Maximum Entropy on the Mean approach to solve inverse problems with an application in computational thermodynamics.

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Abstract:

In the context of computational thermodynamics, we aim at reconstructing a multidimensional function $f : \mathbb{R}^d \to \mathbb{R}^p$ which is solution of an inverse problem. That is, knowing a training set $\{x_l, z_l\}_{l=1,\dots,N}$, we aim at building a regularized $\mathbb{R}^p$-valued function $f = \begin{pmatrix} f^1 & \dots & f^p \end{pmatrix}$ such that

$$\sum_{i=1}^{p} \lambda^i(x_l) f^i(x_l) = z_l, \qquad l = 1, \dots, N, \tag{1}$$

with given functions λ^i. Component f^i represents an energy function. We propose a regularized solution for this problem by a Maximum Entropy on the Mean (MEM) method. Interpolation problem, as problem stated in (1), defines a too "local" constraint and will lead to a trivial reconstruction by MEM methods. Mixed interpolation and moment constraints must be considered to find an appropriate solution.

Motivated by crystallography [1], MEM method has been developed in [2] and [3]. The method aims at the reconstruction on space U of the probability measure P associated with random variables Y when having at hand only a few information on Y.

Let P_0 be a probability measure defined on compact space U. P_0 will be called the reference measure. MEM method derives as solution P the probability measure with highest P_0-entropy, that is the probability measure P which minimizes the divergence (or maximizes the entropy) from measure P_0. Reference measure P_0 can act as a priori information on Y distribution. Letting K be the Kullback-Leibler divergence, this problem is more formally written

$$\begin{aligned} &\min \; K(P, P_0) \\ &P \;:\; \int_U y_l dP(y) = z_l, \qquad z = \begin{pmatrix} z_1 & \dots & z_N \end{pmatrix}^T \in \mathbb{R}^N. \end{aligned} \tag{2}$$

To estimate the solution P, we will work on a sequence of estimators

$$\nu_n = \frac{1}{n} \sum_{i=1}^{n} X_i \delta_{t_i}, \tag{3}$$

where X_i are random amplitudes and δ_{t_i} is the discretization of space U.

In [4] the authors have proposed an extension of MEM method for functional reconstruction instead of probability measure reconstruction. The key idea of MEM method in this case is that

the function to be reconstructed is seen as the expectation of a random function with respect to the unknown probability measure P on the space of functions. The idea is to link a problem in convex optimisation with problem (2).

In convex analysis, the selection of a multidimensional function f can be proceeded by a convex minimization problem. Given a certain convex function γ

$$\begin{aligned} &\min \int_U \gamma(f^1, \ldots, f^p) dP_U \\ &f \ : \ \int_U \sum_{i=1}^{p} \lambda^i(x) f^i(x) \varphi_l(x) dP_U(x) = z_l \qquad 1 \leqslant l \leqslant N. \end{aligned} \tag{4}$$

By a linear transfer principle linking function f to some measure F, we will show that solving (4) can be brought back to solving the following problem on measures taking D_γ, the divergence built in line with convex function γ

$$\begin{aligned} &\min \ D_\gamma(F, F_0) = \min \int_U \gamma\left(\frac{dF^1}{dP_U}, \ldots, \frac{dF^p}{dP_U}\right) dP_U \\ &F \ : \ \int_U \sum_{i=1}^{p} \lambda^i(x) T\left(F^i(x)\right) d\Phi_l(x) = z_l \qquad 1 \leqslant l \leqslant N, \end{aligned} \tag{5}$$

with T is transfer operator from the measure space to the function space. We can go back to a finite dimensional problem by a discrete approximation of F amplitudes. MEM estimator is then obtained as the limit of the discretized estimators for the finite-dimensional problem.

As an energy function, component f^i in the context of thermodynamics must reflect some physical properties and so, it is expected to be regular in a certain sense. Choice of reference measure P_U leads to different levels of regularity for the reconstructed functions f^i. The MEM method described will be applied to a toy example built in agreement with thermodynamics requirements.

References

[1] Jorge Navaza. On the maximum-entropy estimate of the electron density function. *Acta Crystallographica Section A*, 1985.

[2] Didier Dacunha-Castelle and Fabrice Gamboa. Maximum d'entropie et problème des moments. *Annales de l'I.H.P. Probabilités et statistiques*, 1990.

[3] Fabrice Gamboa and Elisabeth Gassiat. Maximum d'entropie et problème des moments: cas multidimensionnel. *Probability and Mathematical Statistics*, 1991.

[4] Imre Csiszár, Fabrice Gamboa, and Elisabeth Gassiat. MEM pixel correlated solutions for generalized moment and interpolation problems. *IEEE Transactions on Information Theory*, 1998.

Short biography – Eva Lawrence graduated from Université Paul Sabatier in 2017 with a Master Degree in Applied Mathematics. She started her PhD at Institut de Mathématiques de Toulouse funded by CEA Saclay in October 2017. PhD project deals with estimating a class of energy functionals in Thermodynamics, namely Gibbs free enthalpy, and studying in this frame uncertainty propagation.