# **Exam on Mathematical tools**

### 3 hours

## Wednesday January 10th

You are allowed to use only your notes and documents distributed during the lectures. Do not mind about not doing everything, the exam is too long and the marking will take that into account.

## Yet another Fresnel integral

We consider the following function, defined for  $x \in \mathbb{R}$  as

$$F(x) = \int_0^{2\pi} \ln(x^2 - 2x\cos\theta + 1)d\theta ,$$
 (1)

but since it is even (just set  $\theta = \pi - \varphi$  in the integral), we will restrict the discussion to  $x \ge 0$  for simplicity.

- a) Show that F obeys to the following relation: F(x) = F(1/x) + 4π ln x for x > 0.
   b) What is F(0)? Show that F is continuous at x = 1 and x = 0.
- 2. a) Show the following relation for  $x \neq 0, 1$ :

$$f(x) = F'(x) = \frac{1}{ix} \oint_{|z|=1} \frac{z^2 - 2xz + 1}{z(z - 1/x)(z - x)} dz$$
(2)

- b) Deduce that  $f(x) = 4\pi/x$  for x > 1.
- c) What is f(x) for  $x \in [0, 1]$ ?
- d) Infer the function F(x) over  $]0, \infty[$ , in particular show that F(1) = 0.
- 3. Compute the following integral  $\int_0^{\pi} \ln(\sin \varphi) d\varphi$ .

### An academic example of the steepest descent method

We check the steepest descent method on an exactly computable integral. We consider

$$f(x) = \int_0^\infty \frac{t^x}{(1+t)^{\alpha x}} dt \quad \text{with} \quad \alpha > 1 .$$
(3)

We recall the definition of Euler's Beta function for  $p, q \in \mathbb{R}$ :

$$B(p,q) = \int_0^1 u^{p-1} (1-u)^{q-1} du = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}$$
(4)

where  $\Gamma(x+1) \sim \sqrt{2\pi} \exp\left(x \ln x - x + \frac{1}{2} \ln x\right)$  for  $x \to \infty$  (Stirling's formula).

- a) In the limit x → ∞, evaluate the asymptotic behavior of f(x) using the steepest descent method.
   b) Discuss the validity of the approximation.
- 2. a) Find an appropriate change of variables to express f(x) in terms of Euler's Beta function B.
  - b) Check that the previous result is recovered using the asymptotic behavior of  $\Gamma$ . Warning! this calculation is long and difficult, skip it if you don't feel like doing it.

## Convolution of Gaussians and Green's function of a random walk

We recall the definition of the convolution product \*: let f and g be two complex functions of the variable  $x \in \mathbb{R}$ , the convolution product f \* g is defined by the relation

$$(f * g)(x) = \int_{-\infty}^{+\infty} f(t) g(x - t) dt .$$
(5)

We use the following definitions for the Fourier transform F(k) of a function f(x):

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx \quad \rightleftharpoons \quad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dx \tag{6}$$

and we will use capital letters for Fourier transforms and small letters for functions. We assume that functions are such that integrals written in the following are always well-defined.

- 1. Show that f \* g = g \* f.
- 2. Let h = f \* g. Show that  $H(k) = \sqrt{2\pi}F(k)G(k)$ .
- 3. Let  $f_{a,\sigma}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-a)^2}{2\sigma^2}}$ . Show that  $F_{a,\sigma}(k) = \frac{e^{-ika}}{\sqrt{2\pi}} e^{-\sigma^2 k^2/2}$ . (7)
- 4. With the same notation for a gaussian as in the previous question, compute the convolution product  $h_{a,a',\sigma,\sigma'}$  of the two gaussians  $f_{a,\sigma}$  and  $f_{a',\sigma'}$ .

We now consider a random-walk in the continuum space: in one-dimension, the walker makes jumps of length y that are distributed according to a given distribution denoted by p(y). Let  $P_t(x)$  be the probability that the walker is at position x at time t. The time is discrete, with time steps of length  $\tau$ , and is put as an index for notation purpose.

5. Draw a sketch for moves between t and  $t + \tau$  and explain, using probability arguments, why one has

$$P_{t+\tau}(x) = \int_{-\infty}^{+\infty} P_t(x-y)p(y) \, dy \,.$$
(8)

6. Infer that for  $n \in \mathbb{N}$ :

$$P_{n\tau} = \underbrace{p \ast \cdots \ast p}_{n \text{ times}} \ast P_0 \tag{9}$$

#### 7. Green's function

- a) What would be the choice for the initial condition  $P_0$  to get the Green function  $G_t(x)$ ?
- b) Give the formal expression of  $G_{n\tau}(x)$  in terms of convolution products.
- c) Give the explicit form of  $G_{n\tau}(x)$  as a function of x and t when  $p(y) = f_{a,\sigma}(y)$  is a gaussian (with notations of question ??).

## Turn page.

### **Stochastic matrices**

We consider a **stochastic matrix A**, which is a  $N \times N$  square matrix with **real and non-negative** entries  $a_{ij} \geq 0$ . It typically appears in markov chains describing the evolution of a **probability** (or stochastic) column vector  $\vec{p}(t)$ . These entries  $a_{ij}$  correspond to the **probability** to have a transition from configuration (or state) j to configuration i, a move  $j \rightarrow i$  in short. The time t is discrete:  $t \in \mathbb{N}$  is an integer and the Markov evolution equation reads

$$\vec{p}(t+1) = \mathbf{A}\vec{p}(t) \ . \tag{10}$$

The entries  $p_i(t)$  of the probability vector  $\vec{p}(t)$  satisfy to the conditions (they are probabilities): for all time t

- (i)  $\forall i, \quad 0 \le p_i(t) \le 1,$ (ii)  $\sum_{i=1}^{N} p_i(t) = 1.$
- 1. Show the following property:

In each column of  $\mathbf{A}$ , the sum of entries is equal to one. (11)

*Hint: check that*  $\vec{p}(t+1)$  *is a stochastic vector and consider a specific*  $\vec{p}(t)$ . In general, the sum of entries in a row is not one.

### Spectral properties

In general, **A** is *not* symmetric. In such case, one usually defines left and right eigenvalues/eigenvectors in the following way ( $\vec{v}^{\dagger}$  is the row vector, hermitian transpose of the column vector  $\vec{v}$ , similarly **A**<sup>T</sup> will denote the transpose of **A**):

- (i) **right** eigenvectors  $\vec{u}_n$  associated to eigenvalues  $\lambda_n \in \mathbb{C}$ :  $\mathbf{A}\vec{u}_n = \lambda_n \vec{u}_n$ .
- (ii) left eigenvectors  $\vec{v}_n$  associated to eigenvalues  $\mu_n \in \mathbb{C}$ :  $\vec{v}_n^{\dagger} \mathbf{A} = \mu_n \vec{v}_n^{\dagger}$ .

We assume that these eigenvectors are all *normalized*. The eigenvalues are ordered in magnitude as  $|\lambda_1| \leq |\lambda_2| \leq \ldots \leq |\lambda_N|$ .

- 2. In terms of ensembles, show that the left and right spectra are the same  $\{\lambda_n\} = \{\mu_n\}$ .
- 3. a) By considering the largest component m of  $\vec{v}_n$ , i.e. such that  $|v_{m,n}| = \max |v_{i,n}|$  show that

$$\forall n, \quad |\lambda_n| \le 1 \ . \tag{12}$$

b) Gerschgorin circles. By considering the largest component m of  $\vec{u}_n$ , i.e. such that  $|u_{m,n}| = \max |u_{i,n}|$ , show also that

$$|\lambda_n - a_{mm}| \le 1 - a_{mm} \,. \tag{13}$$

This is a specific property that we are not going to reuse.

4. Let  $\vec{w}^{\dagger} = (1, ..., 1)/\sqrt{N}$ . Show that  $\vec{w}$  is a left eigenvector of **A** and find the corresponding eigenvalue. What is  $\lambda_N$ ?

### Stationary state

The stationary state  $\vec{p}^{\infty}$  (independent of time) exists provided

$$\lim_{t \to \infty} \vec{p}(t) = \vec{p}^{\infty} \ . \tag{14}$$

with  $\vec{p}^{\infty}$  unique and independent of  $\vec{p}(0)$ . It physically means that the system is ergodic and reaches an equilibrium state independent of the initial conditions.

- 5. After decomposing  $\vec{p}(0)$  in the right eigenvectors basis using some coefficients  $c_n$ , give the expression of  $\vec{p}(t)$  as a function of t, of the  $\lambda_n$  and  $\vec{u}_n$  and the  $c_n$ .
- 6. What can happen if there exist several eigenvalues such that  $|\lambda_n| = 1$ ? Take only  $\lambda_{N-1} = \pm 1$  for simplicity.
- 7. In the following, we consider that  $\lambda_N$  is non-degenerate and such that  $|\lambda_n| < 1$  for all n < N. The Perron-Fröbenius theorem gives the condition to have such a situation.
  - a) Find the relation between  $\vec{p}^{\infty}$  and  $\vec{u}_N$ .
  - b) Show that the leading term in the convergence towards the stationary state is exponential in time, i.e. proportional to  $e^{-t/\tau}$ , and relate the expression of  $\tau$  to the spectral features of **A**. For simplicity, assume that  $\lambda_{N-1}$  is non-degenerate (real).
  - c) Global balance: show that the stationary state necessarily satisfies to the following condition

$$\forall j, \quad \sum_{i} a_{ij} p_j^{\infty} = \sum_{i} a_{ji} p_i^{\infty} . \tag{15}$$

The **detailed balance** is a *sufficient* condition for the global balance to be satisfied. It involves only two states and reads

$$\forall i, j, \quad a_{ij} p_j^{\infty} = a_{ji} p_i^{\infty} \,. \tag{16}$$

#### Metropolis-Hasting rule to construct a stochastic matrix

Here, the goal is to construct a Markov chain, and so a stochastic matrix, which stationary state (as defined above) will be a given one  $\vec{p}^{\infty}$  (the input we give, for instance Boltzmann distribution). In such an algorithm, the transition probabilities are decomposed as

$$a_{ij} = P_{j \to i} A_{j \to i} \text{ for } i \neq j \tag{17}$$

where  $P_{j\to i}$  is the probability to **propose** the move  $j \to i$  and  $A_{j\to i}$  the probability to **accept** it. The Metropolis-Hastings rule is the following prescription for computing the acceptance probabilities of the moves:

$$A_{j \to i} = \min\left(1, \frac{p_i^{\infty} P_{i \to j}}{p_j^{\infty} P_{j \to i}}\right) \tag{18}$$

with some freedom to build the  $P_{j\to i}$  matrix provided it ensures ergodicity of the Markov chain.

- 8. Check that the Metropolis-Hastings rule satisfies to detailed balance. Then, provided that the matrix is such that the stationary state exists, this ensures the convergence of the so-called Monte-Carlo algorithm towards sampling the equilibrium distribution.
- 9. a) What condition can we use to fix the  $a_{ii}$ ?
  - b) Quite often, the  $P_{j\to i}$  matrix is taken symmetrical so that it goes out of the Metropolis rule. In this case, we may take  $P_{j\to i} = P$  uniform for *i* connected to *j*. Is there a constraint on the value of *P*?

## The end.