# Approximation and Quadrature

## 1 Approximation using orthogonal projection

Let $V$ be a vector space with inner product $(u,v)$ and norm $\|u\| = (u,u)^{1/2}$.

We are given $u \in V$ and a subspace $\tilde{V} = \operatorname{span}\left\{v^{(1)},\ldots,v^{(n)}\right\}$ where $v^{(1)},\ldots,v^{(n)}$ are linearly independent. We want to find $p \in \tilde{V}$ such that $\|u-p\|$ is minimal.

**Theorem 1.** *There is a unique $p \in \tilde{V}$ minimizing $\|u-p\|$. It satisfies the "normal equations": $u-p \perp \tilde{V}$, i.e.*

$$\left(u-p, v^{(j)}\right) = 0, \qquad j = 1,\ldots,n$$

**Method 1 to find $p$:** With $p = c_1 v^{(1)} + \cdots + c_n v^{(n)}$ we obtain an $n \times n$ linear system:

$$Mc = b, \qquad M_{jk} = \left(v^{(k)}, v^{(j)}\right), \qquad b_j = \left(u, v^{(j)}\right)$$

**Method 2 to find $p$:** **Step 1:** use Gram-Schmidt orthogonalization to find an orthogonal basis $p^{(1)},\ldots,p^{(n)}$ for $\tilde{V}$:

$$p^{(1)} := v^{(1)}, \qquad p^{(2)} := v^{(2)} - \underbrace{\frac{\left(v^{(2)},p^{(1)}\right)}{\left(p^{(1)},p^{(1)}\right)}}_{s_{12}} p^{(1)}, \qquad p^{(3)} := v^{(3)} - \underbrace{\frac{\left(v^{(3)},p^{(1)}\right)}{\left(p^{(1)},p^{(1)}\right)}}_{s_{13}} p^{(1)} - \underbrace{\frac{\left(v^{(3)},p^{(2)}\right)}{\left(p^{(2)},p^{(2)}\right)}}_{s_{23}} p^{(2)}, \ldots$$

Define the upper triangular matrix $S = \begin{bmatrix} 1 & s_{12} & \cdots & s_{1n} \\ & \ddots & \ddots & \vdots \\ & & \ddots & s_{n-1,n} \\ & & & 1 \end{bmatrix}$. Considering $v^{(j)}, p^{(j)}$ as "column vectors" we can write $\left[v^{(1)},\ldots,v^{(n)}\right] = \left[p^{(1)},\ldots,p^{(n)}\right] S$ and

$$\begin{aligned} p &= c_1 v^{(1)} + \cdots + c_n v^{(n)} = \left[v^{(1)},\ldots,v^{(n)}\right] c \\ &= d_1 p^{(1)} + \cdots + d_n p^{(n)} = \left[p^{(1)},\ldots,p^{(n)}\right] d \end{aligned}$$

so the coefficient vectors $c$ and $d$ are related by $Sc = d$.

**Step 2:** With $p = d_1 p^{(1)} + \cdots + d_n p^{(n)}$ the normal equations give $d_j = \dfrac{\left(u,p^{(j)}\right)}{\left(p^{(j)},p^{(j)}\right)}$.
If we need the coefficient vector $c$ we can solve $Sc = d$ by back substitution.

**Application 1:** Let $V = \mathbb{R}^N$ then we are given a matrix $A := \left[v^{(1)},\ldots,v^{(n)}\right] \in \mathbb{R}^{N\times n}$. Gram-Schmidt gives a decomposition $Q = PS$. Dividing the columns of $P$ by $\left\|p^{(j)}\right\|$ and multiplying the rows or $S$ by $\left\|p^{(j)}\right\|$ gives $A = QR$ where $Q$ has orthonormal columns, i.e., $Q^\top Q = I$. We can then solve the least squares problem $\|Ac-u\|_2 = \min$ by $d := Q^\top u$ and solving $Sc = d$.

**Application 2:** Let $V = L^2_w([a,b])$ which is the space of functions on the interval $[a,b]$ such that $\int_a^b u(x)^2 w(x)dx < \infty$, with a weight function $w(x) \geq 0$. Here $(u,v) := \int_a^b u(x)v(x)w(x)dx$. We consider the subspace $\mathcal{P}_n := \operatorname{span}\{1, x, \ldots, x^n\}$. Applying Gram-Schmidt to $1, x, x^2, \ldots$ gives orthogonal polynomials $p_0, p_1, p_2, \ldots$ where $p_j(x) = x^j +$ lower order terms.
**Example 1:** For the interval $[-1,1]$ and $w(x) = 1$ we obtain the **Legendre polynomials**.

**Example 2:** For the interval $[-1,1]$ and $w(x) = (1-x^2)^{-1/2}$ we obtain the **Chebyshev polynomials**.

We use a different normalization: With $T_0(x) := 1$ and $T_1(x) := x$ we define

$$T_{n+1}(x) := 2x \cdot T_n(x) - T_{n-1}(x)$$

and have with the change of variables $x = \cos t$

$$T_n(x) = \cos(nt)$$

Hence the zeros $\tilde{x}_j$ and extrema $x_j$ on $[-1,1]$ are given by

$$\tilde{x}_j = \cos\left((j - \frac{1}{2})\frac{\pi}{n}\right), \quad j = 1, \ldots, n, \qquad x_j = \cos\left((j-1)\frac{\pi}{n}\right), \quad j = 1, \ldots, n+1 \tag{1}$$

with $T_n(x_j) = (-1)^{j-1}$. Note that

$$(T_k, T_\ell) = \int_{t=0}^{\pi} \cos(kt)\cos(\ell t)dt = \begin{cases} 0 & \text{for } k \neq \ell \\ \pi & \text{for } k = \ell = 0 \\ \frac{\pi}{2} & \text{for } k = \ell > 0 \end{cases} \tag{2}$$

# 2 Approximation of functions by polynomials

We consider a continuous function $u(x)$ on the interval $[-1,1]$ and want to find a polynomial $p_n \in \mathcal{P}_n$ such that

$$\|u - p_n\|_\infty = \max_{x \in [-1,1]} |u(x) - p_n(x)|$$

is small. The **Weierstrass approximation theorem** states that we can make the approximation error arbitrarily small:

**Theorem 2.** *If $u(x)$ is continuous on $[-1,1]$ there exists a sequence $p_n \in \mathcal{P}_n$, $n = 0, 1, 2, \ldots$ such that*

$$\|u - p_n\|_\infty \to 0 \quad as\, n \to \infty$$

**Method 1: Interpolation.** We pick $n+1$ distinct points $x_1, \ldots, x_{n+1} \in [-1,1]$ . Then there is a **unique interpolating polynomial** $p_n \in \mathcal{P}_n$ satisfying $p_n(x_j) = f(x_j)$ for $j = 1, \ldots, n+1$. We can write it in terms of the Lagrange formula:

$$p_n(x) = u(x_1)\ell_1(x) + \cdots + u(x_{n+1})\ell_{n+1}(x) \qquad \text{where } \ell_j(x) := \prod_{\substack{k=1\ldots n+1 \\ k \neq j}} \frac{x - x_k}{x_j - x_k}$$

Note that for equidistant nodes the error can be very large. From now on we will use for $x_j$ the extrema of $T_n(x)$, see (1).

**Method 2: Orthogonal projection with weight function $w(x) = (1-x^2)^{-1/2}$.** We define $u_n \in \mathcal{P}_n$ as the polynomial which minizes $\|u - u_n\|_{L^2_w}$. Using (2) we obtain

$$u_n = a_0 T_0(x) + \cdots + a_n T_n(x), \qquad a_k = \frac{(u, T_k)}{(T_k, T_k)} = \begin{cases} \frac{1}{\pi}(u, T_k) & \text{for } k = 0 \\ \frac{2}{\pi}(u, T_k) & \text{for } k > 0 \end{cases}$$

Note that $(u, T_k) = \int_{-1}^{1} u(x) T_k(x)(1-x^2)^{-1/2} dx = \int_{t=0}^{\pi} u(\cos t)\cos(nt)dt$.

For any $u \in L^2_w$ we have that $\|u - u_n\|_{L^2_w} \to 0$ as $n \to \infty$. If $u$ is continuous we may not have pointwise convergence $u_n(x) \to u(x)$ as $n \to \infty$ in a point $x$. With a stronger assumption on $u$ one can prove nicer convergence properties:

**Theorem 3.** *Assume that $u(x)$ satisfies a Lipschitz condition $|u(x) - u(\tilde{x})| \leq L\,|x - \tilde{x}|$ for $x, \tilde{x} \in [-1,1]$. Then the Chebyshev series $u = \sum_{k=0}^{\infty} a_k T_k$ converges absolutely for each $x \in [-1,1]$ and we have uniform convergence*

$$\|u - u_n\|_\infty \to 0 \quad as\, n \to \infty$$

We can now get a bound for the approximation error for the projection $u_n$ and the interpolation $p_n$ in terms of the Chebyshev coefficients $a_k$:

$$\|u - u_n\|_\infty \leq \sum_{j=n+1}^{\infty} |a_j|$$

$$\|u - p_n\|_\infty \leq 2 \sum_{j=n+1}^{\infty} |a_j|$$

The decay of the coefficients $a_k$ depends on the "smoothness" of the function $u(x)$.

The **total variation** $TV(f)$ of a function is defined as a supremum over all partitions $a = z_0 < z_1 < \cdots < z_m = b$ of the interval $[a,b]$:

$$TV(f) = \sup_{\substack{\text{partitions} \\ z_0,\ldots,z_m}} \sum_{j=1}^{m} |f(z_j) - f(z_{j-1})|$$

If the function $f$ is piecewise continuously differentiable on a partition $a = X_0 < X_1 < \cdots < X_M = b$ with jumps we have

$$TV(f) = \sum_{j=1}^{M} \int_{X_{m-1}}^{X_m} |f'(x)|\, dx + \sum_{j=1}^{M-1} |f(X_j + 0) - f(X_j - 0)|$$

E.g., the total variation of $\operatorname{sign}(x)$ on $[-1,1]$ is 2. Note that we can formally write $TV(f)$ as $\int_a^b |f'(x)|\, dx$ if we understand $f'(x)$ as a generalized function with delta functions at the jumps.

**Theorem 4.** *If the derivative $u^{(\nu)}(x)$ has bounded total variation $TV(u^{(\nu)})$ we have for $\nu \geq 0$ and $k > \nu$*

$$|a_k| \leq \frac{2}{\pi} \frac{TV(u^{(\nu)})}{k(k-1)\cdots(k-\nu)} = O\left(k^{-\nu-1}\right)$$

E.g., for $f(x) = |x|$ we have $\nu = 1$ since $f'(x) = \operatorname{sign}(x)$ has bounded variation: $TV(f') = 2$.

Therefore we obtain for the error of $u_n$ and $p_n$ for $\nu \geq 1$ and $n \geq \nu$

$$\begin{aligned} \|u - u_n\|_\infty &\leq \frac{2}{\pi} \cdot \frac{1}{\nu} \cdot \frac{TV(u^{(\nu)})}{n(n-1)\cdots(n-\nu+1)} = O\left(n^{-\nu}\right) \\ \|u - p_n\|_\infty &\leq \frac{4}{\pi} \cdot \frac{1}{\nu} \cdot \frac{TV(u^{(\nu)})}{n(n-1)\cdots(n-\nu+1)} = O\left(n^{-\nu}\right) \end{aligned} \tag{3}$$

Note that for $u(x) = |x|$ we obtain $\|u - u_n\|_\infty = O(n^{-1})$ and $\|u - p_n\|_\infty = O(n^{-1})$.

We now consider a function $u(x)$ which is **analytic** on $[-1, 1]$, i.e., for each $x_0 \in [-1, 1]$ the Taylor series about $x_0$ converges for $|x - x_0| \leq \epsilon_{x_0}$ with $\epsilon_{x_0} > 0$. This implies that the Taylor series actually converges in the complex plane for $|z - x_0| \leq \epsilon_{x_0}$. Therefore the function $u(x)$ has an analytic continuation to a function $u(z)$ in the complex plane, defined in a region containing the interval $[-1, 1]$. Such a function can be extended in the complex plane until we hit singularities (like e.g. poles). The size of the region in the complex plane where $u(z)$ is analytic determines the decay of $a_k$.

Let $\rho > 1$. The mapping $w = \frac{1}{2}(z + z^{-1})$ maps the circle $|z| = \rho$ to an ellipse $C_\rho$. This ellipse has foci $-1, 1$ and the sum of the semiaxes $a, b$ is $a + b = \rho$. Note that the circle $|z| = \rho^{-1}$ is mapped to the same ellipse.

We define $E_\rho$ as the open region bounded by the curve $C_\rho$.

**Theorem 5.** *Assume that $u(x)$ is analytic on $[-1, 1]$ and has an analytic extension to the open region $E_\rho$ with $\rho > 1$. Let $|u(z)| \leq M$ for $z \in E_\rho$. Then*

$$|a_k| \leq 2M\rho^{-k}$$

Therefore we obtain for the error of $u_n$ and $p_n$ for $\nu \geq 1$

$$\begin{aligned} \|u - u_n\|_\infty &\leq \frac{2M}{\rho - 1}\rho^{-n} \\ \|u - p_n\|_\infty &\leq \frac{4M}{\rho - 1}\rho^{-n} \end{aligned} \tag{4}$$

**Example:** The function $u(x) = (1 + x^2)^{-1}$ is analytic on $[-1, 1]$. The function $u(z) = (1 + z^2)^{-1}$ is analytic everywhere in the complex plane except the two points $z = \pm i$. We want to find the ellipse $C_\rho$ which passes through the point $i$: We must have that the point $z = i\rho$ on the circle gets mapped to the point $w = \frac{1}{2}(z + z^{-1}) = \frac{1}{2}\left(i\rho - (i\rho)^{-1})\right) = i\frac{1}{2}(\rho - \rho^{-1}) \overset{!}{=} i \cdot 1$. Hence we need to find $\rho > 1$ such that $\frac{1}{2}\left(\rho - \rho^{-1}\right) = 1$. This gives a quadratic equation for $\rho$ which we can solve:

$$\rho^2 - 2\rho - 1 = 0, \quad \rho = \frac{2 + \sqrt{8}}{2} = 1 + \sqrt{2}$$

(we use "+" since we want to find $\rho > 1$). Let $\rho_* = 1 + \sqrt{2}$. For any $\rho < \rho_*$ we have that $u(z)$ is bounded on $C_\rho$. Hence we obtain that for any $\rho < \rho_* = 1 + \sqrt{2}$ we have

$$\|u - u_n\|_\infty \leq C_\rho \rho^{-n}, \quad \|u - p_n\|_\infty \leq 2C_\rho \rho^{-n} \tag{5}$$

# 3 Quadrature

For an interval $[a, b]$ and a "weight function" $w(x) \geq 0$ we want to approximate integrals of the form

$$I(f) := \int_a^b f(x)w(x)dx$$

We pick distinct nodes $x_1, \ldots, x_n \in [a, b]$. Let $p(x) = f(x_1)\ell_1(x) + \cdots + f(x_n)\ell_n(x)$ denote the interpolating polynomial, then we define the approximation as

$$Q(f) = \int_a^b p(x)w(x)dx = \sum_{j=1}^{n} w_j f(x_j)$$

where $w_j = I(\ell_j)$. Note that this quadrature rule is exact if $f \in \mathcal{P}_{n-1}$, i.e., $I(f) = Q(f)$.

Usually it is easier to determine $w_1, \ldots, w_n$ by using the $n$ equations $Q(x^j) = I(x^j)$ for $j = 0, \ldots, n-1$. This is a linear system of $n$ equations for $n$ unknowns.

**Example:** For $w(x) = 1$ on $[-1, 1]$ and the nodes $x_1 = -1$, $x_2 = 0$, $x_3 = 1$ we obtain for $f(x) = 1, x, x^2$ the three equations

$$\begin{aligned} w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1 &= \int_{-1}^{1} 1dx = 2 \\ w_1 \cdot (-1) + w_2 \cdot 0 + w_3 \cdot 1 &= \int_{-1}^{1} x\,dx = 0 \\ w_1 \cdot 1 + w_2 \cdot 0 + w_3 \cdot 1 &= \int_{-1}^{1} x^2 dx = \frac{2}{3} \end{aligned}$$

This linear system has the solution $w_1 = \frac{1}{3}$, $w_2 = \frac{4}{3}$, $w_3 = \frac{1}{3}$ which is the well known Simpson rule.

Note that the quadrature rule $Q(f)$ may be exact for polynomials $p \in \mathcal{P}_m$ with $m > n - 1$. But it can never be exact for $\mathcal{P}_{2n}$ since for $f(x) = (x - x_1)^2 \cdots (x - x_n)^2$ we have $Q(f) = 0$ and $I(f) > 0$.

It turns out that we can pick nodes $x_1, \ldots, x_n$ such that the quadrature rule is exact for $p \in \mathcal{P}_{2n-1}$, this is the so-called **Gaussian quadrature**:

**Theorem 6.** *Let $p(x)$ denote the orthogonal polynomial of degree $n$ for the weight function $w(x)$ on $[a, b]$. Let $x_1, \ldots, x_n$ be the zeros of the function $p(x)$, and let $w_1, \ldots, w_n$ denote the corresponding coefficients of the quadrature formula. Then*

- *the nodes $x_1, \ldots, x_n$ are distinct points in $(a, b)$*
- *$w_j > 0$ for $j = 1, \ldots, n$*
- *$Q(p) = I(p)$ for all $p \in \mathcal{P}_{2n-1}$*

**Example:** Approximate $I = \int_0^1 x^{1/3} \cos x\, dx$ by a Gaussian rule with 1 node.
If we use $f(x) = x^{1/3} \cos x$ and $w(x) = 1$ the function $f$ is not very smooth and we will only have very slow convergence of $Q_n(f)$.

Therefore we let $f(x) = \cos x$ and $w(x) = x^{1/3}$. For the Gauss rule we first need to find the orthogonal polynomial of degree 1: $p_1(x) = x - c$ should be orthogonal on 1, i.e.,

$$0 = \int_0^1 (x-c) \cdot 1 \cdot x^{1/3} dx = \left[ \frac{3}{7} x^{7/3} - c\frac{3}{4} x^{4/3} \right]_{x=0}^1 = \frac{3}{7} - c\frac{3}{4}$$

hence $c = \frac{4}{7}$. Now $x_1$ is the zero of $p_1(x) = x - \frac{4}{7}$, so $x_1 = \frac{4}{7}$. We need to determine $w_1$ such that $Q(1) = I(1)$, i.e.,

$$w_1 \cdot 1 = \int_0^1 1 \cdot x^{1/3} dx = \left[ \frac{3}{4} x^{4/3} \right]_{x=0}^1 = \frac{3}{4}$$

hence $w_1 = \frac{3}{4}$. Therefore we have obtain the Gaussian rule

$$\int_0^1 f(x) x^{1/3} dx \approx \frac{3}{4} \cdot f(\frac{4}{7})$$

and we obtain for $f(x) = \cos x$ the approximation $Q(f) = \frac{3}{4} \cos(\frac{4}{7}) = 0.6308$. The exact value is $I(f) = 0.6076$.

**Quadrature error.** The quadrature error satisfies

$$I(f) - Q(f) = \int_a^b (f(x) - p(x))\, w(x) dx$$

where $p(x)$ is the interpolating polynomial through the nodes $x_1, \ldots, x_n$.

For many quadrature rules we have that $w_j \geq 0$ for $j = 1, \ldots, n$, e.g.,

- any Gaussian quadrature rule
- using Chebyshev nodes for $[-1, 1]$ with $w(x) = 1$

We can then express the quadrature error in terms of any approximating polynomial $q(x)$:

**Theorem 7.** *Assume that the quadrature rule $Q(f) = w_1 f(x_1) + \cdots + w_n f(x_n)$ satisfies $w_j \geq 0$ for $j = 1, \ldots, n$ and is exact for all polynomials $p \in \mathcal{P}_m$. Then we have for any $q \in \mathcal{P}_m$*

$$|I(f) - Q(f)| \leq 2I(1) \|f - q\|_\infty \tag{6}$$

Consider the interval $[-1, 1]$. Then we can use for $q(x)$ the Chebyshev projection $u_m \in \mathcal{P}_m$ and our approximation results (3), (4) to obtain bounds for the quadrature error.

**Example:** We consider Gaussian quadrature for $[-1, 1]$ and $w(x) = 1$ with $n$ nodes. Then we have $m = 2n - 1$ and $I(1) = \int_{-1}^1 1 dx = 2$.

**(i)** Let $f(x) = |x|$. Then we have $\nu = 1$ and (6), (3) give

$$|Q_n(f) - I(f)| \leq 2 \cdot 2 \cdot \frac{2}{\pi} \cdot \frac{1}{\nu} \frac{TV(f')}{m} = \frac{8}{\pi} \cdot \frac{2}{2n-1}$$

(This is not a sharp estimate, there actually holds $|Q(f) - I(f)| \leq Cn^{-2}$.)

**(ii)** Let $f(x) = \frac{1}{1+x^2}$. Then $f(z)$ is analytic in $E_\rho$ for $\rho < 1 + \sqrt{2}$. Hence we have for any $\rho < 1 + \sqrt{2}$ using (6), (5)

$$|Q_n(f) - I(f)| \leq 2 \cdot 2 \cdot C_\rho \rho^{-(2n-1)} = C'_\rho e^{-an} \qquad \text{with } a = 2\log(1+\sqrt{2}) = 1.763$$

Here the estimate for $a$ is very sharp: Plotting $\log |Q_n - I|$ vs. $n$ gives a straight line with slope$\approx -1.763$.