Supplementary Document 1: Convergence Analysis

Article Title: Deconvolution via Integral Transform Inversion

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Although in the algorithm as presented in the main paper the splats change in their overall scale over the iterations according to (21), it helps in the analysis of convergence, without altering the numerical identity of the algorithm, if we split the splat definition into two parts: the initial splats (that, in this representation of the algorithm, will never change over the iterations) and a splat scale factor (that does change). We can then analyse how those scale factors change over the iterations. To do this let us change (12) into:

$$\mathrm{Splat}^{0}_{\tilde{f}(r,s)}(x,y)=h_{(r,s)}(x,y)\;\forall\;\text{valid}\;x,y \tag{S1}$$

and then define the splat scale factor as $S^{p}_{(r,s)}(x,y)$ where

$$S^{0}_{(r,s)}(x,y)=\hat{g}\;\forall\;\text{valid}\;x,y \tag{S2}$$

Thus whenever the term $\mathrm{Splat}^{p}_{\tilde{f}(r,s)}$ is used in the algorithm we simply substitute that for $S^{p}_{(r,s)}(x,y)\mathrm{Splat}^{0}_{\tilde{f}(r,s)}(x,y)$ to give exactly the same numerical expression. For example, (13) will be expressed as:

$$\tilde{g}^{p}(x,y)=\frac{1}{N_c(x,y)}\sum_{s=y-B}^{y+B}\sum_{r=x-A}^{x+A}S^{p}_{(r,s)}(x,y)\,\mathrm{Splat}^{0}_{\tilde{f}(r,s)}(x,y) \tag{S3}$$

which, by (S1), is identical to:

$$\tilde{g}^{p}(x,y)=\frac{1}{N_c(x,y)}\sum_{s=y-B}^{y+B}\sum_{r=x-A}^{x+A}S^{p}_{(r,s)}(x,y)\,h_{(r,s)}(x,y) \tag{S4}$$

In this way, the main iteration relation (21) becomes:

$$S^{p+1}_{(r,s)}(x,y)\,\mathrm{Splat}^{0}_{\tilde{f}(r,s)}(x,y)=\delta^{p}(r,s)\,S^{p}_{(r,s)}(x,y)\,\mathrm{Splat}^{0}_{\tilde{f}(r,s)}(x,y)$$

and this reduces to:

$$S^{p+1}_{(r,s)}(x,y)=\delta^{p}(r,s)\,S^{p}_{(r,s)}(x,y) \tag{S5}$$

To analyse convergence I will first put together a complete iteration of the algorithm in a single formula by expressing the estimate $\tilde{g}^{p+1}$ in terms of the previous iteration's estimate i.e. $\tilde{g}^{p}$. Because this will involve amalgamating a lot of the formulae from the main paper into one large formula, I will again revert to using the 1D versions of the formulae for ease of expression. The convention used in the main paper that each PSF will be centred in its position in the *RS* domain (the *R* domain in the 1D case) will also be used to facilitate clarity of indices.

The 1D version of (S4) is:

$$\tilde{g}^{p}(x)=\frac{1}{N_c(x)}\sum_{r=x-A}^{x+A} S_{(r)}^{p}(x)\,h_{(r)}(x) \tag{S6}$$

Now expressing δ^p for the 1D case using the 1D versions of the (13) to (20) we get:

$$\delta^{p}(r)=\frac{1}{H_r}\sum_{x'=x-A}^{x+A}\left(\frac{g(x')h_r(x')\left(1+h_r(x')\left(\frac{g(x')}{\tilde{g}^{p}(x')}-1\right)\right)}{\tilde{g}^{p}(x')+\left(\frac{g(x')}{\tilde{g}^{p}(x')}-1\right)\frac{\sum_{r'=x'-A}^{x'+A} S_{(r')}^{p}(x')\left(h_{r'}(x')\right)^2}{\left(N_c(x')\right)^2}}\right) \tag{S7}$$

So one full iteration from $\tilde{g}^p$ to $\tilde{g}^{p+1}$ using (S4), (S5), (S6) and (S7) will be:

$$\tilde{g}^{p+1}(x)=\frac{1}{N_c(x)}\sum_{r=x-A}^{x+A}\left(\frac{1}{H_r}\sum_{x'=x-A}^{x+A}\left(\frac{g(x')h_r(x')\left(1+h_r(x')\left(\frac{g(x')}{\tilde{g}^{p}(x')}-1\right)\right)}{\tilde{g}^{p}(x')+\left(\frac{g(x')}{\tilde{g}^{p}(x')}-1\right)\frac{\sum_{r'=x'-A}^{x'+A} S_{(r')}^{p}(x')\left(h_{r'}(x')\right)^2}{\left(N_c(x')\right)^2}}\right)\right)S_{(r)}^{p}(x)h_{(r)}(x) \tag{S8}$$

It can easily be seen that if convergence has occurred, i.e. if $\tilde{g}^p=g$, then the summation term in brackets on RHS of (S8) cancels down to 1 so that (S8) becomes (S6).

Now the algorithm will be convergent if the power of the error in the solution at iteration *p* is greater than the power at iteration *p*+1 so we can write a convergence criteria inequality as:

$$\frac{\sum_{\forall x}\left|\tilde{g}^{p}(x)-g(x)\right|^2}{\sum_{\forall x}\left|\tilde{g}^{p+1}(x)-g(x)\right|^2}\geqslant 1 \tag{S9}$$

If it can be shown that (S9) is a ‘greater than’ inequality this proves asymptotic convergence.

If it can be shown that (S9) is an equality this proves lack of divergence.

The numerator of (S9) can be expanded using (S6) to:

$$\left|\tilde{g}^p(x)-g(x)\right|^2=\frac{\left(\sum_{r=x-A}^{x+A}\left(S_{(r)}^p(x)h_{(r)}(x)\right)^2+\sum_{r=x-A}^{x+A}\sum_{s\neq r}^{x+A}S_{(r)}^p(x)S_{(s)}^p(x)h_{(r)}(x)h_{(s)}(x)\right)}{\left(N_c(x)\right)^2}-\frac{2g(x)}{N_c(x)}\sum_{r=x-A}^{x+A}S_{(r)}^p(x)h_{(r)}(x)+\left(g(x)\right)^2$$

(S10)

The denominator of (S9) can be expanded can be expanded using (S8) to:

$$\left|\tilde{g}^{p+1}(x)-g(x)\right|^2=$$
$$\frac{\sum_{r=x-A}^{x+A}\left(\delta^p(r)\right)^2\left(S_{(r)}^p(x)h_{(r)}(x)\right)^2+\sum_{r=x-A}^{x+A}\sum_{s\neq r}^{x+A}\delta^p(r)\delta^p(r)\left(S_{(r)}^p(x)h_{(r)}(x)\right)\left(S_{(s)}^p(x)h_{(r)}(x)\right)}{\left(N_c(x)\right)^2}-$$
$$\frac{2g(x)}{N_c(x)}\sum_{r=x-A}^{x+A}\delta^p(r)S_{(r)}^p(x)h_{(r)}(x)+\left(g(x)\right)^2 \qquad \text{(S11)}$$

Comparing (S10) and (S11) it is clear that convergence, stability or divergence depends on whether the expression $\delta^p(r)$ is less than, equal to or greater than 1, respectively.

If we re-cast (S7) as:

$$\delta^p(r)=\frac{1}{H_r}\sum_{x'=x-A}^{x+A}\frac{h_r(x')g(x')\epsilon_r(x')}{\tilde{g}^p(x')+\zeta(x')} \qquad \text{(S12)}$$

where

$$\epsilon_r(x')=\left(1+h_r(x')\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)\right)$$

and

$$\zeta(x')=\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)\frac{\sum_{r'=x'-A}^{x'+A}S_{(r')}^p(x')\left(h_{r'}(x')\right)^2}{\left(N_c(x')\right)^2}$$

then, for convergence we require that

$$g(x')\epsilon_r(x')\leqslant\tilde{g}^p(x')+\zeta(x')$$

or equivalently that

$$g(x')\epsilon_r(x')-\zeta(x')\leqslant\tilde{g}^p(x')$$

Expressing the latter inequality in full by substituting in ε and ζ we get:

$$g(x')\left(1+h_r(x')\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)\right)-\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)\frac{\sum_{r'=x'-A}^{x'+A} S_{(r')}^p(x')\left(h_{r'}(x')\right)^2}{\left(N_c(x')\right)^2}\leqslant \tilde{g}^p(x') \qquad \text{(S13)}$$

The summation term in (S13) can be expressed as:

$$\frac{1}{N_c(x')}\frac{\sum_{r'=x'-A}^{x'+A} S_{(r')}^p(x')h_{r'}(x')h_{r'}(x')}{N_c(x')} \qquad \text{(S14)}$$

Comparing (S14) to (S6) and remembering that $h_r(x')<1\,\forall\, x'$ (or for all but one x' in the special case where the PSF is a Dirac pulse when it will have a value of 1 at that single x' position and zero elsewhere) it is clear that the complete evaluation of (S14), summing over the range of r', will always result in some value that is less than $\widetilde{g^p}(x')/N_c(x')$. We can express this as:

$$\frac{\sum_{r'=x'-A}^{x'+A} S_{(r')}^p(x')\left(h_{r'}(x')\right)^2}{\left(N_c(x')\right)^2}=\frac{\alpha_{r'}(x')\tilde{g}^p(x')}{N_c(x')}\ \text{where}\ \alpha_{r'}(x')<1\,\forall\, r', x' \qquad \text{(S15)}$$

Note that $\alpha_{r'}(x')$ depends on the shape of the point spread functions which do not change with the iterations. Note also that this $\alpha_{r'}(x')$ function value also depends on $\widetilde{g^p}$ and not g.

Using (S15) we can express (S13) as:

$$g(x')\left(1+h_r(x')\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)\right)-\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)\frac{\alpha_{r'}(x')\tilde{g}^p(x')}{N_c(x')}\leqslant \tilde{g}^p(x')$$

and, re-arranging, gives

$$g(x')\left(h_r(x')\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)+1-\frac{\alpha_{r'}(x')}{N_c(x')}\right)\leqslant \tilde{g}^p(x')\left(1-\frac{\alpha_{r'}(x')}{N_c(x')}\right)$$

then

$$g(x')h_r(x')\left(\frac{g(x')}{\tilde{g}^p(x')}-1\right)+g(x')\left(1-\frac{\alpha_{r'}(x')}{N_c(x')}\right)\leqslant \tilde{g}^p(x')\left(1-\frac{\alpha_{r'}(x')}{N_c(x')}\right) \qquad \text{(S16)}$$

From (S16) it is clear that, if convergence occurs then, at convergence when $g=\widetilde{g^p}$, the left-most term vanishes and the remaining terms become an equality.

For (S16) to define convergence, the relation does not need to hold over all points x' in the range $x' \in x-A \leqslant x' \leqslant x+A$ but only over a sufficient number to make $\delta^p(r)<1$ by (S12). Prior to convergence when, at any point, $\widetilde{g^p}(x')>g(x')$ the left-most term in (S16) becomes a negative amount and the inequality will be satisfied. When $\widetilde{g^p}(x')=g(x')$ then the left-most term in (S16) cancels out and again the inequality is satisfied. When $\widetilde{g^p}(x')<g(x')$ the situation is not so simple to deduce because the shape of the $\alpha_{r'}(x')$ function depends on $\widetilde{g^p}$ and not g, so some of these points may also favour convergence.

Because the algorithm preserves photometry at each iteration using appropriately weighted PSF normalising factors, this means that at each iteration $mean(\widetilde{g^p})=mean(g(x'))\forall x'$ so the situations described above that definitely favour convergence will occur, on average, across up to 50% of the data points at any iteration (the less skewed are the values of g about its mean, the closer this proportion will be to 50%).

While this analysis does not prove the algorithm is convergent in general it may go some way to explaining why convergence is observed in practice in all the experiments conducted for this work.