WELCOME TO MATH 745 –
– TOPICS IN NUMERICAL ANALYSIS

Instructor: Dr. Bartosz Protas
Department of Mathematics & Statistics
Email: bprotas@mcmaster.ca
Office HH 326, Ext. 24116
Course Webpage: http://www.math.mcmaster.ca/~bprotas/MATH745b

PART I

Review of Interpolation and Approximation Theory

Although this may seem a paradox,
all exact science is dominated by the idea of approximation.
— Bertrand Russell (1872–1970)

REVIEW OF INTERPOLATION AND APPROXIMATION THEORY I

- Goal — given a function f, known exactly or only approximately, find its representation that has
  - a more simply computable form, and
  - error of interpolation / approximation is within some prescribed tolerance.
- Interpolation vs. Approximation
- Reduction to an algebraic problem :
  - existence of a solution,
  - its uniqueness,
  - conditioning of the resulting algebraic system
- Error estimates

INTERPOLATION THEORY I
ABSTRACT FRAMEWORK

- Let:
  - V be a normed vector space over a field $\mathbb{K}$ of numbers (real $\mathbb{R}$, or complex $\mathbb{C}$)
  - V' be the dual space , i.e., a space of linear bounded functionals on V
- Statement of an abstract INTERPOLATION PROBLEM:
  - suppose $V_n \in V$ is an n–dimensional subspace of V with a basis $\{v_1,\dots,v_n\}$
  - let $L_i \in V'$, $1 \le i \le n$ be n linear functionals
  - given n numbers $b_i \in \mathbb{R}$, $1 \le i \le n$, find $u_n \in V_n$ such that the following interpolation conditions are satisfied:

$$L_i u_n = b_i, \quad 1 \le i \le n$$

- Questions:
  - Does the interpolation problem have a solutions?
  - If so, is this solution unique?
  - Can we estimate the error?

Interpolation Theory II
Abstract Framework

- Definition — The functionals L_i, $1 \le i \le n$, are linearly independent over V_n if

$$\forall v \in V_n, \quad \sum_{i=1}^{n} \alpha_i L_i(v) = 0 \implies \alpha_i = 0, \quad 1 \le i \le n$$

- Lemma — the linear functionals $L_1, \dots, L_n$ are linearly independent over V_n iff

$$\det(L_i v_j) = \det \begin{bmatrix} L_1 v_1 & \cdots & L_1 v_n \\ \vdots & \ddots & \vdots \\ L_n v_1 & \cdots & L_n v_n \end{bmatrix} \neq 0$$

- *Proof — $L_1, \dots, L_n$ linearly independent over V_n*

$$\iff \sum_{i=1}^{n} \alpha_i L_i(v_j) = 0, \quad 1 \le j \le n \implies \alpha_i = 0, \quad 1 \le i \le n$$

$$\iff \det(L_i v_j) \neq 0.$$

Interpolation Theory III
Abstract Framework

- Theorem — the following statements are equivalent:
  1. The interpolation problem has a unique solution
  2. The functionals $L_1, \dots, L_n$ are linearly independent over V_n
  3. The only element $u_n \in V_n$ satisfying $L_i u_n = 0$, $1 \le i \le n$ is $u_n = 0$
  4. For any data $\{b_i\}_{i=1}^n$, there exists one $u_n \in V_n$ such that

$$L_i u_n = b_i, \quad 1 \le i \le n$$

- *Proof — from linear algebra, for a square matrix $\mathbb{A} \in \mathbb{K}^{x \times n}$, the following statements are equivalent:*
  1. *The system $\mathbb{A}\mathbf{x} = \mathbf{b}$ has a unique solution $\mathbf{x} \in \mathbb{K}^n$ for any $\mathbf{b} \in \mathbb{K}^n$,*
  2. $\det(\mathbb{A}) \neq 0$,
  3. *If $\mathbb{A}\mathbf{x} = \mathbf{0}$, the $\mathbf{x} = \mathbf{0}$,*
  4. *For any $\mathbf{b} \in \mathbb{K}^n$, the system $\mathbb{A}\mathbf{x} = \mathbf{b}$ has a solution $\mathbf{x} \in \mathbb{K}^n$.*

  The results of the theorem follow from the above statements.

Interpolation Theory IV
Abstract Framework

- Given $u \in V$, its interpolant $u_n = \sum_{i=1}^n \alpha_i v_i$ in V_n is defined by the interpolation conditions

$$L_i u_n = L_i u, \quad 1 \le i \le n$$

- The coefficients $\{\alpha_i\}_{i=1}^n$ can be found from the linear system

$$\begin{bmatrix} L_1 v_1 & \cdots & L_1 v_n \\ \vdots & \ddots & \vdots \\ L_n v_1 & \cdots & L_n v_n \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} L_1 u \\ \vdots \\ L_n u \end{bmatrix}$$

  which has a unique solution of the functionals $L_1, \dots, L_n$ are linearly independent over V_n.

- Specific examples of interpolation:
  - Lagrange polynomial interpolation
  - Hermite polynomial interpolation
  - Piecewise polynomial interpolation
  - trigonometric interpolation

Lagrange Polynomial Interpolation I

- Let:
  - $f : [a,b] \to \mathbb{K}$ be a continuous function defined on a finite closed interval $[a,b]$, so that one can choose $V = C[a,b]$
  - $\Delta : a \le x_0 \le x_1 \le \cdots \le x_n \le b$ be a partition of the interval $[a,b]$
  - V_{n+1} be given by $\mathcal{P}_n$, the space of polynomials of degree less then or equal to n

- Defining the interpolation linear functionals as $L_i f = f(x_i)$, $0 \le i \le n$, we obtain the following conditions for the Lagrange polynomial interpolant of degree n

$$p_n(x_i) = f(x_i), \quad 0 \le i \le n, \quad p_n \in \mathcal{P}_n$$

Lagrange Polynomial Interpolation II
Existence of solutions and uniqueness

- Choosing the set of basis functions for $\mathcal{P}_n$ as $v_j(x) = x^j$, $0 \le i \le n$, we obtain $L_i v_j$ in the form of the Vandermonde matrix :

$$L_i v_j = \begin{bmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 1 & x_1 & x_1^2 & \dots & x_1^n \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_{n-1} & x_{n-1}^2 & \dots & x_{n-1}^n \\ 1 & x_n & x_n^2 & \dots & x_n^n \end{bmatrix}$$

The determinant of this matrix can be shown to be

$$\det(L_i v_j) = \prod_{j>i}^{n} (x_j - x_i) \neq 0.$$

Hence, there exists a unique Lagrange interpolation polynomial.

- Caveat — Note that the Vandermonde matrix is extremely ill–conditioned! This mean that in the resulting algebraic system is hard to solve accurately and therefore in practice other methods are preferred.

Lagrange Polynomial Interpolation III

- An alternative approach — Lagrange's formula for the interpolation polynomial:

$$p_n(x) = \sum_{i=0}^{n} f(x_i)\phi_i(x),$$

where $\{\phi_i\}_{i=0}^n$ are the Lagrange basis functions defined as

$$\phi_i(x) = \prod_{j\neq i} \frac{x - x_j}{x_i - x_j},$$

- Note that $\{\phi_i\}_{i=0}^n$ satisfy the interpolation condition

$$\phi_i(x_j) = \delta_{ij} = \begin{cases} 0, & i \neq j, \\ 1, & i = j, \end{cases}$$

and constitute a basis for the space $\mathcal{P}_n$.

- Solution obtained directly (i.e., without solving an algebraic system); Note that for homogeneous data the interpolant is zero which by the above theorem ensures uniqueness of the solution (this is often a very convenient way of proving existence and uniqueness).

Lagrange Polynomial Interpolation IV
Error Estimates

- Theorem — Assume $f \in C^{(n+1)}[a,b]$. Then there exists a ξ_x between $\min(x_i, x)$ and $\max(x_i, x)$ such that the local interpolation error is

$$f(x) - p_n(x) = \frac{\omega_n(x)}{(n+1)!} f^{(n+1)}(\xi_x), \quad \text{where } \omega_n(x) = \prod_{i=0}^{n}(x - x_i)$$

- *Proof:*
  - *The result is obvious for* $x = x_i$, $0 \le i \le n$,
  - *Suppose* $x \neq x_i$, $0 \le i \le n$, *and denote* $E(x) = f(x) - p_n(x)$.
    Consider the function: $g(t) = E(t) - \frac{\omega_n(t)}{\omega_n(x)} E(x)$
    We note that $g(t)$ *has* $(n+2)$ *distinct roots:* $t = x$ *and* $t = x_i$, $0 \le i \le n$.
    By the Mean Value Theorem, $g'(t)$ *has* $(n+1)$ *distinct roots. Repeatedly applying the Mean Value Theorem to derivatives of g we conclude that* $g^{(n+1)}(t)$ *has a root* $\xi_x \in (\min(x_i, x), \max(x_i, x))$. *Thus*

$$g^{(n+1)}(t) = f^{(n+1)}(\xi_x) - \frac{(n+1)!}{\omega_n(x)} E(x) = 0 \qquad \blacksquare$$

Lagrange Polynomial Interpolation V
Remarks

- Runge Phenomenon — Examination of the interpolation error formula shows that there may be points x^* in the interval $[a,b]$ such that

$$\lim_{n\to\infty} |f(x^*) - p_n(x^*)| = \infty,$$

meaning that the sequence of the approximation polynomials $p_n(x)$ does not uniformly converge to f!
Such situation often arises close to the endpoints of the interpolation interval $[a,b]$.

- This difficulty can be mitigated by performing interpolation on sets of non–uniformly spaced grid points — for instance, zeros of Chebyshev polynomials

HERMITE POLYNOMIAL INTERPOLATION I

- General idea — use the values of both $f(x)$ and $f'(x)$ as interpolation conditions
- Assume that $f \in C^1[a,b]$ and let $\Delta : a \le x_1 \le \cdots \le x_n \le b$ be a partition of the interval $[a,b]$
- The Hermite interpolation polynomial $p_{2n-1} \in \mathcal{P}_{2n-1}$ is chosen to satisfy the conditions

$$p_{2n-1}(x_i) = f(x_i), \quad p'_{2n-1}(x_i) = f'(x_i), \quad 1 \le i \le n$$

- More generally, given a set of integers $\{m_i\}_{i=1}^n$ and $f \in C^M[a,b]$, where $M = \max_i(m_i)$, the Hermite interpolation problem can be stated as follows — find an $p_N \in \mathcal{P}_N$, $N = \sum_{i=1}^n (m_i+1) - 1$ such that

$$p_N^{(j)}(x_i) = f^{(j)}(x_i), \quad 0 \le j \le m_i, \quad 1 \le i \le n$$

- Similar results concerning existence and uniqueness of solutions and the corresponding error bounds can be proven as for the Lagrange interpolation.

PIECEWISE POLYNOMIAL INTERPOLATION I

- Assume that $f \in C[a,b]$ and let $\Delta : a \le x_0 \le x_1 \le \cdots \le x_n \le b$ be a partition of the interval $[a,b]$; denote $h_i = x_i - x_{i-1}$, $1 \le i \le n$ and $h = \max_{1 \le i \le n} h_i$.
- The piecewise linear interpolant is defined as follows:
  - for each $i = 1, \dots, n$ $\Pi_\Delta f\big|_{[x_{i-1},x_i]}$ is linear,
  - for $i = 0,1,\dots,n$, $\Pi_\Delta f(x_i) = f(x_i)$
- Is is easy to see that the following unique linear interpolation polynomial exists:

$$\Pi_\Delta f(x) = \frac{x_i - x}{h_i} f(x_{i-1}) + \frac{x - x_{i-1}}{h_i} f(x_i), \quad x \in [x_{i-1}, x_i]$$

- Suppose that $f \in C^2[a,b]$; local interpolation error can be assessed using the estimate derived previously, i.e.

$$\max_{x\in[a,b]} |f(x) - \Pi_\Delta f(x)| \le \frac{h^2}{8} \max_{x\in[a,b]} |f''(x)|$$

- What about global error (i.e., in the integral sense)?

PIECEWISE POLYNOMIAL INTERPOLATION II

- Instead of $f \in C^2[a,b]$, assume now that $f \in H^2(a,b)$
- Consider the interpolation error in the L_2 sense

$$\|f(x) - \Pi_\Delta f(x)\|^2_{L^2(a,b)} = \int_a^b |f(x) - \Pi_\Delta f(x)|^2\,dx = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} |f(x) - \Pi_\Delta f(x)|^2\,dx$$

- Introduce a function $\hat f \in H^2(0,1)$ with its linear interpolant

$$\hat\Pi \hat f(\xi) = \hat f(0)(1-\xi) + \hat f(1)\xi, \quad 0 \le \xi \le 1$$

- By Taylor's theorem

$$\hat f(0) = \hat f(\xi) - \xi \hat f'(\xi) - \int_\xi^0 t \hat f''(t)\,dt$$

$$\hat f(1) = \hat f(\xi) + (1-\xi)\hat f'(\xi) + \int_\xi^1 (1-t)\hat f''(t)\,dt, \quad \text{then}$$

$$|\hat f(\xi) - \hat\Pi \hat f(\xi)| = |\xi \textstyle\int_\xi^1 (1-t)\hat f''(t)\,dt + (1-\xi)\int_0^\xi t \hat f''(t)\,dt| \le \xi(1-\xi)|\int_0^1 \hat f''(\xi)\,d\xi|$$

and therefore (by Cauchy's theorem)

$$\int_0^1 |\hat f(\xi) - \hat\Pi \hat f(\xi)|^2\,d\xi \le c \int_0^1 |\hat f''(\xi)|^2\,d\xi$$

for some c independent of $\hat f$.

PIECEWISE POLYNOMIAL INTERPOLATION III

- On the other hand

$$\int_{x_{i-1}}^{x_i} |f(x) - \Pi_\Delta f(x)|^2\,dx = h_i \int_0^1 |f(x_{i-1}+h_i\xi) - \hat\Pi f(x_{i-1}+h_i\xi)|^2\,d\xi$$

$$\le c h_i \int_0^1 \left|\frac{d^2 f(x_{i-1}+h_i\xi)}{d\xi^2}\right|^2 d\xi$$

$$\le c h_i^5 \int_0^1 |f''(x_{i-1}+h_i\xi)|^2\,d\xi = c h_i^4 \int_{x_{i-1}}^{x_i} |f''(x)|^2\,dx$$

- Therefore

$$\|f(x) - \Pi_\Delta f(x)\|^2_{L^2(a,b)} = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} |f(x) - \Pi_\Delta f(x)|^2\,dx \le c h^4 \|f''\|^2_{L^2(a,b)},$$

or $\quad \|f(x) - \Pi_\Delta f(x)\|_{L^2(a,b)} \le c h^2 \|f''\|_{L^2(a,b)}$

- A similar argument shows that

$$\|f'(x) - (\Pi_\Delta f(x))'\|^2_{L^2(a,b)} \le c_1 h \|f''\|_{L^2(a,b)}$$

TRIGONOMETRIC INTERPOLATION I

- When considering periodic functions, an important class of of interpolating functions is given by trigonometric polynomials

$$p_n(x) = a_0 + \sum_{j=1}^{n} \left[a_j \cos(jx) + b_j \sin(jx)\right]$$

When $|a_n| + |b_n| \neq 0$ $p_n(x)$ is said to be of order n.

- The polynomial can equivalently be written as

$$p_n(x) = \sum_{j=-n}^{n} c_j e^{ijx} = \sum_{j=-n}^{n} c_j z^j = z^{-n} \sum_{k=0}^{2n} c_{k-n} z^k,$$

where $a_0 = c_0$, $a_j = c_j + c_{-j}$, $b_j = i(c_j - c_{-j})$, and $z = e^{ix}$. Note similarity of the last expression to the algebraic polynomials described before.

TRIGONOMETRIC INTERPOLATION II

- Consider a periodic domain $[0, 2\pi)$ with the following partition $\Delta : 0 \leq x_0 \leq x_1 \leq \cdots \leq x_{2n} < 2\pi$, where $x_j = jh$, $j = 0, 1, \ldots, 2n$ and $h = \frac{2\pi}{2n+1}$
- Given the numbers $\{b_j\}_{j=0}^{2n}$ and introducing the complex nodes $z_j = e^{ix_j}$ ($j = 0, 1, \ldots, 2n$), the trigonometric interpolation problem can be stated as follows

$$\sum_{k=0}^{2n} c_{k-n} z_j^k = z_j^n b_j, \quad j = 0, 1, \ldots, 2n$$

- Existence and uniqueness of a solution to this problem can be proven by reducing it to the solution of the complex Lagrange interpolation problem.

APPROXIMATION —ABSTRACT FRAMEWORK I

- The best approximation problem consists in choosing the member of a restricted class of functions that provides the best representation of the given function f when the approximation error is measured in a prescribed norm; Solution of this problem depends on:
  - properties of the function f
  - properties of the set of approximating functions
  - properties of the norm quantifying the approximation error
- More precisely, given a normed vector space V with some $u \in V$ and a set $K \subseteq V$, we are interested in solution of the following minimization problem

$$\inf_{v \in K} \|u - v\|$$

- Remark — recall analogy with the classical theorem by Weierstraß:
  - Theorem — a real–valued continuous function $f : \mathbb{R} \to \mathbb{R}$ on a bounded closed interval $[a, b]$ $(-\infty < a < b < \infty)$ has a maximum and a minimum.

APPROXIMATION —ABSTRACT FRAMEWORK II

- Depending on the setting, existence of a best approximation is addressed by the following two theorems:
  - Theorem — Assume $K \subseteq V$ is a convex and closed finite–dimensional subset of a normed space V. Then there is an element $\hat{u} \in K$ such that $\|u - \hat{u}\| = \inf_{v \in K} \|u - v\|$
  - Theorem — Assume K is a finite–dimensional subspace of a normed space V. Then there is an element $\hat{u} \in K$ such that $\|u - \hat{u}\| = \inf_{v \in K} \|u - v\|$
- Let $V = L^p(a, b)$ and $K = \mathcal{P}_n$, the space of all the polynomials of degree less then or equal to n. Associated with the space V, we may use $L^p(a, b)$ norms with $1 \leq p \leq \infty$. The above results ensure that for any $f \in L^p(a, b)$ there exists a polynomial $f_n \in \mathcal{P}_n$ such that

$$\|f - f_n\|_{L^p(a,b)} = \inf_{q_n \in \mathcal{P}_n} \|f - q_n\|_{L^p(a,b)}$$

For different values of p we have different best approximations. When $p = \infty$, f_n is called a best uniform approximation of f.

Approximation in Hilbert Spaces I

- When V is an inner–product (Hilbert) space, the norm $\|\cdot\|$ is induced by the associated inner product; this significantly simplifies solution of an approximation problem.
- Definition — Let V be a linear space and V_1 and V_2 subspaces of V. We say that V is a direct sum of V_1 and V_2 and write $V = V_1 \oplus V_2$ is any element $v \in V$ can be uniquely decomposed as

$$v = v_1 + v_2, \quad v_1 \in V_1, \quad v_2 \in V_2.$$

  Furthermore, if V is an inner–product space and $(v_1, v_2) = 0$ for any $v_1 \in V_1$ and $v_2 \in V_2$, then V is called the orthogonal direct sum of V_1 and V_2
- Proposition — Let V be a linear space. Then $V = V_1 \oplus V_2$ iff there is a linear operator $P : V \to V$ with $P^2 = P$ such that in the above decomposition $v_1 = Pv$ and $v_2 = (I-P)v$, and also $V_1 = P(V)$ and $V_2 = (I-P)(V)$.
- Note that $V = P(V) \oplus (I-P)(V)$

Approximation in Hilbert Spaces II

- If V is a Banach space , P is called the projection operator
- If V is a Hilbert space and $V = P(V) \oplus (I-P)(V)$ is an orthogonal direct sum , the P is called the orthogonal projection operator
- Is is easy to see that if a projection operator is orthogonal , then

$$(Pv, (I-P)w) = 0, \quad \forall v, w \in V$$

  In other words, when $v = w$ we note that the best approximation in $P(V)$ of an element $v \in V$ and the approximation error are orthogonal !
- Example — Let $V = C[a,b]$, $V_1 = \mathcal{P}_n$ be the space of polynomials of degree less than or equal to n and let $\Delta : a \le x_0 \le x_1 \le \cdots \le x_n \le b$ be a partition of the interval $[a,b]$. For $v \in C[a,b]$, we define $Pv \in \mathcal{P}_n$ to be the Lagrange interpolant of v corresponding to the partition Δ, i.e., Pv satisfies the interpolation conditions $Pv(x_i) = v(x_i)$, $0 \le i \le n$. The interpolant Pv is uniquely determined, hence thus defined operator P is a projector (although not an orthogonal one). Analogous statements can be made for piecewise polynomial interpolation.

Approximation in Hilbert Spaces III

- Let V_n be an n–dimensional subspace of a Hilbert space V. Suppose $\{u_1, \dots, u_n\}$ be an orthogonal basis of V_n. For any $v \in V$, the formula

$$Pv = \sum_{i=1}^{n} (u_i, v) u_i$$

  defines an orthogonal projection from V onto V_n.
- How to find orthogonal systems in function (e.g., polynomial) spaces? — Perform Schmidt orthogonalization procedure on the system $\{1, x, \dots, x^n\}$
- Various families of ORTHOGONAL POLYNOMIALS are obtained depending on the choice of:
  - the domain $[a,b]$ over which the polynomials are defined, and
  - the weight w characterizing the inner product $(u,v) = \int_a^b wuv\,dx$ used for Schmidt orthogonalization

Orthogonal Polynomials I

- Polynomials defined on the interval $[-1,1]$
  - Legendre polynomials $(w = 1)$

$$P_k(x) = \sqrt{\frac{2k+1}{2}} \frac{1}{2^k k!} \frac{d^k}{dx^k} (x^2-1)^k, \;\; k = 0,1,2,\dots$$

  - Jacobi polynomials $(w = (1-x)^{\alpha}(1+x)^{\beta})$

$$J_k^{(\alpha,\beta)}(x) = C_k (1-x)^{-\alpha}(1+x)^{-\beta} \frac{d^k}{dx^k} [(1-x)^{\alpha+k}(1+x)^{\beta+k}] \;\; k = 0,1,2,\dots,$$

    where C_k is a very complicated constant
  - Chebyshev polynomials $(w = \frac{1}{\sqrt{1-x^2}})$

$$T_n(x) = \cos(k \arccos(x)), \;\; k = 0,1,2,\dots,$$

    Note that Chebyshev polynomials are obtained from Jacobi polynomials for $\alpha = \beta = -1/2$

ORTHOGONAL POLYNOMIALS II

- Polynomials defined on the periodic interval $[-\pi,\pi]$
  Trigonometric polynomials ($w=1$)

$$S_k(x) = e^{ikx} \quad k=0,1,2,\dots$$

- Polynomials defined on the interval $[0,+\infty]$
  Laguerre polynomials ($w=e^{-x}$)

$$L_k(x) = \frac{1}{k!}\,e^x\,\frac{d^k}{dx^k}(e^{-x}x^k), \quad k=0,1,2,\dots$$

- Polynomials defined on the interval $[-\infty,+\infty]$
  Hermite polynomials ($w=1$)

$$H_k(x) = \frac{(-1)^k}{(2^k\,k!\,\sqrt{\pi})^{1/2}}\,e^{x^2}\,\frac{d^k}{dx^k}e^{-x^2}, \quad k=0,1,2,\dots$$

ORTHOGONAL POLYNOMIALS III

- Each of the aforementioned families of orthogonal polynomials forms the set of eigenvectors for the following Sturm–Liouville problem

$$\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right] + [q(x)+\lambda r(x)]y = 0$$
$$a_1 y(a) + a_2 y'(a) = 0$$
$$b_1 y(b) + b_2 y'(b) = 0$$

  for appropriately selected domain $[a,b]$ and coefficients p, q, r, a_1, a_2, b_1 and b_2.

- As regards estimates of approximation errors in the different bases, consult
  - for trigonometric polynomials: `http://www.math.mcmaster.ca/~bprotas/MATH745/spectr_01.pdf`, pages 70–72
  - for Chebyshev polynomials: `http://www.math.mcmaster.ca/~bprotas/MATH745/spectr_03.pdf` page 111