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Computing the correlation and other things directly from the raw pairs

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Disclaimer

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Computing the correlation and other things directly from the raw pairs

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We want a faster and more robust way to compute the correlation, expanded in Spherical (or Cartesian) Harmonics. We also want to include the cross-ℓ, m data covariance that are there, but currently ignored. We don't want to get bogged down in fancy binning in $x-y-z$ or $r-\theta-\phi$, just r. Want to just look at $C_{\ell m}$ to decide how many terms to keep – or better yet the pair distributions directly.

First, we need the true pair and mixed pair distributions $T(\mathbf{q})$ and $M(\mathbf{q})$ from which we could compute the correlation $C(\mathbf{q})$:

$$T(\mathbf{q}) = C(\mathbf{q})M(\mathbf{q}) \tag{1}$$

If we expand the pair distributions and the correlation in Spherical Harmonics (for the sake of argument), then we have

$$\sqrt{4\pi}\sum_{\ell m} T_{\ell m}(q)Y_{\ell m}(\Omega_{\hat{\mathbf{q}}}) = \left(\sqrt{4\pi}\sum_{\ell' m'} M_{\ell' m'}(q)Y_{\ell' m'}(\Omega_{\hat{\mathbf{q}}})\right)\left(\sqrt{4\pi}\sum_{\ell'' m''} C_{\ell'' m''}(q)Y_{\ell'' m''}(\Omega_{\hat{\mathbf{q}}})\right) \tag{2}$$

So,

$$\begin{aligned}
T_{\ell m}(q) &= \sqrt{4\pi}\sum_{\ell' m' \ell'' m''} M_{\ell' m'}(q)C_{\ell'' m''}(q)\int_{4\pi} d\Omega_{\hat{\mathbf{q}}} Y^*_{\ell m}(\Omega_{\hat{\mathbf{q}}})Y_{\ell' m'}(\Omega_{\hat{\mathbf{q}}})Y_{\ell'' m''}(\Omega_{\hat{\mathbf{q}}}) && (3)\\
&= \sqrt{4\pi}\sum_{\ell' m' \ell'' m''} M_{\ell' m'}(q)C_{\ell'' m''}(q)(-1)^m\int_{4\pi} d\Omega_{\hat{\mathbf{q}}} Y_{\ell m}(\Omega_{\hat{\mathbf{q}}})Y_{\ell' m'}(\Omega_{\hat{\mathbf{q}}})Y_{\ell'' m''}(\Omega_{\hat{\mathbf{q}}}) && (4)\\
&= \sqrt{4\pi}\sum_{\ell' m' \ell'' m''} M_{\ell' m'}(q)C_{\ell'' m''}(q)(-1)^m\left[\frac{(2\ell+1)(2\ell'+1)(2\ell''+1)}{4\pi}\right]^{1/2}\begin{pmatrix}\ell & \ell' & \ell''\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & \ell' & \ell''\\ -m & m' & m''\end{pmatrix} && (5)\\
&= \sum_{\ell' m' \ell'' m''} M_{\ell' m'}(q)C_{\ell'' m''}(q)(-1)^m\sqrt{(2\ell+1)(2\ell'+1)(2\ell''+1)}\begin{pmatrix}\ell & \ell' & \ell''\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & \ell' & \ell''\\ -m & m' & m''\end{pmatrix} && (6)\\
&\equiv \sum_{\ell'' m''}\tilde{M}_{\ell m \ell'' m''}(q)C_{\ell'' m''}(q) && (7)
\end{aligned}$$

Eq. (7) gives us a was to compute $C_{\ell m}(q)$ directly from the pair distributions expanded in spherical harmonics. All we need to do is invert the matrix in $\ell m \ell'' m''$; Eq. (7) is an imaging problem where $\tilde{M}$ is the kernel, T is the data and C is the model we seek to reconstruct. We can even do error propagation in the obvious way, provided we measure the mixed pair distribution so well that the uncertainties are negligible compared to the true distribution. What's more, when you do the error propagation in the obvious way, you get the cross-ℓm correlations in the covariance matrix by virtue of the cross-ℓm correlations built into the $\tilde{M}$ matrix. All of this can be done with the current imaging code inside of CorAL, provided the appropriate wrappers are written. Also, it is possible to include the covariance in the mixed pair distribution too. This would require writing a new imaging core routine which allows for uncertainties on the kernel.

Now, how to we compute $T_{\ell m}(q)$ (or $M_{\ell' m'}(q)$)? First, we return to the spherical harmonic expansion of the pair distribution:

$$T(\mathbf{q}) = \sqrt{4\pi}\sum_{\ell m} T_{\ell m}(q)Y_{\ell m}(\Omega_{\hat{\mathbf{q}}}) \tag{8}$$

so

$$T_{\ell m}(q) = \int_{4\pi} d\Omega_{\hat{\mathbf{q}}} T(\mathbf{q})Y^*_{\ell m}(\Omega_{\hat{\mathbf{q}}}) \tag{9}$$

We build this up by summing over pairs, which is essentially a Monte-Carlo integration process:

$$T_{\ell m}(q_n) \approx \begin{cases} \frac{1}{N}\sum_{i=1}^N Y^*_{\ell m}(\Omega_{\hat{\mathbf{q}}_i}) & \text{if } q_i \text{ in bin } n\\ 0 & \text{otherwise}\end{cases} \tag{10}$$

with covariance (for if q_i in bin n only:)

$$\Delta^2 T_{\ell m \ell' m'}(q_n) \approx \frac{1}{N-1}\left(\frac{1}{N}\sum_{i=1}^{N} Y^*_{\ell m}(\hat{\mathbf{q}}_i) Y^*_{\ell' m'}(\hat{\mathbf{q}}_i) - T_{\ell m}(q_n) T_{\ell' m'}(q_n)\right) \tag{11}$$

giving (uncorrelated) uncertainties of

$$\Delta T_{\ell m}(q_n) \approx \sqrt{\Delta^2 T_{\ell m \ell m}(q_n)} \tag{12}$$

(Note to reader: check those 1/N type factors. I couldn't find a statistics book to check them)

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