MARCH 23, 2012

3D Radial Symm. tracking.

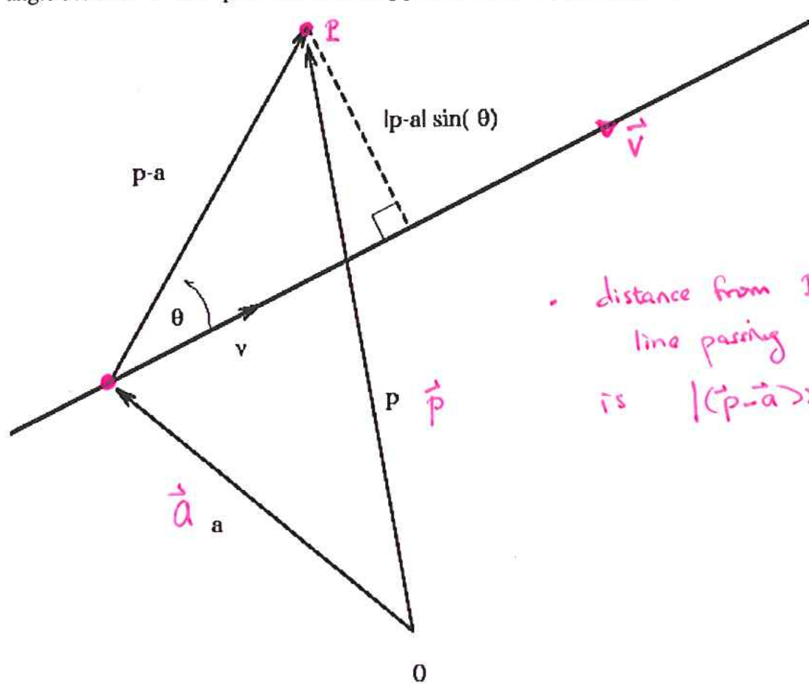
(i) calculate $\vec{\nabla} I$ in 3D

(ii) calculate distance from arbitrary pt to each line passing through lattice points w/ direction // gradient at that pt.

Distance from a Point to a Line

Consider a line in 3D with position vector "a" and direction vector "v" and let "p" be the position vector of an arbitrary point in 3D.

We want to compute the distance from the point "p" to the line. Let us call "theta" the angle between "v" and "p-a". The following picture illustrates the situation,



- distance from P to line passing through $\vec{a}$ w/ (e.g.) gradient $\vec{v}$ is $|(\vec{p}-\vec{a}) \times \vec{v}| / |\vec{v}|$.

Thus, the formula for the distance is given by,

$$| (p-a) \times v | / |v|$$

http://omega.albany.edu:8008/calc3/distance-to-point-di

i.e. the length of the crossprod between the vectors (p-a)

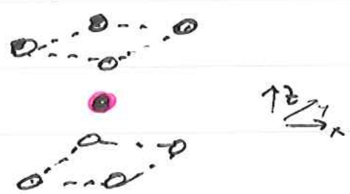
• MARCH 30, 2012

on (i), calculating the gradient. x-y information is more densely sampled than z information ($\approx 0.2\ \mu m$ vs. $1\ \mu m$).

For each 2D slice, get gradient @ grid midpoint as usual

Do this for each slice. Calc $(\vec{\Delta I})_z$ as $\langle \Delta I \rangle_z$ where ΔI_z is the difference in I in z at each x,y pt, averaged over xy points.

So for a grid, will get ∇I at each midpoint



Note that the lattice spacing is different in xy and in z.

Using the above, will get $\vec{\nabla} I$ @ (x_k, y_k, z_k).

can normalize $\hat{m}_k = \frac{\vec{\nabla} I}{|\vec{\nabla} I|}$

arbitrary point (x, y, z) (= P on Mar. 23 notes).

Distance from P to line passing through $\underbrace{(x_k, y_k, z_k)}_{\vec{r}_k}$ w/ direction vector $\hat{m}_k$:

$$d_k = \left| (\vec{p} - \vec{r}_k) \times \hat{m}_k \right|$$

$$= \left| (x - x_k,\ y - y_k,\ z - z_k) \times (m_{kx}, m_{ky}, m_{kz}) \right|$$

$$= \left\| \begin{matrix} \hat{i} & \hat{j} & \hat{k} \\ x - x_k & y - y_k & z - z_k \\ m_x & m_y & m_z \end{matrix} \right\| = \left| \hat{i} \left[(y - y_k) m_{kz} - (z - z_k) m_{ky} \right] + \hat{j} \left[(z - z_k) m_{kx} - (x - x_k) m_{kz} \right] \right.$$

$$\left. + \hat{k} \left[(x - x_k) m_{ky} - (y - y_k) m_{kx} \right] \right|$$

3/30 (2)

$$\Rightarrow \quad d_k^2 = \left[(y-y_k)m_{kz} - (z-z_k)m_{ky}\right]^2 + \left[(z-z_k)m_{kx} - (x-x_k)m_{kz}\right]^2 + \left[(x-x_k)m_{ky} - (y-y_k)m_{kx}\right]^2$$

As before, minimize $\quad \chi^2 = \sum_k d_k^2 w_k$

$$\frac{\partial \chi^2}{\partial x} = \sum_k \Big\{ 2\left[(z-z_k)m_{kx} - (x-x_k)m_{kz}\right](-m_{kz}) + 2\left[(x-x_k)m_{ky} - (y-y_k)m_{kx}\right] m_{ky} \Big\} w_k$$

$$= 2 \sum_k (x-x_k)(m_{kz}^2 + m_{ky}^2)w_k - (y-y_k) m_{kx} m_{ky} w_k - (z-z_k) m_{kx} m_{kz} w_k$$

$$= 0 \quad \Rightarrow$$

$$\cancel{x \sum_k (m_{kz}^2 + m_{ky}^2) = \sum_k \Big\{ x_k (m_{kz}^2 + m_{ky}^2) + y - y_k}$$

$$x \sum_k (m_{kz}^2 + m_{ky}^2)w_k - y \sum_k (m_{kx} m_{ky})w_k - z \sum_k (m_{kx} m_{kz})w_k$$

$$= \sum_k \Big\{ x_k (m_{kz}^2 + m_{ky}^2)w_k - y_k m_{kx} m_{ky} w_k - z_k m_{kx} m_{kz} w_k \Big\} \quad (1)$$

$$\frac{\partial \chi^2}{\partial y} = \sum_k \Big\{ 2\left[(y-y_k)m_{kz} - (z-z_k)m_{ky}\right] m_{kz} w_k + 2\left[(x-x_k)m_{ky} - (y-y_k)m_{kx}\right](-m_{kx}) w_k \Big\}$$

$$= 2 \sum_k (x-x_k)(-m_{ky} m_{kx})w_k + (y-y_k)(m_{kz}^2 + m_{kx}^2)w_k + (z-z_k)(-m_{ky} m_{kz})w_k$$

$$= 0 \Rightarrow -x \sum_k m_{kx} m_{ky} w_k + y \sum_k (m_{kx}^2 + m_{kz}^2) w_k - z \sum_k m_{ky} m_{kz} w_k$$

$$= \sum_k \Big\{ -x_k m_{kx} m_{ky} w_k + y_k (m_{kx}^2 + m_{kz}^2) w_k - z_k m_{ky} m_{kz} w_k \Big\} \quad (2)$$

3/30 (3)

$$\frac{\partial \chi^2}{\partial z} = \sum_k \{ 2[(y-y_k)m_{kz} - (z-z_k)m_{ky}](-m_{ky})w_k + 2[(z-z_k)m_{kx} - (x-x_k)m_{kz}]m_{kx}w_k \}$$

$$= 2\sum_k (x-x_k)(-m_{kz}m_{kx}w_k) + (y-y_k)(-m_{kz}m_{ky}w_k) + (z-z_k)(m_{ky}^2 + m_{kx}^2)w_k$$

$$= 0 \Rightarrow -x\sum_k m_{kx}m_{kz}w_k - y\sum_k m_{kz}m_{ky}w_k + z\sum_k(m_{ky}^2+m_{kx}^2)w_k$$

$$= \sum_k \{ -x_k m_{kz}m_{kx}w_k - y_k m_{kz}m_{ky}w_k + z_k(m_{ky}^2+m_{kx}^2)w_k \} \quad (3)$$

Can solve (1)-(3) for x, y, z ⇒ best-fit symmetry center.

Matrix equation

$$\underbrace{\begin{bmatrix} \sum_k(m_{kz}^2+m_{ky}^2)w_k & -\sum_k m_{kx}m_{ky}w_k & -\sum_k m_{kx}m_{kz}w_k \\ -\sum_k m_{kx}m_{ky}w_k & \sum_k(m_{kx}^2+m_{kz}^2)w_k & -\sum_k m_{ky}m_{kz}w_k \\ -\sum_k m_{kx}m_{kz}w_k & -\sum_k m_{ky}m_{kz}w_k & \sum_k(m_{ky}^2+m_{kx}^2)w_k \end{bmatrix}}_{A} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} \text{RHS of (1)} \\ \text{RHS of (2)} \\ \text{RHS of (3)} \end{bmatrix}}_{b}$$; solve by inversion.

("A\b" in MATLAB)

Implement : radialcenter3D.m

quick test. seems to work!

Should test w/ lots of test images – spheres and shells.