Multi-CCD Point Spread Function Modelling

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ABSTRACT

Context. Galaxy imaging surveys observe a vast number of objects that are affected by the instrument’s Point Spread Function (PSF). Weak lensing missions, in particular, aim at measuring the shape of galaxies, and PSF effects represent an important source of systematic errors which must be handled appropriately. This demands a high accuracy in the modelling as well as the estimation of the PSF at galaxy positions.

Aims. Sometimes referred to as non-parametric PSF estimation, the goal of this paper is to estimate a PSF at galaxy positions, starting from a set of noisy star image observations distributed over the focal plane. To accomplish this, we need our model to first of all, precisely capture the PSF field variations over the Field of View (FoV), and then to recover the PSF at the selected positions.

Methods. This paper proposes a new method, coined MCCD (Multi-CCD PSF modelling), that creates, simultaneously, a PSF field model over all of the instrument’s focal plane. This allows to capture global as well as local PSF features through the use of two complementary models which enforce different spatial constraints. Most existing non-parametric models build one model per Charge-Coupled Device (CCD), which can lead to difficulties in capturing global ellipticity patterns.

Results. We first test our method on a realistic simulated dataset comparing it with two state-of-the-art PSF modelling methods (PSFEx and RCA). We outperform both of them with our proposed method. Then we contrast our approach with PSFEx on real data from CFIS (Canada-France Imaging Survey) that uses the CFHT (Canada-France-Hawaii Telescope). We show that our PSF model is less noisy and achieves a ∼ 22% gain on pixel Root Mean Squared Error (RMSE) with respect to PSFEx.

Conclusions. We present, and share the code of, a new PSF modelling algorithm that models the PSF field on all the focal plane that is mature enough to handle real data.

Key words. Astronomical instrumentation, methods and techniques – Methods: data analysis – Techniques: image processing – Cosmology: observations – Gravitational lensing: weak

1. Introduction

Current galaxy imaging surveys, such as DES (Jarvis et al. 2016), KIDS (Kuijken et al. 2015), CFIS (Ibata et al. 2017) or future surveys such as the Vera C. Rubin Observatory’s LSST (Tyson et al. 2006), the Euclid mission (Laureijs et al. 2011), or the Roman Space Telescope require to estimate the Point Spread Function (PSF) of the instrument. For some scientific applications such as weak gravitational lensing (Kilbinger 2015), low-surface brightness studies (Infante-Sainz 2020), or analysis of diffraction-limited images in crowded stellar fields (Beltramo-Martin et al. 2020), the PSF must be reconstructed with high accuracy. A first approach is to derive a PSF model using known information about the instrument, where the model parameters are then chosen by fitting observed stars in the field to yield a PSF model. This has been widely used for the HST (Hubble Space Telescope) (TinyTim software, Krist 1995), though it was later shown that a relatively simple PSF estimation from the data, which does not assume a model for the instrument, provides better fits to stars for both photometry and astrometry measurements (Hoffmann & Anderson 2017). Furthermore, such a solution can not readily be applied to ground-based observations, where the atmosphere plays an important role and adds stochasticity to the PSF. Other methods, based on imaging-data only, use unresolved stars in the field as direct measurements of the PSF, and reconstruct an accurate PSF from these observed stars. A very impressive range of methodologies have been proposed in the past to perform this task: Moffat modelling (Bendinelli et al. 1988), polynomial models (Piotrowski et al. 2013; Bertin 2011), principal component analysis (Jee et al. 2007; Schrabback et al. 2010; Gentile et al. 2013), sparsity (Ngolè et al. 2015), neural networks (Herbel et al. 2018; Jia et al. 2020b,a), and optimal transport (Ngolè & Starck 2017; Schmitz et al. 2018). The PSFEx software (Bertin 2011) is the most widely used. The Resolved Components Analysis (RCA) method (Ngolè et al. 2016; Schmitz et al. 2020) was proposed in the framework of the Euclid space mission in order to deal with PSFs that are both undersampled and spatially varying in the field. Cameras are often mosaics of several CCDs, but all mentioned methods can only build one PSF model per CCD, with the exception of the approach used by Miller et al. (2013), and the recently proposed approach by Jarvis et al. (2020). Since the models they build within each detector are independent from each other, it is difficult to capture global patterns of variation in the PSF. For example, upon observing PSFEx’s shape residuals maps from the DES Year 1 results (Fig. 8 in Zuntz et al. 2018), we can see global patterns.
2. The observation model

Let us define $\mathcal{H}(u)$ as the PSF field involved in our problem. It is a continuous function of a 2-dimensional position $u = (x, y)$, which in principle could be image coordinates, based on the camera’s CCD pixels, or could also be celestial coordinates such as right ascension and declination. Throughout this paper, we will consider that this PSF field accounts for the contribution of all effects from optical aberrations and diffraction to atmospheric distortions.

Our observation model will consist of images $I_k$, the pixels in one CCD chip $k$, that will contain $n_{\text{star}}^k$ noisy stars at positions $u_i^k$. We define a “stamp” as a square small image cutout centred on a single star. Each star observation stamp $i$ on CCD $k$ can be written as:

$$y_{k,i} = \mathcal{F} \left( \mathcal{H}(u_i^k) \right) + n_{k,i},$$

where $n_{k,i}$ accounts for a noise image that we will consider to be white and Gaussian, and $\mathcal{F}$ is the degradation operator. Three main effects are taken into account in this operator: i) the discrete sampling into a finite number of pixels, namely an image stamp of $n_y \times n_x$ pixels; ii) a sub-pixel shift that depends on where the centroid of the image is placed with respect to the pixel grid; and iii) a downsampling that affects the pixels in the stamp by a factor of $D$ leaving a $D n_y \times D n_x$ stamp. For example, to handle the Euclid mission sampling rate (Cropper et al. 2013), a factor $D = 1/2$ is required to achieve Nyquist sampling rate. From now on, and throughout this article, we will use a unitary value for $D$.

We write each of these stamps into a 1-dimensional column vector and therefore $Y_k = [y_{k,1}, \ldots, y_{k,n_{\text{star}}^k}]$ is the matrix containing all the observed stamps in CCD $k$. It contains $n_{\text{star}}^k$ columns and $D n_y \times D n_x$ rows. Finally, we concatenate all CCD matrices and obtain $Y = \left( Y_1 \cdots Y_K \right)$.

2.2. PSFEx

For a given exposure, this method builds one independent model for each CCD. It was designed as a companion software for SExtractor (Bertin, E. & Arnouts, S. 1996), which builds catalogues of objects from astronomical images. Each object contains several measurements that PSFEx then uses to describe the variability of the PSF. Each selected attribute follows a polynomial law up to some user-defined maximum polynomial degree $d$. The model for CCD $k$ can be written as:

$$\hat{H}_k^{\text{PSFEx}} = S_k A_k,$$

where $A_k$ has $m$ rows corresponding to the number of polynomials used, and $n_{\text{star}}^k$ columns corresponding to the number of observed stars used to train the PSF model. The matrix $S_k$ is learned during training and has $n_y^2$ rows (the number of pixels in each image), and $m$ columns.

For example, if $d$ is set to 2 and the attributes chosen are the pixel coordinates $(x_i, y_i)$, each column $i$ of the $A_k$ matrix corresponding to the star $i$ at location $u_i^k = (x_i, y_i)$ is $a_i^k = [1, x_i, y_i, (x_i)^2, (y_i)^2, x_i y_i]^T$. The number of monomials $m$ corresponding to a maximum degree $d$ can be computed as $(d + 1)(d + 2)/2$. 

2. PSFEx and RCA

PSFEx (Bertin 2011) is a standard and widely-used software\(^1\). RCA (Nicolé et al. 2016) is a more recent method that was developed with the Euclid Visible Imager’s PSF in mind, to deal with the under-sampling of the observed star images. The software is also freely available\(^2\). It is important to remark that these two approaches rely solely on the observed data: they are blind with respect to the optical system involved in the image acquisition process.

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\(^1\) https://github.com/astromatic/psfex
\(^2\) https://github.com/CosmoStat/rca
The training of the model amounts to solving an optimisation problem of the form:

$$\min_{\Delta \sigma_i} \left\{ \sum_{i=1}^{n_{\text{st}}} \left\| y_{i,j} - \mathcal{F} \left( \left( S_{0,k} + \Delta S_k \right) a_k \right) \right\|_2^2 + \| T \Delta S_k \|_F^2 \right\},$$  \tag{3}

where $\Delta \sigma_i$ represents the estimated per-pixel variances, and $T$ is a scalar weighting. The matrix $S_k$ is decomposed as $S_{0,k} + \Delta S_k$, where the first term corresponds to a first guess of the PSF. The optimisation is carried out on the difference between this first guess and the observations. The second term in Eq. (3) acts as a Tikhonov regularisation which, in this case, favours smoother PSF models.

Finally, the PSF recovery at one galaxy position $u_j$ is straightforward and can be done by using the learned $S_k$ matrix and directly calculating a vector $\hat{a}_{k,j}$ corresponding to the monomials of the chosen attributes. The recovered PSF is then computed as

$$\hat{h}_{k,j}^{\text{PSFEx}} = S_k \hat{a}_{k,j}. \tag{4}$$

### 2.3. Resolved Components Analysis

The RCA method is based on a matrix factorisation scheme. It was first presented in Ngolè et al. (2016) and later evaluated on Euclid image simulations in Schmitz et al. (2020). As with PSFEx, this method also builds independent models for each CCD within an exposure and is able to handle under-sampled images. Any observed star $i$ from CCD $k$ is modelled as a linear combination of PSF features, called eigenPSFs in the following, as

$$\hat{h}_{k,j}^{\text{RCA}} = S_k \hat{a}_{k,i}. \tag{5}$$

where $S_k$ is the matrix composed of the eigenPSFs, $a_{k,i}$, a vector containing the set of linear weights and $\hat{h}_{k,j}^{\text{RCA}}$ the reconstructed PSF.

The modelling is recast into an optimisation problem where the $S_k$ and $A_k$ matrices are estimated simultaneously. The problem is ill-posed due to the under-sampling and the noise, meaning that many PSF fields can reproduce the observed stars. In order to break this degeneracy RCA uses a series of regularisers during the optimisation procedure to enforce certain mild assumptions on the PSF field: i) low-rankness of the solution, enforced by setting the number of eigenPSFs learned, $N$, to be small; ii) positivity of the reconstructed PSFs; iii) sparsity of the PSF representation on an appropriate basis; and iv) spatial constraints that account for imposing a certain structure within the $A_k$ matrix. This last constraint is imposed by a further factorisation of $A_k$ into $a_k V_k^T$. The computation of the $V_k^T$ matrix will be addressed in section 3.4. Finally, the PSF model reads:

$$\hat{H}_k^{\text{RCA}} = S_k \alpha_{k} V_k^T, \tag{6}$$

and the optimisation problem that the RCA method solves is

$$\min_{S_k, \alpha_k} \left\{ \frac{1}{2} \left\| Y_k - \mathcal{F} \left( S_k \alpha_k V_k^T \right) \right\|_2^2 + \sum_{i=1}^{N} \left[ (w_{i,j} \odot \Phi s_{k,i})_i + \ell_2(S_k \alpha_k V_k^T) + \ell_1(\alpha_k) \right] \right\}, \tag{7}$$

where $w_{i,j}$ are weights, $\Phi$ represents a transformation allowing the eigenPSFs to have a sparse representation, $\odot$ denotes the Hadamard product, $\ell_1$ is the indicator function of the positive orthant and $\ell_2$ is the indicator function over a set $\Omega$ defined to enforce the spatial constraints.

The PSF recovery at a position $u_j$ is carried out by a Radial Basis Function (RBF) interpolation of the learned columns of the $A_k$ matrix, issuing a vector $a_{k,j}$. In this way, the spatial constraints encoded in the $A_k$ matrix are preserved when estimating the PSF at galaxy positions. Finally, the reconstructed PSF is

$$\hat{h}_{k,j}^{\text{RCA}} = S_k \hat{a}_{k,j}. \tag{8}$$

### 3. A new family of Multi-CCD methods

The MCCD methods we propose here aim at exploiting all of the information available in a single exposure, which requires handling all CCDs simultaneously. The main advantage of this approach is the fact that we can build a more complex model since the number of stars available for training is much larger, compared to a model based on individual CCDs. We aim at a model able to capture PSF features following a global behaviour despite the fact that the PSF field is discontinuous at CCD boundaries. The main reason behind this discontinuity effect is the misalignments between different CCDs. Methods such as PSFEx or RCA, which process each CCD independently, avoid the discontinuity problem by construction, but have difficulties capturing global patterns of PSF variability that occur on scales larger than a single CCD.

The main idea behind our MCCD approach is to include both a global model which provides a baseline estimation of the PSF, and a local model that provides CCD-specific corrections.

#### 3.1. The MCCD data model

In a typical wide-field setting, the PSF field $\mathcal{H}$ exhibits a certain regularity that we translate into spatial correlations of the PSFs. The model we build for a specific CCD $k$ is the matrix $\hat{H}_k \in \mathbb{R}^{n_{\text{pix}} \times n_{\text{star}}}$ composed by the concatenation of the estimations of the different stars encountered in that CCD. Each postage stamp column of length $n_y^2$ corresponds to the model for a specific flattened star from the $n_{\text{star}}$ stars present in CCD $k$.

The PSF field at star positions is reconstructed as a linear combination of PSF features, called eigenPSFs, learned from the observations. As previously stated we want to have both a global and a local component for the model, so we need different eigenPSFs for each component. Hence, the model is based on a matrix factorisation scheme as follows:

$$\hat{H}_k = S_k A_k , \quad \begin{array}{c} \text{Local: } \hat{H}_k^{\text{loc}} \\ \text{Global: } \hat{H}_k^{\text{glob}} \end{array}, \tag{9}$$

where $S_k \in \mathbb{R}^{n_{\text{pix}} \times n_{\text{star}}}$ contains $r_k$ local eigenPSFs and $\hat{S} \in \mathbb{R}^{n_{\text{pix}} \times \tilde{r}}$ contains $\tilde{r}$ global eigenPSFs. The matrices $A_k \in \mathbb{R}^{n_{\text{pix}} \times n_{\text{star}}}$ and $\hat{A}_k \in \mathbb{R}^{n_{\text{pix}} \times \tilde{r}}$ correspond to the local and global weights of the linear combinations, respectively. We can see that for a given CCD $k$, the final model, $\hat{H}_k$, is made up of the sum of the contributions of the local, $\hat{H}_k^{\text{loc}}$, and global, $\hat{H}_k^{\text{glob}}$, models.

Now, let us build a single model for all the $K$ CCDs in the focal plane. We start by building a single matrix containing all
the PSF models by concatenating the model $\hat{H}_k$ for each CCD as follows:

$$\hat{H} = \begin{pmatrix} \hat{H}_1 & \cdots & \hat{H}_K \end{pmatrix},$$

where $\hat{H} \in \mathbb{R}^{r \times N}$ and $N = \sum_{k=0}^{K} n_{\text{star}}^k$ is the total number of stars in one camera exposure. Then, we can concatenate the different eigenPSF matrices $\hat{A}$ into a single matrix:

$$S = \begin{pmatrix} S_1 & \cdots & S_K \end{pmatrix},$$

where $S \in \mathbb{R}^{r \times r}$ and we concatenated the global eigenPSF matrix, $\hat{S}$, at the end. This leaves a total of $r = \sum_{k=1}^{N} r_k + \hat{r}$ columns for the $S$ matrix. We can follow a similar procedure to define $A$ as a block matrix:

$$A = \begin{pmatrix} A_1 & 0 & \cdots & 0 \\ 0 & A_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_K \end{pmatrix},$$

where $A \in \mathbb{R}^{r \times N}$ and 0 is used for matrices made up of zeros. The last row of the $A$ block matrix is composed by the global model weights $\hat{A}_k$. Having already defined the Multi-CCD matrices, $\hat{H}$, $\hat{S}$ and $A$, we can write the final model as:

$$\hat{H} = SA,$$  

where we include all the CCDs. Expanding it leads to a formula like Eq. (9) for each CCD.

### 3.2. Inverse problem and regularisation

The estimation of our model, summarised in the matrices $S$ and $A$ of Eq. (13), is posed as an inverse problem. Given the observation and MCCD data models presented above, this problem amounts to the minimisation of $\| Y - \mathcal{F}(SA) \|_F^2$, where $\| \cdot \|_F$ denotes the Frobenius matrix norm. This problem is ill-posed due to the noise in the observations and to the degradation operator $\mathcal{F}$, meaning that there are many PSF models that would match the star observations. In order to break this degeneracy we enforce several constraints, based on the basic knowledge we dispose of the PSF field, that regularise our inverse problem. Similarly to the ones exploited in the RCA method (Schmitz et al. 2020), we use the following constraints: i) Low-rankness of the model; ii) Positivity of the model; iii) Sparsity in a given domain; iv) Spatial variations. We give a more detailed description of these in Appendix A. These constraints are used by both parts of our model, the global and the local components.

As mentioned above, the spatial constraint is enforced by further factorisation of the coefficient matrices $A$. However, since we want to enforce different properties for the global and the local contributions, the factorisation used will differ for each case.

### 3.3. Global model

We want the global component to provide a baseline estimation of the PSF and for that we propose that the coefficients follow a polynomial variation of the position. The global coefficient matrix $\hat{A}_k$ is factorised into $\hat{A}_k = \tilde{a}\Pi_k$ where $\tilde{a} \in \mathbb{R}^{r \times N}$ is a weight matrix and $\Pi_k \in \mathbb{R}^{r \times n_{\text{star}}^k}$ contains each considered monomials evaluated at global star positions. The dimension, $\tilde{r}$, is determined by the maximum allowed degree in the polynomials: for all monomials of degree less than a given $d$, we have $\tilde{r} = \binom{d+1}{2}$. For example, for $d = 2$ (i.e. $\tilde{r} = 6$), we have:

$$\Pi_k = \begin{pmatrix} 1 & \cdots & 1 \\ x_{k,1} & \cdots & x_{k,n_{\text{star}}^k} \\ y_{k,1} & \cdots & y_{k,n_{\text{star}}^k} \\ x_{k,1}^2 & \cdots & x_{k,n_{\text{star}}^k}^2 \\ y_{k,1}^2 & \cdots & y_{k,n_{\text{star}}^k}^2 \end{pmatrix},$$

where $(x_{k,i}, y_{k,i})_{i=1}^{n_{\text{star}}^k}$ are the global pixel coordinates of the observed stars distributed in the $k$th CCD. The global component of the model for a specific CCD $k$ are as follows:

$$\hat{H}_k^{\text{Glob}} = \hat{S} \tilde{a} \Pi_k.$$  

It is important to mention that despite our choice, throughout this article, to use position polynomials for building the global space constraint, the model is not necessarily restricted to that choice. The $\Pi_k$ matrix could be constructed using other parameters of the observations in order to facilitate the capture of other dependencies and could also follow other types of functions.

### 3.4. Local model

It is possible to define different types of local models. In this article we discuss three options that depend on how we enforce the local spatial constraint. More specifically, they depend on how we factorise the local $A_k$ matrix in the relation:

$$\hat{H}_k^{\text{Loc}} = S_k A_k.$$  

Nevertheless, the MCCD framework does not restrict us to these three options, and it is possible to define other local models.

It is worth remarking that all the framework and optimisation procedures are maintained throughout the different flavours of the MCCD algorithms. The main difference is the way the spatial constraints are enforced in the local and global models.

### 3.4.1. MCCD-RCA

One motivation for the local model is to provide CCD-specific corrections, and to do so our first choice is RCA’s spatial constraint strategy which leads to the MCCD-RCA algorithm. The motivation for this choice is the capability of the RCA spatial constraint to handle different types of PSF variations. On the one hand it can capture smooth variations over the CCD and on the other hand it can account for localised changes that affect a reduced number of PSFs. If the PSFs were sampled on a regular grid this would mean to capture variations occurring at different spatial frequencies. Unfortunately, the PSF locations do not coincide with a regular grid but on what could be seen as a fully connected undirected weighted graph where the weights can be defined as a function of the distance between the different nodes.
(PSF locations). However, the RCA spatial constraint exploits the graph harmonics in order to capture the different PSF variations. These harmonics are represented by the eigenvectors of the graph’s Laplacian matrix (Chung 1997), which will depend on how we define the graph’s weights. A parametric function of the PSF distances can serve as the graph’s weights as in Schmitz et al. (2020) and the selection of the function’s parameters can be done following Ngolè et al. (2016). For each local model (i.e. each CCD in the mosaic), we define \( r_k \) graphs, each corresponding to one of the \( r_k \) local parameters. For each graph, we can extract the \( m_k \) most useful eigenvectors of its Laplacian matrix and gather all of them as columns of a matrix \( V_k^{\text{RCA}} \in \mathbb{R}^{m_k \times r_k m_k} \). This way, we can write:

\[
A_k^{\text{RCA}} = \alpha_k^{\text{RCA}} V_k^{\text{T, RCA}},
\]

where \( \alpha_k^{\text{RCA}} \in \mathbb{R}^{r_k \times r_k m_k} \) is a weight matrix that is used to enforce the spatial constraints. In other words, the sparsity of \( A_k^{\text{RCA}} \)’s rows in the dictionary \( V_k^{\text{T, RCA}} \). Full details are available in Ngolè et al. (2016) and Schmitz et al. (2020).

### 3.4.2. MCCD-POL

The second local model, referred to as MCCD-POL, follows a polynomial spatial constraint. Similar to PSFEx, we factorise the local weights into two matrices as follows:

\[
A_k^{\text{POL}} = \alpha_k^{\text{POL}} \Pi_k^{\text{POL}},
\]

where \( \Pi_k^{\text{POL}} \) has the same form as the matrix in Eq. (14), with the difference that in this case the positions are represented in local coordinates of its corresponding CCD \( k \). As with \( d \) in the global model, a parameter is chosen to define the maximum order of the polynomial used.

### 3.4.3. MCCD-HYB

The third option consists in using the two local models we presented above, RCA and polynomial, to work together in an hybrid algorithm we will refer to as MCCD-HYB. The idea behind it is that the addition of the polynomial space constraint could help the original graph constraint to capture the different features found. In this case we will factorise the local weights with block matrices as

\[
A_k^{\text{HYB}} = \alpha_k^{\text{HYB}} V_k^{\text{T, HYB}} = \begin{pmatrix} \alpha_k^{\text{RCA}} & 0 \\ 0 & \alpha_k^{\text{POL}} \end{pmatrix} V_k^{\text{T}} \Pi_k^{\text{POL}},
\]

where \( \alpha_k^{\text{RCA}} \) and \( \Pi_k^{\text{POL}} \) are the matrices defined in the polynomial version, and \( \alpha_k^{\text{RCA}} \) and \( V_k^{\text{T}} \) are the matrices defined in the original MCCD-RCA algorithm.

Finally, generically including the spatial constraints in Eq. (9) we get the following description of our model for a specific CCD:

\[
\hat{H}_k = S \alpha_k V_k^{\top} + \tilde{S} \tilde{\alpha} \Pi_k,
\]

that we can also write in a global form \( \hat{H} = S \alpha V^\top \), where \( \hat{H} \) and \( S \) have already been defined in Eq. (10) and Eq. (11), and where \( \alpha \) and \( V^\top \) are the following matrices:

\[
\alpha = \begin{pmatrix} \alpha_1 & 0 & \cdots & 0 \\ 0 & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \alpha_N \end{pmatrix}, \quad V^\top = \begin{pmatrix} V_1^\top & 0 & \cdots & 0 \\ 0 & V_2^\top & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & V_N^\top \end{pmatrix}
\]

### 3.5. Optimisation problem

Combining the regularisations enumerated in Sect. 3.2 and the data model described in Sect. 3.1 we can construct the optimisation problem in an elegant way by reformulating the (7). However, we can split the optimisation problem into a more convenient way

\[
\min_{s_{1,\ldots,n},\tilde{s},\alpha} \left\{ \sum_{k=1}^{N} \frac{1}{2} \| Y_k - T_k (S \alpha_k V_k^\top + \tilde{S} \tilde{\alpha} \Pi_k) \|^2_F + \sum_{i=1}^{r_k} \| \mathbf{w}_{i,k} \odot \Phi_i s_i \|_1 + \lambda_i (S \alpha_k V_k^\top + \tilde{S} \tilde{\alpha} \Pi_k + I_{\tilde{\alpha}}(\alpha_i)) + \sum_{i=1}^{f} \| \mathbf{w}_{i} \odot \Phi_i \|_1 + \lambda_i (\tilde{\alpha_i}) \right\}
\]

In the previous equation, the columns of \( Y_k \in \mathbb{R}^{D_{\text{ref}} \times m_k} \) are the stars distributed in the \( k \)th CCD sensor, \( T_k \) is the degradation operator, \( \mathbf{w}_{i,k} \) and \( \mathbf{w}_i \) are weight vectors, \( \Phi \) is a transform that allows a sparse representation of our eigenPSFs, and \( \Omega_k \) and \( \hat{\Omega} \) are sets to enforce sparsity and normalisation of the rows of \( \alpha_k \) and \( \tilde{\alpha} \), respectively. The indicator function of a set \( C \) is written as \( \iota_C(\cdot) \), that is equal to 0 if the argument belongs to \( C \) and +∞ otherwise. For example, \( \iota_i \) is the indicator function over the positive orthant. More explicitly, the sets \( \Omega_k \) and \( \hat{\Omega} \) are defined the following way:

\[
\Omega_k = \{ \alpha_k \mid \forall i \in \{1, \ldots, r_k \}, \| (\alpha_k^i) \|_0 \leq \eta_{\ell_i} \wedge \| (\alpha_k V_k^i) \|_2 = 1 \},
\]

\[
\hat{\Omega} = \{ \tilde{\alpha} \mid \forall i \in \{1, \ldots, f \}, \| (\tilde{\alpha}^i) \|_0 \leq \tilde{\eta}_i \wedge \| (\tilde{\alpha} \Pi_k) \|_2 = 1 \},
\]

where \( (\eta_{\ell_i})_{i \geq 0} \) and \( (\tilde{\eta}_i)_{i \geq 0} \) are appropriately chosen integers, and \( \| \cdot \|_0 \) is the pseudo-norm \( \ell_0 \) that returns the number of non-zero elements of a vector. So we are enforcing, in the global case, the row \( i \) of \( \tilde{\alpha} \) to have at most \( \tilde{\eta}_i \) non-zero elements. An interpretation could be that we are forcing each eigenPSF to follow a small number of positional polynomials as \( \tilde{\alpha} \)’s rows will be sparsely represented over the \( \Omega_k \) matrices.

The \( \Phi \) transform used throughout this paper is the starlet transform (Starck et al. 2011). We enforce the sparsity on the different decomposition levels excluding the coarse scale. The \( \ell_1 \) term promotes the sparsity of the eigenPSFs with respect to \( \Phi \) while the weights \( \mathbf{w}_{i,k} \) and \( \mathbf{w}_i \) regulate the sparsity penalisation against the other constraints and should adapt throughout the optimisation algorithm depending on the noise level.

The second term in each of the \( \hat{\Omega} \) sets (e.g. \( \| (\alpha_k V_k^i) \|_2 = 1 \)) was not mentioned in the regularisation section 3.2, but they are
needed to avoid a degenerated solution, for example $\|S_\delta\|_F \to \infty$ and $\|A_k\|_F \to 0$, due to the usual scale indeterminacy when doing a matrix factorisation. To avoid this, we normalise $A_k$ and $A$. This translates to forcing the normalisation of the eigenPSF weights contributing to model each observed star. This does not mean that the eigenPSF weights will be the same for each star, but that the norms of the weight vectors are equal.

### 3.6. Algorithm

The optimisation in Eq. (22) is non-convex as we are facing a matrix factorisation problem. To overcome this situation we use an alternating minimisation scheme where we optimise one variable at a time, iterating over the variables as studied in Xu & Yin (2013) or Bolette et al. (2014). In consequence, we can at most expect to converge towards a local minima. The main iteration is an alternating minimisation scheme where we optimise one variable at a time, but that the norms of the weight vectors are equal.

The method is shown in Algorithm 1, which contains the four main optimisation problems derived from the alternating scheme. There exists a wide literature on minimisation schemes involving non-smooth terms, specifically proximal methods (Parikh & Boyd 2014), that we can exploit in order to handle the four cases. Notably, we use the algorithm proposed by Condat (2013) for the problems (II), (III) and (IV). For the problem (I) we use the method proposed by Liang et al. (2018) which is an extension of the well-known FISTA algorithm (Beck & Teboulle 2009)

Even though the $\ell_0$ pseudo-norm is non-convex and therefore not adapted to the general scenario of the aforementioned algorithms, we can alleviate this fact by combining the use of its proximal operator and a given heuristic.

Concerning the algorithm’s initialisation, we start by a preprocessing where we reject stars that are strong outliers in terms of shape or size. We run the shape measurement algorithm mentioned in Sect. 4.4 on the train stars and discard the ones that are several sigmas away from nearby stars. At this moment we can assign a specific weight for each train star. There are three available options: i) use a unitary weight for each train star; ii) use a weight provided by the user; iii) compute a weight $\omega_i$ as a function of the star’s Signal-to-Noise-Ratio (SNR) based on $\omega_i \propto \text{SNR}_i (\text{SNR}_i + \text{median} (\text{SNR}))$ and bounded to a specific interval to avoid bright stars from dominating the optimisation.

Next, we continue with all the local eigenPSFs set to zero, as seen in line 4 of Algorithm 1; and the $\vec{a}$ matrix set to the identity, favouring the specialisation of each global eigenPSF to one specific monomial. By following this procedure, we are training a global polynomial model that fits the stars as best as it can. Later on, the local models will work with the residuals between the observed stars and the global model, trying to capture variations missed in the previous step.

There are four iteration loops in algorithm 1. On line 8, the main iteration, and on line 15 the iteration over the CCDs for the training of the local model. The other two iterations on lines 9 and 14 correspond to a refinement of the estimation. Our objective is to correctly estimate the global and the local contributions for the model, and to do this we alternate the minimisation between the global and the local contributions, which we call outer minimisation. On top of that, each of these two contributions include an inner alternating minimisation scheme as we are performing a matrix factorisation for the local and for the global models. For example, we are simultaneously minimising over $S_\delta, \alpha_k$ for the local model and over $S, \vec{a}$ for the global model. We want to refine this inner minimisation, meaning that the optimisation of the two variables separately approaches the joint optimisation of both variables. To accomplish this, we need to go through a small number of iterations, which are described by the superscript variables, before continuing the iteration of the next alternating scheme. The optimisation strategy can be seen as a compound alternating minimisation scheme considering the outer and the inner alternations.

More information about the optimisation strategy can be found in Appendix D.

### 3.7. PSF recovery

Once the training of the model on the observed stars is done, we can continue with the problem of estimating the PSF field at galaxy positions. We call this problem PSF recovery. Gentile et al. (2013) conduct a study on PSF interpolation techniques and Ngolè & Starck (2017) propose a sophisticated approach based on optimal transport theory (Peyré & Cuturi 2018). We will follow a RBF (Radial Basis Function) interpolation scheme with a thin plate kernel$^4$, as in Schmitz et al. (2020), due to its simplicity and good performance. This choice comes with the assumption that the influence of each observation does not depend on the direction but only on the distance to the target which is well described by the RBF kernel.

The RBF interpolation of a function $f$ on a position $u$ works by building a weighted linear combination of RBF kernels $(\phi(v))$ centred in each of the available training star positions $u_i$. The interpolation function reads

$$\hat{f}(u) = \sum_{i=1}^{N_{\text{RBF}}} \lambda_i \phi(\|u - u_i\|) ,$$

(25)

where $\lambda_i^{N_{\text{RBF}}}$ are the linear weights that need to be learnt and $N_{\text{RBF}}$ is the number of elements used to estimate the interpolant. In order to learn the weights, we force the exact reconstruction of the interpolant on the known positions, that is $\hat{f}(u_i) = f(u_i) \forall i \in \{1, \ldots, N_{\text{RBF}}\}$. By fixing the aforementioned constraint we have a system of $N_{\text{RBF}}$ equations with $N_{\text{RBF}}$ unknowns that are the $\lambda_i$ weights. Once the system is solved, it is just a matter of evaluating the interpolant on the desired position $u$ following Eq. (25).

At this point, we need to choose over which function $f$ we will interpolate. A straightforward choice would be to use the reconstructed PSFs at the training positions as the $f(u_i)$. Nevertheless, this would not take into account the specificities and structure of our model. Following the discussion in Sect. 4.2 of Schmitz et al. (2020) we will use the learnt $A_k$ and $A_k^\dagger$ matrices. They encompass all the spatial distribution properties of the learned features, our eigenPSFs, and it is natural for our framework to use these values as the function to interpolate.

We continue with a brief explanation of the interpolation procedure. For one given target position $u$ in CCD $k$, we consider the $N_{\text{RBF}}$ closest observed stars to that position that also belong to the CCD $k$. We call $A_k(N_{\text{RBF}})$ to the $A_k$ matrix composed only with the columns of the aforementioned $N_{\text{RBF}}$ stars. We want to estimate the interpolated column vector $A_k u$. For this, we use a RBF interpolation scheme for each row of the $A_k(N_{\text{RBF}})$ matrix. The elements of the row $t$ represent the $(f^\dagger(u_i))^{N_{\text{RBF}}}$ evaluations and the element $A_k^{t,N_{\text{RBF}}}$ represents the interpolated value $f^\dagger(u)$. The same procedure is repeated for each row of the $A_k(N_{\text{RBF}})$ matrix so as to obtain the column vector $A_k u$.

$^4$ Where the kernel is defined as $\phi(r) = r^2 \ln(r)$. 
Algorithm 1 Multi-CCD Resolved Components Analysis

Initialisation:
1: Preprocessing()
2: for \( k = 1 \) to \( K \) do
3: Harmonic constraint parameters \((e_{k,i}, \alpha_{k,i})_{1 \leq i \leq N} \rightarrow V_k^T, \alpha_k^{(0)}\)
4: \(0_{n \times nr} \rightarrow S_k^{(0,0)}\)
5: end for
6: Global coordinates \(\rightarrow \Pi_k, \tilde{\alpha}_k^{(0,0)}\)
7: \(0_{n \times nr} \rightarrow S^{(0,0)}\)

Alternate minimisation:
8: for \( l = 0 \) to \( l_{\text{max}} \) do
9: \(\text{Noise level, } \tilde{\alpha}_l^{(l,0)} \rightarrow \tilde{W}_l^{(l,0)}\)
10: \(\hat{\alpha}_l^{(l+1,0)} = \min_{\tilde{\alpha}} \{\tilde{W}_l^{(l,0)} V_k^T + \tilde{\alpha}^{(l,0)} \Pi_k \Pi_k^T + \sum_i ||\tilde{W}_l^{(l,0)} \odot \tilde{\Phi}_i ||^2\} \) (I)
11: \(\tilde{S}_l^{(l+1,0)} = \min_{\tilde{\alpha}} \{||Y_k - \tilde{F}_k \tilde{\alpha}_k^{(l,0)} V_k^T + \tilde{S}_l^{(l,0)} \Pi_k \Pi_k^T + \sum_i ||\tilde{W}_l^{(l,0)} \odot \tilde{\Phi}_i ||^2\} \) (II)
12: end for
13: for \( n = 0 \) to \( n_G \) do
14: Noise level, \( \alpha_{l,n}^{(l,0)} \rightarrow W_k^{(l,0)}\)
15: \(\hat{S}_k^{(l+1,n)} = \min_{\tilde{\alpha}_k} \{||Y_k - \tilde{F}_k \tilde{\alpha}_k^{(l,0)} V_k^T + \tilde{S}_k^{(l+1,0)} \Pi_k \Pi_k^T + \sum_i ||\tilde{W}_l^{(l,0)} \odot \tilde{\Phi}_i ||^2\} \) (III)
16: \(\alpha_k^{(l+1,1)} = \min_{\tilde{\alpha}_k} \{||Y_k - \tilde{F}_k \Pi_k \Pi_k^T + \tilde{S}_k^{(l+1,0)} \Pi_k \Pi_k^T + \sum_i ||\tilde{W}_l^{(l,0)} \odot \tilde{\Phi}_i ||^2 + \tilde{\Omega}^{(l)}(\tilde{\alpha}_k)\} \) (IV)
17: end for
18: end for
19: end for
20: end for
21: end for

\[
\hat{H}(u) = \tilde{S} \tilde{A}_{k,n} + S \tilde{A}_{k,n}.
\] (26)

We found that restricting the \( N_{\text{RBF}} \) neighbours to a single CCD for the global components gave better results. This might be due to the fact that the global components are able to capture some of the discontinuities from one CCD to another and therefore the interpolation is degraded when using stars from different CCDs. The number of neighbours \( N_{\text{RBF}} \) should be chosen as a function of the available number of stars per CCD in the training set and as the RBF kernel chosen. From now on, and given the training set we handle in this article, \( N_{\text{RBF}} \) is set to 20.

4. Numerical experiments

4.1. Data

The simulated data set we create to evaluate MCCD set is based on a CFIS\(^5\) (Canada-France Imaging Survey) MegaCam\(^6\) exposure from the CFHT (Canada-France-Hawaii Telescope). It contains 2401 stars distributed along 40 CCDs over a field of view of \( \sim 1 \) deg\(^2\) as shown in Fig. 2. Each CCD consists of a matrix of 2048 by 4612 pixels with some given gaps between the different CCDs. The horizontal gap length consist of \( \sim 70 \) pixels while vertical gaps of \( \sim 425 \) pixels.

\(^5\) http://www.cfht.hawaii.edu/Science/CFIS/
\(^6\) http://www.cfht.hawaii.edu/Instruments/Imaging/MegaPrime/
as it will be added later. Then we distribute them on a mock image of 2048 x 4612 pixels. The corresponding positions will be the pixel coordinates that are presented in Fig. 2. Once the mock image is created, we add the noise value according to the desired SNR to the whole image. When the mock image is created, we run SExtractor in order to have a star catalogue that PSFEx can use as input.

4.3. Testing data set

For the testing, we want to observe how well the different models capture the ellipticity maps when trained on real star positions. Therefore, the positions in each CCD are taken from a regular grid of 20 x 40 and considering that the total amount of CCDs is 40, we finally have a total of 32000 stars to test our model. These stars are simulated following the same ellipticity maps (see Fig. 3), without any sub-pixel shift and without any noise. The goal is now to use the training data (i.e. simulated observed stars) to learn the model, and then to predict the PSFs at positions of test stars. As we have the ground truth at these positions, without noise and sub-pixel shift, it is easy to get a robust evaluation of model predictions.

4.4. Quality criteria

In order to correctly assess the performance of our PSF modelling algorithm, we consider several criteria:

- Pixel Root Mean Square (RMS) error: calculated between the pixel images of the recovered PSFs and the noiseless test stars. The expression of the pixel RMS error is the following:

\[ \text{RMS} = \sqrt{\langle (Y - \hat{Y})^2 \rangle} = \left( \frac{1}{Nn} \sum_{i=1}^{N} \sum_{j=1}^{n} (Y_{i,j} - \hat{Y}_{i,j})^2 \right)^{1/2}, \]  

where \( Y_{i,j} \) is the pixel of test star \( i \) that has a total of \( n \) pixels, \( N \) is the total number of test stars, \( \hat{Y}_{i,j} \) is the estimation of the test star's pixel and \( \langle \cdot \rangle \) denotes the mean over all the elements in the array.

- Shape (ellipticity) error: We estimate the ellipticities of reconstructed stars using the adaptive moments’ ellipticity estimator from Galsim’s HSM module (Hirata & Seljak 2003; Mandelbaum et al. 2005). The shape and size definitions can be found in Appendix B. For each of the ellipticity components, the RMS error is calculated as:

\[ e^{\text{RMS}} = \sqrt{\langle (\varepsilon - \hat{\varepsilon})^2 \rangle} = \left( \frac{1}{N} \sum_{i=1}^{N} (\varepsilon_i - \hat{\varepsilon}_i)^2 \right)^{1/2}. \]  

- Size error: We use the measurements from HSM and the definition in Appendix B to compute the following RMS error:

\[ R^2_{\text{RMS}} = \sqrt{\langle (R^2 - \hat{R}^2) \rangle^2} = \left( \frac{1}{N} \sum_{i=1}^{N} (R^2_i - \hat{R}^2_i)^2 \right)^{1/2}. \]  

- Moment residual maps: To visualise the shape and size errors we plot these quantities as a function of their position on the focal plane.

When comparing two methods we define the relative gain concerning metric \( m \) of method 1 with respect to the method 2 as:

\[ G_{1/2}(m) = \frac{m_2 - m_1}{m_2} \times 100\%. \]
Based on experiments with simulated and real data, we have chosen the following parameters:

- **PSFEx**: we use the following configuration:
  
  ```
  PSF_SAMPLING 1.0
  PSF_SIZE 51,51
  PSFVAR_KEYS XWIN_IMAGE, YWIN_IMAGE
  PSFVAR_GROUPS 1,1
  PSFVAR_DEGREES 2
  ```

  PSFVAR_DEGREES refers to the maximum polynomial degree, and, XWIN_IMAGE and YWIN_IMAGE, to the windowed centroid positions in pixel coordinates. The PSFEx software\(^8\) does not include publicly an interpolation method, so we use an available PSFEx interpolation module\(^9\).

- **RCA**: we set \(r\) equal to 8 local components, the denoising parameters \(K_r^{\text{RCA}}\) to 1, and the other parameters to their default value from its official repository\(^10\).

- **MCCD**: we use the same parameters as RCA for the local component, and a maximum polynomial degree of 8 for the global components. The denoising parameters \(K_r^{\text{Loc}}\) and \(K_r^{\text{Glob}}\) are set to 1 for the local and the global contributions.

The MCCD parameters that most affect its behaviour were mentioned above. Their choice greatly relies on the training data set used. Depending on the number of stars available and the complexity of the instrument’s PSF one may tend to prefer a more complex model by augmenting the number of local components, \(r\), and the maximum polynomial degree. However, if the stars are not enough to constraint the model one may end with a model that is overfitting the training stars. A proper selection of the denoising parameters can control the bias-variance trade-off in the estimation. A high value of the denoising parameter, i.e. 3, will output an extremely denoised model. It will contain a high estimation bias that can be related with a model that cannot capture some spatial variations and fine details of the PSF. On the contrary, if the denoising parameter is close to zero, the only denoising performed by the MCCD is due to the low-rank constraint and therefore the estimations can be rather noisy.

---

\(^8\) [https://www.astromatic.net/software/psfex](https://www.astromatic.net/software/psfex)

\(^9\) [https://github.com/esheldon/psfex](https://github.com/esheldon/psfex)

\(^10\) [https://github.com/CosmoStat/rca](https://github.com/CosmoStat/rca)
4.7. Comparison of computing resources

The MCCD methods take $\sim 2.9 \times$ more CPU-time than PSFEx when compared on the same machine. We evaluate it on the fitting and validation procedures, that is, the estimation of the PSF model and the recovery of PSF at test positions. It is relevant to mention that the PSFEx package is coded in the C programming language, while the MCCD methods are completely coded in Python.

5. UNIONS/CFIS experiments

In this section we compare the MCCD-HYB method with PSFEx using real data from the Ultra-violet Near-Infrared Optical Northern Sky (UNIONS) survey, which is a collaboration between the Panoramic Survey Telescope and Rapid Response System (Pan-STARRS) and CFIS. We use the $r$-band data from the latter.

5.1. Dataset

We analyse a subset of around $50 \text{deg}^2$ from the whole CFIS survey area, that, in total, will span $5000 \text{deg}^2$. It corresponds to the subset named W3 described in Erben et al. (2013), and includes 217 exposures. Each CCD from each exposure has been processed independently with SExtractor. The stars were selected in a size-magnitude diagram, in the magnitude range between 18 and 22, and a Full-Width Half Maximum (FWHM) range between 0.3 and 1.5 arcsec. In order to validate the PSF models, we randomly split the stars into a testing and a training dataset, trying to estimate the first set of stars while constructing the latter.

The ellipticity and the size of the training stars can be seen in Fig. 8. Each bin represents the mean shape measurement over all the stars with a centroid located within the bin.
5.2. Model parameters

The setup of PSFEx for this experiment is similar to the one used for the simulated images that can be found in Sect. 4.5. The MCCD-HYB method uses a maximum global polynomial degree of 3, 16 local components and the denoising parameters $K_\sigma$ set up to 0.1. In order to compare the star images with the different methods (PSFEx and MCCD-HYB), the models need to match the flux as well as the centre of the star. Hence, after estimating a PSF model at a given star location, the PSF is normalised and shifted to match the star. For this purpose, we use the same intra-pixel shift and flux estimation methods for both PSF models: i) we estimate the star and the PSF centroids, ii) we calculate the shift needed by the PSF to match the star and construct a shifting kernel, and iii) the PSFs are convolved by their corresponding shifting-kernel. To match the flux, we calculate an $\alpha$ parameter for each test star and PSF that corresponds to the argument that minimises the function $f(\alpha) = \|I_1 - \alpha I_2\|_2$, where $I_1$ and $I_2$ are the star and the PSF, respectively.
5.3. Metric on real data: the $Q_p$ criteria

Performing a comparison between two PSF models with real data is an arduous task since we do not know the shapes and pixel values of the observed stars. However, subtracting our estimated model from an observed star (i.e. pixel residual) should lead to a residual map containing only noise if the model is perfect. The probability of having our model correlated with the noise is extremely small. Therefore, from this point of view, the method with the smallest pixel RMS residual error can be considered as the best. Using all the test stars $y$, and our estimates $\hat{y}_s$, we calculate the pixel RMS residual error: $\text{Err} = \sqrt{\frac{1}{N_s \cdot N_i} \sum_s \sum_i (y_{s,i} - \hat{y}_{s,i})^2}$, where $N_s$ is the number of stars and $N_i$ is the number of pixels we consider in a given image when we use a 10 pixel radius circle from the centre of the residual images. The noise standard deviation $\sigma_{\text{noise}}$ is calculated from the stars only using the pixels outside the aforementioned circle. For a perfect modelling, we would have $\text{Err} \approx \sigma_{\text{noise}}$, and we define the $Q_{p1}$ metric as:

$$Q_{p1} = \left(\text{Err}^2 - \sigma_{\text{noise}}^2\right)^{1/2}.$$  \hspace{1cm} (32)

We next introduce two metrics to quantify how noisy the models are. The variance of the PSF model for the test stars $s$ reads $\sigma_s^2 = [\text{Var}(y_s - \hat{y}_s) - \sigma_{\text{noise}}^2(y_s)]_+$, where $\text{Var}()$ is a usual variance estimator, the operator $[\cdot]_+$ sets to zero negative values and...
\[ \sigma_{\text{noise}}^2(y_s) \] is the noise variance estimation for a single star. We present the \( Q_{p_2} \) and \( Q_{p_3} \) metrics in the following equations:

\[
Q_{p_2} = \left( \frac{1}{N_s} \sum_{s} \sigma_s^2 \right)^{1/2}, \quad Q_{p_3} = \left( \frac{1}{N_s} \sum_{s} (\sigma_s^2 - Q_{p_2}^2)^2 \right)^{1/4}. \tag{33}
\]

The \( Q_{p_2} \) metric represents the modelling error expectation for a given star, and the \( Q_{p_3} \) metric indicates the fluctuation of the modelling error. A perfect PSF model would give values close to zero for the three metrics.

### 5.4. Results

| Method   | \( Q_{p_2} \) | \( Q_{p_3} \) | \( Q_{p_3} \) |
|----------|---------------|---------------|---------------|
| PSFEx    | 15.56         | 8.13          | 14.31         |
| MCCD-HYB | 12.14         | 6.68          | 10.86         |
| Gain_{PSFEx} | 22\%          | 18\%          | 24\%          |

| Noise Std. Dev. (\( \sigma_{\text{noise}} \)) | 15.83 |

Table 2: \( Q_p \) criterion using all test stars of the W3 dataset from CFIS. The gain of the MCCD-HYB with respect to PSFEx and the noise standard deviation are also presented.

The main results of the experiment are synthesised in Table 2 where the \( Q_p \) criteria are given. In the \( Q_{p_2} \) column, we can observe a 22\% gain of the MCCD-HYB method with respect to PSFEx. From \( Q_{p_3} \) and \( Q_{p_3} \) metrics, we also conclude that the MCCD-HYB model is considerably less noisy than the one from PSFEx.

In order to explore potential remaining structure in the residuals, we stack together the residuals for all 534 test stars from a random exposure. These are shown, along with the stacking of the test stars themselves, in Fig. 9. We can see that PSFEx has a sharper stacked error compared to MCCD-HYB. This could indicate that our algorithm is better at capturing the size of the PSF, as the peak of the residual is directly related to it. Considering that there is no trace of shifting errors and that we are calculating the flux optimally, a greater mismatch in the size of the PSF equals to a greater peak pixel error on the residual. The third row presents the mean of the stacked absolute value of the residuals for both of the PSF models so that the residuals can not cancel themselves. We observe the same behaviour described above with the PSFEx pixel error distribution being sharper but more centred. It is also possible to notice the higher noise PSFEx has when compared to the MCCD-HYB model.

Fig. 10 presents examples of star image reconstructions by the two different PSF models, PSFEx and MCCD-HYB, and their corresponding residuals. The proposed method yields a near noiseless model when compared to PSFEx, as can clearly be seen on the top-left and bottom-right stars of Fig. 10, where the stars have low SNRs of 19.3 and 4.2 respectively. Both models share a good estimation of the bottom-right star, which comes a low-stellar-density region of the focal plane (the bottom-right corner, as can be seen in Fig. 7). On the bottom-left star of Fig. 10, we observe a similar type of error as that appearing in Fig. 9. It is difficult to derive conclusions of different PSF model performances based on the shape measurement of noisy stars due to its high stochasticity. Nevertheless, driven by the comments from DES Y1 (Zuntz et al. 2018) on the residual mean size offset from the PSFEx model, we conducted a study with our data. We measured the size from the training stars and from both calculated PSF models, PSFEx and MCCD-HYB, and then computed the residual. The RMS residual size of the \( \Delta R^2/R^2 \) value gave \( 4.82 \times 10^{-2} \) for PSFEx and \( 4.02 \times 10^{-2} \) for MCCD-HYB. This represents a 16\% gain of our proposed algorithm.

Fig. 11 presents in the left column the histogram of the residuals and in the right column the histograms of the size metrics. We can notice that the MCCD-HYB algorithm has a sharper residual size around zero. The figure also includes the mean of...
the residuals for each PSF model. This shows that both models tend to overestimate the size of the PSF. However, the MCCD-HYB model presents a 30% gain in the mean residual size with respect to PSFEx, indicating a smaller bias in the shape.

6. Reproducible research

In the spirit of reproducible research, the MCCD-RCA algorithm will be publicly available on the CosmoStat’s Github, including the material needed to reproduce the simulated experiences. The MCCD PSF modelling software will be included in the CFIS shape measurement pipeline (Guinot & et al. In Prep.).

7. Conclusion

We have presented a family of non-parametric PSF (Point Spread Function) modelling methods coined MCCD, including its best-performing extension MCCD-HYB, which are built upon the existing RCA (Resolved Component Analysis) method and are capable of constructing PSF models that span all the CCDs (Charge-Coupled Device) from an instrument’s focal plane at once. Naturally, the use of more stars for the training allows us to build more complex models that can capture evasive features. Our model is composed of global components, spanning all the CCDs, and local components that are CCD-specific. By using this structure we can better capture global patterns and features that might be lost when using only a local model like in RCA or, the widely used algorithm, PSFEx.

The method was first tested with a set of simulated PSFs following a real star spatial distribution over MegaCam’s focal plane, an instrument from the CFHT (Canada-France-Hawaii Telescope). Its use leads to better performance in all the evaluated metrics when compared to PSFEx. We then tested the method on a set of real CFIS images, an imaging survey based on CFHT, in order to confirm that it can handle real data. Our method achieves a smaller pixel RMS (Root Mean Square) residual than PSFEx and the estimated model is considerably less noisy.

The performance gain of the MCCD methods over PSFEx is higher when using our simulated dataset than when using the real dataset. This can be explained by the fact that our simulated dataset shows more intricate variations in the PSF than the real data does, and MCCD is better at capturing such strong variations.

The proposed method can naturally handle more complex PSF profiles, such as those expected from space-based instruments. The RCA method was tested with Euclid-like simulated PSFs and has shown a better performance than PSFEx (Ngolè et al. 2016; Schmitz et al. 2020). Therefore, we expect to have an even superior performance in this scenario with MCCD. Thanks to its formulation, it can also handle super-resolution, making it suitable for under-sampled data.

Despite the good performance of the method, there is still room for improvement. A natural straight-forward extension for the MCCD algorithms would be to replace the denoising strategy by one more suited for the specificities of the PSFs we work with. This could be accomplished by using a deep neural network as the denoiser (Ronneberger et al. 2015; Ye et al. 2018).

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This work has made use of the CANDIDE Cluster at the Institut d’Astrophysique de Paris and made possible by grants from the PNCG and the DIM-ACA V. Software: Numpy (van der Walt et al. 2011), Scipy (Virtanen et al. 2020), Astropy (Robitaille et al. 2013; Price-Whelan et al. 2018), GaSim (Rowe et al. 2015), IPython (Perez & Granger 2007), Jupyter (Kluyver et al. 2016), Matplotlib (Hunter 2007), PySAP (Farrens et al. 2020).

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Fig. 9: Stacked star profile from all 534 test stars in a random CFIS exposure (id. 2099948) (top), corresponding stacked residuals after subtraction by the PSFEx (middle left) or MCCD-HYB (middle right) PSF models. The bottom row includes the stacked absolute value of the residuals.
Fig. 10: Examples of real CFIS test stars, the estimations of both methods and the pixel residuals. We used the same exposure as in Fig. 9. We present four test stars with the estimated PSF models and the corresponding residuals. The top-left star corresponds to a star extracted from the top-left corner of the focal plane with a SNR of 19. The top-right star corresponds to a star leading to a high error for both methods. The bottom-left star corresponds to a star located in the centre of the focal, with a relatively high SNR of 160. The bottom-right star corresponds to a star located in the bottom-right corner of the focal plane, with a low SNR of 4.

Fig. 11: Histograms showing the distribution of the size metric over the train stars and their residuals for both PSF models, PSFEx and MCCD-HYB.

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Appendix A: RCA regularisations

In this section we give a more detailed description of each regularisation we use in our local RCA model:

1. **Low rank:** PSF variations can be explained by a small number of eigenPSFs. This constraint can be enforced by the proper choice of two parameters, the number of local, \( r_k \), and global, \( R \), eigenPSFs. These parameters are directly linked with the complexity of the model we will be addressing and its selection will naturally depend on the PSF field we will be facing. It is important to allow the model a certain complexity so that it can correctly capture the PSF field’s variations but it should not be much more complex as the model will tend to overfit the noisy observations and therefore lose its generalising power to estimate the PSF in galaxy positions.

2. **Positivity:** the reconstructed PSFs \( \hat{H} \) should only contain non-negative pixel values.

3. **Sparsity:** the observed PSFs are structured images; a way to promote our model to follow this structured behaviour is to enforce the sparsity of the eigenPSFs in an appropriate basis.

4. **Spatial constraints:** the regularity of the PSF field \( \mathcal{H} \) means that the smaller the distance between two PSFs positions \( u_i, u_j \) the smaller the difference between their representations should be \( \mathcal{H}(u_i), \mathcal{H}(u_j) \). This regularity can be achieved by enforcing a constraint in the coefficient matrices \( A_k, A_k' \); for example, the line \( l \) of \( A_k \) corresponds to the contribution of eigenPSF \( l \) to the \( \rho^{\text{star}}_k \) stars in CCD \( k \) located in positions \( (u_i)^{\text{star}}_k \). The closer the positions, the closer the coefficient values should be.

Appendix B: Shape and size definitions

The ellipticity parameters and the size are defined in terms of the moments of the surface brightness profile \( I(x, y) \) following (Hirata & Seljak 2003):

\[
\begin{align*}
\mu &= \frac{\int \mu I(x, y) w(x, y) \, dx \, dy}{\int I(x, y) w(x, y) \, dx \, dy}, \\
M_{\mu
u} &= \frac{\int I(x, y) (\mu - \bar{\mu}) (v - \bar{v}) w(x, y) \, dx \, dy}{\int I(x, y) w(x, y) \, dx \, dy},
\end{align*}
\]

where \( \mu, \nu \in \{x, y\} \) and \( w(x, y) \) is weight window to avoid noise related issues. The size is defined as:

\[
T = R^2 = M_{xx} + M_{yy},
\]

and the ellipticities are defined as:

\[
e = e_1 + i e_2 = \frac{(M_{xx} - M_{yy}) + i 2M_{xy}}{T}.
\]

The adaptive moment measurement from HSM gives \( \sigma \) as output which relates to our size metric as \( R^2 = 2\sigma^2 \).

Appendix C: Additional figures

In this appendix we include the additional figures, Fig. C.1 and Fig. C.2.
SoftThresh\(_i\)(x) = (|x| - \lambda)\_+ \text{sign}(x) = \begin{cases} x - \lambda, & x \geq \lambda, \\ 0, & |x| < \lambda, \\ x + \lambda, & x \leq -\lambda. \end{cases}
\tag{D.3}

We name \(L_{\nabla S_\lambda F()}\) the Lipschitz constant of \(F\)’s gradient. The next equations resume what we need to use the chosen optimisation algorithm:

\[
\nabla S_\lambda F(S_k) = -F_k^\top (Y_k - F_k(\hat{H}_k))V_k \alpha_k^\top, 
\tag{D.4}
\]

\[
L_{\nabla S_\lambda F()} = \rho(\nabla F_\lambda^\top \circ \nabla F_\lambda) \rho(\alpha_k V_k^\top (\alpha_k V_k^\top)^-)\),
\tag{D.5}
\]

\[
\text{prox}_{\rho S_\lambda F()}(|s_k|) = \text{SoftThreshold}_{\rho}(s_k),
\tag{D.6}
\]

\[
\text{prox}_{\alpha R_F()}(X) = X - (X)_+,
\tag{D.7}
\]

where the proximal operator of \(G\) is defined component-wise, the notation \([s_k]_i\) represents the element \(j\) of the \(i\) column vector of matrix \(S_k\), \(F^\top\) is the adjoint operator of \(F_k\), and \(\rho(\cdot)\) is the spectral radius\(^\text{13}\) that we calculate using the power method (Golub & Van Loan 1996). For the algorithm’s parameters \(\tau\) and \(\sigma\), based on Theorem 3.1 from Condat (2013), we use:

\[
\tau = \frac{1}{\alpha L_{\nabla S_\lambda F()}}, \quad \sigma = \frac{\alpha L_{\nabla S_\lambda F()}}{2\|L\|_\text{op}^2},
\tag{D.8}
\]

where \(\|\cdot\|_\text{op}\) is the operator norm (Aliprantis & Border 2007) and \(\alpha\) is a parameter we set to \(3/2\). Being \(L\) a bounded linear operator we can calculate \(\|L\|_\text{op}\) as \(\sqrt{\rho(L^\top L)}\) being \(L^\top\) its adjoint operator.

We now consider the case where \(\Phi\) is not the identity, but it is orthonormal, \(\Phi^\top \Phi = I\). We can adapt the soft thresholding operator in order to cope with the \(G\) term. This would be \(s_k \rightarrow \Phi^\top \text{SoftThreshold}_{\rho}(\Phi s_k)\). When using undecimated wavelets as the starlets, the orthonormal condition is not met. Nevertheless, they are tight frames whose Gram matrix is close to the identity which means that the presented formulation will be a good approximation. We redirect the reader to Starck et al. (2015) for more information on wavelets.

**Appendix D.2: The remaining optimisation problems**

We deal in a similar way with the problems (II) and (IV) from Algorithm 1 using the same optimisation method proposed in Condat (2013). On the other hand, for problem (I), we use the optimisation algorithm in Liang et al. (2018). This is due to the fact that we are neglecting the positivity constraint as we account for it when optimising over the other variables. In order to use these algorithms we need to compute the gradients of the differentiable term of each problem as follows:

\[
\nabla S_\lambda F_k(x) = -F_k^\top (Y_k - F_k(\hat{H}_k)) V_k \alpha_k^\top, 
\tag{D.9}
\]

\[
\nabla a_k F_k(x) = -S_k^\top F_k^\top (Y_k - F_k(\hat{H}_k)) V_k, 
\tag{D.10}
\]

\[
\nabla g F(x) = \sum_{k=1}^{N} \nabla s_k F_k(x) = \sum_{k=1}^{N} -F_k^\top (Y_k - F_k(\hat{H}_k)) (\alpha \Pi_k)^\top, 
\tag{D.11}
\]

\[
\nabla a F(x) = \sum_{k=1}^{N} \nabla a_k F_k(x) = \sum_{k=1}^{N} -S_k^\top F_k^\top (Y_k - F_k(\hat{H}_k)) \Pi_k^\top, 
\tag{D.12}
\]

\(^{13}\) The spectral radius can be defined as \(\rho(B) = \max \{|\lambda_1(B)|, \ldots, |\lambda_n(B)|\}\) where \(\lambda(B)\) are the eigenvalues of the matrix \(B\).
where \( F = \sum_{k=1}^{N} F_k = \frac{1}{2} \| Y - \mathcal{F}(H + S \tilde{\alpha} \Pi) \|^2_F \). Concerning the global optimisation over \( \tilde{S} \) and \( \tilde{\alpha} \) we need to consider all the CCDs when computing the gradient. So we can reformulate the global formulas as:

\[
\nabla_{\tilde{S}} F(x) = - \mathcal{F}^*(Y - \mathcal{F}(\hat{H})) (\hat{\alpha} \Pi)^\top, \quad (D.13)
\]

\[
\nabla_{\tilde{\alpha}} F(x) = - \tilde{S}^\top \mathcal{F}^*(Y - \mathcal{F}(\hat{H})) \Pi^\top. \quad (D.14)
\]

An approximation for the Lipschitz constants of the different gradients can be calculated as:

\[
L_{S_k} = \rho(\mathcal{F}^* \circ F_k) \rho(\alpha_k V_k^\top (\alpha_k V_k^\top)^\top) \quad (D.15)
\]

\[
L_{w_k} = \rho(\mathcal{F}^* \circ F_k) \rho(S_k S_k^\top) \rho(\alpha_k V_k^\top V_k) \quad (D.16)
\]

\[
L_S = \rho(\mathcal{F}^* \circ F) \rho(\hat{\alpha} \Pi (\hat{\alpha} \Pi)^\top) \quad (D.17)
\]

\[
L_\alpha = \rho(\mathcal{F}^* \circ F) \rho(\tilde{S}^\top \tilde{S}) \rho(\Pi \Pi^\top) \quad (D.18)
\]

where \( \rho(\cdot) \) is the spectral radius.

Finally, we also need the proximal operator of the indicator function over the unit-ball \( \mathcal{B} \), where \( \mathcal{B} = \{ x \in \mathbb{R}^n | \| x \|_2 = 1 \} \). It can be computed as:

\[
\text{prox}_{\mathcal{B}}(x) = \frac{x}{\| x \|_2}. \quad (D.19)
\]

**Appendix D.3: Sparsity enforcement parameters**

There are two moments when we enforce sparsity during the optimisation. First, when we denoise the eigenPSFs by the use of the \( \ell_1 \) norm as in Eq. (22). The \( w \) weights are set depending on a noise estimation of the observed images, and the parameters \( K_{\sigma}^\text{Loc} \) and \( K_{\sigma}^\text{Glob} \). The noise standard deviation is estimated using the median absolute deviation. The higher the \( K_{\sigma} \) parameters are set, the higher the thresholding and the denoising will be. Second, when we enforce the spatial constraints through \( \alpha \) sparsity. In this case, we follow the sparsity enforcement proposed in Ngolè et al. (2016).