Numerical and Scientific Computing with Applications David F. Gleich CS 314, Purdue

In this class you should learn:

- A new type of error that arises in numeric differentiation called truncation error
- And how truncation error and floating point error need to be balanced for accurate computations
- What "high dimensional polynomials" require and why they make it hard.

Numerical differentiation Piecewise & High-d Polys

Next class

Numerical differentiation!

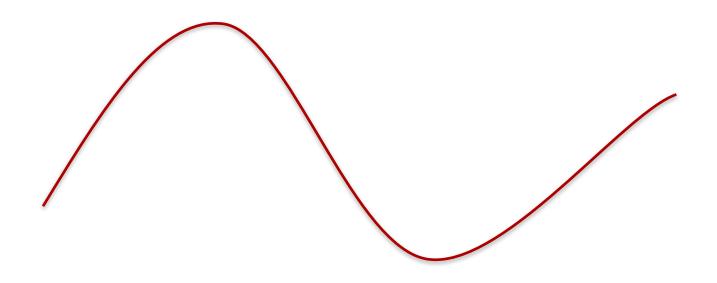
Next next class

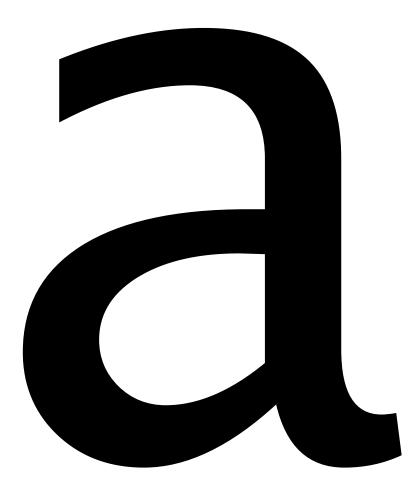
More numerical differentiation

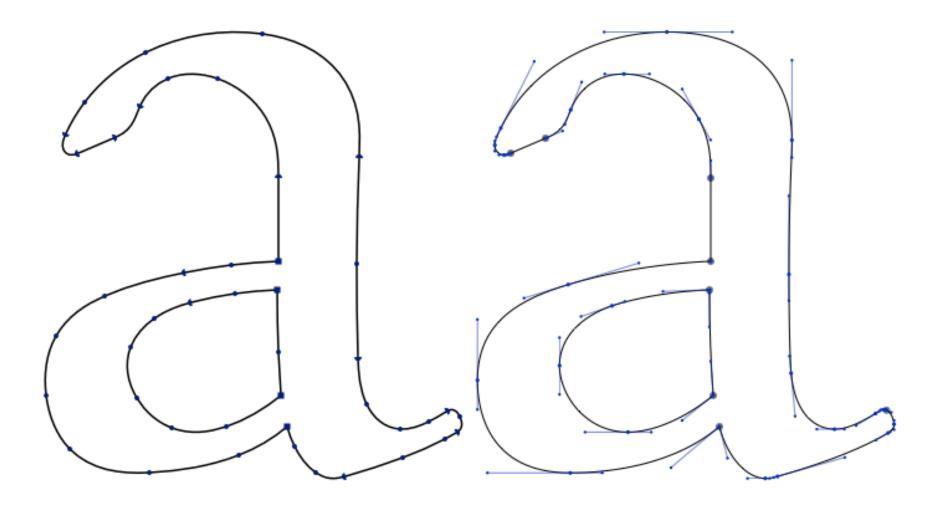
October 31, 2016

Used all over!

Powerpoint curves







$$f(x_{2}) = f(x_{3}) f(x_{4})$$

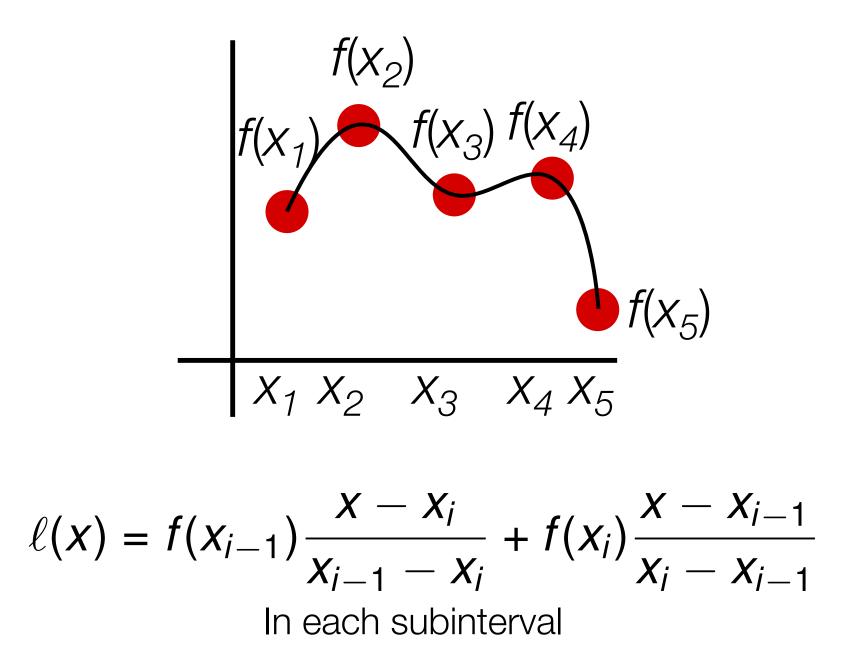
$$f(x_{1}) = f(x_{3}) f(x_{4})$$

$$f(x_{5}) = f(x_{5})$$

$$x_{1} x_{2} x_{3} x_{4} x_{5}$$

$$\ell(x) = f(x_{i-1}) \frac{x - x_i}{x_{i-1} - x_i} + f(x_i) \frac{x - x_{i-1}}{x_i - x_{i-1}}$$

In each subinterval



Linear Uses a set of functions values & points Good if there are *many* points

Quadratic Same info

Can use extra point to match midpoints

Cubic Hermite Uses points, function values, and derivatives

Matches the function values and derivatives!

Cubic Splines Uses points, function values A twice continuously differentiable interpolant!

Linear
$$\ell(x) = f(x_{i-1}) \frac{x - x_i}{x_{i-1} - x_i} + f(x_i) \frac{x - x_{i-1}}{x_i - x_{i-1}}$$

Easy!

Quadratic

Easy!

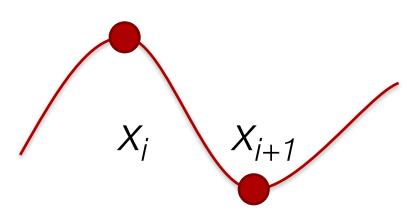
Cubic Hermite

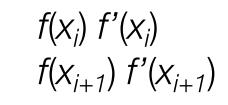
Local work

Cubic Splines

Global work

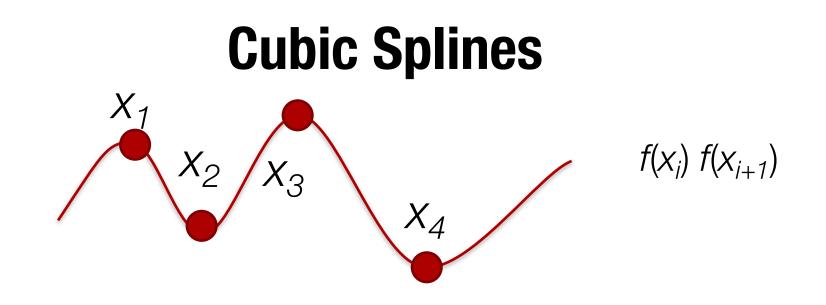
Cubic Hermite





4 parameters, 4 unknowns in the cubic polynomial between x_i , x_{i+1}

Fit via differentiation. One continuous derivative! See the book.

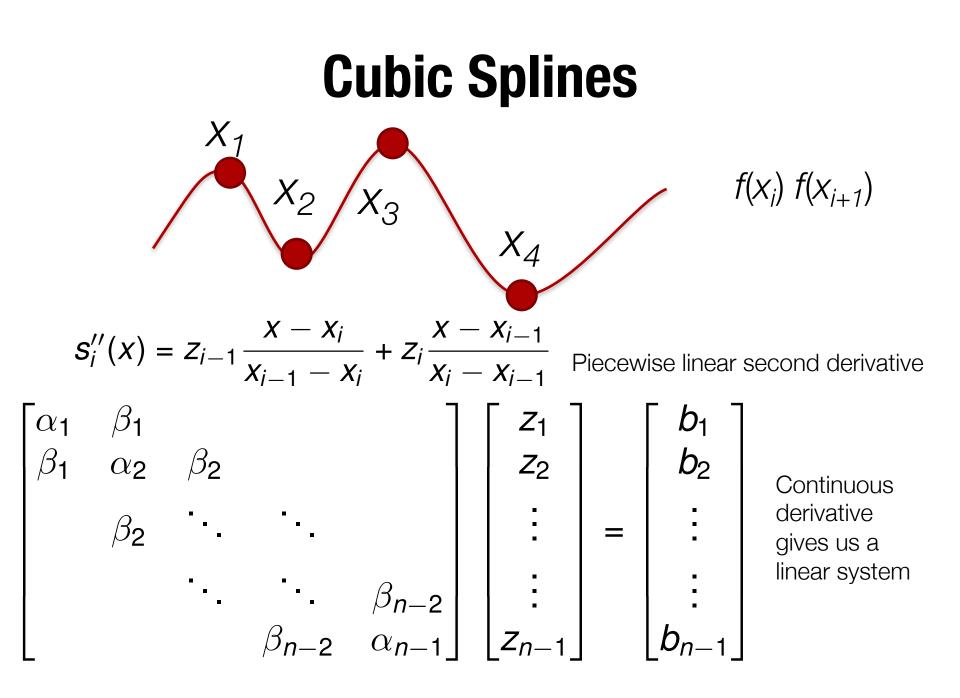


4(n-1) parameters, e.g. 4 unknowns in the cubic polynomial between x_i , x_{i+1}

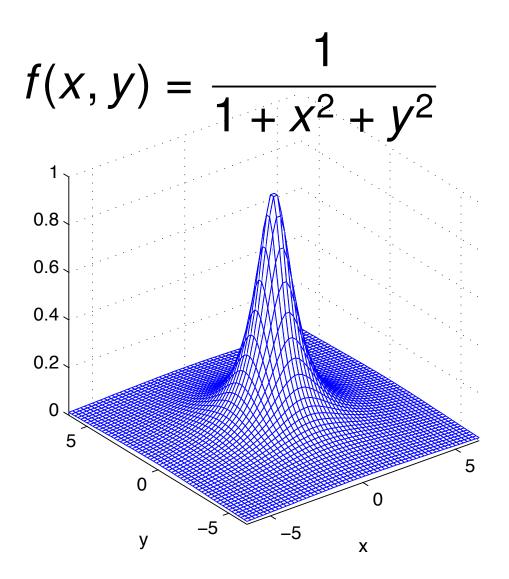
Matching points gives 2(n-1) constraints

Derivatives are continuous (n-3) constraints

2nd derivatives are continuous (n-3) constraints



Multivariate functions



Multivariate polynomials

$$f(x, y) = C_{2,2}x^2y^2 + C_{1,2}xy^2 + C_{0,2}y^2 + C_{2,1}x^2y + C_{1,1}xy + C_{0,1}y + C_{2,0}x^2 + C_{1,0}x + C_{0,0}$$

A bi-variate (2 variable) quadratic has 9 unknown parameters A bi-variate (2 variable) cubic has 16 unknown parameters

A tri-variate (3 variable) quadratic has 27 unknown parameters A tri-variate (3 variable) cubic has ? unknown parameters

Degree of multivariate polynomials

$$f(x, y) = C_{2,2}x^2y^2 + C_{1,2}xy^2 + C_{0,2}y^2 + C_{2,1}x^2y + C_{1,1}xy + C_{0,1}y + C_{2,0}x^2 + C_{1,0}x + C_{0,0}$$

 $x^2 y^2$ has degree "four" $x y^2$ has degree "three"

the degree of a multivar poly is the degree of the largest term

$$f(x, y) = C_{0,2}y^{2} + C_{1,1}xy + C_{0,1}y + C_{2,0}x^{2} + C_{1,0}x + C_{0,0}$$

Quiz

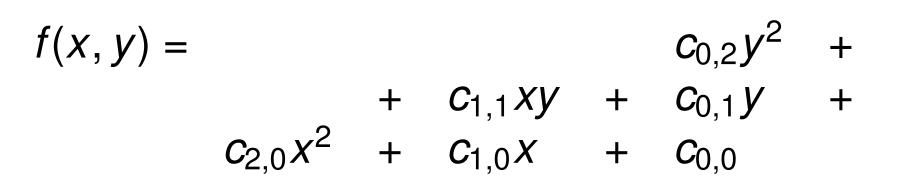
Write down the equations for a multi-linear function in three dimensions:

- (1) where all degrees are less than or equal to 1
- (2) where all "linear" terms of present

$$f(x, y) = C_{2,2}x^2y^2 + C_{1,2}xy^2 + C_{0,2}y^2 + C_{2,1}x^2y + C_{1,1}xy + C_{0,1}y + C_{2,0}x^2 + C_{1,0}x + C_{0,0}$$

$$f(x, y) = C_{2,0}x^2 + C_{1,0}x + C_{0,1}y + C_{2,0}x^2 + C_{1,0}x + C_{0,0}$$

Fitting multivariate polynomials



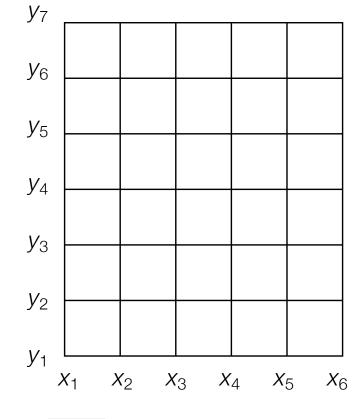
... not nice to write down in general ...

Saniee. "A simple form of the multivariate Lagrange interpolant" SIAM J. Undergraduate Research Online, 2007.

An easier special case

If we have data from our polynomial on a repeated grid then we can fit a sum of 1d polynomials

> "tensor product constructions"



 $p(x, y) = \sum Z_{ij} \varphi_i^x(x) \varphi_j^y(y)$

The big problem

If we have an *m* dimensional function And we want an *n* degree interpolant

We need $(n+1)^m$ samples of our function.

"quadratic" in 10 dimensions – 3¹⁰ samples "quadratic" in 100 dimensions – 3¹⁰⁰ samples Exponential growth or "curse of dimensionality"

Quiz

Write down the equations for a linear interpolant in three dimensions:

(1) where all degrees are less than 1

(2) where all "linear" terms of present

Polynomial approximation

Chebfun implements 1d polynomial interpolation, just use it!

Equally spaced points are bad for interpolation!

There are many mathematically equivalent variations on unique polynomial interpolants but they have different computation properties

Piece-wise polynomials are a highly-flexible model for modeling general smooth curves.

High dimensional interpolation is really hard