NUMERICAL ANALYSIS

- Numerical analysis involves the study of methods of computing numerical data.
- The study actually involves the design, analysis, and implementation of approximation methods for various problems.
- Method classification
  - *Numerical linear algebra topics*: solutions of linear systems $AX = B$, eigenvalues and eigenvectors, matrix factorizations.
  - *Calculus topics*: numerical differentiation and integration, interpolation, solutions of nonlinear equations $f(x) = 0$.
  - *Statistical topics*: polynomial approximation, curve fitting.

NUMERICAL ANALYSIS

- Effective numerical analysis requires several things:
  - An understanding of the computational tool being used, be it a calculator or a computer.
  - An understanding of the problem to be solved.
  - Construction of an algorithm which will solve the given mathematical problem to a given desired accuracy and within the limits of the resources (time, memory, etc) that are available.

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two-sided approach to understanding a subject: the *al* and the *experimental*. More recently, a third approach has has become equally important: the *computational*.

NUMERICAL vs. ANALYTIC SOLUTION

- Numerical methods produce numerical, not analytic, solutions.
  - Used when the problem cannot be solved analytically.
  - A numeric solution is an approximation.
- An analytic solution (e.g. a mathematical function) is more useful than a numeric solution.
  - The properties of the function are more transparent.
  - An analytic solution is exact.
- E.g. the derivative of sin(x) is cos(x) (the analytic solution). There are also many numerical methods to give the answer

$$\frac{d}{dx}\sin\left(\frac{\pi}{4}\right) = 0.7071$$

- There are the trade off between **computational effort** vs. **required accuracy**.

DIRECT vs. ITERATIVE NUMERICAL METHODS

- **Direct methods** (e.g. Gaussian elimination for the solution of systems of linear equations) results in a FIXED number of steps
  - E.g. to solve a system of 2 equations with 2 unknowns (x and y), we can write the steps as:
  - step 1.
  - step 2.
  - ...
- **Iterative methods**, give a sequence of approximate results designed to converge ever closer to the true solution under the proper conditions, where we need to establish:
  - 1. Does the method converge? i.e. do the successive approximations approach the true solution?
  - 2. When do we stop? i.e. what condition do we use to terminate the iterative method?

TERMINATION CONDITIONS

- There are three ways to stop an iterative procedure.
- Suppose we want to find a root of $f(x)=x^3-x-3$.
  - Let x^* be the true root and x^k is be result of our numerical method after k steps. Hence, $f(x^*) = 0$ and we would like $f(x^k)$ to be as close to zero as possible.
- At the kth step of the algorithm
  - **the problem is “sufficiently solved”**
    - function value has reduced to a user specified tolerance, f_{tol}
  - **the iteration has “converged”**
    - **absolute change in x is within specified tolerance, tol**
    - if tol = 10^{-n}, then x^k agrees with x^* to n decimal places rather than using the absolute change.
    - **relative change in x is within specified tolerance, tol**
    - if tol = 10^{-n}, then x^k agrees with x^* to n significant digits.
  - **the iterations have gone on “long enough”**
    - iteration counter exceeds a user specified limit.

COMPUTER ARITHMETIC AND ERRORS

- **Truncation error**
  - Occurs when the summation of an infinite series is approximated using a finite (or truncated) series.
  - Consider the Taylor series for e^x. We might approximate e^x by the polynomial P(x).

$$(e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots) \quad \text{and} \quad P(x) = 1 + x + \frac{x^2}{2!}$$

  - Hence, the approximation P(x) is inexact. The error is $\sum_{n=3}^{\infty} \frac{x^n}{n!}$ and is called a truncation error.
- **Round-off error**
  - A direct consequence of the finite representation of floating point numbers using fixed word lengths employed by computers. Any calculation that produces a non-rational result has to be rounded off by the computer.
- **Other errors**
  - Imprecision of the data, model assumptions, human error

MEASURING ERROR

- There are two common ways to express the size of an error in a computed result. If p^* is an approximation to p,
  - the **absolute error** is

$$| p - p^* |$$

  - the **relative error** is

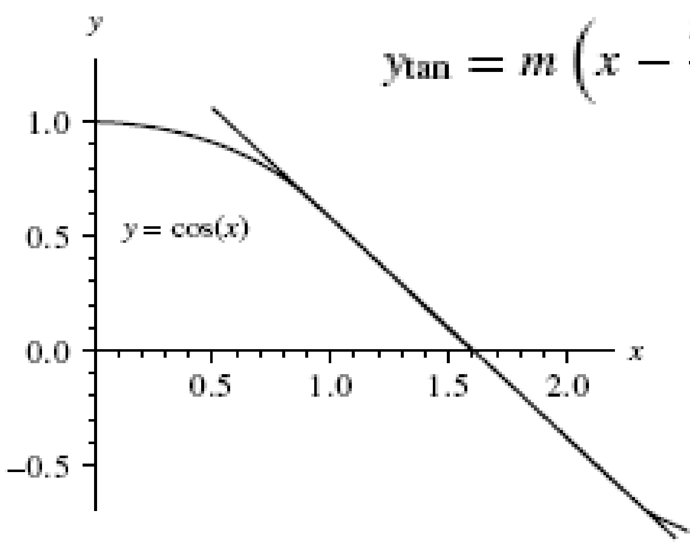
$$\frac{| p - p^* |}{| p |}$$

provided $p \neq 0$ (the relative error is undefined for $p = 0$).

PRELIMINARIES

- Consider the function $f(x)=\cos(x)$, its derivative $f(x)=-\sin(x)$, and its antiderivative $F(x)=\sin(x)+C$.
- The former is used to determine the slope $m=f(x_0)$ of the curve $y=f(x)$ at a point $(x_0,f(x_0))$.
- The slope at the point $(\pi/2,0)$ is $m=f(\pi/2)=-1$ and can be used to find the tangent line at this point.

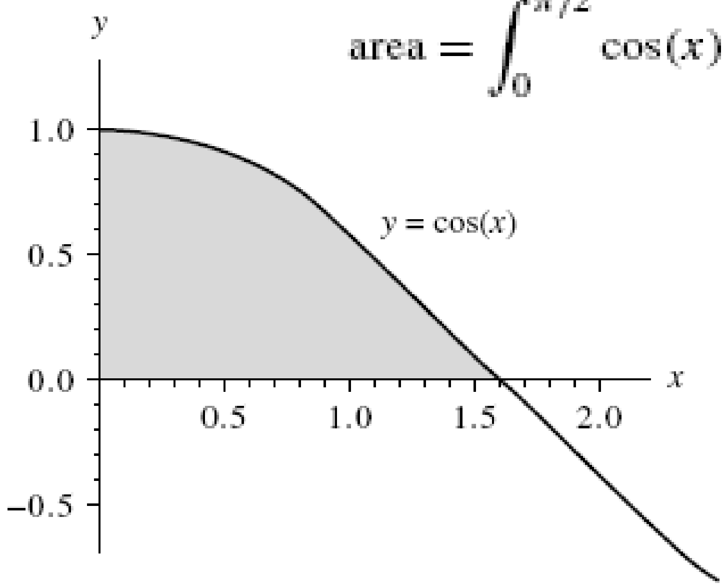
$$y_{\tan} = m\left(x-\frac{\pi}{2}\right)+0 = f'\left(\frac{\pi}{2}\right)\left(x-\frac{\pi}{2}\right) = -x+\frac{\pi}{2}.$$



PRELIMINARIES

- The latter is used to compute the area under the curve for $a \le x \le b$.
- The area under the curve for $0 \le x \le \pi/2$ is computed using an integral

$$\text{area} = \int_0^{\pi/2} \cos(x)\, dx = F\left(\frac{\pi}{2}\right) - F(0) = \sin\left(\frac{\pi}{2}\right) - 0 = 1.$$



LIMITS AND CONTINUITY

- Assume that *f(x)* is defined on an open interval containing $x=x_0$, except possibly a $x=x_0$ itself. Then f is said to have the ***limit*** L at $x=x_0$.

$$\lim_{x \to x_0} f(x) = L,$$

- When the h-increment notation $x=x_0+h$ is used, this equation becomes

$$\lim_{h \to 0} f(x_0 + h) = L.$$

- Assume that *f(x)* is defined on an open interval containing $x=x_0$. Then f is said to be ***continuous*** *at* $x=x_0$ if

$$\lim_{x \to x_0} f(x) = f(x_0).$$

LIMITS AND CONTINUITY

- The function f is said to be continuous on a set S if it is continuous at each point $x \in S$. The notation $C^n(S)$ stands for the set of all functions f such that f and its first n derivatives are continuous on S. When S is an interval, say $[a,b]$, then the notation $C^n[a,b]$ is used.

- As an example, consider the function $f\ x)=x^{4/3}$ on the interval $[-1,1]$. Clearly, $f(x)$ and $f'(x)=(4/3)x^{1/3}$ are continuous on $[-1,1]$, while $f''(x)=(4/9)x^{-2/3}$ is not continuous at $x=0$.

DIFFERENTIABLE FUNCTIONS

- Assume that $f(x)$ is defined on an open interval containing x_0. Then f is said to be *differentiable* at x_0 if

$$\lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

exists. When this limit exists, it is denoted by $f'(x_0)$ and is called the ***derivative*** of f at x_0. An equivalent way to express this limit is to use the h-increment notation:

$$\lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0).$$

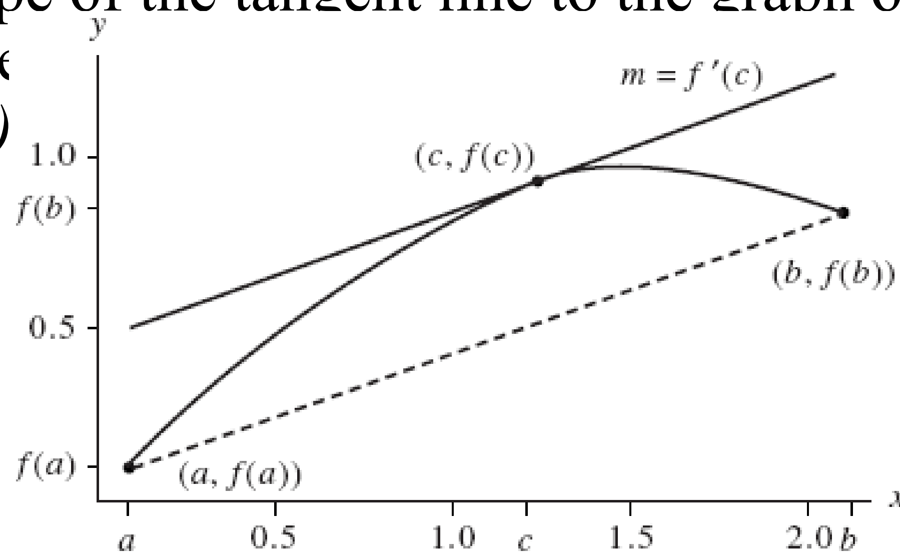
- A function that has a derivative at each point in a set S is said to be ***differentiable*** on S. Note that the number $m=f'(x_0)$ is the slope of the tangent line to the graph of the function $y=f(x)$ at the point $(x_0,f(x_0))$.

DIFFERENTIABLE FUNCTIONS

- **Mean Value Theorem**: Assume that $f \in C[a,b]$ and that $f(x)$ exists for all $x \in (a,b)$. Then there exists a number c, with $c \in (a,b)$, s

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$

- Geometrically, this says that there is at least one number $c \in (a,b)$ such that the slope of the tangent line to the graph of $y=f(x)$ at the point $(c,f(c))$
through the points $(a,f(a))$



$$f'(c) = \frac{f(2.1) - f(0.1)}{2.1 - 0.1} = 0.381688.$$

- is continuous on [0.1,2.1]

is continuous on [0.1,2.1]

- The tangent and secant lines

es
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INTEGRALS

- If f is continuous over $[a,b]$ and F is any antiderivative of f on $[a,b]$, then

$$\int_a^b f(x)\,dx = F(b) - F(a) \qquad \text{where } F'(x) = f(x).$$

- Mean Value Theorem for Integrals: Assume that $f \in C[a,b]$. Then there exists a number c, with $c \in (a,b)$, such that

$$\frac{1}{b-a}\int_a^b f(x)\,dx = f(c).$$

- The value $f(c)$ is the average value of f over the interval $[a,b]$.

INTEGRALS

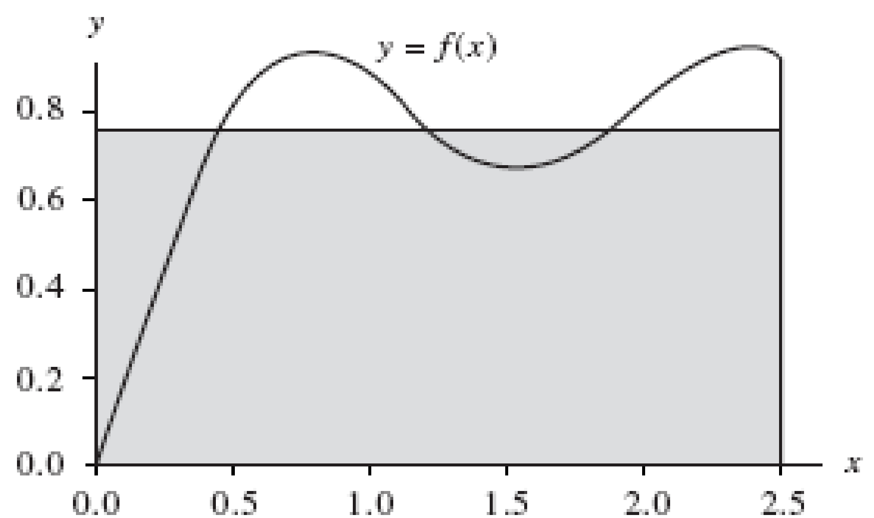
- E.g., the function $f(x)=\sin(x)+(1/3)\sin(3x)$ satisfies the above hypotheses over the interval [0,2.5]. An antiderivative of $f(x)$ is $F(x)=-\cos(x)-(1/9)\cos(3x)$. The average value of the function $f(x)$ over the interval [0,2.5] is

$$\frac{1}{2.5-0}\int_0^{2.5} f(x)\,dx = \frac{F(2.5)-F(0)}{2.5} = 0.749496.$$

- There are three solutions to the equation $f(c)=0.749496$ over the interval [0,2.5]: $c1=0.440566$, $c2=1.268010$, $c3=1.873583$. The area of the rectangle is

$$f(c_j)(b-a) = 0.749496*2.5 = 1.873740.$$

The area of the rectangle has the same numerical value as the integral of $f(x)$ taken over the interval [0,2.5].



MATHEMATICAL MODELS

- A *mathematical* model is a mathematical description of a physical situtation. By means of studying the model, we hope to understand more about the physical situation. Such a model might be very simple. For example,

$$A = 4\pi R_e^2, \qquad R_e \doteq 6,371\ km$$

- is a formula for the surface area of the earth. How accurate is it? First, it assumes the earth is sphere, which is only an approximation. At the equator, the radius is approximately 6,378 km; and at the poles, the radius is approximately 6,357 km. Next, there is experimental error in determining the radius; and in addition, the earth is not perfectly smooth. Therefore, there are limits on the accuracy of this model for the surface area of the earth.

AN INFECTIOUS DISEASE MODEL

- For rubella measles, we have the following model for the spread of the infection in a population (subject to certain assumptions).

$$\frac{ds}{dt} = -a\,s\,i$$
$$\frac{di}{dt} = a\,s\,i - b\,i$$
$$\frac{dr}{dt} = b\,i$$

- In this, s, i, and r refer, respectively, to the proportions of a total population that are susceptible, infectious, and removed (from the susceptible and infectious pool of people). All variables are functions of time t.

AN INFECTIOUS DISEASE MODEL

- The constants can be taken as

$$a = \frac{6.8}{11}, \qquad b = \frac{1}{11}$$

- The same model works for some other diseases (e.g. flu), with a suitable change of the constants a and b. Again, this is an approximation of reality (and a useful one).

- But it has its limits. Solving a bad model will not give good results, no matter how accurately it is solved; and the person solving this model and using the results must know enough about the formation of the model to be able to correctly interpret the numerical results.

THE LOGISTIC EQUATION

- This is the simplest model for population growth. Let *N(t)* denote the number of individuals in a population (rabbits, people, bacteria, etc). Then we model its growth by

$$N'(t) = cN(t), \qquad t \geq 0, \qquad N(t_0) = N_0$$

- The constant *c* is the growth constant, and it usually must be determined empirically. Over short periods of time, this is often an accurate model for population growth. For example, it accurately models the growth of US population over the period of 1790 to 1860, with $c = 0.2975$.

THE PREDATOR-PREY MODEL

- Let *F (t)* denote the number of foxes at time *t*; and let *R(t)* denote the number of rabbits at time *t*. A simple model for these populations is called the *Lotka-Volterra predator-prey* model:

$$\begin{aligned} \frac{dR}{dt} &= a\left[1 - bF(t)\right]R(t) \\ \frac{dF}{dt} &= c\left[-1 + dR(t)\right]F(t) \end{aligned}$$

- with *a, b, c, d* positive constants. If one looks carefully at this, then one can see how it is built from the logistic equation. In some cases, this is a very useful model and agrees with physical experiments. Of course, we can substitute other interpretations, replacing foxes and rabbits with other predator and prey. The model will fail, however, when there are other populations that affect the first two populations in a significant way.

NEWTON'S SECOND LAW

- Newton's second law states that the force acting on an object is directly proportional to the product of its mass and acceleration. With a suitable choice of physical units, we usually write this in its scalar form as

$$F = ma$$

- Newton's law of gravitation for a two-body situation, say the earth and an object moving about the earth is then

$$m\frac{d^2\mathbf{r}(t)}{dt^2} = -\frac{G m\, m_e}{|\mathbf{r}(t)|^2} \cdot \frac{\mathbf{r}(t)}{|\mathbf{r}(t)|}$$

NEWTON'S SECOND LAW

- with *r(t)* the vector from the center of the earth to the center of the object moving about the earth. The constant *G* is the gravitational constant, not dependent on the earth; and *m* and m_e are the masses, respectively of the object and the earth.

- This is an accurate model for many purposes. But what are some physical situations under which it will fail?

NEWTON'S SECOND LAW

- When the object is very close to the surface of the earth and does not move far from one spot, we take $|r(t)|$ to be the radius of the earth. We obtain the new model

$$m\frac{d^2\mathbf{r}(t)}{dt^2} = -mg\mathbf{k}$$

- with **k** the unit vector directly upward from the earth's surface at the location of the object. The gravitational constant

$$g \doteq 9.8 \text{ meters/second}^2$$

- Again this is a model; it is not physical reality.

CALCULATION OF FUNCTIONS

- Using hand calculations, a hand calculator, or a computer, what are the basic operations of which we are capable? In essence, they are addition, subtraction, multiplication, and division (and even this will usually require a truncation of the quotient at some point). In addition, we can make logical decisions for two real numbers a and b as follows:

$$a > b, \quad a = b, \quad a < b$$

- Furthermore, we can carry out only a finite number of such operations. If we limit ourselves to just addition, subtraction, and multiplication, then in evaluating functions *f (x)* we are limited to the evaluation of polynomials (*n* is the degree and $\{a_0, ..., a_n\}$ are the coefficients of the polynomial):

$$p(x) = a_0 + a_1x + \cdots a_nx^n$$

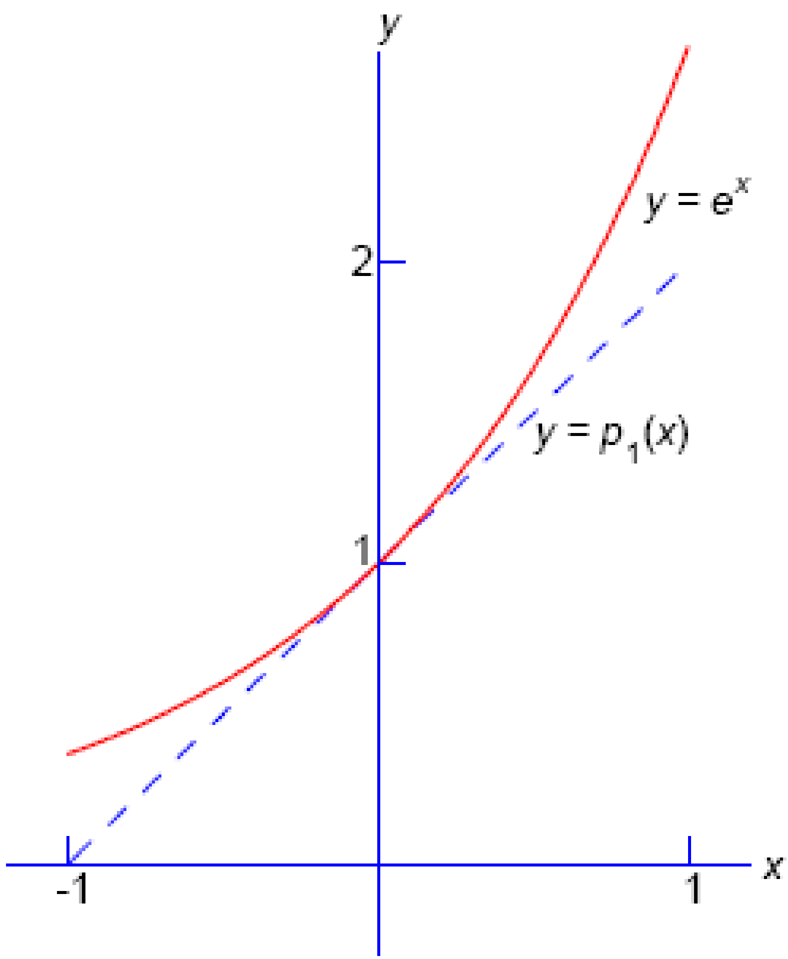
TAYLOR POLYNOMIAL APPROXIMATIONS

- We begin with an example, that of $f(x) = e^x$ from the text. Consider evaluating it for x near to 0. We look for a polynomial $p(x)$ whose values will be the same as those of e^x to within acceptable accuracy.

- Begin with a linear polynomial $p(x) = a_0 + a_1 x$. Then to make its graph look like that of e^x, we ask that the graph of $y = p(x)$ be tangent to that of $y = e^x$ at $x = 0$. Doing so leads to the formula

$$p(x) = 1 + x$$

TAYLOR POLYNOMIAL APPROXIMATIONS



TAYLOR POLYNOMIAL APPROXIMATIONS

- Continue in this manner looking next for a quadratic polynomial

$$p(x) = a_0 + a_1 x + a_2 x^2$$

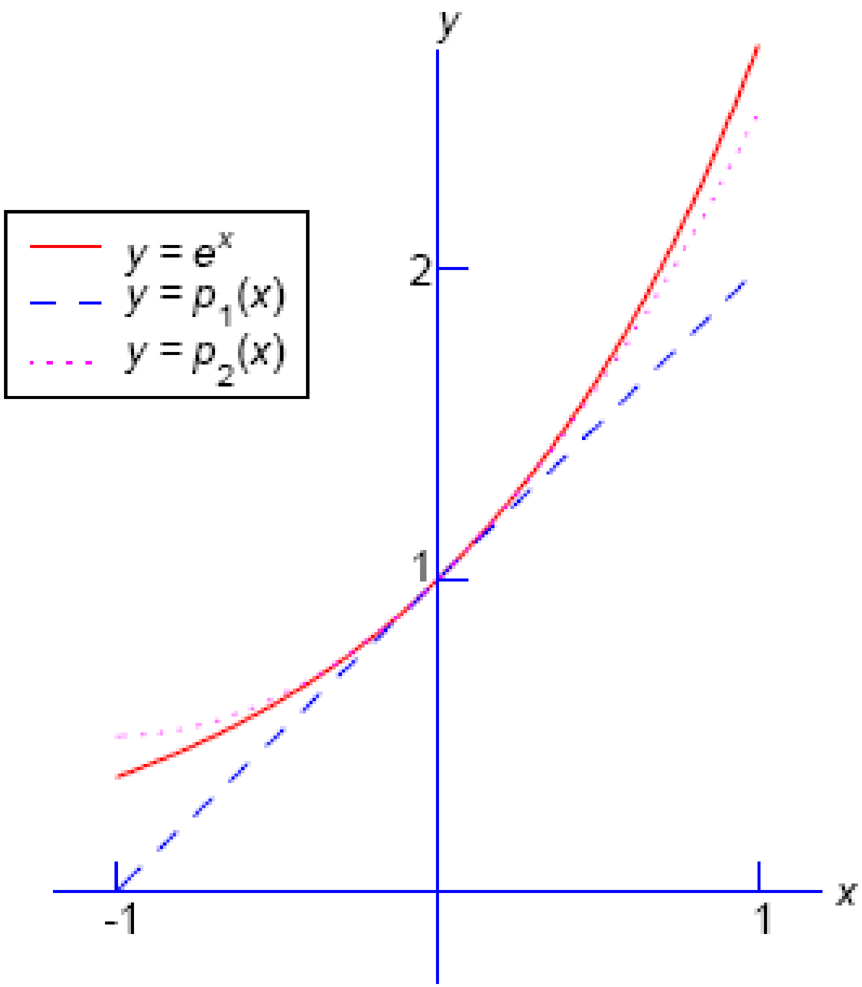
- We again make it tangent; and to determine a_2, we also ask that $p(x)$ and e^x have the same "curvature" at the origin. Combining these requirements, we have for $f(x) = e^x$ that

$$p(0) = f(0), \quad p'(0) = f'(0), \quad p''(0) = f''(0)$$

- This yields the approximation

$$p(x) = 1 + x + \tfrac{1}{2}x^2$$

TAYLOR POLYNOMIAL APPROXIMATIONS



TAYLOR POLYNOMIAL APPROXIMATIONS

- We continue this pattern, looking for a polynomial

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

- We now require that

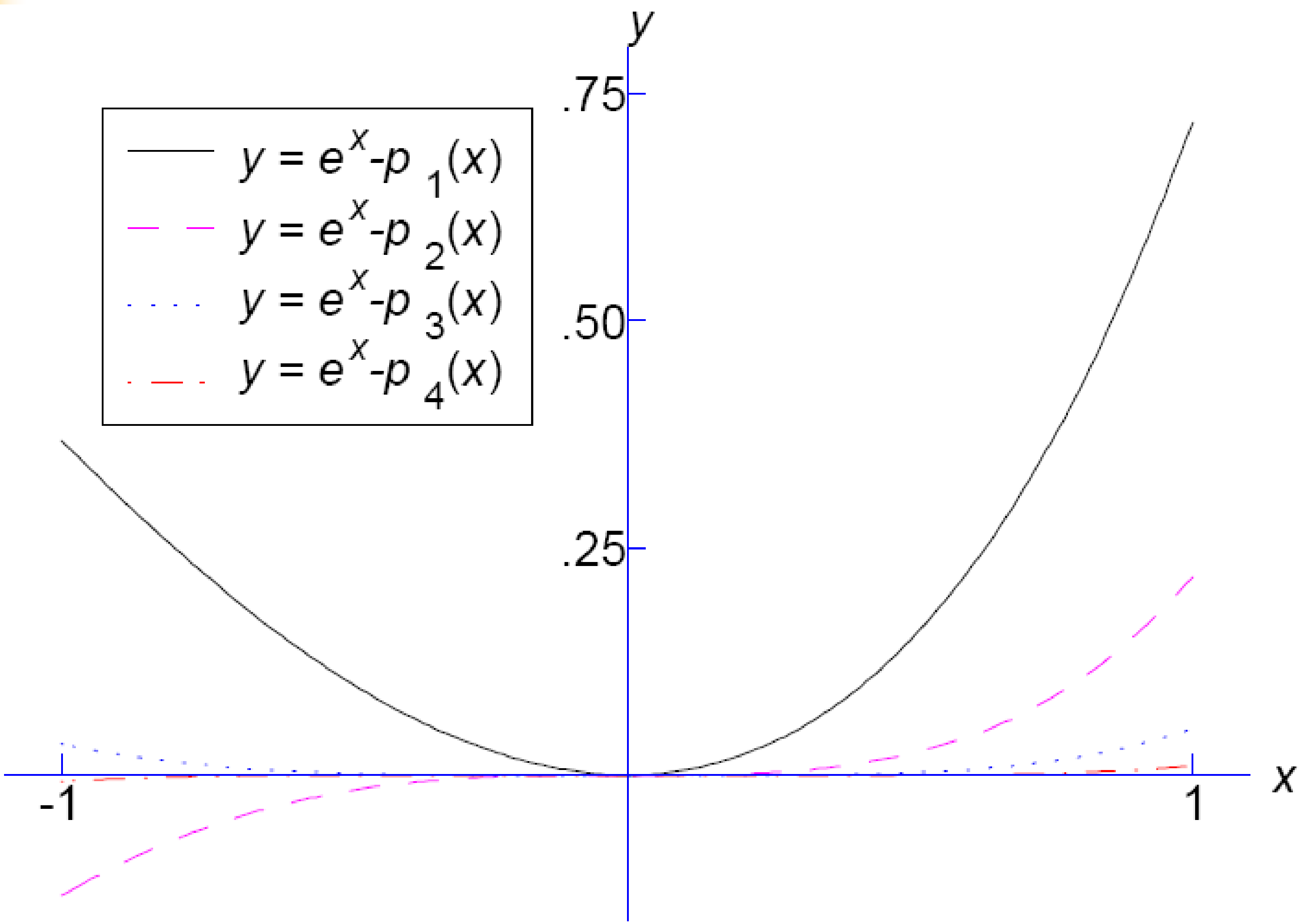
$$p(0) = f(0), \quad p'(0) = f'(0), \quad \cdots, p^{(n)}(0) = f^{(n)}(0)$$

- This leads to the formula

$$p(x) = 1 + x + \tfrac{1}{2}x^2 + \cdots + \tfrac{1}{n!}x^n$$

- What are the problems when evaluating points *x* that are far from 0?

TAYLOR POLYNOMIAL APPROXIMATIONS



TAYLOR'S APPROXIMATION FORMULA

- Let $f(x)$ be a given function, and assume it has derivatives around some point $x = a$ (with as many derivatives as we find necessary). We seek a polynomial $p(x)$ of degree at most n, for some non-negative integer n, which will approximate $f(x)$ by satisfying the following conditions:

$$
\begin{aligned}
p(a) &= f(a) \\
p'(a) &= f'(a) \\
p''(a) &= f''(a) \\
&\vdots \\
p^{(n)}(a) &= f^{(n)}(a)
\end{aligned}
$$

TAYLOR'S APPROXIMATION FORMULA

- The general formula for this polynomial is

$$p_n(x) = f(a) + (x-a)f'(a) + \frac{1}{2!}(x-a)^2 f''(a) + \cdots + \frac{1}{n!}(x-a)^n f^{(n)}(a)$$

- Then $f(x) \approx p_n(x)$ for x close to a.

TAYLOR POLYNOMIALS FOR $f(x) = \log x$

- In this case, we expand about the point $x = 1$,making the polynomial tangent to the graph of $f(x) = \log x$ at the point x = 1. For a general degree $n \geq 1$, this results in the polynomial

$$p_n(x) = (x-1) - \frac{1}{2}(x-1)^2 + \frac{1}{3}(x-1)^3 + \cdots + (-1)^{n-1}\frac{1}{n}(x-1)^n$$

- Note the graphs of these polynomials for varying n.

TAYLOR POLYNOMIALS FOR $f(x) = \log x$