On nonlinear reduced-order modelling: Marginal-constrained modified Wasserstein barycenters

Geneviève Dusson

CNRS & Université Marie et Louis Pasteur

joint work with Maxime Dalery (Univ. Marie et Louis Pasteur),
Virginie Ehrlacher (Ecole des Ponts)

Paris, 30 June 2025

Happy birthday Albert !

Outline

Motivation : model-order reduction for electronic structure calculations

A few results on optimal transport

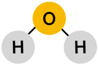
Approach : from density to pair density

Marginal-constrained Wasserstein barycenters between Gaussian mixtures

Numerical results

Context : Modeling a molecular system

Water molecule :



- $K = 3$ nuclei $\rightarrow$ quantum particles

  (2 hydrogen and 1 oxygen)
- $M = 10$ electrons $\rightarrow$ quantum particles

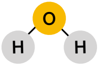
Ground state : state of lowest energy of a system : **energy minimization**

Time-independent Schrödinger equation : (1926)
Parameters : Nuclei configuration $\{\mathbf{R}_k\}_{k=1..K}$.
Unknowns : $\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M)$ wavefunction, E energy.

$$\left(-\frac{1}{2}\sum_{i=1}^{M}\Delta_{\mathbf{r}_i} + V^{ne}_{\mathbf{R}_k}\right)\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, r_M),$$

Context : Modeling a molecular system

Water molecule :



- $K = 3$ nuclei $\rightarrow$ quantum particles

  (2 hydrogen and 1 oxygen)
- $M = 10$ electrons $\rightarrow$ quantum particles

Ground state : state of lowest energy of a system : **energy minimization**

Time-independent Schrödinger equation : (1926)

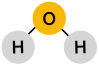
Parameters : Nuclei configuration $\{\mathbf{R}_k\}_{k=1..K}$.

Unknowns : $\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M)$ wavefunction, E energy.

$$\left(-\frac{1}{2}\sum_{i=1}^{M} \Delta_{\mathbf{r}_i} + V^{ne}_{\mathbf{R}_k}\right) \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, r_M),$$

Context : Modeling a molecular system

Water molecule :



- $K = 3$ nuclei (2 hydrogen and 1 oxygen) $\rightarrow$ ~~quantum~~ **classical** particles described by **positions** and **velocities**
- $M = 10$ electrons $\rightarrow$ quantum particles described by a **wavefunction**

Ground state : state of lowest energy of a system : **energy minimization**

Time-independent Schrödinger equation : (1926)
Parameters : Nuclei configuration $\{\mathbf{R}_k\}_{k=1..K}$.
Unknowns : $\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M)$ wavefunction, E energy.

$$\left(-\frac{1}{2}\sum_{i=1}^{M} \Delta_{\mathbf{r}_i} + V^{ne}_{\mathbf{R}_k}\right) \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, r_M),$$

Computational cost :
10^{30} unknowns for the water molecule discretized with 10 points per dimension.

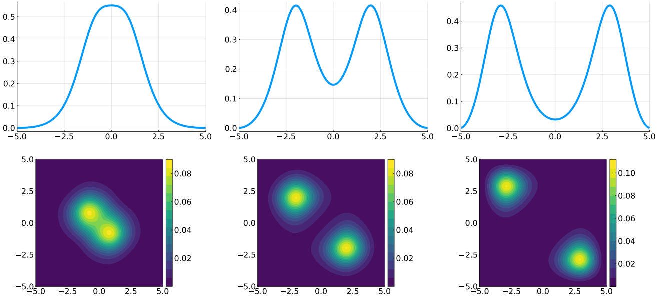
Untractable even for small systems

Density and pair density

R, configuration of the nuclei

$$\text{Density} \quad \rho_{\mathbf{R}}(x) = \int_{\mathbb{R}^{3(N-1)}} |\Psi_{\mathbf{R}}(x, x_2, \dots, x_N)|^2$$

$$\text{Pair density} \quad \tau_{\mathbf{R}}(x, y) = \int_{\mathbb{R}^{3(N-2)}} |\Psi_{\mathbf{R}}(x, y, x_3, \dots, x_N)|^2$$



Aim : Approximate pair density $\tau_{\mathbf{R}}$ from density $\rho_{\mathbf{R}}$

Motivation : Energy efficiently approximated with density, and pair density

$$\text{Fixed number of electrons} \qquad \int_{\mathbb{R}^6} \tau_{\mathbf{R}}(x, y)\, dx\, dy = \int_{\mathbb{R}^3} \rho_{\mathbf{R}}(x)\, dx = 1.$$

Model-order reduction for the pair density

Objective : New reduced-order models

- Database $\tau_{\boldsymbol{R}}$, $\boldsymbol{R} \in \mathcal{R}_{\mathrm{train}}$ with one-body densities $\rho_{\boldsymbol{R}}$
- Construct approximations $\widetilde{\tau}_{\boldsymbol{R}}$ of $\tau_{\boldsymbol{R}}$ using $\rho_{\boldsymbol{R}}$ for $\mathbf{R} \in \mathcal{R}$

Model-order reduction for the pair density

Objective : New reduced-order models

- Database $\tau_{\boldsymbol{R}}$, $\boldsymbol{R} \in \mathcal{R}_{\mathrm{train}}$ with one-body densities $\rho_{\boldsymbol{R}}$
- Construct approximations $\widetilde{\tau}_{\boldsymbol{R}}$ of $\tau_{\boldsymbol{R}}$ using $\rho_{\boldsymbol{R}}$ for $\mathbf{R} \in \mathcal{R}$

Link between one-body and two-body densities

$$\int_{\mathbb{R}^3} \tau_{\boldsymbol{R}}(x,y)\,dy = \rho_{\boldsymbol{R}}(x), \quad \int_{\mathbb{R}^3} \widetilde{\tau}_{\boldsymbol{R}}(x,y)\,dy = \rho_{\boldsymbol{R}}(x)$$

Marginal constraint

Model-order reduction for the pair density

Objective : New reduced-order models

- Database $\tau_{\boldsymbol{R}}$, $\boldsymbol{R} \in \mathcal{R}_{\text{train}}$ with one-body densities $\rho_{\boldsymbol{R}}$
- Construct approximations $\widetilde{\tau}_{\boldsymbol{R}}$ of $\tau_{\boldsymbol{R}}$ using $\rho_{\boldsymbol{R}}$ for $\mathbf{R} \in \mathcal{R}$

Link between one-body and two-body densities

$$\int_{\mathbb{R}^3} \tau_{\boldsymbol{R}}(x, y)\, dy = \rho_{\boldsymbol{R}}(x), \quad \int_{\mathbb{R}^3} \widetilde{\tau}_{\boldsymbol{R}}(x, y)\, dy = \rho_{\boldsymbol{R}}(x)$$

Marginal constraint

Translation invariance

If $\boldsymbol{c} \in \mathbb{R}^3$ is a translation vector, it must hold that

$$\rho_{\boldsymbol{R}+\boldsymbol{c}} = \rho_{\boldsymbol{R}}(\cdot + \boldsymbol{c}), \quad \tau_{\boldsymbol{R}+\boldsymbol{c}} = \tau_{\boldsymbol{R}}(\cdot + \boldsymbol{c}, \cdot + \boldsymbol{c}), \quad \widetilde{\tau}_{\boldsymbol{R}+\boldsymbol{c}} = \widetilde{\tau}_{\boldsymbol{R}}(\cdot + \boldsymbol{c}, \cdot + \boldsymbol{c})$$

Optimal transport

Optimal transport for model order reduction :

[Iollo, Lombardi, 2014] [Ehrlacher, Lombardi, Mula, Vialard, 2020] [Iollo, Taddei, 2022] [Do, Feydy, Mula,2023] [Rim, Peherstorfer, Mandli, 2023]

Outline

Motivation : model-order reduction for electronic structure calculations

A few results on optimal transport

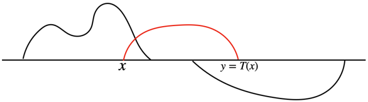
Approach : from density to pair density

Marginal-constrained Wasserstein barycenters between Gaussian mixtures

Numerical results

Wasserstein distance

Originally introduced by Monge : moving a pile of sand efficiently to cover a sinkhole



Wasserstein distance : for $u, v \in \mathcal{P}_2(\Omega)^2$ as

$$W_2(u, v)^2 := \inf_{\pi \in \Pi(u,v)} \int_{\Omega^2} (x - y)^2 \, d\pi(x, y),$$

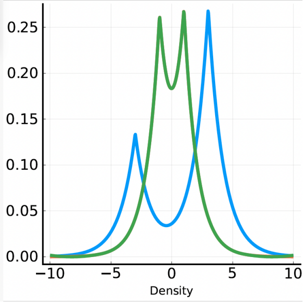
$\Pi(u, v)$: set of probability measures over Ω^2 with marginals u and v.

Wasserstein barycenters

- n probability measures $\rho_1, \ldots, \rho_n$
- n positive weights $\lambda_1, \ldots, \lambda_n$ summing to 1

Barycenter is a solution to the problem

$$\inf_{u \in \mathcal{P}_2(\Omega)} \sum_{i=1}^{n} \lambda_i W_2(u, \rho_i)^2.$$



Agueh, Carlier : Barycenters in the Wasserstein Space. SIAM J. Math. Anal. (2011).

Gangbo, Swiech : Optimal maps for the multidimensional Monge–Kantorovich problem. Commun. Pure Appl. Math. (1998)

Optimal transport between Gaussian measures

Notation : $\mathcal{N}(\mu, S)$

If $\rho_0 = \mathcal{N}(\mu_0, S_0)$ and $\rho_1 = \mathcal{N}(\mu_1, S_1)$, it holds that

$$W_2^2(\rho_0, \rho_1) = \|\mu_0 - \mu_1\|^2 + \mathcal{W}_2(S_0, S_1)^2$$

where $\mathcal{W}_2(S_0, S_1)$ is the **Bures-Wasserstein distance** between S_0 and S_1, defined as

$$\mathcal{W}_2(S_0, S_1)^2 = \mathrm{Tr}\left(S_0 + S_1 - 2\left(\sqrt{S_0}S_1\sqrt{S_0}\right)^{1/2}\right)$$

Wasserstein barycenters between Gaussian measures

Setting :

$M \in \mathbb{N}^\star$
$\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_M) \in \Lambda_M$
$\boldsymbol{\rho} = (\rho_1, \ldots, \rho_M) \in \mathcal{P}_2(\mathbb{R}^n)^M$
for all $i \in \{1, \ldots, M\}$, $\rho_i = \mathcal{N}(\mu_i, S_i)$

Wasserstein barycenter :

$$\mathrm{Bar}^{\boldsymbol{t}}(\boldsymbol{\rho}) = \mathcal{N}(\mu_\star, S_\star)$$

where

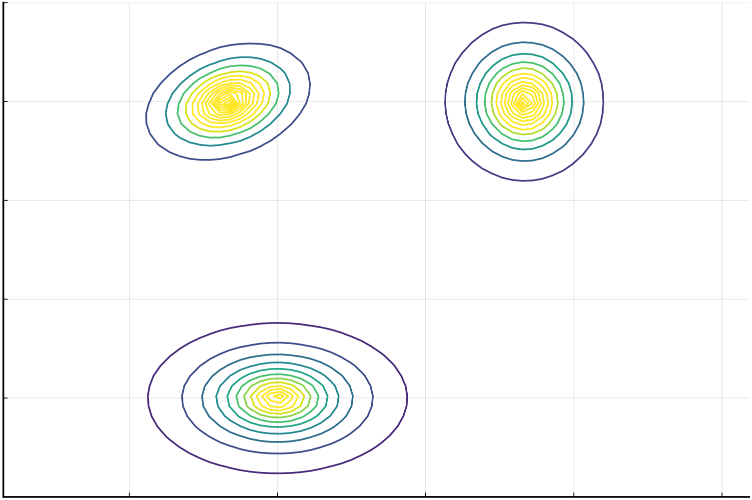
$$\mu_\star = \sum_{m=1}^{M} \lambda_m \mu_m$$

and $S_\star \in \mathcal{S}^n_{+,\star}$ is the unique symmetric positive definite matrix solution to the following equation

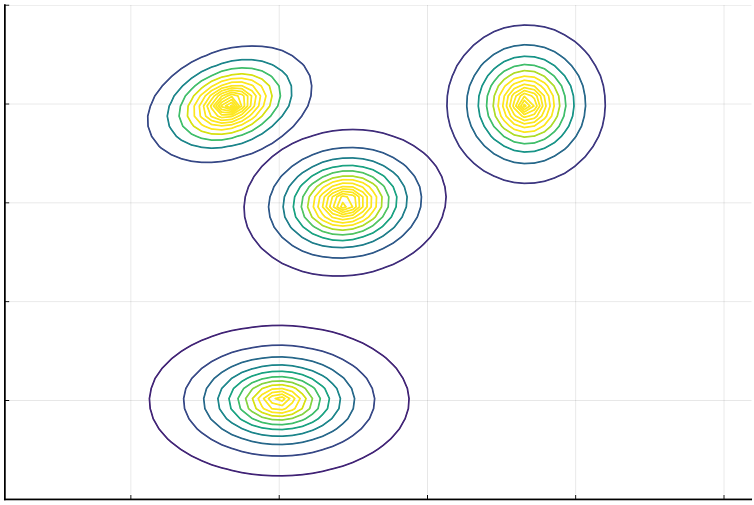
$$\sum_{m=1}^{M} \lambda_m \left(\sqrt{S_\star} S_m \sqrt{S_\star}\right)^{1/2} = S_\star.$$

In the sequel, we will denote $S_\star$ by $\mathrm{Bar}^{\boldsymbol{\lambda}}_{\mathcal{W}_2}(\boldsymbol{S})$ where $\boldsymbol{S} := (S_1, \ldots, S_M)$.

Illustration



Illustration



Outline

Motivation : model-order reduction for electronic structure calculations

A few results on optimal transport

Approach : from density to pair density

Marginal-constrained Wasserstein barycenters between Gaussian mixtures

Numerical results

Approach

- **Offline phase :**
  1. **Database :** Choose values $\mathbf{R} \in \mathcal{R}_{\text{train}}$ and compute
  $$\rho_{\boldsymbol{R}} \quad \text{and} \quad \tau_{\boldsymbol{R}}, \quad \mathbf{R} \in \mathcal{R}_{\text{train}} \qquad \text{(snapshots)}$$
  2. **Greedy algorithm :** Select $\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_M \in \mathcal{R}_{\text{train}}$ with $M \in \mathbb{N}^\star$ (small) so that,
  $$\forall\, \boldsymbol{R} \in \mathcal{R}_{\text{train}}, \quad \tau_{\boldsymbol{R}} \approx \mathrm{Bar}_{W_2}^{\boldsymbol{\lambda}}(\tau_{\boldsymbol{R}_1}, \ldots, \tau_{\boldsymbol{R}_M}) \text{ for some } \boldsymbol{\lambda} \in \Lambda_M. \tag{1}$$
- **Online phase :**

Approach

- **Offline phase :**
  1. **Database :** Choose values $\mathbf{R} \in \mathcal{R}_{\text{train}}$ and compute
  $$\rho_{\boldsymbol{R}} \quad \text{and} \quad \tau_{\boldsymbol{R}}, \quad \mathbf{R} \in \mathcal{R}_{\text{train}} \qquad \text{(snapshots)}$$
  2. **Greedy algorithm :** Select $\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_M \in \mathcal{R}_{\text{train}}$ with $M \in \mathbb{N}^\star$ (small) so that,
  $$\forall\, \boldsymbol{R} \in \mathcal{R}_{\text{train}}, \quad \tau_{\boldsymbol{R}} \approx \text{Bar}_{W_2}^{\boldsymbol{\lambda}}(\tau_{\boldsymbol{R}_1}, \ldots, \tau_{\boldsymbol{R}_M}) \text{ for some } \boldsymbol{\lambda} \in \Lambda_M. \tag{1}$$
- **Online phase :** For a new value $\mathbf{R} \in \mathcal{R}$,
  1. Compute $\rho_{\boldsymbol{R}}$ (out of a one-body density model)
  2. Compute $\boldsymbol{\lambda}_{\boldsymbol{R}} \in \Lambda_M$ so that
  $$\rho_{\boldsymbol{R}} \approx \textbf{Bar}_{W_2}^{\boldsymbol{\lambda}_R}(\rho_{\mathbf{R}_1}, \ldots, \rho_{\mathbf{R}_M}) \text{ for some } \boldsymbol{\lambda}_{\boldsymbol{R}} \in \Lambda_M.$$
  3. Compute $\widetilde{\tau}_{\boldsymbol{R}} \in \Lambda_M$ as
  $$\widetilde{\tau}_{\boldsymbol{R}} = \textbf{Bar}_{W_2}^{\boldsymbol{\lambda}_R}(\tau_{\mathbf{R}_1}, \ldots, \tau_{\mathbf{R}_M}). \tag{2}$$

Approach

- **Offline phase :**
  1. **Database :** Choose values $\mathbf{R} \in \mathcal{R}_{\text{train}}$ and compute
  $$\rho_{\boldsymbol{R}} \quad \text{and} \quad \tau_{\boldsymbol{R}}, \quad \mathbf{R} \in \mathcal{R}_{\text{train}} \qquad \text{(snapshots)}$$
  2. **Greedy algorithm :** Select $\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_M \in \mathcal{R}_{\text{train}}$ with $M \in \mathbb{N}^\star$ (small) so that,
  $$\forall\, \boldsymbol{R} \in \mathcal{R}_{\text{train}}, \quad \tau_{\boldsymbol{R}} \approx \mathrm{Bar}_{W_2}^{\boldsymbol{\lambda}}(\tau_{\boldsymbol{R}_1}, \ldots, \tau_{\boldsymbol{R}_M}) \text{ for some } \boldsymbol{\lambda} \in \Lambda_M. \tag{1}$$
- **Online phase :** For a new value $\mathbf{R} \in \mathcal{R}$,
  1. Compute $\rho_{\boldsymbol{R}}$ (out of a one-body density model)
  2. Compute $\boldsymbol{\lambda}_{\boldsymbol{R}} \in \Lambda_M$ so that
  $$\rho_{\boldsymbol{R}} \approx \mathbf{Bar}_{W_2}^{\boldsymbol{\lambda}_R}(\rho_{\mathbf{R}_1}, \ldots, \rho_{\mathbf{R}_M}) \text{ for some } \boldsymbol{\lambda}_{\boldsymbol{R}} \in \Lambda_M.$$
  3. Compute $\widetilde{\tau}_{\boldsymbol{R}} \in \Lambda_M$ as
  $$\widetilde{\tau}_{\boldsymbol{R}} = \mathbf{Bar}_{W_2}^{\boldsymbol{\lambda}_R}(\tau_{\mathbf{R}_1}, \ldots, \tau_{\mathbf{R}_M}). \tag{2}$$

Issue related to marginals !

Issue related to marginal constraints

We would like that

$$\tau_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\tau_{\mathbf{R}_1}, \ldots, \tau_{\mathbf{R}_M}) \Rightarrow \rho_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\rho_{\mathbf{R}_1}, \ldots, \rho_{\mathbf{R}_M})$$

Not true in general !

Issue related to marginal constraints

We would like that

$$\tau_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\tau_{\mathbf{R}_1}, \ldots, \tau_{\mathbf{R}_M}) \Rightarrow \rho_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\rho_{\mathbf{R}_1}, \ldots, \rho_{\mathbf{R}_M})$$

Not true in general !

Idea : Marginal-constrained modified Wasserstein barycenters

Issue related to marginal constraints

We would like that

$$\tau_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\tau_{\mathbf{R}_1}, \dots, \tau_{\mathbf{R}_M}) \Rightarrow \rho_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\rho_{\mathbf{R}_1}, \dots, \rho_{\mathbf{R}_M})$$

Not true in general !

Idea : Marginal-constrained modified Wasserstein barycenters

So far (and talk of today) : marginal-constrained modified Wasserstein barycenters for

- Gaussian distributions
- Gaussian mixtures

Issue related to marginal constraints

We would like that

$$\tau_{\mathbf{R}} \approx \mathrm{Bar}_{W_2}^{\lambda}(\tau_{\mathbf{R}_1}, \ldots, \tau_{\mathbf{R}_M}) \Rightarrow \rho_{\mathbf{R}} \approx \mathrm{Bar}_{W_2}^{\lambda}(\rho_{\mathbf{R}_1}, \ldots, \rho_{\mathbf{R}_M})$$

Not true in general !

Idea : Marginal-constrained modified Wasserstein barycenters

So far (and talk of today) : marginal-constrained modified Wasserstein barycenters for

- Gaussian distributions
- Gaussian mixtures

Extension to general distributions is work in progress !

Issue related to marginal constraints

We would like that

$$\tau_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\tau_{\mathbf{R}_1}, \ldots, \tau_{\mathbf{R}_M}) \Rightarrow \rho_{\mathbf{R}} \approx \mathrm{Bar}^{\lambda}_{W_2}(\rho_{\mathbf{R}_1}, \ldots, \rho_{\mathbf{R}_M})$$

Not true in general !

Idea : Marginal-constrained modified Wasserstein barycenters

So far (and talk of today) : marginal-constrained modified Wasserstein barycenters for

- Gaussian distributions
- Gaussian mixtures

Extension to general distributions is work in progress !

[Abraham, Abraham, Bergounioux, Carlier, 2017] Marginal constraint enforced using penalization

Outline

Motivation : model-order reduction for electronic structure calculations

A few results on optimal transport

Approach : from density to pair density

Marginal-constrained Wasserstein barycenters between Gaussian mixtures

Numerical results

Marginals of Gaussian measures

Setting : $n = n_x + n_y$ for some $n_x, n_y \in \mathbb{N}^\star$.

Marginals of Gaussian measures

Setting : $n = n_x + n_y$ for some $n_x, n_y \in \mathbb{N}^\star$.

If $\tau = \mathcal{N}(\mu, S)$

$$\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad S = \begin{pmatrix} S_x & S_{xy} \\ S_{xy}^T & S_y \end{pmatrix},$$

Marginals of Gaussian measures

Setting : $n = n_x + n_y$ for some $n_x, n_y \in \mathbb{N}^\star$.

If $\tau = \mathcal{N}(\mu, S)$

$$\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad S = \begin{pmatrix} S_x & S_{xy} \\ S_{xy}^T & S_y \end{pmatrix},$$

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y)$$

Marginals of Gaussian measures

Setting : $n = n_x + n_y$ for some $n_x, n_y \in \mathbb{N}^\star$.

If $\tau = \mathcal{N}(\mu, S)$

$$\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad S = \begin{pmatrix} S_x & S_{xy} \\ S_{xy}^T & S_y \end{pmatrix},$$

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y)$$

Question : Find the closest Gaussian distribution $\tau = \mathcal{N}(\mu, S)$ to $\tau_{\mathrm{ref}} = \mathcal{N}(\mu_{\mathrm{ref}}, T)$ with marginals

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y),$$

that is

$$\inf W_2(\tau_{\mathrm{ref}}, \tau)^2$$

Marginals of Gaussian measures

Setting : $n = n_x + n_y$ for some $n_x, n_y \in \mathbb{N}^\star$.

If $\tau = \mathcal{N}(\mu, S)$

$$\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad S = \begin{pmatrix} S_x & S_{xy} \\ S_{xy}^T & S_y \end{pmatrix},$$

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y)$$

Question : Find the closest Gaussian distribution $\tau = \mathcal{N}(\mu, S)$ to $\tau_{\mathrm{ref}} = \mathcal{N}(\mu_{\mathrm{ref}}, T)$ with marginals

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y),$$

that is

$$\inf W_2(\tau_{\mathrm{ref}}, \tau)^2$$

Partial answer : Necessarily,

$$\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad S = \begin{pmatrix} S_x & Z \\ Z^T & S_y \end{pmatrix}$$

for some $Z \in \mathbb{R}^{n_x \times n_y}$.

Main result

Theorem [Dalery, GD, Ehrlacher, 2025]
Let $n_x, n_y \in \mathbb{N}^*$ and let $T \in \mathcal{S}_{+,\star}^{n_x+n_y}$ with block decomposition

$$T = \begin{pmatrix} T_x & T_{xy} \\ T_{xy}^\intercal & T_y \end{pmatrix} \tag{3}$$

Denote for $Z \in \mathcal{C}_{S_x,S_y} := \left\{ Z \in \mathbb{R}^{n_x \times n_y},\ \|S_x^{-1/2} Z S_y^{-1/2}\|_2 < 1 \right\}$

$$S(Z) := \begin{pmatrix} S_x & Z \\ Z^\intercal & S_y \end{pmatrix}. \tag{4}$$

The function F defined as

$$F : \mathcal{C}_{S_x,S_y} \ni Z \longmapsto \mathcal{W}_2(T, S(Z))^2$$

is strictly convex. Moreover, the minimization problem

$$Z^*_{T,S} \in \operatorname*{argmin}_{Z \in \mathcal{C}_{S_x,S_y}} \mathcal{W}_2^2(T, S(Z))$$

has a unique minimizer which is given by

$$Z^*_{T,S} = ({T_x}^{-1} \# S_x) T_{xy} ({T_y}^{-1} \# S_y)$$

Geometric mean of covariance matrices

Geometric mean of covariance matrices For $S, T \in \mathcal{S}^n_{+,\star}$, the geometric mean of S and T is given by

$$S\#T := S^{1/2}\left(S^{1/2}T^{-1}S^{1/2}\right)^{-1/2}S^{1/2}$$

Lemma [Bhatia, 2009] It holds that

(i) $S\#T$ is the unique matrix $C \in \mathcal{S}^n_{+,\star}$ solution to the equation $CS^{-1}C = T$;

(ii) $S\#T = T\#S$;

(iii) $(S\#T)^{-1} = S^{-1}\#T^{-1}$.

Marginal-constrained modified Wasserstein barycenter

Question : Find the closest Gaussian distribution for Wasserstein distance $\tau = \mathcal{N}(\mu, S)$ to $\tau_{\mathrm{ref}} = \mathcal{N}(\mu_{\mathrm{ref}}, S_{\mathrm{ref}})$ with marginals

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y).$$

Marginal-constrained modified Wasserstein barycenter

Question : Find the closest Gaussian distribution for Wasserstein distance $\tau = \mathcal{N}(\mu, S)$ to $\tau_{\mathrm{ref}} = \mathcal{N}(\mu_{\mathrm{ref}}, S_{\mathrm{ref}})$ with marginals

$$\mathrm{marg}_x(\tau) = \mathcal{N}(\mu_x, S_x) \quad \text{and} \quad \mathrm{marg}_y(\tau) = \mathcal{N}(\mu_y, S_y).$$

Full answer :

$$\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad S = \begin{pmatrix} S_x & Z^*_{S_{\mathrm{ref}},S} \\ (Z^*_{S_{\mathrm{ref}},S})^T & S_y \end{pmatrix}$$

for some $Z \in \mathbb{R}^{n_x \times n_y}$.

Marginal-constrained barycenters (arbitrary number of Gaussians) :
Choose τ_{ref} as a Wasserstein barycenter

Extension to Gaussian mixtures

We consider Gaussian mixtures :

$$\forall 1 \leq m \leq M, \quad \tau_m = \sum_{k_m=1}^{K_m} \alpha_{k_m}^{(m)} \mathcal{N}(\mu_{k_m}^{(m)}, S_{k_m}^{(m)})$$

with $(\alpha_1^{(m)}, \dots, \alpha_{K_m}^{(m)}) \in \Lambda_{K_m}$ for some $K_m \in \mathbb{N}^*$.

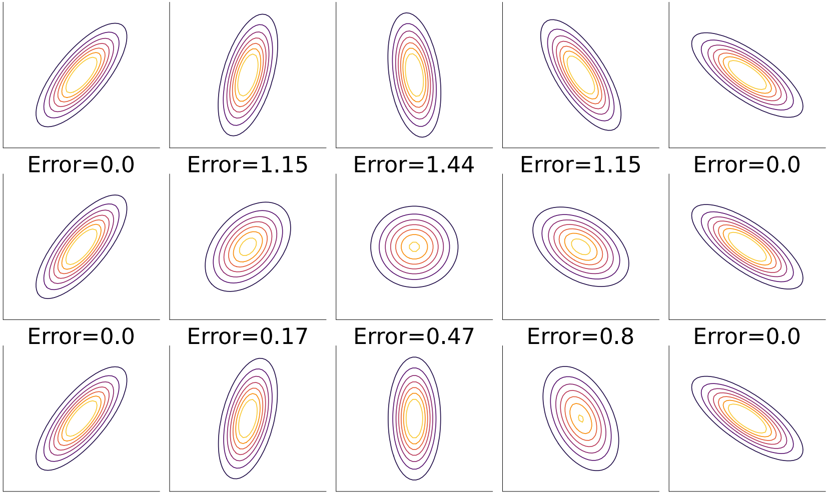
Main steps :

- Write down a similar optimization problem (using mixture distance [Delon, Desolneux, 2020])
- Simplify this problem by specific choice of Gaussians
- Numerical resolution by postprocessing the mixture Wasserstein barycenter.

More details in [Dalery, GD, Ehrlacher, 2025]

Outline

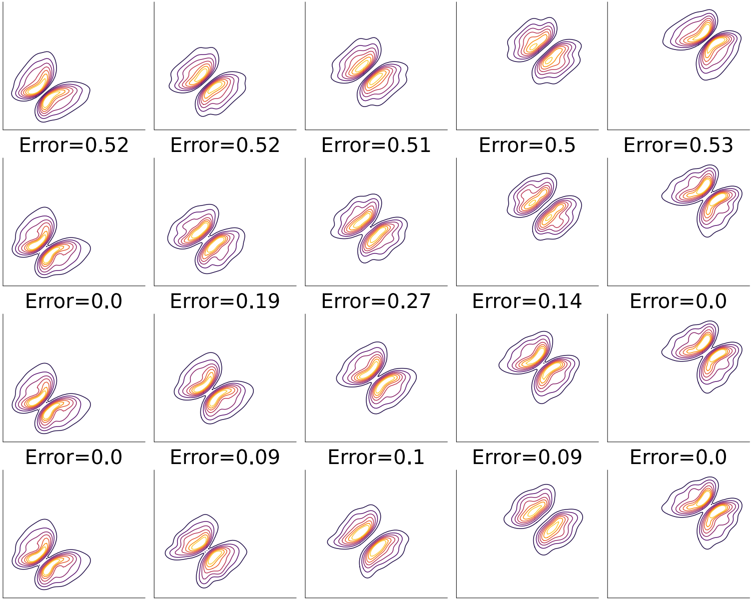
Toy gaussian model



Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = -\nabla_{x,y} \cdot \left(A \begin{pmatrix} x \\ y \end{pmatrix} \rho \right) + D \Delta_{x,y} \psi \quad \text{with } D > 0 \text{ and } A = \Omega \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Preliminary results for electronic structure calculations



Conclusion and perspectives

Conclusion :

- Definition of marginal-constrained (and marginal-preserving) modified Wasserstein barycenters between Gaussian measures and Gaussian mitures which can be easily computed
- Encouraging preliminary towards the design of new reduced-order models results for electronic structure calculations

Perspectives :

- Gaussian fit of electronic one or two-body densities lead to quite large errors !
  - Improve on gaussian fit algorithms
  - Extend the definition/computation of marginal-constrained modified Wasserstein barycenters to arbitrary measures

Conclusion and perspectives

Conclusion :

- Definition of marginal-constrained (and marginal-preserving) modified Wasserstein barycenters between Gaussian measures and Gaussian mitures which can be easily computed
- Encouraging preliminary towards the design of new reduced-order models results for electronic structure calculations

Perspectives :

- Gaussian fit of electronic one or two-body densities lead to quite large errors !
  - Improve on gaussian fit algorithms
  - Extend the definition/computation of marginal-constrained modified Wasserstein barycenters to arbitrary measures

Open postdoc position on nonlinear reduced order modelling (Jan. 2026).

Conclusion and perspectives

Conclusion :

- Definition of marginal-constrained (and marginal-preserving) modified Wasserstein barycenters between Gaussian measures and Gaussian mitures which can be easily computed
- Encouraging preliminary towards the design of new reduced-order models results for electronic structure calculations

Perspectives :

- Gaussian fit of electronic one or two-body densities lead to quite large errors !
  - Improve on gaussian fit algorithms
  - Extend the definition/computation of marginal-constrained modified Wasserstein barycenters to arbitrary measures

Open postdoc position on nonlinear reduced order modelling (Jan. 2026).

Thank you for your attention.

Dalery, Dusson, Ehrlacher, 2025 : hal-04696783v2