UNIVERSIDAD COMPLUTENSE DE MADRID
FACULTAD DE CIENCIAS FISICAS

4 de Septiembre de 2015 (3,4A)

Examen de Física Computacional - 2014/2015

Nombre y Apellidos:

DNI y Firma:

Advertencias: La calculadora en modo de **radianes**. Respuestas sin la debida justificación no puntúan.

1. [2.5 puntos] a) Estimar la integral
$$\int_{-x}^{x} e^{\sin t}\,dt$$
mediante la *regla de Simpson extendida* dividiendo el intervalo en subintervalos de $h = x/2$ (hay que aplicar Simpson dos veces, ya se lo aclaro) y llame al resultado $S(x)$, S de Simpson.

   b) Escribir explícitamente el *método de Newton* para resolver la ecuación trascendente
$$\int_{-x}^{x} e^{\sin t}\,dt = 1$$
utilizando la estimación del apartado a) donde sea necesario. La solución pedida existe y es única.

   c) Tomando en el Newton como input $x_0 = 0$, calcule x_1 y x_2 con al menos **ocho** cifras significativas.

2. [2.25 puntos] Sean las matrices
$$A = \begin{pmatrix} 1 & 2 & -1 \\ 2 & 20 & -12 \\ -1 & -12 & 9 \end{pmatrix}, \quad B = \begin{pmatrix} 4 & 2 & 4 \\ 2 & 5 & 6 \\ 4 & 6 & 9 \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 2 & 0 \\ 2 & 20 & 12 \\ 0 & 12 & 10 \end{pmatrix}.$$

   a) Decir cuáles de estas matrices admiten una factorización de la forma U^tU, donde U es una matriz triangular superior con entradas positivas en la diagonal principal. La t indica matriz transpuesta. Encontrar U para cada caso posible.

   Ayuda: La descomposición es única. Puede usar el método de **factorización** que prefiera siempre que sea manipulación de filas, o sea eliminación Gaussiana. No hace falta pivoteo parcial. Ojo! Método de 'cuenta de la vieja' no puntuará en el examen. Sólo contarán los de factorización de matrices.

   b) Los libros dicen que cuando $M = U^tU$, el número $\mathbf{v}^t\,M\,\mathbf{v}$ es **positivo** y que es igual a cero sólo si $\mathbf{v} = 0$. Siendo M la matriz, o matrices, del apartado anterior y $\mathbf{v}$ el vector columna $(x, y, z)^t$, demostrar mediante esta propiedad que todos los valores propios de M son positivos. No hay que calcularlos.

3. [2.25 puntos] a) Usando técnicas simples de Monte Carlo evaluar la integral
$$\int\int_{\Omega} (x^2 + y^2)\,dxdy,$$

Sigue a la vuelta...

donde Ω es el triángulo definido por $1/2 \leq x \leq 1$ y $0 \leq y \leq 2x - 1$. Para ello se han tirado aleatoriamente los $N = 20$ puntos (x, y) que siguen

$$
\begin{gathered}
(0.835, 0.516),\ (0.826, 0.869),\ (0.849, 0.604),\ (0.663, 0.884),\ (0.784, 0.723),\\
(0.628, 0.844),\ (0.993, 0.066),\ (0.859, 0.197),\ (0.977, 0.434),\ (0.954, 0.874),\\
(0.746, 0.401),\ (0.685, 0.010),\ (0.758, 0.789),\ (0.538, 0.151),\ (0.660, 0.268),\\
(0.560, 0.002),\ (0.651, 0.280),\ (0.723, 0.116),\ (0.932, 0.879),\ (0.558, 0.712).
\end{gathered}
$$

En estos puntos la x está distribuida uniformemente entre 0.5 y 1 como pide el enunciado y no hay que hacerle nada, mientras que la y está uniformemente distribuida entre 0 y 1. Aunque no lo va a usar en ningún cálculo, la integral pedida vale exactamente 7/32.

b) Calcule la desviación standard como viene en el libro de Press (recuerde que lo vimos en clase) e interprete el resultado a 1, 2 y 3 desviaciones.

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① Facts about $\int_{-x}^{x} dt\, e^{\sin t}$.

This is obviously a function of x. But no one knows the primitive of $e^{\sin t}$ in terms of "elementary functions". How to calculate then $\int_{-x}^{x} dt\, e^{\sin t}$? One answer is: use an approximation method to evaluate it. This is done in a) using an "extended Simpson's method".

Besides, $\int_{-x}^{x} dt\, e^{\sin t}$ is an odd function

[call it g(x) and show that $g(x) = -g(-x)$.
obviously $g(0)=0$.

The derivative of an odd fction is an even function. Then, if needed,

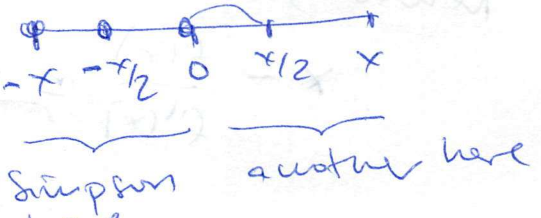
$$g'(x) = e^{\sin x} + e^{-\sin x} \qquad g(x) \equiv \int_{-x}^{x} dt\, e^{\sin t}$$

Back to the exam!! It starts here.

a)

$$\int_{-x}^{x} dt\, e^{\sin t} = \int_{-x}^{0} + \int_{0}^{x} e^{\sin t}$$

h = x/2



$$\simeq \frac{h}{3}\left[e^{-\sin x} + 4e^{-\sin\left(\frac{x}{2}\right)} + 1\right]$$

4h=2x

$$+ \frac{h}{3}\left[1 + 4e^{\sin\frac{x}{2}} + e^{\sin x}\right]$$

$$= \frac{h}{3}\left[e^{-\sin x} + 4e^{-\sin\frac{x}{2}} + 2 + 4e^{\sin\frac{x}{2}} + e^{\sin x}\right]$$

approximation! Not exact!!!

Thus

$$\int_{-x}^{x} e^{\sin t}\,dt \simeq \underbrace{\frac{x}{6}\left[e^{-\sin x}+4e^{-\sin\frac{x}{2}}+2+4e^{\sin\frac{x}{2}}+e^{\sin x}\right]}_{\text{this is } S(x)}$$

b) Need to solve $f(x)=0$ with

$$f(x)\equiv\int_{-x}^{x}dt\,e^{\sin t}-1.$$

and Newton's method

Take

$$f(x)\simeq S(x)-1 \quad \text{" with } S(x) \text{ as there.}$$

$$f'(x)=e^{\sin x}+e^{-\sin x} \quad [\text{exact!!}] \quad [*]$$

⌈Of course one can use $f'(x)\simeq S'(x)$ instead of $e^{\sin x}+e^{-\sin x}$. Which approximation does afford a better result? [more accurate...] Hmmm... Our exam is not a suitable place to treat this point... continue... please.

⌊Para el examen doy por bueno ambos, uno u otro... ver números atrás.

Newton's method:

$$x-\frac{f(x)}{f'(x)}$$

$$\simeq x-\frac{\frac{x}{6}\left[e^{-\sin x}+4e^{-\sin\frac{x}{2}}+2+4e^{\sin x/2}+e^{\sin x}\right]-1}{e^{\sin x}+e^{-\sin x}}$$

$$=\frac{5x}{6}+\frac{1-x/3\left[2(e^{-\sin x/2}+e^{\sin x/2})+1\right]}{e^{\sin x}+e^{-\sin x}}.$$

[*] Fundamental theorem of calculus.

c) $$x_1 = \frac{5x_0}{6} + \frac{1 - \frac{x_0}{3}\left[2(e^{-\sin x_0/2} + e^{\sin x_0/2}) + 1\right]}{e^{\sin x_0} + e^{-\sin x_0}}$$

If

$x_0 = 0$

$x_1 = \frac{1}{2} = 0.5$

$x_2 = 0.482083326 \ldots$

$x_3 = 0.4820156661 \ldots$

$x_4 = 0.4820156478 \ldots$

using $x - \frac{S(x)-1}{S''(x)}$ instead of $x - \frac{S(x)-1}{e^{\sin x} + e^{-\sin x}}$,

the result is

$x_0 = 0$

$x_1 = 0.5$

$x_2 = 0.48207802 \ldots$

$x_3 = 0.482015649 \ldots$

$x_4 = 0.4820156478 \ldots$

Up to 9-10 digits both results do agree...
... in x_4...

If needed,

$$S'(x) = \frac{1}{6}\Big[(1 - x\cos x)e^{-\sin x} + (1 + x\cos x)e^{\sin x} + 4\left(1 - \frac{x}{2}\cos\frac{x}{2}\right)e^{-\sin x/2} + 4\left(1 + \frac{x}{2}\cos\frac{x}{2}\right)e^{\sin x/2} + 2\Big]$$

②

$$A=\begin{pmatrix}1&2&-1\\2&20&-12\\-1&-12&9\end{pmatrix}$$

U^tU is a symmetric matrix, A too. Let us see then what factorization gives.

$$L_1A=\underbrace{\begin{pmatrix}1&0&0\\-2&1&0\\1&0&1\end{pmatrix}}_{L_1}\begin{pmatrix}1&2&-1\\2&20&-12\\-1&-12&9\end{pmatrix}=\begin{pmatrix}1&2&-1\\0&16&-10\\0&-10&8\end{pmatrix}$$

$$L_2L_1A=\underbrace{\begin{pmatrix}1&0&0\\0&1&0\\0&\frac{10}{16}&1\end{pmatrix}}_{L_2}\begin{pmatrix}1&2&-1\\0&16&-10\\0&-10&8\end{pmatrix}=\begin{pmatrix}1&2&-1\\0&16&-10\\0&0&7/4\end{pmatrix}$$

$\frac{5}{8}$

Note: L_1^{-1} L_2^{-1} are very simple to obtain [very very simple...]

Thus

$$A=L_1^{-1}L_2^{-1}\begin{pmatrix}1&2&-1\\0&16&-10\\0&0&7/4\end{pmatrix}$$

$$=\begin{pmatrix}1&0&0\\2&1&0\\-1&-\frac{10}{16}&1\end{pmatrix}\begin{pmatrix}1&2&-1\\0&16&-10\\0&0&7/4\end{pmatrix}$$

$$=\begin{pmatrix}1&0&0\\2&1&0\\-1&-\frac{5}{8}&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&16&0\\0&0&7/4\end{pmatrix}\begin{pmatrix}1&2&-1\\0&1&-5/8\\0&0&1\end{pmatrix}$$

yes!!! we can write A as demanded... see 1, 16, 7/4 (all are +ve)

$$=\underbrace{\begin{pmatrix}1&0&0\\2&4&0\\-1&-5/2&\sqrt{7}/2\end{pmatrix}}_{U^t}\underbrace{\begin{pmatrix}1&2&-1\\0&4&-5/2\\0&0&\sqrt{7}/2\end{pmatrix}}_{U}$$

$$v^tAv=v^tU^tUv=(Uv)^t(Uv)=(x+2y-z)^2+\left(4y-\frac{5}{2}z\right)^2+\frac{7}{4}z^2\geq 0$$ always.

(1) is zero if and only if $x=y=z=0$.

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conclusion: A admits the decomposition U^tU and U satisfies the conditions demanded.

$$B = \begin{pmatrix}4&2&4\\2&5&6\\4&6&9\end{pmatrix}$$

B is symmetric too.

$$L_1 B = \underset{\overset{\shortparallel}{L_1}}{\begin{pmatrix}1&0&0\\-1/2&1&0\\-1&0&1\end{pmatrix}}\begin{pmatrix}4&2&4\\2&5&6\\4&6&9\end{pmatrix} = \begin{pmatrix}4&2&4\\0&4&4\\0&4&5\end{pmatrix}$$

$$L_2 L_1 B = \underset{\overset{\shortparallel}{L_2}}{\begin{pmatrix}1&0&0\\0&1&0\\0&-1&1\end{pmatrix}}\begin{pmatrix}4&2&4\\2&5&6\\4&6&9\end{pmatrix} = \begin{pmatrix}4&2&4\\0&4&4\\0&0&1\end{pmatrix}$$

$$B = L_1^{-1} L_2^{-1} \begin{pmatrix}4&2&4\\2&5&6\\4&6&9\end{pmatrix} = \begin{pmatrix}1&0&0\\1/2&1&0\\1&1&1\end{pmatrix}\begin{pmatrix}4&2&4\\0&4&4\\0&0&1\end{pmatrix}$$

L_1^{-1} is $\begin{pmatrix}1&0&0\\1/2&1&0\\1&0&1\end{pmatrix}$ $\quad$ L_2^{-1} is $\begin{pmatrix}1&0&0\\0&1&0\\0&1&1\end{pmatrix}$

$$= \begin{pmatrix}1&0&0\\1/2&1&0\\1&1&1\end{pmatrix}\begin{pmatrix}4&0&0\\0&4&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&1/2&1\\0&1&1\\0&0&1\end{pmatrix}$$

transpose of each other

$$= \underset{U^t}{\begin{pmatrix}2&0&0\\1&2&0\\2&2&1\end{pmatrix}}\underset{U}{\begin{pmatrix}2&1&2\\0&2&2\\0&0&1\end{pmatrix}}$$; yes $B = U^tU$!!

$$v^tBv = v^tU^tUv = (Uv)^t(Uv) = (2x+y+2z)^2 + 4(y+z)^2 + z^2 \geq 0$$

It is zero iff $x=y=z=0$.

$$C=\begin{pmatrix}1&2&0\\2&20&12\\0&12&10\end{pmatrix}$$, C is symmetric

$$L_1C=\underset{\overset{\shortparallel}{L_1}}{\begin{pmatrix}1&0&0\\-2&1&0\\0&0&1\end{pmatrix}}\begin{pmatrix}1&2&0\\2&20&12\\0&12&10\end{pmatrix}=\begin{pmatrix}1&2&0\\0&16&12\\0&12&10\end{pmatrix}$$

$$L_2L_1C=\underset{\overset{\shortparallel}{L_2}}{\begin{pmatrix}1&0&0\\0&1&0\\0&-3/4&1\end{pmatrix}}\begin{pmatrix}1&2&0\\0&16&12\\0&12&10\end{pmatrix}=\begin{pmatrix}1&2&0\\0&16&12\\0&0&1\end{pmatrix}$$

$$C=L_1^{-1}L_2^{-1}\begin{pmatrix}1&2&0\\0&10&12\\0&0&1\end{pmatrix}=\begin{pmatrix}1&&\\2&1&\\0&3/4&1\end{pmatrix}\begin{pmatrix}1&2&0\\0&10&12\\0&0&1\end{pmatrix}$$

$$=\begin{pmatrix}1&&\\2&1&\\0&3/4&1\end{pmatrix}\begin{pmatrix}1&&\\&16&\\&&1\end{pmatrix}\begin{pmatrix}1&2&0\\0&1&3/4\\0&0&1\end{pmatrix}$$

$$=\underset{\overset{\shortparallel}{U^t}}{\begin{pmatrix}1&0&0\\2&4&0\\0&3&1\end{pmatrix}}\underset{\overset{\shortparallel}{U}}{\begin{pmatrix}1&2&0\\0&4&3\\0&0&1\end{pmatrix}}=U^tU$$

C can be decomposed as indicated.

$$v^tCv=(Uv)^tUv=(x+2y)^2+(4y+3z)^2+z^2\geq0$$

only zero iff $x=y=z=0$.

All matrices A, B, C satisfy U^tU decomposition with U with positive entries in the main diagonal.

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let M be A, B or C. For certain λ and $u \not\equiv 0$ ↑ vector!!
it is satisfied the relation

$$Mu = \lambda u$$

↑ & eigenvector with $u \not\equiv 0$
eigenvalue.

Since $v^t M v \geq 0$ (remember that M admits a factorization as $U^t U$ with positive entries in the diagonal of U), when $v = u$ (an eigenvector),

$$u^t M u > 0$$ **strictly** (why? because $u \not\equiv 0$)

that is also

$$\lambda \underbrace{u^t u}_{\text{always true}} > 0$$

↗ conclusion: has to be strictly positive
(and is real since M is symmetric)

This is an important result, obtained without calculating λ.

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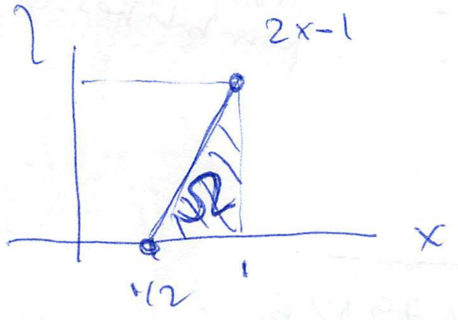
③



$$\int dx \int_{\Omega} dy \, (x^2+y^2) = 7/32$$ exact value.

$$= 0.21875$$

First we check the points given in the exercise that are in Ω. 'yes' means that we calculate x^2+y^2 for those points too.
If the points are not in Ω, do nothing (≡ or assigne a 0 to those points)

x	y	in Ω?	x^2+y^2	
0.835	0.516	yes	0.963481	$\rightarrow$ this is f_1 (if you want)
0.826	0.869	no	2nd 0	$\rightarrow f_2$
0.849	0.604	yes	1.085617	$\rightarrow f_3$
0.663	0.884	no	4th 0	⋮
0.784	0.723	no	5th 0	
0.628	0.844	no	6th 0	
0.993	0.066	yes	0.990405	— f_7
0.859	0.197	yes	0.776690	
0.977	0.434	yes	1.142885	
0.954	0.874	yes	1.673992	
0.746	0.401	yes	0.717317	
0.685	0.010	yes	0.469325	
0.758	0.789	no	13th 0	
0.538	0.151	no	14th 0	
0.660	0.268	yes	0.507424	
0.560	0.002	yes	0.313604	
0.651	0.280	yes	0.502201	
0.723	0.116	yes	0.536185	
0.932	0.879	no	19th 0	
0.558	0.719	no	20th 0	

12 points (x+y) out of 20 are in Ω.

Ω is a triangle (easy area to compute).

A_{box} = area of Ω = 1/4

↑

if you want. There are more possibilities...

$$\sum_1^{20} f_i = 9.679126$$

$$\sum_1^{20} f_i^2 = 9.929781$$

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Call I the integral to be computed, $I \equiv \int_{1/2}^{1} dx \int_{0}^{2x-1} dy\,(x^2+y^2)$

You know that $I_{MC} \sim A_{box} \langle f \rangle$

<u>one method</u>: Since Ω is a simple area (1/4), count only the points (x,y) inside Ω:

$$\underset{MC}{I} \sim \underset{\underset{0.25}{\parallel}}{A_{box}} \times \frac{f_1+f_3+f_7+\cdots+f_{18}}{12} = 0.201648$$

$$\sigma = A_{box} \times \sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}} = 0.026538$$

N is 12

$\langle f^2 \rangle = (f_1^2 + f_3^2 + \cdots + f_{18}^2)/12 = 0.785815$

$\langle f \rangle = (f_1 + f_3 + \cdots + f_{18})/12 = \frac{9.679126}{12}$

compute: $[I_{MC}-\sigma, I_{MC}+\sigma]$, $[I_{MC}-2\sigma, I_{MC}+2\sigma]$, and obtain: $[I_{MC}-3\sigma, I_{MC}+3\sigma]$:

$[0.175110, 0.228187]$: → ~aprox un 68% a tu favor.

$[0.148572, 0.254725]$:

$[0.122034, 0.281263]$: ↓ es "casi imposible" que el valor verdadero de I no esté en este intervalo... Y lo está!!! (97,... %) Felicidades

↙ "muy difícil" pero está aquí [lo está tb]

$I_{exact} = 0.21875$

Se admiten otros MC tb. Ex: ;

, $A_{box} = \frac{1}{2}$

↑ en el examen tb se admiten.

$N = 20$

$\langle f \rangle = \frac{f_1+f_2+\cdots+f_{20}}{20}$ → los mismos 12 de antes son los no 0's

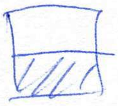
Sale otro I_{MC}, otro σ.

Solo los intervalos dicen si es mejor el método anterior o este. <u>Son los que mandan</u>

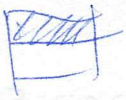
Para mí:

$\int_{1/2}^{1} dx \int_{0}^{2x-1} dy \, (x^2+y^2) = 7/32 = 0.21875$

$\int_{1/2}^{1} dx \int_{2x-1}^{1} dy \, (x^2+y^2) = \frac{23}{96} = 0.2395\overline{83}$



$\int_{1/2}^{1} dx \int_{0}^{1/2} dy \, (x^2+y^2) = \frac{1}{6} = 0.1\overline{6}$



$\int_{1/2}^{1} dx \int_{1/2}^{1} dy \, (x^2+y^2) = \frac{7}{24} = 0.291\overline{6}$

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