

Hessian terms

The idea now is that for every energy term i will add the Hessian terms that will be needed.

I already have the Hessian of the area i also need to add later the hessian of the Dihedral angle

$$u = p_2 - p_1 \quad v = p_3 - p_1 \quad w = p_4 - p_1 \quad (1)$$

The idea now is to write the terms of the Hessian here

We consider also that

$$g = \det(u, v, w) \|u\| \quad (2)$$

$$h = \langle u \times w, v \times u \rangle \quad (3)$$

$$f = \arctan 2(g, h) \quad (4)$$

$$r = g^2 + h^2 \quad (5)$$

Now we calculate the derivatives

$$f_u = f_h h_u + f_g g_u \quad (6)$$

$$= \frac{1}{r} \left(-g u^T ([w]_x [v]_x + [v]_x [w]_x) + h (\|u\| (v \times w)^T + \det(u, v, w) \frac{u^T}{\|u\|}) \right) \quad (7)$$

$$f_v = f_h h_v + f_g g_v \quad (8)$$

$$= \frac{1}{r} \left(-g w^T [u]_x^2 + h \|u\| (w \times u)^T \right) \quad (9)$$

$$f_w = f_h h_w + f_g g_w \quad (10)$$

$$= \frac{1}{r} \left(-g v^T [u]_x^2 + h \|u\| (u \times v)^T \right) \quad (11)$$

Now that we have differentiated with all the variables we can say how is the gradient for every point.

$$f_{p_1} = -f_u - f_v - f_w \quad f_{p_2} = f_u \quad f_{p_3} = f_v \quad f_{p_4} = f_w \quad (12)$$

And those are the terms of the gradient of f . Lets remember that f is the dihedral angle.

Now we will do the Hessian of the dihedral angle

Considering

$$l = v \times w \quad B = [w]_x[v]_x + [v]_x[w]_x \quad \alpha = \det(u, v, w) \quad (13)$$

$$f_{p_2 p_2} = \frac{g^2 - h^2}{r^2} \left[\|u\| (Bu \otimes l + l \otimes Bu) + \frac{\alpha}{\|u\|} (Bu \otimes u + u \otimes Bu) \right] \quad (14)$$

$$- \frac{2gh}{r^2} [Bu \otimes Bu + \|u\|^2 l \otimes l] + \frac{1}{r^2} \left(-2gh\alpha + \frac{hr}{\|u\|} \right) (l \otimes u + u \otimes l) \quad (15)$$

$$- \left(\frac{2gh\alpha^2}{r^2\|u\|^2} - \frac{h\alpha r}{r^2\|u\|^3} \right) (u \otimes u) - \frac{g}{r} B + \frac{h\alpha}{\|u\|r} \mathcal{I} \quad (16)$$

This one is the ugliest actually, the other ones are nicer

First $f_{p_3 p_3}$ courtesy of Christian, assuming this

$$a = w \times u \quad b = u \times (u \times w) = a \times u \quad (17)$$

$$f_{p_3 p_3} = \frac{2gh}{r^2} (b \otimes b - \|u\|^2 a \otimes a) + \frac{\|u\|(g^2 - h^2)}{r^2} (a \otimes b + b \otimes a) \quad (18)$$

The next one is $f_{p_4 p_4}$. In this case we consider

$$d = u \times v \quad k = u \times (u \times v) = u \times d \quad (19)$$

And the terms are

$$f_{p_4 p_4} = \frac{2gh}{r^2} (k \otimes k - \|u\|^2 d \otimes d) + \frac{\|u\|(g^2 - h^2)}{r^2} (d \otimes k + k \otimes d) \quad (20)$$

And those are the diagonal terms, now we will do the off diagonals.

We will define some things also

$$C = (-2[w]_x[u]_x + [u]_x[w]_x) \quad (21)$$

So the next term is $f_{p_2 p_3}$

$$f_{p_2 p_3} = \frac{g^2 - h^2}{r^2} \left[-||u|| C v \otimes a + ||u|| l \otimes b + \frac{\alpha}{||u||} u \otimes b \right] \quad (22)$$

$$+ \frac{2gh}{r^2} \left[C v \otimes b + ||u||^2 l \otimes a + \alpha u \otimes a \right] - \frac{g}{r} C \quad (23)$$

And now we have $f_{p_2 p_4}$

We define a matrix as

$$D = -2[v]_x[u]_x + [u]_x[v]_x \quad (24)$$

$$f_{p_2 p_4} = \frac{g^2 - h^2}{r^2} \left[||u|| D w \otimes d + ||i|| l \otimes (u \times d) + \frac{\alpha}{||u||} u \otimes (u \times d) \right] \quad (25)$$

$$+ \frac{2gh}{r^2} [D w \otimes (u \times d) - ||u|| l \otimes d - \alpha u \otimes d] - \frac{g}{r} D + \frac{h}{r} \left(||u|| [v]_x + \frac{1}{||u||} u \otimes d \right) \quad (26)$$

And now we have $f_{p_4 p_3}$

$$f_{p_4 p_3} = \frac{g^2 - h^2}{r^2} [||u|| k \otimes a + ||u|| c \otimes b] \quad (27)$$

$$+ \frac{2gh}{r^2} [-||u||^2 c \otimes a + k \otimes b] - \frac{g}{r} [u]_x^2 + \frac{h||u||}{r} [u]_x \quad (28)$$

Now we can do the rest of the terms

$$f_{p_1 p_1} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p_1} \quad (29)$$

$$= f_{p_2 p_2} + f_{p_2 p_3} + f_{p_2 p_4} + f_{p_3 p_2} + f_{p_3 p_3} + f_{p_3 p_4} + f_{p_4 p_2} + f_{p_4 p_3} + f_{p_4 p_4} \quad (30)$$

Lets do the rest

$$f_{p_1 p_2} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p_2} \quad (31)$$

$$= -f_{p_2 p_2} - f_{p_3 p_2} - f_{p_4 p_2} \quad (32)$$

$$f_{p_1 p_3} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p_3} \quad (33)$$

$$= -f_{p_2 p_3} - f_{p_3 p_3} - f_{p_4 p_3} \quad (34)$$

$$f_{p_1 p_4} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p_4} \quad (35)$$

$$= -f_{p_2 p_4} - f_{p_3 p_4} - f_{p_4 p_4} \quad (36)$$

Ok, now lets write the rest of the Hessians. To take a small break i will write the Hessian of an edge

Let $u = p_2 - p_1$

$$l(u) = ||u|| \quad (37)$$

From out previous experience we know

$$l_{p1} = -l_u \quad l_{p2} = l_u \quad (38)$$

Thefore the term of the gradient is

$$l_u = \frac{u^T}{||u||} \quad l_{p1} = -\frac{u^T}{||u||} \quad l_{p2} = \frac{u^T}{||u||} \quad (39)$$

And now the for the Hessian we now

$$l_{uu} = l_{p_1 p_1} = l + p_2 p_2 = \frac{1}{||u||} \left(\mathcal{I} - \frac{u \otimes u}{||u||^2} \right) \quad (40)$$

Now for the off diagonal terms, hmm... in this case i think they just have a minus sign at the front.

$$l_{p_1 p_2} = -(l_u)_u = -\frac{1}{||u||} \left(\mathcal{I} - \frac{u \otimes u}{||u||^2} \right) \quad (41)$$

Now we can do the Hessian of the area, we will use the same notation as before, so we have

$$u = p_2 - p_1 \quad v = p_3 - p_1 \quad u_{p_1} = -id \quad u_{p_2} = id \quad v_{p_1} = -id \quad v_{p_3} = id \quad (42)$$

Let $z = u \times v$ $z_v = [u]_{\times}$ $z_u = -[v]_{\times}$

Considering $A = ||z||$ (This is actually twice the area but we just need to remember to divide the results by two at the the end)

$$A_z = \frac{z^T}{||z||} \quad (43)$$

$$A_u - A_z z_u = -\frac{1}{||z||} z^T [v]_{\times} = \frac{1}{||z||} ([v]_{\times} z)^T \quad (44)$$

$$= \frac{1}{||z||} (v \times z)^T \quad (45)$$

$$A_v = A_z z_v = \frac{1}{||z||} z^T [u]_{\times} = \frac{1}{||z||} ([u]_{\times}^T z)^T \quad (46)$$

$$= -\frac{1}{||z||} (u \times z)^T \quad (47)$$

Now that we have the partial derivatives we can write the gradient of the area

$$A_{p_1} = A_u u_{p_1} + A_v v_{p_1} \quad (48)$$

$$= -A_u - A_v \quad (49)$$

$$= -\frac{1}{||z||} ((u - v) \times z)^T \quad (50)$$

$$= -\frac{1}{||z||} ((p_2 - p_3) \times z)^T \quad (51)$$

$$A_{p_2} = \frac{1}{||z||_{vert}} ((p_3 - p_1) \times z)^T \quad (52)$$

$$A_{p_3} = \frac{1}{||z||} ((p_1 - p_2) \times z)^T \quad (53)$$

Perfect, now that we have the first derivatives its time to write down the second derivatives.

Thanks to Christian we got this

$$A_{p_1 p_1} = \frac{1}{\|z\|} \left(\frac{-((u-v) \times z) \cdot ((u-v) \times z)^T}{\|z\|^2} - [u-v]_{\times}^2 \right) \quad (54)$$

$$A_{p_2 p_2} = -\frac{1}{\|z\|} \left(\frac{1}{\|z\|^2} ((p_3 - p_1) \times z)((p_3 - p_1) \times z) + [p_3 - p_1]_{\times}^2 \right) \quad (55)$$

$$A_{p_3 p_3} = -\frac{1}{\|z\|} \left(\frac{1}{\|z\|^2} ((p_1 - p_2) \times z)((p_1 - p_2) \times z) + [p_1 - p_2]_{\times}^2 \right) \quad (56)$$

$$A_{p_2 p_3} = \frac{1}{\|z\|} \left([p_3 - p_1]_{\times} (id - \frac{zz}{\|z\|^2}) [p_2 - p_1]_{\times} - [z]_{\times} \right) \quad (57)$$

$$A_{p_3 p_1} = \frac{1}{\|z\|} \left([p_1 - p_2]_{\times} (id - \frac{zz}{\|z\|^2}) [p_3 - p_2]_{\times} - [z]_{\times} \right) \quad (58)$$

$$A_{p_1 p_2} = \frac{1}{\|z\|} \left([p_2 - p_3]_{\times} (id - \frac{zz}{\|z\|^2}) [p_1 - p_3]_{\times} - [z]_{\times} \right) \quad (59)$$

I think those are all the terms that i need for now. I still need to add the interactions with the Bead but lets do that later because we require considering dot products :(

Assembling the Hessian

Ok so this is the part where we dialog the structure of the code to get my Hessian.

According to Christian I should create functions that take a vector and return the Block Hessians.

For the area hessian i should have

- **gradient_{area}**([p1p2,p3]) *This function takes a 9-dimensional vector with the coordinates of the three vertices and returns a vector that contains the gradient of the area with respect to each of the vertices.*

This functions should be implemented simply because there will be a bigger function that will ensemble the rest of the info.