Least Squares Polynomials

Suppose we want to approximate the set of data $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with a polynomial of degree less than or equal to d. In the least squares sense, the answer is the polynomial $p(x) = \sum_{j=0}^{d} c_j x^j$, whose coefficients are determined from

$$\min_{deg p \leq d} \sum_{i=1}^{n} (y_i - p(x_i))^2 \;\equiv\; \min_{c_0, c_1, \ldots, c_d} \sum_{i=1}^{n} (y_i - \sum_{j=0}^{d} c_j x_i^j)^2.$$

There are lots of ways to compute p; one is to use the standard ordered basis as above. Let $g(c) = \sum_{i=1}^{n} (y_i - \sum_{j=0}^{d} c_j x_i^j)^2$. Requiring $\nabla g = 0$ gives:

$$2 \sum_{i=1}^{n} (y_i - \sum_{j=0}^{d} c_j x_i^j)(-x_i^k) = 0, \quad k = 0, 1, \ldots, d$$

or

$$\sum_{j=0}^{d} c_j \sum_{i=1}^{n} x_i^{k+j} = \sum_{i=1}^{n} x_i^k y_i, \quad k = 0, 1, \ldots, d.$$

These are the *normal equations* for the discrete linear least squares polynomial problem.

If we define $x \equiv (x_1, x_2, \ldots, x_n)$ and $x^{\underline{k}} \equiv (x_1^k, x_2^k, \ldots, x_n^k)$, then these normal equations can be written as

$$Hc = f, \text{ where}$$

$H = [h_{ij}]_{i,j=0}^{d}$, where $h_{ij} = \sum_{k=1}^{n} x_k^i x_k^j \equiv x^{\underline{i}} \cdot x^{\underline{j}}$, and $f = [f_i]$, $f_i = \sum_{j=1}^{n} x_j^i y_j \equiv x^{\underline{k}} \cdot y$. Notice that $x^{\underline{i}}$ is the i^{th} row of an $n \times (d+1)$ Vandermonde matrix V, and that $Hc = f$ can also be written as $V^t V c = V^t y$.

Now suppose we want a polynomial approximation to a *function* $y = y(x)$, integrable over an inverval $[a, b]$. We can define a degree d least squares polynomial p whose coefficients satisfy

$$\min_{c_0, c_1, \ldots, c_d} \int_a^b (y(x) - \sum_{j=0}^{d} c_j x^j)^2,$$

and proceed as above. Let $g(c) = \int_a^b (y(x) - \sum_{j=0}^{d} c_j x^j)^2 dx$. Setting $\nabla g = 0$:

$$\int_a^b 2(y(x) - \sum_{j=0}^{d} c_j x^j))(-x^k) = 0, \quad k = 0, 1, \ldots, d,$$

giving the continuous least squares normal equations

$$\sum_{j=0}^{d} c_j \int_a^b x^{k+j} dx = \int_a^b x^k y(x) dx, \quad k = 0, 1, \ldots, d.$$

Let $H = [h_{ij}]_{i,j=0}^{d}$, where $h_{ij} = \int_a^b x^{i+j} dx \equiv < x^i, x^j >$, and $f_i = \int_a^b x^i y(x) dx = < x^i, y >$, and the normal equations are

$$Hc = f.$$