Fast $SO(3)$ Fourier Transforms at nonequispaced nodes and its Application to Protein-Protein Docking

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A brief outline

1. About $SO(3)$, $L^2(SO(3))$ and $\mathbb{D}_B$

2. Nonequispaced Discrete Fourier Transforms on $SO(3)$ (NDSOFT)

3. The discrete Wigner transform

4. The fast Wigner transform

5. The Nonequispaced Fast $SO(3)$ Fourier Transform (NFSOFT)

6. The Docking Problem
**The rotation group \( SO(3) \)**

**Special Orthogonal group \( SO(3) \):**
- rotations in \( \mathbb{R}^3 \)
- \( SO(3) = \{ R \in \mathbb{R}^{3 \times 3} : \det(R) = 1, R^T R = I_3 \} \)
- Parametrization (Euler angles):

Given three angles \( \alpha, \gamma \in [0, 2\pi) \) and \( \beta \in [0, \pi] \), the corresponding rotation \( R(\alpha, \beta, \gamma) \) is given by

\[
R(\alpha, \beta, \gamma) = R_{ZYZ}(\alpha, \beta, \gamma) = R_Z(\alpha) R_Y(\beta) R_Z(\gamma)
\]

where

\[
R_Z(\varphi) = \begin{pmatrix}
\cos \varphi & -\sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix}, \quad R_Y(\theta) = \begin{pmatrix}
\cos \theta & 0 & \sin \theta \\
0 & 1 & 0 \\
-\sin \theta & 0 & \cos \theta
\end{pmatrix}
\]
A Basis System for $L^2(SO(3))$

We denote

- a rotation $g \in SO(3)$ by $g(\alpha, \beta, \gamma) = R_{ZYX}(\alpha, \beta, \gamma)$
- a function $f : SO(3) \to \mathbb{C}$ by $f(g(\alpha, \beta, \gamma)) = f(\alpha, \beta, \gamma)$.

We now consider the Hilbert space $L^2(SO(3))$ with the inner product of two functions $f_1, f_2 \in L^2(SO(3))$ given by

$$
\langle f_1, f_2 \rangle = \int_{SO(3)} f_1(g) \overline{f_2(g)} \, dg
$$

$$
= \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} f_1(\alpha, \beta, \gamma) \overline{f_2(\alpha, \beta, \gamma)} \sin(\beta) \, d\alpha d\beta d\gamma
$$

and the corresponding norm

$$
\| f \|_{L^2(SO(3))} = \sqrt{\langle f, f \rangle}.
$$

We are looking for a basis system of $L^2(SO(3))$. 
Wigner-D and Wigner-d functions

The Wigner-D functions $D_{lm}^m(g)$ are the eigenfunctions of the Laplace operator for $SO(3)$.
They are given for $|m|, |n| \leq l \in \mathbb{N}_0$ by

$$D_{lm}^m(\alpha, \beta, \gamma) = e^{-im\alpha}e^{-in\gamma}d_{lm}^m(\cos \beta)$$

where

$$d_{lm}^m(x) = \frac{(-1)^{l-m}}{2^l} \sqrt{\frac{(l + m)!}{(l - n)!(l + n)!(l - m)!}} \sqrt{\frac{(1 - x)^{n-m}}{(1 + x)^{m+n}}} \frac{d^{l-m}}{dx^{l-m}} \frac{(1 + x)^{n+l}}{(1 - x)^{n-l}}$$

are called Wigner-d functions.
The $D_{lm}^m$ are not normalized with respect to the inner product $\langle \cdot, \cdot \rangle$:

$$\|D_{lm}^m(g)\|_{L^2(SO(3))}^2 = \frac{4\pi^2}{l + \frac{1}{2}}.$$ 

A special case:

$$Y_l^m(\xi) = Y_l^m(\beta, \alpha) = (-1)^{\delta_{m|m|}} \sqrt{\frac{2l - 1}{4\pi}} D_{l}^{0,-m}(\alpha, \beta, \gamma)$$

where $(\beta, \alpha) \in [0, \pi] \times [0, 2\pi)$ are the polar coordinates of the point $\xi \in \mathbb{S}^2$.
An orthogonal basis

By means of the Peter-Weyl-Theorem the harmonic spaces

\[ \text{Harm}_l(SO(3)) = \text{span} \{ D_{lmn} : m, n = -l, \ldots , l \} \]

spanned by the Wigner-D functions satisfy

\[ L^2(SO(3)) = \text{clos}_{L^2} \bigoplus_{l=0}^{\infty} \text{Harm}_l(SO(3)). \]

Hence the collection of Wigner-D functions \( \{ D_{lmn}(g) : l \in \mathbb{N}_0, m, n = -l, \ldots , l \} \) forms an orthogonal basis system in \( L^2(SO(3)) \).

Every function \( f \in L^2(SO(3)) \) has a unique series expansion in terms of the Wigner-D functions

\[ f(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \hat{f}_{lmn} D_{lmn}(g), \]

where \( g \in SO(3) \) and the \( SO(3) \) Fourier coefficients \( \hat{f}_{lmn} \) are given by the integral

\[ \hat{f}_{lmn} = \frac{l + \frac{1}{2}}{4\pi^2} \langle f, D_{lmn} \rangle. \]
The function spaces $\mathbb{D}_B$

Moreover we define the function spaces

$$\mathbb{D}_B = \bigoplus_{l=0}^{B} \text{Harm}_l(\text{SO}(3))$$

for arbitrary $B \in \mathbb{N}$. The dimension of these spaces is given by

$$\dim(\mathbb{D}_B) = \sum_{l=0}^{B} (2l + 1)^2 = \frac{1}{3} (B + 1)(2B + 1)(2B + 3).$$

B-bandlimited functions $f \in \mathbb{D}_B$ can be written as their own finite Fourier partial sum

$$f(g) = \sum_{l=0}^{B} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \hat{f}_{l}^{mn} D_{l}^{mn}(g).$$
Nonequispaced Discrete Fourier Transforms on SO(3) (NDSOFT)

Consider sampling sets of three-dimensional non-equispaced data

$$\mathcal{X}_M = \{g(\alpha_q, \beta_q, \gamma_q) : q = 0, \ldots, M - 1\}$$

where $0 \leq \alpha_q, \gamma_q < 2\pi$ and $0 \leq \beta_q \leq \pi$ are Euler angles.

The Fourier sum of a $B$-band-limited function $f \in \mathbb{D}_B$ reads as

$$f(\alpha_q, \beta_q, \gamma_q) = \sum_{l=0}^{B} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \hat{f}_l^{mn} D_l^{mn}(\alpha_q, \beta_q, \gamma_q)$$

for $q = 0, \ldots, M - 1$.

$\Rightarrow$ nonequispaced discrete Fourier transform on the rotation group (NDSOFT)

$$f = D\hat{f}$$

with

- $f = (f(g))_{g \in \mathcal{X}_M} \in \mathbb{C}^M$, the function samples
- $\hat{f} = (\hat{f}_l^{mn})_{(l,m,n) \in \mathcal{I}_B} \in \mathbb{C}^{\frac{1}{3}(B+1)(2B+1)(2B+3)}$, the SO(3) Fourier coefficients
- $D = (D_l^{mn}(\alpha_q, \beta_q, \gamma_q))_{(\alpha_q, \beta_q, \gamma_q) \in \mathcal{X}_M; (l,m,n) \in \mathcal{I}_B} \in \mathbb{C}^{M \times \frac{1}{3}(B+1)(2B+1)(2B+3)}$ the nonequispaced SO(3) Fourier matrix
A note on complexity

Computing

\[ f = D\hat{f} \]

- lower bound: \( \mathcal{O}(B^3) \) Fourier coefficients and \( \mathcal{O}(M) \) nodes as input values
  \[ \Rightarrow \mathcal{O}(M + B^3) \] flops

- naive approach: matrix-multiplication with \( D \in \mathbb{C}^{M \times \frac{1}{3}(B+1)(2B+1)(2B+3)} \)
  \[ \Rightarrow \mathcal{O}(MB^3) \] flops

- our approach on nonequispaced grids on the \( SO(3) \):
  - generalizing an algorithm for the Fourier transform of scattered data on the sphere \( S^2 \) presented in the works of Kunis, Potts
  - use the nonequispaced fast Fourier transform (NFFT) algorithm from Potts, Steidl, Tasche and a fast polynomial transform
  \[ \Rightarrow \mathcal{O}(B^3 \log^2 B + M) \]
Getting faster, Step 1: Rearranging sums

We split up the Wigner-D functions according to the Euler angles of \( f(\alpha_q, \beta_q, \gamma_q) \in D_B \) for \( q = 0, \ldots, M - 1 \):

\[
\begin{align*}
\hat{f} \left( \alpha_q, \beta_q, \gamma_q \right) &= \sum_{l=0}^{B} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \hat{f}^{mn}_l D^{mn}_l (\alpha_q, \beta_q, \gamma_q) \\
&= \sum_{l=0}^{B} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \hat{f}^{mn}_l e^{-i m \alpha_q} d^{mn}_l (\cos \beta_q) e^{-i n \gamma_q}.
\end{align*}
\]

The next step is to rearrange these sums into

\[
\begin{align*}
\hat{f} \left( \alpha_q, \beta_q, \gamma_q \right) &= \sum_{m=-B}^{B} e^{-i m \alpha_q} \sum_{n=-B}^{B} e^{-i n \gamma_q} \sum_{l=\max(|m|,|n|)}^{B} \hat{f}^{mn}_l d^{mn}_l (\cos \beta_q).
\end{align*}
\]
The discrete Wigner transform

Wigner-d functions:

\[ d_{l,m}^{n,n}(x) = \frac{(-1)^{l-m}}{2^l} \sqrt{\frac{(l+m)!}{(l-n)!(l+n)!(l-m)!}} \sqrt{\frac{(1-x)^{n-m}}{(1+x)^{m+n}}} \frac{dl-m}{dx^{l-m}} \frac{(1+x)^{n+l}}{(1-x)^{n-l}} \]

- for \( m + n \) even: \( d_{l,m}^{n,n}(x) \) are polynomials of degree at most \( l \)
- for \( m + n \) odd: \( (1 - x^2)^{-1/2} d_{l,m}^{n,n}(x) \) are polynomials of degree \( l - 1 \)

\[
\sum_{l=\max(|m|,|n|)}^{B} \hat{f}_{l,m}^{n,n}(\cos \theta) = \begin{cases} 
\sum_{l=0}^{B} t_{l,m}^{n,n} T_l(\cos \theta) & \text{for } m + n \text{ even}, \\
\sin \theta \sum_{l=0}^{B-1} t_{l,m}^{n,n} T_l(\cos \theta) & \text{for } m + n \text{ odd}
\end{cases}
\]

in matrix-vector notation:

\[ \mathbf{t}_{mn} = \mathbf{W}_{mn}^{mn} \hat{\mathbf{f}}^{mn} \]

with \( \hat{\mathbf{f}}^{mn} = \left( \hat{f}_{\max(|m|,|n|)}^{mn}, \ldots, \hat{f}_{B}^{mn} \right)^T \) and \( \mathbf{t}_{mn} = (t_0^{mn}, \ldots, t_B^{mn})^T \) for fixed \( m, n \)
The matrix \( W^{mn} \in \mathbb{C}(B+1) \times (B - \max(|m|,|n|)) \) can be separated into

\[
W^{mn} = \begin{cases} 
T\tilde{D}^{mn} & \text{for } m + n \text{ even}, \\
ST\tilde{D}^{mn} & \text{for } m + n \text{ odd}
\end{cases}
\]

where we consider for the \( B + 1 \) nodes of an equispaced grid \( \chi_C = \left\{ \frac{(2k+1)\pi}{2(B+1)} : k = 0, \ldots, B \right\} \) the matrices

\[
T = \left( \frac{2 - \delta_{0k}}{B + 1} \cos \frac{(2l + 1)k \pi}{2(B + 1)} \right)_{k,l=0,\ldots,B},
\]

\[
\tilde{D}^{mn} = \left( d_l^{mn} \cos \frac{(2k + 1)\pi}{2(B + 1)} \right)_{(k=0,\ldots,B);(l=\max(|m|,|n|),\ldots,B)}
\]

and

\[
S = \text{diag} \left( \left( \sin \frac{(q + 1)\pi}{B + 2} \right)^{-1} \right)_{q=0,\ldots,B}.
\]
The separation of $W^{mn}$

A simple calculation shows that the inverse of $T$ and $S$ are given by

$$T^{-1} = \left( \cos \left( \frac{(2k + 1)l \pi}{2(B + 1)} \right) \right)_{k,l=0,...,B}$$

and

$$S^{-1} = \text{diag} \left( \sin \left( \frac{(q + 1)\pi}{B + 2} \right) \right)_{q=0,...,B}.$$

We have

$$\tilde{D}^{mn}f^{mn} = \begin{cases} 
T^{-1}t^{mn} & \text{for } m + n \text{ even,} \\
T^{-1}S^{-1}t^{mn} & \text{for } m + n \text{ odd}
\end{cases}$$

We obtain the unique solution of

$$t^{mn} = T\tilde{D}^{mn}f^{mn} = W^{mn}f^{mn}$$

for even orders $m + n$, and

$$t^{mn} = ST\tilde{D}^{mn}f^{mn} = W^{mn}f^{mn}$$

for odd orders $m + n$. 
The discrete Wigner transform

Notes on the complexity

\[ W^{mn} = \begin{cases} T \tilde{D}^{mn} & \text{for } m + n \text{ even}, \\ S T \tilde{D}^{mn} & \text{for } m + n \text{ odd} \end{cases} \]

- matrix vector multiplication with \( T \): with the discrete cosine transform (DCT) in \( O(B \log B) \) flops
- matrix vector multiplication with \( S \): a diagonal matrix multiplication in \( O(B) \) flops
- matrix vector multiplication with \( \tilde{D}^{mn} \): for fixed \( m \) and \( n \) recursive computation in \( O(B^2) \) flops with the Clenshaw algorithm
- \((2B + 1)^2\) many vectors \( t^{mn} \) to be computed
  \[ \Rightarrow \text{total complexity of this transformation step: } O(B^4) \text{ flops.} \]
  \[ \Rightarrow \text{speed up the multiplication with } \tilde{D}^{mn} \text{ by adopting the fast polynomial transform (Driscoll/Healy, Potts/Steidl/Tasche)} \]
Dealing with the matrices $\tilde{D}^{mn}$

- evaluate the following three-term recurrence relation: for $|m|, |n| \leq l$

$$d_{l+1}^{mn}(x) = (u_l^{mn} x + v_l^{mn})d_{l}^{mn}(x) + w_l^{mn}d_{l-1}^{mn}(x), \quad x = \cos \theta,$$

with the recurrence coefficients

$$u_l^{mn} = \frac{(l + 1)(2l + 1)}{\sqrt{((l + 1)^2 - m^2)((l + 1)^2 - n^2)}},$$

$$v_l^{mn} = \frac{-mn(2l + 1)}{l \sqrt{((l + 1)^2 - m^2)((l + 1)^2 - n^2)}},$$

$$w_l^{mn} = \frac{-(l + 1) \sqrt{(l^2 - m^2)(l^2 - n^2)}}{l \sqrt{((l + 1)^2 - m^2)((l + 1)^2 - n^2)}},$$

where we set $d_l^{mn}(x) = 0$ for all $l < \max(|m|, |n|)$ and $d_{\max(|m|,|n|)}^{mn}$ are given to start the recurrence.
Towards the Fast Wigner Transform

Step 1: A new three term recurrence for better stability
For \( m, n = -B, \ldots, B \) and \( l \in \mathbb{N}_0 \) (for \( |m|, |n| > l \), too.):

\[
d_{l+1}^{mn}(x) = (\alpha_l^{mn} x + \beta_l^{mn})d_l^{mn}(x) + (\gamma_l^{mn})d_{l-1}^{mn}(x), \quad x = \cos \theta,
\]

where for \( \mu = \min(|m|, |n|) \) and \( \nu = \max(|m|, |n|) \) we get

\[
\alpha_0^{mn} = \begin{cases} 
1 & \text{for } m = n, \\
-1 & \text{for } m + n \text{ even}, \\
0 & \text{otherwise},
\end{cases} \quad \alpha_l^{mn} = \begin{cases} 
(-1)^{m+n+1} & \text{for } l \leq \nu - \mu, \\
\frac{mn}{|mn|} & \text{for } \nu - \mu < l < \nu, \\
u_l^{mn} & \text{otherwise},
\end{cases}
\]

\[
\beta_l^{mn} = \begin{cases} 
1 & \text{for } 0 \leq l < \nu, \\
0 & \text{for } m = n = 0, \\
v_l^{mn} & \text{otherwise}
\end{cases} \quad \text{and} \quad \gamma_l^{mn} = \begin{cases} 
0 & \text{for } l \leq \nu, \\
w_l^{mn} & \text{otherwise},
\end{cases}
\]

using \( u_l^{mn}, v_l^{mn} \) and \( w_l^{mn} \), the old recurrence coefficients. We set \( d_{-1}^{mn} = 0 \) and

\[
d_0^{mn}(x) = \begin{cases} 
\sqrt{(2\mu)!} & \text{for } m + n \text{ even}, \\
\frac{\sqrt{(2\mu)!}}{2^\mu \mu!} & \text{for } m + n \text{ odd}.
\end{cases}
\]
Towards the Fast Wigner Transform

Step 2: Associated Wigner-d functions
Following Kunis/Potts we perform the fast polynomial multiplication based on discrete cosine transforms (DCT).

- associated Wigner-d functions $d_{i}^{mn}(\cdot, c)$

$$
\begin{align*}
  d_{-1}^{mn}(x, c) &= 0, \\
  d_{0}^{mn}(x, c) &= 1, \\
  d_{i+1}^{mn}(x, c) &= (\alpha_{i+c}^{mn} x + \beta_{i+c}^{mn})d_{i}^{mn}(x, c) + \gamma_{i+c}^{mn}d_{i-1}^{mn}(x, c)
\end{align*}
$$

- shift the degree $l$ of $d_{i}^{mn}$ by $c \in \mathbb{N}_0$ step instead of only one at a time

$$
  d_{i+c}^{mn}(x) = d_{c}^{mn}(x, l)d_{i}^{mn}(x) + \gamma^{mn}d_{c-1}^{mn}(x, l + 1)d_{i-1}^{mn}(x).
$$

- reorganization leads to a cascade summation

- perform the fast polynomial transform (Driscoll/Healy, Potts/Steidl/Tasche) in $\mathcal{O}(B \log^2 B)$ flops per set of orders $m, n$

$\Rightarrow$ total complexity of $\mathcal{O}(B^3 \log^2 B)$ flops instead of the previous $\mathcal{O}(B^4)$ flops
Getting faster, Step 2: Basis transforms

\[ f(\alpha_q, \beta_q, \gamma_q) = \sum_{m=-B}^{B} \sum_{n=-B}^{B} \sum_{l=\max(|m|,|n|)}^{B} \hat{f}_{mn}^l d_{mn}^l (\cos \beta_q). \]

Performing the change of basis described by the matrices \(W_{mn}\):

\[ f(\alpha_q, \beta_q, \gamma_q) = \sum_{m=-B}^{B} \sum_{n=-B}^{B} \sum_{l=0}^{B} t_{mn}^l T_l(\cos \beta_q)(\sin \beta_q)^{\text{mod}(m+n,2)}. \]

The matrices \(A_{mn}\) then provide the change from Chebychev coefficients to standard Fourier coefficients,

\[ f(\alpha_q, \beta_q, \gamma_q) = \sum_{m=-B}^{B} \sum_{n=-B}^{B} \sum_{l=-B}^{B} e^{-im\alpha_q} e^{-in\gamma_q} \sum_{l=-B}^{B} h_{mn}^l e^{-i\beta_q} h_{mn}^l. \]

\[ = \sum_{m=-B}^{B} \sum_{n=-B}^{B} \sum_{l=-B}^{B} h_{mn}^l e^{-i(m\alpha_q+n\gamma_q+l\beta_q)} \]

for \(q = 0, \ldots, M - 1\). Thus we obtain a three-dimensional Fourier transform.
Using \( \cos l \beta = \frac{1}{2}(e^{il\beta} + e^{-il\beta}) \) and \( \sin \beta = \frac{i}{2}(e^{-i\beta} - e^{i\beta}) \) we get

\[
H_{mn} = \begin{pmatrix}
1 & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{pmatrix},
O_{mn} = \frac{i}{2} \begin{pmatrix}
0 & 1 \\
-1 & \cdots & \cdots \\
\cdots & \cdots & 1 \\
-1 & 0
\end{pmatrix}
\in \mathbb{C}^{(2B+1) \times (B+1)}.
\]

(4.1)

such that

\[
A_{mn} = \begin{cases}
H_{mn} & \text{for } m + n \text{ even}, \\
O_{mn}H_{mn} & \text{for } m + n \text{ odd}.
\end{cases}
\]

satisfying

\[
h_{mn} = A_{mn}t_{mn}.
\]

The multiplication of \( A_{mn} \) can be done in \( \mathcal{O}(B) \) steps as it is a sparse one. So for all possible \( m, n \) this yields \( \mathcal{O}(B^3) \) flops in total.
The Nonequispaced Fast SO(3) Fourier Transform (NFSOFT)

Theorem

The matrix $\hat{D}$ with $f = \hat{D} \hat{f}$ representing the NDSOFT can be splitted into the matrix product $D = FAW$ with

- the block diagonal matrix consisting of the matrices $W^{mn}$:

$$W = \text{diag} \left( W^{mn} \right)_{m,n=-B,...,B} \in \mathbb{C}^{(2B+1)^2(B+1) \times (2B+1)^2(B+1)}$$

- the diagonal block matrix composed of blocks $A^{mn}$:

$$A = \text{diag} \left( A^{mn} \right)_{m,n=-B,...,B} \in \mathbb{C}^{(2B+1)^3 \times (2B+1)^2(B+1)}$$

- a three-dimensional Fourier matrix $F \in \mathbb{C}^{M \times (2B+1)^3}$:

$$F = \left( e^{-i \left( (m,l,n)(\alpha_q,\beta_q,\gamma_q)^T \right)} \right)_{q=0,...,M-1; (l,m,n) \in \mathcal{I}_B}.$$
The Nonequispaced Fast SO(3) Fourier Transform (NFSOFT)

The whole algorithm

Algorithm 1 Nonequispaced Fast SO(3) Fourier Transform (NFSOFT)

<table>
<thead>
<tr>
<th>Input:</th>
<th>$B \in \mathbb{N}$ the bandwidth</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>$\mathcal{X}_M$ a sampling set</td>
</tr>
<tr>
<td></td>
<td>$\tilde{f} = (\tilde{f}^mn)$ the $\frac{1}{3}(B+1)(2B+1)(2B+3)$ SO(3) Fourier coefficients of $f \in \mathbb{D}_B$</td>
</tr>
</tbody>
</table>

1. Compute $t = W\tilde{f}$, the vector of $(B+1)(2B+1)^2$ Chebychev coefficients $t_i^{mn}$ in $O(B^3 \log^2 B)$ flops.

2. Compute $h = A t$, the vector of $(2B+1)^3$ Fourier coefficients $h_i^{mn}$ in $O(B^3)$ flops.

3. Compute $f = F h$ by means of a trivariate NFFT in $O(B^3 \log B + M)$ flops.

Output: $f = (f(\alpha_q, \beta_q, \gamma_q))_{q=0, \ldots, M-1}$ the function samples of $f \in \mathbb{D}_B$

Complexity: $O(B^3 \log^2 B + M)$ flops
Some numerical results: The NDSOFT and NFSOFT at different bandwidths $B$ and $M = B^3$ nodes
The NDSOFT and NFSOFT at different number of nodes $M$ and bandwidth $B = 24$
The Docking Problem

**Input:** coordinates of the atoms of two single protein molecules

**Docking:** modelling $\rightarrow$ matching $\rightarrow$ refined scoring

**Output:** coordinates of the atoms of the new molecule

**Stage 1: Modelling**

**Affinity function** for $\mathbf{x} \in \mathbb{R}^3$:

$$Q(\mathbf{x}) = \sum_{k=1}^{M} \gamma_k \kappa(\mathbf{x} - \mathbf{z}_k)$$

with weights $\gamma_k$ and $\kappa(\mathbf{x} - \mathbf{z}_k)$ being the electron density of the $k$-th atom at $\mathbf{x} \in \mathbb{R}^3$.

**Task for Stage 2:** Find the maximal overlap of the two molecular skins.
Fast Rotational Matching

Molecules are assumed to be inflexible:

- manipulation by rigid body motion
- 6D-search space:
  - 3 degrees of freedom for the rotation $R \in SO(3)$ of the molecule $A$
  - 3 degrees of freedom for the motion of molecule $B$:
    - compute fastly the two remaining rotation parameter of $R'$ by fast Fourier transforms
    - perform a global search the optimal value $\rho$ of the translation of molecule $B$ along one axis

$$
\arg \max_{\rho, R, R'} C_\rho(R, R') = \arg \max_{\rho, R, R'} \int_{\mathbb{R}^3} \Lambda_R Q^A(\vec{x}) \quad T^\rho \Lambda_{R'} Q^B(\vec{x}) \, d\vec{x}
$$
Adapting the modell for fast rotational Matching

For all $x \in \mathbb{R}^3$ where $x = ru$ mit $r = |x|$ and $u \in S^2$:

$$\tilde{Q}^A(x) = \tilde{Q}^A(ru) = \sum_{l=0}^{B-1} \sum_{m=-l}^{l} \hat{a}_l^m(r) Y_l^m(u)$$

- Translation along the z-axis: $t = (0, 0, \rho)^T$

$$T^\rho \tilde{Q}^B \left( r \begin{pmatrix} \vartheta \\ \phi \end{pmatrix} \right) = \tilde{Q}^B \left( r' \begin{pmatrix} \vartheta' \\ \phi' \end{pmatrix} \right)$$

- Rotation:

$$\Lambda_R \tilde{Q}^A(ru) = \sum_{l=0}^{B-1} \sum_{m=-l}^{l} \hat{a}_l^m(r) Y_l^m(R^{-1}u)$$

$$= \sum_{l=0}^{B-1} \sum_{k=-l}^{l} \sum_{m=-l}^{l} \hat{a}_l^m(r) D_{l}^{km}(R) Y_l^k(u)$$

with Wigner-D-function $D_{l}^{km}$. 
The solution of the docking problem

\[ \arg \max_{\rho, R, R'} C_{\rho}(R, R') = \arg \max_{\rho, R, R'} \int_{\mathbb{R}^3} (\Lambda_{\rho} Q^A)(\vec{x}) \quad (T_{\rho}(\Lambda_{R'} Q^B)(\vec{x}) )d\vec{x}. \]

becomes

\[ C_{\rho}(R, R') = \int_{\mathbb{R}} \int_{\mathbb{S}^2} \sum_{lkm} \hat{a}^m_l (r) D^k_m (R) Y_l^k (u) \sum_{l'm'} \hat{b}^{m'}_{l'}(r') D^{k'}_{l'} (R') Y_{l'}^{k'} (u') r^2 dr du \]

\[ = \sum_{ll'kk'mm'} D^k_m (R) D^{k'}_{l'} (R') \underbrace{\int_{\mathbb{R}} \int_{\mathbb{S}^2} \hat{a}^m_l (r) \hat{b}^{m'}_{l'}(r') Y_l^k (u) Y_{l'}^{k'} (u') r^2 dr du}_{J^{kk',mm'}_{ll',mm'}(\rho)} \]

\[ = \sum_{ll'km'm'} D^k_m (R) D^{k'}_{l'} (R') J^{k',mm'}_{ll',mm'}(\rho) \]
The five rotation parameter

Splitting up $D_i^{km}(R)$ according to its Euler angles $(\phi, \theta, \psi)$ of $R \in SO(3)$

$$D_i^{km}(R) = D_i^{km}(\phi, \theta, \psi) = e^{-ik\phi} d_i^{km}(\theta) e^{-im\psi}$$

with real-valued Wigner-d function $d_i^{km}(\theta)$ leads to

$$C_{\rho}(R, R') = \sum_{ll'kmm'} J_{ll'}^{k,m'm'}(\rho) D_i^{km}(\phi, \theta, \psi) D_{l'}^{-km'}(\phi', \theta', \psi')$$

$$= \sum_{ll'kmm'} J_{ll'}^{k,m'm'}(\rho) D_i^{km}(\xi, \theta, \psi) d_{l'}^{-km'}(\theta') e^{-im'\psi'}$$

$$= C_{\rho}(\xi, \theta, \psi, \theta', \psi')$$

using one translation parameter $\rho$ and five rotation parameter $\psi, \psi', \theta, \theta'$ and $\xi = \phi - \phi'$. 
Docking Example

Thank you for your attention.
The Docking Problem

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