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

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#### In this class:

- A quick overview of the numerical methods perspective on applied mathematics
- Overview of Unit 3.
- Interpolation "grids"
- Polynomial interpolation via least squares.
- APPROXFUN

#### Numerical Methods, Applied Mathematics, and Polynomial interpolation

Next class

Lagrange polynomials

Next next class

QUIZ Piecewise interpolants & Splines

#### **Applied mathematics**

*functions* not *numbers* 

Find a function with this property Find a function that satisfies this equation Find a property of this function

#### **Applied mathematics**

What is the value of the integral of a function? What is the derivative function of a given function? What function solves a given differential equation?

### **Problems in applied math**

In this part of the course, it is much harder to find "simple real world" examples as the complexities of realistic problems multiply.

Many of the problems we'll study are abstractions of more intricate real-world problems.

# **Numerical Methods for Applied Math**

- Error 1/Approx 1 1. Take the continuous problem. e.g. integral
- Error 2/Approx 2 2. Compute a discrete representation.
- Error 3/Approx 3 3. Determine where to apply continuous & discrete properties to derive a *tractable* problem. e.g. linear system
- Error 4/Approx 4 4. Solve the tractable problem. e.g. LU factorization

### **Key assumption**

# There is something in the problem we can evaluate exactly.

where exactly means up to floating point error

e.g.

#### f(x) in an integral or derivative the boundary condition of an ODE

# **Outline of Topics**

- Polynomial approximations & piecewise polynomial approximations (Chapter 8)
- 2. Numerical differentiation (Chapter 9)
- 3. Numerical integration (Chapter 10)
- 4. ODEs and PDEs (Chapter 11, 13, 14)
- 5. Optimization (Chapter 4)

#### **Reading outline on website**

<u>www.cs.purdue.edu/homes/dgleich/</u> <u>cs314-2016/syllabus.html</u>

# **Polynomial approximation**

Polynomials are one of the most useful ways of representing 1d functions on a computer.

#### **Alternatives**

*grid of points* images *sins/cosines* signals/MP3s *radial basis functions* machine learning

# Polynomial approximation.

#### **Key points**

Not all sets of point to "evaluate" are equal. 1d case is "solved"

Many different ways to write polynomials that "fit" a set of points exactly, *but they have different numerical properties*.

Piecewise polynomials are flexible models

Polynomial methods do not generalize to higher dimensions easily.

### **Numerical differentiation**

Given a computer representation of a function, how can we determine or approximate it's derivative?

fis	1d	2d	X-d
A regular/uniform grid of points			
A polynomial			
A set of sines/cosines			
A scattered set of data			

### **Numerical differentiation**

#### **Key points**

Numerical accuracy is tricky with regular grids

Polynomial representations make differentiation "easy"

There are some standard approaches to improve the accuracy of numerical derivatives on regular grids. (Richardson extrapolation) ... numerical integration ... ... ODES and PDES ... ... optimization ...

coming soon!

# Why polynomial approximation?

#### Weierstrass approximation theorem

Every continuous function on an interval [a,b] can be *uniformly approximated* by as closely as desired by a polynomial -



uniform error =  $\max_{x \in [a,b]} |f(x) - p(x)|$ 

# How to do polynomial interpolation?

We'll see a bunch of different ways to do this!

The easiest – via Least squares!

Given  $(y_1, x_1), (y_2, x_2), ..., (y_m, x_m)$ Find  $c_0, ..., c_n$ such that  $y_i \approx c_0 + c_1 x_i + c_2 x_i^2 + ... + c_n x_i^n$ .

> Galileo wanted to find a mathematical relationship between ball height and horizontal distance in the following experiment.



# QUIZ

**Q1.** If we could choose where to "see" the function *f*, would it make a difference to how well we can interpolate it with polynomials?

**Q2.** How can we fit a degree *n* polynomial to *n*+1 points?

**Q3.** Which set of points is better to interpolate *f*, Cluster red/uniform or blue/clustered?



# How to do polynomial interpolation?

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# How to do polynomial interpolation?

```
"""c = polyfit(x,y,n): fit the coefficients of a poly
interp. fits a degree n polynomial to the data x,y"""
function polyfit(x,y,n)
  m = length(x) # datapoints
  A = zeros(m, n+1) \# matrix
  for i=1:m
    xi = 1.
    for j=1:n+1
      A[i,j] = xi
      xi *= x[i]
     end
   end
                    # least-squares or linsys
  return A\y
end
```

#### **Polynomial interpolation**

... demo ... Lecture-26 on Juliabox!

# **Error in polynomial interpolation**

#### THEOREM 8.4.1

#### Assume

that *f* is n + 1 times cont. diff. in a region [*a*, *b*], and that  $x_0, \ldots, x_n$  are distinct points in [*a*, *b*].

#### Let

p(x) be the unique polynomial of degree n that interpolates f at  $x_0, \ldots, x_n$ .

#### Then

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{j=0}^n (x - x_j)$$

for some point  $\xi_x$  in [a, b] that depends on x.

#### Analysis Hard to control if the n+1 derivative isn't well behaved. Goes down with n n $[(X - X_i)]$ $f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=1}^{n}$ *i*=0 A polynomial that is zero at each $x_i$ if this is necessarily large, we'll study this!

# **Interpolation at Chebyshev points**

#### **THEOREM 8.5.1**

#### Let

f be a continuous function on [-1, 1]

 $p_n$  its degree *n* interpolant at Chebyshev points

 $p_n^*$  its best approximation among *n* degree polynomials in the uniform error

#### Then

uniform error in  $p_n \le (2 + \frac{2}{\pi} \log n)$  uniform error in  $p_n^*$  $p_n$  converges exponentially fast to *f* if *f* is smooth

# Analysis

If we interpolate f at Chebyshev points, we get something close to the *best possible result* 

and if *f* is smooth, the polynomial approximation always converges "fast"

#### ApproxFun demo