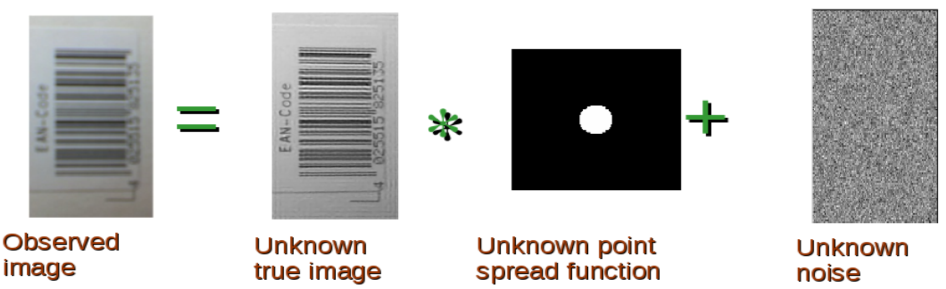
Initiation à la Recherche & à l'Innovation

École des Ponts ParisTech

Universitat de les Illes Balears

Introduction to research by innovation



u_{obs} u_{orig} k η

Goal: Given u_{obs}, recover both u_{orig} and k *up to a noise* η

Numerical Modeling, inverse problems

Steady progress but no real revolution !

Unapprochable inverse problems?

Robust solutions ?

Computer Science and Applied Mathematics Workshop

10 - 14 september 2018

Objectives of this workshop

Scientific Committee : Bartomeu Coll, Pascal Monasse, Gabriel Stoltz, Eric Duceau and Mohammed El Rhabi.
Teacher's Team : see page 6
Webpage : https://imi2018.enpc.fr/ (in progress)

I- Objectives :

This creative workshop will allow to initiate our students, second year (master's degree) from Computer Science and Applied Mathematics (IMI) of École des Ponts and students from last year of Bachelor's and master's degree in Advanced Physics and Applied Mathematics-University of the Balearic Islands, to "research for innovation". At the end of this week, students will acquire (or confirm) the necessary skills: there are a number of questions that must be addressed before tackling a project. Ideally, they will be able to propose the first step towards a solution.

"Real-life" problem are often ill-posed problems. A real challenge for the engineer is to reframe these difficult problems and turn them into a "more tractable one". However, applied mathematics engineers need to engage with all the actors (other engineers or sometimes customers). An opportunity to engage these dialogues: to be able to ensure a well-honed ability to explain complex concepts, to understand the problems of each contact and to suggest the tools that best meet their needs.

9 projects are proposed by researchers or industrials. The students should decide on a topic. Each project is handled by a group of 5-6 students. **Deadline: 11 June 2018**.

Another interesting viewpoint is the intercultural work. Spanish students (bachelor's and master's degree, UIB) will work with French students (master's, École des Ponts).

This workshop is valued at 1.5 **credits (ECTS)** for our students.

Last, this week may be the opportunity to give rise to vocations.

II-Workshop program:

Two morning sessions will be devoted to conferences or site visits.
The rest of the week takes place in a workshop by groups of students: case study in small groups (6) on a project of your choice.

III- Validation :

Full and active participation in the programme.
9 projects were proposed to students (max 6 students per project).

It is expected:

- For each project : A poster
- In the Posters each participant displays the different steps :

  - 1 page for the introduction.
  - 6 pages: describing the work of the group (analysis and main contributions according to the instructions of the supervisors).
  - 1 page « conclusion and future work ». Be sure, you don't forget the bibliography.
  - Tuesday 19/09, the supervisor gives instructions for the poster.
  - Students prepare their poster then send their first version to their supervisor before **1 October 2018**. Deadline: **5 October 2018**.

The week of October 15, 2018**:**

Posters sessions : at least one student of each group must present to lay out the work to others students and professors each day from **12h00 to 14h00**.

Posters session: **20 points**: This part will be evaluated by professors/teachers of the School (and / or) the directorate of studies (academic directors / managers). They will choose “their” projects:

- Quality of the presentation
- Scientific and technical content
- Approach

Practical issues : From 8 October until **12 October 2018**:

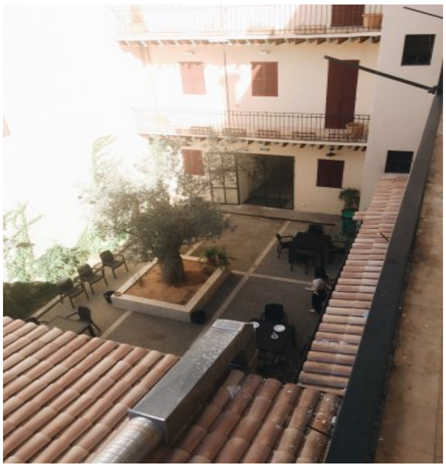
- B/W printing : Prony wing, 4th floor (computer room).
- Color printing ; Vicat wing, V216, V217 and V219.
- If you need any further information, please contact Ms Mortier (V216).

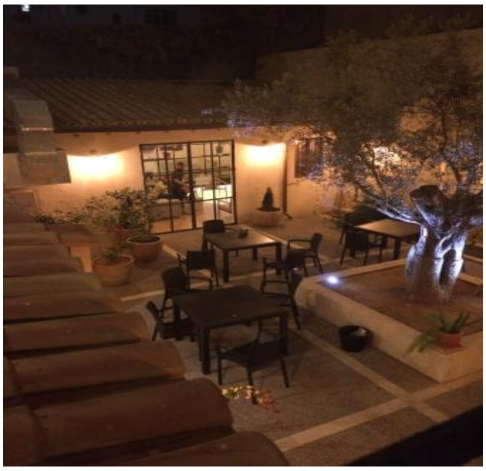
Schedule

Dates Horaires	**Monday 10/09/18**	**Tuesday 11/09/18**	**Wednesday 12/09/18**	**Thursday 13/09/18**	**Friday 14/09/18**
9H00 9h15	Workshop presentation		Visit of **a research center**	Work in groups (without supervisor)	**Departure for the airport**
9h15 9h45	**C1** Research @UIB	Work in groups (with supervisor)			
9H45 10h15	**C2** Research for innovation? **Eric Duceau**				
10h15 12h00	Project presentation, Work in groups (with supervisor)				
12h00 13h30	lunch	lunch	lunch	lunch	
13h45 18h30	Work in groups (with supervisor)	Work in groups (with supervisor)	Work in groups (without supervisor)	Work in groups (without supervisor)	

Residence : Hostel Fleming

https://www.booking.com/hotel/es/hostel-fleming.fr.htm





The Team

Conferences

	Title	Speaker
C1	Research @ UIB	Prof @ UIB
C2	Research for innovation ?	Eric Duceau

Projects

	Title	Supervisors
P1	Numerical Resolution of Martingale Optimal Transport Problems	William Margheriti (Cermics[1])
P2	Simulation of rare events with the Adaptive Multilevel Splitting method	Laura Lopes (Cermics)
P3	Simulating Metastable Dynamics	Mouad Ramil (Cermics)
P4	Optimal Transportation: Numerical Methods and Applications to Finance and Quantum Chemistry	Rafaël Coyaud (Cermics)
P5	Topological phases of matter	Sami Siraj-Dine (Cermics)
P6	Blur reduction in a photograph of a document	Pascal Monasse (Imagine[2]) and Mohammed El Rhabi(IMI[3])
P7	Blind source separation and applications	Mohammed El Rhabi and Pascal Monasse
P8	The color constancy problem and some solutions	Jose-Luis Lisani (TAMI[4])
P9	Aircraft noise by Simulation: does the additional knowledge worth the investment?	Eric Duceau (Airbus, IMI)

1 Cermics: Applied Mathematics Lab. - Ecole des Ponts ParisTech
2 Imagine: Gaspard-Monge Computer Science Laboratory, Ecole des Ponts Team
3 IMI : Applied Mathematics and Computer Science department, Ecole des Ponts
4 TAMI: Mathematical Processing and Analysis of Images, Universitat de les Illes Balears

P1: Numerical Resolution of Martingale Optimal Transport Problems

Supervisor: William Margheriti
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Description

The optimal transport (OT) problem was initially formulated by Monge at the end of the 18th century and then developed by Kantorovich in the middle of the 20th century. It has applications in semigeostrophic equations, meteorology, isoperimetric problems, granular materials, statistical physics, Sobolev inequalities and many other fields. Basically, it consists in minimising or maximising the expected value $E[c(X,Y)]$ among all random variables X, Y such that X follows μ and Y follows ν, where μ and ν are two given probability measures and $c:\mathbb{R}\times\mathbb{R}\to\mathbb{R}_+$ is a cost function.

However, despite all these connections between numerous field, practitioners in financial mathematics had the need to modify the initial formulation of the OT problem as follows. In the minimisation (or maximisation) of $E[c(X,Y)]$, the couple (X, Y) must be a martingale, which means (among other things) that X and Y have same expected values. This additional constraint is the exact mathematical transcription of the no-arbritrage framework, which is the name of the reasonable assumption according to which there cannot be any risk-free making money opportunity.

The OT problem added with the martingale constraint is called the martingale optimal transport (MOT) problem, and its resolution is a major issue in the financial sphere. Since it is an infinite dimensional problem, the first step is to consider a discretization of the MOT problem so that this problem becomes a basic linear programming problem for which we have powerful solvers such that GLPK. But this approximation will lead to various theoretical issues which will be explained during the project.

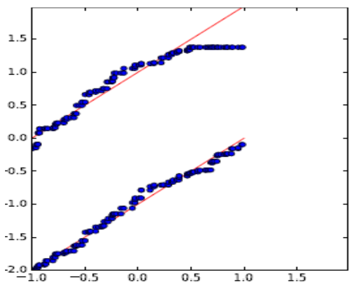

Figure 1: Comparison between the approximation (blue points) and the explicit solution (red line) of a particular soluble case

Project Goal

The goal of this project is to implement a numerical method to solve the MOT problem, with the following subtasks:
Present a simplified MOT problem with a one-time step martingale;
Discretisation of the MOT problem:
)1 Experience the failure of a naïve method with empirical measures;
)2 Test a dedicated method;
)3Validate the method on an analytically soluble case. **Students will need a computer with a programming language of their choice, typically C++, R or Python.** If time permits, various extensions will be investigated.

Bibliography

- [A. Alfonsi, J. Corbetta, and B. Jourdain. *Sampling of probability measures in the convex order and approximation of Martingale Optimal Transport problems*. ArXiv e-prints:1709.05287, Sept. 2017.
- V. Strassen. *The existence of probability measures with given marginal*. Ann. Math. Statist., 36:423-439, 1965.
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P2: Simulation of rare events with the Adaptive Multilevel Splitting method

Supervisor: Laura Lopes

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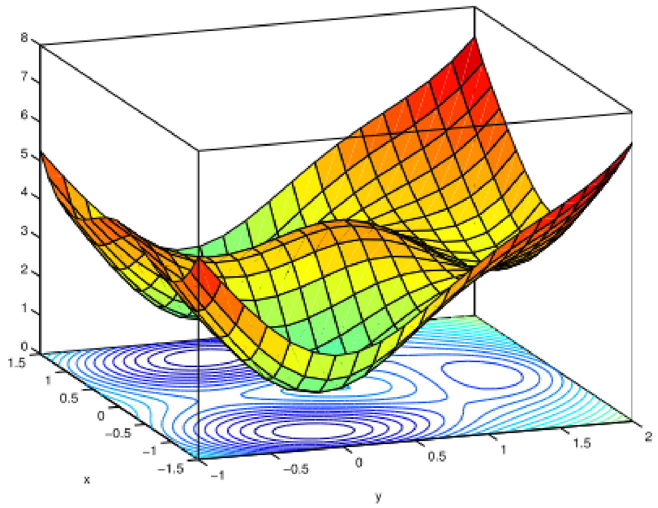
Description

The simulation of rare events has been an important field of research for the past decades. Rare events often play an important role in a wide range of natural phenomen, and are are present in different fields of research, from earthquakes to condensation of matter [1]. Because of their low probability of occurrence they are difficult to simulate and the use of a simple Monte Carlo method is not possible. One of the appropriate simulation methods is the Adaptive Multilevel Splitting (AMS) [2], which is a multilevel splitting method, where the event of interest is split into successive more likely, and thus easier to simulate, events. This is done using surfaces, defined such that the probability of transition between them is constant. The optimality of this approach can be proved in a certain sense. The Adaptive Multilevel Splitting is a powerful rare event method that is currently used in different fields of research, like chemistry [3], for example.

Project Goal

The goal of this project is to implement and test the performance of the AMS method on a simple two dimensional example (see figure below) [4], for a stochastic differential equation.



For this we will use the overdamped Langevin dynamics (equation below).

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t, X_t \in \mathbb{R}^n$$

We will see how to numerically solve this equation. The only requirements for this project is to have some familiarity with ordinary differential equations and their discretization.

Bibliography

- [1] F. A. Escobedo, E. E. Borrero, and J. C. Araque. Transition path sampling and forward flux sampling. applications to biological systems. J. Phys: Condensed Matter, 21, 2009.
- [2] F. Cérou and A. Guyader. Adaptive multilevel splitting for rare event analysis. Stoch. Anal. Appl., 25(2):417–443, 2007.
- [3] Ivan Teo, Christopher G. Mayne, Klaus Schulten, and Tony Lelièvre. Adaptive multilevel splitting method for molecular dynamics calculation of benzamidine-trypsin dissociation time. J. Chem. Theory Comput., 12(6):2983– 2989, 2016.
- [4] Charles-Edouard Bréhier, Maxime Gazeau, Ludovic Goudenège, Tony Lelièvre, and Mathias Rousset. Unbiasedness of some generalized adaptive multilevel splitting algorithms. Ann. Appl. Probab., 26(6):3559–3601, 12 2016.

P3: Simulating Metastable Dynamics

Supervisor: Mouad Ramil

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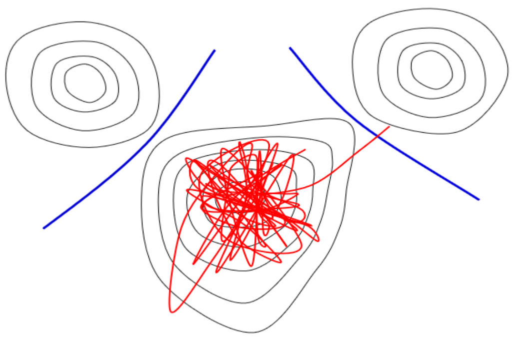
Description

Atomistic simulations provide a convenient tool to predict properties of materials. Average behaviors are obtained by simulating ordinary differential equations perturbed by a random process like a Brownian motion, as is the case for the **Overdamped Langevin** (OL) dynamics given below which simulates the position of a particle under under a potential V:

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}\,dW_t$$

Simulating this process numerically is often done using known numerical schemes such as the classic **Euler Scheme**, also used for deterministic behaviors. The OL dynamics also correspond to what we call **Metastable dynamics:** systems that get trapped in some regions of the phase space for very long times. As a result, simulating naively these dynamics with our numerical schemes is no longer relevant, as most of the computation will lead to vibrations in wells of the potential V.



However, the jumps from one metastable state to the other provide the most interesting information on the system as they characterize profund changes in the physical system. One way to simulate such transition happen is to resort to Accelerated Method Dynamics like **Parallel Replica** (ParRep), developed at Los Alamos National Laboratory, which aim at simulating the long time-scale behaviour of a process for **state-to-state dynamics**, using some stochastic properties of metastable dynamics.

Project Goal

As a first step here, we are going to introduce metastable dynamics and their properties. Secondly we will simulate a simple 1-dimension metastable diffusion using a Euler scheme. We will next implement the ParRep algorithm for this example. Finally we will extend this study to more complex 1-D diffusions using a Generalized ParRep algorithm which resorts to the so-called Fleming-Viot process.

Bibliography

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- Binder, A; Lelievre, T.; Simpson, G. A Generalized Parallel Replica Dynamics. *Journal of Computational Physics* 284 – March 2014

P4: Optimal Transportation: Numerical Methods and Applications to Finance and Quantum Chemistry

Supervisor: Rafaël Coyaud
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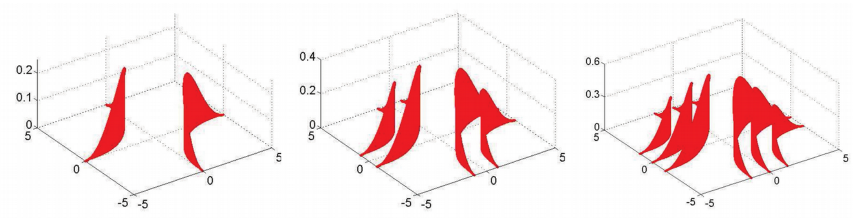
Description

The aim of this project is to study and implement numerical methods using optimal transportation in two contexts: the computation of option bounds in finance and the computation of the electronic density in a molecule with radial symmetry in quantum chemistry.
Optimal transportation problems have received great attention in several applied mathematics domains, and have numerous applications in physics, imaging, economy or finance. Most of the time an optimal transportation problem has no analytical solution. That is why numerical methods must be implemented to use it.
In finance, the price of an asset at time t is only known probabilistically. The evolution of this price with time can be modelled in different ways. An option on this asset at time t_1 and price K_1 is the possibility to buy or sell this asset at time t_1 and at price K_1, whatever the real price of the asset when time t_1 comes. The price of a financial product built on several options on one asset at different times depends on the chosen model for the asset. Martingale optimal transport allows to compute bounds on that price, independent from the modeling, which allow to evaluate the model quality.
In quantum chemistry, the computation of the shape of a molecule requires solving several minimization sub-problems in order to find the nucleus configuration and the electronic density associated with the lowest energy; the computation of the energy associated to the electronic density is one of them. In this sub-problem, the computation of the interaction energy between electrons is only doable with some approximations. One of them consists in considering that electrons positions are perfectly correlated, and can be formulated as an optimal transportation problem with a Coulombian cost.



Pair densities with 2, 3 and 4 electrons.

Project Goal

After an introduction to optimal transportation, students will implement its resolution on a grid, using a linear programming solver for the problem with two marginal laws. Then, two half-groups will work on the two applications:
After an introduction to the Cox-Ross-Rubinstein model (discrete approximation of the Black-Scholes model), students will implement the computation of the martingale optimal transport and will compute price bounds.
After an introduction to the DFT (Density Functional Theory), and its optimal transport formulation, students will implement the computation of a multimarginal optimal transport and will represent pair densities with 3 and 4 electrons.

Bibliography

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- Chen, H., & Friesecke, G. (2015). Pair densities in density functional theory. *Multiscale Modeling & Simulation*, *13*(4), 1259-1289.

P5: Topological phases of matter

Supervisor: Sami Siraj-Dine
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Description:

Solid-state physics is the branch of Quantum Mechanics that studies the behavior of electrons in crystals. In the standard approach, one considers that the electrons are independent, so that each one follows the Schrödinger equation, which is a time-dependent PDE. Here, we will further simplify by considering that electrons stay in their state of lowest energy, which are given by the eigenspaces of the Schrödinger operator.
The discovery of the Quantum Hall effect by Klaus von Klitzing [1], in which the conductivity of a 2D electron gas (free electrons) is quantized (i.e. an integer to an accuracy of a billionth), challenged the previously widely held idea in solid-state physics that electronic properties had a regular dependence on parameters. Rather, it showed that they can undergo sharp phase transitions. It was in fact the first identified topological quantum effect and was later observed in room temperature graphene [2]. Topological quantum computers would possibly rely on similar effects.

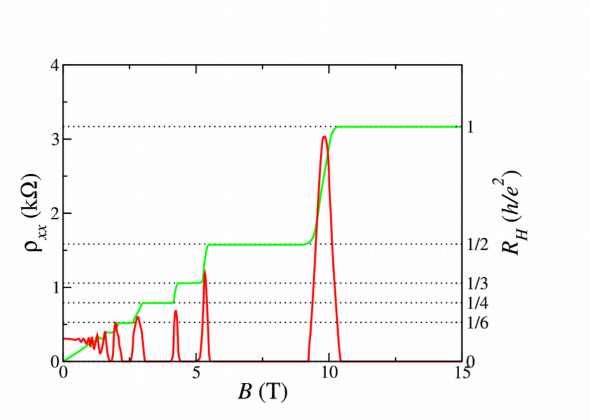

Figure 2: Quantized transverse resistance (in green) against magnetic field
(Picture: courtesy of Niels Walet, http://oer.physics.manchester.ac.uk/AQM2/)

The theoretical explanation of this phenomenon was provided by Thouless et al [3], making the link between the conductivity and a topological invariant, called the Chern number, of the eigenspaces of the Schrödinger operator.

Although these experiments rely on the application of a strong magnetic field, a class of new materials, called topological insulators, display these properties without any external magnetic field.

Project goal:

First, the students will get an introduction to the relevant quantum mechanics, (Schrödinger equation and eigenspaces of the Schrödinger operator), and to the topological concepts. Then, they will proceed to compute numerically the Chern number of Haldane's model of topological insulator [4], in which the Schrödinger operator reduces to an explicit matrix-valued function, and draw the topological phase diagram. Integrating the semi-classical laws of motion (a simple system of ODEs), they will verify that the conductivity converges to the Chern number. (Language: Julia/Python).

Bibliography

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- [2] K. S. Novoselov et al., "Room-Temperature Quantum Hall Effect in Graphene," *Science* 315, no. 5817 (March 9, 2007): 1379–1379.
- [3] D. J. Thouless et al., "Quantized Hall Conductance in a Two-Dimensional Periodic Potential," *Physical Review Letters* 49, no. 6 (August 9, 1982): 405-8.
- [4] F. D. M. Haldane, "Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the 'Parity Anomaly,'" *Physical Review Letters* 61, no. 18 (October 31, 1988): 2015–18.

P6: Blur reduction in a photograph of a document

Supervisors: Pascal Monasse and Mohammed El Rhabi
monasse@imagine.enpc .fr and mohammed.el-rhabi@enpc.fr

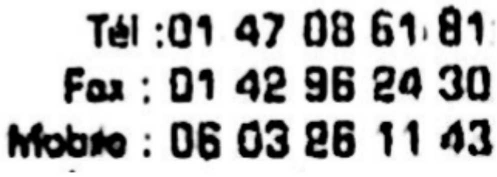
Description

The goal of this study is to help in the interpretation of information in an image captured by a smartphone or hand-held camera. The process is technically challenging. The main difficulty is in the quality of the optical pipeline. It translates into an image that is sub-resolved and possibly blurry. In our study, we will assume the blur is due to the camera itself (focal plane aberration). For example in barcodes, the unidimensional bars merge. Another problem, due to the imaging conditions, is the noise level, depending on hardware, luminosity, etc. It is also unknown.

The biggest challenge of such an inverse problem resides in the estimation of the blur level and of an approximation of the noise-free image.

The blur level estimation is necessary for the interpretation of the data in the image. It has numerous applications, which are obvious in the case of text or barcode documents. In a first stage, students will deal with a simplified model when the blur is known, before attacking the general problem, that is, with unknown blur level.

From the mathematical standpoint, the model is written $u_0 = k*u+n$, where u_0 is the observed image, k is the noise kernel, supposed defined by a single parameter r, the radius of the uniform kernel. The star represents a convolution and n is the noise, supposed to be independent from the data. Recovering the ideal image u from such an equation is called an inverse problem, such problems are usually ill-posed by themselves, because there is no unique solution. Therefore, a regularization term is introduced in an energy optimization problem, encoding the desired regularity properties of the solution.



Original Image: captured with a smartphone without autofocus (Nokia N70).

Deblurred Image

Goal of the project

After a short theoretical exploration of the problem, the goal of the project will be to propose a numerical algorithm to determine a solution to the blur removal problem for a document image (containing only text or bar codes).

Bibliography

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P7: Blind Source Separation and applications

Supervisors : Mohammed El Rhabi and Pascal Monasse
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Description:

In this project, the problem of blind source separation separation (BSS) is considered. The BSS problem has several applications in different areas including feature extraction, brain imaging, telecommunications, vibratory analysis, industrial reliability … etc.
The problem consists in retrieving unobserved signals (called sources) from unknown mixtures of them (called observations). When the components of the source signals are independent, a solution to this problem exists up to a permutation and scale indeterminacies, and many algorithms have been proposed to obtain the solution with applications in many area

BSS problem can be modeled as follows. Denoting **A[.]** the (unknown) mixing operator, the relationship between the observed and source signals can be written as

$$\mathbf{x(t) := A[s(t)] + n(t)}$$

where **s(t)** is the unknown vector of source signals to be estimated, and **x(t)** represents the observed signal vector at time **t**. The goal of BSS, is therefore to estimate the unknown sources **s(t)** from the observed mixtures **x(t).** The presence of additive noise **n(t)** with in the mixing model complicates significantly the BSS problem. It is reduced by applying some form of preprocessing such as denoising the observed signals through regularization approach.

The estimation is performed with no prior information about either the sources or the mixing operator **A[**.]. Specific restrictions are made on both the mixing model and the source signals. We will restrict our self to the case where the number of source components and the number of observed mixture ones are equal, and we assume, in the present paper, that the mixtures are linear and instantaneous, so that the mixing operator A can be considered as a matrix of order p. In this case, supposing in addition that **A** is invertible, the candidate estimates of the sources will be obviously of the form

$$\mathbf{y(t) := Bx(t)}$$

where **B** represents an appropriate demixing matrix. In other words, the problem is to obtain an estimate, denote it **B'**, \closing" as much as possible to the ideal solution $\mathbf{B = A^{-1}}$, by the use of only the observed vector signal **x(t),** leading to accurate estimate **s'(t)** of the source vector signal **s(t),**

$$\mathbf{s'(t) := B'\,x(t)}$$

Project Goal

After a brief theoretical overview of the method, our objective is to propose a numerical one to resolve the problem of blind source separation in the case where the mixture is supposed to be instantaneous and the noise negligible. We will then, apply it to a BSS application of your choice.

Bibliography

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P8: The color constancy problem and some solutions

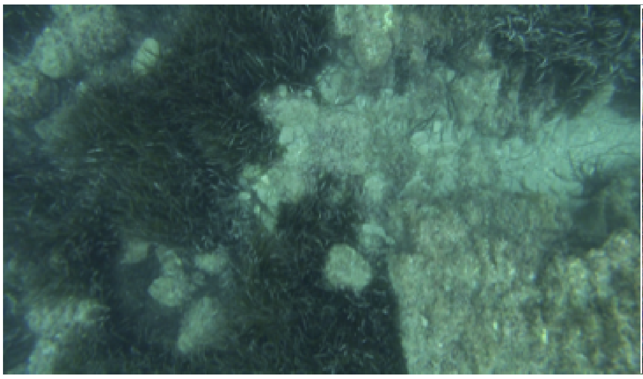
Supervisor : Jose-Luis Lisani

Descriptif

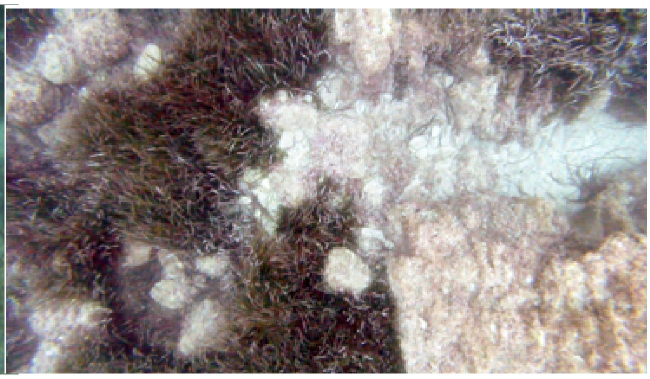
From [1]:
"*Color can be an important cue for computer vision or image processing related topics, like human–computer interaction, color feature extraction, and color appearance models. The colors that are present in images are determined by the intrinsic properties of objects and surfaces as well as the color of the light source. For a robust color-based system, these effects of the light source should be filtered out. This ability to account for the color of the light source is called color constancy*."

Project Goal

In this project we are going to discuss different solutions to the color constancy problem [1, 3], ranging from the basic white balance method to more sophisticated techniques involving transformations of the 3D color space. In particular, we will apply the methods to correct the colors of underwater images, as in [2].



Original Image



Color correction result

Bibliography

- *[1] A. Gijsenij, T. Gevers, J. van de Weijer, "Computational Color Constancy: Survey and Experiments", IEEE Transactions on Image Processing archive, Volume 20 Issue 9, September 2011, Page 2475-2489*.
- *[2] T. Baba, K. Nakamura, S. Kyochi and M. Okuda, "Image enhancement method for underwater images based on discrete cosine eigenbasis transformation", IEEE International Conference on Image Processing (ICIP), Beijing, 2017, pp. 4272-4276.*
- *[3] J.L. Lisani, A.B. Petro, E. Provenzi, C, Sbert, "A generalized white-patch model for fast color cast detection in natural images", IS&T International Symposium on Electronic Imaging, 2016.*

P9: Aircraft noise by Simulation: does the additional knowledge worth the investment?

Supervisor : Eric Duceau
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Description:

The problem is to support a decision making process in a design loop. The use case deals with aircraft noise on the one hand and the available simulation capability to predict either the noise or the potential of a device or a design to lower the level of noise on the other hand. The project team will have to mirror the preliminary phase in R&T leading to a decision to use (or develop) a simulation test bench or not. To make it short: “*the scientific bricks to be used are known –more or less- but the industrial potential that the simulation can provide has to be challenged*”. The deliverable of the project shall be “*yes or no*” with a methodology to explain the recommendation.

Actually, the team will be split in (at least) 3 groups: the first one will be in charge of “analyzing” the aerodynamic models and understand the choices behind, including numerical analysis and performance; a second one will have to look at the same problem from the acoustic point of view; the last (and not least!) subgroup will have to deal with industrial constrains such as uncertainties, quantities of interest etc. The supervisor will introduce the industrial problem and a brainstorming session will be organized to shape the problem to tackle. Then, the group will address a couple of scientific questions in parallel and loop together; then a session will be dedicated to a “negotiation” to find out the strengths and weaknesses of the simulation approaches we will be investigating.

Project Goal

decompose a very complex industrial system (multiphysics, multi actors, multi constrains) - =the aircraft noise production- and provide an Analyse to recommend or not the development of a simulation tool (and which one).

NB: from a pedagogical point of view, this “exercise” aims at highlighting the various criteria showing up in a decision making phase during systems engineering analysis… and not only the pure scientific one.
It’s also a very representative configuration for “young engineers” facing very complicated situation with a huge legacy (eg aeronautic) and so, some skills and knowledge may be missing. How comfortable are you in such a situation?

References

In French : SFA_Bruit_Avions.pdf http://www.google.fr/url?sa=t&rct=j&q=&esrc=s&source=web&cd=1&cad=rja&uact=8&ved=0ahUKEwjjq-2Gg-naAhVByKQKHa--AA8QFggnMAA&url=http%3A%2F%2Fwww.iroqua.fr%2Firoqua%2Fsites%2Fsites.onera.fr.iroqua%2Ffiles%2Firoquoa%2FZone%2520Publique%2520Externe%2FSFA_Bruit_Avions.pdf&usg=AOvVaw0eEk_j-nWUhXEG7amUAZGf

and have a look to Wikipedia articles:
Computational aeroacoustics; Navier stokes & Euler Equations; wave equation & integral equation

Other stuff will be given “on the fly” in Palma

« Oser ; le progrès est à ce prix.
Toutes les conquêtes sublimes sont plus ou moins des prix de hardiesse.»
Victor Hugo, *Les Contemplations*, 1856