FittingMethods

May 1, 2023

1 Fitting Methods

Here we will explore the various fitting methods in AutoProf. You have already encountered some of the methods, but here we will take a more systematic approach and discuss their strengths/weaknesses. Each method will be applied to the same problem with the same initial conditions so you can see how they operate.

[1]:
```python
import torch
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.patches import Ellipse
from scipy.stats import gaussian_kde as kde
from scipy.stats import norm

%matplotlib inline
import autoprof as ap
```

[2]:
```python
# Setup a fitting problem. You can ignore this cell to start, it just makes␣
↪some test data to fit

def true_params():

    # just some random parameters to use for fitting. Feel free to play around␣
↪with these to see what happens!
    sky_param = np.array([1.5])
    sersic_params = np.array([
        [ 68.44035491,  65.58516735,   0.54945988, 127.19794926*np.pi/180,   2.
↪14513004,   22.05219055,   2.45583024],
        [ 54.00353786,  41.54430634,   0.40203928,  82.03862521*np.pi/180,   2.
↪88613347,   12.095631,     2.76711163],
        [ 43.13601431,  58.3422508,    0.71894728, 167.07973506*np.pi/180,   3.
↪964371,     5.3767236,     2.41520244],
    ])

    return sersic_params, sky_param

def init_params():
    sky_param = np.array([1.4])
    sersic_params = np.array([
        [ 67.,  66.,   0.6, 130.*np.pi/180,   1.5,   25.,   2.],
        [ 55.,  40.,   0.5,  80.*np.pi/180,   2.,   10.,     3.],
        [ 41.,  60.,    0.8, 170.*np.pi/180,   3.,     4.,     2.],
    ])

    return sersic_params, sky_param

def initialize_model(target, use_true_params = True):

    # Pick parameters to start the model with
    if use_true_params:
        sersic_params, sky_param = true_params()
    else:
        sersic_params, sky_param = init_params()

    # List of models, starting with the sky
    model_list = [ap.models.AutoProf_Model(
        name = "sky",
        model_type = "flat sky model",
        target = target,
        parameters = {"sky": sky_param[0]},
    )]
    # Add models to the list
    for i, params in enumerate(sersic_params):
        model_list.append([
            ap.models.AutoProf_Model(
                name = f"sersic {i}",
                model_type = "sersic galaxy model",
                target = target,
                parameters = {
                    "center": [params[0],params[1]],
                    "q": params[2],
                    "PA": params[3],
                    "n": params[4],
                    "Re": params[5],
                    "Ie": params[6],
                },
                #psf_mode = "full", # uncomment to try everything with PSF␣
↪blurring (takes longer)
            )
        ])

    MODEL = ap.models.Group_Model(
        name = "group",
        model_list = model_list,
        target = target,
    )
    # Make sure every model is ready to go
    MODEL.initialize()

    return MODEL

def generate_target():

    N = 100
    pixelscale = 1.
    rng = np.random.default_rng(42)

    # PSF has sigma of 2x pixelscale
    PSF = ap.utils.initialize.gaussian_psf(2, 21, pixelscale)
    PSF /= np.sum(PSF)

    target = ap.image.Target_Image(
        data = np.zeros((N,N)),
        pixelscale = pixelscale,
        psf = PSF,
    )

    MODEL = initialize_model(target, True)

    # Sample the model with the true values to make a mock image
    img = MODEL().data.detach().cpu().numpy()
    # Add poisson noise
    target.data = torch.Tensor(img + rng.normal(scale = np.sqrt(img)/2))
    target.variance = torch.Tensor(img/4)

    fig, ax = plt.subplots(figsize = (8,8))
    ap.plots.target_image(fig, ax, target)
    ax.axis("off")
    plt.show()

    return target


def corner_plot(chain, labels=None, bins=None, true_values=None,␣
↪plot_density=True, plot_contours=True, figsize=(10, 10)):
    ndim = chain.shape[1]

    fig, axes = plt.subplots(ndim, ndim, figsize=figsize)
    plt.subplots_adjust(wspace=0., hspace=0.)
    if bins is None:
        bins = int(np.sqrt(chain.shape[0]))

    for i in range(ndim):
        for j in range(ndim):
            ax = axes[i, j]

            i_range = (np.min(chain[:, i]), np.max(chain[:, i]))
            j_range = (np.min(chain[:, j]), np.max(chain[:, j]))
            if i == j:
                # Plot the histogram of parameter i
                #ax.hist(chain[:, i], bins=bins, histtype="step", range =␣
↪i_range, density=True, color="k", lw=1)

                if plot_density:
                    # Plot the kernel density estimate
                    kde_x = np.linspace(i_range[0], i_range[1], 100)
                    kde_y = kde(chain[:, i])(kde_x)
                    ax.plot(kde_x, kde_y, color="green", lw=1)

                if true_values is not None:
                    ax.axvline(true_values[i], color='red', linestyle='-', lw=1)
                ax.set_xlim(i_range)

            elif i > j:
                # Plot the 2D histogram of parameters i and j
                #ax.hist2d(chain[:, j], chain[:, i], bins=bins, cmap="Greys")

                if plot_contours:
                    # Plot the kernel density estimate contours
                    kde_ij = kde([chain[:, j], chain[:, i]])
                    x, y = np.mgrid[j_range[0]:j_range[1]:100j, i_range[0]:
↪i_range[1]:100j]
                    positions = np.vstack([x.ravel(), y.ravel()])
                    kde_pos = np.reshape(kde_ij(positions).T, x.shape)
                    ax.contour(x, y, kde_pos, colors="green", linewidths=1,␣
↪levels=3)


                if true_values is not None:
                    ax.axvline(true_values[j], color='red', linestyle='-', lw=1)
                    ax.axhline(true_values[i], color='red', linestyle='-', lw=1)
                ax.set_xlim(j_range)
                ax.set_ylim(i_range)

            else:
                ax.axis("off")

            if j == 0 and labels is not None:
                ax.set_ylabel(labels[i])
            ax.yaxis.set_major_locator(plt.NullLocator())

            if i == ndim - 1 and labels is not None:
                ax.set_xlabel(labels[j])
            ax.xaxis.set_major_locator(plt.NullLocator())

    plt.show()

def corner_plot_covariance(cov_matrix, mean, labels=None, figsize=(10, 10),␣
 ↪true_values = None, ellipse_colors='g'):
    num_params = cov_matrix.shape[0]
    fig, axes = plt.subplots(num_params, num_params, figsize=figsize)
    plt.subplots_adjust(wspace=0., hspace=0.)

    for i in range(num_params):
        for j in range(num_params):
            ax = axes[i, j]

            if i == j:
                x = np.linspace(mean[i] - 3 * np.sqrt(cov_matrix[i, i]),␣
 ↪mean[i] + 3 * np.sqrt(cov_matrix[i, i]), 100)
                y = norm.pdf(x, mean[i], np.sqrt(cov_matrix[i, i]))
                ax.plot(x, y, color='g')
                ax.set_xlim(mean[i] - 3 * np.sqrt(cov_matrix[i, i]), mean[i] +␣
 ↪3 * np.sqrt(cov_matrix[i, i]))
                if true_values is not None:
                    ax.axvline(true_values[i], color='red', linestyle='-', lw=1)
            elif j < i:
                cov = cov_matrix[np.ix_([j, i], [j, i])]
                lambda_, v = np.linalg.eig(cov)
                lambda_ = np.sqrt(lambda_)
                angle = np.rad2deg(np.arctan2(v[1, 0], v[0, 0]))
                for k in [1, 2]:
                    ellipse = Ellipse(xy=(mean[j], mean[i]),
                                      width=lambda_[0] * k * 2,
                                      height=lambda_[1] * k * 2,
                                      angle=angle,
                                      edgecolor=ellipse_colors,
                                      facecolor='none')
                    ax.add_artist(ellipse)

                # Set axis limits
                margin = 3
                ax.set_xlim(mean[j] - margin * np.sqrt(cov_matrix[j, j]),␣
 ↪mean[j] + margin * np.sqrt(cov_matrix[j, j]))
```

```
                ax.set_ylim(mean[i] - margin * np.sqrt(cov_matrix[i, i]),␣
↪mean[i] + margin * np.sqrt(cov_matrix[i, i]))

                if true_values is not None:
                    ax.axvline(true_values[j], color='red', linestyle='-', lw=1)
                    ax.axhline(true_values[i], color='red', linestyle='-', lw=1)

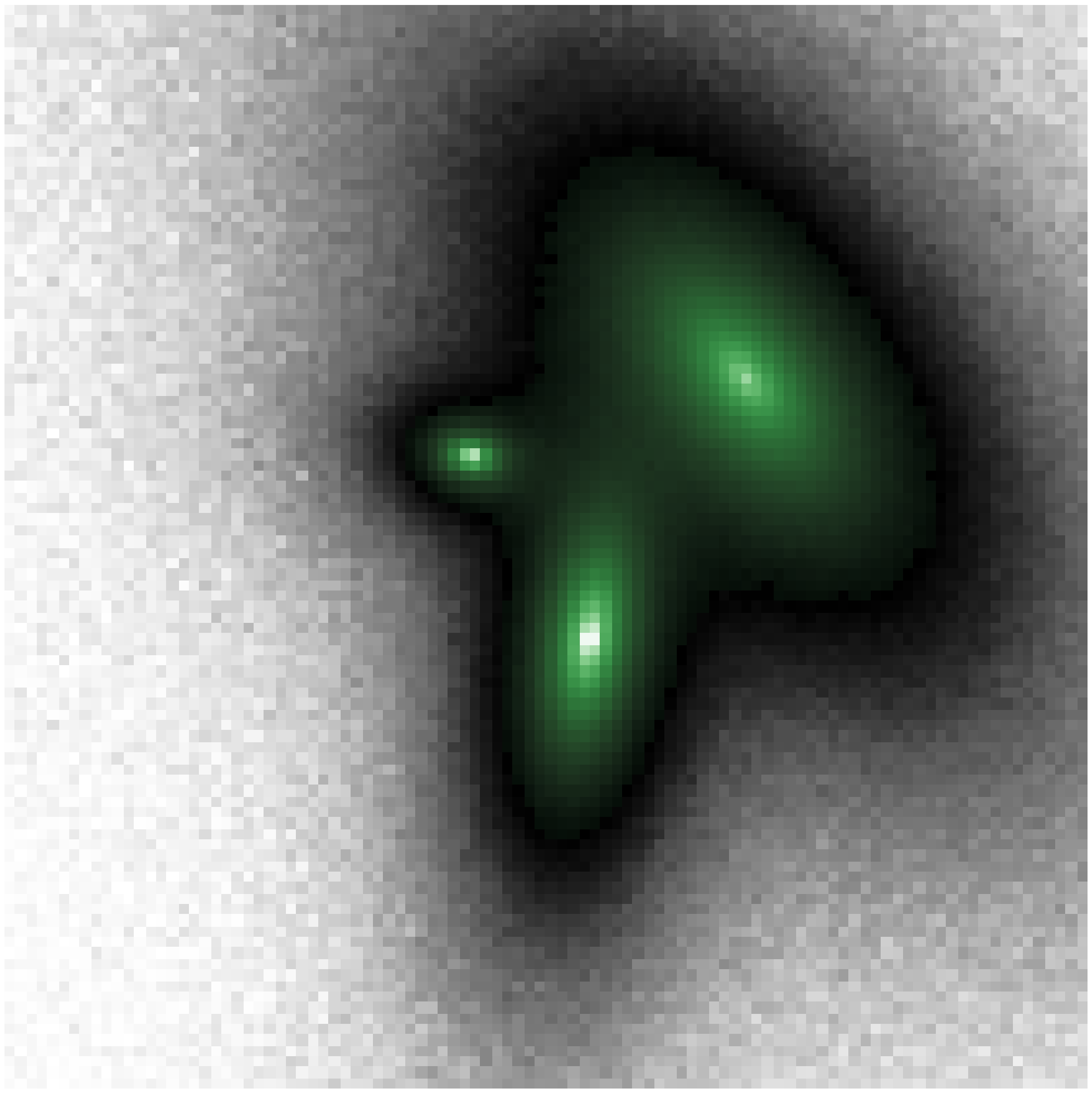
            if j > i:
                ax.axis('off')

            if i < num_params - 1:
                ax.set_xticklabels([])
            else:
                if labels is not None:
                    ax.set_xlabel(labels[j])
            ax.yaxis.set_major_locator(plt.NullLocator())

            if j > 0:
                ax.set_yticklabels([])
            else:
                if labels is not None:
                    ax.set_ylabel(labels[i])
            ax.xaxis.set_major_locator(plt.NullLocator())

    plt.show()


target = generate_target()
```



1.1 Levenberg-Marquardt

This fitter is identitied as `ap.fit.LM` and it employs a variant of the second order Newton's method to converge very quickly to the local minimum. This is the generally accepted best algorithm for most use cases in χ^2 minimization. If you don't know what to pick, start with this minimizer. The LM optimizer bridges the gap between first-order gradient descent and second order Newton's method. When far from the minimum, Newton's method is unstable and can give wildly wrong results, so LM takes gradient descent steps. However, near the minimum it switches to the Newton's method which has "quadratic convergence" this means that it takes only a few iterations to converge to several decimal places. This can be represented as:

$(H + LI)h = g$

Where H is the Hessian matrix of second derivatives, L is the damping parameter, I is the identity matrix, h is the step we will take in parameter space, and g is the gradient. We solve this linear system for h to get the next update step. The "L" scale parameter goes from L >> 1 which represents gradient descent to L << 1 which is Newton's Method. When L >> 1 the hessian is effectively zero and we get $h = g/L$ which is just gradient descent with $1/L$ as the learning rate. In AutoProf the damping parameter is treated somewhat differently, but the concept is the same.

LM can handle a lot of scenarios and converge to the minimum. Keep in mind, however, that it is seeking a local minimum, so it is best to start off the algorithm as close as possible to the best fit parameters. AutoProf can automatically initialize, as discussed in other notebooks, but even that needs help sometimes (often in the form of a segmentation map).

The main drawback of LM is its memory consumption which goes as $\mathcal{O}(PN)$ where P is the number of pixels and N is the number of parameters.

[3]:
```
MODEL = initialize_model(target, False)
fig, axarr = plt.subplots(1,4, figsize = (24,5))
plt.subplots_adjust(wspace= 0.1)
ap.plots.model_image(fig, axarr[0], MODEL)
axarr[0].set_title("Model before optimization")
ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
axarr[1].set_title("Residuals before optimization")

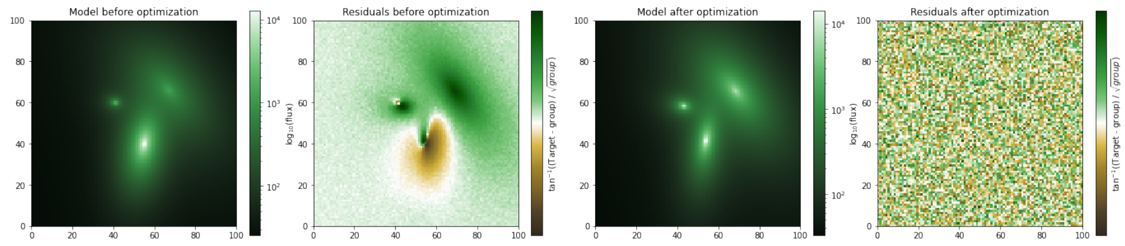
res_lm = ap.fit.LM(MODEL, verbose = 1).fit()

ap.plots.model_image(fig, axarr[2], MODEL)
axarr[2].set_title("Model after optimization")
ap.plots.residual_image(fig, axarr[3], MODEL, normalize_residuals = True)
axarr[3].set_title("Residuals after optimization")
plt.show()
```

```
L: 1.0
---------init---------
LM loss: 283.81094319158024
L: 1.0
---------iter---------
LM loss: 849.0109828400438
reject
L: 11.0
---------iter---------
LM loss: 192.57226752058315
accept
L: 1.2222222222222223
---------iter---------
LM loss: 69.76483619240399
accept
L: 0.1358024691358025
---------iter---------
LM loss: 24.256005308222395
accept
```

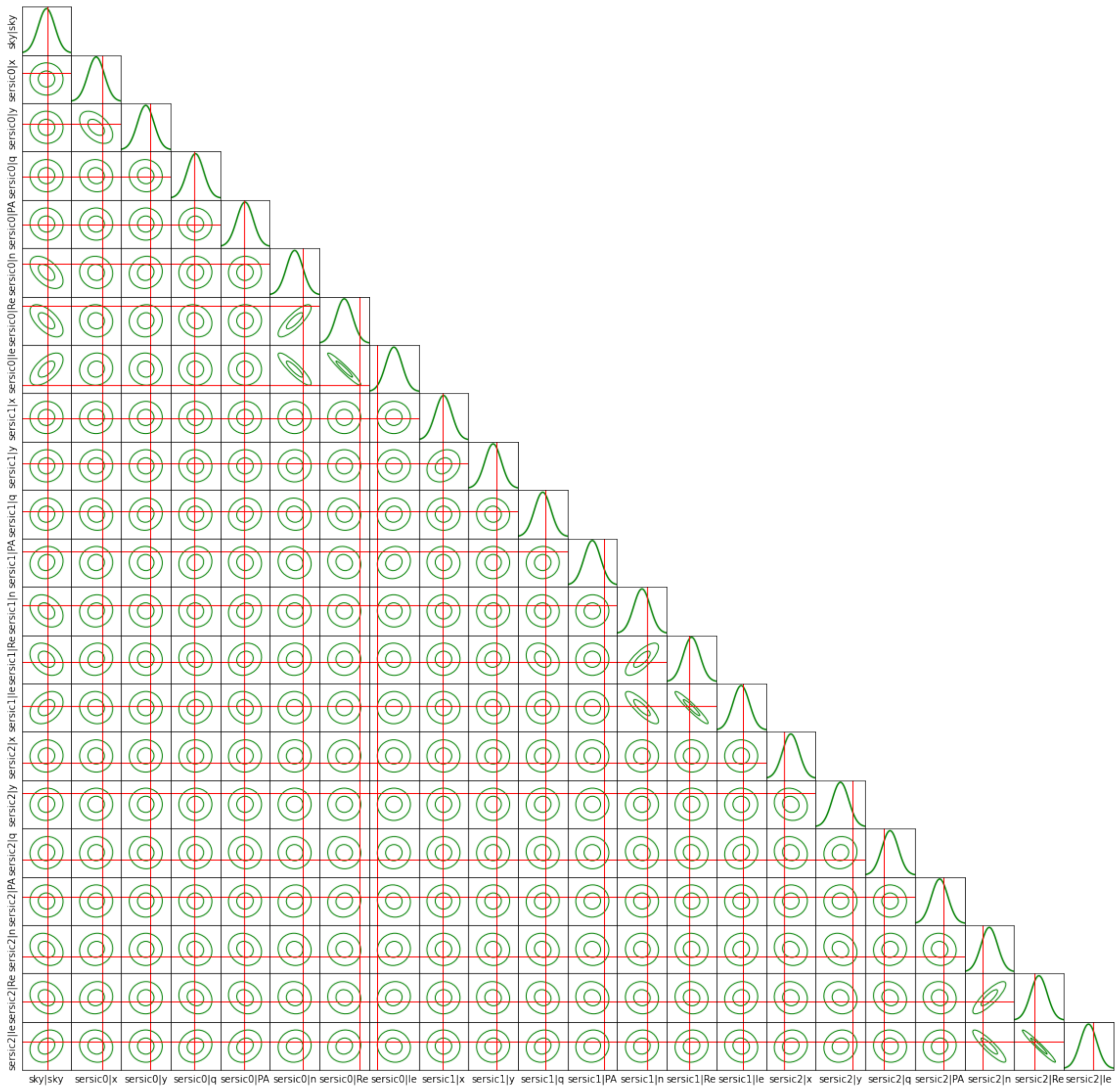
```
L: 0.015089163237311388
---------iter---------
LM loss: 30.071938222875325
reject
L: 0.16598079561042528
---------iter---------
LM loss: 27.261758221743143
reject
L: 1.825788751714678
---------iter---------
LM loss: 18.69506679958759
accept
L: 0.20286541685718645
---------iter---------
LM loss: 28.386073296858303
reject
L: 2.231519585429051
---------iter---------
LM loss: 15.242646605322426
accept
L: 0.2479466206032279
---------iter---------
LM loss: 22.387939636837555
reject
L: 2.727412826635507
---------iter---------
LM loss: 12.461517579583184
accept
L: 0.3030458696261674
---------iter---------
LM loss: 12.126933297954073
reject
L: 3.3335045658878415
---------iter---------
LM loss: 10.564772629729806
accept
L: 0.3703893962097602
---------iter---------
LM loss: 6.123883804201112
accept
L: 0.04115437735664002
---------iter---------
LM loss: 3.3033211897345005
accept
L: 0.004572708595182225
---------iter---------
LM loss: 1.9106270717708704
accept
```

```
L: 0.000508078732798025
---------iter---------
LM loss: 1.4800231508207649
accept
L: 5.6453192533113885e-05
---------iter---------
LM loss: 1.012878922723731
accept
L: 6.272576948123765e-06
---------iter---------
LM loss: 1.0127841836614357
accept
L: 6.969529942359739e-07
---------iter---------
LM loss: 1.0127841824837123
accept
```



Now that LM has found the χ^2 minimum, we can do a really neat trick. Since LM needs the hessian matrix, we have access to the hessian matrix at the minimum. This is in fact equal to the negative Fisher information matrix. If we take the matrix inverse of this matrix then we get the covariance matrix for a multivariate gaussian approximation of the χ^2 surface near the minimum. With the covariance matrix we can create a corner plot just like we would with an MCMC. We will see later that the MCMC methods (at least the ones which converge) produce very similar results!

```
[4]: param_names = list(MODEL.parameter_order())
     i = 0
     while i < len(param_names):
         param_names[i] = param_names[i].replace(" ", "")
         if "center" in param_names[i]:
             center_name = param_names.pop(i)
             param_names.insert(i, center_name.replace("center", "y"))
             param_names.insert(i, center_name.replace("center", "x"))
         i += 1
     ser, sky = true_params()
     corner_plot_covariance(
         res_lm.covariance_matrix.detach().cpu().numpy(),
         MODEL.get_parameter_vector().detach().cpu().numpy(),
         labels = param_names,
         figsize = (20,20),
         true_values = np.concatenate((sky,ser.ravel()))
     )
```



1.2 Iterative Fit (models)

An iterative fitter is identified as `ap.fit.Iter`, this method is generally employed for large models where it is not feasible to hold all the relevant data in memory at once. The iterative fitter will cycle through the models in a `Group_Model` object and fit them one at a time to the image, using the residuals from the previous cycle. This can be a very robust way to deal with some fits, especially if the overlap between models is not too strong. It is however more dependent on good initialization than other methods like the Levenberg-Marquardt. Also, it is possible for the Iter method to get stuck in a local minimum under certain circumstances.

Note that while the Iterative fitter needs a `Group_Model` object to iterate over, it is not necessarily true that the sub models are `Component_Model` objects, they could be `Group_Model` objects as well. In this way it is possible to cycle through and fit "clusters" of objects that are nearby, so long as it doesn't consume too much memory.

By only fitting one model at a time it is possible to get caught in a local minimum. For this reason it can be good to mix-and-match the iterative optimizers so they can help each other get unstuck.

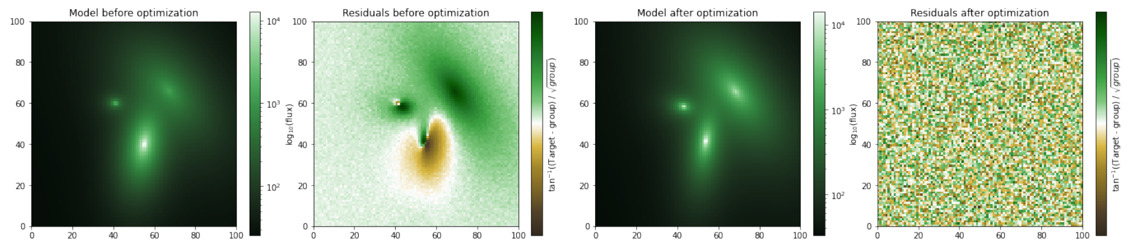
[5]:
```
MODEL = initialize_model(target, False)
fig, axarr = plt.subplots(1,4, figsize = (24,5))
plt.subplots_adjust(wspace= 0.1)
ap.plots.model_image(fig, axarr[0], MODEL)
axarr[0].set_title("Model before optimization")
ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
axarr[1].set_title("Residuals before optimization")

res_iter = ap.fit.Iter(MODEL, verbose = 1).fit()

ap.plots.model_image(fig, axarr[2], MODEL)
axarr[2].set_title("Model after optimization")
ap.plots.residual_image(fig, axarr[3], MODEL, normalize_residuals = True)
axarr[3].set_title("Residuals after optimization")
plt.show()
```

```
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 7.205865375699771
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 2.4705932063631284
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.5805326550442294
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.2512768478124128
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.1127864669960037
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0530447882827145
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0282650623186584
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0184151513545818
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0147107760651968
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0134398452263913
--------iter-------
sky
```

```
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0129958243247057
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.012848036312808
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.0128020490769345
--------iter-------
sky
sersic 0
sersic 1
sersic 2
Update Chi^2 with new parameters
Loss: 1.012788813135204
```



1.3 Iterative Fit (parameters)

This is an iterative fitter identified as `ap.fit.Iter_LM` and is generally employed for large models where it is not feasible to hold all the relevant data in memory at once. This iterative fitter will cycle through chunks of parameters and fit them one at a time to the image. This can be a very robust way to deal with some fits, especially if the overlap between models is not too strong. This is very similar to the other iterative fitter, however it is necessary for certain fitting circumstances when the problem can't be broken down into individual component models. This occurs, for example, when the models have many shared (constrained) parameters and there is no obvious way to break down sub-groups of models (an example of this is discussed in the AutoProf paper).

Note that this is iterating over the parameters, not the models. This allows it to handle parameter covariances even for very large models (if they happen to land in the same chunk). However, for this to work it must evaluate the whole model at each iteration making it somewhat slower than the regular `Iter` fitter, though it can make up for it by fitting larger chunks at a time which makes the whole optimization faster.

By only fitting a subset of parameters at a time it is possible to get caught in a local minimum. For this reason it can be good to mix-and-match the iterative optimizers so they can help each other get unstuck.

```
[6]: MODEL = initialize_model(target, False)
     fig, axarr = plt.subplots(1,4, figsize = (24,5))
     plt.subplots_adjust(wspace= 0.1)
     ap.plots.model_image(fig, axarr[0], MODEL)
     axarr[0].set_title("Model before optimization")
     ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
     axarr[1].set_title("Residuals before optimization")

     res_iterlm = ap.fit.Iter_LM(MODEL, chunks = 11, verbose = 1).fit()

     ap.plots.model_image(fig, axarr[2], MODEL)
     axarr[2].set_title("Model after optimization")
     ap.plots.residual_image(fig, axarr[3], MODEL, normalize_residuals = True)
     axarr[3].set_title("Residuals after optimization")
     plt.show()
```

```
--------iter-------
['140099848431264:0' '140100290926240:0' '140099852362176:0'
 '140103645984896:0' '140099848431360:0' '140099848432320:0'
 '140099848430880:0' '140099848430112:0' '140099848430976:0'
 '140099848399696:0' '140099848398544:0']
chunk loss: 35.836873026504335
['140099848432224:0' '140099848431264:1' '140100290925376:0'
 '140103645984704:0' '140099848431360:1' '140099848433040:0'
 '140099848430352:0' '140099848430352:1' '140099848431552:0'
 '140099848399648:0' '140099848400800:0']
chunk loss: 14.562455505279104
Loss: 14.562455505279104
--------iter-------
['140099848431264:0' '140100290925376:0' '140100290926240:0'
 '140103645984704:0' '140103645984896:0' '140099848431360:0'
 '140099848432320:0' '140099848433040:0' '140099848430352:1'
 '140099848399648:0' '140099848400800:0']
chunk loss: 13.152171158257392
['140099848432224:0' '140099848431264:1' '140099852362176:0'
 '140099848431360:1' '140099848430880:0' '140099848430112:0'
 '140099848430976:0' '140099848430352:0' '140099848431552:0'
 '140099848399696:0' '140099848398544:0']
```

```
chunk loss: 3.510773458706077
Loss: 3.510773458706077
--------iter-------
['140099848432224:0' '140099848431264:1' '140100290925376:0'
 '140099848431360:0' '140099848430880:0' '140099848433040:0'
 '140099848430352:0' '140099848430352:1' '140099848399648:0'
 '140099848399696:0' '140099848398544:0']
chunk loss: 3.353452269676198
['140099848431264:0' '140100290926240:0' '140099852362176:0'
 '140103645984704:0' '140103645984896:0' '140099848431360:1'
 '140099848432320:0' '140099848430112:0' '140099848430976:0'
 '140099848431552:0' '140099848400800:0']
chunk loss: 3.0961597807131325
Loss: 3.0961597807131325
--------iter-------
['140099848432224:0' '140099848431264:0' '140099848431264:1'
 '140100290925376:0' '140103645984896:0' '140099848431360:1'
 '140099848430112:0' '140099848433040:0' '140099848430352:0'
 '140099848399648:0' '140099848398544:0']
chunk loss: 2.8631077057761045
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 '140099848431360:0' '140099848432320:0' '140099848430880:0'
 '140099848430976:0' '140099848430352:1' '140099848431552:0'
 '140099848399696:0' '140099848400800:0']
chunk loss: 2.7339689038865473
Loss: 2.7339689038865473
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 '140099848431552:0' '140099848398544:0']
chunk loss: 1.5444639707866126
Loss: 1.5444639707866126
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 '140099848399696:0' '140099848398544:0']
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 '140099848430112:0' '140099848430976:0' '140099848430352:1'
 '140099848431552:0' '140099848400800:0']
```

```
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Loss: 1.432121259627228
--------iter-------
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 '140099848399696:0' '140099848398544:0']
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 '140099848430880:0' '140099848430976:0' '140099848430352:0'
 '140099848430352:1' '140099848400800:0']
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Loss: 1.3726253391697867
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 '140099848431552:0' '140099848399648:0']
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Loss: 1.3197302033549454
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Loss: 1.2850000299916242
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 '140099848433040:0' '140099848430352:0' '140099848430352:1'
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```
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Loss: 1.0489710124807763
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 '140099848399648:0' '140099848398544:0']
chunk loss: 1.0285384354855114
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Loss: 1.0196543663874342
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 '140099848399696:0' '140099848400800:0']
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 '140099848430352:0' '140099848430352:1' '140099848431552:0'
 '140099848399648:0' '140099848398544:0']
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Loss: 1.018786867713684
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Loss: 1.0180926607221428
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 '140099848399696:0' '140099848398544:0']
```

```
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Loss: 1.0163310631654936
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 '140099848398544:0' '140099848400800:0']
chunk loss: 1.0152477444592884
['140099848431264:0' '140100290925376:0' '140100290926240:0'
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 '140099848431360:0' '140099848431360:1' '140099848433040:0'
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chunk loss: 1.0151040664642486
Loss: 1.0151040664642486
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 '140099848399696:0' '140099848400800:0']
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Loss: 1.0149317275999186
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 '140099848399696:0' '140099848398544:0']
chunk loss: 1.0131967739454029
Loss: 1.0131967739454029
--------iter-------
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 '140099848431360:1' '140099848432320:0' '140099848430880:0'
 '140099848430112:0' '140099848430976:0' '140099848431552:0'
 '140099848398544:0' '140099848400800:0']
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 '140099848399648:0' '140099848399696:0']
```

```
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Loss: 1.0130944490316525
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 '140099848430112:0' '140099848430976:0' '140099848433040:0'
 '140099848430352:0' '140099848399696:0']
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 '140099848398544:0' '140099848400800:0']
chunk loss: 1.0129278984762435
Loss: 1.0129278984762435
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 '140099848430112:0' '140099848400800:0']
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 '140099848399696:0' '140099848398544:0']
chunk loss: 1.0128991377677936
Loss: 1.0128991377677936
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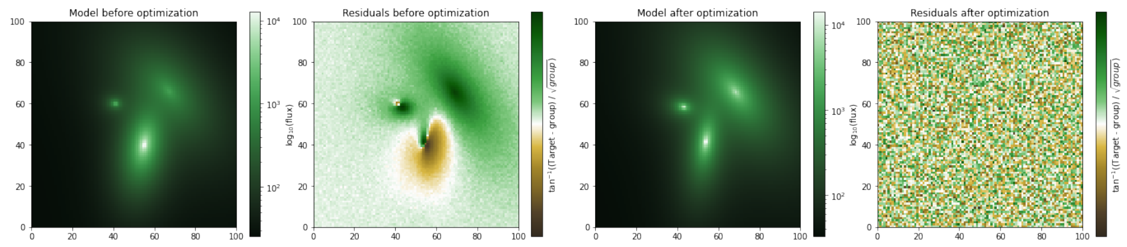
 '140099848430880:0' '140099848430976:0' '140099848433040:0'
 '140099848399696:0' '140099848398544:0']
chunk loss: 1.012888742507812
Loss: 1.012888742507812
```



1.4 Gradient Descent

A gradient descent fitter is identified as `ap.fit.Grad` and uses standard first order derivative methods as provided by PyTorch. These gradient descent methods include Adam, SGD, and LBFGS to name a few. The first order gradient is faster to evaluate and uses less memory, however it is considerably slower to converge than Levenberg-Marquardt. The gradient descent method with a small learning rate will reliably converge towards a local minimum, it will just do so slowly.

In the example below we let it run for 1000 steps and even still it has not converged. In general you should not use gradient descent to optimize a model. However, in a challenging fitting scenario the small step size of gradient descent can actually be an advantage as it will not take any unedpectedly large steps which could mix up some models, or hop over the χ^2 minimum into impossible parameter space. Just make sure to finish with LM after using Grad so that it fully converges to a reliable minimum.

[7]:
```
MODEL = initialize_model(target, False)
fig, axarr = plt.subplots(1,4, figsize = (24,5))
plt.subplots_adjust(wspace= 0.1)
ap.plots.model_image(fig, axarr[0], MODEL)
axarr[0].set_title("Model before optimization")
ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
axarr[1].set_title("Residuals before optimization")

res_grad = ap.fit.Grad(MODEL, verbose = 1, max_iter = 1000, optim_kwargs =␣
 ↪{"lr": 5e-3}).fit()

ap.plots.model_image(fig, axarr[2], MODEL)
axarr[2].set_title("Model after optimization")
ap.plots.residual_image(fig, axarr[3], MODEL, normalize_residuals = True)
axarr[3].set_title("Residuals after optimization")
plt.show()
```

```
loss: 283.81094319158024
loss: 275.0393610548054
loss: 268.85931406428676
loss: 263.2779117938314
loss: 257.877334915675
loss: 252.5360252575934
loss: 247.22217833403124
loss: 241.9701048873146
loss: 236.72684346247385
loss: 231.53330760658764
loss: 226.40130852071508
loss: 221.33173382541167
loss: 216.3513607420002
loss: 211.46963084714196
loss: 206.67612250453496
```

```
loss: 201.96134579688248
loss: 197.32261129787932
loss: 192.78048552272938
loss: 188.33554270003418
loss: 183.9870655839911
loss: 179.73410690859117
loss: 175.57551803358464
loss: 171.51038920453948
loss: 167.53759711396364
loss: 163.65617554818527
loss: 159.8652348940428
loss: 156.163961996483
loss: 152.61719579475093
loss: 149.11110570683581
loss: 145.69366428214747
loss: 142.36503784991376
loss: 139.12461441907936
loss: 135.96429158199467
loss: 132.89874932029176
loss: 129.91871581018518
loss: 127.02642003435994
loss: 124.21990899280156
loss: 121.49877852316133
loss: 118.86847043127084
loss: 116.31611907280967
loss: 113.80266466016582
loss: 111.41655078144984
loss: 109.15484193103487
loss: 106.9293482488707
loss: 104.7819205352155
loss: 102.71124240337855
loss: 100.71290152999458
loss: 98.78799440108169
loss: 96.93523238749158
loss: 95.15292247895407
loss: 93.43757297433952
loss: 91.78849248086725
loss: 90.20322758570488
loss: 88.67957914006332
loss: 87.03614800064638
loss: 85.81043348397667
loss: 84.46036613864449
loss: 83.16223606790172
loss: 81.91533305248507
loss: 80.71778309850568
loss: 79.56593553098415
loss: 78.46037031794732
loss: 77.39901928454577
```

```
loss: 76.37742165934047
loss: 75.39555461692545
loss: 74.45128094558623
loss: 73.54272029656175
loss: 72.6682689512887
loss: 71.81121247776811
loss: 71.02388000140472
loss: 70.24056824710891
loss: 69.4839204427075
loss: 68.75459843132698
loss: 68.05645002551107
loss: 67.37906975291364
loss: 66.71981403719367
loss: 66.0942237172398
loss: 65.47331700431742
loss: 64.87915583932175
loss: 64.3038006813147
loss: 63.7459644252015
loss: 63.20449157233736
loss: 62.53774380579923
loss: 62.169108825074545
loss: 61.672264256625084
loss: 61.18858973442914
loss: 60.71738663820906
loss: 60.25805923181737
loss: 59.809655957768854
loss: 59.37223591832943
loss: 58.944248330795034
loss: 58.525495300818555
loss: 58.11487993634246
loss: 57.71301049142119
loss: 57.31885724775598
loss: 56.93180595750731
loss: 56.551543197369455
loss: 56.177264935117805
loss: 55.80847977794872
loss: 55.44460186401591
loss: 55.084907720845045
loss: 54.72925132391115
loss: 54.37588112105742
loss: 54.02539449414436
loss: 53.67682707601258
loss: 53.329785064119534
loss: 52.98378258450447
loss: 52.639044128128894
loss: 52.295253129444646
loss: 51.952976370315184
loss: 51.61205414241519
```

```
loss: 51.27252856110209
loss: 50.934747865042254
loss: 50.5985548983575
loss: 50.264039362003096
loss: 49.931297280319605
loss: 49.600269875927665
loss: 49.2674138611058
loss: 48.939602307062366
loss: 48.613473003544506
loss: 48.28898704889232
loss: 47.96586138920102
loss: 47.64416182217012
loss: 47.322474831830334
loss: 47.00352778989465
loss: 46.68597373413877
loss: 46.369315791492
loss: 46.053805459858154
loss: 45.73948105898749
loss: 45.42636992681638
loss: 45.11452835217678
loss: 44.80389092169222
loss: 44.494640306921994
loss: 44.18665689335939
loss: 43.88009320802736
loss: 43.57300103609254
loss: 43.269319897660814
loss: 42.967352933933704
loss: 42.66687638203881
loss: 42.36803948768871
loss: 42.070700831677904
loss: 41.77749176343157
loss: 41.4838492051131
loss: 41.19215037929946
loss: 40.90212985135737
loss: 40.61384125058809
loss: 40.32701664578645
loss: 40.04188080592544
loss: 39.75742063032564
loss: 39.475049527702176
loss: 39.19316102686258
loss: 38.91173068350094
loss: 38.630702972639845
loss: 38.348117697231395
loss: 38.066677305914574
loss: 37.784982799531356
loss: 37.504383317654785
loss: 37.22090068636923
loss: 36.922914854807736
```

```
loss: 36.6442725930131
loss: 36.387938590407764
loss: 36.112693315210436
loss: 35.83279221413085
loss: 35.5404101757898
loss: 35.24256727571578
loss: 34.96345927640203
loss: 34.47763320039172
loss: 34.35928090153894
loss: 34.069276938216056
loss: 33.78209347404544
loss: 33.49745712575716
loss: 33.2265587982232
loss: 32.94606064304948
loss: 32.66807479769871
loss: 32.391804391030526
loss: 32.11838394994759
loss: 31.835146837977668
loss: 31.563544791458085
loss: 31.293544861131974
loss: 31.02560369537414
loss: 30.759498009430544
loss: 30.49521834110536
loss: 30.23211303627716
loss: 29.971263386632568
loss: 29.712149632832134
loss: 29.455069626947868
loss: 29.1992114676351
loss: 28.945010041845382
loss: 28.691153555277147
loss: 28.440239908115455
loss: 28.190899397199754
loss: 27.943150591194307
loss: 27.697141632364985
loss: 27.4528360089844
loss: 27.210236379731242
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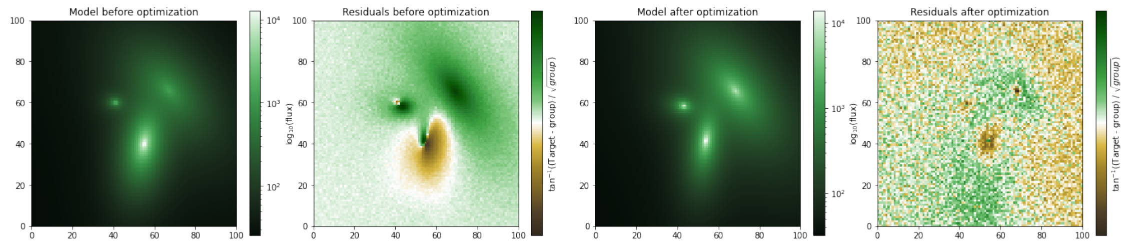
loss: 1.7526358710174013
loss: 1.7499395248183351
loss: 1.7510255941390762
loss: 1.7470633864542393
loss: 1.749544691894521
loss: 1.7468447746784626
loss: 1.7479304560879168
loss: 1.7452374836327005
loss: 1.7463301341763504
loss: 1.7436429088173435
loss: 1.7447413437734993
loss: 1.7420590499442392
loss: 1.7431623938980105
loss: 1.74048438480713
loss: 1.7415919869130043
loss: 1.7389177579923647
loss: 1.740029125238227
loss: 1.7373582881796104
loss: 1.7384730381921822
loss: 1.7358052977196055
loss: 1.7369231258616409
loss: 1.7342582601148766
loss: 1.7353789167650537
loss: 1.7327167612332752
loss: 1.733840036183025
loss: 1.731180470772833
loss: 1.73230618252155
loss: 1.7296491212581493
loss: 1.7307771096393028
loss: 1.7281224925246033
loss: 1.7292526135757527
loss: 1.7266004001895074
loss: 1.727732522524705
loss: 1.7250826870233873
loss: 1.7262166892099464
loss: 1.7235692164412524
loss: 1.724704985051259
loss: 1.7220598675563816
loss: 1.7231972956783366
loss: 1.7205545313992965
```

```
loss: 1.7216935174724703
loss: 1.7190622732431213
loss: 1.7201935562851502
loss: 1.7175646624194174
loss: 1.7187044568905698
loss: 1.7172537691872514
loss: 1.7158414595482758
loss: 1.7132151958541104
loss: 1.7143779956781056
loss: 1.7129215134761113
loss: 1.712828139310406
loss: 1.7102084276471685
loss: 1.7113750583792615
loss: 1.7087570695147463
loss: 1.709926152964093
loss: 1.7084721594406176
loss: 1.708391358222552
loss: 1.7057795883714904
loss: 1.706952711053431
loss: 1.7055014501032688
loss: 1.704141242789741
loss: 1.702792105854768
loss: 1.7026421723465028
loss: 1.7013094903996464
loss: 1.7011550839412715
loss: 1.699826383464564
loss: 1.6991091841826054
loss: 1.698359058152422
loss: 1.6976444709685174
loss: 1.6968970276451594
loss: 1.6961743285039201
loss: 1.6954404360267157
loss: 1.69472076348199
loss: 1.693988324380067
loss: 1.6932705905893128
loss: 1.6925400980075174
loss: 1.6918242199225295
loss: 1.6910955886988797
loss: 1.690381502617122
loss: 1.6896546691494152
loss: 1.688942325062543
loss: 1.6882172404046103
loss: 1.6875065981897708
loss: 1.6867832236551565
loss: 1.6860742505639392
loss: 1.6853525549467616
loss: 1.6846559680368351
loss: 1.6839250703250686
```

```
loss: 1.6832300941509544
loss: 1.6825116739757269
loss: 1.6818075593318353
loss: 1.6810907545626455
loss: 1.6803882230276483
loss: 1.679673018828669
loss: 1.6789720583862997
loss: 1.6782584431347618
loss: 1.6775590440671047
loss: 1.676847008615624
loss: 1.6761491633033039
loss: 1.6754387007420704
loss: 1.6747424035773575
loss: 1.6740335091171112
loss: 1.673338756503739
loss: 1.672631427476623
loss: 1.6719382179290352
loss: 1.6712324539127033
loss: 1.6705407882722154
loss: 1.6698365913519302
loss: 1.6691464731446175
loss: 1.668443848339766
loss: 1.6677552843125494
loss: 1.6670542402092052
loss: 1.6663672410970014
loss: 1.66566779074851
loss: 1.6649823723484412
loss: 1.6642845345336477
loss: 1.663600719194365
loss: 1.662904520161548
loss: 1.6622223388409463
loss: 1.6615278147189367
loss: 1.6614001342352485
loss: 1.6601504645557705
loss: 1.660023579200089
loss: 1.6587761403412662
loss: 1.6586500627143093
loss: 1.6574048245379838
loss: 1.656728399072158
loss: 1.6560398482961343
loss: 1.6559155714966647
loss: 1.6546746447686145
loss: 1.654551171793466
loss: 1.6533123973145778
loss: 1.6531897351546685
loss: 1.6519530934192956
loss: 1.651831245744091
loss: 1.6505967203055683
```

```
loss: 1.6499274494511 89
loss: 1.6492461891395451
loss: 1.649126173837288
loss: 1.6478958643406396
loss: 1.647776651548971
loss: 1.646548436830631
loss: 1.6464300305014075
loss: 1.6452038969227052
loss: 1.6450862984647026
loss: 1.6438622338493942
loss: 1.643745443933312
loss: 1.6425234375135938
loss: 1.6424074568626885
loss: 1.6411874996041054
loss: 1.6410723298647851
loss: 1.639854415252756
loss: 1.639196259936101
loss: 1.6385262372702691
loss: 1.6384128603093893
loss: 1.637199012656819
loss: 1.6370864275714128
loss: 1.6358746082643436
loss: 1.6357628208676782
loss: 1.6345530248955886
loss: 1.63444204311657
```



1.5 No U-Turn Sampler (NUTS)

Unlike the above methods, `ap.fit.NUTS` does not stricktly seek a minimum χ^2, instead it is an MCMC method which seeks to explore the likelihood space and provide a full posterior in the form of random samples. The NUTS method in AutoProf is actually just a wrapper for the Pyro implementation (**link here**). Most of the functionality can be accessed this way, though for very advanced applications it may be necessary to manually interface with Pyro (this is not very challenging as AutoProf is fully differentiable).

The first iteration of NUTS is always very slow since it compiles the forward method on the fly, after that each sample is drawn much faster. The warmup iterations take longer as the method is exploring the space and determining the ideal step size and mass matrix for fast integration with minimal numerical error (we only do 20 warmup steps here, if something goes wrong just try rerunning). Once the algorithm begins sampling it is able to move quickly (for an MCMC) throught the parameter space. For many models, the NUTS sampler is able to collect nearly completely uncorrelated samples, meaning that even 100 is enough to get a good estimate of the posterior.

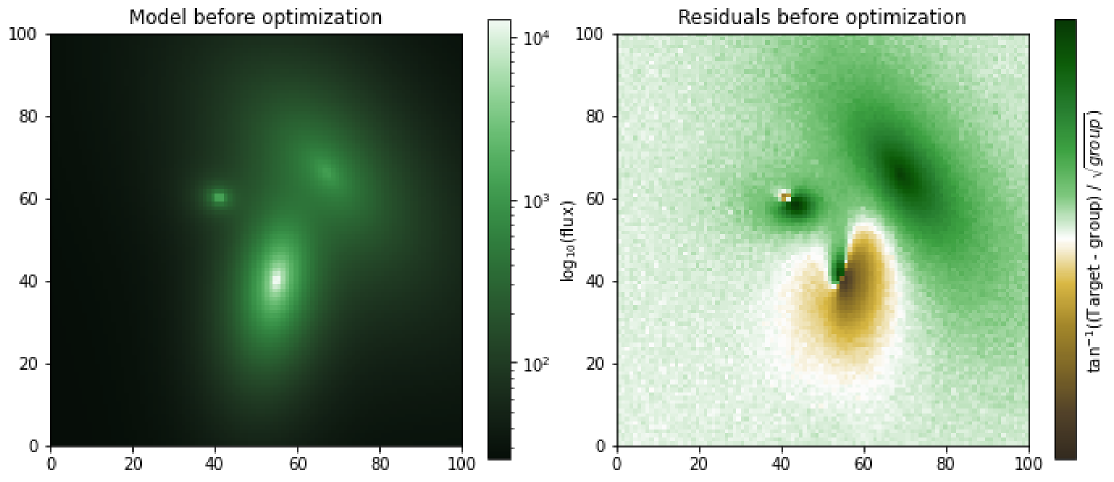
NUTS is far faster than other MCMC implementations such as a standard Metropolis Hastings MCMC. However, it is still a lot slower than the other optimizers (LM) since it is doing more than seeking a single high likelihood point, it is fully exploring the likelihood space. In simple cases, the automatic covariance matrix from LM is likely good enough, but if one really needs access to the full posterior of a complex model then NUTS is the best way to get it.

For an excellent introduction to the Hamiltonian Monte-Carlo and a high level explanation of NUTS see this review: **Betancourt 2018**

[8]:
```
MODEL = initialize_model(target, False)
fig, axarr = plt.subplots(1,2, figsize = (12,5))
plt.subplots_adjust(wspace= 0.1)
ap.plots.model_image(fig, axarr[0], MODEL)
axarr[0].set_title("Model before optimization")
ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
axarr[1].set_title("Residuals before optimization")
plt.show()

# Use LM to start the sampler at a high likelihood location, no burn-in needed!
# In general, NUTS is quite fast to do burn-in so this is often not needed
res1 = ap.fit.LM(MODEL).fit()

# Run the NUTS sampler
res_nuts = ap.fit.NUTS(MODEL, warmup = 20, max_iter = 100).fit()
```

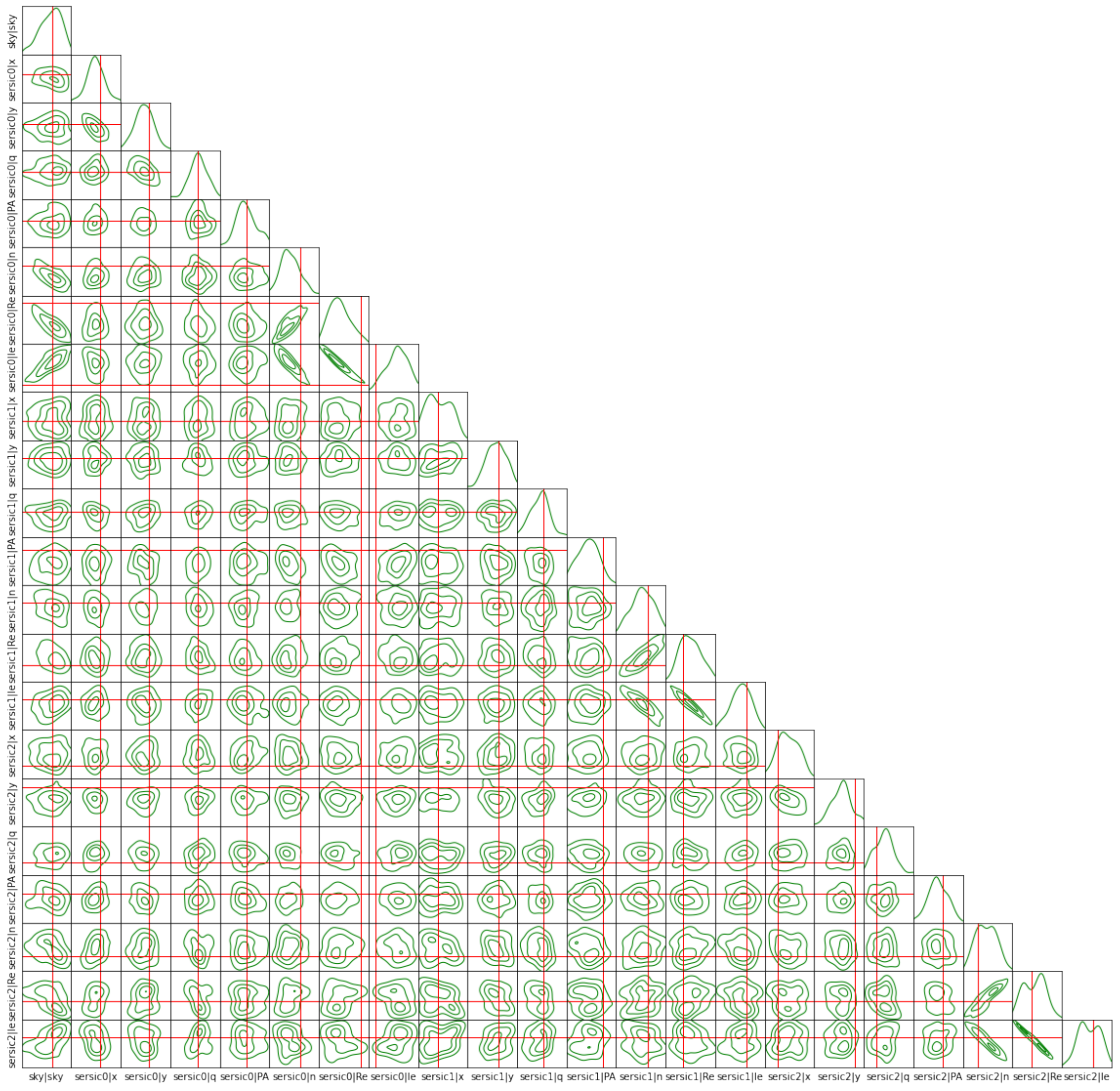


```
Sample: 100%|      | 120/120 [06:03,  3.03s/it, step size=2.45e-02, acc.
prob=0.653]
```

Note that there is no “after optimization” image above, because optimization was not done, it was full likelihood exploration. We can now create a corner plot with 2D projections of the 22 dimensional space that NUTS was exploring. The resulting corner plot is about what you would expect to get with 100 samples drawn from the multivariate gaussian found by LM above. If you run it again with more samples then the results will get even smoother.

[9]:
```
# corner plot of the posterior
# observe that it is very similar to the corner plot from the LM optimization␣
↪since this case can be roughly
# approximated as a multivariate gaussian centered on the maximum likelihood␣
↪point
param_names = list(MODEL.parameter_order())
i = 0
while i < len(param_names):
    param_names[i] = param_names[i].replace(" ", "")
    if "center" in param_names[i]:
        center_name = param_names.pop(i)
        param_names.insert(i, center_name.replace("center", "y"))
        param_names.insert(i, center_name.replace("center", "x"))
    i += 1

ser, sky = true_params()
corner_plot(
    res_nuts.chain.detach().cpu().numpy(),
    labels = param_names,
    figsize = (20,20),
    true_values = np.concatenate((sky,ser.ravel()))
)
```



1.6 Hamiltonian Monte-Carlo (HMC)

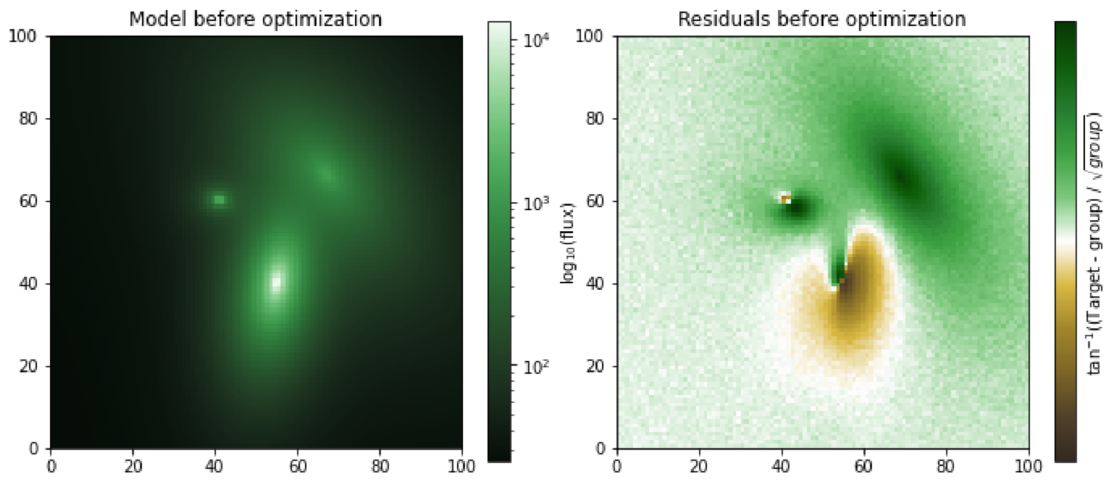
The `ap.fit.HMC` is a simpler variant of the NUTS sampler. HMC takes a fixed number of steps at a fixed step size following Hamiltonian dynamics. This is in contrast to NUTS which attempts to optimally choose these parameters. HMC may be suitable in some cases where NUTS is unable to find ideal parameters. Also in some cases where you already know the pretty good step parameters HMC may run faster. If you don't want to fiddle around with parameters then stick with NUTS, HMC results will still have autocorrelation which will depend on the problem and choice of step parameters.

[10]:
```
MODEL = initialize_model(target, False)
fig, axarr = plt.subplots(1,2, figsize = (12,5))
plt.subplots_adjust(wspace= 0.1)
ap.plots.model_image(fig, axarr[0], MODEL)
```

```
axarr[0].set_title("Model before optimization")
ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
axarr[1].set_title("Residuals before optimization")
plt.show()

# Use LM to start the sampler at a high likelihood location, no burn-in needed!
res1 = ap.fit.LM(MODEL).fit()

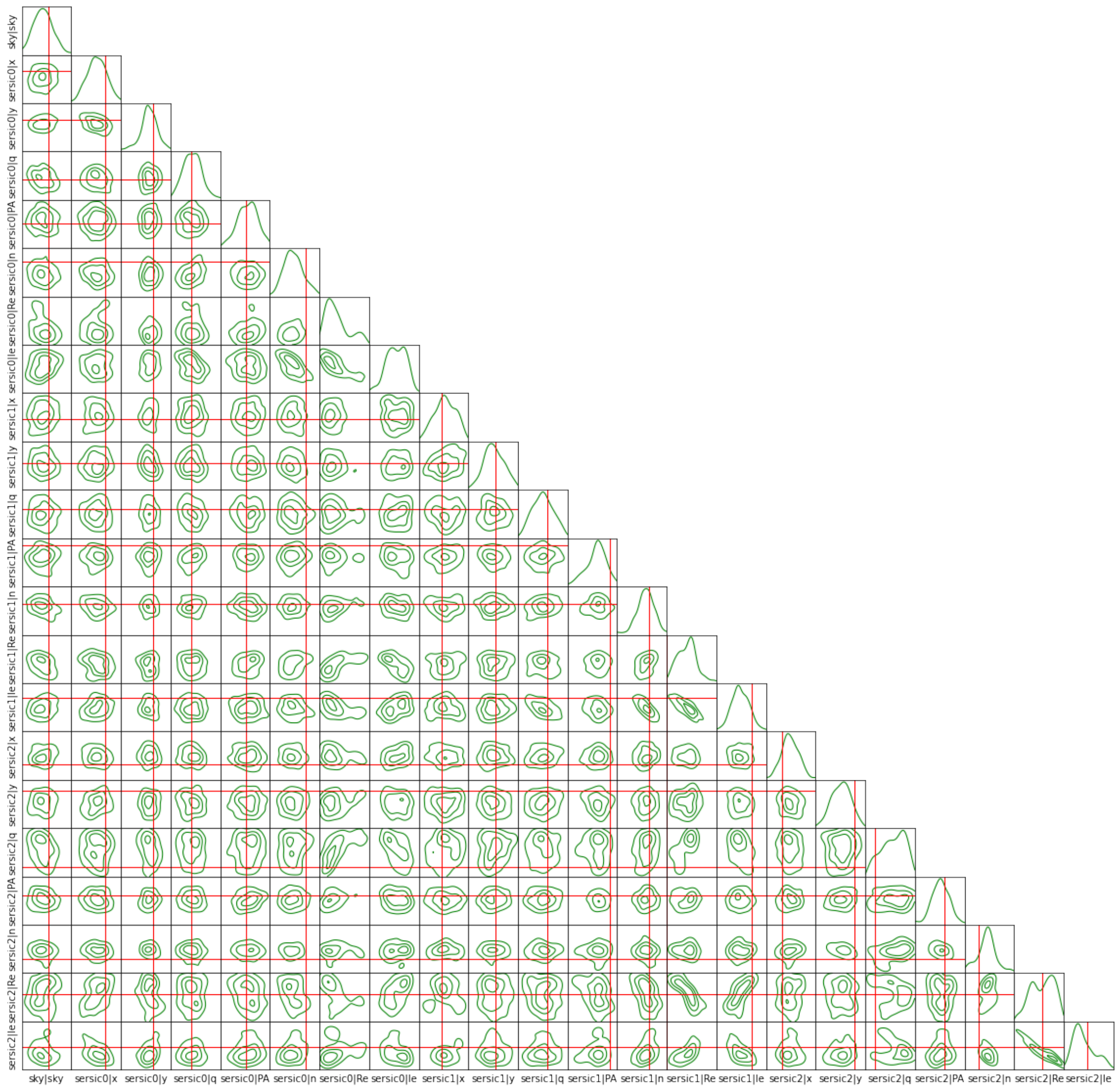
# Run the HMC sampler
res_hmc = ap.fit.HMC(MODEL, warmup = 20, max_iter = 200, epsilon = 1e-2,␣
 ↪leapfrog_steps = 20).fit()
```



```
Sample: 100%|      | 220/220 [02:26,  1.50it/s, step size=1.00e-02, acc.
prob=0.939]
```

[11]:
```
# corner plot of the posterior
# note that for the HMC, 200 samples is not enough to overcome the␣
 ↪autocorrelation so the posterior has not converged
param_names = list(MODEL.parameter_order())
i = 0
while i < len(param_names):
    param_names[i] = param_names[i].replace(" ", "")
    if "center" in param_names[i]:
        center_name = param_names.pop(i)
        param_names.insert(i, center_name.replace("center", "y"))
        param_names.insert(i, center_name.replace("center", "x"))
    i += 1

ser, sky = true_params()
corner_plot(
    res_hmc.chain.detach().cpu().numpy(),
    labels = param_names,
    figsize = (20,20),
    true_values = np.concatenate((sky,ser.ravel()))
)
```



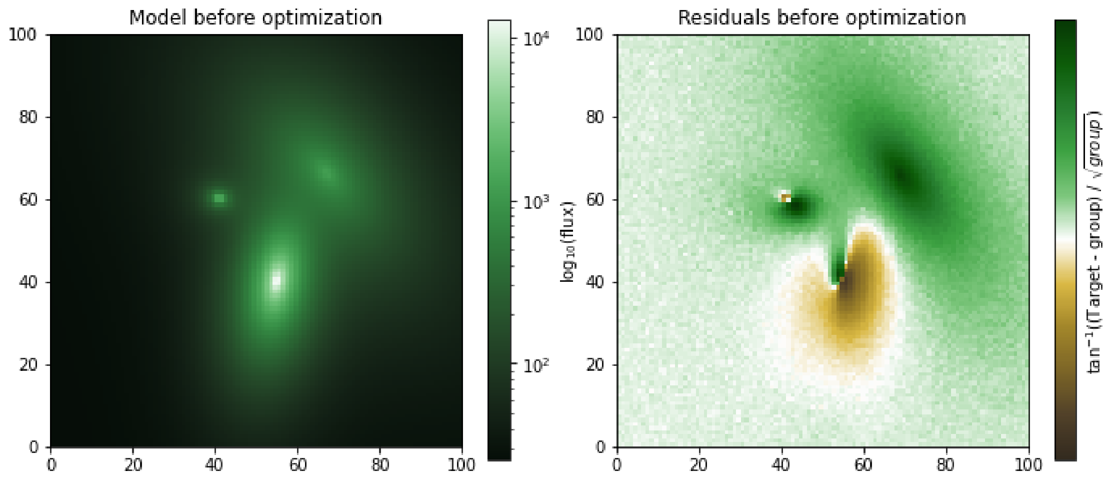
1.7 Metropolis Hastings

This is the classic MCMC algorithm using the Metropolis Hastngs accept step identified with `ap.fit.MHMCMC`. One can set the gaussian random step scale and then explore the posterior. While this technically always works, in practice it can take exceedingly long to actually converge to the posterior. This is because the step size must be set very small to have a reasonable likelihood of accepting each step, so it never moves very far in parameter space. With each subsequent sample being very close to the previous sample it can take a long time for it to wander away from its starting point. In the example below it would take an extremely long time for the chain to converge. Instead of waiting that long, we demonstrate the functionality with 5000 steps, but suggest using NUTS for any real world problem. Still, if there is something NUTS can't handle (a function that isn't differentiable) then MHMCMC can save the day (even if it takes all day to do it).

[12]:
```
MODEL = initialize_model(target, False)
fig, axarr = plt.subplots(1,2, figsize = (12,5))
plt.subplots_adjust(wspace= 0.1)
ap.plots.model_image(fig, axarr[0], MODEL)
axarr[0].set_title("Model before optimization")
ap.plots.residual_image(fig, axarr[1], MODEL, normalize_residuals = True)
axarr[1].set_title("Residuals before optimization")
plt.show()

# Use LM to start the sampler at a high likelihood location, no burn-in needed!
res1 = ap.fit.LM(MODEL).fit()

# Run the HMC sampler
res_mh = ap.fit.MHMCMC(MODEL, verbose = 1, max_iter = 5000, epsilon = 1e-4,␣
 ↪report_after = np.inf).fit()
```



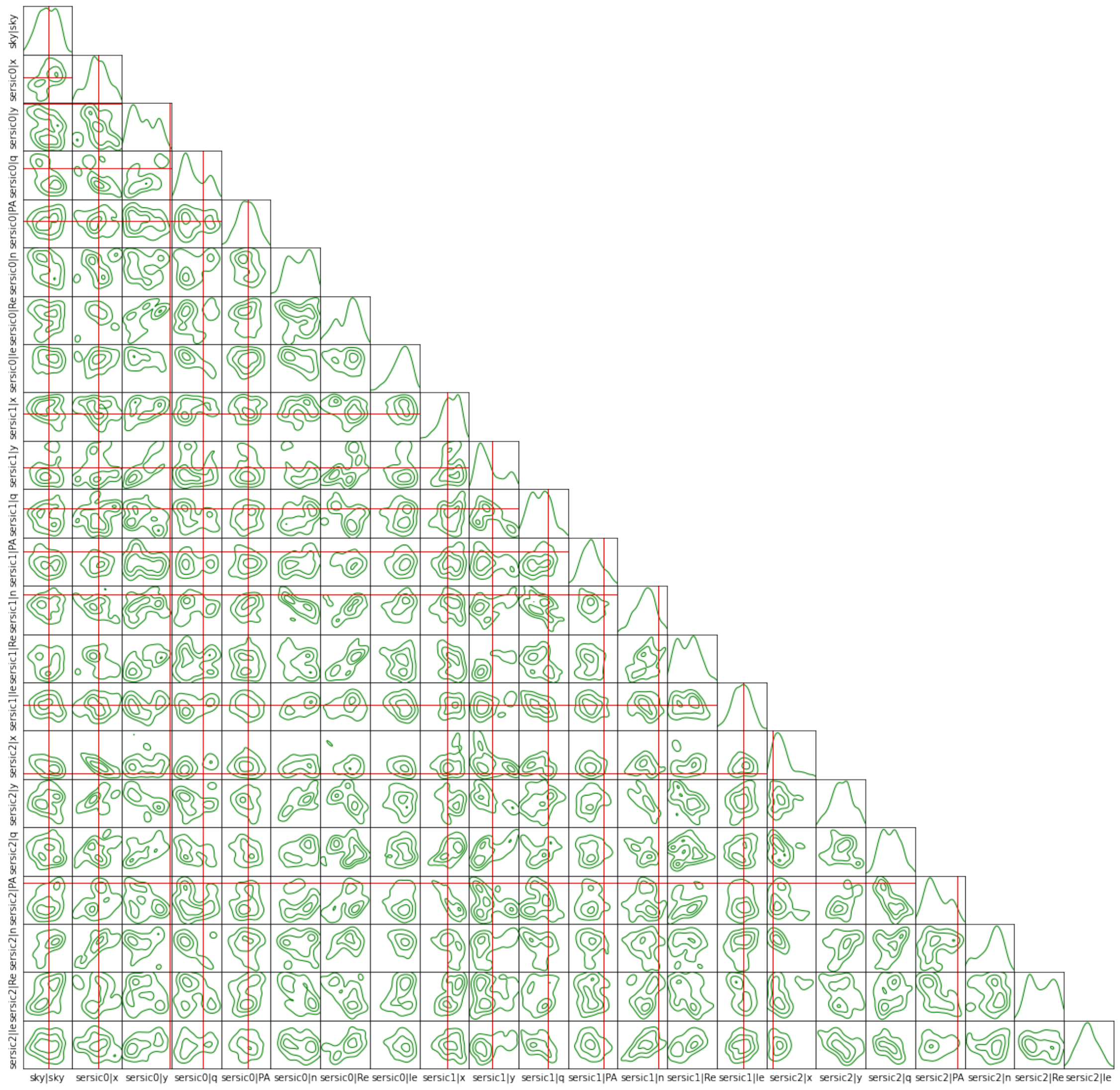
```
100%|          | 5000/5000 [02:41<00:00, 31.04it/s]

Acceptance: 0.765999972820282
```

[13]:
```
# corner plot of the posterior
# note that, even 5000 samples is not enough to overcome the autocorrelation so␣
 ↪the posterior has not converged.
# In fact it is not even close to convergence as can be seen by the multi-modal␣
 ↪blobs in the posterior since this
```

```
# problem is unimodal (except the modes where models are swapped). It is almost␣
↪never worthwhile to use this
# sampler except as a sanity check on very simple models.
param_names = list(MODEL.parameter_order())
i = 0
while i < len(param_names):
    param_names[i] = param_names[i].replace(" ", "")
    if "center" in param_names[i]:
        center_name = param_names.pop(i)
        param_names.insert(i, center_name.replace("center", "y"))
        param_names.insert(i, center_name.replace("center", "x"))
    i += 1

ser, sky = true_params()
corner_plot(
    res_mh.chain[::10], # thin by a factor 10 so the plot works in reasonable␣
↪time
    labels = param_names,
    figsize = (20,20),
    true_values = np.concatenate((sky,ser.ravel()))
)
```


sky|sky
sersic0|x
sersic0|y
sersic0|q
sersic0|PA
sersic0|n
sersic0|Re
sersic0|le
sersic1|x
sersic1|y
sersic1|q
sersic1|PA
sersic1|n
sersic1|Re
sersic1|le
sersic2|x
sersic2|y
sersic2|q
sersic2|PA
sersic2|n
sersic2|Re
sersic2|le

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[ ]:
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