pPXF: Full Spectrum and SED Fitting of Galactic and Stellar Spectra

(Package v8.1, June 2022)

This pPXF package contains a Python implementation of the Penalized PiXel-Fitting (pPXF) method to fit the stellar and gas kinematics, as well as the stellar population and the photometry (SED) of galaxies. The method was originally described in Cappellari & Emsellem (2004) and was substantially upgraded in subsequent years and particularly in Cappellari (2017).

Attribution

If you use this software for your research, please cite at least Cappellari (2017), or both pPXF papers above. The BibTeX entry for the paper is:

```
@ARTICLE{Cappellari2017,
    author = {{Cappellari}, M.},
    title = "{Improving the full spectrum fitting method:
        accurate convolution with Gauss-Hermite functions}",
    journal = {MNRAS},
    eprint = {1607.08538},
    year = 2017,
    volume = 466,
    pages = {798-811},
    doi = {10.1093/mnras/stw3020}
}
```

Installation

install with:

pip install ppxf

Without write access to the global site-packages directory, use:

pip install --user ppxf

To upgrade pPXF to the latest version use:

pip install --upgrade ppxf

Usage Examples

To learn how to use the pPXF package, copy, modify and run the example programs in the ppxf/examples directory. It can be found within the main ppxf package installation folder inside site-packages. The detailed documentation is contained in the docstring of the file ppxf.py, or on PyPi or as PDF from https://purl.org/cappellari/software.

Examples as Jupyter Notebooks are also available on my GitHub repository.

pPXF Purpose

Extract the galaxy stellar and gas kinematics, stellar population and gas emission by fitting a set of templates to an observed spectrum, or to a combination of a spectrum and photometry (SED), via full-spectrum fitting, using the Penalized PiXel-Fitting (pPXF) method originally described in

Cappellari & Emsellem (2004)

and substantially upgraded in subsequent years and particularly in

Cappellari (2017).

The following key optional features are also available:

- 1) An optimal template, positive linear combination of different input templates, can be fitted together with the kinematics.
- 2) One can enforce smoothness on the template weights during the fit. This is useful to attach a physical meaning to the weights e.g. in terms of the star formation history of a galaxy.
- 3) One can fit multiple kinematic components for both the stars and the gas emission lines. Both the stellar and gas LOSVD can be penalized and can be described by a general Gauss-Hermite series.
- 4) One can fit simultaneously a spectrum and a set of photometric measurements (SED fitting).
- 5) Any parameter of the LOSVD (e.g. sigma) for any kinematic component can either be fitted or held fixed to a given value, while other parameters are fitted. Alternatively, parameters can be constrained to lie within given limits or tied by nonlinear equalities to other parameters.
- 6) One can enforce linear equality/inequality constraints on either the template weights or the kinematic parameters.
- 7) Additive and/or multiplicative polynomials can be included to adjust the continuum shape of the template to the observed spectrum.
- 8) Iterative sigma clipping can be used to clean the spectrum.
- 9) It is possible to fit a mirror-symmetric LOSVD to two spectra at the same time. This is useful for spectra taken at point-symmetric spatial positions with respect to the center of an equilibrium stellar system.
- 10) One can include sky spectra in the fit, to deal with cases where the sky dominates the observed spectrum and an accurate sky subtraction is critical.
- 11) One can derive an estimate of the reddening in the spectrum. This can be done independently for the stellar spectrum or the gas emission lines.
- 12) The covariance matrix can be input instead of the error spectrum, to account for correlated errors in the spectral pixels.

- 13) One can specify the weights fraction between two kinematics components, e.g. to model bulge and disk contributions.
- 14) One can use templates with higher resolution than the galaxy, to improve the accuracy of the LOSVD extraction at low dispersion.

Calling Sequence

```
from ppxf.ppxf import ppxf
```

```
print(pp.sol) # print best-fitting kinematics (V, sigma, h3, h4)
pp.plot() # Plot best fit with gas lines and photometry
```

Example programs are in the ppxf/examples directory. It can be found within the main ppxf package installation folder inside site-packages.

Examples as Jupyter Notebooks are also available on my GitHub repository.

Input Parameters

templates: array_like with shape (n_pixels_temp, n_templates) Vector containing a single optimized spectral template, or an array of dimensions templates[n_pixels_temp, n_templates] containing different stellar or gas emission spectral templates to be optimized during the fit of the galaxy spectrum. It has to be n_pixels_temp >= galaxy.size.

To apply linear regularization to the weights via the keyword regul, templates should be an array of

- 2-dim: templates[n_pixels_temp, n_age],
- 3-dim: templates[n_pixels_temp, n_age, n_metal]
- 4-dim: templates[n_pixels_temp, n_age, n_metal, n_alpha]

depending on the number of population variables one wants to study. This can be useful to try to attach a physical meaning to the output weights, in term of the galaxy star formation history and chemical composition distribution. In that case the templates may represent single stellar population SSP models and should be arranged in sequence of increasing age, metallicity or alpha (or alternative population parameters) along the second, third or fourth dimension of the array respectively.

IMPORTANT: The templates must be normalized to unity order of magnitude, to avoid numerical instabilities.

When studying stellar population, the relative fluxes of the templates are important. For this reason one must scale all templates by a scalar. This can be done with a command like:

templates /= np.median(templates)

When using individual stars as templates, the relative fluxes are generally irrelevant and one can normalize each template independently. This can be done with a command like:

templates /= np.median(templates, 0)

galaxy: array_like with shape (n_pixels,) Vector containing the spectrum of the galaxy to be measured. The star and the galaxy spectra have to be logarithmically rebinned but the continuum should not be subtracted. The rebinning may be performed with the log_rebin routine in ppxf.ppxf_util. The units of the spectrum flux are arbitrary. One can use e.g. erg/(s cm^2 A) or erg/(s cm^2 pixel) as long as the same are used for templates. But see the note at the end of this section.

For high redshift galaxies, it is generally easier to bring the spectra close to the restframe wavelength, before doing the pPXF fit. This can be done by dividing the observed wavelength by (1 + z), where z is a rough estimate of the galaxy redshift. There is no need to modify the spectrum in any way, given that a red shift corresponds to a linear shift of the log-rebinned spectrum. One just needs to compute the wavelength range in the rest-frame and adjust the instrumental resolution of the galaxy observations. See Section 2.4 of Cappellari (2017) for details.

galaxy can also be an array of dimensions galaxy[n_pixels, 2] containing two spectra to be fitted, at the same time, with a reflection-symmetric LOSVD. This is useful for spectra taken at point-symmetric spatial positions with respect to the center of an equilibrium stellar system. For a discussion of the usefulness of this two-sided fitting see e.g. Section 3.6 of Rix & White (1992).

IMPORTANT: (1) For the two-sided fitting the vsyst keyword has to be used. (2) Make sure the spectra are rescaled to be not too many order of magnitude different from unity, to avoid numerical instability. E.g. units of $erg/(s cm^2 A)$ may cause problems!

noise: array_like with shape (n_pixels,) Vector containing the 1*sigma uncertainty (per spectral pixel) in the galaxy spectrum, or covariance matrix describing the correlated uncertainties in the galaxy spectrum. Of course this vector/matrix must have the same units as the galaxy spectrum.

The overall normalization of the **noise** does not affect the location of the **chi2** minimum. For this reason one can measure reliable kinematics even when the noise is not accurately know.

If galaxy is a n_pixels*2 array, noise has to be an array with the same dimensions.

When noise has dimensions n_pixels*n_pixels it is assumed to contain the covariance matrix with elements cov(i, j). When the errors in the spectrum are uncorrelated it is mathematically equivalent to input in pPXF an error vector noise=errvec or a n_pixels*n_pixels diagonal matrix noise = np.diag(errvec**2) (note squared!).

IMPORTANT: the penalty term of the **pPXF** method is based on the *relative* change of the fit residuals. For this reason, the penalty will work as expected even if the normalization of the **noise** is arbitrary. See Cappellari & Emsellem (2004) for details. If no reliable noise is available this keyword can just be set to:

noise = np.ones_like(galaxy) # Same uncertainty for all pixels

velscale: float Velocity scale of the spectra in km/s per pixel. It has to be the same for both the galaxy and the template spectra. An exception is when the **velscale_ratio** keyword is used, in which case one can input **templates** with smaller **velscale** than **galaxy**.

velscale is precisely defined in pPXF by velscale = c*np.diff(np.log(lambda)), which is approximately velscale ~ c*np.diff(lambda)/lambda. See Section 2.3 of Cappellari (2017) for details.

start: Vector, or list/array of vectors [start1, start2, ...], with the initial estimate for the LOSVD parameters.

When LOSVD parameters are not held fixed, each vector only needs to contain start = [velStart, sigmaStart] the initial guess for the velocity and the velocity dispersion in km/s. The starting values for h3-h6 (if they are fitted) are all set to zero by default. In other words, when moments=4:

start = [velStart, sigmaStart]

is interpreted as:

start = [velStart, sigmaStart, 0, 0]

When the LOSVD for some kinematic components is held fixed (see fixed keyword), all values for [Vel, Sigma, h3, h4,...] can be provided.

Unless a good initial guess is available, it is recommended to set the starting sigma >= 3*velscale in km/s (i.e. 3 pixels). In fact, when the sigma is very low, and far from the true solution, the chi^2 of the fit becomes weakly sensitive to small variations in sigma (see pPXF paper). In some instances, the near-constancy of chi^2 may cause premature convergence of the optimization.

In the case of two-sided fitting a good starting value for the velocity is velStart = 0.0 (in this case vsyst will generally be nonzero). Alternatively on should keep in mind that velStart refers to the first input galaxy spectrum, while the second will have velocity -velStart.

With multiple kinematic components **start** must be a list of starting values, one for each different component.

EXAMPLE: We want to fit two kinematic components. We fit 4 moments for the first component and 2 moments for the second one as follows:

```
component = [0, 0, ... 0, 1, 1, ... 1]
moments = [4, 2]
start = [[V1, sigma1], [V2, sigma2]]
```

Optional Keywords

bias: float, optional When moments > 2, this parameter biases the (h3, h4, ...) measurements towards zero (Gaussian LOSVD) unless their inclusion significantly decreases the error in the fit. Set this to bias=0 not to bias the fit: the solution (including [V, sigma]) will be noisier in that case. This parameter is ignored if moments <= 2. The default bias should provide acceptable results in most cases, but it would be safe to test it with Monte Carlo simulations as described in the section "How to Set the Kinematic Penalty Keyword" near the end of the documentation. This keyword precisely corresponds to the parameter lambda in the Cappellari & Emsellem (2004) paper. Note that the penalty depends on the *relative* change of the fit residuals, so it is insensitive to proper scaling of the noise vector. A nonzero bias can be safely used even without a reliable noise spectrum, or with equal weighting for all pixels.

bounds: Lower and upper bounds for every kinematic parameter. This is an array, or list of arrays, with the same dimensions as **start**, except for the last dimension, which is 2. In practice, for every element of **start** one needs to specify a pair of values [lower, upper].

EXAMPLE: We want to fit two kinematic components, with 4 moments for the first component and 2 for the second (e.g. stars and gas). In this case:

```
moments = [4, 2]
start_stars = [V1, sigma1, 0, 0]
start_gas = [V2, sigma2]
start = [start_stars, start_gas]
```

then we can specify boundaries for each kinematic parameter as:

component: When fitting more than one kinematic component, this keyword should contain the component number of each input template. In principle, every template can belong to a different kinematic component.

EXAMPLE: We want to fit the first 50 templates to component 0 and the last 10 templates to component 1. In this case:

component = [0]*50 + [1]*10

which, in Python syntax, is equivalent to:

 $component = [0, 0, \dots 0, 1, 1, \dots 1]$

This keyword is especially useful when fitting both emissions (gas) and absorption (stars) templates simultaneously (see the example for the moments keyword).

constr_kinem: dictionary, optional It enforces linear constraints on the kinematic parameters during the fit. This is specified by the following dictionary, where A_ineq and A_eq are arrays (have A.ndim = 2), while b_ineq and b_eq are vectors (have b.ndim = 1). Either the _eq or the _ineq keys can be omitted if not needed:

constr_kinem = {"A_ineq": A_ineq, "b_ineq": b_ineq, "A_eq": A_eq, "b_eq": b_eq}

The resulting pPXF kinematics solution will satisfy the following linear matrix inequalities and/or equalities:

params = np.ravel(pp.sol) # Unravel for multiple components
A_ineq @ params <= b_ineq
A_eq @ params == b_eq</pre>

IMPORTANT: the starting guess start must satisfy the constraints, or in other words, it must lie in the feasible region.

Inequalities can be used e.g. to force one kinematic component to have larger velocity or dispersion than another one. This is useful e.g. when extracting two stellar kinematic components or when fitting both narrow and broad components of gas emission lines.

EXAMPLES: We want to fit two kinematic components, with two moments for both the first and second component. In this case:

moments = [2, 2]
start = [[V1, sigma1], [V2, sigma2]]

then we can set the constraint sigma1 >= 3*sigma2 as follows:

A_ineq = [[0, -1, 0, 3]] # 0*V1 - 1*sigma1 + 0*V2 + 3*sigma2 <= 0 b_ineq = [0]

constr_kinem = {"A_ineq": A_ineq, "b_ineq": b_ineq}

We can set the constraint sigma1 >= sigma2 + 2*velscale as follows:

We can set both the constraints V1 >= V2 and sigma1 >= sigma2 + 2*velscale as follows:

We can constrain the velocity dispersion of the second kinematic component to differ less than 10% from that of the first component sigma1/1.1 <= sigma2 <= sigma1*1.1 as follows:

EXAMPLE: We want to fit three kinematic components, with four moments for the first and two for the rest. In this case:

moments = [4, 2, 2]
start = [[V1, sigma1, 0, 0], [V2, sigma2], [V3, sigma3]]

then we can set the constraints sigma3 >= sigma1 + 2*velscale and V1 <= V2 <= V3 as follows:

NOTE: When possible, it is more efficient to set equality constraints using the tied keyword, instead of setting A_eq and b_eq in constr_kinem.

constr_templ: dictionary, optional It enforces linear constraints on the template weights
 during the fit. This is specified by the following dictionary, where A_ineq and A_eq are
 arrays (have A.ndim = 2), while b_ineq and b_eq are vectors (have b.ndim = 1). Either
 the _eq or the _ineq keys can be omitted if not needed:

constr_templ = {"A_ineq": A_ineq, "b_ineq": b_ineq, "A_eq": A_eq, "b_eq": b_eq}

The resulting pPXF solution will satisfy the following linear matrix inequalities and/or equalities:

A_ineq @ pp.weights <= b_ineq
A_eq @ pp.weights == b_eq</pre>

Inequality can be used e.g. to constrain the fluxes of emission lines to lie within prescribed ranges. Equalities can be used e.g. to force the weights for different kinematic components to contain prescribed fractions of the total weights.

EXAMPLES: We are fitting a spectrum using four templates, the first two templates belong to one kinematic component and the rest to the other. (NOTE: This 4-templates example is for illustration, but in real applications one will use many more than two templates per component!) This implies we have:

component=[0, 0, 1, 1]

then we can set the equality constraint that the sum of the weights of the first kinematic component is a given fraction of the total:

pp.weights[component == 0].sum()/pp.weights.sum() == fraction

as follows [see equation 30 of Cappellari (2017)]:

A_eq = [[fraction - 1, fraction - 1, fraction, fraction]] b_eq = [0] constr_templ = {"A_eq": A_eq, "b_eq": b_eq}

An identical result can be obtained in this case using the legacy fraction keyword, but constr_templ additionally allows for general linear constraints for multiple kinematic components.

Similarly, we can set the inequality constraint that the total weights of each of the two kinematic components is larger than fraction:

fraction <= pp.weights[component == 0].sum()/pp.weights.sum()
fraction <= pp.weights[component == 1].sum()/pp.weights.sum()
as follows:
A_ineq = [[fraction - 1, fraction - 1, fraction, fraction],</pre>

```
[fraction i, fraction i, fraction, fraction],
[fraction, fraction, fraction - 1, fraction - 1]]
b_ineq = [0, 0]
constr_templ = {"A_ineq": A_ineq, "b_ineq": b_ineq}
```

We can constrain the ratio of the first two templates weights to lie in the interval ratio_min <= w[0]/w[1] <= ratio_max as follows:

If we have six templates for three kinematics components:

component=[0, 0, 1, 1, 2, 2]

we can set the fractions for the first two components to be fraction1 and fraction2 (of the total weights) respectively as follows (the third components will be 1 - fraction1 - fraction2):

clean: bool, optional Set this keyword to use the iterative sigma clipping method described in Section 2.1 of Cappellari et al. (2002). This is useful to remove from the fit unmasked bad pixels, residual gas emissions or cosmic rays.

IMPORTANT: This is recommended *only* if a reliable estimate of the **noise** spectrum is available. See also note below for .chi2.

- **degree:** int, optional Degree of the *additive* Legendre polynomial used to correct the template continuum shape during the fit (default: 4). This uses the standard mathematical definition where e.g. degree=2 is a quadratic polynomial. Set degree=-1 not to include any additive polynomial.
- fixed: Boolean vector set to True where a given kinematic parameter has to be held fixed with the value given in start. This is an array, or list, with the same dimensions as start.

EXAMPLE: We want to fit two kinematic components, with 4 moments for the first component and 2 for the second. In this case:

moments = [4, 2]
start = [[V1, sigma1, h3, h4], [V2, sigma2]]

then we can held fixed e.g. the sigma (only) of both components using:

fixed = [[0, 1, 0, 0], [0, 1]]

NOTE: Setting a negative moments for a kinematic component is entirely equivalent to setting fixed = 1 for all parameters of the given kinematic component. In other words:

moments = [-4, 2]

is equivalent to:

moments = [4, 2] fixed = [[1, 1, 1, 1], [0, 0]]

fraction: float, optional This keyword allows one to fix the ratio between the first two kinematic components. This is a scalar defined as follows:

This is useful e.g. to try to kinematically decompose bulge and disk.

The remaining kinematic components (component > 1) are left free, and this allows, for example, to still include gas emission line components. More general linear constraints, for multiple kinematic components at the same time, can be specified using the more general and flexible constr_templ keyword.

- ftol: float, optional Fractional tolerance for stopping the non-linear minimization (default 1e-4).

EXAMPLE: In the common situation where component = 0 are stellar templates and the rest are gas emission lines, one will set:

gas_component = component > 0

This keyword is also used to plot the gas lines with a different color.

- gas_names: String array specifying the names of the emission lines (e.g. gas_names=["Hbeta",
 "[OIII]",...], one per gas line. The length of this vector must match the number of
 nonzero elements in gas_component. This vector is only used by pPXF to print the line
 names on the console.
- $gas_reddening:$ float, optional Set this keyword to an initial estimate of the gas reddening $E(B-V) \geq 0$ to fit a positive gas reddening together with the kinematics and the templates. This reddening is applied only to the gas templates, namely to the templates with the corresponding element of $gas_component=True$. The typical use of this keyword is when using a single template for all the Balmer lines, with assumed intrinsic ratios for the lines. In this way the gas fit becomes sensitive to redening. The fit assumes by default the extinction curve of Calzetti et al. (2000) but any other prescription can be passed via the reddening_func keyword. By default gas_reddening=None and this parameter is not fitted.
- global_search: bool or dictionary, optional Set to True to perform a global optimization of the nonlinear parameters (kinematics) before starting the usual local optimizer. Alternatively, one can pass via this keyword a dictionary of options for the function scipy.optimize.differential_evolution. Default options are global_search={'tol': 0.1, 'disp': 1}.

The fixed and tied keywords, as well as constr_kinem are properly supported when using global_search and one is encouraged to use them to reduce parameters degeneracies.

NOTE: This option is computationally intensive and completely unnecessary in most situations. It should *only* be used in special situations where there are obvious multiple local **chi2** minima. An example is when fitting multiple stellar or gas kinematic components with well-resolved velocity differences.

IMPORTANT: when using this keyword it is recommended *not* to use multiplicative polynomials but only additive ones to avoid unnecessarily long computation times. After converging to a global solution, if desired one can repeat the pPXF fit with multiplicative polynomials but without setting global_search.

- goodpixels: array_like of int with shape (n_pixels,), optional Integer vector containing the indices of the good pixels in the galaxy spectrum (in increasing order). Only these spectral pixels are included in the fit.
- lam: array_like with shape (n_pixels,), optional Vector with the *restframe* wavelength in Angstrom of every pixel in the input galaxy spectrum. This keyword is required when using the keyword reddening or gas_reddening.

If one uses my ppxf_util.log_rebin routine to rebin the spectrum before the pPXF fit, the wavelength can be obtained as lam = np.exp(ln_lam) below:

from ppxf.ppxf_util import log_rebin
specNew, ln_lam, velscale = log_rebin(lamRange, galaxy)

When lam is given, the wavelength is shown in the best-fitting plot, instead of the pixels.

lam_temp: array_like with shape (n_pixels_temp,), optional Vector with the
 restframe wavelength in Angstrom of every pixel in the input templates spectra.

When both the wavelength of the templates lam_temp and of the galaxy lam are given, the templates are automatically truncated to the minimal range required, for the adopted input velocity guess. In this case it is unnecessary to use the vsyst keyword.

If phot is also given, the final plot will include a best fitting spectrum estimated using the full template, before truncation, together with the photometric values and the truncated best fit to the galaxy spectrum. This is useful to see the underlying best fitting spectrum, in the wavelength range where only photometry (SED) was fitted.

- **linear: bool, optional** Set to **True** to keep *all* nonlinear parameters fixed and *only* perform a linear fit for the templates and additive polynomials weights. The output solution is a copy of the input one and the errors are zero.
- linear_method: {'nnls', 'lsq_box', 'lsq_lin', 'cvxopt'} optional Method used for the solution of the linear least-squares subproblem to fit for the templates weights (default 'lsq_box' fast box-constrained).

The computational speed of the four alternative linear methods depends on the size of the problem, with the default 'lsq_box' generally being the fastest without linear inequality constraints. Note that 'lsq_lin' is included in ppxf, while 'cvxopt' is an optional external package. The 'nnls' option (the only one before v7.0) is generally slower and for this reason is now deprecated.

The inequality constraints in constr_templ are only supported with linear_method='lsq_lin' or linear_method='cvxopt'.

- mask: array_like of bool with shape (n_pixels,), optional Boolean vector of length galaxy.size specifying with True the pixels that should be included in the fit. This keyword is just an alternative way of specifying the goodpixels.
- **mdegree:** int, optional Degree of the *multiplicative* Legendre polynomial (with a mean of 1) used to correct the continuum shape during the fit (default: 0). The zero degree multiplicative polynomial (i.e. constant) is always included in the fit as it corresponds to the multiplicative weights assigned to the templates. Note that the computation time is longer with multiplicative polynomials than with the same degree of additive polynomials.

method: {'capfit', 'trf', 'dogbox', 'lm'}, optional. Algorithm to perform the non-linear minimization step. The default 'capfit' is a novel linearly-constrained non-linear least-squares optimization program, which combines the Sequential Quadratic Programming and the Levenberg-Marquardt methods. For a description of the other methods ('trf', 'dogbox', 'lm'), see the documentation of scipy.optimize.least_squares.

The use of linear constraints with constr_kinem is only supported with the default method='capfit'.

moments: Order of the Gauss-Hermite moments to fit. Set this keyword to 4 to fit [h3, h4] and to 6 to fit [h3, h4, h5, h6]. Note that in all cases the G-H moments are fitted (non-linearly) *together* with [V, sigma].

If moments=2 or moments is not set then only [V, sigma] are fitted.

If moments is negative then the kinematics of the given component are kept fixed to the input values. NOTE: Setting a negative moments for a kinematic component is entirely equivalent to setting fixed = 1 for all parameters of the given kinematic component.

EXAMPLE: We want to keep fixed component = 0, which has a LOSVD described by [V, sigma, h3, h4] and is modelled with 100 spectral templates; At the same time, we fit [V, sigma] for component = 1, which is described by 5 templates (this situation may arise when fitting stellar templates with pre-determined stellar kinematics, while fitting the gas emission). We should give in input to pPXF the following parameters:

```
component = [0]*100 + [1]*5  # --> [0, 0, ... 0, 1, 1, 1, 1]
moments = [-4, 2]
start = [[V, sigma, h3, h4], [V, sigma]]
```

phot: dictionary, optional Dictionary of parameters used to fit photometric data (SED fitting) together with a spectrum. This is defined as follows:

The keys of this dictionary are analogue to the pPXF parameters galaxy, templates, noise and lam for the spectra. However, the ones in this dictionary contain photometric data instead of spectra and will generally consist just a few values (one per photometric band) instead of thousands of elements like the spectra. Specifically:

• phot_templates: array_like with shape (n_phot, n_templates) -Mean flux of the templates in the observed photometric bands. This array has the same number of dimension as the templates input parameter. The same description applies. The only difference is that the first dimension is n_phot instead of n_pixels_temp. This array can have 2-4 dimensions and all dimensions must match those of the spectral templates, except for the first dimension. These templates must have the same units and normalization as the spectral templates. If the spectral templates cover the ranges of the photometric bands, and filter responses resp are available, the mean fluxes for each template can be computed as (e.g. equation A11 of Bessell & Murphy 2012):

One can use the function ppxf_util.photometry_from_spectra as an illustration of how to compute the phot_templates. This function can be easily modified to include any additional filter.

Alternatively, the fluxes may be tabulated by the authors of the SSP models, for the same model parameters as the spectral SSP templates. However, this can only be used for redshift $z \sim 0$.

- phot_galaxy: array_like with shape (n_phot) Observed photometric measurements for the galaxy in linear flux units. These values must be matched to the same spatial aperture used for the spectra and they must have the same units (e.g. erg/(s cm² A)). This means that these values must be like the average fluxes one would measure on the fitted galaxy spectrum if it was sufficiently extended. One can think of these photometric values as some special extra pixels to be added to the spectrum. The difference is that they are not affected by the polynomials nor by the kinematics.
- phot_noise: array_like with shape (n_phot) -Vector containing the 1*sigma uncertainty of each photometric measurement in phot_galaxy. One can change the normalization of these uncertainties to vary the relative influence of the photometric measurements versus the spectral fits.
- phot_lam: array_like with shape (n_phot) or (n_phot, n_templates)

- Mean *restframe* wavelength for each photometric band in phot_galaxy. This is only used to estimate reddening of each band and to produce the plots. It can be computed from the system response function **resp** as (e.g. equation A17 of Bessell & Murphy 2012):

If spectral templates are available over the full extent of the photometric bands, then one can compute a more accurate effective wavelength for each template separately. In this case phot_lam must have the same dimensions as phot_templates. For each templates the effective wavelength can be computed as (e.g. equation A21 of Bessell & Murphy 2012):

plot: bool, optional Set this keyword to plot the best fitting solution and the residuals at the end of the fit.

One can also call separately the class function pp.plot() after the call to pp = ppxf(...).

- **quiet: bool, optional** Set this keyword to suppress verbose output of the best fitting parameters at the end of the fit.
- reddening: float, optional Set this keyword to an initial estimate of the stellar reddening E(B-V) >= 0 to fit a positive stellar reddening together with the kinematics and the templates. This reddening is applied only to the stellar templates (both spectral and photometric ones), namely to the templates with the corresponding element of gas_component=False, or to all templates, if gas_component is not set. The fit assumes by default the extinction curve of Calzetti et al. (2000) but any other prescription can be passed via the reddening_func keyword. By default reddening=None and this parameter is not fitted.

regul: float, optional If this keyword is nonzero, the program applies first or second-order linear regularization to the weights during the pPXF fit. Regularization is done in one, two or three dimensions depending on whether the array of templates has two, three or four dimensions respectively. Large regul values correspond to smoother weights output. When this keyword is nonzero the solution will be a trade-off between the smoothness of weights and goodness of fit.

Section 3.5 of Cappellari (2017) gives a description of regularization.

When fitting multiple kinematic component the regularization is applied only to the first component = 0, while additional components are not regularized. This is useful when fitting stellar population together with gas emission lines. In that case, the SSP spectral templates must be given first and the gas emission templates are given last. In this situation, one has to use the reg_dim keyword (below), to give pPXF the dimensions of the population parameters (e.g. n_age, n_metal, n_alpha). A usage example is given in the file ppxf_example_population_gas_sdss.py.

The effect of the regularization scheme is the following:

- With reg_ord=1 it enforces the numerical first derivatives between neighbouring weights (in the 1-dim case) to be equal to w[j] w[j+1] = 0 with an error Delta = 1/regul.
- With reg_ord=2 it enforces the numerical second derivatives between neighboring weights (in the 1-dim case) to be equal to w[j-1] 2*w[j] + w[j+1] = 0 with an error Delta = 1/regul.

It may be helpful to define regul = 1/Delta and think of Delta as the regularization error.

IMPORTANT: Delta needs to be smaller but of the same order of magnitude of the typical weights to play an effect on the regularization. One quick way to achieve this is:

1. Divide the full templates array by a scalar in such a way that the typical template has a median of one:

templates /= np.median(templates)

2. Do the same for the input galaxy spectrum:

```
galaxy /= np.median(galaxy)
```

In this situation, a sensible guess for Delta will be a few percent (e.g. Delta=0.01
 --> regul=100).

Alternatively, for a more rigorous definition of the parameter **regul**:

A. Perform an un-regularized fit (regul=0) and then rescale the input noise spectrum so that:

Chi²/DOF = Chi²/goodPixels.size = 1.

This is achieved by rescaling the input **noise** spectrum as:

noise = noise*np.sqrt(Chi**2/DOF) = noise*np.sqrt(pp.chi2);

B. Increase regul and iteratively redo the pPXF fit until the Chi² increases from the unregularized value Chi² = goodPixels.size by DeltaChi² = np.sqrt(2*goodPixels.size).

The derived regularization corresponds to the maximum one still consistent with the observations and the derived star formation history will be the smoothest (minimum curvature or minimum variation) that is still consistent with the observations.

reg_dim: tuple, optional When using regularization with more than one kinematic component (using the component keyword), the regularization is only applied to the first one (component=0). This is useful to fit the stellar population and gas emission together.

In this situation, one has to use the reg_dim keyword, to give pPXF the dimensions of the population parameters (e.g. n_age, n_metal, n_alpha). One should creates the initial array of population templates like e.g. templates [n_pixels, n_age, n_metal, n_alpha] and define:

reg_dim = templates.shape[1:] # = [n_age, n_metal, n_alpha]

The array of stellar templates is then reshaped into a 2-dim array as:

templates = templates.reshape(templates.shape[0], -1)

and the gas emission templates are appended as extra columns at the end. An usage example is given in ppxf_example_population_gas_sdss.py.

When using regularization with a single component (the **component** keyword is not used, or contains identical values), the number of population templates along different dimensions (e.g. **n_age**, **n_metal**, **n_alpha**) is inferred from the dimensions of the **templates** array and this keyword is not necessary.

- **reg_ord: int, optional** Order of the derivative that is minimized by the regularization. The following two rotationally-symmetric estimators are supported:
 - reg_ord=1: minimizes the integral over the weights of the squared gradient:

Grad[w] @ Grad[w].

• **reg_ord=2**: minimizes the integral over the weights of the squared curvature:

Laplacian[w]**2.

sigma_diff: float, optional Quadratic difference in km/s defined as:

```
sigma_diff**2 = sigma_inst**2 - sigma_temp**2
```

between the instrumental dispersion of the galaxy spectrum and the instrumental dispersion of the template spectra.

This keyword is useful when the templates have higher resolution than the galaxy and they were not convolved to match the instrumental dispersion of the galaxy spectrum. In this situation, the convolution is done by pPXF with increased accuracy, using an analytic Fourier Transform.

sky: vector containing the spectrum of the sky to be included in the fit, or array of dimensions
sky[n_pixels, nSky] containing different sky spectra to add to the model of the observed
galaxy spectrum. The sky has to be log-rebinned as the galaxy spectrum and needs to
have the same number of pixels.

The sky is generally subtracted from the data before the **pPXF** fit. However, for observations very heavily dominated by the sky spectrum, where a very accurate sky subtraction is critical, it may be useful *not* to subtract the sky from the spectrum, but to include it in the fit using this keyword.

templates_rfft: When calling pPXF many times with an identical set of templates, one can use this keyword to pass the real FFT of the templates, computed in a previous pPXF call, stored in the pp.templates_rfft attribute. This keyword mainly exists to show that there is no need for it...

IMPORTANT: Use this keyword only if you understand what you are doing!

tied: A list of string expressions. Each expression "ties" the parameter to other free or fixed parameters. Any expression involving constants and the parameter array p[j] are permitted. Since they are totally constrained, tied parameters are considered to be fixed; no errors are computed for them.

This is an array, or list of arrays, with the same dimensions as **start**. In practice, for every element of **start** one needs to specify either an empty string '' implying that the parameter is free, or a string expression involving some of the variables p[j], where j represents the index of the flattened list of kinematic parameters.

EXAMPLE: We want to fit three kinematic components, with 4 moments for the first component and 2 moments for the second and third (e.g. stars and two gas components). In this case:

moments = [4, 2, 2]
start = [[V1, sigma1, 0, 0], [V2, sigma2], [V3, sigma3]]
then we can force the equality constraint V2 = V3 as follows:
tied = [['', '', '', ''], ['', ''], ['p[4]', '']] # p[6] = p[4]
or we can force the equality constraint sigma2 = sigma3 as follows:

tied = [['', '', '', ''], ['', ''], ['', 'p[5]']] # p[7] = p[5]

One can also use more general formulas. For example one could constrain V3 = (V1 + V2)/2 as well as sigma1 = sigma2 as follows:

p[5] = p[1]
p[6] = (p[0] + p[4])/2
tied = [['', '', '', ''], ['', 'p[1]'], ['(p[0] + p[4])/2', '']]

NOTE: One could in principle use the tied keyword to completely tie the LOSVD of two kinematic components. However, this same effect is more efficient achieved by assigning them to the same kinematic component using the component keyword.

trig: Set trig=True to use trigonometric series as an alternative to Legendre polynomials, for both the additive and multiplicative polynomials. When trig=True the fitted series below has N = degree/2 or N = mdegree/2:

poly = A_0 + sum_{n=1}^{N} [A_n*cos(n*th) + B_n*sin(n*th)]

IMPORTANT: The trigonometric series has periodic boundary conditions. This is sometimes a desirable property, but this expansion is not as flexible as the Legendre polynomials.

velscale_ratio: int, optional Integer. Gives the integer ratio >= 1 between the velscale
 of the galaxy and the templates. When this keyword is used, the templates are convolved
 by the LOSVD at their native resolution, and only subsequently are integrated over the
 pixels and fitted to galaxy. This keyword is generally unnecessary and mostly useful for
 testing.

Note that in realistic situations the uncertainty in the knowledge and variations of the intrinsic line-spread function becomes the limiting factor in recovering the LOSVD well below velscale.

vsyst: float, optional Reference velocity in km/s (default 0). The input initial guess and the output velocities are measured with respect to this velocity. This keyword can be used to account for the difference in the starting wavelength of the templates and the galaxy spectrum as follows:

vsyst = c*np.log(wave_temp[0]/wave_gal[0])

As alternative to using this keyword, one can pass the wavelengths lam and lam_temp of both the galaxy and templates spectra. In that case vsyst is computed automatically and should not be given.

The value assigned to this keyword is *crucial* for the two-sided fitting. In this case vsyst can be determined from a previous normal one-sided fit to the galaxy velocity profile. After that initial fit, vsyst can be defined as the measured velocity at the galaxy center. More accurately vsyst is the value which has to be subtracted to obtain a nearly anti-symmetric velocity profile at the two opposite sides of the galaxy nucleus.

IMPORTANT: this value is generally *different* from the systemic velocity one can get from the literature. Do not try to use that!

Output Parameters

Stored as attributes of the pPXF class:

.apoly: Vector with the best fitting additive polynomial.

- .bestfit: Vector with the best fitting model for the galaxy spectrum. This is a linear combination of the templates, convolved with the best fitting LOSVD, multiplied by the multiplicative polynomials and with subsequently added polynomial continuum terms or sky components.
- .chi2: The reduced chi^2 (namely chi^2/DOF) of the fit, where DOF = pp.dof (approximately
 DOF ~ pp.goodpixels.size).

IMPORTANT: if Chi²/DOF is not ~1 it means that the errors are not properly estimated, or that the template is bad and it is *not* safe to set the clean keyword.

.error: This variable contains a vector of *formal* uncertainty (1*sigma) for the fitted parameters in the output vector sol. They are computed from the estimated covariance matrix of the standard errors in the fitted parameters assuming it is diagonal at the minimum. This option can be used when speed is essential, to obtain an order of magnitude estimate of the uncertainties, but we *strongly* recommend to run bootstrapping simulations to obtain more reliable errors. In fact, these errors can be severely underestimated in the region where the penalty effect is most important (sigma < 2*velscale). These errors are meaningless unless $Chi^2/DOF \sim 1$. However if one *assumes* that the fit is good, a corrected estimate of the errors is:

error_corr = error*sqrt(chi^2/DOF) = pp.error*sqrt(pp.chi2).

IMPORTANT: when running Monte Carlo simulations to determine the error, the penalty (bias) should be set to zero, or better to a very small value. See Section 3.4 of Cappellari & Emsellem (2004) for an explanation.

- .gas_bestfit: If gas_component is not None, this attribute returns the best-fitting gas emission-lines spectrum alone. The best-fitting stellar spectrum alone can be computed as stars_bestfit = pp.bestfit - pp.gas_bestfit
- .gas_bestfit_templates: If gas_component is not None, this attribute returns the individual best-fitting gas emission-lines templates as columns of an array. Note that pp.gas_bestfit = pp.gas_bestfit_templates.sum(1)
- .gas_flux: Vector with the integrated flux (in counts) of all lines set as True in the input gas_component keyword. This is the flux of individual gas templates, which may include multiple lines. This implies that, if a gas template describes a doublet, the flux is that of both lines. If the Balmer series is input as a single template, this is the flux of the entire series.

The returned fluxes are not corrected in any way and in particular, no reddening correction is applied. In other words, the returned .gas_flux should be unchanged, within the errors, regardless of whether reddening or multiplicative polynomials were fitted by pPXF or not.

IMPORTANT: pPXF makes no assumptions about the input flux units: The returned .gas_flux has the same units and values one would measure (with lower accuracy) by summing the pixels values, within the given gas lines, on the continuum-subtracted input galaxy spectrum. This implies that, if the spectrum is in units of erg/(s cm^2 A), the .gas_flux returned by pPXF should be multiplied by the pixel size in Angstrom at the line wavelength to obtain the integrated line flux in units of erg/(s cm^2).

NOTE: If there is no gas reddening and each input gas templates was normalized to sum = 1, then pp.gas_flux = pp.weights[pp.gas_component].

When a gas template is identically zero within the fitted region, then pp.gas_flux = pp.gas_flux_error = np.nan. The corresponding components of pp.gas_zero_template are set to True. These np.nan values are set at the end of the calculation to flag the undefined values. These flags generally indicate that some of the gas templates passed to pPXF consist of gas emission lines that fall outside the fitted wavelength range or within a masked spectral region. These np.nan do *not* indicate numerical issues with the actual pPXF calculation and the rest of the pPXF output is reliable.

.gas_flux_error: Formal uncertainty (1*sigma) for the quantity pp.gas_flux, in the same units as the gas fluxes.

This error is approximate as it ignores the covariance between the gas flux and any non-linear parameter. Bootstrapping can be used for more accurate errors.

These errors are meaningless unless $Chi^2/DOF \sim 1$. However if one *assumes* that the fit is good, a corrected estimate of the errors is:

gas_flux_error_corr = gas_flux_error*sqrt(chi^2/DOF)

= pp.gas_flux_error*sqrt(pp.chi2).

.gas_mpoly: vector with the best-fitting gas reddening curve.

- .gas_reddening: Best fitting E(B-V) value if the gas_reddening keyword is set. This is especially useful when the Balmer series is input as a single template with an assumed theoretically predicted decrement e.g. using emission_lines(..., tie_balmer=True) in ppxf.ppxf_util to compute the gas templates.
- .gas_zero_template: vector of size gas_component.sum() set to True where the gas template
 was identically zero within the fitted region. For those gas components pp.gas_flux
 = pp.gas_flux_error = np.nan. These flags generally indicate that some of the gas
 templates passed to pPXF consist of gas emission lines that fall outside the fitted wavelength
 range or within a masked spectral region.
- .goodpixels: Integer vector containing the indices of the good pixels in the fit. This vector is a copy of the input goodpixels if clean = False otherwise it will be updated by removing the detected outliers.
- .matrix: Prediction matrix[n_pixels, degree+n_templates] of the linear system.

pp.matrix[n_pixels, :degree] contains the additive polynomials if degree >= 0.

pp.matrix[n_pixels, degree:] contains the templates convolved by the LOSVD, and multiplied by the multiplicative polynomials if mdegree > 0.

.mpoly: Best fitting multiplicative polynomial (or reddening curve when reddening is set).

.mpolyweights: This is largely superseded by the .mpoly attribute above.

When mdegree > 0 this contains in output the coefficients of the multiplicative Legendre polynomials of order 1, 2,... mdegree. The polynomial can be explicitly evaluated as:

```
from numpy.polynomial import legendre
x = np.linspace(-1, 1, len(galaxy))
mpoly = legendre.legval(x, np.append(1, pp.mpolyweights))
```

When trig = True the polynomial is evaluated as:

mpoly = pp.trigval(x, np.append(1, pp.mpolyweights))

- .phot_bestfit: array_like with shape (n_phot) When phot is given, then this attribute contains the best fitting fluxes in the photometric bands given as input in phot_galaxy.
- .plot: function Call the method function pp.plot() after the call to pp = ppxf(...) to
 produce a plot of the best fit. This is an alternative to calling pp = ppxf(..., plot=True).

Use the command pp.plot(gas_clip=True) to scale the plot based on the stellar continuum alone, while allowing for the gas emission lines to go outside the plotting region. This is useful to inspect the fit to the stellar continuum, in the presence of strong gas emission lines. This has effect only if gas_component is not None.

.polyweights: This is largely superseded by the .apoly attribute above.

When degree >= 0 contains the weights of the additive Legendre polynomials of order 0, 1,... degree. The best fitting additive polynomial can be explicitly evaluated as:

from numpy.polynomial import legendre

x = np.linspace(-1, 1, len(galaxy))
apoly = legendre.legval(x, pp.polyweights)

When trig=True the polynomial is evaluated as:

apoly = pp.trigval(x, pp.polyweights)

When doing a two-sided fitting (see help for galaxy parameter), the additive polynomials are allowed to be different for the left and right spectrum. In that case, the output weights of the additive polynomials alternate between the first (left) spectrum and the second (right) spectrum.

.reddening: Best fitting E(B-V) value if the reddening keyword is set.

.sol: Vector containing in output the parameters of the kinematics.

- If moments=2 this contains [Vel, Sigma]
- If moments=4 this contains [Vel, Sigma, h3, h4]
- If moments=N this contains [Vel, Sigma, h3,... hN]

When fitting multiple kinematic component, pp.sol contains a list with the solution for all different components, one after the other, sorted by component: pp.sol = [sol1, sol2,...].

Vel is the velocity, Sigma is the velocity dispersion, h3 - h6 are the Gauss-Hermite coefficients. The model parameters are fitted simultaneously.

IMPORTANT: The precise relation between the output pPXF velocity and redshift is Vel = c*np.log(1 + z). See Section 2.3 of Cappellari (2017) for a detailed explanation.

These are the default safety limits on the fitting parameters (they can be changed using the **bounds** keyword):

- Vel is constrained to be +/-2000 km/s from the input guess
- velscale/100 < Sigma < 1000 $\rm km/s$
- -0.3 < [h3, h4, ...] < 0.3 (extreme value for real galaxies)

In the case of two-sided LOSVD fitting the output values refer to the first input galaxy spectrum, while the second spectrum will have by construction kinematics parameters [-Vel, Sigma, -h3, h4, -h5, h6]. If vsyst is nonzero (as required for two-sided fitting), then the output velocity is measured with respect to vsyst.

- .status: Contains the output status of the optimization. Positive values generally represent success (the meaning of status is defined as in scipy.optimize.least_squares).
- .weights: Receives the value of the weights by which each template was multiplied to best fit the galaxy spectrum. The optimal template can be computed with an array-vector multiplication:

bestemp = templates @ weights

These .weights do not include the weights of the additive polynomials which are separately stored in pp.polyweights.

When the sky keyword is used weights[:n_templates] contains the weights for the templates, while weights[n_templates:] gives the ones for the sky. In that case the best fitting galaxy template and sky are given by:

```
bestemp = templates @ weights[:n_templates]
bestsky = sky @ weights[n_templates:]
```

When doing a two-sided fitting (see help for galaxy parameter) *together* with the sky keyword, the sky weights are allowed to be different for the left and right spectrum. In that case the output sky weights alternate between the first (left) spectrum and the second (right) spectrum.

How to Set the Kinematic Penalty Keyword

The bias keyword is only used if moments > 2, otherwise it is ignored.

The pPXF routine can give sensible quick results with the default bias parameter, however, like in any penalized/filtered/regularized method, the optimal amount of penalization generally depends on the problem under study.

The general rule here is that the penalty should leave the line-of-sight velocity-distribution (LOSVD) virtually unaffected, when it is well sampled and the signal-to-noise ratio (S/N) is sufficiently high.

EXAMPLE: If you expect a LOSVD with up to a high h4 ~ 0.2 and your adopted penalty (bias) biases the solution towards a much lower h4 ~ 0.1, even when the measured sigma > 3*velscale and the S/N is high, then you are *misusing* the pPXF method!

THE RECIPE: The following is a simple practical recipe for a sensible determination of the penalty in pPXF:

- 1. Choose a minimum (S/N)_min level for your kinematics extraction and spatially bin your data so that there are no spectra below (S/N)_min;
- 2. Perform a fit of your kinematics *without* penalty (keyword bias=0). The solution will be noisy and may be affected by spurious solutions, however, this step will allow you to check the expected mean ranges in the Gauss-Hermite parameters [h3, h4] for the galaxy under study;
- 3. Perform a Monte Carlo simulation of your spectra, following e.g. the included ppxf_example_montecarlo_simulation.py routine. Adopt as S/N in the simulation the chosen value (S/N)_min and as input [h3, h4] the maximum representative values measured in the non-penalized pPXF fit of the previous step;
- 4. Choose as the penalty (bias) the *largest* value such that, for sigma > 3*velscale, the mean difference delta between the output [h3, h4] and the input [h3, h4] is well within (e.g. delta ~ rms/3) the rms scatter of the simulated values (see an example in Fig. 2 of Emsellem et al. 2004).

Problems with Your First Fit?

Common problems with your first pPXF fit are caused by incorrect wavelength ranges or different velocity scales between galaxy and templates. To quickly detect these problems try to overplot the (log rebinned) galaxy and the template just before calling the pPXF procedure.

You can use something like the following Python lines while adjusting the smoothing window and the pixels shift. If you cannot get a rough match by eye it means something is wrong and it is unlikely that pPXF (or any other program) will find a good match:

```
import numpy as np
import matplotlib.pyplot as plt
from scipy import ndimage
sigma = 2  # Velocity dispersion in pixels
shift = -20  # Velocity shift in pixels
template = np.roll(ndimage.gaussian_filter1d(template, sigma), shift)
plt.plot(galaxy, 'k')
plt.plot(template*np.median(galaxy)/np.median(template), 'r')
```