|CH 7 - P1|

Numerical Integration

$f : \mathbb{R} \to \mathbb{R}$, many times differentiable

aim: compute $\int_a^b f(x)\,dx$

Exploit

$$\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx$$

$p_n(x)$ – Lagrange interpolation polynomial for $f(x)$ at interpolation points $x_0, x_1, \ldots, x_n$

Hence,

$$\int_a^b f(x)\,dx \approx \int_a^b \sum_{k=0}^{n} L_k(x) f(x_k)\,dx$$

$$(*) \quad = \sum_{k=0}^{n} \underbrace{\left\{ \int_a^b L_k(x)\,dx \right\}}_{w_k} f(x_k)\,dx$$

TERMINOLOGY

(*) — a quadrature formula

$w_0, w_1, \ldots, w_n$ — quadrature weights

$x_0, x_1, \ldots, x_n$ — quadrature points

Note: $w_0, \ldots, w_n$ only depends on $x_0, \ldots, x_n$ (in particular they are independent of f)

Newton-Cotes Quadrature Formulas

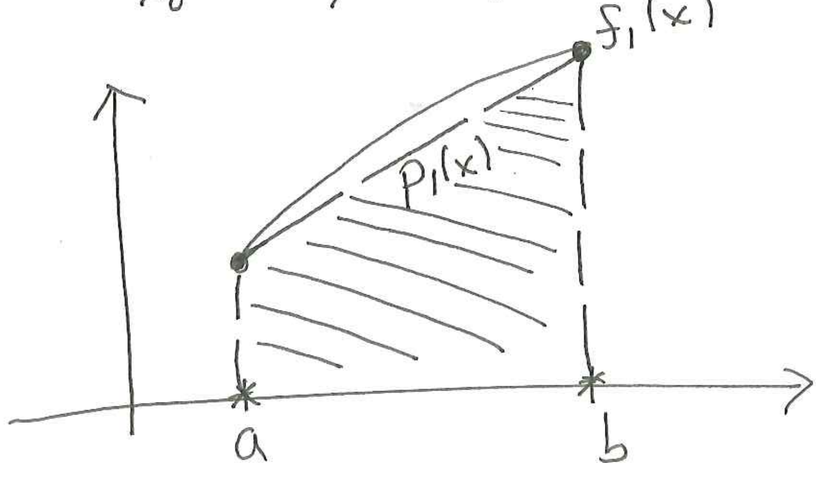
Employs equally spaced points on $[a, b]$ as $x_0, \ldots, x_n$, that is

$$x_j = a + jh \qquad j = 0, 1, \ldots, n$$

where $h := (b-a)/n$

n = 1 (Trapezoidal Rule)

$x_0 = a, \quad x_1 = b$



$$\int_a^b f(x)\,dx \approx \left\{ \int_a^b \frac{x-a}{b-a}\,dx \right\} f(b)$$

$$+$$

$$\left\{ \int_a^b \frac{x-b}{a-b}\,dx \right\} f(a)$$

$$= \frac{1}{b-a}\,\frac{(x-a)^2}{2}\Bigg|_a^b f(a) + \frac{1}{a-b}\,\frac{(x-b)^2}{2}\Bigg|_a^b f(b)$$

$$\boxed{= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)}$$

$n=2$ (Simpson's Rule)

$$x_0 = a \qquad x_1 = \frac{a+b}{2} \qquad x_2 = b$$

$$\int_a^b f(x)\,dx \approx \int_a^b P_2(x)\,dx$$

$$= \underbrace{\left\{ \int_a^b \frac{\left(x - \frac{a+b}{2}\right)(x-b)}{\left(a - \frac{a+b}{2}\right)(a-b)}\,dx \right\}}_{\to w_0} f(a)$$

$$+ \underbrace{\left\{ \int_a^b \frac{(x-a)(x-b)}{\left(\frac{a+b}{2}-a\right)\left(\frac{a+b}{2}-b\right)}\,dx \right\}}_{\to w_1} f\left(\frac{a+b}{2}\right)$$

$$+ \underbrace{\left\{ \int_a^b \frac{(x-a)\left(x - \frac{a+b}{2}\right)}{(b-a)\left(b - \frac{a+b}{2}\right)}\,dx \right\}}_{\to w_2} f(b)$$

To compute w_0, w_1, w_2 change the integration variable; use t s.t.

$$x = \frac{b+a}{2} + \frac{(b-a)}{2} t. \quad \left(\begin{array}{l} \text{that is} \\ x(-1) = a \\ x(1) = b, \\ x(t) \text{ is the} \\ \text{line through} \\ (-1, a) \text{ and } (1, b) \end{array} \right.$$

We have

$$w_0 = \int_{-1}^{1} \frac{\left\{(b-a)/_2\, t\right\} \left\{(b-a)/_2 (t-1)\right\}}{-\left(\frac{b-a}{2}\right)(a-b)} \left(\frac{b-a}{2}\right) dt$$

$$= + \frac{(b-a)}{4} \left(\frac{t^3}{3} - \frac{t^2}{2}\right)\Bigg|_{-1}^{1} = \frac{b-a}{6}$$

$$w_1 = \int_{-1}^{1} \frac{\left\{(b-a)/_2 (t+1)\right\} \left\{(b-a)/_2 (t-1)\right\}}{-\frac{(b-a)}{2} (b-a)/_2} \left(\frac{b-a}{2}\right) dt$$

$$= -\frac{(b-a)}{2} \left(\frac{t^3}{3} - t\right)\Bigg|_{-1}^{1} = \frac{4(b-a)}{6}$$

$$w_2 = \int_{-1}^{1} \frac{\left\{(b-a)/_2 (t+1)\right\} \left\{(b-a)/_2\, t\right\}}{(b-a)\left(\frac{b-a}{2}\right)} \left(\frac{b-a}{2}\right) dt$$

$$= \left(\frac{b-a}{4}\right) \left(\frac{t^3}{3} + \frac{t^2}{2}\right)\Bigg|_{-1}^{1} = \frac{b-a}{6}$$

$$\boxed{\int_a^b f(x)\,dx \approx \frac{b-a}{6} f(a) + 4\frac{(b-a)}{6} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b)}$$

$n=3$ (Simpson's 3/8 rule)

$$x_0 = a \qquad x_1 = a + \frac{(b-a)}{3} = \frac{b+2a}{3}$$

$$x_2 = a + \frac{2(b-a)}{3} = \frac{2b+a}{3} \qquad x_3 = b$$

$$\int_a^b f(x)\,dx \approx \int_a^b p_3(x)\,dx$$

$$= \frac{b-a}{8} f(a) + 3\frac{(b-a)}{8} f\left(\frac{b+2a}{3}\right)$$

details exercise

$$+ 3\frac{(b-a)}{8} f\left(\frac{2b+a}{3}\right) + \frac{(b-a)}{8} f(b)$$

Ex

$$\int_0^1 \underbrace{e^{-x^2}}_{f(x)}\,dx = 0.7468$$

exact up to 4 decimal digits

$$\approx \frac{1}{2}\left[f(0) + f(1)\right] = 0.6840 \quad \left(\text{Trapezoidal rule}\right)$$

$$\approx \frac{1}{6}\left[f(0) + 4f(1/2) + f(1)\right] = 0.7472 \quad \left(\text{Simpson's rule}\right)$$

$$\approx \frac{1}{8}\left[f(0) + 3f(1/3) + 3f(2/3) + f(1)\right] = 0.7470 \quad \left(\text{Simpson's 3/8 rule}\right)$$

Error of Quadrature Formulas

Suppose f is $(n+1)$ times differentiable on $[a,b]$, indeed suppose $f^{(n+1)}(x)$ is continuous on $[a,b]$.

Let $M_{n+1} := \max_{x \in [a,b]} |f^{(n+1)}(x)|$.

$$\left| \int_a^b f(x)\,dx - \sum_{k=0}^{n} w_k f(x_k) \right|$$

$$= \left| \int_a^b f(x) - p_n(x)\,dx \right|$$

$$= \left| \int_a^b \underbrace{\frac{f^{(n+1)}(\xi(x))}{(n+1)!}}_{|f^{(n+1)}(\xi(x))| \leq M_{n+1}} \pi_{n+1}(x)\,dx \right|$$

$$\leq \frac{M_{n+1}}{(n+1)!} \int_a^b |\underbrace{\pi_{n+1}(x)}_{=(x-x_0)(x-x_1)\cdots(x-x_n)}|\,dx$$

Trapezoidal Rule

$$E_T := \left| \int_a^b f(x)\,dx - \frac{(b-a)}{2}[f(a)+f(b)] \right|$$

$$\leq \frac{M_2}{2} \int_a^b |(x-a)(x-b)|\,dx$$

where $M_2 := \max\limits_{x \in [a,b]} |f''(x)|$.

Again, using the substitution

$$x = \frac{b+a}{2} + \frac{(b-a)}{2} t$$

we have

$$\int_a^b -(x-a)(x-b)\,dx = \int_{-1}^{1} -\left(\frac{b-a}{2}\right)^2 (t^2-1) \left(\frac{b-a}{2}\right) dt$$

$$= -\left(\frac{b-a}{2}\right)^3 \left(\frac{t^3}{3} - t\right)\Big|_{-1}^{1} = +\frac{(b-a)^3}{6}.$$

Hence,

$$E_T \leqslant \frac{M_2}{12}(b-a)^3.$$

Simpson's rule

$$E_S := \left| \int_a^b f(x)\,dx - \left(\frac{b-a}{6}\right)\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \right|$$

$$\leqslant \frac{M_3}{3!} \int_a^b \left|(x-a)\left(x - \frac{a+b}{2}\right)(x-b)\right| dx = M_3 \frac{(b-a)^4}{196}$$

details, exercise

with $M_3 := \max\limits_{x \in [a,b]} |f'''(x)|$.

A tighter bound (assumes the continuity of $\xi(x)$ below)

$$E_S = \left| \int_a^b \frac{f'''(\xi(x))}{3!} (x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,dx \right|$$

Lemma

Suppose $h, g : \mathbb{R} \to \mathbb{R}$ are continuous on $[a, b]$, and $g(x) \geqslant 0 \ \forall x \in [a, b]$ or $g(x) \leqslant 0 \ \forall x \in [a, b]$. There exists $\mu \in [a, b]$ such that

$$\int_a^b h(x) g(x) dx = h(\mu) \int_a^b g(x) dx \quad \exists \mu \in [a, b].$$

Proof

Assume $g(x) \geqslant 0 \ \forall x \in [a, b]$. The proof if $g(x) \leqslant 0 \ \forall x \in [a, b]$ is similar. Let $\underset{\sim}{x}, \tilde{x} \in [a, b]$ be such that

$$h(\underset{\sim}{x}) = \min_{x \in [a,b]} h(x), \quad h(\tilde{x}) = \max_{x \in [a,b]} h(x).$$

and define

$$H(x) := h(x) \int_a^b g(t) dt.$$

Now observe

$$\underbrace{\int_a^b h(\underset{\sim}{x}) g(x) dx}_{H(\underset{\sim}{x})} \leqslant \underbrace{\int_a^b h(x) g(x) dx}_{\sigma :=} \leqslant \underbrace{\int_a^b h(\tilde{x}) g(x) dx}_{H(\tilde{x})}.$$

Since $H(x)$ is continuous,

$$H(\mu) = h(\mu) \int_a^b g(t) dt = \sigma$$

hence the result. $\square$

Employing the lemma

$$E_s = \left| \int_a^{(a+b)/2} \frac{f'''(\varepsilon(x))}{6} (x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,dx \right.$$

$$\left. + \int_{(a+b)/2}^{b} \frac{f'''(\varepsilon(x))}{6} (x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,dx \right|$$

$$= \left| \frac{f'''(\varepsilon_1)}{6} \int_a^{(a+b)/2} (x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,dx \right.$$

$$\left. + \frac{f'''(\varepsilon_2)}{6} \int_{(a+b)/2}^{b} (x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,dx \right|$$

$$= \left| \frac{f'''(\varepsilon_1)}{24}\left(\frac{b-a}{2}\right)^4 - \frac{f'''(\varepsilon_2)}{24}\left(\frac{b-a}{2}\right)^4 \right|$$

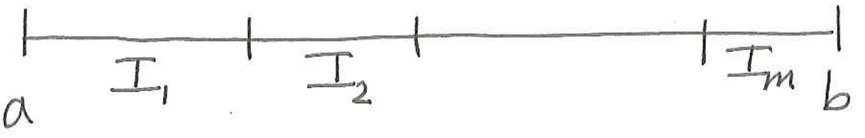
for some $\varepsilon_1, \varepsilon_2 \in [a,b]$. Finally, by the mean value thm

$$E_s = \frac{1}{24}\left(\frac{b-a}{2}\right)^4 \left| f^{(4)}(\varepsilon) \underbrace{(\varepsilon_1 - \varepsilon_2)}_{|\varepsilon_1 - \varepsilon_2| \leq b-a} \right|$$

$$\leq \frac{(b-a)^5}{384} \left| f^{(4)}(\varepsilon) \right|$$

for some $\varepsilon \in (a,b)$.

Composite Quadrature Formulas



Divide $[a,b]$ into m subintervals of equal length, $I_1, I_2, \ldots, I_m$

Apply the same quadrature formula in each of $I_1, I_2, \ldots, I_m$.

Composite trapezoidal rule

$$h := \frac{b-a}{m}$$

$$x_j := a + jh \qquad j = 0, 1, \ldots, m.$$

$$\int_a^b f(x)\,dx = \sum_{j=1}^{m} \int_{x_{j-1}}^{x_j} f(x)\,dx$$

$$\approx \sum_{j=1}^{m} \frac{h}{2}\left[f(x_{j-1}) + f(x_j)\right]$$

$$= \frac{h}{2}\left[f(x_0) + 2\sum_{j=1}^{m-1} f(x_j) + f(x_m)\right]$$

Error

$$E_{CT} = \left| \int_a^b f(x)\,dx - \left\{ \frac{h}{2} \left[f(x_0) + 2\sum_{j=1}^{m-1} f(x_j) + f(x_m) \right] \right\} \right|$$

$$\leqq \sum_{j=1}^{m} \frac{M_2}{12} h^3 = \frac{M_2}{12} \frac{(b-a)^3}{m^2}$$

<u>Remark</u> $E_{CT} \to 0$ as $m \to \infty$.

Composite Simpson's rule

$$h := \frac{b-a}{2m}$$

$$x_j := a + jh \qquad j = 0, 1, \cdots, 2m$$

$$(I_j = [x_{2j-2}, x_{2j}])$$

$$\int_a^b f(x)\,dx = \sum_{j=1}^{m} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx$$

$$\approx \sum_{j=1}^{m} \frac{2h}{6} \left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \right]$$

$$= \frac{2h}{6} \left[f(x_0) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(x_{2m}) \right]$$

Error

$$E_{cs} = \left| \int_a^b f(x)\,dx - \frac{2h}{6}\left\{ f(x_0) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(x_{2m}) \right\} \right|$$

$$\leq \sum_{j=1}^{m} \frac{(2h)^5}{384} \left| f^{(4)}(\xi_j) \right|$$

$$\leq \frac{1}{384} \frac{(b-a)^5}{m^4} M_4$$

for some $\xi_j \in (x_{2j-2}, x_{2j})$ $j = 1, \dots, m$, and

where $M_4 := \max_{x \in [a,b]} \left| f^{(4)}(x) \right|$.

Best polynomial approximation

Problem

Given n and $f \in C[a,b]$, find $p_n \in P_n$ such that

$$\|f - p_n\| \rightarrow \text{a norm on } C[a,b]$$

is as small as possible.

$C[a,b]$ - vector space of continuous functions $f: \mathbb{R} \to \mathbb{R}$ on $[a,b]$.

A norm $\|\cdot\|$ on $C[a,b]$ satisfies

(i) $\|f\| > 0 \quad \forall f \in C[a,b]$, except $f(x) \equiv 0$

(ii) $\|\alpha f\| = |\alpha| \, \|f\| \quad \forall f \in C[a,b], \ \forall \alpha \in \mathbb{R}$

(iii) $\|f+g\| \leq \|f\| + \|g\| \quad \forall f, g \in C[a,b]$

We will consider the following norms:

(1) (∞-norm) $\quad \|f\|_\infty := \max\limits_{x \in [a,b]} |f(x)|$

(2) (2-norm) given $w: \mathbb{R} \to \mathbb{R}$ positive, continuous integrable on (a,b)

$$\|f\|_2 := \sqrt{\int_a^b w(x) f(x)^2 \, dx}$$

Infinite dimensional versions of ∞-norm

$$\|v\|_\infty := \max_{j=1,\dots,n} |v_j|$$

and 2-norm

$$\|v\|_2 := \sqrt{v_1^2 + \cdots + v_n^2}$$

on $\mathbb{R}^n$.

Ex

$f(x) = \cos x$ on $[0, \pi]$

$$\|f\|_\infty = 1$$

With $w(x) = 1$

$$\|f\|_2 = \sqrt{\int_0^\pi \cos^2 x \, dx} = \sqrt{\int_0^\pi \frac{\cos 2x + 1}{2} \, dx}$$

$$= \sqrt{\left(\frac{\sin 2x}{4} + \frac{x}{2}\right)\Bigg|_0^\pi} = \sqrt{\pi/2}$$

Observe

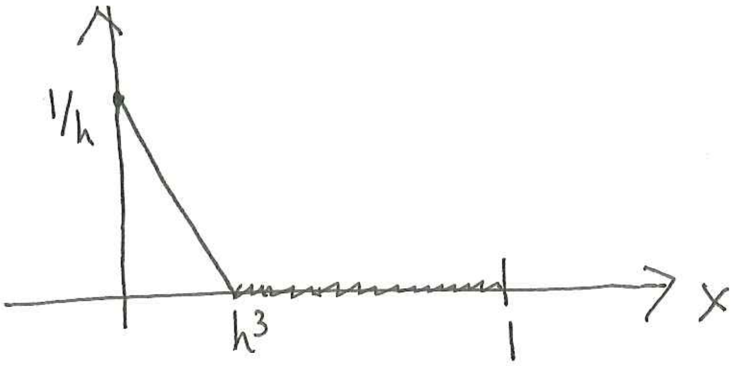
$$\|f\|_2 \leq \sqrt{\int_a^b w(x) \, \|f\|_\infty^2 \, dx}$$

$$= \|f\|_\infty \sqrt{\int_a^b w(x) \, dx}$$

Converse is not true; it may not be possible to bound $\|\cdot\|_\infty$ in terms of $\|\cdot\|_2$.

e.g.
$$f(x) = \begin{cases} \frac{1}{h} - \frac{1}{h^4}x & x \leqslant h^3 \\ 0 & x \in (h^3, 1] \end{cases}$$

on $[0, 1]$. (with $w(x) \equiv 1$)



(h is small, as small as we wish)

$$\|f\|_\infty = 1/h$$

$$\|f\|_2 = \sqrt{\int_0^{h^3} \left(\frac{1}{h} - \frac{1}{h^4} x\right)^2 dx}$$

$$= \sqrt{\left(\frac{1}{h^4}x - \frac{1}{h}\right)^3 / 3 \cdot h^4 \Big|_0^{h^3}} = \sqrt{h/3}$$

THM

For every $\varepsilon > 0$ (no matter how small), and for every $M > 0$ (no matter how large), there exists $f \in C[a, b]$ s.t.

$$\|f\|_2 \leqslant \varepsilon \quad \text{and} \quad \|f\|_\infty \geqslant M.$$

A function $f \in C[a,b]$ can be approximated by a polynomial $p_n \in P_n$ as accurately as we wish provided n is chosen large enough.

<u>THM</u> (Weierstrass Best Approximation Thm)
Let $f \in C[a,b]$. For every $\epsilon > 0$, there exists a polynomial $p : \mathbb{R} \to \mathbb{R}$ such that

$$\|f - p\|_\infty \leq \epsilon .$$

Analogaus result holds for the 2-norm.

For a proof, see exercise 8.12 in the textbook. In particular, show that for each $\epsilon > 0$ there exists $n = n(\epsilon)$ such that

$$p_n(x) = \sum_{k=0}^{n} p_{nk}(x) f(k/n) \qquad x \in [0,1]$$

$$p_{nk}(x) = \binom{n}{k} x^k (1-x)^{n-k}$$

satisfies

$$\|f - p_n\| \leq \epsilon \quad \text{on } [0,1].$$

Best approximation in the ∞-norm

Find $p_n \in P_n$ such that $\left(\begin{array}{l} \text{Given } f \in C[a,b] \\ \text{and } n \end{array} \right.$

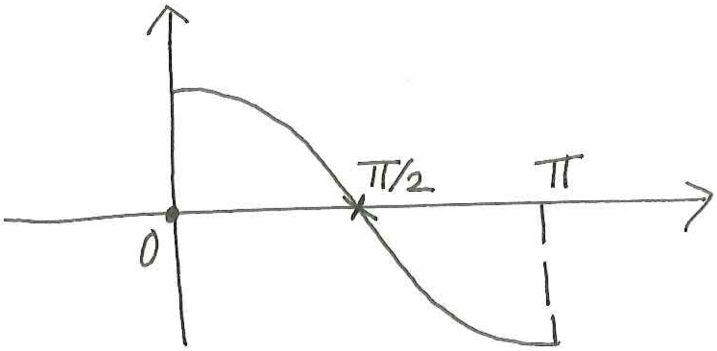
$$\| f - p_n \|_\infty$$

is as small as possible.

e.g.

$f(x) = \cos x$ on $[0, \pi]$

$n = 0$



$p_0(x) \equiv c$

if $c < 0$

$$| f(0) - p_0(0) | > 1$$

if $c > 0$

$$| f(\pi) - p_0(\pi) | > 1$$

and for $c = 0$

$$\| f - p_0 \| = | f(0) - p_0(0) | = | f(\pi) - p_0(\pi) | = 1$$

Hence, $p_0(x) \equiv 0$ is the solution.

THM (Existence)

Let $f \in C[a,b]$, and n be a nonnegative integer. There exists $p_n \in \mathcal{P}_n$ such that

$$\| f - p_n \|_\infty \leqslant \| f - \tilde{p}_n \|_\infty \quad \forall \tilde{p}_n \in \mathcal{P}_n .$$

Proof

Define $E : \mathbb{R}^{n+1} \to \mathbb{R}$ by

$$E(c_0, \ldots, c_n) = \| f - \tilde{p}_n \|_\infty$$

where

$$\tilde{p}_n(x) = c_0 + c_1 x + \cdots + c_n x^n .$$

First we prove E is continuous. Given an $\varepsilon > 0$, define $\delta := \varepsilon / \{1 + K + \cdots + K^n\}$ where $K_n := \max\{|a|, |b|\}$ and consider any $\delta_i \in \mathbb{R}$ s.t. $|\delta_i| \leqslant \delta$ as well as

$$\eta(x) := \delta_0 + \delta_1 x + \cdots + \delta_n x^n .$$

By triangle inequality.

$$E(c_0 + \delta_0, \ldots, c_n + \delta_n) = \| f - (\tilde{p}_n + \eta) \|_\infty$$

$$\leqslant \| f - \tilde{p}_n \|_\infty + \| \eta \|_\infty$$

$$\leqslant E(c_0, \ldots, c_n) + \underbrace{(\delta_0 + |\delta_1||x| + \cdots + |\delta_n||x|^n)}_{\leqslant \delta(1 + |x| + \cdots + |x|^n) \leqslant \varepsilon}$$

$$\Longrightarrow | E(c_0 + \delta_0, \ldots, c_n + \delta_n) - E(c_0, \ldots, c_n) | \leqslant \varepsilon$$

Similarly,

$$E(c_0, \dots, c_n) = \|\{f - (\tilde{p}+n)\} + n\|_\infty$$
$$\leq \|f - (\tilde{p}+n)\|_\infty + \|n\|_\infty$$
$$\leq E(c_0+\delta_0, \dots, c_n+\delta_n) + \varepsilon$$
$$\Longrightarrow E(c_0, \dots, c_n) - E(c_0+\delta_0, \dots, c_n+\delta_n) \leq \varepsilon.$$

Consequently, for every $\varepsilon > 0$ there exists a $\delta > 0$ such that

$$|E(c_0+\delta_0, \dots, c_n+\delta_n) - E(c_0, \dots, c_n)| \leq \varepsilon$$
$$\forall \tilde{\delta} := (\delta_0, \dots, \delta_n) \in \mathbb{R}^{n+1} \text{ s.t. } \|\tilde{\delta}\|_\infty \leq \delta$$

proving continuity.

Now consider the set

$$S := \{(c_0, \dots, c_n) \in \mathbb{R}^{n+1} \mid E(c_0, \dots, c_n) \leq \|f\|_\infty + 1\}.$$

This set is closed, bounded and nonempty (as $E(0, \dots, 0) = \|f\|_\infty$ meaning $0 \in S$). Hence, there exists $c_* \in S$ such that

$$E(c_*) \leq E(c) \quad \forall c \in S.$$

Moreover,

$$E(c_*) \leq \|f\|_\infty < \|f\|_\infty + 1 < E(c) \quad \forall c \in \mathbb{R}^{n+1} \setminus S$$

implying

$$E(c_*) \leq E(c) \quad \forall c \in \mathbb{R}^{n+1}.$$

Consequently, letting $p_n(x) := c_{*,0} + c_{*,1}x + \dots + c_{*,n}x^n$ for $c_* = (c_{*,1}, \dots, c_{*,n})$, we deduce

$$\|f - p_n\|_\infty = E(c_*) \leq E(c) = \|f - (c_0 + \dots + c_n x^n)\|_\infty \quad \forall c = (c_0, \dots, c_n) \in \mathbb{R}^{n+1}$$

$$\Longrightarrow \quad \|f - p_n\|_\infty \leq \|f - \tilde{p}_n\| \quad \forall \tilde{p}_n \in \mathcal{P}_n. \qquad \square$$