Unmixing dynamic PET images: combining spatial heterogeneity and non-Gaussian noise

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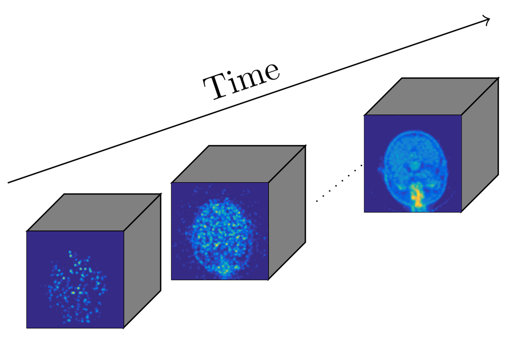
1 - Introduction

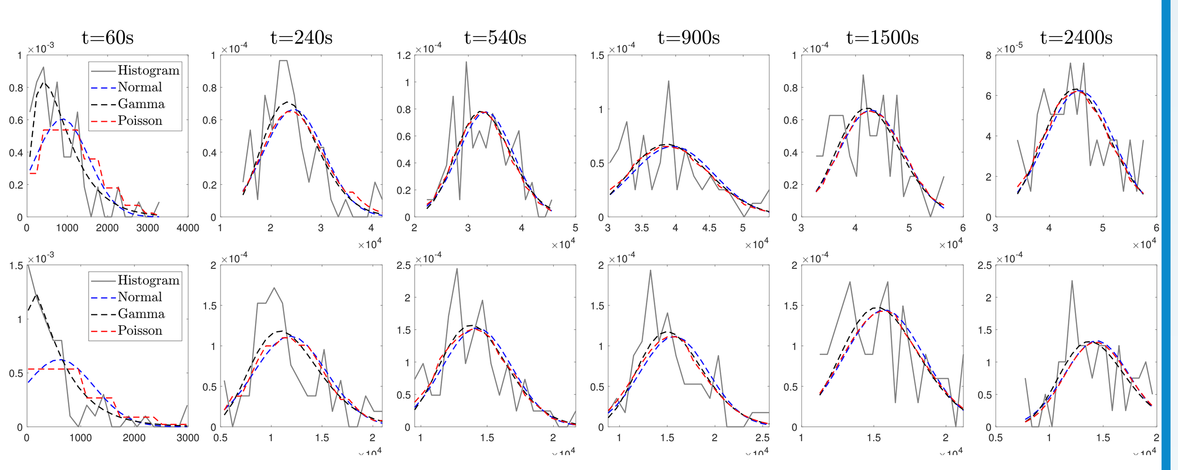
Dynamic positron emission tomography (PET)

- non-invasive nuclear imaging technique;
- time-activity curves (TACs): variation of the radiotracer concentration over time.

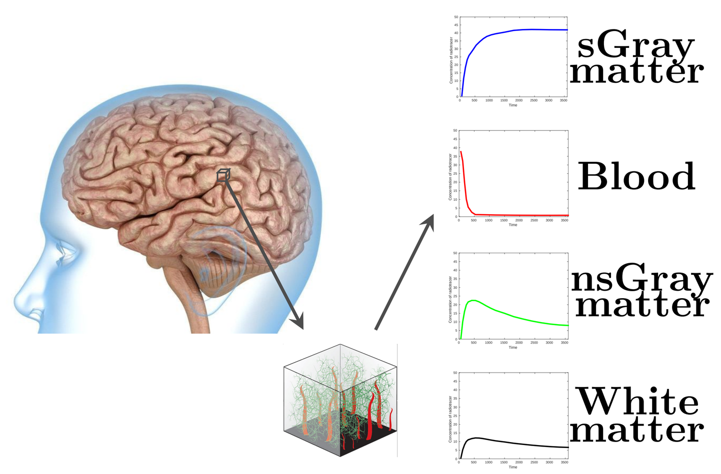


Noise distribution in PET images

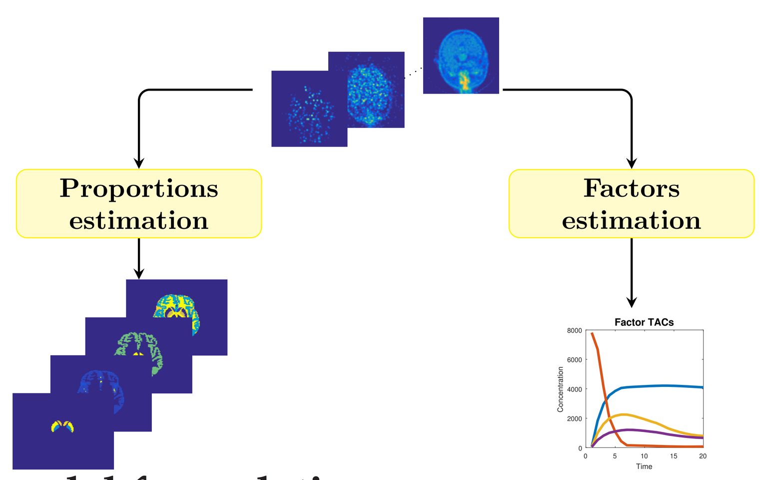
- acquisition conditions, postprocessing corrections and reconstruction settings alter the initial Poisson distribution of the count rates;
- literature has assumed the noise to be Gaussian, Poisson, Gamma or even hybrid (Poisson-Gaussian, Poisson-Gamma).



Voxel decomposition



2 - Factor analysis models



General model formulation

$$\mathbf{Y} \approx \mathbf{X}(\underline{\boldsymbol{\theta}}), \qquad (1)$$

- $\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_N]$: $L \times N$ matrix of the N measured TACs;
- $\mathbf{X}(\underline{\boldsymbol{\theta}})$: approximation model;
- $\underline{\boldsymbol{\theta}} = \{\boldsymbol{\theta}_1, \cdots, \boldsymbol{\theta}_P\}$: P physically interpretable variables.

Optimization problem

$$\hat{\underline{\boldsymbol{\theta}}} \in \arg\min_{\underline{\boldsymbol{\theta}} \in \mathcal{C}} \left\{ \mathcal{D}(\mathbf{Y}|\mathbf{X}(\underline{\boldsymbol{\theta}})) + \boldsymbol{\lambda}^{\mathrm{T}} \mathbf{R}(\underline{\boldsymbol{\theta}}) \right\}, \qquad (2)$$

- $\mathcal{D}(\cdot|\cdot)$: loss function;
- $\mathbf{R}(\underline{\boldsymbol{\theta}}) = [r_1(\underline{\boldsymbol{\theta}}), \dots, r_T(\underline{\boldsymbol{\theta}})]^{\mathrm{T}}$: T penalizations;
- $\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_T]^{\mathrm{T}}$: parameters weighting the penalizations;
- $\mathcal{C}$: set of constraints.

Table 1: Summary of NMF, LMM and SLMM.

	$\underline{\boldsymbol{\theta}}$	$\mathbf{X}(\underline{\boldsymbol{\theta}})$	$\mathcal{C}$	$\mathbf{R}(\underline{\boldsymbol{\theta}})$
NMF	$\{\mathbf{M}, \mathbf{A}\}$	$\mathbf{X} = \mathbf{MA}$	$\mathbf{A} \succeq \mathbf{0}_{K,N}$ $\mathbf{M} \succeq \mathbf{0}_{L,K}$	-
LMM	$\{\mathbf{M}, \mathbf{A}\}$	$\mathbf{X} = \mathbf{MA}$	$\mathbf{A} \succeq \mathbf{0}_{K,N}$ $\mathbf{M} \succeq \mathbf{0}_{L,K}$ $\mathbf{A}^{\mathrm{T}}\mathbf{1}_K = \mathbf{1}_N$	-
SLMM	$\{\mathbf{M}, \mathbf{A}, \mathbf{B}\}$	$\mathbf{X} = \mathbf{MA}$ $+ \left[\mathbf{E}_1\mathbf{A} \cdot \mathbf{VB}\right]$	$\mathbf{A} \succeq \mathbf{0}_{K,N}$ $\mathbf{M} \succeq \mathbf{0}_{L,K}$ $\mathbf{B} \succeq \mathbf{0}_{N_v,N}$ $\mathbf{A}^{\mathrm{T}}\mathbf{1}_K = \mathbf{1}_N$	$\lVert\mathbf{B}\rVert_{2,1}$

- $\mathbf{M}$: $L \times K$ matrix of factors;
- $\mathbf{A}$: $K \times N$ matrix of factor proportions;
- $\mathbf{E}_1$: matrix $[\mathbf{1}_{\mathbf{L},\mathbf{1}}\mathbf{0}_{\mathbf{L},\mathbf{K-1}}]$;
- $\mathbf{V}$: dictionary describing the variability;
- $\mathbf{B}$: matrix of variability coefficients in each voxel.

3 - The β-divergence

Divergence measure

$$\mathcal{D}_\beta(\mathbf{Y}|\mathbf{X}) = \sum_{\ell=1}^{L}\sum_{n=1}^{N} d_\beta(y_{\ell,n}|x_{\ell,n}), \qquad (3)$$

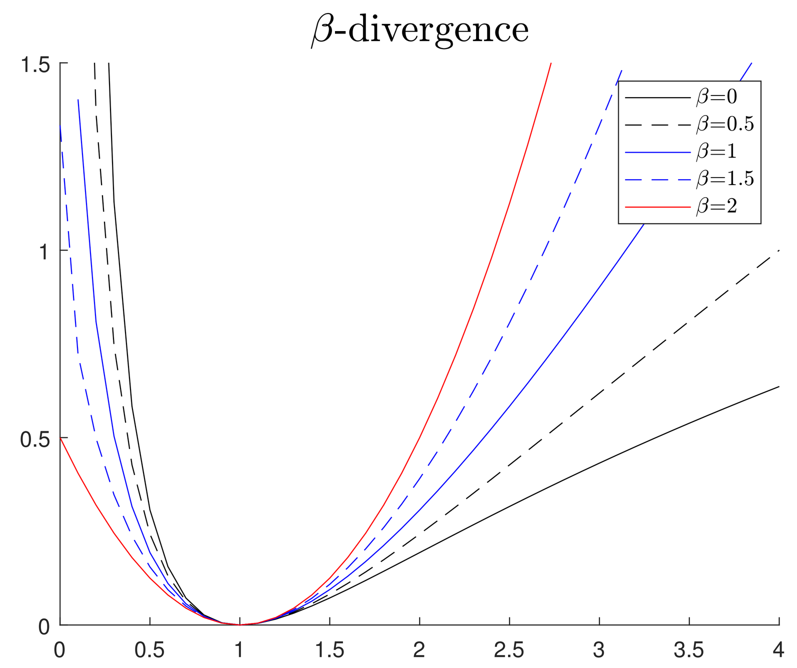
with

$$d_\beta(y|x) = \frac{1}{\beta(\beta-1)}(y^\beta + (\beta-1)x^\beta - \beta y x^{\beta-1}). \qquad (4)$$

Limit cases

$$d_\beta(y|x) = \begin{cases} \frac{1}{2}(y^2 + x^2 - 2yx) & \beta = 2, \\ y \log\frac{y}{x} - y + x & \beta = 1, \\ \frac{y}{x} - \log\frac{y}{x} - 1 & \beta = 0. \end{cases} \qquad (5)$$

- $\beta = 2$: Euclidian distance;
- $\beta = 1$: Kullback-Leibler divergence;
- $\beta = 0$: Itakura-Saito divergence.



Tweedie distributions

$$-\log p(y|x) = \varphi^{-1} d_\beta(y|x) + \text{const.} \qquad (6)$$

- p(y | x): probability density function;
- φ: dispersion parameter.

- in the special cases $\beta = 2, 1, 0$, the β-divergence is related to additive Gaussian, and multiplicative Poisson and Gamma observation noises.

4 - Optimization algorithm

Block-coordinate descent algorithm

- majorization-minimization algorithms;
- multiplicative updates;
- β-NMF algorithm is widely used in the literature and β-LMM is a depreciated version of β-SLMM.

β-SLMM unmixing

Input: $\mathbf{Y}, \mathbf{A}, \mathbf{M}, \mathbf{B}, \lambda$

Initialize:
$\tilde{\mathbf{X}} \leftarrow \mathbf{MA} + \left[\mathbf{E}_1\mathbf{A} \cdot \mathbf{VB}\right]$

while stopping criterion not satisfied **do**

% Update variability matrix

$$\mathbf{B} \leftarrow \mathbf{B} \cdot \left[\frac{\mathbf{1}_{N_v}^{\mathrm{T}}\mathbf{A}_{1,:} \cdot (\mathbf{V}^{\mathrm{T}}(\mathbf{Y} \cdot \tilde{\mathbf{X}}^{\beta-2}))}{\mathbf{1}_{N_v}^{\mathrm{T}}\mathbf{A}_{1,:} \cdot (\mathbf{V}^{\mathrm{T}}\tilde{\mathbf{X}}^{\beta-1}) + \lambda\mathbf{B}^k\boldsymbol{\Gamma}_{\mathbf{B}}}\right]^{\frac{1}{3-\beta}}$$

$\tilde{\mathbf{X}} \leftarrow \mathbf{MA} + \left[\mathbf{E}_1\mathbf{A} \cdot \mathbf{VB}\right]$

% Update factor TACs

$$\mathbf{M}_{2:K} \leftarrow \mathbf{M}_{2:K} \cdot \left[\frac{(\mathbf{Y} \cdot \tilde{\mathbf{X}}^{\beta-2})\mathbf{A}_{2:K}^T}{\tilde{\mathbf{X}}^{\beta-1}\mathbf{A}_{2:K}^T}\right]$$

$\tilde{\mathbf{X}} \leftarrow \mathbf{MA} + \left[\mathbf{E}_1\mathbf{A} \cdot \mathbf{VB}\right]$

% Update SBF factor proportion

$$\mathbf{A}_1 \leftarrow \mathbf{A}_1 \cdot \left[\frac{\mathbf{1}_L^{\mathrm{T}}((\mathbf{M}_1\mathbf{1}_N^{\mathrm{T}} + \mathbf{VB}) \cdot (\mathbf{Y} \cdot \tilde{\mathbf{X}}^{\beta-2}) + \tilde{\mathbf{x}}^\beta)}{\mathbf{1}_L^{\mathrm{T}}((\mathbf{M}_1\mathbf{1}_N^{\mathrm{T}} + \mathbf{VB}) \cdot \tilde{\mathbf{X}}^{\beta-1} + \mathbf{Y} \cdot \tilde{\mathbf{X}}^{\beta-1})}\right]$$

% Update other factor proportions

$$\mathbf{A}_{2:K} \leftarrow \mathbf{A}_{2:K} \cdot \left[\frac{\mathbf{M}_{2:K}^T(\mathbf{Y} \cdot \tilde{\mathbf{X}}^{\beta-2}) + \mathbf{1}_{K-1,L}\tilde{\mathbf{X}}^\beta}{\mathbf{M}_{2:K}^{\mathrm{T}}\tilde{\mathbf{X}}^{\beta-1} + \mathbf{1}_{K-1,L}(\mathbf{Y} \cdot \tilde{\mathbf{X}}^{\beta-1})}\right]$$

$\tilde{\mathbf{X}} \leftarrow \mathbf{MA} + \left[\mathbf{E}_1\mathbf{A} \cdot \mathbf{VB}\right]$

end while

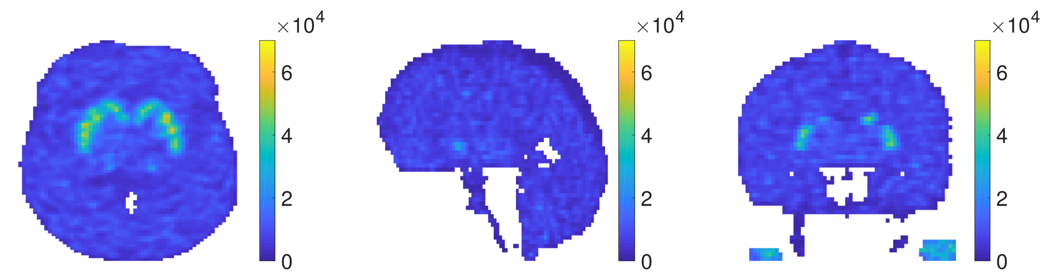
Output: $\mathbf{A}, \mathbf{M}, \mathbf{B}$

- $\mathbf{1}_{K,L}$: $K \times L$-matrix of ones;
- $\boldsymbol{\Gamma}_{\mathbf{B}} \triangleq \mathrm{diag}[\lVert\mathbf{b}_1\rVert_1, \cdots, \lVert\mathbf{b}_1\rVert_N]^{-1}$.

5 - Results

Data generation:

- Dynamic PET phantom with $128 \times 128 \times 64$ voxels and $L = 20$ time-frames;
- Two phantoms:
  - Phantom I TACs derived from a clinical PET image using the ^{11}C-PE2I radioligand;
  - Phantom II derived from Phantom I but applying a variability to the high-uptake tissue.
- Generation process: analytical simulations with realistic count-rate properties: reconstruction based on ordered-subset expectation-maximization algorithm (with 3 and 30 iterations).



Parameters choice: stopping criterion $\varepsilon = 10^{-4}$.

Table 2: Variability penalization parameters.

	λ		
	β=0	β=1	β=2
3it	2.10^{-4}	1.10^{-3}	1.10^{-3}
30it	1.10^{-4}	1.10^{-3}	1.10^{-3}

Results

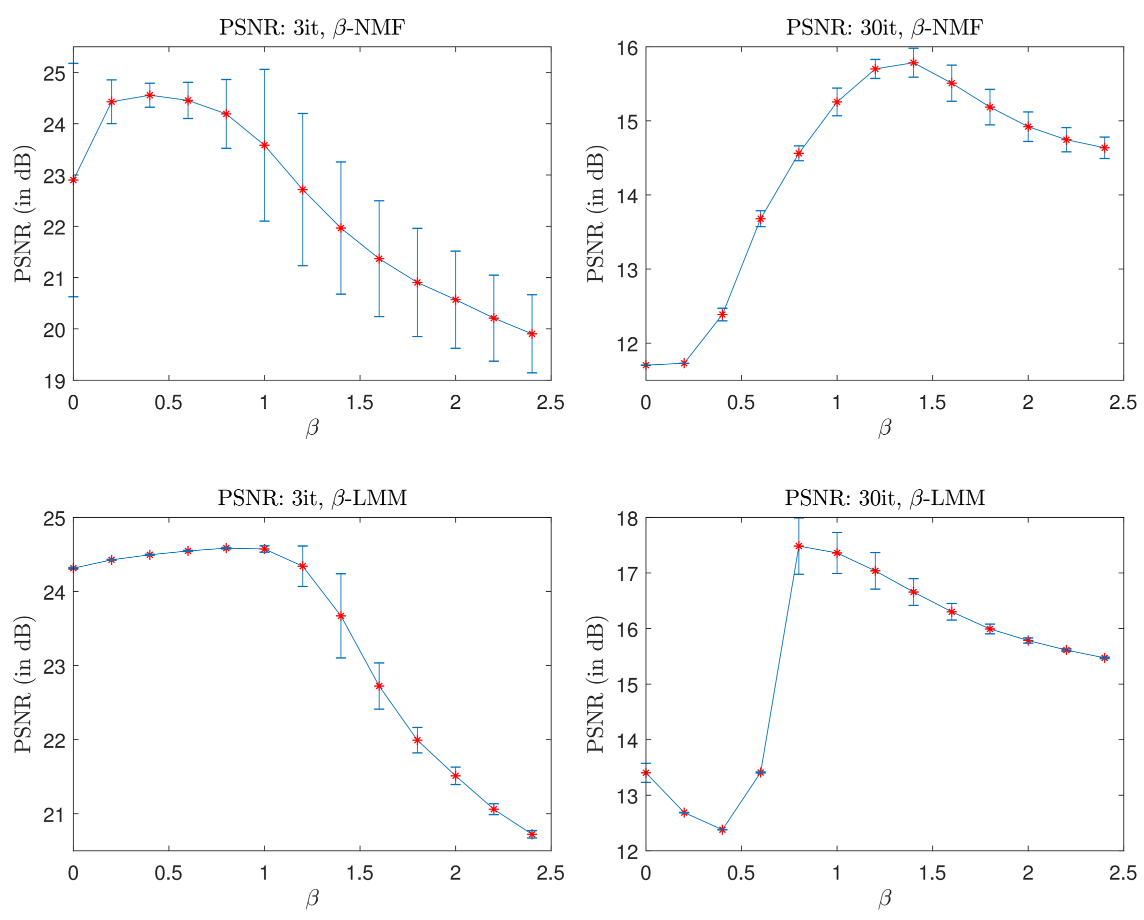


Table 3: Mean NMSE of $\mathbf{A}_1$, $\mathbf{A}_{2:K}$, $\tilde{\mathbf{M}}^1$, $\mathbf{M}^{2:K}$ and $\mathbf{A}_1 \cdot \mathbf{B}$ and PSNR of estimated image estimated by β-LMM and β-SLMM for different values of β.

		β-LMM			β-SLMM		
	β	0	1	2	0	1	2
3it	$\mathbf{A}_1$	0.31	0.29	0.30	0.30	0.30	0.31
	$\mathbf{A}_{2:K}$	0.52	0.51	**0.51**	0.53	0.53	**0.52**
	$\tilde{\mathbf{M}}^1$	**0.10**	0.19	0.27	**0.01**	**0.01**	0.01
	$\mathbf{M}^{2:K}$	0.39	0.37	**0.31**	0.38	0.37	**0.32**
	$\mathbf{A}_1 \cdot \mathbf{B}$	-	-	-	0.49	**0.48**	0.53
	PSNR	22.2	25.3	**28.3**	30.0	**30.2**	27.9
30it	$\mathbf{A}_1$	0.58	0.63	**0.56**	**0.68**	0.78	0.70
	$\mathbf{A}_{2:K}$	0.58	**0.56**	0.59	**0.58**	0.59	0.59
	$\tilde{\mathbf{M}}^1$	0.76	0.51	**0.41**	0.01	**0.01**	0.01
	$\mathbf{M}^{2:K}$	0.27	0.28	**0.24**	0.26	0.25	**0.24**
	$\mathbf{A}_1 \cdot \mathbf{B}$	-	-	-	0.87	**0.72**	0.80
	PSNR	20.4	25.5	**26.1**	25.8	**27.4**	27.0

6 - Conclusion

Main contributions

- Introduction of the β-divergence for the factor analysis of dynamic PET images;
- Derivation of a new algorithm for the SLMM model, using the β-divergence.

Future work

- Validate the approach on real data;
- Propose an optimal value of β for different reconstruction iterations in this setting;
- Apply the β-divergence into different steps of the PET imaging pipeline, such as denoising and reconstruction.