}} - \cancel{\frac{\sqrt{2}}{2}} + \frac{2}{4} \\ \hline 3 \qquad\qquad + 1 = 4 \end{array}$$

with error $\frac{4}{4!} f''''(\xi) = \frac{4}{(\xi+1)^5}$

Considering that $I_{exact} = 0.59635$ and $I_{Gauss-Laguerre} = 0.57143$ the error is $\simeq 0.0249$.

(2) a) $x_n = x_{n-1} + x_{n-2}$, mod 12

$0, \underline{1, 1}, 2, 3, 5, 8, 1, 9, 10, 7, 5, 0, 5, 5, 10, 3, 1,$

$4, 5, 9, 2, 11, 1, 0, \underline{1, 1}, 2, 3, \ldots$

amouw, porsqnesto!

x_{10} (for instance) $\quad x_{34} \quad 34-10=24$

$\boxed{\text{Period is } 24}$

1b) $a = 3141592621$, $c = 2718281829$

$m = 10^{10} = 2^{10} \cdot 5^{10}$, $\quad p = 2, 5$: primes that factorize m.

ok c cannot be divided by 2 or 5, hence relatively prime to m

ok $a-1$ = multiple of 2 and 5.

ok m is divisible by 4, $a-1$ is divisible by 4 because ends with a 20.

$\boxed{\text{Period}: m = 10^{10}}$ (maximum)

2b) $m = 29$ is prime

5 is ~~not a~~ primitive root of 29 since $5^{14} = 1$, mod 29 before then $5^{28} = 1$, mod 29.

Flo new...

$5^0 = 1$

$5^1 = 5$

$5^2 = 25 = -4$

x_1

$5^3 = -20 + 29 = 9$

$5^4 = 45 = 30 + 15 = 1 + 15 = 16$

$5^5 = 50 + 30 = 20 + 30 + 30 = 22 = -7$

$5^6 = -35 = -30 - 5 = -29 - 1 - 5 = -6 = 23$

$5^7 = -30 = -29 - 1 = -1 + 29 = 28$

$5^8 = -5 = 24$

$5^9 = -25 + 29 = 4$

$5^{10} = 20 = -9$

$5^{11} = -45 = -30 - 15 = -16 + 29 = 13$

$5^{12} = 50 + 15 = 1 + 20 + 15 = 7$

$5^{13} = 35 = 6$

$5^{14} = 30 = 1$

$5^{15} = 5$

The period is 14 and not $28 = m-1$.
No maximum period.

c) $aabc = a \cdot 1000 + a\,100 + b \cdot 10 + c$

$10 = 13 - 3 = -3$, mod 13

$100 = 10 \cdot 10 = (-3)(-3) = 9$,

$1000 = 9(13-3) = -27 + 26 = -1$

then $-a + a \cdot 9 - 3b + c$ has to be zero or multiple of 13

nine

Conclusion: $aabc$ is divided by 13 if

$$8a - 3b + c$$

is 0 or a multiple of 13.

Examples: 1105, 4472, 9945.

[con Maple y un do + if: tb se sacan todos los que empiezan por 11, por ej:
1105, 1118, 1131, 1144, 1157, $\underbrace{1170}_{13}$, $\underbrace{1183}_{13}$, $\underbrace{1196}_{13}$. No hay más con 11bc.]

[Tb se sacarlos a mano!!!: sumo 13 a cada uno para sacar el siguiente...]

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(3) $x_n = F(x_n)$ // $x_n = G(x_n)$

$$F(x) = \frac{x^3 + 33x}{3x^2 + 11}, \quad G(x) = \frac{x^2 + 11}{2x}$$

Ambos métodos iterativos calculan $\sqrt{11}$. si x_0 es $+$vo.
lo veo con uno de ellos: $F(p) = p$ // p = fixed point

$$p = \frac{p^3 + 33p}{3p^2 + 11},$$

$$3p^3 + 11p - p^3 - 33p = 0$$

$$0 = 2p^3 - 22p = 2p(p^2 - 11)$$

$\boxed{p = 0}$ sin interés

$\boxed{p = \sqrt{11}}$

Tb sale $-\sqrt{11}$, sí, pero nuestro interés es calcular muito $\sqrt{11}$.

b) El segundo, $G(x) = \frac{x^2+11}{2x}$, tb calcula la $\sqrt{11}$.
Y es un Newton aplicado a

$$f(x) = x^2 - 11$$

lo vemos:

$$f'(x) = 2x$$

$$x - \frac{f(x)}{f'(x)} = x - \frac{x^2-11}{2x}$$

$$= \frac{x^2+11}{2x}. \quad \underline{\underline{ok}}$$

c) $x_{n+1} = F(x_n)$

n	x_n
	2.000000000
1	3.217391304
2	3.316601554
3	3.316624790
4	3.316624791

$x_{n+1} = G(x_n)$

n	
	2.0000000
1	3.750000000
2	3.411666666
3	3.316718620
4	3.316624791
5	3.316624790

d) This seems faster than (Newton's) !!!!!
what happens?

e) why?
Remember that $x_{n+1} = F(x_n)$:

true for all F analytic in p.

$$F(x) = F(p) + F'(p)(x-p) + \frac{F''}{2!}(p)(x-p)^2 + \frac{F'''}{3!}(p)(x-p)^3 + \dots$$

substitute x by x_n and p for the fixed point $F(p) = p$

$$\underset{x_{n+1}}{\overset{\shortparallel}{F(x_n)}} = \underset{p}{\overset{\shortparallel}{F(p)}} + F'(p)(x_n-p) + \frac{F''}{2!}(p)(x_n-p)^2 + \dots$$

Substract p on both sides and use $e_{n+1} \equiv x_{n+1} - p$, $e_n \equiv x_n - p$

$$e_{n+1} = F'(p)\,e_n + \frac{F''}{2!}(p)\,e_n^2 + \frac{F'''}{3!}(p)\,e_n^3 + \dots$$

→ This is our convergence order equation (or whatever...)

We now investigate this convergence order equation for our $F(x)$ and $G(x)$.
Remember that

$$F(x) = \frac{x^3+33x}{3x^2+11} \quad , \quad G(x) = \frac{x^2+11}{2x}$$

and

$$p = \sqrt{11}$$

Starting with $G(x) = \frac{1}{2}\left(x + \frac{11}{x}\right)$

$$G'(x) = \frac{1}{2}\left(1 - \frac{11}{x^2}\right) \quad \text{''} \quad G'(p) = 0$$ as expected (is Newton!!)

$$G''(x) = \frac{11}{x^3} \quad , \quad G''(p) = \frac{1}{\sqrt{11}}$$ (not zero)

Newton has quadratic convergence,

$$e_{n+1} \simeq \frac{1}{2\sqrt{11}} e_n^2 + \dots$$ smaller than e_n^2 if things are OK.

Now $F(x) = \frac{x^3+33x}{3x^2+11}$

$$F'(x) = \frac{3(x^4-22x^2+121)}{(3x^2+11)^2} = \frac{3(x^2-11)^2}{(3x^2+11)^2}$$

here

so $F'(p) = 0$; now

$$F''(x) = \frac{528x(x^2-11)}{(3x^2+11)^3}$$ so $F''(p) = 0$ as well

a difference

the method $x_{n+1} = F(x_n)$ is a third order convergence method, faster than Newton!!!! that is second order. Now $F'''(p) \neq 0$.