Homotopy

Suppose we are trying to find a root $\mathbf{x}^*$ of a nonlinear, vector-valued function $F(\mathbf{x})$:

$$F(\mathbf{x}^*) = \mathbf{0}$$

Suppose further that we have an initial guess $\mathbf{x}_0$ that approximates the root.

A *homotopy* is a vector-valued function $G(\lambda,\mathbf{x})$ of a parameter λ and $\mathbf{x}$ with the following characteristics.

1. When $\lambda = 0$, the function $G(0,\mathbf{x})$ has a root at $\mathbf{x}_0$.
2. When $\lambda = 1$, the function $G(1,\mathbf{x})$ has a root at $\mathbf{x}^*$.

Here is a homotopy that has the desired characteristics.

$$G(\lambda,\mathbf{x}) = \lambda\, F(\mathbf{x}) + (1 - \lambda)\, \left(F(\mathbf{x}) - F(\mathbf{x}_0)\right)$$

Continuation

The *continuation problem* is the problem of constructing a function $\mathbf{x}(\lambda)$ that can map smoothly from $\mathbf{x}(0) = \mathbf{x}_0$ to $\mathbf{x}(1) = \mathbf{x}^*$.

If we were able to compute $\mathbf{x}(\lambda)$, its defining characteristic is that

$$G(\lambda,\mathbf{x}(\lambda)) = 0$$

for all λ between 0 and 1.

Differentiating this equation with respect to λ gives

$$\frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \lambda} + \frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \mathbf{x}}\, \mathbf{x}'(\lambda) = 0$$

or

$$\mathbf{x}'(\lambda) = -\left(\frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \mathbf{x}}\right)^{-1} \frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \lambda}$$

This is a nonlinear system of first order differential equations with initial condition $\mathbf{x}(0) = \mathbf{x}_0$.

Setting up and solving the system

Bearing in mind that $G(\lambda,\mathbf{x})$ is defined in terms of $F(\mathbf{x})$, the first step in setting up and solving the continuation equations is to substitute the definition

$$G(\lambda,\mathbf{x}) = \lambda\, F(\mathbf{x}) + (1 - \lambda)\, \big(F(\mathbf{x}) - F(\mathbf{x}_0)\big)$$

into the equation

$$\mathbf{x}'(\lambda) = -\left(\frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \mathbf{x}}\right)^{-1} \frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \lambda}$$

When we do this we discover two things.

$$\frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \mathbf{x}} = \lambda\, \frac{\partial F(\mathbf{x}(\lambda))}{\partial \mathbf{x}} + (1 - \lambda)\, \frac{\partial F(\mathbf{x}(\lambda))}{\partial \mathbf{x}} = \frac{\partial F(\mathbf{x}(\lambda))}{\partial \mathbf{x}} = J(\mathbf{x}(\lambda))$$

$$\frac{\partial G(\lambda,\mathbf{x}(\lambda))}{\partial \lambda} = F(\mathbf{x}) - \big(F(\mathbf{x}) - F(\mathbf{x}_0)\big) = F(\mathbf{x}_0)$$

Thus, the system simplifies down to

$$\mathbf{x}'(\lambda) = -\big(J(\mathbf{x}(\lambda))\big)^{-1}\, F(\mathbf{x}_0)$$

Once we have set up the system of equations, we can solve it by any of our usual methods, such as the Runge-Kutta method.