Numerical Analysis Hilary Term 2020
Lecture 11: Least-Squares Approximation

For the problem of least-squares approximation, $\langle f, g\rangle = \int_a^b w(x) f(x) g(x)\,\mathrm{d}x$ and $\|f\|_2^2 = \langle f, f\rangle$ where $w(x) > 0$ on (a, b).

Theorem. If $f \in \mathrm{L}^2_w(a, b)$ and $p_n \in \Pi_n$ is such that

$$\langle f - p_n, r\rangle = 0 \qquad \forall r \in \Pi_n, \tag{1}$$

then

$$\|f - p_n\|_2 \le \|f - r\|_2 \qquad \forall r \in \Pi_n,$$

i.e., p_n is a best (weighted) least-squares approximation to f on $[a, b]$.

Proof.

$$\begin{aligned}
\|f - p_n\|_2^2 &= \langle f - p_n, f - p_n\rangle \\
&= \langle f - p_n, f - r\rangle + \langle f - p_n, r - p_n\rangle \qquad \forall r \in \Pi_n \\
&\ \text{Since } r - p_n \in \Pi_n \text{ the assumption (1) implies that} \\
&= \langle f - p_n, f - r\rangle \\
&\le \|f - p_n\|_2 \|f - r\|_2 \ \text{ by the Cauchy–Schwarz inequality.}
\end{aligned}$$

Dividing both sides by $\|f - p_n\|_2$ gives the required result. □

Remark: the converse is true too (see problem sheet 4).

This gives a direct way to calculate a best approximation: we want to find $p_n(x) = \sum_{k=0}^{n} \alpha_k x^k$ such that

$$\int_a^b w(x) \left(f - \sum_{k=0}^{n} \alpha_k x^k\right) x^i \,\mathrm{d}x = 0 \ \text{ for } \ i = 0, 1, \ldots, n. \tag{2}$$

[Note that (2) holds if, and only if,

$$\int_a^b w(x) \left(f - \sum_{k=0}^{n} \alpha_k x^k\right) \left(\sum_{i=0}^{n} \beta_i x^i\right) \mathrm{d}x = 0 \qquad \forall q = \sum_{i=0}^{n} \beta_i x^i \in \Pi_n.]$$

However, (2) implies that

$$\sum_{k=0}^{n} \left(\int_a^b w(x) x^{k+i} \,\mathrm{d}x\right) \alpha_k = \int_a^b w(x) f(x) x^i \,\mathrm{d}x \ \text{ for } \ i = 0, 1, \ldots, n$$

which is the component-wise statement of a matrix equation

$$A\alpha = \varphi, \tag{3}$$

to determine the coefficients $\alpha = (\alpha_0, \alpha_1, \ldots, \alpha_n)^{\mathrm{T}}$, where $A = \{a_{i,k}, i, k = 0, 1, \ldots, n\}$, $\varphi = (f_0, f_1, \ldots, f_n)^{\mathrm{T}}$,

$$a_{i,k} = \int_a^b w(x) x^{k+i} \,\mathrm{d}x \ \text{ and } \ f_i = \int_a^b w(x) f(x) x^i \,\mathrm{d}x.$$

The system (3) are called the **normal equations**.

Example: the best least-squares approximation to e^x on $[0,1]$ from Π_1 in $\langle f,g\rangle = \int_a^b f(x)g(x)\,\mathrm{d}x$. We want

$$\int_0^1 [\mathrm{e}^x - (\alpha_0 1 + \alpha_1 x)]1\,\mathrm{d}x = 0 \text{ and } \int_0^1 [\mathrm{e}^x - (\alpha_0 1 + \alpha_1 x)]x\,\mathrm{d}x = 0.$$

$\iff$

$$\alpha_0 \int_0^1 \mathrm{d}x + \alpha_1 \int_0^1 x\,\mathrm{d}x = \int_0^1 \mathrm{e}^x\,\mathrm{d}x$$

$$\alpha_0 \int_0^1 x\,\mathrm{d}x + \alpha_1 \int_0^1 x^2\,\mathrm{d}x = \int_0^1 \mathrm{e}^x x\,\mathrm{d}x$$

i.e.,

$$\begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \mathrm{e}-1 \\ 1 \end{bmatrix}$$

$\implies \alpha_0 = 4\mathrm{e} - 10$ and $\alpha_1 = 18 - 6\mathrm{e}$, so $p_1(x) := (18-6\mathrm{e})x + (4\mathrm{e} - 10)$ is the best approximation.

Proof that the coefficient matrix A is nonsingular will now establish existence and uniqueness of (weighted) $\|\cdot\|_2$ best-approximation.

Theorem. The coefficient matrix A is nonsingular.

Proof. Suppose not $\implies \exists \alpha \neq 0$ with $A\alpha = 0 \implies \alpha^{\mathrm{T}} A \alpha = 0$

$$\iff \sum_{i=0}^{n} \alpha_i (A\alpha)_i = 0 \iff \sum_{i=0}^{n} \alpha_i \sum_{k=0}^{n} a_{ik}\alpha_k = 0,$$

and using the definition $a_{ik} = \int_a^b w(x) x^k x^i\,\mathrm{d}x$,

$$\iff \sum_{i=0}^{n} \alpha_i \sum_{k=0}^{n} \left(\int_a^b w(x) x^k x^i\,\mathrm{d}x \right) \alpha_k = 0.$$

Rearranging gives

$$\int_a^b w(x) \left(\sum_{i=0}^{n} \alpha_i x^i \right) \left(\sum_{k=0}^{n} \alpha_k x^k \right) \mathrm{d}x = 0 \text{ or } \int_a^b w(x) \left(\sum_{i=0}^{n} \alpha_i x^i \right)^2 \mathrm{d}x = 0$$

which implies that $\sum_{i=0}^{n} \alpha_i x^i = 0$ and thus $\alpha_i = 0$ for $i = 0, 1, \ldots, n$. This contradicts the initial supposition, and thus A is nonsingular. □

Remark: This result does not imply that the normal equations are usable in practice: the method would need to be stable with respect to small perturbations. In fact, difficulties arise from the "ill-conditioning" of the matrix A as n increases. The next lecture looks at a fix.