1102 Calculus II 11.12 Application of Taylor Series

Taylor series can be used to show that theories reduce to other theories under certain values of parameters. There is a beautiful example in the text relating special relativity to classical mechanics under the assumption that the speed of light is very large. Used in this way, the Taylor series are not calculational at all, but more a theoretical tool.

Taylor series can be used to simplify calculations when the function being studied is complicated. Typically, only the first few terms of the Taylor series are kept, and the general pattern is not sought. The main problem with this is that the radius of convergent cannot be determined (to determine the radius of convergence, we need the general Taylor series expansion $\sum a_n(x)$). Estimation of the error in an interval can be done visually by using a graph. In this type of use, the Taylor series is most definitely a calculational tool.

If we are using Taylor series as a calculational tool involving $T_n(x)$, we need ways to estimate error:

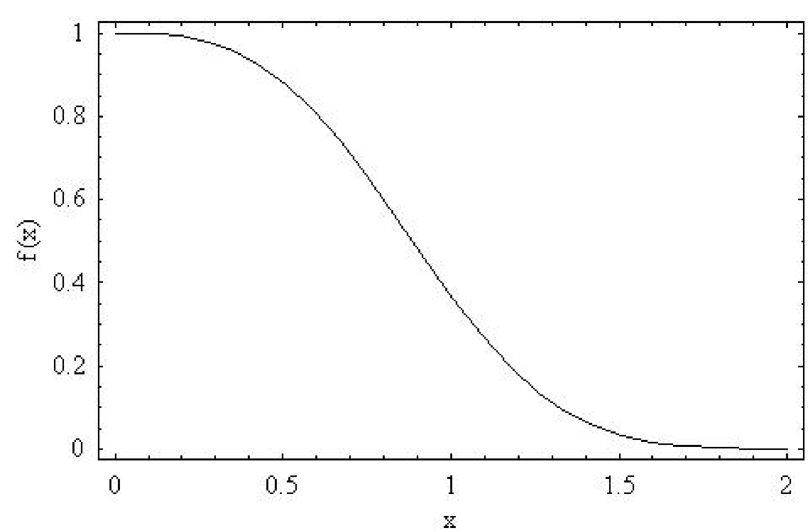
- use a graph to estimate error over an interval,
- if series is alternating, use alternating series estimation theorem,
- use Taylor's Inequality,
- use larger n until the result doesn't change.

Example: Statistics Given $f(x) = Ne^{-x^3}$, $0 < x < 2$, which is going to be used as an approximation to a probability density function in statistics. If this is going to be a probability density function, then we must have that $\int_0^2 f(x)\,dx = 1$, the normalization condition that will determine the value of the constant N.

This integral is not one that can be done using standard techniques, so we need a numerical approximation to it. Let's use Taylor series to do this.

First, we need to decide what a to expand about. Let's sketch the function when $N = 1$ (if this was coming from statistics, we would have a sketch of the probability density function to begin with):

```
f[x_] =  Exp[-x^3]
Plot[f[x], {x, 0, 3}, Frame -> True, FrameLabel -> {"x", "f(x)"}]
```



From the sketch, it looks like $a = 1$ would be a good choice to expand about, since the function is symmetric.

The Taylor polynomial approximation $T_n(x)$ is given by

$$f(x) \sim T_n(x) \quad = \quad \sum_{i=0}^{n} \frac{f^{(i)}(1)}{i!}(x-1)^i$$

Since we are <u>not</u> looking for a pattern, it may be easier to work out the derivatives by hand outside of a table. For complicated derivatives, not using a table is probably going to be easier.

There is a super awesome *Mathematica* command for derivatives:

```
f[x_] = Exp[-x^3]
Derivative[3][f][x]
```

Let's use that and the form for $T_n(x)$ from above:

```
a = 1
f[x_] = Exp[-x^3]
T[n_, x_] = Sum[Derivative[i][f][a]/i! (x - a)^i, {i, 0, n}]

Series[f[x],{x,a,10}]
T[10,x]
```

This is pretty cool–it uses *Mathematica* to do the derivatives and create the Taylor series! It replaces the intrinsic `Series` command.

Let's use *Mathematica* to do the integral, and we should take n large enough so the result stops changing.

```
Table[{n, N[Integrate[T[n, x], {x, 0, 2}]]}, {n, 10, 100, 10}] // TableForm
```

So it looks like $\int_0^2 e^{-x^3}\,dx = 0.892954$, so we should choose $N = 1/0.892954 = 1.11988$ for Ne^{-x^3} over $0 < x < 2$ to be a valid probability density function.

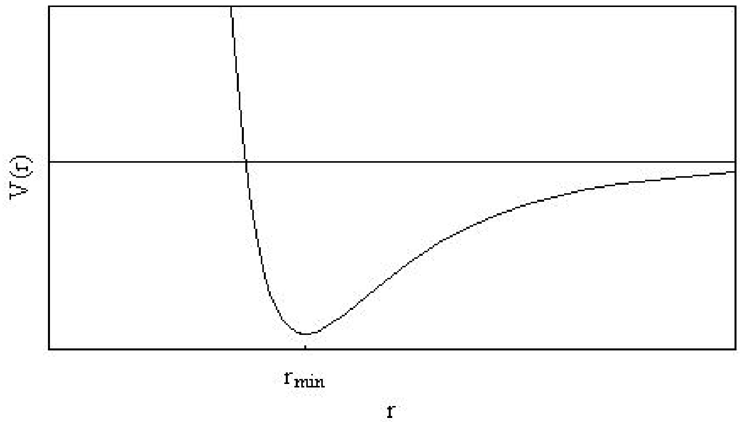
If you plot $T_{30}(x)$ against $f(x)$, you will see very little difference between them for $0 < x < 2$.

```
Plot[{f[x], T[30, x]}, {x, 0, 2}, PlotRange -> {{0, 2}, {0, 1}}, PlotStyle -> {Red, Blue}]
```

Knowing this, you could then use $T_{30}(x)$ for the probability distribution, since it would be much easier to calculate means, medians, skewness–all the usual statistical properties of a probability distribution.

Example: Lennard-Jones Potential In molecular chemistry (from physical chemistry), you would study potential energy surfaces that tell you how molecules vibrate. One common potential energy surface is the Lennard-Jones 6-12 potential:

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



The distance between two atoms in a molecule is given by the distance r. The molecule vibrates, since the length of this distance changes. The more energy you put into the molecule, the more it can vibrate, and for large enough energies the molecule can be broken apart ($r \to \infty$). For small energies, the molecule vibrates in a very predictable and well understood way–as if it was a harmonic oscillator. In this problem, we will find the associated harmonic oscillator potential for the Lennard-Jones 6-12 potential.

(a) Find the r coordinate that produces the minimum of the potential.
(b) Construct the Taylor polynomial of order 2 about the minimum.
(c) Plot the $V(r)$ and the Taylor polynomial when $\epsilon = 2.3$ and $\sigma = 3.6$.

Solution

(a) We need to solve $V'(r) = 0$ for r:

```
V[r_] = 4 epsilon ((sigma/r)^12 - (sigma/r)^6)
Solve[V'[r] == 0, r]
```

We get $r_{\text{min}} = 2^{1/6}\sigma$.

(b) We need the Taylor polynomial $T_2(r)$ about $r = 2^{1/6}\sigma$. We don't need the infinite series here.

$$V(r) \sim T_2(r) = \sum_{i=0}^{2} \frac{V^{(i)}(r_{\text{rmin}})}{i!}(r - r_{\text{min}})^i = V(r_{\text{min}}) + V'(r_{\text{min}})(r - r_{\text{min}}) + \frac{1}{2}V''(r_{\text{min}})(r - r_{\text{min}})^2.$$

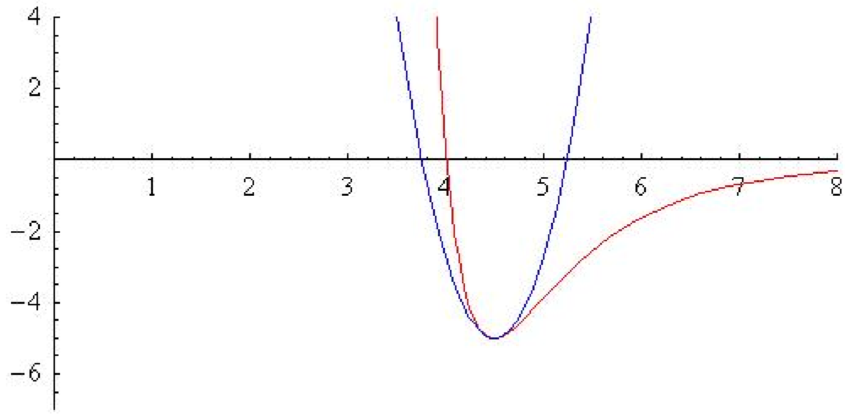
Let *Mathematica* do the work for us:

```
rmin = 2^(1/6) sigma
a = rmin
T[n_, r_] = Sum[Derivative[i][V][a]/i!(r - a)^i, {i, 0, n}]
T[2, r]
```

$$V(r) \sim T_2(r) = -\epsilon + \frac{18 \cdot 2^{2/3}\epsilon}{\sigma^2}(r - 2^{1/6}\sigma)^2$$

(c) The plots can be found from

```
epsilon = 5;
sigma = 4;
Plot[{V[r], T[2, r]}, {r, 0, 15}, PlotRange -> {{0, 8}, {-7, 4}},
  PlotStyle -> {Red, Blue}]
```



What you have found is the harmonic oscillator approximation to the molecular vibration, in terms of the general parameters for the Lennard-Jones potential ϵ, σ. Notice that ϵ is the depth of the potential, and σ is related to the location of the minimum.

Example: Special Relativity Einstein's special relativity is used for particles that are moving at speeds which are close the speed of light. In special relativity, the energy of the particle is given by

$$E(\beta) = Mc^2 = \frac{mc^2}{\sqrt{1-\beta^2}}$$

where c is the speed of light, M is the relativistic mass, m is the rest mass, and $\beta = v/c$ where v is the velocity of the particle.

This relationship between the relativistic mass and the rest mass is given by

$$M = \frac{m}{\sqrt{1-(v/c)^2}}$$

and is based on the Lorentz transformation $T = \gamma t$ where $\gamma = \dfrac{1}{\sqrt{1-(v/c)^2}}$, which was known to mathematicians before Einstein developed the theory of special relativity. This particular relationship tells us that to an outside observer, the mass of a particle in motion increases with the speed of the particle, and is infinite in the limit $v \to c$.

What if the speed v is small compared to the speed of light? The energy equation of special relativity should reduce to the energy equation of Newtonian (classical) mechanics $E = \frac{1}{2}mv^2$ when $v/c \sim 0$ (this is the familiar kinetic energy you see in high school physics).

We can use Taylor series to show this. Let's expand $E(\beta)$ in a Taylor series in β about $\beta = 0$.

$$E(\beta) \sim T_2(\beta) = \sum_{i=0}^{2} \frac{E^{(i)}(0)}{i!}(\beta - 0)^i = E(0) + E'(0)(\beta - 0) + \frac{1}{2}E''(0)(\beta - 0)^2$$

```
Clear[beta]
```

```
Energy[beta_] = 1/Sqrt[1 - beta^2]*m c^2

a = 0
T[n_, beta_] = Sum[Derivative[i][Energy][a]/i!(beta - a)^i, {i, 0, n}]
T[2, beta]
```

From this, we can write:

$$\begin{aligned} E(\beta) &\sim mc^2 + \frac{1}{2}mc^2\beta^2 \qquad \text{(what \textit{Mathematica} told us)} \\ &\sim mc^2 + \frac{1}{2}mc^2\left(\frac{v}{c}\right)^2 \\ &\sim mc^2 + \frac{1}{2}mv^2 \end{aligned}$$

The quantity mc^2 is called the rest energy, since we are only interested in energy difference between particles moving at different velocities:

$$E_1 - E_2 = mc^2 + \frac{1}{2}mv_1^2 - mc^2 - \frac{1}{2}mv_2^2 = \frac{1}{2}mv_1^2 - \frac{1}{2}mv_2^2$$

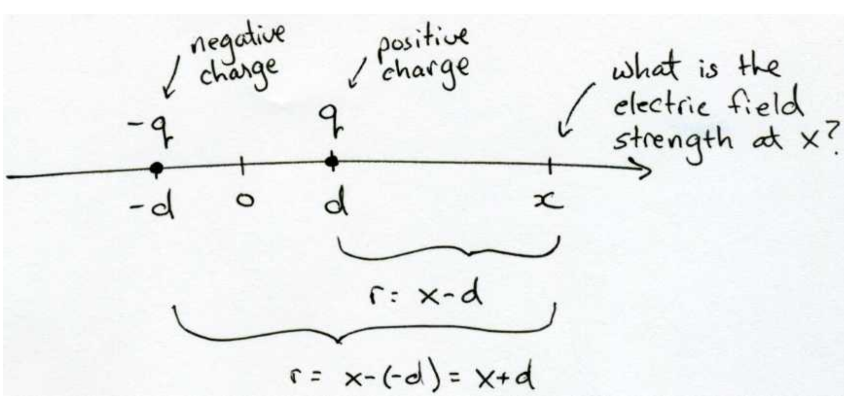
so the classical energy is given by $E = \frac{1}{2}mv^2$ (which gives the same value for $E_1 - E_2$).

This theoretical analysis shows how special relativity reduces to classical mechanics when the particle is moving at speeds which are small compared to the speed of light.

Example: Electromagnetism In electromagnetism, the electric field strength at a distance r from a point charge q is given by $E = \frac{kq}{r^2}$ where

- k is a constant,
- q is the charge,
- r is the distance,
- E is the strength of the electric field.

Consider the following situation, which is called an *electric dipole*:



The electric field strength at the point x is given by the following:

$$E = \frac{kq}{(x-d)^2} - \frac{kq}{(x+d)^2}$$

Let's show the electric field strength is proportional to x^{-3} when $x >> d$. This means the two charges tend to cancel each other out when they are far away, and reduce the field strength.

$$\begin{aligned}
E &= \frac{kq}{(x-d)^2} - \frac{kq}{(x+d)^2} \\
&= \frac{kq}{x^2((1+(-d/x))^2} - \frac{kq}{x^2(1+d/x)^2} \qquad \text{use binomial series} \\
&= \frac{kq}{x^2}\sum_{n=0}^{\infty}\frac{(-2)!}{(-2-n)!n!}(-d/x)^n - \frac{kq}{x^2}\sum_{n=0}^{\infty}\frac{(-2)!}{(-2-n)!n!}(d/x)^n
\end{aligned}$$

If $x >> d$, then let's just keep the first two terms in the infinite series and see what happens (if we just keep the first term, we get $E \sim 0$, which doesn't help us).

$$\begin{aligned}
E &\sim \frac{kq}{x^2}\sum_{n=0}^{\infty}\frac{(-2)!}{(-2-n)!n!}(-d/x)^n - \frac{kq}{x^2}\sum_{n=0}^{\infty}\frac{(-2)!}{(-2-n)!n!}(d/x)^n \\
&\sim \frac{kq}{x^2}\sum_{n=0}^{\infty}\frac{(-2)!}{(-2-n)!n!}(-d/x)^n - \frac{kq}{x^2}\sum_{n=0}^{\infty}\frac{(-2)!}{(-2-n)!n!}(d/x)^n
\end{aligned}$$

This looks good, but we will run into a problem here. Remember, the factorial function had vertical asymptotes, so $(-2)!$ was not defined. There is a also a quantity like $(-1)!$ in the denominator, so they cancel somehow to give us an answer. What we know, however, is that the factorial representation will not work here. Let's switch to the binomial coefficient representation:

$$E \sim \frac{kq}{x^2}\sum_{n=0}^{\infty}\binom{-2}{n}(-d/x)^n - \frac{kq}{x^2}\sum_{n=0}^{\infty}\binom{-2}{n}(d/x)^n$$

```
T[n_, x_] := k*q/x^2(Sum[Binomial[-2, i]*(-d/x)^i, {i, 0, n}]
        - Sum[Binomial[-2, i]*(d/x)^i, {i, 0, n}])

Table[{n, T[n, x]}, {n, 0, 6}] // TableForm
```

We see that $T_1(x)$ is the first nonzero approximation, and it gives us

$$E \sim T_1(x) = \frac{4dqk}{x^3} \text{ when } x >> d.$$

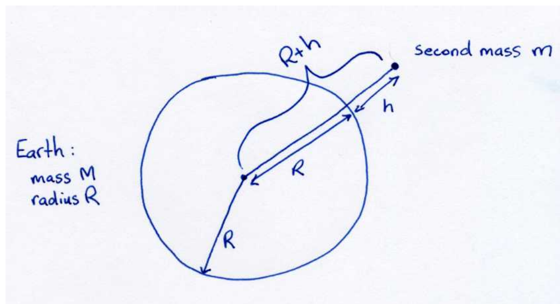
So this shows the electric field strength is reduced from an x^{-2} dependency for a single charge to an x^{-3} dependency for the dipole when $x >> d$. The two charges cancel each other out somewhat (not surprisingly). But this analysis shows *how the canceling out occurs*, so we know the field strength goes as x^{-3} and not as x^{-4}, for example.

Example: Gravitational Potential Energy The gravitational attraction (ie, potential energy) between two masses is given by the formula:

$$PE = -\frac{Gm_1m_2}{r}$$

where m_1 and m_2 are the masses of the objects, G is the gravitational constant, and r is the distance between the two objects.

Consider the following picture:



When the two objects are the earth and something near the surface of the earth, this equation should simplify to the familiar $PE = mgh$, the gravitational potential energy near the earth's surface where h is the height above the surface and $g = GM/R^2 \sim 9.8$ m/s^2. Let's show this using power series, where we will assume $R >> h$.

$$\begin{aligned}
PE(h) &= -\frac{Gm_1m_2}{r} \\
&= -\frac{GMm}{R+h} \\
&= -\frac{GMm}{R(1+h/R)} \\
&= -\frac{GMmR}{R^2} \times \frac{1}{1+h/R} \\
&= -gmR \times \frac{1}{1-(-h/R)} \quad \text{geometric series} \\
&= -mgR\sum_{n=0}^{\infty} |-h/R|\,, \quad |-h/R| < 1 \longrightarrow |h| < R \quad \text{converges since we assumed } R >> h \\
&= -mgR\left(1 - \frac{h}{R} + \frac{h^2}{R^2} - \cdots\right) \sim -mgR\left(1 - \frac{h}{R}\right) = -mgR + mgh
\end{aligned}$$

Potential energy is always defined as a difference in potential energy between two heights (similar to our approximate kinetic energy in special relativity being a difference between two speeds), so we can say $PE(h) = mgh$. The $-mgR$ is a constant that would disappear whenever we looked at potential energy differences.

But even better than that, since we had an alternating series, we have an error bound on this approximation!

$$PE(h) = mgh, \quad |\text{error}| < \frac{mgh^2}{R}$$