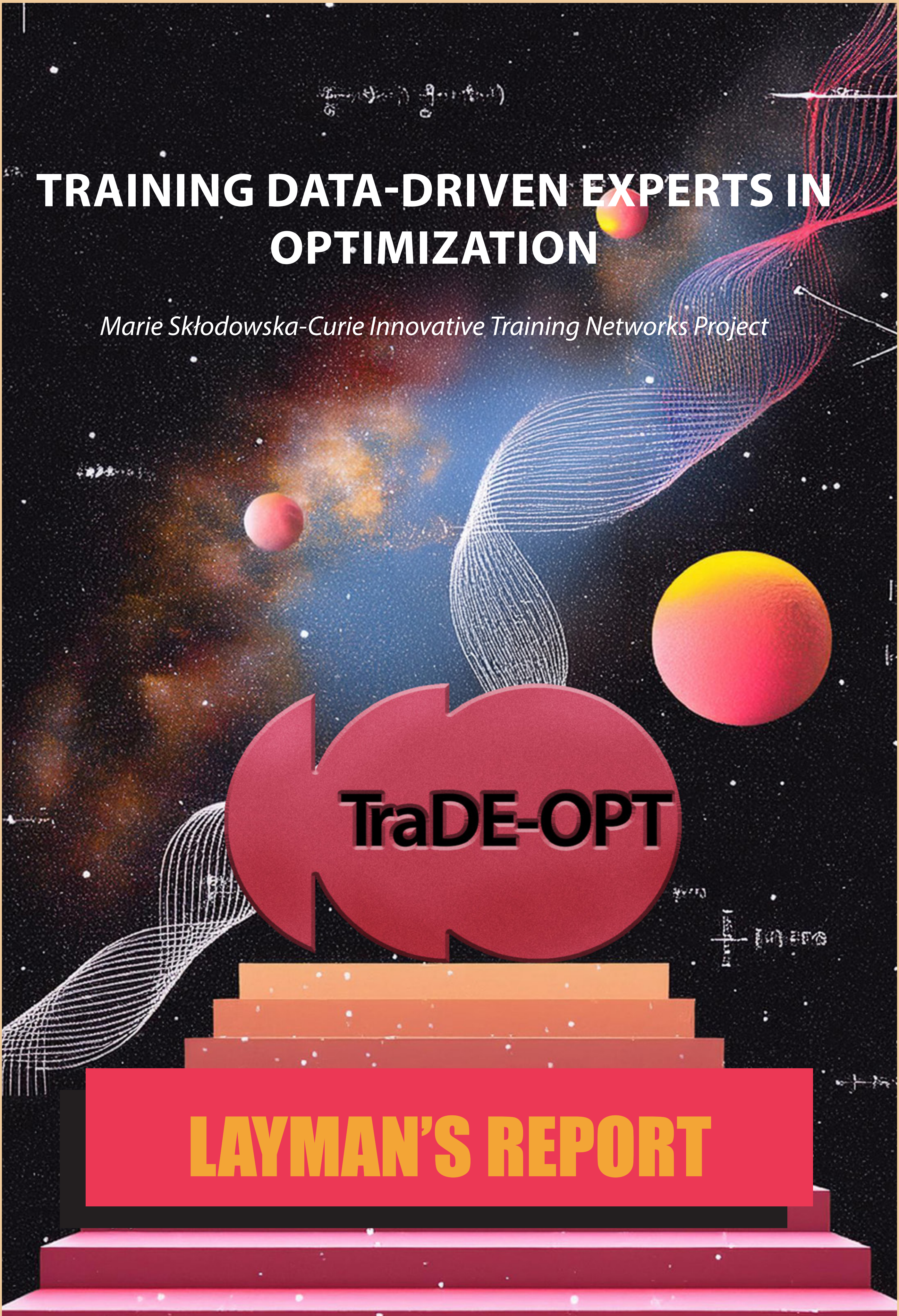
TRAINING DATA-DRIVEN EXPERTS IN OPTIMIZATION

Marie Skłodowska-Curie Innovative Training Networks Project



LAYMAN'S REPORT

Funded by
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TraDE-OPT AT A GLANCE

PROJECT TITLE: Training Data-driven Experts in OPTimization

DURATION: 1 June 2020-31 November2024

EU FINANCIAL CONTRIBUTION: € 3 774 874,32

FUNDED UNDER: MSCA-ITN-2019 - Innovative Training Networks

PROJECT COORDINATOR: professor Silvia Villa, Università degli Studi di Genova, Italy

PROJECT NUMBER: 861137

Members of the consortium:

Università degli Studi di Genova, Italy

CentraleSupélec, France

Universität Graz, Austria

Technische Universität Braunschweig Germany

Universitatea Politehnica Din Bucuresti, Romania

Systems Research Institute, Polish Academy of Sciences, Poland

Université catholique de Louvain, Belgium

Camelot Biomedical Systems, Italy

Why Optimization in data analysis matters

The **TraDe-Opt** project has been designed from the observation that data-driven systems have become more complex than the numerical tools available for managing them. The main scientific objective of the TraDE-Opt research program is to develop a theoretical — optimization based — framework to derive and analyze new efficient optimization algorithms for solving data-driven problems, i.e. for the extraction of high-level information and the subsequent identification of optimal decisions.

Currently, optimization, and especially convex optimization, is at the core of many theoretical and algorithmic methods underpinning solver technology for a myriad of data-driven problems. Furthermore, convex optimization has been intimately tied to the development of image processing, computer vision, and machine learning algorithms.

Despite many remarkable achievements, the fast technical progress continuously poses new challenges due to: 1) constant development of new sensors and measurement devices, 2) need of automatic data processing in new fields (smart mobility sector, smart industries, new scanner devices) 3) heavily constrained computational environments, which can be found on CPUs embedded in sensors devices 4) privacy, security, and ethics issues arising for user-generated data.

The construction of mathematically-sound models featuring one or several of these aspects will allow the extraction of rich information and underlying knowledge, with the help of dedicated machine learning techniques. Optimization will play a central role in every stage of this project, as the main computational technique.

To achieve this goal the validation and testing of the devised algorithms on real data is a key part of the **TraDE-Opt** endeavor. The applications has a multidisciplinary flavor, addressing urgent problems in three key areas: smart mobility sector (vehicle track interactions for railway systems and smart highways), imaging devices (4D flow velocity encoding in MRI, high precision optical measurement techniques in an industrial environment, related also to smart industries), smart industries.

A LAYMAN HITCHHIKER'S GUIDE TO THE OPTIMIZATION GALAXY

Inverse Problem - a mathematical problem where you try to determine the underlying causes or parameters of a system based on the observed effects or results. We can abstractly formulate inverse problems as finding the solution $u \in U$ to the operator equation

$$K(u)=f$$

$K:U \to F$ is called the forward operator, which models the underlying physical process and simulates the measurements for a given u. u is the original signal (image, cause), and $f \in F$ are the measurements (mathematical representation of the measured data).

Regularization - inverse problems are usually solved as the optimization problem:

$$\text{minimize}_u \ \tfrac{1}{2}\|K(u)-f\|^2$$

often noisy, incomplete or ill-posed, making it difficult to directly reconstruct the original signal. A technique used to address these issues is regularization, which relies on introducing additional constraints or assumptions about the original signal. These constraints help to stabilize the reconstruction process and prevent the model from overfitting to the noisy data. Regularization involves adding a penalty term to the objective function that is used to optimize the reconstruction. This penalty term encourages the solution to have certain properties, such as smoothness, sparsity, or low-rankness. By incorporating these prior assumptions, the regularization can help to improve the quality and reliability of the reconstructed signal. In the case of image reconstruction, regularization might involve assuming that the original image is smooth or has a sparse representation in a certain basis. This helps to prevent the reconstruction from being overly sensitive to the noise in the data and can lead to a more accurate and visually appealing result.

In essence, regularization of inverse problem is a powerful tool that can be used to improve the quality and reliability of reconstructions from noisy or incomplete data. By incorporating prior knowledge or assumptions about the original signal, regularization can help to mitigate the effects of noise and artifacts, leading to more accurate and meaningful results.

Total Variation Regularization - Total variation regularization is a mathematical regularization technique used to constrain solutions in optimization problems. It is particularly effective in applications where the desired solution exhibits sharp discontinuities or edges, such as image processing, signal processing, and machine learning. The core idea behind total variation regularization is to minimize a functional $T(u)$ that consists of two terms: general data fidelity term (how well the solution fits the given data or observations), and regularization term (penalizes solutions with large variations or discontinuities). Formaly the total variaton regularization can be expressed as

$$T(u)=\underbrace{F(f/K(u))}_{\text{general data fidelity term}}+\underbrace{\lambda}_{\text{regularization parameter}}\underbrace{\|\nabla u\|_1}_{\text{total variation regularization term}}$$

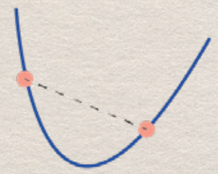
Imaging Problems - a general term for all issues related to the generation of images in different fields, these might include noise, blur, incomplete data.

Splitting Methods - a class of algorithms applied to optimization problems in which the original minimized function can be represented as the sum of two (or more) simple functions as in

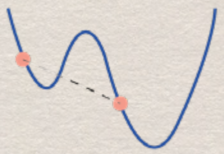
$$\text{minimize}_u \ F(u)+G(u)$$

then the splitting algoritms are defined via an iterative update that deals with the two functions $F(u)$ and $G(u)$ separately. Common splitting methods include: Alternating direction method of multipliers (ADMM), Proximal gradient methods, and Augmented Lagrangian methods.

Convex Optimization - a field of mathematics that deals with finding the minimum value of a convex function subject to convex constraints. A convex function is one that curves upward like a bowl, and a convex constraint is one that defines a convex region. The most useful property of convex optimization is global optimality, meaning that each local minimum is a global one. Convex optimization can be applied to a wide range of problems, including machine learning, signal processing, and control theory.

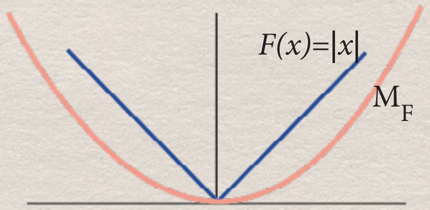


Non Convex Optimization - deals with finding the minimum or maximum value of a non-convex function subject to constraints. A non-convex function is one that can have multiple local minima or maxima that are not global. Non-convex optimization is a challenging problem because of multiple local optima (there might be many local minima or maxima, making it difficult to find the global optimum), and non-convex optimization problems can be computationally expensive to solve.



Proximal Operator - is an operator $prox_F(v)$, that helps solve optimization problems. It's particularly useful when the optimized convex function F is non-diferentiable. Fixed points of the proximal operator are minimizers of F. It is used in definition of proximal type algorithms.

Moreau envelope - denoted as M_F is a smoothed and regularized form of F. Its domain is the whole space and it is continusly differentiable even if F is not. The set of minimizers of F and M_F are the same. The problem of minimizing F and M_F are equivalent and the latter is always an optimization problem with differentiable functions.



TRADE-OPT: OPTIMIZATION IN ACTION

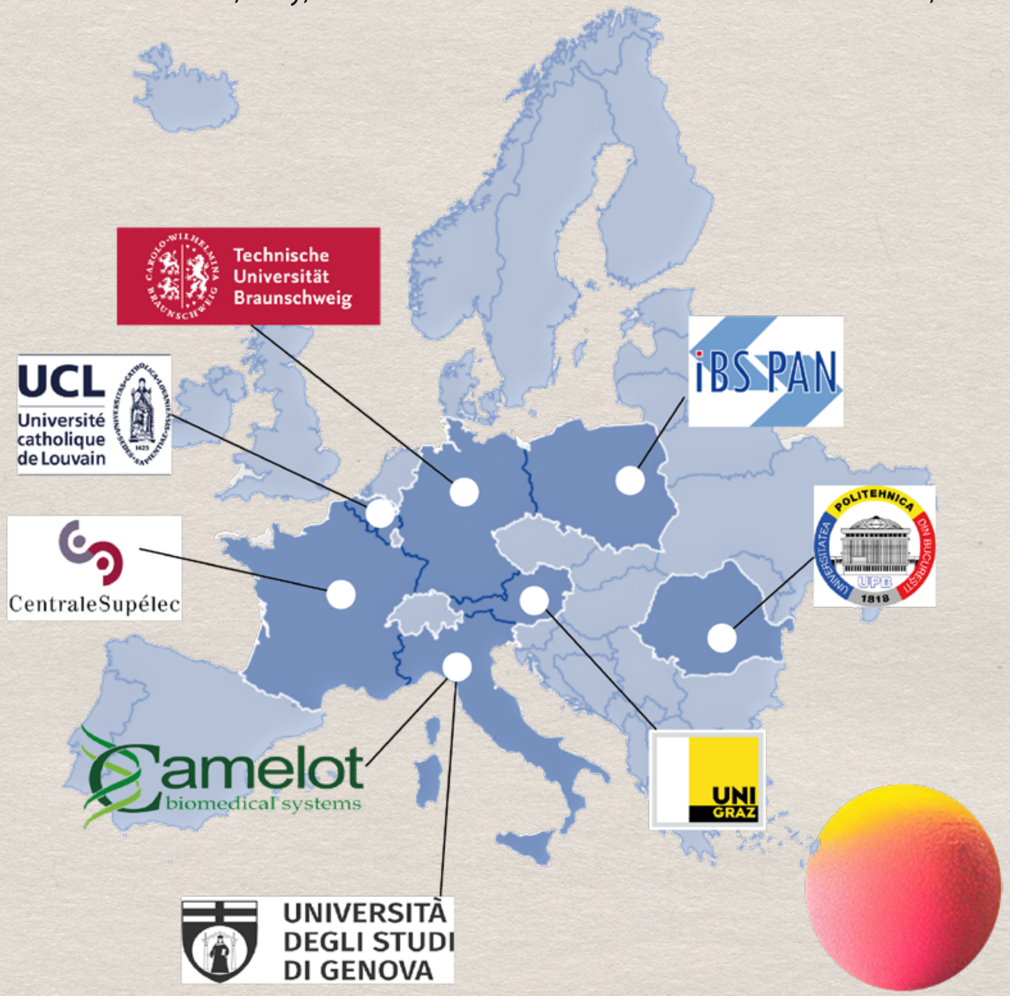
The main goal of **TraDE-Opt** is the education of 15 experts (Early Stage Researchers) in optimization for data science, with a solid multidisciplinary background, able to advance the state-of-the-art. This field is fast-developing and its reach on our life is growing both in pervasiveness and impact.

To achieve this goal, we have offered an innovative training program, giving a solid technical background combined with employability skills: management, fund raising, communication, and career planning skills. Integrated training of the ESR's took place at the host institute and by secondments, workshops, and schools. As a result, **TraDE-Opt** alumni will be prepared for outstanding careers in academia or industry.

To pursue our objectives, we rely on the strong expertise of the members of the consortium, which gather many of the most prominent researchers working in data-driven convex optimization in Europe and on the expertise on specific appilication domains of the industrial partners. The academic institutions of the consortium served as hosts to the ESR's. These institutions provided supervision and local PhD courses to the ESR's.

Three schools and two workshops have been organized. School #1 served as a kick-off for the ESR's, being the first oportunity to get to know each other. It offred a compact convex optimization course, and presentation of industrial partner problems. School #2 offered training in form of a course in machine learning and inverse problems. It focused especially on methods for huge problems. School #3 was devoted to a course on quality management and structured problem solving.

During Workshop#1 ESR's presented their ongoing research and lines of progress. Workshop #2 took place in Sestri Levante, Italy, was in the form of an international conference, closing the project.



PROJECT OBJECTIVES -WORK PACKAGES

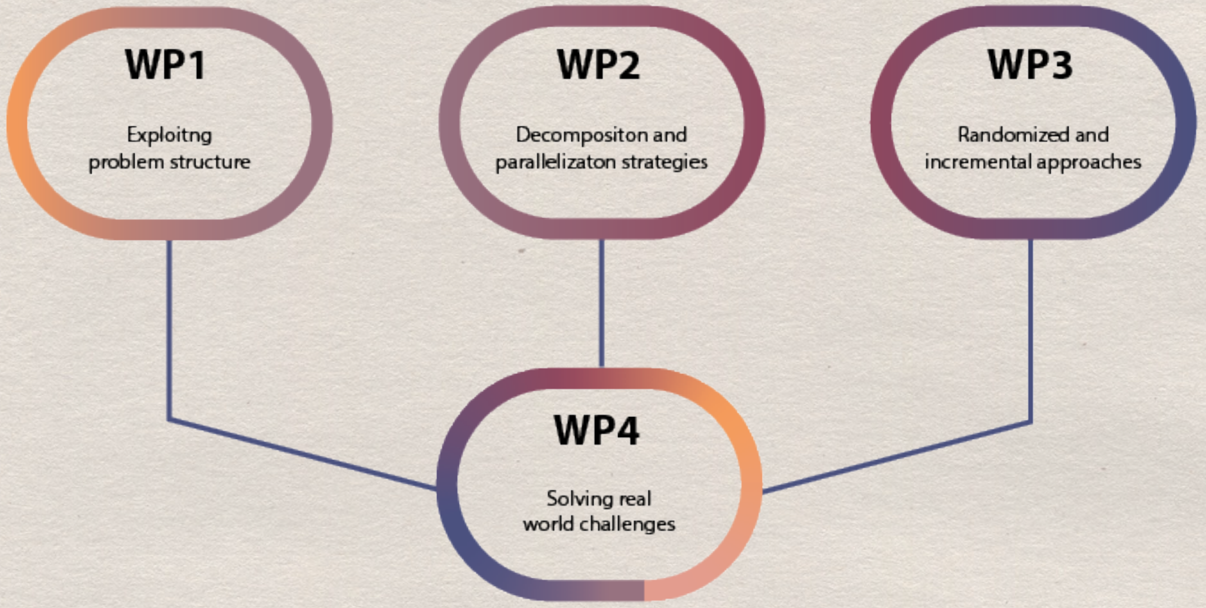
The research program of **TraDe-OPt** is organized in three theoretical workpackages (WP1, WP2, WP3) and one applied workpackage (WP4).

The goal of WP1 is to exploit structural properties of data driven problems to derive algorithms adapted to the modeling assumptions both from the design and convergence standpoint . This viewpoint will also allow to go beyond convexity, and successfully solve some nonconvex, but structured, problems.

The goal of WP2 is to leverage the intrinsic acceleration provided by recent multicore computing architectures or GPUs by developing new decomposition strategies that ideally adapt to the problem structure (in the data, in the objective function, and in the computational platform). We investigated parallel methods for adaptive/distributed processing based on majorization-minimization (MM) techniques and proximal tools.

A class of methods that recently received a lot of attention, especially in machine learning applications, is the class of stochastic methods. The advantage of these methods is in the drastic reduction of the cost per iteration. An example is given by incremental methods, where the gradient of a sum of functions is replaced by the gradient of a single component. In addition, this is the only option for stochastic optimization problems, where data are corrupted by stochastic perturbations and the true gradient is not accessible. Stochastic and incremental methods are the subject of WP3, whose main goal is to apply these methods as low cost regularization procedures to solve huge scale linear inverse problems.

The goal of WP4 is to build bridges between the new advances that results from WP1-WP3 and what is currently deployed by practitioners using enterprise-ready tools and components.



MEET THE TEAM: SENIOR RESEARCHERS

Silvia Villa

- Role: Project Coordinator, Supervisor (ESR1, ESR2)
- Institution: Università degli Studi di Genova
- Interests: optimization, convex analysis, machine learning

Lorenzo Rosasco

- Role: Coordinator, Supervisor(ESR2)
- Institution: Università degli Studi di Genova
- Interests: learning theory, machine learning

Jean-Christophe Pesquet

- Role: Supervisor (ESR3)
- Institution: CentraleSupélec
- Interests: signal and image processing, optimization, inverse problems

Émilie Chouzenoux

- Role: Supervisor (ESR4)
- Institution: CentraleSupélec
- Interests: inverse problems, image processing, optimization

Dirk Lorenz

- Role: Supervisor (ESR5, ESR6)
- Institution: Technische Universität Braunschweig
- Interests: applied analysis, inverse problems, convex optimization

Kristian Bredies

- Role: Supervisor (ESR7, ESR8)
- Institution: Universität Graz
- Interests: inverse problems, oprimization, image processing

Ion Necoara

- Role: Supervisor (ESR9, ESR10)
- Institution: Universitatea Politehnica din București
- Interests: optimization theory, bigdata, machine learning

Ewa Bednarczuk

- Role: Supervisor (ESR11, ESR12)
- Institution: Systems Research Institute, PAS
- Interests: variational analysis, optimization, solution methods

Francois Glineur

- Role: Supervisor (ESR13, ESR14)
- Institution: Université catholique de Louvain
- Interests: Optimization, nonnegative matrix factorization

Curzio Basso

- Role: Supervisor (ESR15)
- Institution: Camelot Biomedical Systems
- Interests: Medical image analysis, machine learning

MEET THE TEAM
EARLY STAGE RESEARCHERS

ESR 1: *Cristian Vega*

- Thesis: "Implicit Regularization: Insights from Iterative Regularization and Overparameterization"
- Supervisor: Silvia Villa
- Co-Supervisor: Lorenzo Rosasco
- Primary host institution: Università degli Studi di Genova
- Secondments: CAMELOT, Technische Universität Braunschweig, CentraleSupelec
- Involvment in work packages: WP3, WP4
- Other achievements during the project: 2 articles, 7 conference presentations

ESR 2: *Cheik Traoré*

- Thesis: "Large-scale convex optimization: parallelization and variance reduction"
- Supervisor: Silvia Villa
- Primary host institution: Università degli Studi di Genova
- Secondments: N-SIDE, Universitatea Politehnica din București
- Involvment in work packages: WP1, WP2, WP4
- Other achievements during the project: 3 publications, 7 conference talks

ESR 3: *Gabriele Scrivanti*

- Thesis: „Some strategies Addressing Non-Convex Variational Problems in Image Processing"
- Supervisor: Jean-Christophe Pesquet
- Co-Supervisor: Ewa Bednarczuk
- Primary host institution: Centrale Supelec
- Secondments: Designers, SRI PAS
- Involvment in work packages: WP1, WP4
- Other achievements during the project: published 3 papers

ESR 4: *Mouna Gharbi*

- Thesis: "Unrolled Majorization-Minimization Approaches for Sparse Signal Reconstruction in Analytical Chemistry"
- Supervisor: Émilie Chouzenoux
- Co-Supervisor: Laurent Duval
- Primary host institution: CentraleSupélec
- Secondments: IFPEN, Università degli Studi di Genova
- Involvment in work packages: WP2, WP4
- Other achievements during the project: published 3 papers

ESR 5: *Lionel Tondji*

- Thesis: "Advances in Bregman-Kaczmarz methods : Accelerations and Inconsistency"
- Supervisor: Dirk Lorenz
- Primary host institution: Technische Universität Braunschweig
- Secondments: GOM, Universitatea Politehnica din București
- Involvment in work packages: WP3, WP4
- Other achievements during the project: Published 7 articles, pariticipated in 5 conferences

ESR 6: *Emanuele Naldi*

- Thesis: "Investigating degenerate preconditioners for proximal point algorithms"
- Supervisor: Dirk Lorenz
- Primary host institution: Technische Universität Braunschweig
- Secondments: GE, Universität Graz
- Involvment in work packages: WP2, WP4
- Other achievements during the project: Published 6 papers, 7 conference presentations, 2 conference posters

ESR 7: *Rodolfo Assereto*

- Thesis: "Total Variation denoising: new techniques and definitions with applications to medical imaging"
- Supervisor: Kristian Bredies
- Primary host institution: Universität Graz
- Secondments: GE, Università degli studi di Genova
- Involvment in work packages: WP1, WP4
- Other achievements during the project: 4 conference presentations, participation "Lange Nacht der Forschung" in Graz

ESR 8: *Enis Chenchene*

- Thesis: "Splitting Methods in Nonsmooth Convex Degenerate Optimization"
- Supervisor: Kristian Bredies
- Primary host institution: Universität Graz
- Secondments: VIF, Technische Universität Braunschweig
- Involvment in work packages: WP1, WP3, WP4
- Other achievements during the project: published 5 papers, 4 invited talks

ESR 9: *Flavia Chorobura*

- Thesis: "Adaptive first-order methods for structured optimization"
- Supervisor: Ion Necoara
- Primary host institution: Universitatea Politehnica din București
- Secondments: CAMELOT, Université catholique de Louvain, CentraleSupelec
- Involvment in work packages: WP2, WP3, WP4
- Other achievements during the project: published 4 papers, participated in 2 conferences,

ESR 10: *Yassine Naboue*

- Thesis: "Higher-order methods for composite optimization and applications"
- Supervisor: Ion Necoara
- Primary host institution: Universitatea Politehnica din București
- Secondments: N-SIDE, Università degli Studi di Genova, Université catholique de Louvain
- Involvment in work packages: WP3, WP4
- Other achievements during the project: published 3 papers

ESR 11: *Giovanni Bruccola*

- Thesis: „Outer Approximation Scheme for Weakly Convex Constrained Optimization Problems"
- Supervisor: Ewa Bednarczuk
- Co-Supervisor: Jean-Christophe Pesquet
- Primary host institution: Systems Research Institute, PAS
- Secondments: CentraleSupelec, Designers
- Involvment in work packages: WP 1, WP 2, WP 4
- Other achievements during the project: published 3 papers

ESR 12: *The Hung Tran*

- Thesis: „Abstract Convexity: Duality, Primal-dual and proximal based Algorithms"
- Supervisor: Ewa Bednarczuk
- Co-Supervisor: Dirk Lorenz
- Primary host institution: Systems Research Institute, PAS
- Secondments: Technische Universität Braunschweig, GOM
- Involvment in work packages: WP 2, WP 4
- Other achievements during the project: published 4 papers

ESR 13: *Yassine Kamri*

- Thesis: "Worst-Case Analysis and Design of First-Order Algorithms"
- Supervisor: François Glineur, Julien Hendrickx
- Primary host institution: Université catholique de Louvain
- Secondments: N-SIDE, Universitatea Politehnica din București
- Involvment in work packages: WP1, WP4
- Other achievements during the project: 1 paper published, 3 papers in preparation, participated in 4 conferences

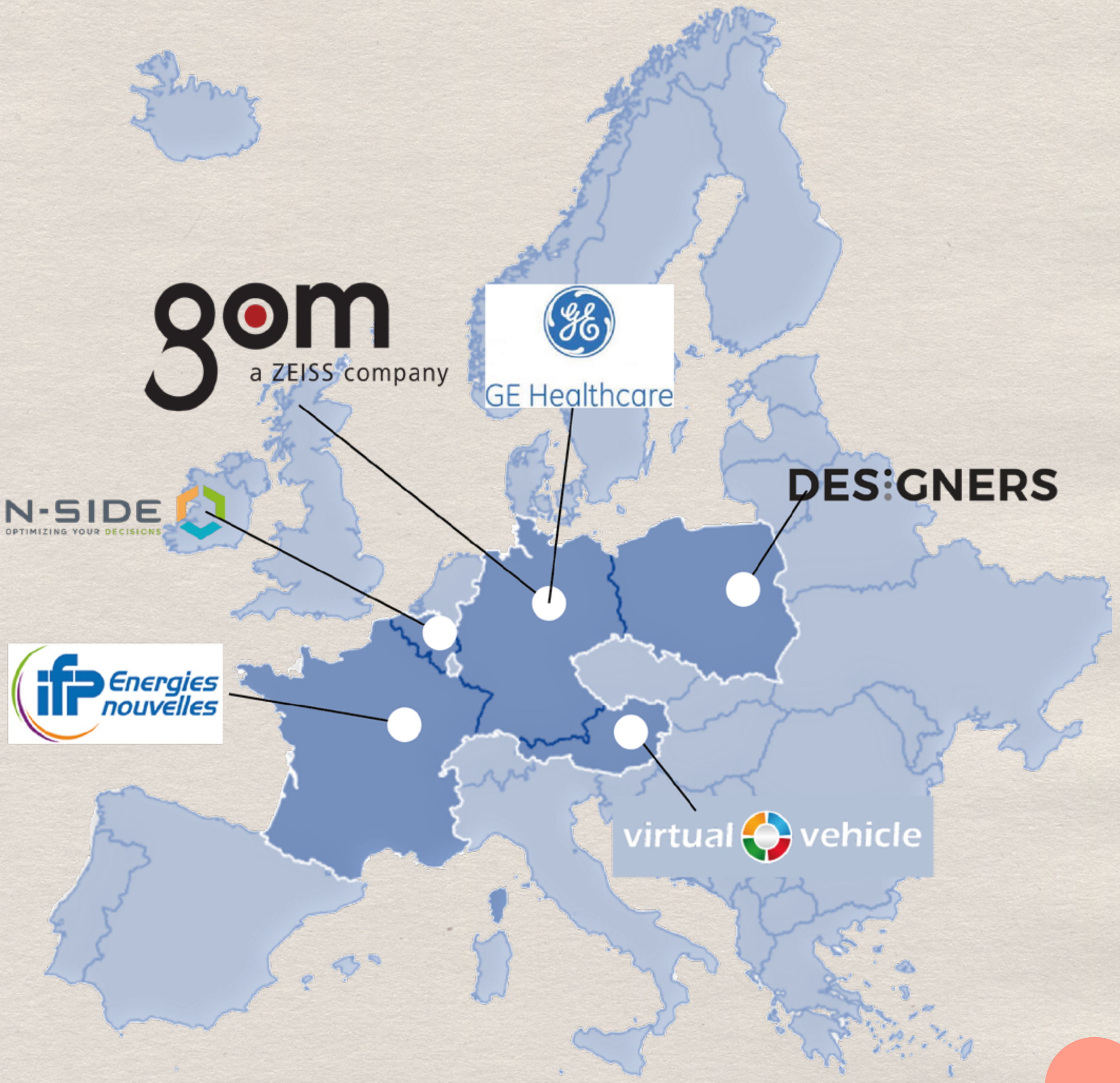
ESR 14: *Sofiane Tanji*

- Thesis: "Recommendation of first-order methods: Theory and Applications"
- Supervisor: François Glineur
- Primary host institution: Université catholique de Louvain
- Secondments: N-SIDE
- Involvment in work packages: WP1, WP4
- Other achievements during the project: published 1 paper, participated in 7 conferences

ESR 15: *Jonathan Chirinos Rodriguez*

- Thesis: "Machine learning techniques for inverse problems"
- Supervisor: Curzio Basso
- Co-Supervisor: Silvia Villa
- Primary host institution: Camelot Biomedical Systems, UNIGE
- Secondments: VIF, Universität Graz
- Involvment in work packages: WP1, WP2, WP3, WP4
- Other achievements during the project: published 2 papers and 1 submitted, 2 invited seminars

BUSSINES PARTNERS



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virtual vehicle

The Virtual Vehicle Competence Center (VIF) was founded in 2002 as an international research center that develops technologies to achieve affordable, safe and environmentally friendly vehicles for road and rail. Since 2008, VIF has been a holding company of the Austrian COMET K2 research program K2-Mobility. With 200+ full-time equivalent employees today, of which almost 80% are involved in R&D, VIF has many years of experience in setting up and coordinating projects in collaboration with industry and research facilities. Website: https://www.virtual-vehicle.at

IFP Energies nouvelles

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OPTIMIZATION IN APPLICATIONS

Tha main focus of the project is methodological. We focused on the design and convergence analysis of algorithms. Our approaches are applied to solve real-world problems faced by our business partners.

Optimization in brain MRI

Magnetic resonance imaging (MRI) is a powerful tool that has revolutionized the way we study the human brain. By using magnetic fields and radio waves, MRI can create detailed images of the brain's structure and function. An MRI scanner draws information from biological tissue by exciting hydrogen nuclei, and then measures the resulting signals. However, despite its capabilities, MRI faces certain limitations when it comes to examining the brain at a microscopic level.

One of the main challenges is the trade-off between spatial resolution and data acquisition time. To obtain high-resolution images, MRI machines need to collect more data, which can take longer. This can be problematic for studying the brain in real-time or for individuals who have difficulty staying still for extended periods. As a result, most MRI studies are limited to millimetre-scale voxels, which are still relatively large compared to the size of individual cells.

To address this limitation, scientists have developed various techniques to extract information about subvoxel microstructure from MRI data.

One approach involves multicomponent modelling, which assumes that each voxel consists of multiple compartments, each with its unique properties. By analyzing the decay of the MRI signal over time, it is possible to identify these different compartments and estimate their relative contributions to the overall signal.

A second approach to extracting information from MRI is through Diffusion-weighted MRI, where each voxel "contains" a probability distribution. Therefore, we want to reconstruct a "matrix" of distributions, or the object called

Ensemble Average Propagator (EAP) - u(x, y)

which represents the likelihood that a particle within a voxel x undergoes a displacement along the vector y during a given time interval. In practice, we measure the so called Fourier transform of the

EAP: $S = F(u) = np.fft.fftn(u)$

Several techniques have been employed in the past for such a reconstruction, but they all reconstruct a simpler object than the full EAP!

The signal is subject to noise η and undersampling: the measured signal is

$$b = \mathbf{K}u_0 + \eta$$

In the field of Inverse Problems, a common approach to restore the data u_0, is to solve the optimization problem

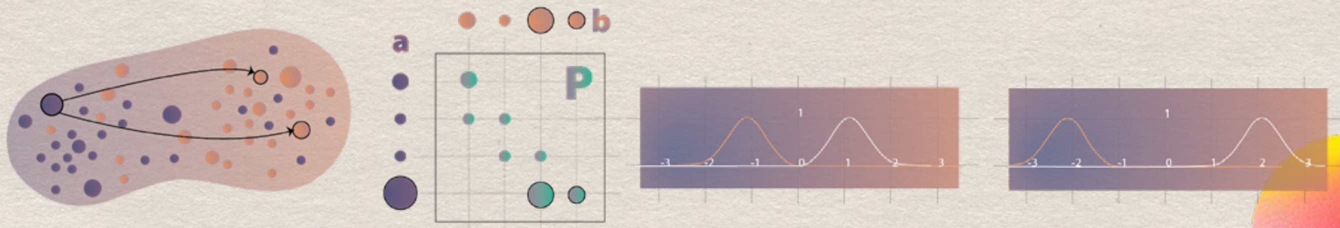
$$\min_u \tfrac{1}{2} \|\mathbf{K}u - b\|^2 + R(u)$$

the idea: to stay "loyal" to the data b, but at the same time to keep the measure of noise R as low as possible.

A common regularizers (for simple images) are Total-Variation-type regularizers (TV). In our research we have combined Total Variation Regularizer with the Wasserstein distance.

Idea: use tools from Optimal Transport theory: for $u_1, u_2 \in \mathcal{P}(Y)$, the Wasserstein-1 distance is

$$W_1(u_1, u_2) = \inf_{\pi \in \Pi(u1,\, u2)} \int_{Y \times Y} \|x - y\| \, d\pi(x, y)$$



and one can introduce the TV-Wasserstein regularization

$$\min_u \underbrace{\tfrac{1}{2} \|\mathbf{K}u - b\|^2}_{\text{fidelity}} + \underbrace{\alpha TV_W(u)}_{\text{regularizer}}$$

where $TV_W(u) = \Sigma_{i,j} W_1(u_{i+1,j}, u_{ij}) + W_1(u_{i+1,j}, u_{ij})$

Idea: the W1 admits a so-called "dual formulation": $u_1, u_2 \in \mathcal{P}(Y)$

$$W_1(u_1, u_2) = \sup_{Lip(v) \le 1} \langle v, u1 - u2 \rangle$$

It still involves a subproblem, but the subproblem is simpler, and it can be encorporated in existing formulations for the solution of problems like

$$\min_x F(x) + G(Lx)$$

or equivalently of the form

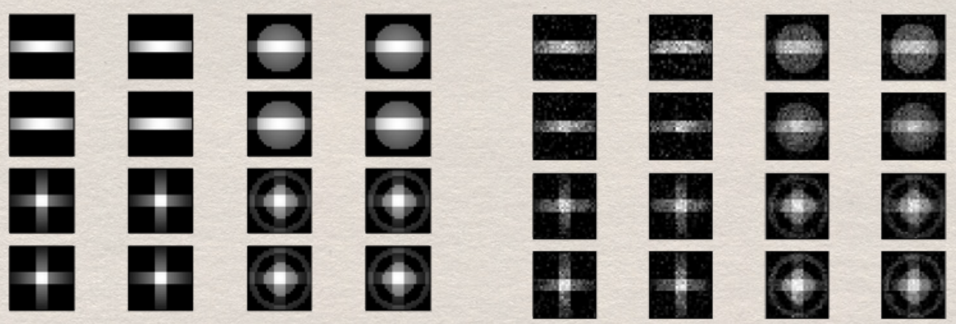
$$\min_x \max_y F(x) - G^*(y) + \langle \mathcal{L}x, y \rangle$$

We also provide different formulations of the same problem :

$$\begin{array}{lll} \inf_{\nabla_x u = div_y \gamma} \|\gamma\|_{21} & (primal) & \\ = \sup_v \inf_\gamma \|\gamma\|_{21} + \langle v, \nabla_x u + div_y \gamma \rangle & & \nabla_y\text{-voxelwise gradient} \\ = \sup_v \inf_\gamma \|\gamma\|_{21} + \langle v, \nabla_x u \rangle - \langle \nabla_y v, \gamma \rangle & (primal\text{-}dual) & \\ = \sup_v \langle v, \nabla_x u \rangle - \sup_\gamma \langle \nabla_y v, \gamma \rangle - \|\gamma\|_{21} & & (div_y = -\nabla^*_y) \\ TV_W(u) = \sup_{Lip_y(v) \le 1} \langle div_x v, u \rangle & (dual) & \end{array}$$

This approach, relying on incorporating Wasserstein Distance into the regularization term, has given very promising results in the test phase, and is now being verified on data coming from real life applications, provided by GE Healthcare.

Toy Model | TV regularized

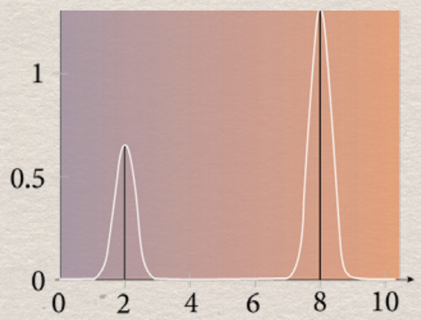


Optimization in Analytical Chemistry

Analytical chemistry or physico-chemical analysis chiefly seeks to decipher chemical compositions or properties of natural and artificial materials, by providing measurement methods and computational tools to gain insight into those substances. A typical goal in analytical chemistry is to identify, within a sample, existing compounds and their associated abundances. To do so, chemical analysis relies on qualitative and quantitative inspection. Analytical chemistry is useful in many practical fields. For instance, it serves in medicine for clinical laboratory tests, in industrial quality assurance tests on pharmaceutical drugs or fuels, as well as for food examination. Among the chemical analysis measurement techniques, let us cite: gas, liquid or ion chromatography, ultraviolet (UV), infrared (IR) and X-ray diffraction or absorption, nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry (MS).

Among these techniques, separative methods hold particular significance. These methods produce monodimensional or multidimensional signals that provide valuable information about the chemical composition of the sample. By focusing on generic peak models, analytical chemists can extract meaningful features related to the components of the chemical mixture. However, the raw measurements often deviate from ideal conditions. In complex mixtures, peaks may overlap, and even with advancements in acquisition devices, measurements can be affected by instrumental or external disturbances. To overcome these challenges and accurately recover the desired signal, sophisticated computational data processing techniques are essential. Advanced analytical chemistry benefits greatly from the application of state-of-the-art machine learning algorithms.

A simplified one-dimensional representation can be visualized in figure below. Ideally, the resulting signal would consist of a series of distinct peaks, where the location and height of each peak would directly correspond to the identity and quantity of the components. However, in practice, overlapping peaks are more commonly observed.

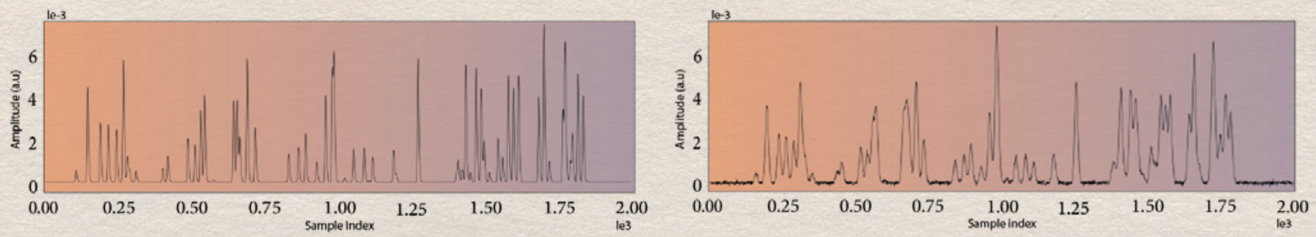


Synthetic representation of a chemical analysis signal, displaying two Gaussian peaks (white) surrounding two spikes (black).

In our research we denote p the ground-truth signal. This signal is modeled as a linear combination of peaks obtained through convolving a chemically informative spiky signal s (as the black signal in Figure) and a parametric model π, through

$$p = \pi * s$$

On the figure below we show an example studied in this context, with the sought ground truth signal (after processing), to compare with the raw acquired signal. The inverse problem consists in providing an estimate of p (and possibly, of s), knowing z, H and some statistical assumptions on the noise e. Such problem is common to various 1D and 2D analytical chemistry applications.



Example of a signal p (left) and observed spectrum z (right).

Inverse problem in analytical chemistry is as follows:

$z = Hp + e$

$z \in R^M$: observed acquisition

$p \in R^N$: original sparse positive-valued signal

$H \in R^{M \times N}$: measurement degradation, typically convolution with Gaussian, Voigt, ..., kernel shapes

e : corrupting noise, typically additive Gaussian iid

Our goal is to retrieve an estimate of $x \in R^N$ knowing H and z.

Challenges: heterogenous signals, high dimensionality, large databases.

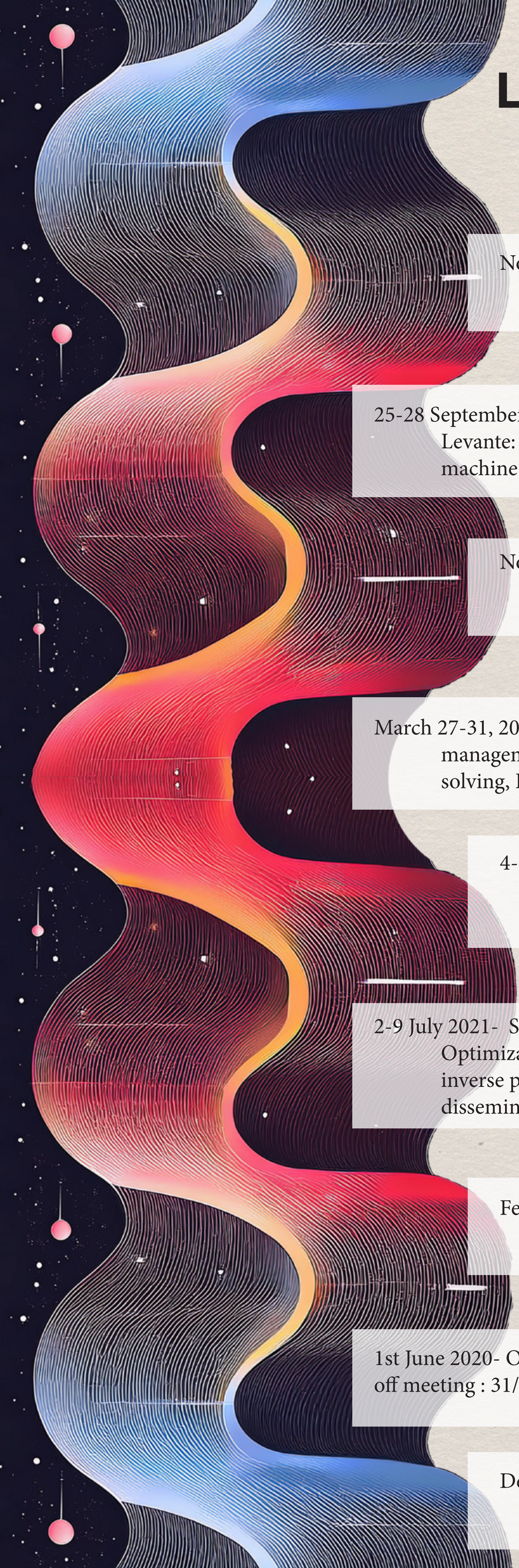
Such problem is common to various 1D and 2D analytical chemistry applications. It is a crucial problem for chemists, that is necessary to tackle to have readable and interpretable spectra. Several approaches in literature are available, mainly relying on two classes, (i) model-based approaches using iterative optimization algorithms and (ii) deep learning methods relying on learnt deep neural networks architectures. However, both struggle with shortcomings, and a recent paradigm, called deep unfolding (or unrolling) has been introduced in the field of inverse problems to overcome these issues.

The goal is to provide a comprehensive study of deep unfolding methods for the resolution of the inverse problem arising in chemical analysis. We focus our study on the case where the baseline term b is almost constant and can be assumed null, or removed by preprocessing.

Our contributions are as follows.

- We deploy three model-based iterative methods, and their deep unrolled counterpart, for solving the inverse problem arising in analytical chemistry data restoration. We develop an original simulator for building realistic databases with adjustable parameters. This yields the construction of seven realistic databases for the learning and testing of the proposed methods.
- We perform an extensive benchmarking of the methods on these databases, implementing an original chemically-inspired evaluation procedure.
- We finally assess our proposed approaches on real data arising from chromatography acquisitions , proving the potential of our methods in real settings for chemists.

All the proposed tools, from the database simulation to the algorithm implementation and validation, are shared through a comprehensive toolbox, for reproducibility purposes.



LIFE OF THE PROJECT

November 2024 - End of project

25-28 September 2024: Final workshop in Sestri Levante: a meeting on optimization for machine learning and inverse problems

November 2022 and 2023: Participation to Science's Festival in Genoa

March 27-31, 2023 School at UniGraz: Quality management, structured problem solving, PhD defense rehearsal

4-8 July 2022: Louvain: Workshop on Algorithmic and Continuous Optimization

2-9 July 2021- School at Central Supelec: Optimization in machine learning and inverse problems + course for dissemination to a Lay audience

February 2021 First TraDE-OPT School hosted by TUBS: (15-19 February)

1st June 2020- Official start of the project! kick off meeting : 31/07/2020

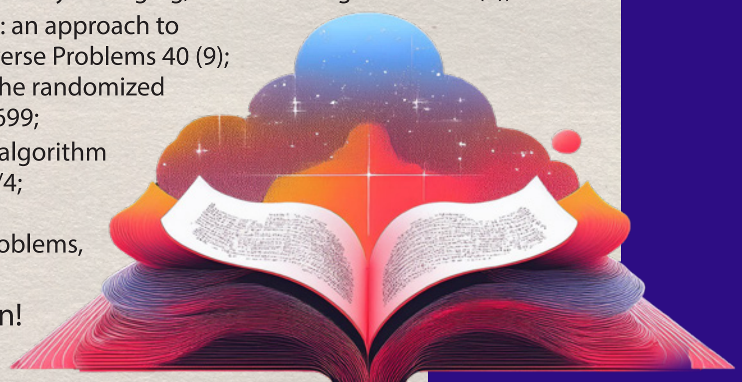
December 2019- in December TraDE-OPT ITN was granted financing!

LIST OF PUBLICATIONS

A list of selscted articles published as of October 2024:

1. C. Brauer, D. Lorenz, L. Tondji, Group equivariant networks for leakage detection in vacuum bagging, 2022 30th European Signal Processing Conference (EUSIPCO);
2. K. Bredies, E. Chenchene, D. Lorenz, E. Naldi, Degenerate preconditioned proximal point algorithms, SIAM Journal on Optimization, 32(3);
3. K. Bredies, J. Chirinos Rodriguez, E. Naldi, On extreme points and representer theorems for the Lipschitz unit ball on finite metric spaces, Archiv der Mathematik, 122(6);
4. K. Bredies, E. Chenchene, J. Fuchs, B. Luber, Proximal Gauss-Newton Method for Box-constrained Parameter Identification of a Nonlinear Railway Suspension System, International Journal of Prognostics and Health Management, 15;
5. K. Bredies, E. Chenchene, E. Naldi. Graph and distributed extensions of the Douglas–Rachford method. SIAM Journal on Optimization 34 (2), 1569-1594 (2024);
6. E. M. Bednarczuk, G. Bruccola, On global solvability of a class of possibly nonconvex QCQP problems in Hilbert spaces, Optimisation;
7. E. M. Bednarczuk; T. H. Tran, Duality for composite optimization problem within the framework of abstract convexity, Optimization: A Journal of Mathematical Programming and Operations Research, Volume 72, 2023 - Issue 1;
8. L. Briceño-Arias, J. Deride, C. Vega, Random Activations in Primal-Dual Splittings for Monotone Inclusions with a Priori Information, Journal of Optimization Theory and Applications volume 192, issue 1, pages 56–81 (2022);
9. G Carlier, E. Chenchene, K Eichinger, Wasserstein Medians: Robustness, PDE Characterization, and Numerics, SIAM Journal on Mathematical Analysis 56 (5), 6483-6520;
10. E. Chenchene, K. Bredies, A. Hosseini, A hybrid proximal generalized conditional gradient method and application to total variation parameter learning, 2023 European Control Conference (ECC);
11. F. Chorobura, D. Lupu, I. Necoara, Coordinate projected gradient descent minimization and its application to orthogonal nonnegative matrix factorization, IEEE 61st Conference on Decision and Control (CDC);
12. F. Chorobura, F. Glineur and I. Necoara, Can random proximal coordinate descent be accelerated on nonseparable convex composite minimization problems?, European Control Conference (ECC);
13. F.Chorobura, I. Necoara, Coordinate descent methods beyond smoothness and separability, Computational Optimization and Applications, 88, 107–149, 2024;
14. F. Chorobura, I. Necoara, Random coordinate descent methods for nonseparable composite optimization, SIAM Journal on Optimization, 33(3), 2160–2190, 2023;
15. S. Endt, M. Engel, E. Naldi, R. Assereto, M. Molendowska, L. Mueller, C. Mayrink Verdun, C.M. Pirkl, M. Palombo, D. K. Jones, M. I. Menzel, In Vivo Myelin Water Quantification Using Diffusion–Relaxation Correlation MRI: A Comparison of 1D and 2D Methods, Applied Magnetic Resonance, 54(11-12):1-18;
16. M. Gharbi, E. Chouzenoux, J.-C. Pesquet, L. Duval, GPU-based Implementations of MM Algorithms. Application to Spectroscopy Signal Restoration, Proceedings of the 29th European Signal Processing Conference, EUSIPCO 2021;
17. Gharbi, M., Chouzenoux, E., Pesquet, J. C. (2024). An unrolled half-quadratic approach for sparse signal recovery in spectroscopy. Signal Processing, no. 218;
18. Gharbi, M., Villa, S., Chouzenoux, E., Pesquet, J.-C., Duval, L. (2024). Unrolled deep networks for sparse signal restoration in analytical chemistry. In the 34th International workshop on Machine Learning for Signal Processing (MLSP 2024), Sept. 22–25, 2024, London, UK ;
19. D. Lorenz, F. Schneppe, and L. Tondji, Linearly convergent adjoint free solution of least squares problems by random descent, Inverse Problems, Volume 39, Number 12;
20. D. Lorenz, J. Marquardt, E. Naldi. The Degenerate Variable Metric Proximal Point Algorithm and Adaptive Stepsizes for Primal-Dual Douglas-Rachford. Optimization, 1-27 (2024);
21. Y. Nabou, I. Necoara, Efficiency of higher-order algorithms for minimizing composite functions, Computational Optimization and Applications, 87(2):1-33;
22. Y Nabou, L Toma and I Necoara, Modified projected Gauss-Newton method for constrained nonlinear least-squares: application to power flow analysis, European Control Conference (ECC);
23. E. Naldi, G. Savaré. Weak topology and Opial property in Wasserstein spaces, with applications to gradient flows and proximal point algorithms of geodesically convex functionals. Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. 32, 725-750 (2021);
24. L. Tondji, D. Lorenz and I. Necoara, An accelerated randomized Bregman-Kaczmarz method for strongly convex linearly constraint optimization*, 2023 European Control Conference (ECC);
25. L. Tondji, D Lorenz, Faster randomized block sparse Kaczmarz by averaging, Numerical Algorithms 93 (4);
26. L. Tondji, I. Tondji, D. Lorenz, Adaptive Bregman–Kaczmarz: an approach to solve linear inverse problems with independent noise exactly, Inverse Problems 40 (9);
27. L. Tondji, I Necoara, D Lorenz Acceleration and restart for the randomized Bregman-Kaczmarz method, Linear Algebra and its Applications 699;
28. C. Traoré, E. Pauwels, Sequential convergence of AdaGrad algorithm for smooth convex optimization, Operations Research Letters, 49/4;
29. C. Vega, C. Molinari, S. Villa, and L. Rosasco, Fast iterative regularization by reusing data, Journal of Inverse and Ill-posed Problems, 2023.

...and even more in preparation!



Kristian Bredies with Rodolfo Assereto and Enis Chenchene at the Austrian Long Night of Research 2022

Participants of the Workshop on Algorithmic and Continuous Optimization, Louvain, 4-8 July 2022.

The TraDE-Opt station at the Science Festival in 2023 in Genova

Participants of the TraDE-OPT Final workshop in Sestri Levante: a meeting on optimization for machine learning and inverse problems, 25-28 September 2024:

Looking back

What the ESR's say

84,6 % ESRs rated their overall participation in the ITN a success

"The company secondment helped me take a look at what happens in companies. This was really helpful"

75 % ESRs are satisfied with the publication outcomes of their PhD

"The fact of being part of a wide network already at the beginning of of my PhD and research career was the most helpful part of the ITN"

84,6 % of ESR think that being part of the ITN was helpful to find a job in academia

75 % of ESRs think that the ITN was helpful to form a scientific network

"The ITN was helpful on many levels, in terms of renumeration, resources, providing a network of skilled scientists to learn from, orginizingsummer and winter schools, pushing towards scientifif dissemination, giving the chance to go to secondments, giving some guidance, insight and support for the after-PhD carreer opportunities"

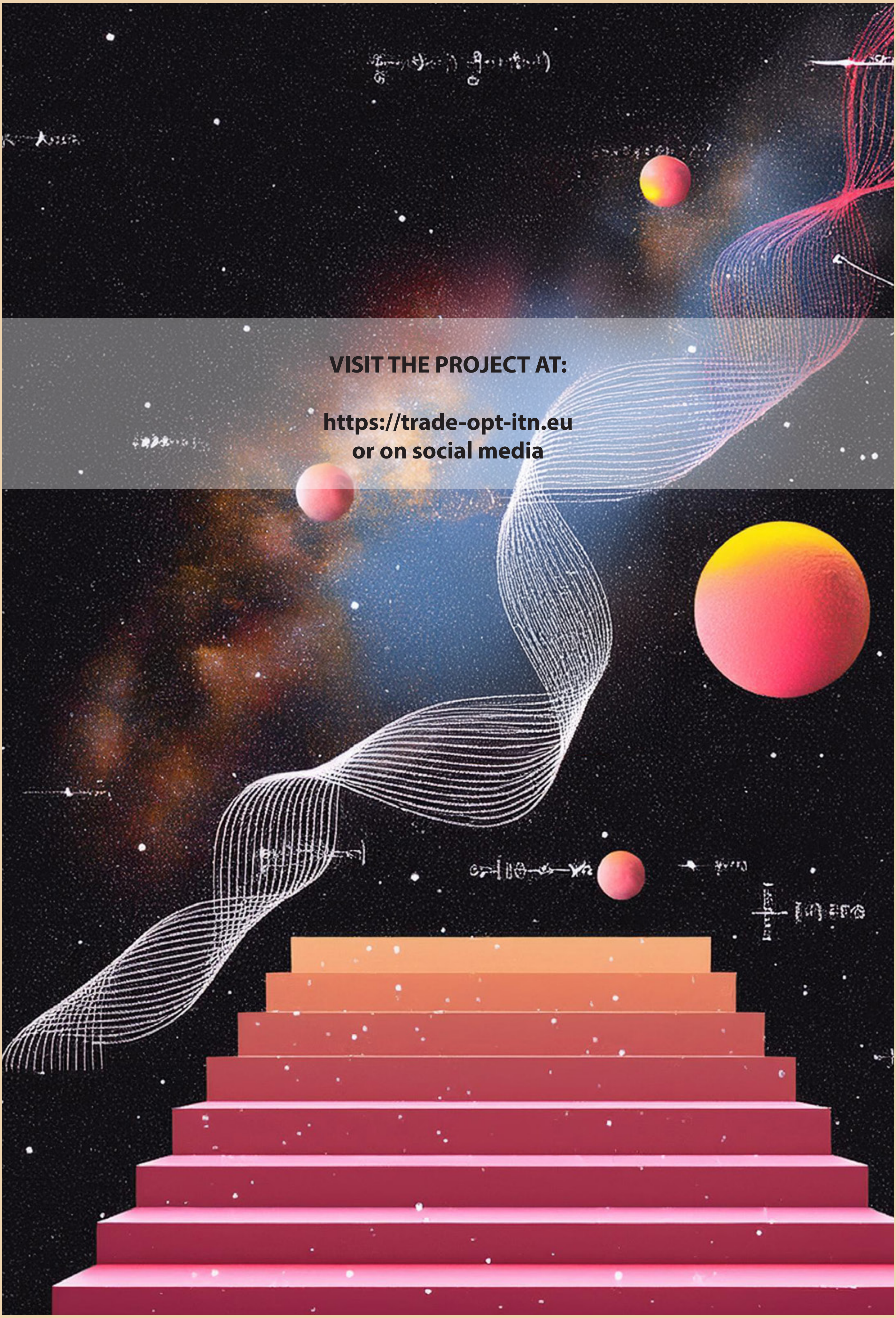
"The secondment at the university was great. Both for networking and scientifically".

61 % ESRs have already started a new position in Academia!

"I liked the fact that the workshops were intimate. Students +professors +few invited speakers I think it works well"

92,3 % of ESRs said that given the choice to do a PhD again they would choose a ITN

Quotes and responses based on Deliverable 5.9: 4th Evaluation Questionnaires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or on social media