# Fitting 3D Data with a Helix

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This document describes an algorithm for fitting a 3D point set with a helix. The assumption is that the underlying data is modeled by an elliptical helix. The algorithm will produce useless results for a random data set or data sets with intrinsic dimension of 2 or 3.

## 1 Reconstructing a Standard Elliptical Helix

An elliptical helix with the $z$–axis as axis and cross–section being an axis–aligned ellipse is specified parametrically by

$$\begin{aligned} x(t) &= a\cos(\omega t + \phi), \\ y(t) &= b\sin(\omega t + \phi), \\ z(t) &= t \end{aligned}$$

where $a > 0$, $b > 0$, $\omega > 0$, $\phi \in [0, 2\pi)$, and $t \in \mathbb{R}$. The helix lies on the elliptical cylinder $(x/a)^2 + (y/b)^2 = 1$.

Given two points $(x_0, y_0, z_0)$ and $(x_1, y_1, z_1)$ on the helix such that $\Delta := x_0^2 y_1^2 - x_1^2 y_0^2 \neq 0$, the ellipse axis lengths are determined by the system of equations

$$\begin{bmatrix} x_0^2 & y_0^2 \\ x_1^2 & y_1^2 \end{bmatrix} \begin{bmatrix} 1/a^2 \\ 1/b^2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

The solution leads to $a = \sqrt{(y_1^2 - y_0^2)/\Delta}$ and $b = \sqrt{(x_0^2 - x_1^2)/\Delta}$.

For the same two helix points, $x_i/a = \cos(\omega z + \phi)$ and $y_i/b = \sin(\omega z + \phi)$. Taking the ratios and applying inverse tangent yields

$$\begin{bmatrix} z_0 & 1 \\ z_1 & 1 \end{bmatrix} \begin{bmatrix} \omega \\ \phi \end{bmatrix} = \begin{bmatrix} \tan^{-1}((ay_0)/(bx_0)) \\ \tan^{-1}((ay_1)/(bx_1)) \end{bmatrix}.$$

Defining $\theta_0 = \tan^{-1}((ay_0)/(bx_0))$ and $\theta_1 = \tan^{-1}((ay_1)/(bx_1))$, the solution to the system of equations is $\omega = (\theta_1 - \theta_0)/(z_1 - z_0)$ and $\phi = (\theta_0 z_1 - \theta_1 z_0)/(z_1 - z_0)$.

## 2 Reconstructing a General Elliptical Helix

Generally, the data points might be approximated by a helix whose axis is a line other than the z–axis. The elliptical cylinder containing the helix satisfies the general quadratic equation

$$\vec{x}^t A\vec{x} + \vec{b}^t\vec{x} + c = 0$$

where $A$ is a $3 \times 3$ symmetric matrix, $\vec{b}$ and $\vec{x}$ are $3 \times 1$ vectors, and $c$ is a scalar. Moreover, exactly one of the eigenvalues of $A$ must be zero and the other two eigenvalues are positive. The other eigenvalues could both be negative, but in that case the quadratic equation could be multiplied by $-1$ to obtain the case we consider here. In fact there is one additional constraint as described below.

Using an eigendecomposition, let $A = RDR^t$ where $R$ is an orthonormal matrix and $D = \mathrm{Diag}\{d_0, d_1, 0\}$. Let $\vec{y} = (y_0, y_1, y_2) = R^t\vec{x}$ and $\vec{e} = (e_0, e_1, e_2) = R^t\vec{b}$. The quadratic equation becomes

$$\vec{y}^t D\vec{y} + \vec{e}^t\vec{y} + c = 0.$$

The additional constraint is that $e_2 = 0$. In this case we get

$$d_0 y_0^2 + d_1 y_1^2 + e_0 y_0 + e_1 y_1 + c = 0.$$

Completing the square on both $y_0$ and $y_1$ terms yields

$$d_0\left(y_0 + \frac{e_0}{2d_0}\right)^2 + d_1\left(y_1 + \frac{e_1}{2d_1}\right)^2 = \frac{e_0^2}{4d_0} + \frac{e_1^2}{4d_1} - c =: \lambda.$$

The right–hand side $\lambda$ must be positive. In standard form, the equation is

$$\frac{\left(y_0 + \frac{e_0}{2d_0}\right)^2}{\lambda/d_0} + \frac{\left(y_1 + \frac{e_1}{2d_1}\right)^2}{\lambda/d_1} = 1.$$

This is the equation for an elliptical cylinder whose axis is in the direction of the $y_2$ axis and passes through $(e_0/(2d_0), e_1/(2d_1))$. The lengths of the ellipse axes are $a = \sqrt{\lambda/d_0}$ and $b = \sqrt{\lambda/d_1}$. A final change of variables is $\vec{u} = (u_0, u_1, u_2) = (y_0 + e_0/(2d_0), y_1 + e_1/(2d_1), y_2)$. This produces the standard elliptical cylinder $(u_0/a)^2 + (u_1/b)^2 = 1$. Given points on the helix, the helix can be reconstructed as shown in the previous section by first transforming the data points indicated by this section's discussion.

## 3 Fitting a Standard Elliptical Helix

If the data points are not exactly on the helix, then the parameters $a$, $b$, $\omega$, and $\phi$ must be estimated. One possibility is to sort the data points by $z$–value, then compute the parameters for each pair of consecutive points using the reconstruction of the first section. A summary statistic could be used to make the final selection (average, median, generalized order statistics, etc.)

Another approach is to use a least–squares method. The energy function is

$$\begin{aligned} E(a, b, \omega, \phi) &= \textstyle\sum_{i=0}^{N-1} |(x_i, y_i, z_i) - (a\cos(\omega z_i + \phi), b\sin(\omega z_i + \phi), z_i)|^2 \\ &= \textstyle\sum_{i=0}^{N-1} (x_i - a\cos(\omega z_i + \phi))^2 + (y_i - b\sin(\omega z_i + \phi))^2 . \end{aligned}$$

The global minimum occurs when $\nabla E = \vec{0}$. Define $\psi_i = \omega z_i + \phi$. The derivatives are

$$\begin{aligned}
\frac{1}{2}\frac{\partial E}{\partial a} &= a \sum_i \cos^2\psi_i - \sum_i x_i \cos\psi_i \\
\frac{1}{2}\frac{\partial E}{\partial b} &= b \sum_i \sin^2\psi_i - \sum_i y_i \cos\psi_i \\
\frac{1}{2}\frac{\partial E}{\partial \omega} &= \sum_i (x_i - a\cos\psi_i)(z_i a \sin\psi_i) + (y_i - b\sin\psi_i)(-z_i b\cos\psi_i) \\
\frac{1}{2}\frac{\partial E}{\partial \phi} &= \sum_i (x_i - a\cos\psi_i)(a \sin\psi_i) + (y_i - b\sin\psi_i)(-b\cos\psi_i)
\end{aligned}$$

The first two equations determine $a$ and $b$ in terms of $\omega$ and $\phi$:

$$\begin{aligned}
a &= \frac{\sum_i x_i \cos\psi_i}{\sum_i \cos^2\psi_i} \\
b &= \frac{\sum_i y_i \sin\psi_i}{\sum_i \sin^2\psi_i}
\end{aligned}$$

These can be plugged into the last two equations to produce two nonlinear equations in the two unknowns $\omega$ and $\phi$. This system can be numerically solved by a multidimensional root finder, perhaps by a Newton–Jacobi method.

If the cylinder is circular, say $a = b = r$ for some $r > 0$, then the equations may be reduced to a simpler numerical problem. The derivatives are

$$\begin{aligned}
\frac{1}{2}\frac{\partial E}{\partial r} &= Nr - \sum_i x_i \cos\psi_i - \sum_i y_i \sin\psi_i \\
\frac{1}{2r}\frac{\partial E}{\partial \omega} &= \sum_i x_i z_i \sin\psi_i - y_i z_i \cos\psi_i \\
\frac{1}{2r}\frac{\partial E}{\partial \phi} &= \sum_i x_i \sin\psi_i - y_i \cos\psi_i
\end{aligned}$$

The first equation determines $r$,

$$r = \frac{1}{N}\sum_i x_i \cos\psi_i + y_i \sin\psi_i.$$

The other two equations may be separated by expanding $\sin\psi_i = \sin(\omega z_i)\cos(\phi) + \cos(\omega z_i)\sin(\phi)$ and $\cos\psi_i = \cos(\omega z_i)\cos(\phi) - \sin(\omega z_i)\sin(\phi)$. Define $\Psi_i = \omega z_i$. The two equations from setting derivatives equal to zero are

$$\begin{aligned}
0 &= (\cos\phi)\sum_i z_i(x_i \sin\Psi_i - y_i\cos\Psi_i) + (\sin\phi)\sum_i z_i(x_i\cos\Psi_i + y_i \sin\Psi_i) \\
0 &= (\cos\phi)\sum_i x_i \sin\Psi_i - y_i\cos\Psi_i + (\sin\phi)\sum_i x_i\cos\Psi_i + y_i \sin\Psi_i
\end{aligned}$$

Abstractly these represent two orthogonality conditions. If $u(\phi) = (\cos\phi, \sin\phi)$, then the two equations are of the form $u \cdot (p_0, p_1) = 0$ and $u \cdot (q_0, q_1) = 0$. Both $(p_0, p_1)$ and $(q_0, q_1)$ are orthogonal to the $u$, so they must be parallel vectors. Thus, we need $p_0 q_1 - p_1 q_0 = 0$. This last equation is a function only of the unknown $\omega$. A standard root finder for a function of one variable may be applied, for example, a Newton's method. An initial guess could be obtained by choosing two data points and computing $\omega$ as indicated in the first section. Once a root is found, the vector $(p_0, p_1)$ is computed. The value for $\phi = \tan^{-1}(p_1/p_0)$.

# 4 Fitting a General Elliptical Helix

The elliptical cylinder of best fit is computed according to the method in section 2. The cylinder and data points are transformed into standard position so that we have an elliptical cylinder whose axis is the z–axis and whose cross section is an axis–aligned ellipse. The fitting methods of section 3 can then be applied. The parametric equation of the fitting helix can then be inverse transformed back to the original coordinate system.