Scientific Computing: An Introductory Survey Chapter 7 – Interpolation

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Selected subset of slides for CS 357 - page numbers will not necessarily be correct



Outline

- Interpolation
- Polynomial Interpolation
- 3 Piecewise Polynomial Interpolation



Interpolation

Basic interpolation problem: for given data

$$(t_1, y_1), (t_2, y_2), \dots (t_m, y_m)$$
 with $t_1 < t_2 < \dots < t_m$

determine function $f: \mathbb{R} \to \mathbb{R}$ such that

$$f(t_i) = y_i, \quad i = 1, \dots, m$$

- f is interpolating function, or interpolant, for given data
- Additional data might be prescribed, such as slope of interpolant at given points
- Additional constraints might be imposed, such as smoothness, monotonicity, or convexity of interpolant
- f could be function of more than one variable, but we will consider only one-dimensional case



Purposes for Interpolation

- Plotting smooth curve through discrete data points
- Reading between lines of table
- Differentiating or integrating tabular data
- Quick and easy evaluation of mathematical function
- Replacing complicated function by simple one



Interpolation vs Approximation

- By definition, interpolating function fits given data points exactly
- Interpolation is inappropriate if data points subject to significant errors
- It is usually preferable to smooth noisy data, for example by least squares approximation
- Approximation is also more appropriate for special function libraries



Issues in Interpolation

Arbitrarily many functions interpolate given set of data points

- What form should interpolating function have?
- How should interpolant behave between data points?
- Should interpolant inherit properties of data, such as monotonicity, convexity, or periodicity?
- Are parameters that define interpolating function meaningful?
- If function and data are plotted, should results be visually pleasing?



Choosing Interpolant

Choice of function for interpolation based on

- How easy interpolating function is to work with
 - determining its parameters
 - evaluating interpolant
 - differentiating or integrating interpolant
- How well properties of interpolant match properties of data to be fit (smoothness, monotonicity, convexity, periodicity, etc.)



Functions for Interpolation

- Families of functions commonly used for interpolation include
 - Polynomials
 - Piecewise polynomials
 - Trigonometric functions
 - Exponential functions
 - Rational functions
- For now we will focus on interpolation by polynomials and piecewise polynomials
- We will consider trigonometric interpolation (DFT) later



Basis Functions

- Family of functions for interpolating given data points is spanned by set of *basis functions* $\phi_1(t), \dots, \phi_n(t)$
- Interpolating function f is chosen as linear combination of basis functions,

$$f(t) = \sum_{j=1}^{n} x_j \phi_j(t)$$

• Requiring f to interpolate data (t_i, y_i) means

$$f(t_i) = \sum_{j=1}^{n} x_j \phi_j(t_i) = y_i, \quad i = 1, \dots, m$$

which is system of linear equations Ax = y for n-vector x of parameters x_j , where entries of $m \times n$ matrix A are given by $a_{ij} = \phi_j(t_i)$



Existence, Uniqueness, and Conditioning

- ullet Existence and uniqueness of interpolant depend on number of data points m and number of basis functions n
- If m > n, interpolant usually doesn't exist
- If m < n, interpolant is not unique
- If m = n, then basis matrix A is nonsingular provided data points t_i are distinct, so data can be fit exactly
- Sensitivity of parameters x to perturbations in data depends on $\mathrm{cond}(A)$, which depends in turn on choice of basis functions



Polynomial Interpolation

- Simplest and most common type of interpolation uses polynomials
- Unique polynomial of degree at most n-1 passes through n data points (t_i, y_i) , i = 1, ..., n, where t_i are distinct
- There are many ways to represent or compute interpolating polynomial, but in theory all must give same result

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Monomial Basis

Monomial basis functions

$$\phi_j(t) = t^{j-1}, \quad j = 1, \dots, n$$

give interpolating polynomial of form

$$p_{n-1}(t) = x_1 + x_2t + \dots + x_nt^{n-1}$$

with coefficients x given by $n \times n$ linear system

$$oldsymbol{Ax} = egin{bmatrix} 1 & t_1 & \cdots & t_1^{n-1} \ 1 & t_2 & \cdots & t_2^{n-1} \ dots & dots & \ddots & dots \ 1 & t_n & \cdots & t_n^{n-1} \end{bmatrix} egin{bmatrix} x_1 \ x_2 \ dots \ x_n \end{bmatrix} = egin{bmatrix} y_1 \ y_2 \ dots \ y_n \end{bmatrix} = oldsymbol{y}$$

Matrix of this form is called Vandermonde matrix



Example: Monomial Basis

- Determine polynomial of degree two interpolating three data points (-2, -27), (0, -1), (1, 0)
- Using monomial basis, linear system is

$$oldsymbol{A}oldsymbol{x} = egin{bmatrix} 1 & t_1 & t_1^2 \ 1 & t_2 & t_2^2 \ 1 & t_3 & t_3^2 \end{bmatrix} egin{bmatrix} x_1 \ x_2 \ x_3 \end{bmatrix} = egin{bmatrix} y_1 \ y_2 \ y_3 \end{bmatrix} = oldsymbol{y}$$

For these particular data, system is

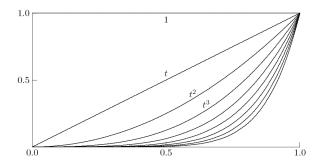
$$\begin{bmatrix} 1 & -2 & 4 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -27 \\ -1 \\ 0 \end{bmatrix}$$

whose solution is $x = \begin{bmatrix} -1 & 5 & -4 \end{bmatrix}^T$, so interpolating polynomial is

$$p_2(t) = -1 + 5t - 4t^2$$



Monomial Basis, continued



< interactive example >

• Solving system Ax = y using standard linear equation solver to determine coefficients x of interpolating polynomial requires $\mathcal{O}(n^3)$ work



Monomial Basis, continued

- For monomial basis, matrix A is increasingly ill-conditioned as degree increases
- Ill-conditioning does not prevent fitting data points well, since residual for linear system solution will be small
- But it does mean that values of coefficients are poorly determined
- Both conditioning of linear system and amount of computational work required to solve it can be improved by using different basis
- Change of basis still gives same interpolating polynomial for given data, but representation of polynomial will be different



Monomial Basis, continued

 Conditioning with monomial basis can be improved by shifting and scaling independent variable t

$$\phi_j(t) = \left(\frac{t-c}{d}\right)^{j-1}$$

where, $c=(t_1+t_n)/2$ is midpoint and $d=(t_n-t_1)/2$ is half of range of data

- ullet New independent variable lies in interval [-1,1], which also helps avoid overflow or harmful underflow
- Even with optimal shifting and scaling, monomial basis usually is still poorly conditioned, and we must seek better alternatives

< interactive example >



Evaluating Polynomials

When represented in monomial basis, polynomial

$$p_{n-1}(t) = x_1 + x_2t + \dots + x_nt^{n-1}$$

can be evaluated efficiently using *Horner's nested* evaluation scheme

$$p_{n-1}(t) = x_1 + t(x_2 + t(x_3 + t(\cdots(x_{n-1} + tx_n)\cdots)))$$

which requires only n additions and n multiplications

For example,

$$1 - 4t + 5t^2 - 2t^3 + 3t^4 = 1 + t(-4 + t(5 + t(-2 + 3t)))$$

 Other manipulations of interpolating polynomial, such as differentiation or integration, are also relatively easy with monomial basis representation



Lagrange Interpolation

• For given set of data points (t_i, y_i) , i = 1, ..., n, Lagrange basis functions are defined by

$$\ell_j(t) = \prod_{k=1, k \neq j}^n (t - t_k) / \prod_{k=1, k \neq j}^n (t_j - t_k), \quad j = 1, \dots, n$$

For Lagrange basis,

$$\ell_j(t_i) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}, \quad i, j = 1, \dots, n$$

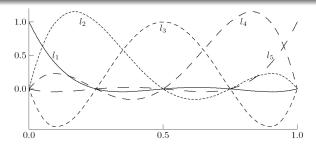
so matrix of linear system $\boldsymbol{A}\boldsymbol{x}=\boldsymbol{y}$ is identity matrix

• Thus, Lagrange polynomial interpolating data points (t_i,y_i) is given by

$$p_{n-1}(t) = y_1 \ell_1(t) + y_2 \ell_2(t) + \dots + y_n \ell_n(t)$$



Lagrange Basis Functions



< interactive example >

- Lagrange interpolant is easy to determine but more expensive to evaluate for given argument, compared with monomial basis representation
- Lagrangian form is also more difficult to differentiate, integrate, etc.



Example: Lagrange Interpolation

- Use Lagrange interpolation to determine interpolating polynomial for three data points (-2, -27), (0, -1), (1, 0)
- Lagrange polynomial of degree two interpolating three points (t_1, y_1) , (t_2, y_2) , (t_3, y_3) is given by $p_2(t) =$

$$y_1 \frac{(t-t_2)(t-t_3)}{(t_1-t_2)(t_1-t_3)} + y_2 \frac{(t-t_1)(t-t_3)}{(t_2-t_1)(t_2-t_3)} + y_3 \frac{(t-t_1)(t-t_2)}{(t_3-t_1)(t_3-t_2)}$$

For these particular data, this becomes

$$p_2(t) = -27 \frac{t(t-1)}{(-2)(-2-1)} + (-1) \frac{(t+2)(t-1)}{(2)(-1)}$$



Newton Interpolation

• For given set of data points (t_i, y_i) , i = 1, ..., n, Newton basis functions are defined by

$$\pi_j(t) = \prod_{k=1}^{j-1} (t - t_k), \quad j = 1, \dots, n$$

where value of product is taken to be 1 when limits make it vacuous

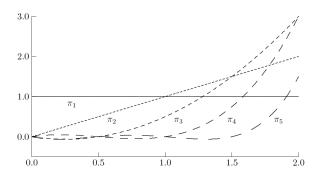
Newton interpolating polynomial has form

$$p_{n-1}(t) = x_1 + x_2(t-t_1) + x_3(t-t_1)(t-t_2) + \cdots + x_n(t-t_1)(t-t_2) \cdots (t-t_{n-1})$$

• For i < j, $\pi_j(t_i) = 0$, so basis matrix \boldsymbol{A} is lower triangular, where $a_{ij} = \pi_j(t_i)$



Newton Basis Functions



< interactive example >



Newton Interpolation, continued

- Solution x to system Ax = y can be computed by forward-substitution in $\mathcal{O}(n^2)$ arithmetic operations
- Moreover, resulting interpolant can be evaluated efficiently for any argument by nested evaluation scheme similar to Horner's method
- Newton interpolation has better balance between cost of computing interpolant and cost of evaluating it



Example: Newton Interpolation

- Use Newton interpolation to determine interpolating polynomial for three data points (-2, -27), (0, -1), (1, 0)
- Using Newton basis, linear system is

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & t_2 - t_1 & 0 \\ 1 & t_3 - t_1 & (t_3 - t_1)(t_3 - t_2) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

For these particular data, system is

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 & 3 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -27 \\ -1 \\ 0 \end{bmatrix}$$

whose solution by forward substitution is

 $x = \begin{bmatrix} -27 & 13 & -4 \end{bmatrix}^T$, so interpolating polynomial is

$$p(t) = -27 + 13(t+2) - 4(t+2)t$$



Newton Interpolation, continued

• If $p_j(t)$ is polynomial of degree j-1 interpolating j given points, then for any constant x_{j+1} ,

$$p_{j+1}(t) = p_j(t) + x_{j+1}\pi_{j+1}(t)$$

is polynomial of degree j that also interpolates same j points

• Free parameter x_{j+1} can then be chosen so that $p_{j+1}(t)$ interpolates y_{j+1} ,

$$x_{j+1} = \frac{y_{j+1} - p_j(t_{j+1})}{\pi_{j+1}(t_{j+1})}$$

• Newton interpolation begins with constant polynomial $p_1(t) = y_1$ interpolating first data point and then successively incorporates each remaining data point into interpolant < interactive example >



Divided Differences

• Given data points (t_i, y_i) , i = 1, ..., n, divided differences, denoted by $f[\]$, are defined recursively by

$$f[t_1, t_2, \dots, t_k] = \frac{f[t_2, t_3, \dots, t_k] - f[t_1, t_2, \dots, t_{k-1}]}{t_k - t_1}$$

where recursion begins with $f[t_k] = y_k$, k = 1, ..., n

 Coefficient of jth basis function in Newton interpolant is given by

$$x_j = f[t_1, t_2, \dots, t_j]$$

ullet Recursion requires $\mathcal{O}(n^2)$ arithmetic operations to compute coefficients of Newton interpolant, but is less prone to overflow or underflow than direct formation of triangular Newton basis matrix



Orthogonal Polynomials

• Inner product can be defined on space of polynomials on interval [a,b] by taking

$$\langle p, q \rangle = \int_{a}^{b} p(t)q(t)w(t)dt$$

where w(t) is nonnegative weight function

- Two polynomials p and q are *orthogonal* if $\langle p, q \rangle = 0$
- Set of polynomials $\{p_i\}$ is *orthonormal* if

$$\langle p_i, p_j \rangle = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

 Given set of polynomials, Gram-Schmidt orthogonalization can be used to generate orthonormal set spanning same space



Orthogonal Polynomials, continued

• For example, with inner product given by weight function $w(t) \equiv 1$ on interval [-1,1], applying Gram-Schmidt process to set of monomials $1,t,t^2,t^3,\ldots$ yields Legendre polynomials

1,
$$t$$
, $(3t^2 - 1)/2$, $(5t^3 - 3t)/2$, $(35t^4 - 30t^2 + 3)/8$,
$$(63t^5 - 70t^3 + 15t)/8$$
, ...

first n of which form an orthogonal basis for space of polynomials of degree at most n-1

 Other choices of weight functions and intervals yield other orthogonal polynomials, such as Chebyshev, Jacobi, Laguerre, and Hermite



Orthogonal Polynomials, continued

- Orthogonal polynomials have many useful properties
- They satisfy three-term recurrence relation of form

$$p_{k+1}(t) = (\alpha_k t + \beta_k) p_k(t) - \gamma_k p_{k-1}(t)$$

which makes them very efficient to generate and evaluate

 Orthogonality makes them very natural for least squares approximation, and they are also useful for generating Gaussian quadrature rules, which we will see later



Chebyshev Polynomials

• kth Chebyshev polynomial of first kind, defined on interval [-1,1] by

$$T_k(t) = \cos(k \arccos(t))$$

are orthogonal with respect to weight function $(1-t^2)^{-1/2}$

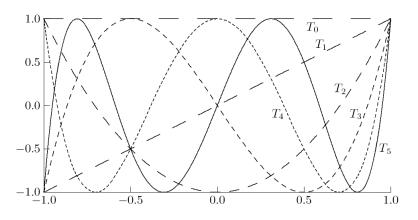
First few Chebyshev polynomials are given by

1,
$$t$$
, $2t^2 - 1$, $4t^3 - 3t$, $8t^4 - 8t^2 + 1$, $16t^5 - 20t^3 + 5t$, ...

ullet Equi-oscillation property: successive extrema of T_k are equal in magnitude and alternate in sign, which distributes error uniformly when approximating arbitrary continuous function



Chebyshev Basis Functions



< interactive example >



Chebyshev Points

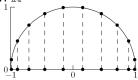
• Chebyshev points are zeros of T_k , given by

$$t_i = \cos\left(\frac{(2i-1)\pi}{2k}\right), \quad i = 1, \dots, k$$

or extrema of T_k , given by

$$t_i = \cos\left(\frac{i\pi}{k}\right), \quad i = 0, 1, \dots, k$$

• Chebyshev points are abscissas of points equally spaced around unit circle in \mathbb{R}^2



 Chebyshev points have attractive properties for interpolation and other problems



High-Degree Polynomial Interpolation

- Interpolating polynomials of high degree are expensive to determine and evaluate
- In some bases, coefficients of polynomial may be poorly determined due to ill-conditioning of linear system to be solved
- High-degree polynomial necessarily has lots of "wiggles," which may bear no relation to data to be fit
- Polynomial passes through required data points, but it may oscillate wildly between data points



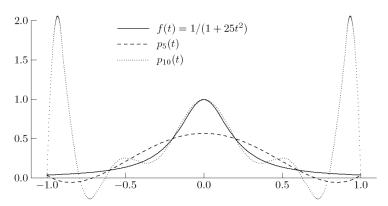
Convergence

- Polynomial interpolating continuous function may not converge to function as number of data points and polynomial degree increases
- Equally spaced interpolation points often yield unsatisfactory results near ends of interval
- If points are bunched near ends of interval, more satisfactory results are likely to be obtained with polynomial interpolation
- Use of Chebyshev points distributes error evenly and yields convergence throughout interval for any sufficiently smooth function



Example: Runge's Function

 Polynomial interpolants of Runge's function at equally spaced points do not converge

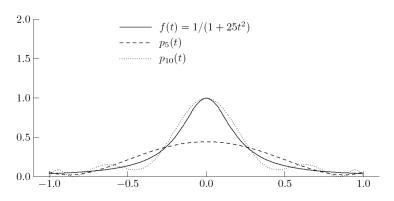


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Example: Runge's Function

 Polynomial interpolants of Runge's function at Chebyshev points do converge



< interactive example >



Piecewise Polynomial Interpolation

- Fitting single polynomial to large number of data points is likely to yield unsatisfactory oscillating behavior in interpolant
- Piecewise polynomials provide alternative to practical and theoretical difficulties with high-degree polynomial interpolation
- Main advantage of piecewise polynomial interpolation is that large number of data points can be fit with low-degree polynomials
- In piecewise interpolation of given data points (t_i, y_i) , different function is used in each subinterval $[t_i, t_{i+1}]$
- Abscissas t_i are called *knots* or *breakpoints*, at which interpolant changes from one function to another



Piecewise Interpolation, continued

- Simplest example is piecewise linear interpolation, in which successive pairs of data points are connected by straight lines
- Although piecewise interpolation eliminates excessive oscillation and nonconvergence, it appears to sacrifice smoothness of interpolating function
- We have many degrees of freedom in choosing piecewise polynomial interpolant, however, which can be exploited to obtain smooth interpolating function despite its piecewise nature

< interactive example >



Hermite Interpolation

- In Hermite interpolation, derivatives as well as values of interpolating function are taken into account
- Including derivative values adds more equations to linear system that determines parameters of interpolating function
- To have unique solution, number of equations must equal number of parameters to be determined
- Piecewise cubic polynomials are typical choice for Hermite interpolation, providing flexibility, simplicity, and efficiency



Hermite Cubic Interpolation

- Hermite cubic interpolant is piecewise cubic polynomial interpolant with continuous first derivative
- Piecewise cubic polynomial with n knots has 4(n-1) parameters to be determined
- Requiring that it interpolate given data gives 2(n-1) equations
- Requiring that it have one continuous derivative gives n-2 additional equations, or total of 3n-4, which still leaves n free parameters
- Thus, Hermite cubic interpolant is not unique, and remaining free parameters can be chosen so that result satisfies additional constraints



Cubic Spline Interpolation

- *Spline* is piecewise polynomial of degree k that is k-1 times continuously differentiable
- For example, linear spline is of degree 1 and has 0 continuous derivatives, i.e., it is continuous, but not smooth, and could be described as "broken line"
- Cubic spline is piecewise cubic polynomial that is twice continuously differentiable
- As with Hermite cubic, interpolating given data and requiring one continuous derivative imposes 3n-4 constraints on cubic spline
- Requiring continuous second derivative imposes n-2 additional constraints, leaving 2 remaining free parameters



Cubic Splines, continued

Final two parameters can be fixed in various ways

- ullet Specify first derivative at endpoints t_1 and t_n
- Force second derivative to be zero at endpoints, which gives natural spline
- Enforce "not-a-knot" condition, which forces two consecutive cubic pieces to be same
- Force first derivatives, as well as second derivatives, to match at endpoints t₁ and t_n (if spline is to be periodic)



Example: Cubic Spline Interpolation

- Determine natural cubic spline interpolating three data points (t_i,y_i) , i=1,2,3
- Required interpolant is piecewise cubic function defined by separate cubic polynomials in each of two intervals $[t_1,t_2]$ and $[t_2,t_3]$
- Denote these two polynomials by

$$p_1(t) = \alpha_1 + \alpha_2 t + \alpha_3 t^2 + \alpha_4 t^3$$

$$p_2(t) = \beta_1 + \beta_2 t + \beta_3 t^2 + \beta_4 t^3$$

 Eight parameters are to be determined, so we need eight equations



Example, continued

• Requiring first cubic to interpolate data at end points of first interval $[t_1,t_2]$ gives two equations

$$\alpha_1 + \alpha_2 t_1 + \alpha_3 t_1^2 + \alpha_4 t_1^3 = y_1$$

$$\alpha_1 + \alpha_2 t_2 + \alpha_3 t_2^2 + \alpha_4 t_2^3 = y_2$$

• Requiring second cubic to interpolate data at end points of second interval $[t_2, t_3]$ gives two equations

$$\beta_1 + \beta_2 t_2 + \beta_3 t_2^2 + \beta_4 t_2^3 = y_2$$

$$\beta_1 + \beta_2 t_3 + \beta_3 t_3^2 + \beta_4 t_3^3 = y_3$$

• Requiring first derivative of interpolant to be continuous at t_2 gives equation

$$\alpha_2 + 2\alpha_3 t_2 + 3\alpha_4 t_2^2 = \beta_2 + 2\beta_3 t_2 + 3\beta_4 t_2^2$$



Example, continued

 Requiring second derivative of interpolant function to be continuous at t₂ gives equation

$$2\alpha_3 + 6\alpha_4 t_2 = 2\beta_3 + 6\beta_4 t_2$$

 Finally, by definition natural spline has second derivative equal to zero at endpoints, which gives two equations

$$2\alpha_3 + 6\alpha_4 t_1 = 0$$

$$2\beta_3 + 6\beta_4 t_3 = 0$$

• When particular data values are substituted for t_i and y_i , system of eight linear equations can be solved for eight unknown parameters α_i and β_i



Hermite Cubic vs Spline Interpolation

- Choice between Hermite cubic and spline interpolation depends on data to be fit and on purpose for doing interpolation
- If smoothness is of paramount importance, then spline interpolation may be most appropriate
- But Hermite cubic interpolant may have more pleasing visual appearance and allows flexibility to preserve monotonicity if original data are monotonic
- In any case, it is advisable to plot interpolant and data to help assess how well interpolating function captures behavior of original data

< interactive example >



Hermite Cubic vs Spline Interpolation

