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ARTIFICIAL & NATURAL INTELLIGENCE
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AI and physical models

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September 28-29 2020

Université Fédérale
Toulouse Midi-Pyrénées

Agenda

MEMBERS

Definition/scientific perimeter of the theme

Thread 1 Accelerating physical models

Thread 2 Improving learning with physics

On-going work

Highlight & main results

Scientific animation of the theme

Publications

MEMBERS I

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Chairs

- Fabrice Gamboa: AI for physical models with geometric tools
- Serge Gratton: Data Assimilation and Machine Learning
- Thomas Schiex: Design using intuition[1] and logic[2]
- Jérôme Bolte: Large scale optimization for AI
- Nicolas Dobigeon: Fusion-based inference from heterogeneous data

Co chairs

- AI for physical models with geometric tools: Reda Chhaibi (IMT) and Thomas Pellegrini (IRIT)
- Data Assimilation and Machine Learning: Pierre Boudier (Nvidia), Alfredo Buttari (IRIT), Selime Gurol (Cerfacs), Corentin Lapeyre (Cerfacs)
- Design using intuition and logic: S. Barbe (INSA/INRAE), D. Simoncini (IRIT/UT1), G. Katsirelos & S. de Givry (INRAE)
- Large scale optimization for AI: J. Bolte (UT1) and external collaborators A. Blanchet (UT1), L. Miclo (CNRS), M. Fathi (P7), S. Villeneuve (UT1).
- Fusion-based inference from heterogeneous data: M. Fauvel (INRAe)

MEMBERS II

ANITI Resources

- AI for physical models with geometric tools: Virgile Foy Ph.D (ANITI SAFRAN)
- Data Assimilation and Machine Learning: Anthony Fillion PD (ANITI), 4 interns $\rightarrow$ 3 CIFRE PhD, Philippe Toint (Visitor)
- Design using intuition and logic: D. Allouche & N. Rousse (INRAe),
- Large scale optimization for AI: J. Bolte

MEMBERS III

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Other Resources

- AI for physical models with geometric tools: Louis Berry and Faouzi Hakimi CEA Cadarache Bayesian data assimilation, Clément Benesse (IMT-ENS Lyon scholarship) Fairness and sensitivity
- Data Assimilation and Machine Learning: Ehouarn Simon (IRIT), Elisa Riccietti (IRIT TOTAL)
- Design using intuition and logic: M. Defresne (PhD, SEVAB)
- Large scale optimization for AI: none yet

AI and physical models-Scientific Perimeter

Can ML techniques be extended to solve problems, involving Physics represented by raw data or by partial differential equations?

- Thread 1 Improve (accuracy, time, explainability,stability,...) physical models simulation and optimization via ML, statistical and geometric, approaches
  How physical information can be used to train machine learning algorithms?
  Replace (totally, partially) numerical simulations with ML ?
  Energy based models
- Thread 2 Improving learning models with physical constraints
  Propagate sensor information in training method, provide reduced models
  Enhance Data Assimilation with ML
  Develop ML models ensuring biophysical constraints

Thread 1 Accelerating physical models I

ML techniques = complex classification or regression tasks (images, text, audio signals, 3D objects..)

Wish to hybrid these methods with physical reality

Tranversality physical modelling and applied maths

- data assimilation
- optimisation
- geometry
- complex simulation
- statistical learning
- uncertainty quantification and sensitivity analysis
- high performance computing in large scale systems, aggressive reduction of computing accuracy

Thread 1 Accelerating physical models II

- Can ML improve standard modelling techniques?
  - Numerically solve PDE's with data centric approaches using ML techniques
  - Approximate PDE solutions by deep learning functions
  - Learn from data suitable approximations of physical quantities (fluxes in finite volumes, energy..)
- How physical information can train machine learning algorithms?
  - Penalizing by physical equation
  - Introduce smart parametrization related to physics
- Performance achieved compared to standard methods?
  - HPC and non convex programming
  - Online learning of physical processes

Thread I Improving learning with physics III

Dynamical systems from physics are inspirational for optimization: steepest descent and heat equations, Newton's law with friction and heavy ball descent, simulated annealing and thermodynamics

Goal: pursue this research line with new physical models & solve ML problems

Optimization through measure spaces

- Embed and regularize problems in measure spaces
- Apply classical dynamics/algorithms (e.g. steepest descent) in the embedding space
- Model the problem through discrete systems (e.g. Markov chains, Metropolis algorithms)
- Quantify convergence: rates, role of hyperparameters
- Analyze the impact for ML problems

Data assimilation = putting heterogeneous observed data in physical models

Wish to systematise and implement smartly

Tranversality physical modelling and applied maths

- optimisation
- geometry
- complex simulation
- statistical learning
- uncertainty quantification

Thread 2 Improving learning with physics II

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- How can data assimilation reinforce physical approaches?
  - Filtering and ensemble techniques
  - Variational algorithms
- How can ML provide better data assimilation then existing DA approaches?
  - Use of recurrent Elman networks to (out)perform DA
  - Go beyond Gaussianity and nonlinearity
  - Fresh look on the analysis-propagation DA paradigm
- Are extensions to non highly linear dynamic achievable?
  - HPC and neural networks modelling
- How designing ML models satisfying physical constraints?
  - To reduce dependence of the algorithms on the learning sets
  - To provide explainable and interpretable models

On-going work I

On-going collaboration between chairs

- AI for physical models with geometric tools **with**
  - Data Assimilation and Machine Learning (Ph.D Project)
  - Fair & Robust Methods in Machine Learning (Ph.D Benesse)
  - Deep Learning with semantic, cognitive and biological constraints (Ph. D co advisors Filbet and Pellegrini)
- Data Assimilation and Machine Learning
  - Discussion with AI for physical models with geometric tools (March 2020, cancelled)
- Design using intuition and logic & Large scale optimization for AI
  - None at this point. Happy to discuss.

On-going work II

On-going collaboration with ANITI Industrial partners

- AI for physical models with geometric tools
  - SAFRAN accelerating fluid simulation by machine learning
  - THALES uncertainty machine learning and GPS
  - EDF Geometry, Robustness, explainability
  - in progress NPX, VITESCO CONTINENTAL
- Data Assimilation and Machine Learning
  - BRLi accelerating flood prediction by machine learning
  - Airbus and ATOS accelerating solvers for time dependent PDEs
  - ATOS robustsness of large scale computations/inference in a multi-precision context
  - Liebherr Optimal sampling of physical models in data-centric ML approaches
- Design using intuition and logic
  - Collaborations with Biotech companies that did not participate to ANITI when Environment/Heath were out of scope (TWB, CARBIOs, ENOBRAQ): improving enzymes for plastic recycling or CO_2 fixation. Also with INSERM on antibody design (patent pending).

On-going work III

On-going collaboration with external projects

- AI for physical models with geometric tools
  - Project ANR RISCOPE Risk-based system for coastal flooding early warning with BRGM
  - SAMSI `https://www.samsi.info/`
- Data Assimilation and Machine Learning
  - (with Z. Zhang) Hong Kong RCS grant on space decompositon, coarse space corrections and randomization
  - Contrat with JCSDA (Boulder, USA) on large scale covariance estimation and ensemble DA
- Design using intuition and logic
  - ANR SPACEHEX: designing orthogonal symmetrical protein to organize enzymes in space (with INSA/CNRS/CEA)
- Large scale optimization for AI
  - ANR MasDol (Gadat), US Air Force Grant (Bolte & Pauwels)

On-going work IV

On-going ANITI Phd & Post doc

- AI for physical models with geometric tools
  - With SAFRAN begining Ph. D Virgile Foy
  - In discussion Sadok Gerad and Saif Eddine Ghribi
- Data Assimilation and Machine Learning
  - 2 CIFRE PhD's under construction With ATOS (M. Peyron, Th. Beuzewill), 1 Phd with BRLi (Valentin Mercier)
  - GRAINE project with Liebherr for a PG
  - 1 PhD on second order methods for non-convex optimization (cofunding with Region)
  - In discussion Sadok Gerad and AI for physical models with geometric tools (co-funding with Region)
- Design using intuition and logic
  - SEVAB funded PhD of Marianne DEFRESNE starting. Not ANITI funded but could have been.

Highlight & main results

Scientific event organisation or participation

- Co-organisation Indo-French Workshop on Statistics and Artificial Intelligence for Data Science (Calcutta January 2020)
- Organisation Workshop mathematical statistics and artificial intelligence. ANITI Toulouse-ISM Tokyo (July 2020 Canceled)
- ICTS conference on Statistical Physics of Machine Learning (Bangalore Janary 2020)

Scientific animation of the theme

Description of the theme agenda (weekly seminar,. . .)

- Half day bimonthly meeting with all the members of *AI for physical models with geometric tools* and *Data Assimilation and Machine Learning* chairs.

Emerging collaboration between chairs & industrial partner

- *AI for physical models with geometric tools* with NXP (mean field model) and Laplace/Vitesco on hydrogen fuel cell

Publications- AI for physical models with geometric tools

1. Daouda, T., Chhaibi, R., Tossou, P., & Villani, A. C. (2020). Geodesics in fibered latent spaces: A geometric approach to learning correspondences between conditions. arXiv preprint arXiv:2005.07852.
2. Gamboa, F., Klein, T., Lagnoux, A., & Moreno, L. (2020). Sensitivity analysis in general metric spaces. arXiv preprint arXiv:2002.04465.
3. Fraiman, R., Gamboa, F., & Moreno, L. (2020). Sensitivity indices for output on a Riemannian manifold. International Journal for Uncertainty Quantification, 10(4).
4. Gamboa, F., Gremaud, P., Klein, T., & Lagnoux, A. (2020). Global Sensitivity Analysis: a new generation of mighty estimators based on rank statistics. arXiv preprint arXiv:2003.01772.
5. Gamboa, F., Gueneau, C., Klein, T., & Lawrence, E. (2020). Maximum entropy on the mean approach to solve generalized inverse problems with an application in computational thermodynamics.
6. Idier, D., *et al.*(2020). Toward a user-based, robust and fast running method for coastal flooding forecast, early warning, and risk prevention. Journal of Coastal Research, 95 (sp1), 1111-1116.
7. Roustant, O., Gamboa, F., & Iooss, B. (2020). Parseval inequalities and lower bounds for variance-based sensitivity indices. Electronic Journal of Statistics, 14(1), 386-412.
8. Stenger, J., Gamboa, F., Keller, M., & Iooss, B. (2020). Optimal Uncertainty Quantification of a risk measurement from a thermal-hydraulic code using Canonical Moments. International Journal for Uncertainty Quantification, 10(1).
9. Stenger, J., Gamboa, F., & Keller, M. (2019). Optimization Of Quasi-convex Function Over Product Measure Sets. arXiv preprint arXiv:1907.07934.
10. Stenger, J., Gamboa, F., Keller, M., & Iooss, B. (2019, August). Canonical Moments for Optimal Uncertainty Quantification on a Variety. In International Conference on Geometric Science of Information (pp. 571-578). Springer, Cham.

Publications- Data Assimilation and Machine Learning

1. Serge Gratton, Ehouarn Simon, Philippe Toint An algorithm for the minimization of nonsmooth and nonconvex functions using inexact evaluations and its worst-case complexity in Mathematical Programming, Series A, Springer, 2020
2. Serge Gratton, Philippe L. Toint: A note on solving nonlinear optimization problems in variable precision. Comput. Optim. Appl. 76(3): 917-933 (2020)
3. Serge Gratton, Ehouarn Simon, David Titley-Péloquin, Philippe L. Toint: Exploiting variable precision in GMRES, (https://arxiv.org/abs/1907.10550), 2019
4. Henry Calandra, Serge Gratton, Elisa Riccietti and Xavier Vasseur, On iterative solution of the extended normal equations, SIAM Journal on Matrix Analysis and Applications, acepted 2020
5. Henry Calandra, Serge Gratton, Elisa Riccietti and Xavier Vasseur, On a multilevel Levenberg-Marquardt method for the training of artificial neural networks and its application to the solution of partial differential equations, Optimization Methods and Software, accepted 2020
6. Anthony Fillion, Marc Bocquet, Serge Gratton, Selime Gurol, Pavel Sakov, An iterative ensemble Kalman smoother in presence of additive model error, accepted in SIAM JUQ
7. Serge Gratton, Ehouarn Simon, David Titley-Peloquin, Ph. Toint. Minimizing convex quadratics with variable precision conjugate gradients, Numer. Linear Algebra Appl., in press
8. Henry Calandra, Serge Gratton, Elisa Riccietti and Xavier Vasseur, On high-order multilevel optimization strategies , in review for SIAM Journal on Optimization, 2019.
9. Antoine Bernigaud, Serge Gratton, Flavia Lenti, Ehouarn Simon, Oumeima Sohab. p-norm regularization in variational data assimilation, submitted, 2020
10. Serge Gratton, Ehouarn Simon, David Titley-Peloquin. Computing optimal empirical covariance matrices from multi-ensembles with application to ensemble-based Kalman filters, submitted, 2019

Publications- Design using intuition and logic

- Brouard, Céline, Simon de Givry, and Thomas Schiex. "Pushing data into CP models using Graphical Model Learning and Solving." (2020). Proc. CP'2020. Pages 811-826, LNCS 12333, Springer.

Publications- Large scale optimization for AI

- None on this thread!