FFTs in Graphics and Vision

Correlation of Spherical Functions

Outline

- Math Review
- Fast Spherical Harmonic Transform
- Spherical Correlation

Review

Dimensionality:

Given a complex n-dimensional array $\mathbf{a} \in \mathbb{C}^n$ representing regular samples of a function on the circle, we can express the array in terms of its Fourier decomposition:

$$\mathbf{a} = \frac{1}{\sqrt{2\pi}} \sum_j \hat{a}_j \cdot e^{-\frac{ik2\pi j}{n}}$$

Review

Dimensionality:

How many complex exponentials do we use?

Because the array is of dimension n, we need n Fourier coefficients to capture all the data:

$$\mathbf{a} = \frac{1}{\sqrt{2\pi}} \sum_j \hat{a}_j \cdot e^{-\frac{ik2\pi j}{n}}$$

$$\Downarrow$$

$$\mathbf{a} = \frac{1}{\sqrt{2\pi}} \sum_{j=-n/2}^{n/2-1} \hat{a}_j \cdot e^{-\frac{ik2\pi j}{n}}$$

Review

<u>Dimensionality</u>:

How many complex exponentials do we use?

Because the array is of dimension n, we need n Fourier coefficients to capture all the data:

The value of the largest frequency is the *bandwidth* of the function.

$\Downarrow$

$$\mathbf{a} = \frac{1}{\sqrt{2\pi}} \sum_{j=-n/2}^{n/2-1} \hat{a}_j \cdot e^{-\frac{ik2\pi j}{n}}$$

Review

<u>Dimensionality</u>:

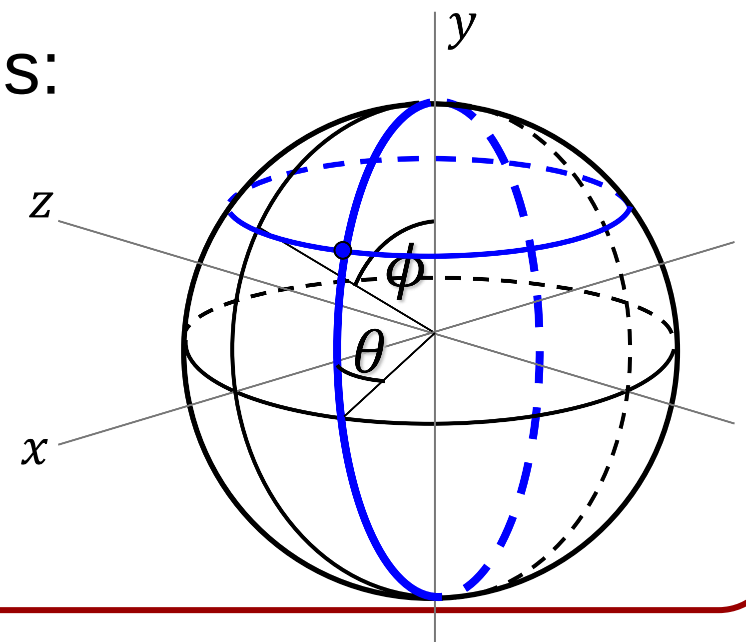
We represent a spherical function by an $n \times n$ grid whose entries are the regular samples of the function along the lines of latitude and longitude:

$$f_{jk} = f\left(\cos\theta_j \cdot \sin\phi_k, \cos\phi_k, \sin\theta_j \cdot \sin\phi_k\right)$$

where θ_j and ϕ_k are the angles:

$$\theta_j = \frac{2\pi j}{n}$$

$$\phi_k = \frac{\pi(2k+1)}{2n}$$



Review

Dimensionality:

We can express the spherical function as a sum of spherical harmonics:

$$\mathbf{f} = \sum_{l} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \mathbf{Y}_l^m$$

Review

Dimensionality:

How many frequencies should we use?

As in the case of functions on a circle, we use a bandwidth that is half the resolution:

$$\mathbf{f} = \sum_{l} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \mathbf{Y}_l^m$$

$$\Downarrow$$

$$\mathbf{f} = \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \mathbf{Y}_l^m$$

Review

Dimensionality:

$$\mathbf{f} = \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \mathbf{Y}_l^m$$

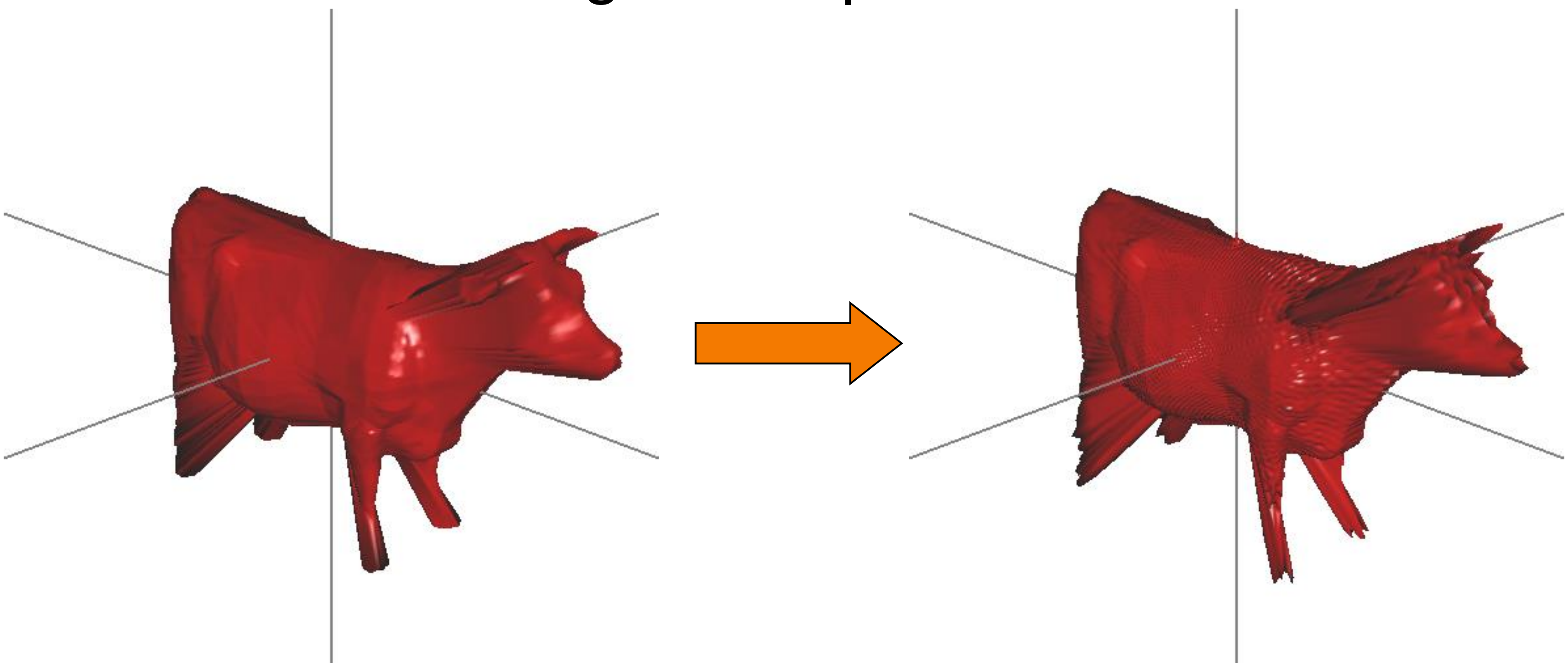
In this case, the number of coefficients is:

$$\sum_{l=0}^{n/2-1} (2l+1) = \left(\frac{n}{2}\right)^2$$

Review

Dimensionality:

Since we go from n^2 spherical samples to $(n/2)^2$ spherical harmonic coefficients, there is a loss of information at the higher frequencies:



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Spherical Harmonic Decomposition

Given a function $f: S^2 \to \mathbb{C}$, we would like to compute the spherical harmonic coefficients of f:

$$\hat{f}_{lm} = \langle f, \mathbf{Y}_l^m \rangle$$

Or, in spherical coordinates:

$$\hat{f}_{lm} = \int_0^{\pi} \int_0^{2\pi} f(\theta, \phi) \cdot \overline{\mathbf{Y}_l^m(\theta, \phi)} \cdot \sin(\phi) \ d\theta \ d\phi$$

Done naively over a sphere sampled at $O(n^2)$ positions:

- Each $\hat{f}_{lm}$ can be computed in $O(n^2)$ time.

$\Rightarrow$ All $\hat{f}_{lm}$ can be computed in $O(n^4)$ time.

Spherical Harmonic Decomposition

$$\hat{f}_{lm} = \int_0^{\pi} \int_0^{2\pi} f(\theta,\phi) \cdot \overline{\mathbf{Y}_l^m(\theta,\phi)} \cdot \sin(\phi)\ d\theta\, d\phi$$

To compute this more efficiently, we will:

- Use the fact that the spherical harmonics are separable (products of functions in θ and ϕ)
- Leverage the FFT

Spherical Harmonic Decomposition

$$\hat{f}_{lm} = \int_0^{\pi} \int_0^{2\pi} f(\theta, \phi) \cdot \overline{\mathbf{Y}_l^m(\theta, \phi)} \cdot \sin(\phi)\ d\theta\ d\phi$$

Using the definition of spherical harmonics:

$$\hat{f}_{lm} = \int_0^{\pi} \int_0^{2\pi} f(\theta, \phi) \cdot \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \cdot \overline{e^{im\theta}}\ d\theta\ d\phi$$

$$= \int_0^{\pi} \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \int_0^{2\pi} f(\theta, \phi) \cdot \overline{e^{im\theta}} \cdot\ d\theta\ d\phi$$

Spherical Harmonic Decomposition

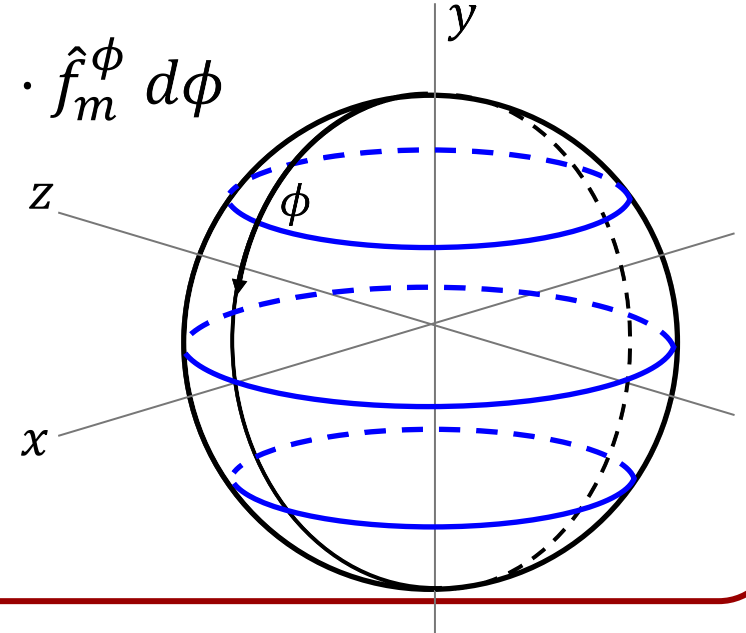
$$\hat{f}_{lm} = \int_0^{\pi} \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \int_0^{2\pi} f(\theta,\phi) \cdot \overline{e^{im\theta}} \cdot \; d\theta \, d\phi$$

Consider the restriction of f to the parallels with angle ϕ:

$$f^{\phi}(\theta) = f(\theta,\phi)$$

$$\hat{f}_{lm} = \int_0^{\pi} \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \int_0^{2\pi} f^{\phi}(\theta) \cdot \overline{e^{im\theta}} \cdot \; d\theta \, d\phi$$

$$= \frac{1}{\sqrt{2\pi}} \int_0^{\pi} \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \cdot \hat{f}_m^{\phi} \, d\phi$$



Spherical Harmonic Decomposition

$$\hat{f}_{lm} = \frac{1}{\sqrt{2\pi}} \int_0^{\pi} \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \cdot \hat{f}_m^{\phi} \, d\phi$$

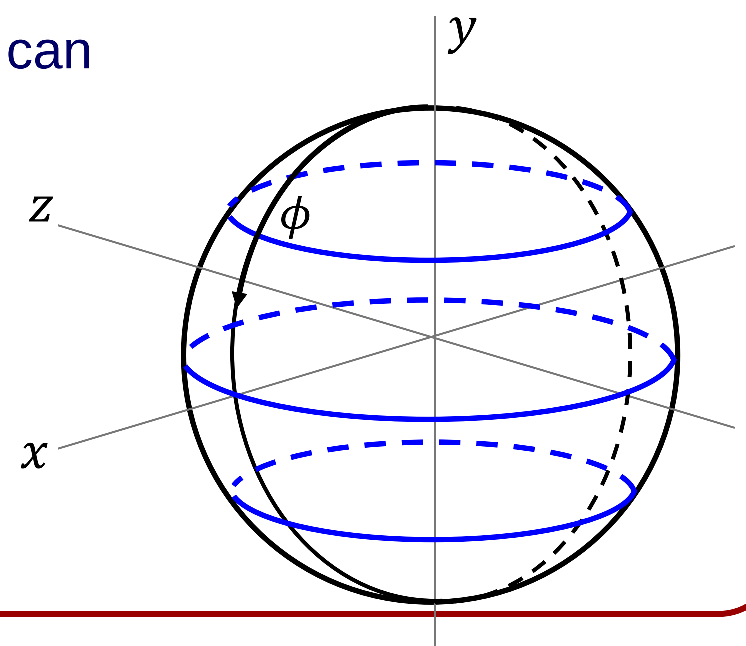
- For each ϕ and all m, we can compute the Fourier coefficients $\hat{f}_m^{\phi}$ in $O(n \log n)$ time.

⇒ We can compute all the $\hat{f}_m^{\phi}$ in $O(n^2 \log n)$ time.

- For each l and m (with $|m| \leq l$), we can compute $\hat{f}_{lm}$ in $O(n)$ time.

⇒ We can compute all the $\hat{f}_{lm}$ in $O(n^3)$ time.

⇒ We can compute the spherical harmonic transform in $O(n^3)$ time.



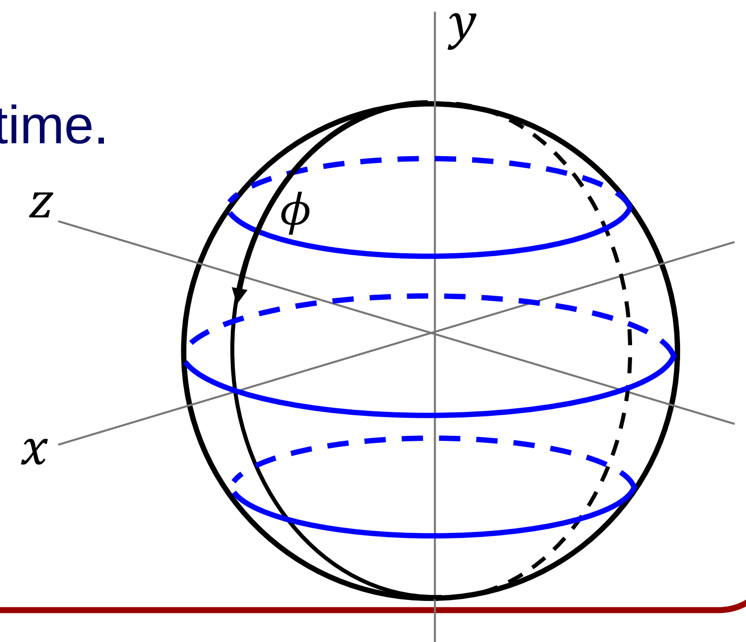
Spherical Harmonic Decomposition

$$\hat{f}_{lm} = \frac{1}{\sqrt{2\pi}} \int_0^\pi \mathbf{P}_l^{|m|}(\cos\phi) \cdot \sin(\phi) \cdot \hat{f}_m^\phi \, d\phi$$

- For each ϕ and all m, we can compute the Fourier coefficients $\hat{f}_m^\phi$ in $O(n \log n)$ time.

⇒ We can compute all the $\hat{f}_m^\phi$ in $O(n^2 \log n)$ time.

- With some more work, we can compute all the $\hat{f}_{lm}$ in $O(n^2 \log^2 n)$ time.



⇒ We can compute the spherical harmonic transform in $O(n^2 \log^2 n)$ time.

Outline

- Math Review
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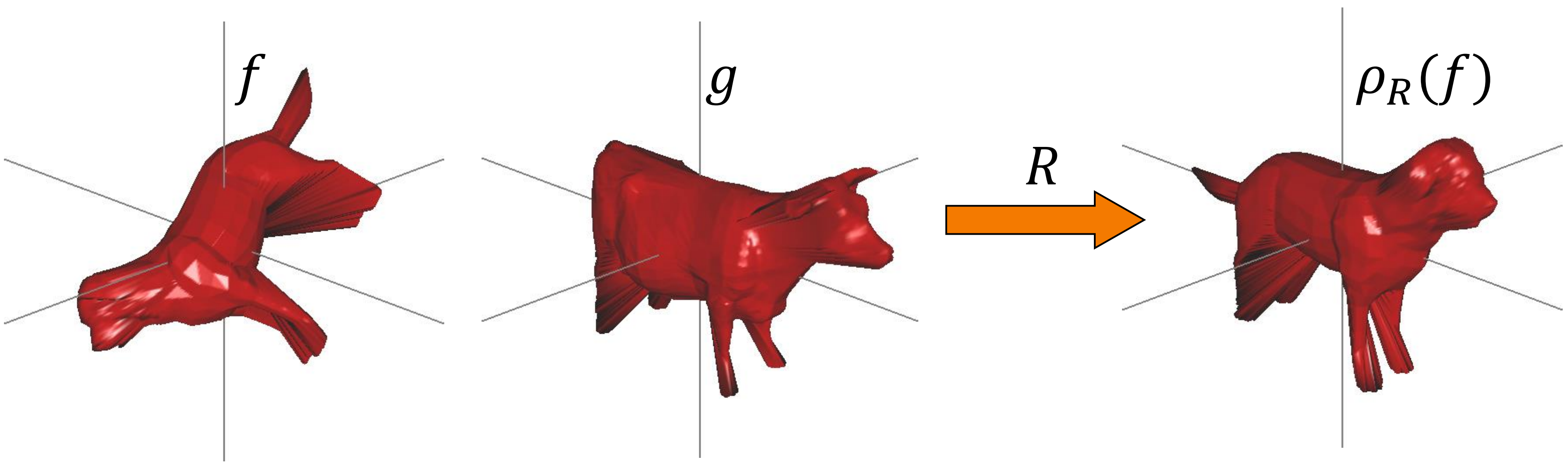
Goal

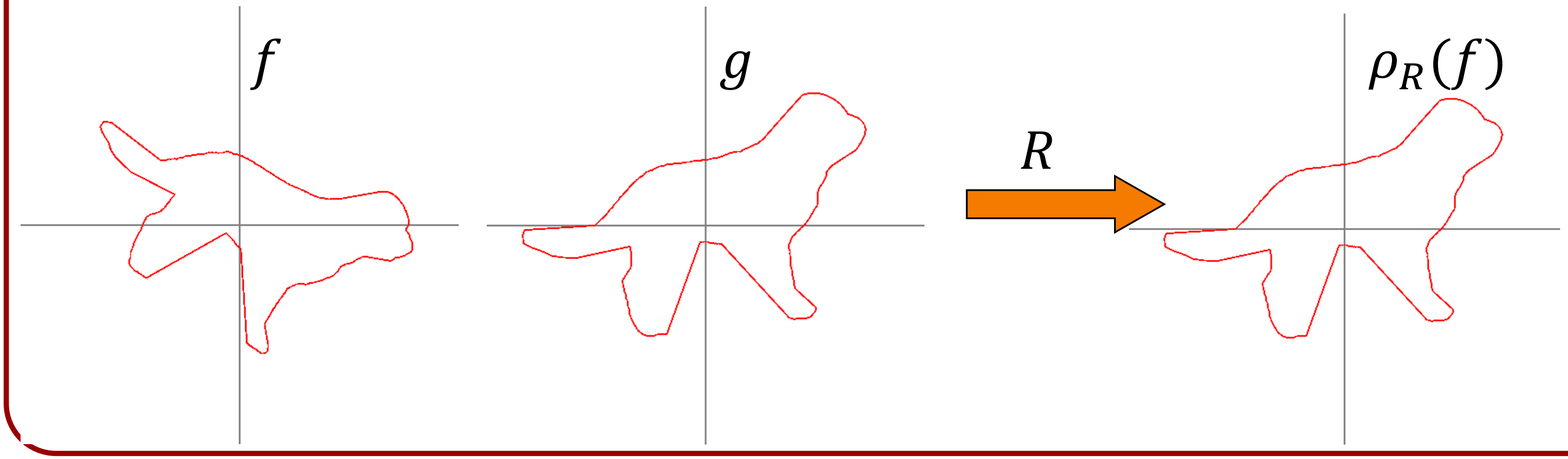
Given real-valued functions on the sphere f and g, find the rotation R that optimally aligns f to g:

$$R = \arg\min_{R \in SO(3)} \|\rho_R(f) - g\|^2$$



Recall

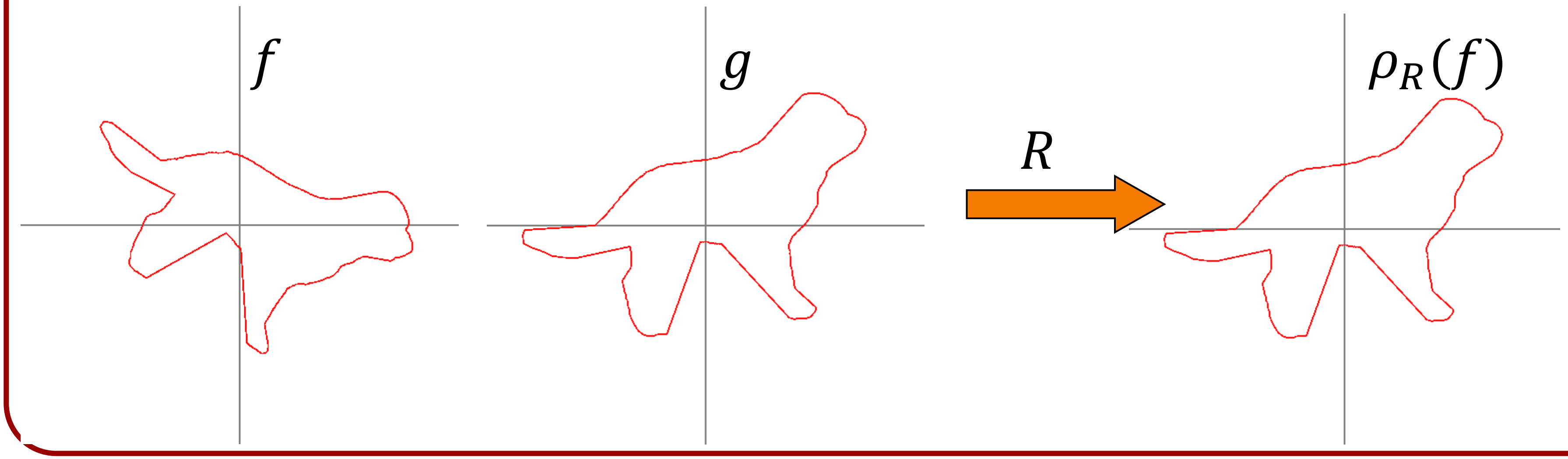
Given real-valued functions on the circle f and g, we would like to find the rotation R that optimally aligns f to g.



Reduction to a Moving Dot-Product

Expressing the norm in terms of the dot-product, we get:

$$\|\rho_R(f) - g\|^2 = \langle \rho_R(f) - g, \rho_R(f) - g \rangle$$
$$= \langle \rho_R(f), \rho_R(f) \rangle + \langle g, g \rangle - \langle g, \rho_R(f) \rangle - \langle \rho_R(f), g \rangle$$
$$= \|f\|^2 + \|g\|^2 - 2\langle \rho_R(f), g \rangle$$

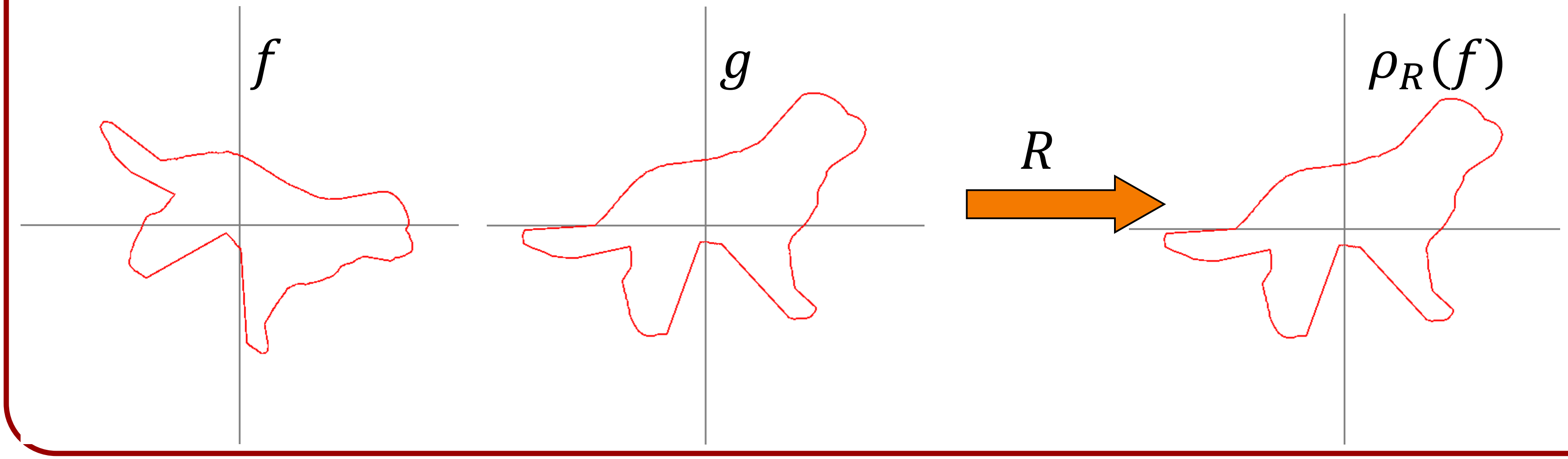


Reduction to a Moving Dot-Product

Expressing the norm in terms of the dot-product, we get:

$$\|\rho_R(f) - g\|^2 = \|f\|^2 + \|g\|^2 - 2\langle \rho_R(f), g \rangle$$

$\Rightarrow$ Finding the rotation minimizing the norm is equivalent to finding the rotation maximizing the dot-product.

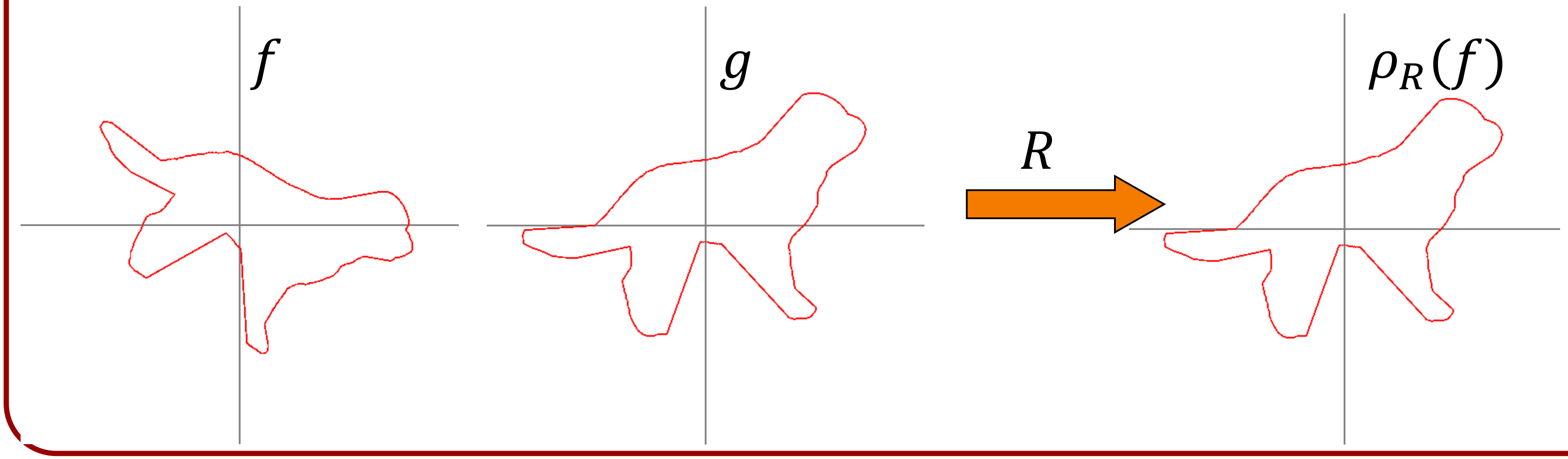


General Approach

If we define the function $D_{f,g}(\alpha)$ giving the dot-product of the rotation of f by angle α with g:

$$D_{f,g}(\alpha) = \langle \rho_\alpha(f), g \rangle$$

we can find the aligning rotation by finding the value of α maximizing $D_{f,g}(\alpha)$.



Brute-Force

To compute $D_{f,g}(\alpha)$, we could explicitly compute the value at each angle of rotation α.

If we represent a function on a circle by the values at n regular samples, this would give an algorithm whose complexity is $O(n^2)$

Fourier Transform

We do better by using the Fourier transform:

- We leverage the irreducible representations to minimize the number of multiplications that need to be performed.
- We use the FFT to compute the Inverse Fourier Transform efficiently.

Irreducible Representations

Given the functions f and g on the circle, we can express the functions in terms of their Fourier decomposition:

$$f(\theta) = \frac{1}{\sqrt{2\pi}} \sum_k \hat{f}_k \cdot e^{ik\theta}$$

$$g(\theta) = \frac{1}{\sqrt{2\pi}} \sum_k \hat{g}_k \cdot e^{ik\theta}$$

Irreducible Representations

In terms of this decomposition, the expression for the dot-product becomes:

$$D_{f,g}(\alpha) = \left\langle \rho_\alpha\left(\frac{1}{\sqrt{2\pi}}\sum_k \hat{f}_k \cdot e^{ik\theta}\right), \frac{1}{\sqrt{2\pi}}\sum_{k'} \hat{g}_{k'} \cdot e^{ik'\theta} \right\rangle$$

$$= \left\langle \frac{1}{\sqrt{2\pi}}\sum_k \hat{f}_k \cdot \rho_\alpha\left(e^{ik\theta}\right), \frac{1}{\sqrt{2\pi}}\sum_{k'} \hat{g}_{k'} \cdot e^{ik'\theta} \right\rangle$$

$$= \frac{1}{2\pi}\sum_{k,k'} \hat{f}_k \cdot \overline{\hat{g}_{k'}} \cdot \left\langle \rho_\alpha\left(e^{ik\theta}\right), e^{ik'\theta} \right\rangle$$

Irreducible Representations

Let $\mathbf{D}_{k,k'}(\alpha)$ be the function giving the dot-product of the rotation of the k-th complex exponential by an angle of α with the k'-th complex exponential:

$$\mathbf{D}_{k,k'}(\alpha) = \left\langle \rho_\alpha\left(e^{ik\theta}\right), e^{ik'\theta} \right\rangle$$

Then the equation for the dot-product becomes:

$$D_{f,g}(\alpha) = \frac{1}{2\pi} \sum_{k,k'} \hat{f}_k \cdot \overline{\hat{g}_{k'}} \cdot \left\langle \rho_\alpha\left(e^{ik\theta}\right), e^{ik'\theta} \right\rangle$$

$$\Downarrow$$

$$D_{f,g}(\alpha) = \frac{1}{2\pi} \sum_{k,k'} \hat{f}_k \cdot \overline{\hat{g}_{k'}} \cdot \mathbf{D}_{k,k'}(\alpha)$$

Irreducible Representations

$$D_{f,g}(\alpha) = \frac{1}{2\pi} \sum_{k,k'} \hat{f}_k \cdot \overline{\hat{g}_{k'}} \cdot \mathbf{D}_{k,k'}(\alpha)$$

Up to this point, the algorithm looks like:

- Compute the Fourier coefficients of f and g.
- Cross-multiply the Fourier coefficients to get the coefficients of the correlation in terms of the functions $D_{k,k'}(\alpha)$

This doesn't seem particularly promising since it in the second step, we need to perform $O(n^2)$ multiplies – which is no better than brute force.

Irreducible Representations

We know that the space of functions on a circle of frequency k are:

- Fixed by rotation (i.e. a sub-representation)
- Perpendicular to the space of functions of frequency k' (for $k \neq k'$)

Thus, for $k \neq k'$, we know that:

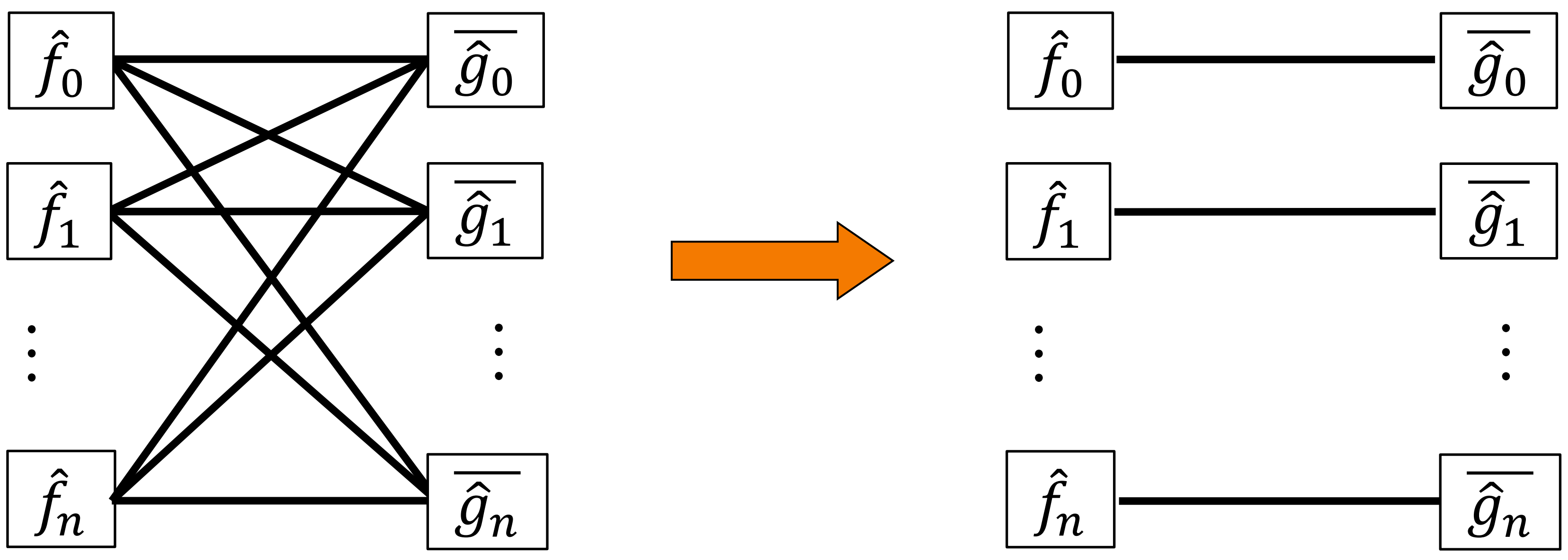
$$\mathbf{D}_{k,k'}(\alpha) = \left\langle \rho_\alpha\left(e^{ik\theta}\right), e^{ik'\theta} \right\rangle = 0$$

Irreducible Representations

So the expression for the correlation becomes:

$$D_{f,g}(\alpha) = \frac{1}{2\pi} \sum_k \hat{f}_k \cdot \overline{\hat{g}_k} \cdot \mathbf{D}_k(\alpha)$$

Reducing the number of cross-multiplications that need to be performed from $O(n^2)$ to $O(n)$:



Change of Basis

At this point, we have an expression for the correlation as a linear sum of the function $\mathbf{D}_k(\alpha)$:

$$D_{f,g}(\alpha) = \frac{1}{2\pi}\sum_k \hat{f}_k \cdot \overline{\hat{g}_k} \cdot \mathbf{D}_k(\alpha)$$

To evaluate the correlation at α we need to get the value of each of the $\mathbf{D}_k(\alpha)$, and take the linear combination, using weights $\frac{1}{2\pi} \cdot \hat{f}_k \cdot \overline{\hat{g}_k}$.

That, is evaluating the correlation at any single angle requires $O(n)$ computations and evaluating at all angles would take $O(n^2)$.

Change of Basis

Set $\mathbf{c} \in \mathbb{C}^n$ to be the n-dimensional array:

$$c_k = \frac{1}{2\pi} \cdot \hat{f}_k \cdot \overline{\hat{g}_k}$$

and set $\mathbf{a} \in \mathbb{C}^n$ to be the n-dimensional array:

$$a_k = D_{f,g}\left(\frac{2k\pi}{n}\right)$$

Then we get:

$$\mathbf{a} = \begin{pmatrix} D_0(0) & \cdots & D_{n-1}(0) \\ \vdots & \ddots & \vdots \\ D_0\left(\frac{2(n-1)\pi}{n}\right) & \cdots & D_{n-1}\left(\frac{2(n-1)\pi}{n}\right) \end{pmatrix} \cdot \mathbf{c}$$

Change of Basis

Set $\mathbf{c} \in \mathbb{C}^n$ to be the n-dimensional array:

$$c_k = \frac{1}{2\pi} \cdot \hat{f}_k \cdot \overline{\hat{g}_k}$$

and set $\mathbf{a} \in \mathbb{C}^n$ to be the n-dimensional array:

$$a_k = D_c \left(\frac{2k\pi}{\cdots} \right)$$

Th

To get the desired expression for the correlation, we need to do a matrix vector multiply!

$$\mathbf{a} = \begin{pmatrix} \vdots & \ddots & \vdots \\ D_0\left(\frac{2(n-1)\pi}{n}\right) & \cdots & D_{n-1}\left(\frac{2(n-1)\pi}{n}\right) \end{pmatrix} \cdot \mathbf{c}$$

Change of Basis

Computing this change of basis amounts to computing the Inverse Fourier Transform.

$$\mathbf{D}_k(\alpha) = \langle e^{ik(\theta-\alpha)}, e^{ik\theta} \rangle = e^{-ik\alpha}$$

Algorithm for Circular Functions

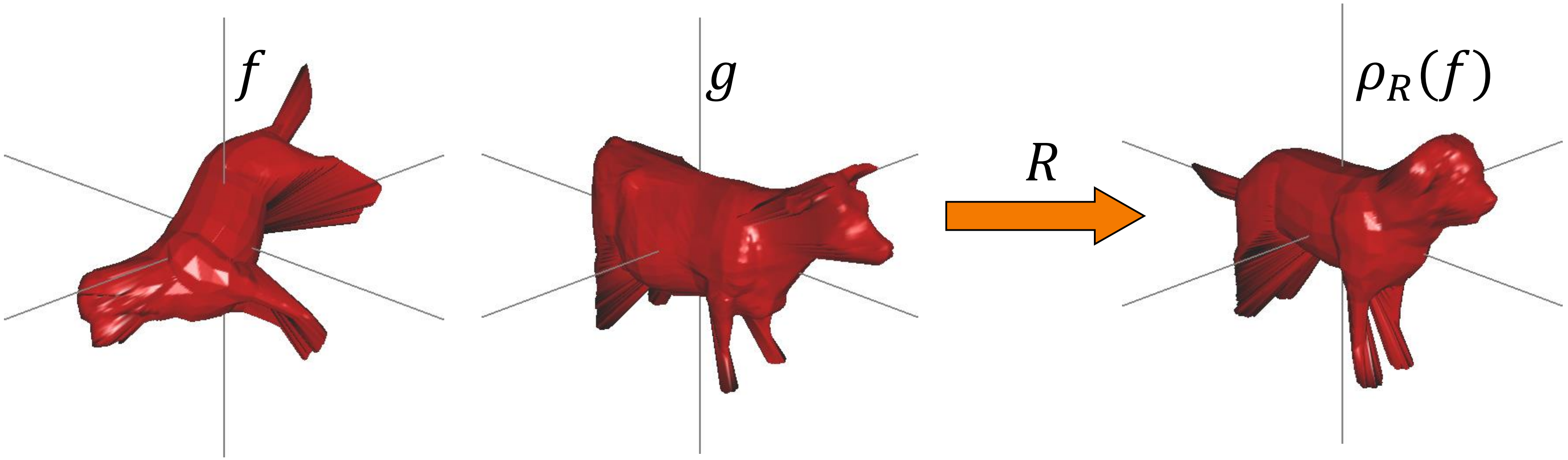
In sum, we get an algorithm for computing the value of the correlation of f with g:

1. Compute the Fourier coefficients of f and g:
   $O(n \log n)$
2. Cross-multiply the Fourier coefficients:
   $O(n)$
3. Compute the inverse Fourier transform:
   $O(n \log n)$

Goal

Given real-valued functions on the sphere f and g, find the rotation R that optimally aligns f to g:

$$R = \arg\min_{R \in SO(3)} \|\rho_R(f) - g\|^2$$



Expanding the Norm

Given real-valued functions on the sphere f and g, find the rotation R that optimally aligns f to g:

$$R = \underset{R \in SO(3)}{\arg\min} \|\rho_R(f) - g\|^2$$

Expanding the norm, we get:

$$\|\rho_R(f) - g\|^2 = \|f\|^2 + \|g\|^2 - 2\langle \rho_R(f), g \rangle$$

Expanding the Norm

$$\|\rho_R(f) - g\|^2 = \|f\|^2 + \|g\|^2 - 2\langle \rho_R(f), g\rangle$$

Thus, to find the rotation minimizing the norm of the difference, we need to find the rotation maximizing the dot-product:

$$D_{f,g}(R) = \langle \rho_R(f), g\rangle$$

Brute-Force

Again, we can try to compute the value of the dot-product using a brute force algorithm:

For each rotation R, we could compute the dot-product of the rotated function $\rho_R(f)$ with g.

If n is the resolution of the spherical function:

- the “size” of a spherical function is $O(n^2)$
- the “size” of the space of rotations is $O(n^3)$.

This means that a brute force algorithm would take on the order of $O(n^5)$ time.

Approach

As in the case of functions on a circle, we take a two-step approach:

1. We use the irreducible representations to minimize the number of cross multiplications.
2. We compute an efficient change of basis.

Irreducible Representations

Expanding the functions f and g in terms of their spherical harmonic decompositions, we get:

$$f(\theta,\phi) = \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \mathbf{Y}_l^m(\theta,\phi)$$

$$g(\theta,\phi) = \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{g}_{lm} \cdot \mathbf{Y}_l^m(\theta,\phi)$$

Irreducible Representations

Expanding the dot-product in terms of the spherical harmonics, we get:

$$D_{f,g}(R) = \left\langle \rho_R \left(\sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \mathbf{Y}_l^m(\theta,\phi) \right), \sum_{l'=0}^{n/2-1} \sum_{m'=-l'}^{l'} \hat{g}_{l'm'} \cdot \mathbf{Y}_{l'}^{m'}(\theta,\phi) \right\rangle$$

Using the linearity of ρ_R, we can pull the linear summation outside of the rotation:

$$D_{f,g}(R) = \left\langle \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \rho_R\left(\mathbf{Y}_l^m(\theta,\phi)\right), \sum_{l'=0}^{n/2-1} \sum_{m'=-l'}^{l'} \hat{g}_{l'm'} \cdot \mathbf{Y}_{l'}^{m'}(\theta,\phi) \right\rangle$$

Irreducible Representations

Expanding the dot-product in terms of the spherical harmonics, we get:

$$D_{f,g}(R) = \left\langle \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{f}_{lm} \cdot \rho_R\left(\mathbf{Y}_l^m(\theta,\phi)\right), \sum_{l'=0}^{n/2-1} \sum_{m'=-l'}^{l'} \hat{g}_{l'm'} \cdot \mathbf{Y}_{l'}^{m'}(\theta,\phi) \right\rangle$$

Using the conjugate-linearity of the inner product, we can pull out the linear summation:

$$D_{f,g}(R) = \sum_{l,l'=0}^{n/2-1} \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \hat{f}_{lm} \cdot \overline{\hat{g}_{l'm'}} \left\langle \rho_R\left(\mathbf{Y}_l^m(\theta,\phi)\right), \mathbf{Y}_{l'}^{m'}(\theta,\phi) \right\rangle$$

Irreducible Representations

$$D_{f,g}(R) = \sum_{l,l'=0}^{n/2-1} \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \hat{f}_{lm} \cdot \overline{\hat{g}_{l'm'}} \left\langle \rho_R\left(\mathbf{Y}_l^m(\theta,\phi)\right), \mathbf{Y}_{l'}^{m'}(\theta,\phi) \right\rangle$$

Recall that:

1. Rotations of l-th frequency functions are l-th frequency functions
2. The space of l-th frequency functions is orthogonal to the space of l'-th frequency functions (for $l \neq l'$)

We get:

$$D_{f,g}(R) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \left\langle \rho_R\left(\mathbf{Y}_l^m(\theta,\phi)\right), \mathbf{Y}_l^{m'}(\theta,\phi) \right\rangle$$

Change of Basis

$$D_{f,g}(R) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \left\langle \rho_R\left(\mathbf{Y}_l^m(\theta,\phi)\right), \mathbf{Y}_l^{m'}(\theta,\phi) \right\rangle$$

Set $\mathbf{D}_l^{m,m'}$ to be the functions on the space of rotations defined by:

$$\mathbf{D}_l^{m,m'}(R) = \left\langle \rho_R(\mathbf{Y}_l^m), \mathbf{Y}_l^{m'} \right\rangle$$

This gives:

$$D_{f,g}(R) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{D}_l^{m,m'}(R)$$

The $\mathbf{D}_l^{m,m'}$ are called *Wigner-D* functions.

Change of Basis

$$D_{f,g}(R) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{D}_l^{m,m'}(R)$$

Given the spherical harmonic coefficients of f and g, we can express the correlation as a sum of the functions $\mathbf{D}_l^{m,m'}$ by cross-multiplying the harmonic coefficients within each frequency.

Change of Basis

$$D_{f,g}(R) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{D}_l^{m,m'}(R)$$

The problem is that this expression for the correlation is not easy to evaluate.

To compute the value at a particular rotation R, we need to:

- Evaluate $\mathbf{D}_l^{m,m'}(R)$ at every frequency l and every pair of indices $-l \leq m, m' \leq l$,
- And then take the linear sum weighted by the product of the harmonic coefficients

Change of Basis

$$D_{f,g}(R) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{D}_l^{m,m'}(R)$$

That is, for each of $O(n^3)$ rotations, we would need to evaluate:

$$\sum_{l=0}^{O(n)} (2l+1)^2 = O(n^3)$$

different functions.

This is worse than brute force method since it requires $O(n^6)$ while brute force requires $O(n^5)$.

Change of Basis

What is that we really want to do?

We would like to take a function expressed as a linear sum of the $\mathbf{D}_l^{m,m'}$ and get an expression of the function, "regularly" sampled at n^3 rotations.

As in the case of circular correlation, this amounts to a change of basis. Only in the spherical case:

- The vectors themselves are of dimension n^3
- So the matrices are of $n^3 \times n^3 = n^6$.

Change of Basis

If we represent rotations in terms of the triplet of Euler angles $(\theta,\phi,\psi) \in [0,2\pi) \times [0,\pi] \times [0,2\pi)$:

$$R(\theta,\phi,\psi) = \underbrace{\begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\text{Rotation sending } (0,1,0) \to p = \Phi(\theta,\phi)} \underbrace{\begin{pmatrix} \cos\psi & 0 & -\sin\psi \\ 0 & 1 & 0 \\ \sin\psi & 0 & \cos\psi \end{pmatrix}}_{\text{Rotation about the } y\text{-axis by } \psi}$$

what do the function $\mathbf{D}_l^{m,m'}\left(R(\theta,\phi,\psi)\right)$ look like?

Change of Basis

Recall that the spherical harmonics can be expressed as a complex exponential in θ times a "polynomial" in $\cos\phi$:

$$\mathbf{Y}_l^m(\theta,\phi) = \mathbf{P}_l^{|m|}(\cos\phi)\cdot e^{im\theta}$$

So a rotation by an angle of α about the y-axis acts on the (l,m)-th spherical harmonics by:

$$\rho_{R_y(\alpha)}(\mathbf{Y}_l^m) = e^{-im\alpha}\cdot\mathbf{Y}_l^m$$

Change of Basis

Thus, writing out the functions $\mathbf{D}_l^{m,m'}$ as functions of the Euler angles, we get:

$$\begin{aligned}
\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) &= \left\langle \left(\rho_{R_{y(\theta)}} \circ \rho_{R_{z(\phi)}} \circ \rho_{R_{y(\psi)}}\right)(\mathbf{Y}_l^m), \mathbf{Y}_l^{m'} \right\rangle \\
&= \left\langle \rho_{R_{z(\phi)}}\left(\rho_{R_{y(\psi)}}(\mathbf{Y}_l^m)\right), \rho_{R_y^{-1}(\theta)}\left(\mathbf{Y}_l^{m'}\right) \right\rangle \\
&= \left\langle \rho_{R_{z(\phi)}}(e^{-im\psi} \cdot \mathbf{Y}_l^m), e^{im'\theta} \cdot \left(\mathbf{Y}_l^{m'}\right) \right\rangle \\
&= e^{-im\psi} \cdot e^{-im'\theta} \left\langle \rho_{R_{z(\phi)}}(\mathbf{Y}_l^m), \mathbf{Y}_l^{m'} \right\rangle
\end{aligned}$$

Change of Basis

$$\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) = e^{-im\psi} \cdot e^{-im'\theta} \left\langle \rho_{R_{z(\phi)}}(\mathbf{Y}_l^m), \mathbf{Y}_l^{m'} \right\rangle$$

Denoting:

$$\mathbf{d}_l^{m,m'}(\phi) = \left\langle \rho_{R_{z(\phi)}}(\mathbf{Y}_l^m), \mathbf{Y}_l^{m'} \right\rangle$$

we can express the functions $\mathbf{D}_l^{m,m'}$ as:

$$\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) = e^{-im'\theta} \cdot \mathbf{d}_l^{m,m'}(\phi) \cdot e^{-im\psi}$$

$$\mathbf{d}_l^{m,m'}(\phi) = \sum_k (-1)^k \frac{\sqrt{(l+m)! \cdot (l-m)! \cdot (l+m')! \cdot (l-m')!}}{(l-m'-k)! \cdot (l+m-k)! \cdot k! \cdot (k+m'-m)!} \cos^{2l+m-m'-2k}\left(\frac{\phi}{2}\right) \cdot \sin^{2k+m'-m}\left(\frac{\phi}{2}\right)$$

The $\mathbf{d}_l^{m,m'}$ are sometimes called *Wigner-small-d* functions.

Change of Basis

$$\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) = e^{-im'\theta} \cdot \mathbf{d}_l^{m,m'}(\phi) \cdot e^{-im\psi}$$

The advantage of this representation is that the basis functions are separable so instead of doing a single $O(n^3 \times n^3)$ we need to do $3n^2$ different $O(n \times n)$ matrix multiplies.

We can make things even faster noting that in two of the dimensions we are performing a Fourier transform.

Change of Basis

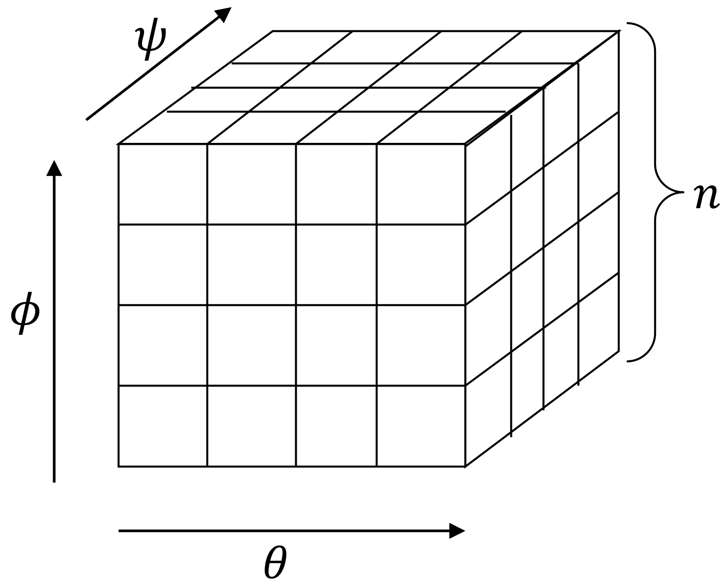
$$\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) = e^{-im'\theta} \cdot \mathbf{d}_l^{m,m'}(\phi) \cdot e^{-im\psi}$$

We can think of the sampled correlation function as an $n \times n \times n$ grid, whose (p,q,r)-th entry corresponds to the value of the correlation at the Euler angle $(\theta_p, \phi_q, \psi_r)$

$$\theta_p = \frac{2\pi p}{n}$$

$$\phi_q = \frac{\pi(2q+1)}{2n}$$

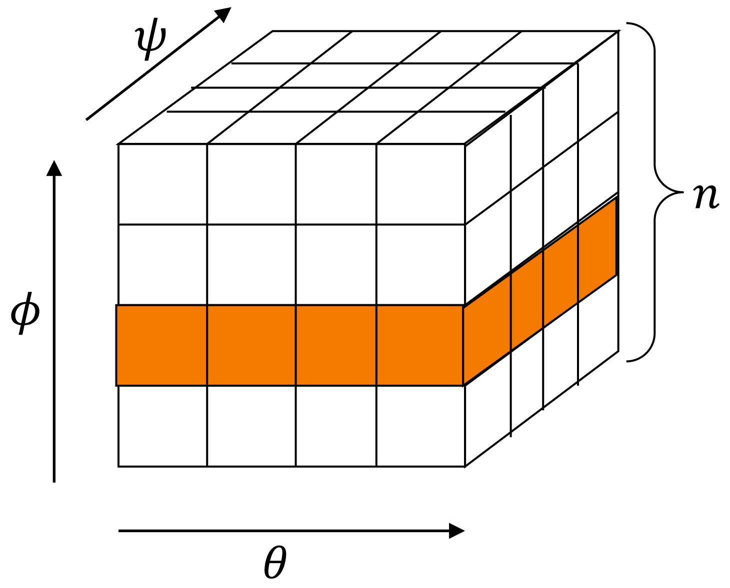
$$\psi_r = \frac{2\pi r}{n}$$



Change of Basis

$$\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) = e^{-im'\theta} \cdot d_l^{m,m'}(\phi) \cdot e^{-im\psi}$$

Fixing the angle ϕ, we restrict ourselves to a 2D slice of the correlation values.



Change of Basis

$$\mathbf{D}_l^{m,m'}(\theta,\phi,\psi) = e^{-im'\theta} \cdot d_l^{m,m'}(\phi) \cdot e^{-im\psi}$$

Fixing the angle ϕ, we restrict ourselves to a 2D slice of the correlation values.

On this 2D slice, the values of the correlation are:

$$\begin{aligned} D_{f,g}^{\phi}(\theta,\psi) &= \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{D}_l^{m',m}(\theta,\phi,\psi) \\ &= \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot e^{-im'\theta} \cdot \mathbf{d}_l^{m,m'}(\phi) \cdot e^{-im\psi} \end{aligned}$$

Change of Basis

$$D_{f,g}^{\phi}(\theta,\psi) = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot e^{-im'\theta} \cdot \mathbf{d}_l^{m,m'}(\phi) \cdot e^{-im\psi}$$
$$= \sum_{m,m'=-n/2-1}^{n/2-1} e^{-im'\theta} \cdot e^{-im\psi} \left(\sum_{l=\max(|m|,|m'|)}^{n/2-1} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{d}_l^{m,m'}(\phi) \right)$$

That is, for fixed ϕ we get a 2D function which is the sum of complex exponentials, with (m, m')-th Fourier coefficient defined by:

$$\left(\widehat{\mathbf{D}}_{f,g}^{\phi}\right)_{mm'} = \sum_{l=\max(|m|,|m'|)}^{n/2-1} \hat{f}_{l,-m} \cdot \overline{\hat{g}_{l,-m'}} \cdot \mathbf{d}_l^{-m,-m'}(\phi)$$

⇒ We can get the values in this 2D slice by running the 2D inverse FFT.

Change of Basis

$$D_{f,g}^{\phi}(\theta,\psi) = \sum_{m,m'=-n/2-1}^{n/2-1} e^{-im'\theta} \cdot e^{-im\psi} \left(\sum_{l=\max(|m|,|m'|)}^{n/2-1} \hat{f}_{lm} \cdot \overline{\hat{g}_{lm'}} \cdot \mathbf{d}_l^{m,m'}(\phi) \right)$$

This allows us evaluate the correlation on a slice-by-slice basis.

For every sampled value of ϕ:

- We compute the Fourier coefficients:

$$\left(\widehat{\mathbf{D}}_{f,g}^{\phi}\right)_{mm'} = \sum_{l=\max(|m|,|m'|)}^{n/2-1} \hat{f}_{l,m} \cdot \overline{\hat{g}_{l,-m'}} \cdot \mathbf{d}_l^{-m,-m'}(\phi)$$

- And then we compute the 2D inverse FFT.

Change of Basis

Since we sample ϕ at n different values, there are n different 2D slices.

For each slice there are $n \times n$ different Fourier coefficients, requiring $O(n)$ calculations per coefficient:

$$\left(\widehat{\mathbf{D}}_{f,g}^{\phi}\right)_{mm'} = \sum_{l=\max(|m|,|m'|)}^{n/2-1} \hat{f}_{l,m} \cdot \overline{\hat{g}_{l,-m'}} \cdot \mathbf{d}_l^{-m,-m'}(\phi)$$

Change of Basis

Since we sample ϕ at n different values, there are n different 2D slices.

For each slice there are $n \times n$ different Fourier coefficients, requiring $O(n)$ calculations per coefficient.

And each inverse FFT takes $O(n^2 \log n)$ time.

Thus, the computational complexity becomes:

- $O(n^4)$ for computing all the 2D slice Fourier coefficients
- $O(n^3 \log n)$ to compute all the 2D inverse FFTs.

Change of Basis

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In particular, we can do much better than the brute force algorithm

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Thus, the computational complexity becomes:

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General Overview

To make the computation of the correlation efficient, we used the fact that in two of the three coefficients – θ and ψ – the functions $\mathbf{D}_l^{m,m'}$ could be expressed as complex exponentials.

This allowed us to replace the $n^2 \times n^2$ matrix multiplication in two of the variables by an $O(n^2 \log n)$ inverse FFT.

In the third variable – ϕ – we still end up doing a full $n \times n$ matrix multiplication:

$$n^3 \times n^3 \rightarrow \underbrace{n^2 \cdot (n \times n)}_{\phi} + \underbrace{(n^2 \log n) \cdot n}_{\theta,\psi}$$

General Overview

In practice, the change of basis in ϕ can also be performed using an FFT like approach, giving rise to an algorithm with complexity $O(n\log^2 n)$.

Thus, the total complexity of computing the correlation drops down to $O(n^3\log^2 n)$.

Aligning 3D Functions

What kind of penalty hit do we pay for aligning functions defined in 3D?

Correlating 3D Functions

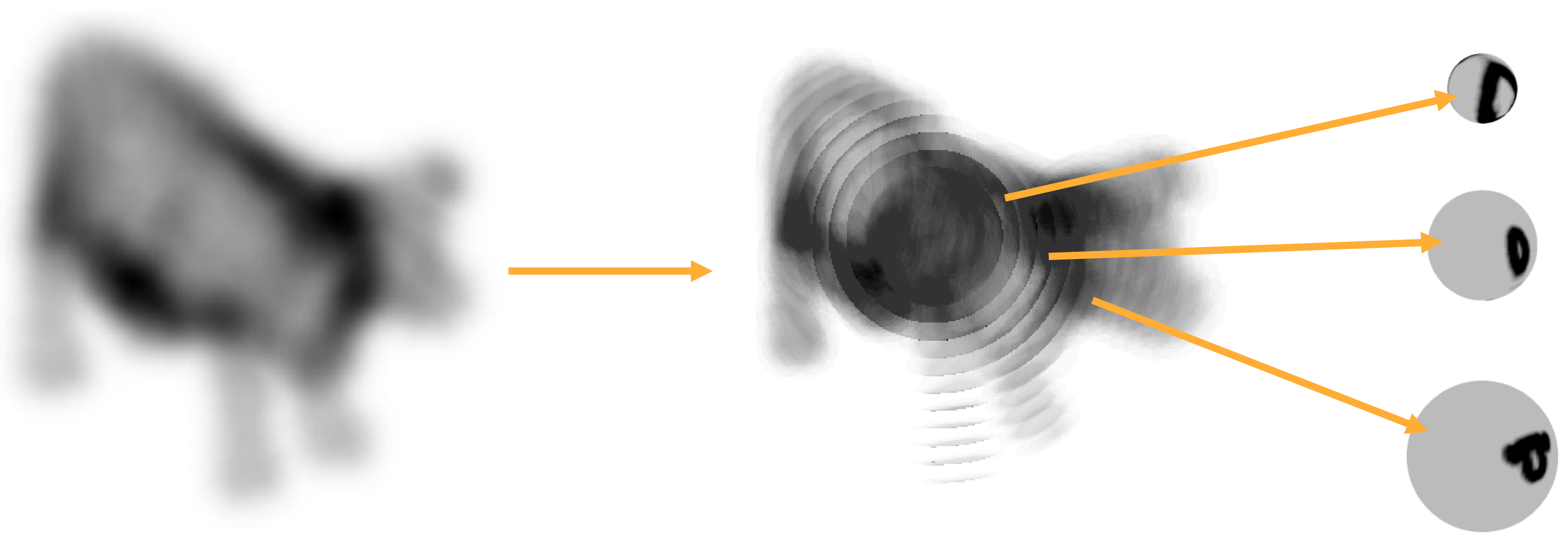
Given two functions F and G defined on the unit ball (i.e. (x, y, z) with $\|(x, y, z)\| \leq 1$) we would like to compute the distance between the functions at every rotation:

$$\|\rho_R(F) - G\|^2 = \|F\|^2 + \|G\|^2 - 2\langle\rho_R(F), G\rangle$$

Correlating 3D Functions

Using the fact that rotations fix spheres about the origin, we express the functions as a set of spherical functions:

$$F^r(\theta,\phi) = F(r \cdot \cos\theta \cdot \sin\phi\,, r \cdot \cos\phi\,, r \cdot \sin\theta \cdot \sin\phi)$$
$$G^r(\theta,\phi) = G(r \cdot \cos\theta \cdot \sin\phi\,, r \cdot \cos\phi\,, r \cdot \sin\theta \cdot \sin\phi)$$



Correlating 3D Functions

The value of the correlation then becomes:

$$\langle \rho_R(F), G \rangle = \int_0^1 \langle \rho_R(F^r), G^r \rangle \cdot r^2 \, dr$$

Thus, if we express each radial restriction in terms of its spherical harmonics:

$$F^r = \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{F}_{lm}(r) \cdot \mathbf{Y}_l^m \qquad G^r = \sum_{l=0}^{n/2-1} \sum_{m=-l}^{l} \hat{G}_{lm}(r) \cdot \mathbf{Y}_l^m$$

we get:

$$\langle \rho_R(F), G \rangle = \int_0^1 \left(\sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot \mathbf{D}_l^{m,m'}(R) \right) r^2 \, dr$$

Correlating 3D Functions

$$\langle \rho_R(F), G \rangle = \int_0^1 \left(\sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot \mathbf{D}_l^{m,m'}(R) \right) r^2 \, dr$$

This implies that we can compute the correlation, by performing a correlation for each radial restriction and then take the (area weighted) sum.

Assuming that we sample the radius at $O(n)$ different values, this would given an algorithm with complexity $O(n^5)$ / $O(n^4 \log^2 n)$.

Correlating 3D Functions

We can do better.

The functions $\mathbf{D}_l^{m,m'}$ do not depend on the radius, so we can pull them out of the integral:

$$\langle \rho_R(F), G \rangle = \int_0^1 \left(\sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot \mathbf{D}_l^{m,m'}(R) \right) r^2 \, dr$$

$$\Downarrow$$

$$\langle \rho_R(F), G \rangle = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \left(\int_0^1 \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot r^2 \, dr \right) \cdot \mathbf{D}_l^{m,m'}(R)$$

Correlating 3D Functions

$$\langle \rho_R(F), G \rangle = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \left(\int_0^1 \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot r^2 \, dr \right) \cdot \mathbf{D}_l^{m,m'}(R)$$

The advantage of this expression, is that by gathering values across different radii first, we only need to perform a single change of basis.

Correlating 3D Functions

$$\langle \rho_R(F), G \rangle = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \left(\int_0^1 \boxed{\hat{F}_{lm}(r)} \cdot \boxed{\overline{\hat{G}_{lm'}(r)}} \cdot r^2\, dr \right) \cdot \mathbf{D}_l^{m,m'}(R)$$

Algorithm: (Assuming $O(n)$ radial samples)

1. Compute the spherical harmonic transform of each radial restriction: $O(n) \cdot O(n^2 \log^2 n)$

Correlating 3D Functions

$$\langle \rho_R(F), G \rangle = \sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \boxed{\left(\int_0^1 \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot r^2 \, dr \right)} \cdot \mathbf{D}_l^{m,m'}(R)$$

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1. Compute the spherical harmonic transform of each radial restriction: $O(n) \cdot O(n^2 \log^2 n)$
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Correlating 3D Functions

$$\langle \rho_R(F), G \rangle = \boxed{\sum_{l=0}^{n/2-1} \sum_{m,m'=-l}^{l} \left(\int_0^1 \hat{F}_{lm}(r) \cdot \overline{\hat{G}_{lm'}(r)} \cdot r^2 \, dr \right) \cdot \mathbf{D}_l^{m,m'}(R)}$$

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1. Compute the spherical harmonic transform of each radial restriction: $O(n) \cdot O(n^2 \log^2 n)$
2. Cross multiply intra-frequency harmonic coeffs. and sum over the radii: $O(n) \cdot O(n^3)$
3. Do the change of basis: $O(n^3 \log^2 n)$ / $O(n^4)$

$\Rightarrow$ In 3D, correlations can be done in $O(n^4)$ time.