Numerical Methods I Polynomial Interpolation

> Aleksandar Donev Courant Institute, NYU¹ donev@courant.nyu.edu

¹Course G63.2010.001 / G22.2420-001, Fall 2010

October 28th, 2010



- 2 Piecewise Polynomial Interpolation
- 3 Higher Dimensions

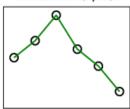


- Find a **numerical** application or theoretical problem that **interests you**. Examples:
 - Incompressible fluid dynamics.
 - Web search engines (google) and database indexing in general.
 - Surface reconstruction in graphics.
 - Proving that linear programming can be solved in polynomial time.
- Then learn more about it (read papers, books, etc) and find out what **numerical algorithms** are important. Examples:
 - Linear solvers for projection methods in fluid dynamics.
 - Eigenvalue solvers for the google matrix.
 - Spline interpolation or approximation of surfaces.
 - The interior-point algorithm for linear programming.
- **Discuss** your selection with me via email or in person.

- Learn how the numerical algorithm works, and what the **difficulties are** and how they can be addressed. Examples:
 - Slow convergence of iterative methods for large meshes (preconditioning, multigrid, etc.).
 - Matrix is very large but also very sparse (power-like methods).
 - ???
 - Simplex algorithm has finite termination but not polynomial.
- Possibly **implement some part of the numerical algorithm** yourself and show some (sample) **results**.
- In the **15min presentation** only explain what the problem is, the mathematical formulation, and what algorithm is used.
- In the **10-or-so page writeup**, explain the details effectively (think of a scientific paper).

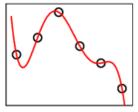
Polynomial Interpolation in 1D

Interpolation in 1D (Cleve Moler)

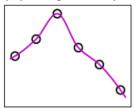


Piecewise linear interpolation

Full degree polynomial interpolation



Shape-preserving Hermite interpolation



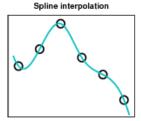


Figure 3.8. Four interpolants.

Interpolation

The task of interpolation is to find an interpolating function φ(x) which passes through m + 1 data points (x_i, y_i):

$$\phi(\mathbf{x}_i) = y_i = f(\mathbf{x}_i)$$
 for $i = 0, 2, \dots, m$,

where \mathbf{x}_i are given **nodes**.

• The type of interpolation is classified based on the form of $\phi(\mathbf{x})$:

- Full-degree **polynomial** interpolation if $\phi(\mathbf{x})$ is globally polynomial.
- **Piecewise polynomial** if $\phi(\mathbf{x})$ is a collection of local polynomials:
 - Piecewise linear or quadratic
 - Hermite interpolation
 - Spline interpolation
- Trigonometric if φ(x) is a trigonometric polynomial (polynomial of sines and cosines).
- Orthogonal polynomial intepolation (Chebyshev, Legendre, etc.).
- As for root finding, in dimensions higher than one things are more complicated!

Polynomial Interpolation in 1D

Polynomial interpolation in 1D

• The interpolating polynomial is degree at most m

$$\phi(x) = \sum_{i=0}^m a_m x^m = \sum_{i=0}^m a_m p_m(x),$$

where the monomials $p_m(x) = x^m$ form a basis for the space of polynomial functions.

• The coefficients $\mathbf{a} = \{a_1, \dots, a_m\}$ are solutions to the square linear system:

$$\phi(x_i) = \sum_{j=0}^m a_j x_i^j = y_i \text{ for } i = 0, 2, \dots, m$$

• In matrix notation, if we start indexing at zero:

$$[\mathbf{V}(x_0, x_1, \dots, x_m)] \, \mathbf{a} = \mathbf{y}$$

where the **Vandermonde matrix** $\mathbf{V} = \{v_{i,j}\}$ is given by

$$v_{i,j} = x_i^j$$
.

The Vandermonde approach

 $\mathbf{V}\mathbf{a} = \mathbf{x}$

• One can prove by induction that

$$\det \mathbf{V} = \prod_{j < k} (x_k - x_j)$$

which means that the Vandermonde system is non-singular and thus: The intepolating polynomial is **unique if the nodes are distinct**.

- Polynomail interpolation is thus equivalent to solving a linear system.
- However, it is easily seen that the Vandermonde matrix can be very ill-conditioned.
- Solving a full linear system is also not very efficient because of the special form of the matrix.

Choosing the right basis functions

• There are many mathematically equivalent ways to rewrite the unique interpolating polynomial:

$$x^2 - 2x + 4 = (x - 2)^2.$$

One can think of this as choosing a different polynomial basis
 {φ₀(x), φ₁(x),..., φ_m(x)} for the function space of polynomials of
 degree at most m:

$$\phi(x) = \sum_{i=0}^m a_i \phi_i(x)$$

• For a given basis, the coefficients **a** can easily be found by solving the linear system

$$\phi(x_j) = \sum_{i=0}^m a_i \phi_i(x_j) = y_j \quad \Rightarrow \quad \mathbf{\Phi}\mathbf{a} = \mathbf{y}$$

Lagrange basis

$$\Phi a = y$$

• This linear system will be trivial to solve if $\mathbf{\Phi} = \mathbf{I}$, i.e., if

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

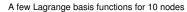
- The φ_i(x) is itself a polynomial interpolant on the same nodes but with function values δ_{ij}, and is thus unique.
- Note that the **nodal polynomial**

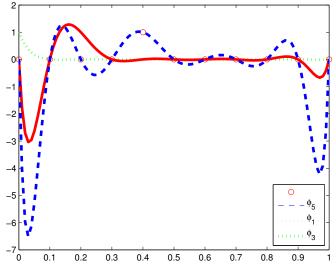
$$w_{m+1}(x) = \prod_{i=0}^m (x - x_i)$$

vanishes at all of the nodes but has degree m + 1.

Polynomial Interpolation in 1D

Lagrange basis on 10 nodes





Lagrange interpolant

$$\phi_i(x_j) = \delta_{ij}$$

• It can easily be seen that the following **characteristic polynomial** provides the desired basis:

$$\phi_i(x) = \frac{\prod_{j \neq i} (x - x_j)}{\prod_{j \neq i} (x_i - x_j)} = \frac{w_{m+1}(x)}{(x - x_i)w'_{m+1}(x_i)}$$

• The resulting Lagrange interpolation formula is

$$\phi(x) = \sum_{i=0}^{m} y_i \phi_i(x) = \sum_{i=0}^{m} \left[\frac{y_i}{\prod_{j \neq i} (x_i - x_j)} \right] \prod_{j \neq i} (x - x_j)$$

• This is useful analytically but **expensive and cumbersome** to use computationally!

Newton's interpolation formula

• By choosing a different basis we get different representations, and Newton's choice is:

$$\phi_i(x) = w_i(x) = \prod_{j=0}^{i-1} (x - x_j)$$

• There is a simple recursive formula to calculate the coefficients **a** in this basis, using Newton's **divided differences**

$$D_i^0 f = f(x_i) = y_i$$

$$D_i^k = \frac{D_{i+1}^{k-1} - D_i^{k-1}}{x_{i+1} - x_i}.$$

• Note that the first divided difference is

$$D_i^1 = rac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \approx f'(x_i),$$

and D_i^2 corresponds to second-order derivatives, etc.

Polynomial Interpolation in 1D Convergence, stability, etc.

- We have lost track of our goal: How good is polynomial interpolation?
- Assume we have a function f(x) that we are trying to **approximate** over an interval $I = [x_0, x_m]$ using a polynomial interpolant.
- Using Taylor series type analysis it is not hard to show that

$$\exists \xi \in I \text{ such that } E_m(x) = f(x) - \phi(x) = \frac{f^{(m+1)}(\xi)}{(m+1)!} \left[\prod_{i=0}^m (x - x_i) \right]$$

Question: Does $||E_m(x)||_{\infty} = max_{x \in I} |f(x)| \to 0$ as $m \to \infty$.

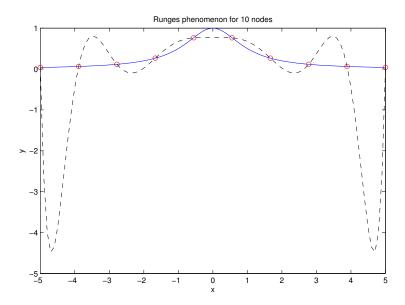
• For equi-spaced nodes, $x_{i+1} = x_i + h$, a bound is

$$\left\|E_{m}(x)\right\|_{\infty} \leq \frac{h^{n+1}}{4(m+1)} \left\|f^{(m+1)}(x)\right\|_{\infty}$$

• The problem is that higher-order derivatives of seemingly nice functions can be unbounded!

Polynomial Interpolation in 1D

Runge's counter-example: $f(x) = (1 + x^2)^{-1}$



A. Donev (Courant Institute)

Uniformly-spaced nodes

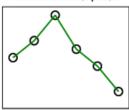
- Not all functions can be approximated well by an interpolating polynomial with equally-spaced nodes over an interval.
- Interpolating polynomials of higher degree tend to be **very oscillatory** and **peaked**, especially near the endpoints of the interval.
- Even worse, the **interpolation is unstable**, under small perturbations of the points $\tilde{y} = y + \delta y$,

$$\left\|\delta\phi(\mathbf{x})\right\|_{\infty} \leq rac{2^{m+1}}{m\log m} \left\|\delta\mathbf{y}\right\|_{\infty}$$

- It is possible to improve the situation by using **specially-chosen nodes** (e.g., Chebyshev nodes, discussed later), or by **interpolating derivatives** (Hermite interpolation).
- In general however, we conclude that interpolating using high-degree polynomials is a bad idea!

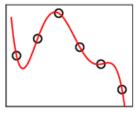
Piecewise Polynomial Interpolation

Interpolation in 1D (Cleve Moler)

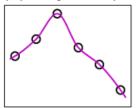


Piecewise linear interpolation

Full degree polynomial interpolation



Shape-preserving Hermite interpolation



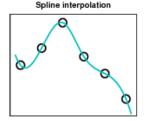


Figure 3.8. Four interpolants.

Piecewise Lagrange interpolants

- The idea is to use a different low-degree polynomial function φ_i(x) in each interval l_i = [x_i, x_{i+1}].
- **Piecewise-constant** interpolation: $\phi_i^{(0)}(x) = y_i$.
- Piecewise-linear interpolation:

$$\phi_i^{(1)}(x) = y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}(x - x_i)$$
 for $x \in I_i$

• For node spacing *h* the error estimate is now bounded and stable:

$$\left\| f(x) - \phi^{(1)}(x) \right\|_{\infty} \le \frac{h^2}{8} \left\| f^{(2)}(x) \right\|_{\infty}$$

Piecewise Hermite interpolants

• If we are given not just the function values but also the first derivatives at the nodes:

$$z_i=f'(x_i),$$

we can find a cubic polynomial on every interval that interpolates both the function and the derivatives at the endpoints:

$$\phi_i(x_i) = y_i$$
 and $\phi'_i(x_i) = z_i$

$$\phi_i(x_{i+1}) = y_{i+1}$$
 and $\phi'_i(x_{i+1}) = z_{i+1}$.

- This is called the **piecewise cubic Hermite interpolant**.
- If the derivatives are not available we can try to estimate z_i ≈ φ'_i(x_i) (see MATLAB's pchip).

Splines

Note that in piecewise Hermite interpolation φ(x) has is continuously differentiable, φ(x) ∈ C¹_I:
 Both φ(x) and φ'(x) are continuous parage the interpol nodes

Both $\phi(x)$ and $\phi'(x)$ are continuous across the **internal nodes**.

- We can make this even stronger, φ(x) ∈ C_I², leading to piecewise cubic spline interpolation:
 - The function φ_i(x) is cubic in each interval I_i = [x_i, x_{i+1}] (requires 4m coefficients).
 - We interpolate the function at the nodes: φ_i(x_i) = φ_{i-1}(x_i) = y_i. This gives m + 1 conditions plus m − 1 conditions at interior nodes.
 - The first and second derivatives are continous at the interior nodes:

$$\phi'_i(x_i) = \phi'_{i-1}(x_i)$$
 and $\phi''_i(x_i) = \phi''_{i-1}(x_i)$ for $i = 1, 2, ..., m-1$,

which gives 2(m-1) equations, for a total of 4m-2 conditions.

Types of Splines

- We need to specify two more conditions arbitrarily (for splines of order k ≥ 3, there are k − 1 arbitrary conditions).
- The most appropriate choice depends on the problem, e.g.:
 - **Periodic** splines, if $y_0 \equiv y_m$ and we think of node 0 and node *m* as one interior node.
 - **Natural** spline: $\phi''(x_0) = \phi''(x_0) = 0$.
 - Not-a-knot condition: Enforce third-derivative continuity at x_1 and x_{m-1} .
- Once the type of spline is chosen, finding the coefficients of the cubic polynomials requires solving a **tridiagonal linear system**, which can be done very fast (O(m)).

Nice properties of splines

• Minimum curvature property:

$$\int_{I} \left[\phi''(x)\right]^2 dx \leq \int_{I} \left[f''(x)\right]^2 dx$$

• The spline approximation converges for zeroth, first and second derivatives (also third for uniformly-spaced nodes):

$$\|f(x) - \phi(x)\|_{\infty} \le \frac{5}{384} \cdot h^{4} \cdot \left\|f^{(4)}(x)\right\|_{\infty}$$
$$\|f'(x) - \phi'(x)\|_{\infty} \le \frac{1}{24} \cdot h^{3} \cdot \left\|f^{(4)}(x)\right\|_{\infty}$$
$$\|f''(x) - \phi''(x)\|_{\infty} \le \frac{3}{8} \cdot h^{2} \cdot \left\|f^{(4)}(x)\right\|_{\infty}$$

In MATLAB

- c = polyfit(x, y, n) does least-squares polynomial of degree n which is interpolating if n = length(x).
- Note that MATLAB stores the coefficients in reverse order, i.e., c(1) is the coefficient of xⁿ.
- y = polyval(c, x) evaluates the interpolant at new points.
- y1 = interp1(x, y, x_{new},' method') or if x is ordered use interp1q. Method is one of 'linear', 'spline', 'cubic'.
- The actual piecewise polynomial can be obtained and evaluated using *ppval*.

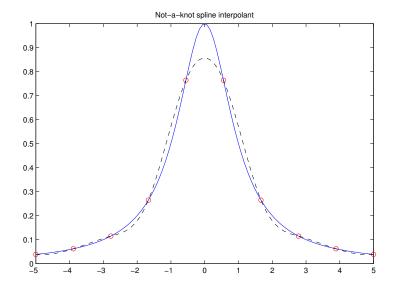
Piecewise Polynomial Interpolation

Interpolating $(1 + x^2)^{-1}$ in MATLAB

```
n = 10:
x = linspace(-5.5.n);
y = (1 + x^2)^{(-1)}
plot(x,y,'ro'); hold on;
x_fine = linspace(-5, 5, 100);
y_fine = (1 + x_fine.^2).^(-1);
plot(x_fine, y_fine, 'b-');
c=polyfit(x,y,n);
v_{interp} = polvval(c.x_{fine}):
plot(x_fine,y_interp,'k—');
y_interp=interp1(x,y,x_fine, 'spline');
plot(x_fine, y_interp, 'k—');
% Or equivalently:
pp=spline(x,y);
y_interp=ppval(pp, x_fine)
```

Piecewise Polynomial Interpolation

Runge's function with spline



Regular grids

- Now x = {x₁,...,x_n} ∈ Rⁿ is a multidimensional data point. Focus on 2D since 3D is similar.
- The easiest case is when the data points are all inside a rectangle

$$\Omega = [x_0, x_{m_x}] \times [y_0, y_{m_y}]$$

where $m = m_x m_y$ and the nodes lie on a regular grid

$$\mathbf{x}_{i,j} = \{x_i, y_j\}, \quad f_{i,j} = f(\mathbf{x}_{i,j}).$$

• We can use separable basis functions:

$$\phi_{i,j}(\mathbf{x}) = \phi_i(x)\phi_j(y).$$

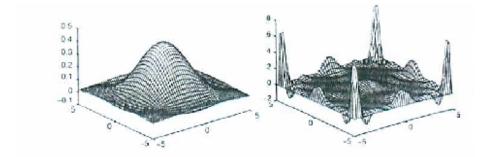
Higher Dimensions

Full degree polynomial interpolation

We can directly apply Lagrange interpolation to each coordinate separately:

$$\phi(\mathbf{x}) = \sum_{i,j} f_{i,j} \phi_{i,j}(\mathbf{x}, \mathbf{y}) = \sum_{i,j} f_{i,j} \phi_i(\mathbf{x}) \phi_j(\mathbf{y}),$$

but this still suffers from Runge's phenomenon:



Piecewise-Polynomial Interpolation

• Juse as in 1D, one can use a different interpolation function $\phi_{(i,j)}: \Omega_{i,j} \to \mathbb{R}$ in each rectange of the grid

$$\Omega_{i,j}=[x_i,x_{i+1}]\times[y_j,y_{j+1}].$$

• For separable polynomials, the equivalent of piecewise linear interpolation in 1D is the **piecewise bilinear interpolation**

$$\phi_{(i,j)}(x,y) = \phi_{(i)}^{(x)}(x) \cdot \phi_{(j)}^{(y)}(y),$$

where $\phi_{(i)}^{(x)}$ and $\phi_{(j)}^{(y)}$ are linear function.

- There are 4 unknown coefficients in $\phi_{(i,j)}$ that can be found from the 4 data (function) values at the corners of rectangle $\Omega_{i,j}$.
- Note that the pieces of the interpolating function φ_(i,j)(x, y) are not linear since they contain quadratic product terms xy: bilinear functions.

This is because there is not a plane that passes through 4 generic points in 3D.

Bilinear Interpolation

It is better to think in terms of a basis set {\(\phi_{i,j}(x, y)\)}\), where each basis functions is itself piecewise bilinear, and

$$\phi_{i,j}(\mathbf{x}_{i'},\mathbf{y}_{j'}) = \delta_{i,i'}\delta_{j,j'} \quad \Rightarrow \quad$$

$$\phi(x) = \sum_{i,j} f_{i,j} \phi_{i,j}(x,y).$$

• Furthermore, it is sufficient to look at a **unit reference rectangle** $\hat{\Omega} = [0,1] \times [0,1]$ since any other rectangle or even **parallelogram** can be obtained from the reference one via a linear transformation:

$$\mathbf{B}_{i,j}\hat{\Omega}+\mathbf{b}_{i,j}=\Omega_{i,j},$$

and the same transformation can then be applied to the interpolation function:

$$\phi_{i,j}(\mathbf{x}) = \hat{\phi}(\mathbf{B}_{i,j}\hat{\mathbf{x}} + \mathbf{b}_{i,j}).$$

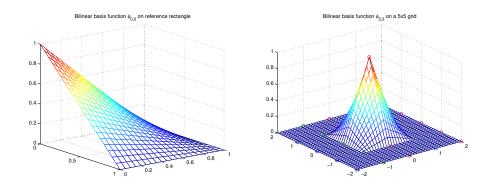
Bilinear Basis Functions

• Consider one of the corners (0,0) of the reference rectangle and the corresponding basis $\hat{\phi}_{0,0}$ restricted to $\hat{\Omega}$:

$$\hat{\phi}_{0,0}(\hat{x},\hat{y}) = (1-\hat{x})(1-\hat{y})$$

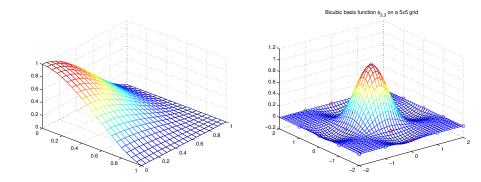
- For an actual grid, the basis function corresponding to a given interior node is simply a composite of 4 such bilinear terms, one for each rectangle that has that interior node as a vertex: Often called a **tent function**.
- If higher smoothness is required one can consider, for example, **bicubic Hermite interpolation** (when derivatives f_x , f_y and f_{xy} are known at the nodes as well).

Bilinear basis functions



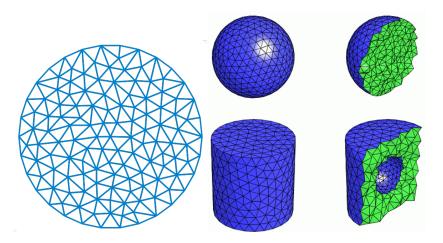
Higher Dimensions

Bicubic basis functions



Irregular (Simplicial) Meshes

Any polygon can be triangulated into arbitrarily many **disjoint triangles**. Similarly **tetrahedral meshes** in 3D.

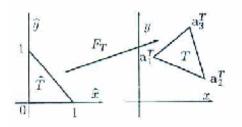


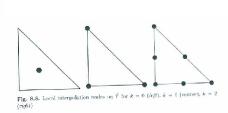
Basis functions on triangles

• For irregular grids the x and y directions are no longer separable.

Higher Dimensions

- But the idea of using basis functions φ_{i,j}, a reference triangle, and piecewise polynomial interpolants still applies.
- For a linear function we need 3 coefficients (x, y, const), for quadratic 6 (x, y, x², y², xy, const):





Higher Dimensions

Piecewise constant / linear basis functions

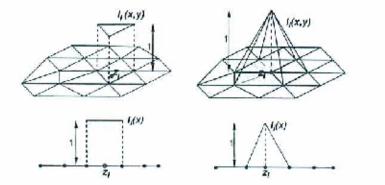


Fig. 8.7. Characteristic piecewise Lagrange polynomial, in two and one space dimensions. Left, k = 0; right, k = 1

• For regular grids the function

$$qz = interp2(x, y, z, qx, qy,' linear')$$

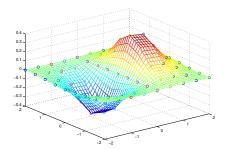
will evaluate the piecewise bilinear interpolant of the data x, y, z = f(x, y) at the points (qx, qy).

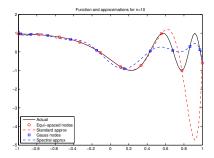
- Other method are 'spline' and 'cubic', and there is also *interp*3 for 3D.
- For irregular grids one can use the old function *griddata* which will generate its own triangulation or there are more sophisticated routines to manipulate triangulations also.

Regular grids

Higher Dimensions

MATLAB's *interp*2

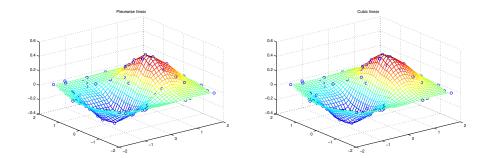




Irregular grids

Higher Dimensions

MATLAB's griddata



Conclusions/Summary

- Interpolation means approximating function values in the interior of a domain when there are **known samples** of the function at a set of **interior and boundary nodes**.
- Given a **basis set** for the **interpolating functions**, interpolation amounts to solving a linear system for the coefficients of the basis functions.
- Polynomial interpolants in 1D can be constructed using several basis.
- Using polynomial interpolants of **high order is a bad idea**: Not accurate and not stable!
- Instead, it is better to use **piecewise polynomial** interpolation: constant, linear, Hermite cubic, cubic spline interpolant on each **interval**.
- In higher dimensions one must be more careful about how the domain is split into disjoint elements (analogues of intervals in 1D): regular grids (separable basis such as bilinear), or simplicial meshes (triangular or tetrahedral).