Computational methods-Lecture 3

Least squares approximation

Problem: Consider $f \in C[a,b]$. Let $\{\phi_0(x), \phi_1(x), \cdots, \phi_n(x)\}$ be linearly independent functions defined on $[a,b]$. We aim to find a function $S(x)$ in the space V spanned by them such that

$$\|f-S\|^2_{L^2(w)} := \int_a^b w(x)|f(x)-S(x)|^2\,dx,\ S \in V = span\{\phi_0(x), \phi_1(x), \cdots, \phi_n(x)\}$$

is minimized. Here, $w(x)$ is called the weight function.

1 Least squares approximating polynomial

1.1 A simple case

Let us consider a simple case $w \equiv 1$ and $\phi_k(x) = x^k$ so that V is the set of all polynomials with degree at most n. Then,

$$S(x) = a_0 + a_1 x + \cdots + a_n x^n.$$

Then, we aim to minize the following function of $a_0, \cdots, a_n$:

$$I(a_0, \cdots, a_n) := \int_a^b (f(x) - \sum_{k=0}^n a_k x^k)^2\,dx.$$

This function is quadratic in a_k and it must has a minimizer. To find the minimizer, we have

$$\frac{\partial I}{\partial a_j} = 0, \quad \forall j = 0, \cdots, n.$$

Hence,

$$\int_a^b 2(f(x) - \sum_{k=0}^n a_k x^k)(-\sum_{k=0}^n \delta_{kj} x^k)\,dx = 0.$$

This simplifies to the **normal equations**

$$\sum_{k=0}^n a_k \int_a^b x^j x^k\,dx = \int_a^b f(x) x^j\,dx,\ \ j = 0, \cdots, n.$$

Remark 1. *The normal equations have clear geometric meaning. In fact, let S be the best approximation. Then, $f(x) - S(x)$ should be perpendicular (or "normal") to the subspace V. Hence,*

$$\langle f(x) - S(x), x^j \rangle = 0, \forall j = 0, \cdots, n.$$

This perpendicular condition is exactly the normal conditions.

This then gives a linear system for the coefficients $\{a_0, \cdots, a_n\}$:

$$H\vec{a} = \vec{d}$$

where H is an $(n+1) \times (n+1)$ matrix with $H_{ij} = \int_a^b x^{i+j-2}\,dx$, and $d_j = \int_a^b f(x)x^{j-1}\,dx$.

Example Let $a = 0, b = 1$.

1. Find the matrix H for this case. This matrix is called the **Hilbert matrix**.

2. Let $f(x) = \sqrt{1+x^2}$ and $n = 1$. Find the least squares approximating polynomial.

If $a = 0, b = 1$, it is easy to find $H_{ij} = \frac{1}{i+j-1}$.
In the question, we have

$$d_1 = \int_0^1 \sqrt{1+x^2}\,dx = \frac{1}{2}\ln(1+\sqrt{2}) + \frac{\sqrt{2}}{2} \approx 1.147.$$

$$d_2 = \int_0^1 \sqrt{1+x^2}x\,dx = \frac{2\sqrt{2}-1}{3} \approx 0.609.$$

Hence, $a_0 \approx 0.934$ and $a_1 \approx 0.426$.
There are several issues using $\{x^k\}$ as basis.

- The matrix H is a full matrix. Then, solving the linear system is expensive, which often takes $O(n^3)$.

- The condition number is big, i.e. $\max(|\lambda_i|)/\min(|\lambda_i|)$ is big. This is a big issue while we see later.

- After we obtain $a_0, \cdots, a_n$. If we want one more coefficient a_{n+1}, we have to solve the whole system again, wasting the previously computed results.

1.2 Orthogonal polynomials

Let us consider the basis functions $\{\phi_k\}$ such that

$$\int_a^b w(x)\phi_i(x)\phi_j(x)\,dx = 0,\ i \neq j.$$

This is much better. Why?

Consider $S(x) = \sum_{k=0}^n a_k\phi_k(x)$. Then, following similar approach, one has

$$\sum_{k=0}^n a_k \int_a^b w(x)\phi_k(x)\phi_j(x)\,dx = \int_a^b w(x)f(x)\phi_j(x)\,dx,\ j = 0, \cdots, n.$$

The left hand side now becomes $a_j \int_a^b w(x)\phi_j^2(x)\,dx$. Hence, the matrix now is a diagonal matrix. Moreover, if we want one more coefficient, the previously computed coefficients will be unchanged. This resolves the first and the third issues! How about the second one? If we multiply ϕ_j by some constant to make $\int_a^b w(x)\phi_j^2 \approx 1$, then the second issue can also be resolved.

Hence, it is highly desirable to use orthogonal polynomials to find least sqaure approximating polynomials. To obtain the orthogonal functions, one can apply the **Gram-Schmidt** process, which we omit here.

If $w(x) \equiv 1$ and $[a,b] = [-1,1]$, the orthogonal polynomials are given by by **Legendre polynomials**:

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\{(x^2-1)^n\}.$$

Hence,

$$P_0(x) = 1, P_1(x) = x, P_2(x) = \frac{1}{2}(3x^2-1), \cdots.$$

In particular,

$$P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - nP_{n-1}(x).$$

One has

$$\int_{-1}^1 P_n(x)P_m(x)\,dx = \frac{2}{2n+1}\delta_{m,n}.$$

If

$$w(x) = \frac{1}{\sqrt{1-x^2}},$$

the orthogonal polynomials are given by

$$T_0(x) = 1,\ T_1(x) = x, T_2(x) = 2x^2-1,$$

and in general given by

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x).$$

These are called the **Chebyshev polynomials** and one has

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} T_n(x)T_m(x) = \begin{cases} 0 & m \neq n \\ \frac{\pi}{2} & n = m \neq 0 \\ \pi, & n = m = 0. \end{cases}$$

In fact, the Chebyshev polynomials are given by

$$T_n(x) = \cos(n \arccos x).$$

Hence, if we do change of variables $\theta = \arccos x$ for $\theta \in [0, \pi]$, one then has

$$f_n(\theta) = T_n(\cos\theta) = \cos(n\theta).$$

Also, $\frac{1}{\sqrt{1-x^2}}dx = \frac{1}{\sin\theta}(-\sin\theta)d\theta = -d\theta,\ \theta : \pi \to 0$. In other words, the Chebyshev polynomials are just the cosine modes on the unit circle. The Chebyshev points will then be the equi-spaced points in θ.

What if the interval is not $[-1, 1]$? One can do linear transform to change it into $[-1, 1]$ first and then use these orthogonal polynomials.

Using the theory of Hilbert space, one can show that

Theorem 1. *Let $w = 1$. Suppose $f \in C[a, b]$ (in fact, more generally $L^2[a, b]$) and $S_n(x)$ is the best least square approximating polynomial with degree at most n, then*

$$\|f - S_n\|_2 \to 0,\ n \to \infty.$$

Example Find the best least square polynomial approximation using orthogonal basis for $f(x) = \sqrt{1 + x^2},\ x \in [0, 1]$.

We use the Legendre polynomials. However, the interval now is $[0, 1]$ instead of $[-1, 1]$. Define

$$\alpha = \frac{1 - (-1)}{1 - 0} = 2.$$

Then, we use

$$\tilde{P}_n(x) = \sqrt{\alpha} P_n\left(\alpha(x - \frac{1}{2})\right).$$

Hence, we find

$$\tilde{P}_0(x) = \sqrt{2},\ \tilde{P}_1(x) = 2\sqrt{2}(x - \frac{1}{2})$$

are orthogonal polynomials on $[0, 1]$.

Hence, we find

$$a_0 = \int_0^1 \tilde{P}_0(x)\sqrt{1+x^2}\,dx / \int_0^1 \tilde{P}_0^2(x)\,dx = \frac{\sqrt{2}}{2}(\frac{1}{2}\ln(1+\sqrt{2}) + \frac{\sqrt{2}}{2}) \approx 0.812.$$

Similarly,

$$a_1 = \int_0^1 \sqrt{1+x^2}(2\sqrt{2}(x - \frac{1}{2}))\,dx/(2/3) = 3\sqrt{2}\int_0^1 \sqrt{1+x^2}(x - \frac{1}{2})\,dx \approx 0.151.$$

Hence, the approximation is

$$0.812 * \sqrt{2} + 0.151 * 2\sqrt{2}(x - \frac{1}{2}) \approx 0.935 + 0.427x.$$

This is in fact the same as before. The difference is clearly due to roundoff error.

2 Trigonometric polynomial approximation

If the target function f is periodic, like on $[0, 2\pi]$ with periodic boundary condition. We can use trigonomietric polynomiasl, i.e. $\{1, \cos x, \sin x, \cos(2x), \sin(2x), \cdots\}$.

One can consider the space

$$V_n := span\{\frac{1}{2}, \cos x, \sin x, \cdots, \cos(nx), \sin(nx)\}.$$

These functions are orthogonal on $[0, 2\pi]$.

The approximation is given by

$$S_n(x) = \frac{1}{2}a_0 + \sum_{k=1}^{n}(a_k\cos(kx) + b_k\sin(kx)).$$

Using similar technique, one finds

$$a_k = \frac{1}{\pi}\int_0^{2\pi} f(x)\cos(kx)\,dx, \quad b_k = \frac{1}{\pi}\int_0^{2\pi} f(x)\sin(kx)\,dx.$$

This is called the **Fourier series**. A more frequently used basis function is given by $\{e^{ikx}\}_{k=-\infty}^{\infty}$. Then,

$$S_n(x) = \sum_{k=-n}^{n} c_k e^{ikx},$$

and

$$c_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx}\, dx.$$

Recall that

$$e^{ikx} = \cos(kx) + i \sin(kx).$$

This gives the same approximation. This is in fact more often used form of Fourier series.

Similarly,

Theorem 2. *Suppose $f \in C[0, 2\pi]$ (in fact, more generally $L^2[0, 2\pi]$) and $S_n(x)$ is the best least square Fourier series with degree at most n, then*

$$\|f - S_n\|_2 \to 0, \ n \to \infty.$$

Note that the convergence is not pointwise convergence.