Optimal Transport and PSF Modeling

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French-Chinese Days on Weak Lensing



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Motivation



Inverse problem

Dependency on position

$$\min_{X} \frac{1}{2} \|\boldsymbol{Y} - \boldsymbol{M}\boldsymbol{X}\|_{2}^{2}$$

• $X \in \mathbb{R}^{N \times K}_+$: true PSFs at different positions of the FOV.

•
$$M = [M_1, \cdots, M_K], M_k \in \mathbb{R}^{N' \times N}_+$$
: decimation and shifting.

•
$$oldsymbol{Y} \in \mathbb{R}^{N' imes K}_+$$
 : observed PSFs.

Inverse problem

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$$\boldsymbol{Y} \in \mathbb{R}^{N' imes K}_+$$
 : observed PSFs.



Fig: PSF variation for different wavelengths (400 to 900 nm)



• $\boldsymbol{Y} \in \mathbb{R}^{N' imes K}_+$: observed PSFs.



Fig: PSF variation for different wavelengths (400 to 900 nm)





Optimal Transport

The Monge-Kantorovich problem



Fig: Graphical representation of mass transportation problem: find the optimal way of transporting a heap of sand α into the shape of a heap of sand β , knowing the cost of moving grains of sand to and from any position.

Optimal Transport

Discrete formalism



between two discrete distributions.¹

$$\boldsymbol{lpha} = \sum_{i=1}^{N} \alpha_i \delta_{\boldsymbol{p}_i} \qquad \boldsymbol{\beta} = \sum_{i=1}^{N} \beta_i \delta_{\boldsymbol{p}_i}$$

•
$$\boldsymbol{\alpha}, \boldsymbol{\beta} \in \sum_{N} \qquad \sum_{N} := \left\{ \boldsymbol{d} \in \mathbb{R}^{N}_{+}; \sum_{i} d_{i} = 1 \right\}$$

• $[\boldsymbol{p}_1,\cdots,\boldsymbol{p}_N]\in\mathbb{R}^{d imes N}$



¹ Cuturi & Peyré, Computational Optimal Transport



Optimal Transport

Discrete formalism

• Given that $C_{i,j} = [d(i,j)]^d$ where d(i,j) is a distance:

Wasserstein distance $W_2(\boldsymbol{lpha}, \boldsymbol{eta}) \coloneqq \left(\min_{\boldsymbol{\Gamma} \in \boldsymbol{\Pi}(\boldsymbol{lpha}, \boldsymbol{eta})} < \boldsymbol{C}, \boldsymbol{\Gamma} >
ight)^{1/2}$

Optimal Transport

Displacement interpolation

• Given that $C_{i,j} = [d(i,j)]^d$ where d(i,j) is a distance:

Wasserstein distance
$$W_2(oldsymbol{lpha},oldsymbol{eta}) \coloneqq \left(\min_{oldsymbol{\Gamma}\in oldsymbol{\Pi}(oldsymbol{lpha},oldsymbol{eta})} < oldsymbol{C},oldsymbol{\Gamma} >
ight)^{1/2}$$

Wasserstein barycenter

$$oldsymbol{P}((oldsymbol{d}_1,\cdots,oldsymbol{d}_S),oldsymbol{\lambda}) = rgmin_{oldsymbol{u}}\sum_{i=1}^S \lambda_i W_2^2(oldsymbol{u},oldsymbol{d}_i)$$

•
$$oldsymbol{d}_i \in \sum_N$$
 , $oldsymbol{\lambda} \in \sum_S$



Transport tools $\bullet \bullet \bullet \circ \circ \circ$

Optimal Transport

Displacement interpolation

• Given that
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Wasserstein distance $W_2(\boldsymbol{\alpha}, \boldsymbol{\beta}) \coloneqq \left(\min_{\boldsymbol{\Gamma} \in \boldsymbol{\Pi}(\boldsymbol{\alpha}, \boldsymbol{\beta})} < \boldsymbol{C}, \boldsymbol{\Gamma} > \right)^{1/2}$

ATTRACTIVE TOOL, BUT COSTLY TO COMPUTE: $\mathcal{O}(N^3)$

Wasserstein barycenter

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Transport tools

Optimal Transport

Wasserstein distance approximations

Entropic regularization² $W_2^2(\boldsymbol{\alpha},\boldsymbol{\beta}) = \inf_{\boldsymbol{\Gamma}\in\boldsymbol{\Pi}(\boldsymbol{\alpha},\boldsymbol{\beta})} < \boldsymbol{C}, \boldsymbol{\Gamma} > -\gamma H(\boldsymbol{\Gamma})$ • $W(\boldsymbol{\Gamma}) := -\sum_{i,j} \Gamma_{i,j} \log(\Gamma_{i,j} - 1)$

Advantages:

- **1.** Problem γ -strongly convex.
- **2.** Gain in stability. The greater γ , more smooth the coupling matrix.
- **3.** Solution is a diagonal scaling of $e^{-C/\gamma} \rightarrow$ allows the use of Bregman's optimization tools, wich are easily paralellizable.

Transport tools

Optimal Transport

Wasserstein distance approximations

Entropic regularization: a Kulback-Leibler projection

 $W_2^2(\boldsymbol{\alpha},\boldsymbol{\beta}) = \min_{\boldsymbol{\Gamma}\in\boldsymbol{\Pi}(\boldsymbol{\alpha},\boldsymbol{\beta})} \operatorname{KL}(\boldsymbol{\Gamma}|\boldsymbol{K})$

•
$$K = \exp(-C/\gamma)$$

• $\Pi(\alpha, \beta) = \underbrace{\{\Gamma \in \mathbb{R}^{N \times N}, \quad \Gamma \mathbb{1}_N = \alpha\}}_{C^1} \cap \underbrace{\{\Gamma \in \mathbb{R}^{N \times N}, \quad \Gamma^T \mathbb{1}_N = \beta\}}_{C^2}$

Sinkhorn iterations

$$egin{aligned} m{b}^0 &\coloneqq \mathbbm{1}_N \ m{1.} & m{\Gamma}^l &\coloneqq \Delta(m{b}^l) m{K}^{\mathrm{T}} \Delta(m{a}^l) \ m{2.} & m{a}^l &\coloneqq rac{m{eta}}{m{K} m{b}^{l-1}} \ m{3.} & m{b}^l &\coloneqq rac{m{lpha}}{m{K}^{\mathrm{T}} m{a}^l} \end{aligned}$$



Transport tools

Optimal Transport

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Sinkhorn iterations

$$b^{0} := \mathbb{1}_{N}$$
1. $\Gamma^{l} := \Delta(b^{l})K^{T}\Delta(a^{l})$
2. $a^{l} := \frac{\beta}{Kb^{l-1}}$
3. $b^{l} := \frac{\alpha}{K^{T}a^{l}}$



Notes:

- If cost the squared Euclidean distance, K dot product can be replaced by convolution with Gaussian kernel with std equals to γ.
- Small values of γ can lead to instabilities.
 Alternatively , we can perform sinkhorn iterations in log domain.

Transport tools

Optimal Transport

Wasserstein barycenter approximation

Extending to the barycenter computation..

$$oldsymbol{P}(oldsymbol{D},oldsymbol{\lambda}) = rgmin_{oldsymbol{u}} \sum_{s=1}^{S} \lambda_s W_{\gamma}(oldsymbol{u},oldsymbol{d}_s)^4$$





Schmitz at al.,2018

⁴Agueh & Carlier, 2011; Benamou et al., 2015; Chizat et al., 2016

λ -RCA

Transporting mass over wavelengths

Back to the PSF estimation problem:

$$\boldsymbol{Y} = \boldsymbol{M} \sum_{v} \beta_{v} \boldsymbol{X}_{v} + b$$





λ -RCA

Transporting mass over wavelengths

Back to the PSF estimation problem:

$$oldsymbol{Y} = oldsymbol{M} \sum_v eta_v oldsymbol{X}_v + b$$
 How to break the degeneracy?



λ -RCA

Transporting mass over wavelengths

Back to the PSF estimation problem:



Hypothesis: monochromatic PSFs of a intermediary wavelength are Wasserstein barycenters of the extremes.





 λ -RCA

λ -RCA

Transporting mass over wavelengths

Hypothesis: monochromatic PSFs of a intermediary wavelength are Wasserstein barycenters of the extremes.

Experiment results:

Barycenters

Simulated





λ -RCA

Transporting mass over wavelengths

Is linear projection of λ 's into [0,1] really the best option?





 $\begin{array}{c} \lambda \text{-RCA} \\ \bullet \bullet \bullet \bullet \bullet \bullet \circ \circ \circ \circ \circ \circ \end{array}$

λ -RCA

Inverse problem: RCA background (cf. Morgan's talk)

$$\min_{X} \frac{1}{2} \| m{Y} - m{M} m{X} \|_{2}^{2}$$



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λ -RCA

Inverse problem: RCA background (cf. Morgan's talk)

$$\min_{X} \frac{1}{2} \| \boldsymbol{Y} - \boldsymbol{M} \boldsymbol{X} \|_{2}^{2} \quad \text{s.t.} \quad x_{i,j} > 0$$

• Positivity constraint: $X_{i,j} \ge 0$

 $\begin{array}{c} \lambda \text{-RCA} \\ \bullet \bullet \bullet \bullet \bullet \bullet \circ \circ \circ \circ \circ \circ \end{array}$

λ -RCA

Inverse problem: RCA background (cf. Morgan's talk)

$$\min_{\boldsymbol{A},\boldsymbol{S}} \frac{1}{2} \sum_{k}^{K} \|\boldsymbol{Y}_{k} - \boldsymbol{M} \sum_{i}^{r} a_{i,k} \boldsymbol{s}_{i}\|_{2}^{2} \quad \text{s.t.} \quad x_{i,j} > 0$$

- Positivity constraint: $X_{i,j} \ge 0$
- Low-rank constraint: X = SA eigen-PSFs $S = [s_1, \cdots, s_r], s_i \in \mathbb{R}^{N \times r}, r << K$ coefficients $A \in \mathbb{R}^{r \times K}$

 λ -RCA $\bullet \bullet \bullet \bullet \circ \circ \circ \circ \circ \circ$

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Smoothness constraint: imposed on the atoms s_i .

 λ -RCA $\bullet \bullet \bullet \bullet \circ \circ \circ \circ \circ \circ$

λ -RCA

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- Smoothness constraint: imposed on the atoms s_i.
 Graph constraint: imposed on the rows of A . A = αV^T
 Graph matrix.

 $\begin{array}{c} \lambda \text{-RCA} \\ \bullet \bullet \bullet \bullet \bullet \bullet \circ \circ \circ \circ \circ \circ \end{array}$

λ -RCA

Inverse problem: RCA background (cf. Morgan's talk)

$$\min_{A,S} \frac{1}{2} \sum_{k}^{K} \|Y_{k} - M \sum_{i}^{r} a_{i,k} s_{i}\|_{2}^{2} + \|\Phi S\|_{1} \quad \text{s.t.} \quad x_{i,j} > 0$$

Graph matrix.

- Positivity constraint: $X_{i,j} \ge 0$
- Low-rank constraint: X = SA eigen-PSFs $S = [s_1, \cdots, s_r], s_i \in \mathbb{R}^{N \times r}, r << K$ coefficients $A \in \mathbb{R}^{r \times K}$
- Smoothness constraint: imposed on the atoms s_i . Coefficients learned from data.
- Graph constraint: imposed on the rows of A . $A=lpha V^{ ext{T}}$
- **Sparsity constraint:** PSF is sparse in starlet domain.

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λ -RCA

Inverse problem: introduction of barycenters

$$\begin{split} \min_{\boldsymbol{A},\boldsymbol{D}} \frac{1}{2} \sum_{k}^{K} \|\boldsymbol{Y}_{k} - \boldsymbol{M} \sum_{i}^{r} a_{i,k} \underbrace{\sum_{v} \beta_{v} \boldsymbol{P}_{i}(\boldsymbol{D}, \boldsymbol{w}_{v})}_{S_{i}} \|_{2}^{2} & + \|\boldsymbol{\Phi}\boldsymbol{D}\|_{1} \quad \text{s.t.} \quad \boldsymbol{D} \in \sum_{N} \\ & \bullet \quad \boldsymbol{D} = \left(\boldsymbol{d}_{0}^{i}, \boldsymbol{d}_{1}^{i}\right)_{1 \leq i \leq S}, \quad \boldsymbol{d}_{0}^{i} \in \mathbb{R}^{N}_{+} \\ \text{Eigen-PSF extreme left} & \bullet \quad \text{Eigen-PSF extreme right} \end{split}$$

•
$$\boldsymbol{w} = (1 - t_v, t_v)_{1 \le v \le \text{nb-wvls}}$$

λ -RCA

Alternated optimization

Algorithm 1 λ -RCA

- 1: Parameters estimation and initialization :
- 2: First guess super resolution $\rightarrow D$
- 3: Spatial constraints parameters $\rightarrow \alpha, V$
- 4: Noise estimation \rightarrow sigmas, threshold weights \boldsymbol{W} , shifts
- 5: Power method \rightarrow gradient descent step

7: for
$$l = 0, ..., L$$
 do

8: (I) dictionary update:

9:
$$\boldsymbol{D}_{\text{new}} := \text{Condat-Vu} \left(\underset{\boldsymbol{D}}{\operatorname{argmin}} \sum_{k} \frac{1}{2} \| \boldsymbol{y}_{k} - \sum_{i} a_{i,k} \sum_{v} \beta_{v} \boldsymbol{P}_{i}(\boldsymbol{D}, \boldsymbol{w}_{v}) \|_{2}^{2} + \| \boldsymbol{W} \boldsymbol{\Phi} \boldsymbol{D} \|_{1} + \delta_{\boldsymbol{D} \in \sum_{N}} \right)$$

10: (II) coefficients update:

11:
$$\boldsymbol{\alpha}_{\text{new}} \coloneqq \text{Forward-Backward} \left(\underset{\boldsymbol{\alpha}}{\operatorname{argmin}} \sum_{k} \frac{1}{2} \| \boldsymbol{y}_{k} - \sum_{i} a_{i,k} \sum_{v} \beta_{v} \boldsymbol{P}_{i}(\boldsymbol{D}, \boldsymbol{w}_{v}) \|_{2}^{2} + \| \boldsymbol{\alpha} \|_{0} \right)$$

12: $A_{\text{new}} = \alpha_{\text{new}} V^{\text{T}}$ 13: (III) update parameters and threshold weights.

14: return $\boldsymbol{A}, \boldsymbol{D}$



λ -RCA $\bullet \bullet \bullet \bullet \bullet \circ \circ \circ$

λ -RCA





Data description:

- 100 stars in Euclid resolution 22x22p.
- Spatial positions in FOV.
- SEDs in 11 wavelengths. [550-900nm]





 λ -RCA $\bullet \bullet \bullet \bullet \bullet \bullet \bullet \circ$

λ -RCA

Preliminary results

Dictionary first guess: ground-truth PSFs





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λ -RCA

Preliminary results

Dictionary first guess: ground-truth PSFs





λ -RCA

Perspectives

- Test different dictionary first guess using observed information.
- Optimize λ -RCA algorithm to its full potential.
- Reconstruct PSFs of Euclid-like simulated galaxies on galsim and perform shape measurement.
- Evaluate sensibility with respect to SED uncertainty.
- Evaluate impact of band leakage in the barycenter estimation.