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Representing the Intersection of Two Ellipsoids as a Gaussian

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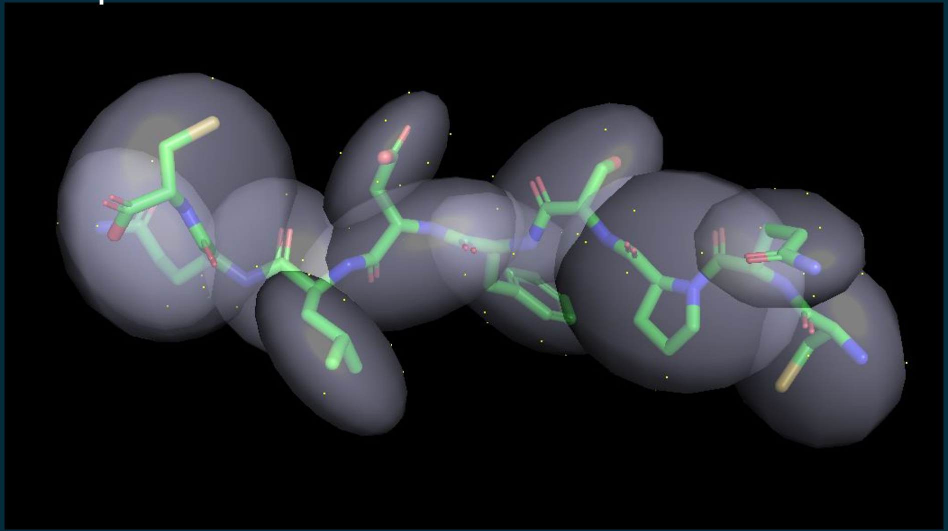
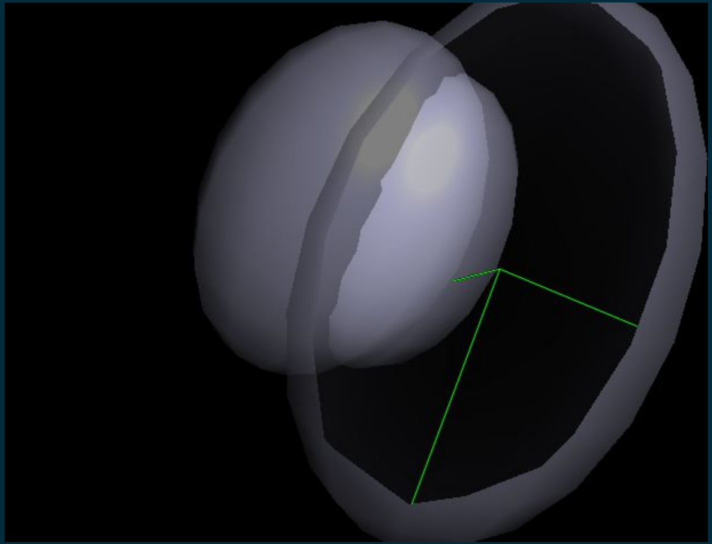
This project aimed to find a fast and efficient way to represent the intersection of two ellipsoids.

- In the summer of 2023, we worked on representing molecule structures with ellipsoids.
- We used minimum volume enclosing ellipsoid (MVEE). This takes all points used to represent a form and represents them in the smallest possible ellipsoid shape.
- We also created systems for separating into branches and other customizable parts of the visualization.





An alternative to calculating the volume of an ellipsoid by the mathematical route is by using a Gaussian approximation. An ellipsoid can be approximately represented by a Gaussian, and the integral of said Gaussian can return an approximate volume. If we represent two ellipsoids by Gaussian distributions, we can calculate the product of the two, which is also a Gaussian.

Quadratic Formula for an Ellipsoid

$$(x-u)^T \mathbf{A}(x-u) = 1$$

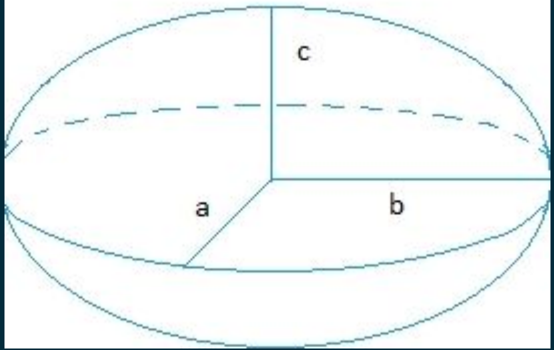
The symmetric matrix A is the covariance inverse matrix, and we can also get the axes from it.

$$|\mathbf{A}| = |\mathbf{UDV^T}| = |\mathbf{U}||\mathbf{D}||\mathbf{U^T}| = |\mathbf{D}| = \frac{1}{a^2b^2c^2}$$

We get A from MVEE.

To check the volume of a single ellipsoid gaussian, we used the mathematical equation for the volume of an ellipsoid.

$$V = \frac{4}{3} \times \pi \times a \times b \times c$$



Gaussian Formula for an Ellipsoid

$$f(x) = e^{-n(x-u)^T \mathbf{A}(x-u)}$$

u is the center, and A is the inverse covariance matrix from the other slide.

We're specifically using a asymmetric Gaussian. The skew and asymmetry allows us to capture ellipsoid.
A Gaussian function is a distribution, but by taking the integral we can get the volume.

Volume Constant

$$f(x) = e^{-n(x-u)^T \mathbf{A}(x-u)}$$

$$C\int_x f(x)dx = \sqrt{\frac{\pi^3}{n^3|\mathbf{A}|}} = abc\sqrt{\frac{\pi^3}{n^3}}$$

In the first step for finding the volume constant, we can substitute the magnitude of matrix A with a relationship to abc (the axes).

Volume Constant

Volume constant

$$C\int_x f(x)dx = \frac{4}{3}\pi abc$$

$$C = \frac{4\pi n^{\frac{3}{2}}}{3\pi^{\frac{3}{2}}} = \frac{4n^{\frac{3}{2}}}{3\sqrt{(\pi)}} = 0.75225n^{\frac{3}{2}}$$

By running multiple tests comparing the volume to abc we were able to also prove the value for C is 0.75225.

n is a constant that will later be used to scale our integers, to create a normal distribution with intersections.

With one singular ellipsoid, n doesn’t impact volume.

Using the Product of Two Ellipsoid Gaussians to Find the Intersection Gaussian

To the right is the math for the intersection Gaussian.

This is based off a paper with all math checked and some changes made.

One of these Gaussians, Gaussian B, will be placed at the origin for convenience. B refers to the symmetric matrix that represents Gaussian B, whereas A refers to the symmetric matrix that represents Gaussian A.

P is sum of A and B. It is representative of the shape of the intersection, but does not depend on u, the distance between ellipsoids.

$$
\begin{aligned}
f(x) &= Ce^{-n(x-u)^T A(x-u)} Ce^{-nx^T Bx} \\
&= C^2 e^{-n(x-u)^T A(x-u) - nx^T Bx} \\
&= C^2 e^{-n\alpha} \\
\alpha &= (x-u)^T A(x-u) + x^T Bx \\
&= x^T Ax - x^T Au - u^T Ax + u^T Au + x^T Bx \\
&= x^T Ax + x^T Bx - x^T Au - x^T A^T u + u^T Au \\
&= x^T (A+B) - 2x^T Au + u^T Au \\
P &= A + B \\
v &= P^{-1} Au \\
u &= A^{-1} Pv \\
\alpha &= x^T Px - 2xTAA^{-1} Pv + u^T Au \\
&= x^T Px - 2x^T Pv + u^T Au \\
&= x^T Px - x^T Pv - v^T Px + v^T Pv - v^T Pv + u^T Au \\
&= (x-v)^T P(x-v) - v^T Pv + u^T Au \\
f(x) &= C^2 e^{n(v^T Pv - u^T Au)} e^{-n(x-v)^T P(x-v)}
\end{aligned}
$$

$$
\int_x f(x)dx = \sqrt{\frac{\pi^3}{n^3 |P|}} C^2 e^{n(v^T Pv - u^T Au)}
$$

There were multiple ways we checked our Gaussian.

- To check ellipsoids pre-intersection, we used the mathematical equation for the volume of an ellipsoid.
- To get an estimate of if our intersection volumes were correct, we created a grid to measure intersection volume.
- For any point, if the left side of the quadratic ellipse equation was less than 1, the point is within the ellipsoid. We looped through points and appended those within each ellipse.

$$(\mathbf{x}-\mathbf{v})^T\mathbf{A}(\mathbf{x}-\mathbf{v})$$

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- We also checked this in an octave/matlab grid function.

Determining Maximum Axes for Grid

$$(x_{max}, y_{max}, z_{max}) = \left(\sqrt{(A^{-1})_{11}}, \sqrt{(A^{-1})_{22}}, \sqrt{(A^{-1})_{33}}\right)$$

Using this we could find the maximum three axes of the two ellipsoids, and minimize the size of our coordinate grid.

There were multiple ways we checked our Gaussian.

We also ran the intersection volume function of an ellipsoid with itself. We needed the intersection of an ellipsoid with itself to equal its grid volume. When it didn't come back as equal, we could use the relationship to find the constant needed.

Using math we were able to determine a constant for n.

Using the intersection of an ellipsoid with itself, we would find that the sum of the inverse covariance matrix would be two times one of them. This would make the value of the magnitude of P 8 times that of A.

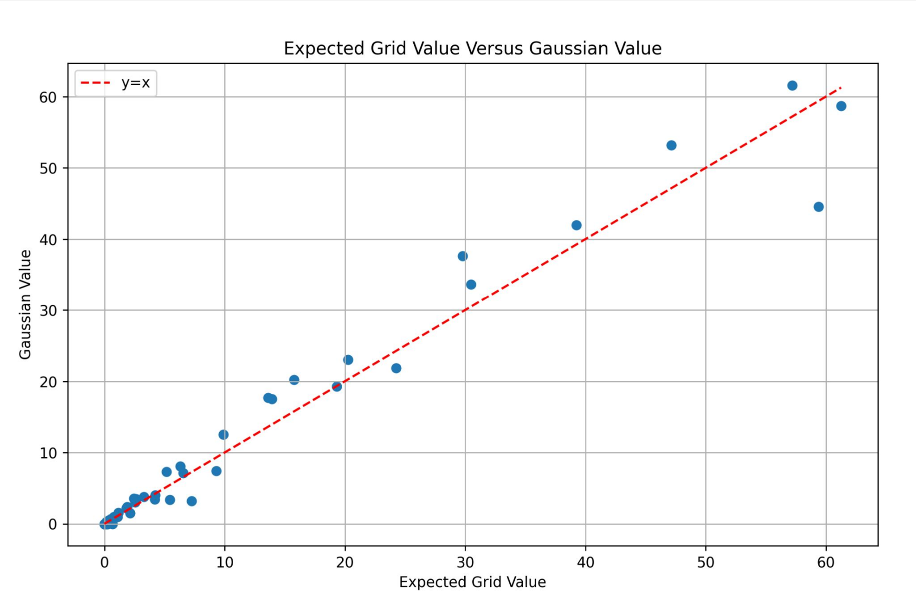
From this information, and testing, we modified n to become 2.418 when C is still 0.7225 times $n^{3/2}$.

$$
\begin{aligned}
\int_x f(x)dx =& \sqrt{\frac{\pi^3}{n^3|P|}} C^2 e^{n(v^T P v - u^T A u)} \\
A =& B \\
u =& O \\
v =& O, P = 2A, |P| = 8|A| \\
\int_x f(x)dx =& \sqrt{\frac{\pi^3}{n^3|P|}} C^2 \\
=& \sqrt{\frac{\pi^3}{n^3 8|A|}} \cdot [\frac{4n^{\frac{3}{2}}}{3\sqrt{\pi}}]^2 \\
=& \frac{4}{9} abc\sqrt{2\pi n^3} \\
=& \frac{4}{3}\pi abc n^{\frac{3}{2}} \sqrt{\frac{2}{9\pi}} \\
=& volume \times 0.2660 \times n^{\frac{3}{2}}
\end{aligned}
$$

Testing On A Larger Scale

We then created a function that generates two random ellipsoids in order to test this approximation.
Find it generated three orthonormal axis. For the first x was a randomly generated number and y and z were zero. And so on.
Then it created a random center (if necessary).
After that it rotated the axis by a random rotation using quaternion.
We generated hundreds of pairs of ellipsoids, and compared their grid and gaussian intersection volumes.

Grid intersection versus Gaussian intersection using ln 100 points



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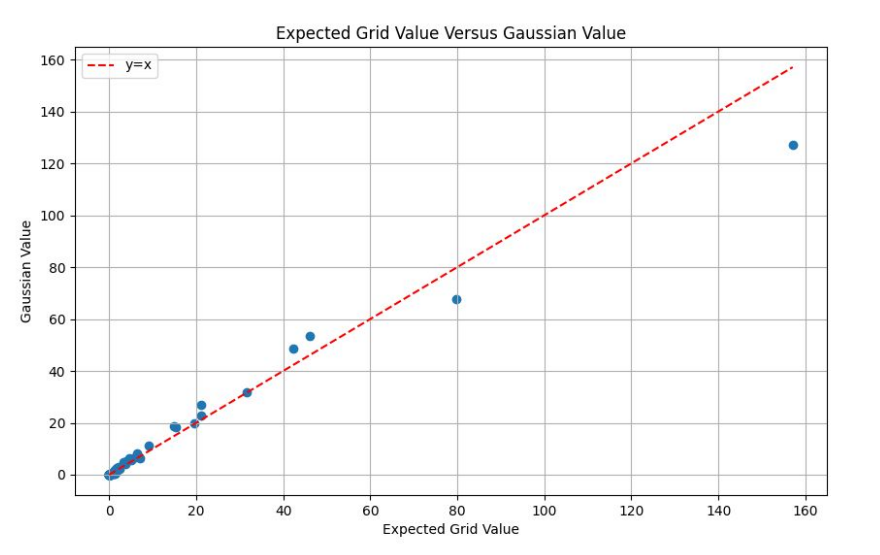
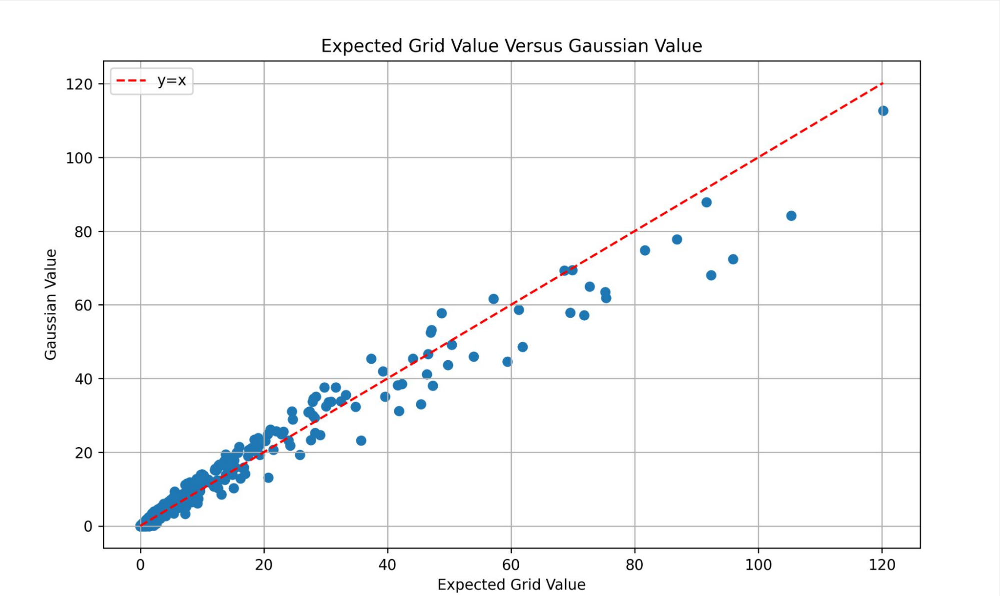


Grid intersection versus Gaussian intersection using ln 1000 points



What could the next steps be for this project?

One other thing to pursue would be determining a different way to scale the intersection gaussian. We could try normalizing by scaling the inverse covariance matrix so that it reflects magnitude.

We could also calculate molecular overlap and maximize the overlay of one molecule with another.