Applications of Calculus I

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Preface

From the beginning Nature has led the way and established the pattern which mathematics, the language of nature, must follow.

George D. Birkhoff

Calculus is really exciting . . . Calculus must become a pump instead of a filter in the pipeline.

Robert White, Past President of the National Academy of Engineering

Welcome to the fascinating world of Calculus and its applications. Throughout this course you will learn that although Calculus was invented to study problems in astronomy, it has grown into a very sophisticated and powerful tool with almost universal use. Calculus enables us to analyze and solve many of our current daily problems and thus to not only understand, but ultimately control the world around us. It not only revolutionized science and technology but it changed the way we view our relation to the universe, it gave way to the “Age of Enlightenment”, overseas commerce, the industrial revolution, and the rise of new social orders that made possible our present way of life.

This book is exciting because it opens the door to the cutting edge science that is being developed here at the University of Central Florida. You will get a glimpse of how Calculus is used in the forefront of science and technology. Throughout this book the faculty will show you how mathematics, and Calculus in particular, has fundamentally influenced their research and facilitated their discoveries. You will also have the opportunity to get to know and talk to the authors on what’s needed to get the most out of your college experience and help you succeed in your future career.

The applications covered in this course were chosen to reinforce Calculus concepts that the students typically have difficulty with. Each chapter follows the same format, starting with examples taken directly from your Calculus text and based on material already covered in class. These problems will set the reference point for the chapter application. In the background section, the authors set up the governing equations from physical principles. The solution technique using Calculus is carefully developed. The mathematical results are then given physical interpretation. Chapters list future courses where you might see these concepts again and alerts you to the significance of the material being covered and the connections to your major of choice.

A brief description of each chapter’s content has been provided by the authors:
Chapter 1 by Dr. Kassab, a Professor of Mechanical Engineering, with interests in inverse problems, computational heat transfer and fluid flow, explains limits and rates of change. The underlying power of Calculus is the concept of the limit in defining the instantaneous rate of change of a function, its derivative, and the area under the graph of the curve of that function, its integral. Both operations were recognized by Newton to be the inverse of each other. What we mean by taking a limit of a function is to evaluate the behavior of that function as the variable on which it depends tends towards a particular value. Often the value of the variable is a finite constant, however, in many cases we are interested in what happens when the constant is zero or when the value of the constant tends to positive or negative infinity.

From a physical point of view, if for example, the function of interest describes the displacement of a moving body as a function of time, then the time rate of change of the body’s displacement, which is provided by the derivative, is the body’s velocity. Moreover, if we were to determine the rate of change of the body’s velocity we would then obtain its acceleration. In heat transfer, if the function of interest describes the variation of temperature with the position between a hot wall and a cold wall, then, the instantaneous spatial rate of change of that function would be related to the flow of energy from the high temperature wall to the low temperature wall. Calculus is thus part of the mathematical toolbox we utilize routinely in science and engineering to build models that help us describe, analyze, and understand physical processes.

In this chapter, we approach the concept of the limit from a practical point of view of its application in heat transfer. Specifically, we first arrive at the constant $e$ as a limit of a sequence, and we then define the exponential function and examine its behavior in the limits of very large and very small arguments. Armed with these results, we consider the general solution for the temperature distribution in a cooling fin and utilize the limit to arrive at a physically realistic solution. Finally, we use the limit to determine the instantaneous spatial rate of change of the temperature and relate that result to the amount of heat removed by the fin. We also examine what happens when we undertake the limiting process computationally, and we come to the conclusion that we can approximate a limit on the computer but can never evaluate it exactly. Topics in this chapter will be considered in differential equations (MAP 2302), electrical engineering (EGN 3373 and EEL 3304), dynamics(EGN 3321) and EML 4142 (Heat Transfer).

In Chapter 2 Dr. Clausen, a Professor of Chemistry, with 38 years of experience teaching at UCF, talks about kinetics and catalysis of industrial and environmental remediation processes. Chemical kinetics is the branch of physical chemistry that deals with the rates of chemical reactions and with the factors on which the rates depend. Catalysis is the area of study concerned with the discovery of materials and methods to make reactions go towards completion faster. Both kinetics and catalysis rely heavily on mathematical principles that are covered in Calculus. In particular, the topic that is covered in this chapter concerns the beginning of your study of differential calculus which deals with how one quantity changes in relation to another quantity. The central concept of differential calculus is the derivative which is related to such topics as velocity and slopes of tangents to curves that you will study in Chapter 2 of your calculus text. After learning how to calculate derivatives, you will use
them to solve problems involving rates of change, which is the area of chemical kinetics.

In Chapter 3 Dr. da Vitória Lobo, an Associate Professor of Computers Science, with interests in computer vision, the area that gives machines the power to see and sense their environments, explains that computer vision can be used in autonomous vehicles, medical image analysis, industrial manufacturing and inspection, security and crime prevention systems, homeland security, satellite monitoring of the environment, optical character recognition, motion capture for computer games, and many other exciting spheres of life. You will first see how to estimate derivatives for practical situations. Then, you will be shown how computing derivatives for images produces edges of regions in an image. This process will be examined in detail, including the use of the gradient, and second derivatives.

Dr. Brueckner, a Lecturer in Physics, presents the task in Chapter 4 that researchers encounter in real life situations, where calculating a derivative numerically can be challenging. The application areas are derivative constraints and minimization on the wave function for a quantum star. He also introduces a short bonus topic, the general idea of vector-as-derivative, and discusses the tangents to a sphere in the context of curved spacetime.

In Chapter 5 Dr. Chopra, an Associate Professor of Civil and Environmental Engineering, Chair of the UCF Faculty Senate, and a Member of the UCF Board of Trustees, talks about real-world engineering problems in the various areas of engineering practice where the topics that you are learning in Calculus on the use of derivatives are applied. The concepts dealing with finding the global and local extreme values and its application to optimization are very commonly used in engineering. It could be the optimization of the shape of a structure, a transportation system, shape of a component or machinery or a process that moves humans and goods. The diverse applications discussed in this chapter provide an insight into the world of engineering design and practice. In this chapter, we will apply the methods you have learned in the calculus course to determine the global and local maxima/minima of a function. This technique is then applied to solving optimization problems. This chapter will give you a preview of some of the advanced concepts you are likely to see in later courses. Mechanical and civil engineers use it for the optimal design of components and structural systems. They also use the concept of minimization of energy and analysis of the stability of systems. Industrial engineers are involved extensively in optimization of systems that may deal with management of manufactured goods or movement of humans such as theme-park management. Electrical and computer engineers require these principles to analyze the energy and power requirements and an optimal system for miniaturization of components.

In Chapter 6 Dr. Self, an Assistant Professor of Molecular Biology and Microbiology, talks about how the ability to quantify a given amount of any biological molecule is critical in the analysis of biology and the fundamental study of living systems. Calculus is needed to determine the exact concentration of a substance after separation by chromatography in order to gain information on the amount of that substance in a given sample. In this chapter we will apply several methods to determine 'area under the curve' and show how this is needed for biomedical applications. We will survey the types of chromatography used in research and testing labs, emphasizing the relevant uses in real world problems. This chapter will then integrate the mathematics of calculus to current biomedical applications, and give you a sneak peak on concepts you are likely to see in later courses. Finally we will
introduce the use of computer modeling to chromatography that is enabling early detection of cancer in proteomic research. The concepts covered are broad but should strengthen your appreciation for the utility of mathematics in science and engineering.
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This book would not have been possible without the hard work and dedication of the EXCEL faculty: Drs. Georgiopoulos and Young (Directors), who have been involved with all aspects of this project from planning, writing, coordinating, scheduling, handling of the project’s finances and have provided the leadership and commitment necessary for the success of any project; Drs. Geiger, Hagen, Islas, and Winningham (Coordinators), all of which spent uncountable hours planning and directing this project; Drs. Kassab, Clausen, da Vitoria Lobo, Brueckner, Chopra, and Self (Chapter Authors), who contributed their knowledge and expertise which gives life to this project;

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Chapter 1

Limits and Rates of Change: heat transfer

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Weeks
Limits and Rates of Change

Introduction

The various notions that lead to the modern developments of Calculus were known to the ancient Greeks, for instance, to Archimedes (287 BC - 212 BC) who utilized the concept of infinitesimals to compute areas and volumes and to Indian mathematicians who also employed infinitesimals to study the motions of the moon. While several French, German, English and Dutch mathematicians contributed seminal concepts of what was to become modern Calculus, it was Isaac Newton (1643 - 1727 AD) and Gottfried Leibniz (1646 - 1716 AD), who are credited to have independently arrived at the Fundamental Theorem of Calculus, and defined and codified Calculus, its rules and its notations.

Calculus is principally concerned with differentiation, which, for the case of a function of a single real variable, can be thought of as the evaluation of the instantaneous rate of change (slope) of the curve described by that function, and integration, that can be thought of as the evaluation of the area under that curve. What Newton and Leibniz determined is that the two processes are related, and that integration is the inverse of differentiation. Furthermore, they established certain notations as well rigorous rules and procedures to carry out both operations which taken all together constitute Calculus.

The great contribution of Isaac Newton is his extensive application of Calculus to physics as reflected in his monumental publication in 1687 of Philosophiae Naturalis Principia Mathematica, which is considered by all scientists, mathematicians, and engineers to be one of the greatest and defining accomplishments in human history. Relying heavily on Calculus, Newton laid out, amongst other things, the basic principles describing gravitational attraction and the three laws of motion that are the groundwork of classical mechanics and the basis of modern engineering. Ever since, we have become very adept at utilizing differentials and integrals to build mathematical models describing the physical processes around us, and these models allow us to predict a wide variety of physical behaviors. The applications of Calculus pervade our lives, and they range for example, from understanding how a toy top spins and gyroscopes work, to how to make spaceships reach the moon and return, how to predict the future behavior of the weather, how to model and control how fluids and heat flow, and how to model and harness electricity and magnetism.

From a physical point of view, if for example, the function of interest describes the displacement of a moving body as a function of time, then the time rate of change of the body’s displacement which is provided by the derivative is the body’s velocity. Moreover, if we were to determine the rate of change of the body’s velocity we would then obtain the its acceleration. In heat transfer, if the function of interest describes the variation of temperature with the position between a hot wall and a cold wall, then, the instantaneous spatial rate of change of that function would be related to the flow of energy from the high temperature wall to the low temperature wall. Calculus is thus part of the mathematical toolbox we utilize routinely in science and engineering to build models that help us describe, analyze and understand physical processes.
The notion of the limit is central to understanding the two basic operations in calculus: the derivative and the integral. What we mean by taking a limit of a function is to evaluate the behavior of that function as the variable on which it depends tends towards a particular value. Often the value of the variable is a finite constant, however, in many cases we are interested in what happens when the constant is zero or value of the constant tends to positive or negative infinity. We will consider the notion of the limit in the context of its applications to mathematical definitions and to physical problems.

**Limits and Rates of Change**

**Example Problem 1.**

Section 2.2, Exercise 1

Evaluate the value of the function

\[ f(x) = \frac{x - 1}{x^2 - 1} \]  

as \( x \) approaches 1, that is evaluate

\[ \lim_{x \to 1} \frac{x - 1}{x^2 - 1} \]  

At \( x = 1 \), the denominator goes to zero, and the function is not defined. However, if we tabulate the function close to 1 but not 1 we see from the tables below

<table>
<thead>
<tr>
<th>( x_i )</th>
<th>( f(x_i) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.666667</td>
</tr>
<tr>
<td>0.9</td>
<td>0.526316</td>
</tr>
<tr>
<td>0.99</td>
<td>0.502513</td>
</tr>
<tr>
<td>0.999</td>
<td>0.500025</td>
</tr>
<tr>
<td>0.9999</td>
<td>0.5000025</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( x_i )</th>
<th>( f(x_i) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>0.4</td>
</tr>
<tr>
<td>1.1</td>
<td>0.47619</td>
</tr>
<tr>
<td>1.01</td>
<td>0.497512</td>
</tr>
<tr>
<td>1.001</td>
<td>0.49975</td>
</tr>
<tr>
<td>1.0001</td>
<td>0.499975</td>
</tr>
</tbody>
</table>

that the function seems to approach the value of 0.5 as \( x \) approaches the value of 1 from the left and from the right. Examining the function more closely, we note that we can write

\[
\lim_{x \to 1} \frac{x - 1}{x^2 - 1} = \lim_{x \to 1} \frac{x - 1}{(x - 1)(x + 1)} = \lim_{x \to 1} \frac{1}{x + 1} = 0.5
\]  

(1.3)
and, indeed the limit of the function in equation (1.1) at \( x = 1 \) is 0.5. So that we can plot the continuous variation of \( f(x) \) say on \([0,5]\),

Interestingly, if we were to ask what is the limit of \( f(x) \) as \( x \to -1 \), then we would find that

\[
\lim_{x \to -1} \frac{x - 1}{x^2 - 1} = \lim_{x \to -1} \frac{x - 1}{(x - 1)(x + 1)}
\]

\[
= \lim_{x \to -1} \frac{1}{x + 1}
\]

which is undefined. Examining from the left and the right of \( x = -1 \),

we find that the function tends to \(-\infty\) when approaching \( x = -1 \) from the left and \(+\infty\) when approaching \( x = -1 \) from the right. Taking these limits symbolically utilizing MATHCAD we indeed find that this is the case:

Indeed, since the limit of \( f(x) \) from the left does not equal the limit from the right at \( x = -1 \), then the limit of \( f(x) \) as \( x \) approaches \(-1\) is undefined. The limit of \( f(x) \) as \( x \to -1 \) has to be interpreted depending on how \( x = -1 \) is approached.
Example Problem 2

The following temperature distribution occurs in a nuclear fuel element that is $2L$ thick in the $x$-direction, and whose edges are at a temperature $T_w$,

$$T(x) = T_w + c \left[ 1 - \left( \frac{x}{L} \right)^2 \right] \quad (1.5)$$

The constant $c$ depends on the amount of heat generated in the nuclear element, its thickness, and a property of the material measuring its ability to conduct heat. Taking $c = 50^\circ C$ and the wall edge temperature at $T_w = 100^\circ C$, then the temperature profile is shown below along with a table of value for the temperature for $x \in [0, L]$.

![Temperature profile and table](image)

The average rate of change of temperature with respect to $x$ from $x_1 = 0.5m$ to $x_2 = 0.6m$ is

$$\frac{\Delta T}{\Delta x} = \frac{T(0.6) - T(0.5)}{0.6m - 0.5m} = -55^\circ C/m \quad (1.6)$$

while the instantaneous rate of change of the temperature with $x$ is evaluated as

<table>
<thead>
<tr>
<th>x</th>
<th>$T(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>150</td>
</tr>
<tr>
<td>0.1</td>
<td>149.5</td>
</tr>
<tr>
<td>0.2</td>
<td>148</td>
</tr>
<tr>
<td>0.3</td>
<td>145.5</td>
</tr>
<tr>
<td>0.4</td>
<td>142</td>
</tr>
<tr>
<td>0.5</td>
<td>137.5</td>
</tr>
<tr>
<td>0.6</td>
<td>132</td>
</tr>
<tr>
<td>0.7</td>
<td>125.5</td>
</tr>
<tr>
<td>0.8</td>
<td>119</td>
</tr>
<tr>
<td>0.9</td>
<td>103.5</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
</tr>
</tbody>
</table>
\[ m_T(x) = \lim_{\Delta x \to 0} \frac{\Delta T}{\Delta x} \]

\[ = \lim_{h \to 0} \frac{T(x + h) - T(x)}{h} \]

\[ = \lim_{h \to 0} \frac{(T_w + c\left[1 - \left(\frac{x+h}{L}\right)^2\right]) - (T_w + c\left[1 - \left(\frac{x}{L}\right)^2\right])}{h} \]

\[ = \lim_{h \to 0} \frac{c\left(-\frac{2xh}{L^2} - \frac{h^2}{L^2}\right)}{h} \]

\[ = -\frac{2cx}{L^2} \]

where we used rule number 3 of the limit laws in Section 2.3 of your book. Evaluating the instantaneous rate of change of the temperature \( m_T(x) \) at \( x = 0.5m \) we find

\[ m_T(x = 0.5m) = -50^\circ C/m \] (1.8)

while at \( x = 0.6m \) we find

\[ m_T(x = 0.6m) = -60^\circ C/m \] (1.9)

So that we recognize that the average rate of change over the interval \([0.5m, 0.6m]\) is, in this case, well approximated in equation (1.6).

**Applications of Limits to Heat Transfer: determining the temperature in a cooling fin**

Limits can be applied to sequences and to functions. When studying the temperature distributions in bodies that are cooling or heating, the function of the constant \( e \) is often encountered. The definition of the constant \( e \) is actually the limit of the following sequence

\[ e = \lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^n \] (1.10)

This limit, attributed to the Swiss mathematician and physicist Jacob Bernoulli(1654-1705), states that the value of \( e \) is approached as \( n \) tends to infinity (\( \infty \)). Alternatively, \( e \) can also be defined as the limit of the sequence (which you will see in Calculus II),

\[ e = \lim_{n \to \infty} \left(\frac{1}{0!} + \frac{1}{1!} + \frac{1}{2!} + \frac{1}{3!} + \ldots + \frac{1}{n!}\right) \] (1.11)
where \( n! = 1 \cdot 2 \cdot 3 \ldots n \), denotes \( n \) factorial, and \( 0! = 1 \). Symbolically, we can write the above as

\[
e = \lim_{M \to \infty} \sum_{n=0}^{M} \left( \frac{1}{n!} \right)
\]  

(1.12)

The Greek capital sigma (\( \Sigma \)) was introduced by Leibniz as the notation for summation. A table and plot of this limit computed and plotted with the software package MATHCAD show that to 15 digits

\[
e = 2.71828 \; 18284 \; 5905 \ldots
\]

(1.13)

This number \( e \) is irrational, just like \( \pi \) which can also be defined as a limit, and it occurs so often in analysis and physical systems that is called the “natural base” of logarithms. As such, logarithms to the base \( e \) are given the special notation: \( \log_e(x) = \ln(x) \).

The constant \( e \) can be used to define an exponential function,

\[
f(x) = e^x
\]

(1.14)
that appears often in practice in heat transfer (EML 4142), in electrical engineering (EGN 3373 and EEL 3304), and in dynamics (EGN 3321). Plots of the exponential function are provided below

\[
\lim_{x \to +\infty} (e^x) = \infty \quad \text{and} \quad \lim_{x \to -\infty} (e^x) = 0 \quad (1.15)
\]

Anywhere in between \([-\infty, +\infty]\) we can see that if we ask what is the value of \(e^x\) for any \(x_o\), then we have a unique and finite value. You will learn that you can represent the exponential function by an infinite polynomial, and that according to the rules of section 2.3, you can evaluate that limit by substitution. For example,

\[
e^2 = \lim_{x \to 2} (e^x) = 7.389 \quad (1.16)
\]

We often use limits to check and guide us in our solutions. For example, suppose that we are interested to determine the temperature distribution in a cooling fin. Such devices are designed to help improve the removal of heat and are ubiquitous in our world, serving to remove heat from a wide variety of devices, ranging from our car engine cooling system where fins are attached to the car radiator to our computers where fins are attached to certain electronic chips to aid in removing waste heat. Suppose a fin of length, \(x = L\), is being cooled by air at a temperature \(T_c\) that is being forced over the fin by a fan.

By applying the principles of conservation of energy and using methods you will learn in differential equations (MAP 2302), we can solve for the temperature to obtain the general solution for the temperature, namely,

\[
T(x) = T_c + C_1 e^{-\lambda x} + C_2 e^{+\lambda x} \quad (1.17)
\]

where \(C_1\) and \(C_2\) are arbitrary constants and \(\lambda\) depends on the fin geometry and material property as well as how fast the air is blowing over the fin. From our experience with the exponential function, we know that for a very long fin \((x \to \infty)\), the temperature in equation...
(1.18) tends to infinity unless $C_2 = 0$. Thus, using the limiting behavior of the exponential function, we arrive at the conclusion that the general solution to the very long fin problem is

$$T(x) = T_c + C_1 e^{-\lambda x}$$

The remaining solution tells us that as the fin becomes very long, the temperature tends to that of the cooling air which makes physical sense, as plotted below for a hot wall temperature of $T_w = 150^\circ C$, a cooling air temperature of $T_c = 25^\circ C$, the constant $C_1 = T_w - T_c = 125^\circ C$, and taking a characteristic value of $\lambda = 4.414 \, [m^{-1}]$. We also find that as $x \to 0$ the temperature approaches $T_w$, which is also physically correct. So that our solution satisfies,

$$\lim_{x \to \infty} T(x) = T_c \quad \text{and} \quad \lim_{x \to 0} T(x) = T_w$$

Application of Rates of Change to Heat Transfer: evaluating the heat flow into the cooling fin

In heat transfer the rate of change of the temperature is related to the heat flow according to the relation discovered by Jean-Baptiste Fourier (1768-1830) whom we will revisit in our applications in Calc. II lectures. Namely, Fourier showed that in a solid where the temperature varies in a single direction, say $x$, the energy per unit time flowing through the cross sectional area, $A$, which is called the heat flow rate, $Q \, [W]$, is related to the instantaneous rate of change of the temperature at that position as,

$$Q = -kA \times m_T$$

(1.20)
where, $m_T$ is the instantaneous rate of change of the temperature at the position, $x$, that is

$$m_T = \lim_{h \to 0} \left[ \frac{T(x + h) - T(x)}{h} \right]$$

(1.21)

Here, $k$ is a physical property of the material. It is called the thermal conductivity, and it is measured and known for many materials. The thermal conductivity for the fin we considered above was that of Copper, and its value is: $k = 385 \text{ W/m}^\circ\text{C}$. We also considered a $1\text{cm} \times 2\text{cm}$ cross-sectional area, $A = 2 \times 10^{-4} \text{[m]}^2$ to find a value of $\lambda = 4.414$. Utilizing equation 1.18, rules 3 and 7 of the limits laws from section 2, and the law of exponents, we have,

$$m_T = \lim_{h \to 0} \left[ -kA \left[ (T_c + C_1 e^{-\lambda(x+h)}) - (T_c + C_1 e^{-\lambda x}) \right] \right]$$

$$= -kAC_1 \left\{ \lim_{h \to 0} \left[ e^{-\lambda(x+h)} - e^{-\lambda x} \right] \right\}$$

$$= -kAC_1 \left\{ e^{-\lambda x} \lim_{h \to 0} \left[ e^{-\lambda h} - 1 \right] \right\}$$

(1.22)

what is this term?

So that we are now required to evaluate the limit in the square brackets to determine $m_T$ for our problem and ultimately our heat flow rate. The results from a numerical computation using MATHCAD (and from the symbolic manipulator in MATHCAD) are shown below:

**Computing the limit numerically:**

<table>
<thead>
<tr>
<th>$h_i$</th>
<th>Function($h_i$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-3.568</td>
</tr>
<tr>
<td>0.01</td>
<td>-4.318</td>
</tr>
<tr>
<td>$1 \times 10^{-3}$</td>
<td>-4.404</td>
</tr>
<tr>
<td>$1 \times 10^{-4}$</td>
<td>-4.413</td>
</tr>
<tr>
<td>$1 \times 10^{-5}$</td>
<td>-4.414</td>
</tr>
<tr>
<td>$1 \times 10^{-6}$</td>
<td>-4.414</td>
</tr>
<tr>
<td>$1 \times 10^{-7}$</td>
<td>-4.414</td>
</tr>
<tr>
<td>$1 \times 10^{-8}$</td>
<td>-4.414</td>
</tr>
<tr>
<td>$1 \times 10^{-9}$</td>
<td>-4.414</td>
</tr>
<tr>
<td>$1 \times 10^{-10}$</td>
<td>-4.414</td>
</tr>
</tbody>
</table>

**Evaluating the limit symbolically with MATHCAD's symbolic manipulator:**

$$\lim_{h \to 0} \frac{e^{-\lambda h} - 1}{h}$$

results in:

$$-\lambda$$

and in our case, we have set

$$-\lambda = -4.414$$

Both lead us to the result that,
\[ \lim_{h \to 0} \left[ \frac{e^{-\lambda h} - 1}{h} \right] = -\lambda \quad (1.23) \]

You will learn later how to determine this result by several different means. Furthermore, with our excursion into this heat transfer problem we have established that for the function \( f(x) = e^{-\lambda x} \), the instantaneous rate of change is

\[ \lim_{h \to 0} \left[ \frac{e^{-\lambda (x+h)} - e^{-\lambda x}}{h} \right] = -\lambda e^{-\lambda x} \quad (1.24) \]

and we recognize when we set \( \lambda = -1 \), we find the extraordinary general result that the instantaneous rate of change of the function \( f(x) = e^x \) is

\[ \lim_{h \to 0} \left[ \frac{e^{x+h} - e^x}{h} \right] = e^x \quad (1.25) \]

itself! As a matter of fact it is the only function of \( x \) that has this property.

Another interesting results is established from equation (1.23), that the following limit applies,

\[ \lim_{h \to 0} \left[ \frac{e^h - 1}{h} \right] = 1 \quad (1.26) \]

So that we are now in a position to evaluate the heat flow rate due to the fin, and utilizing our results we find that

\[ Q(x) = +kA\lambda C_1 e^{-\lambda x} \quad (1.27) \]

which at \( x = 0 \) gives us, with our constants, an amount of heat of

\[ Q(0) = 42.48161 W \]

removed by the fin. From a plot of \( Q(x) \), we see that the amount of heat flowing through the fin decreases significantly as we progress further from the wall to a point where there is little and almost no flow of heat through the fin. This has design implications.

It is also interesting to see what happens when we compute the heat flow rate at \( x = 0 \) using the temperature in equation (1.18) and the definitions of equation (1.20) and (1.21). Let us do this on the computer using MATHCAD, that is compute

\[ Q(0) = \lim_{h \to 0} \left[ -kA \left( \frac{T(x_o + h) - T(x_o)}{h} \right) \right]_{x_o=0} \quad (1.28) \]

The results are provided in a table along with a plot of the computed heat flow rate versus the exact value we found as we drive the value of \( h \) towards zero on the computer. It is noticeable that the correct value of 42.48161 is found as \( h \) takes on smaller values, however, at some point, close to \( h \sim 10^{-9} \) (which is pretty small but not zero), things begin to go wrong: (1) the value of the heat flow rate begins to depart from the exact value, and (2) as \( h \) reduces even more, around \( h \sim 10^{-16} \), things go terribly wrong and we compute zero!
We can plot and compute the absolute error in a log-log plot so that we can see the trend, and we find an interesting pattern: the error first reduces with diminishing value of $h$ as expected, then it increases as $h$ reduces in magnitude, and finally the error stay constant at a maximum value of 42.48161 or 100% error.

This exemplifies why you cannot take the limit that $h \rightarrow 0$ on the computer and why analytical methods of Calculus are important. What happened is that the computer (and any electronic means of calculating) makes small mistakes due to the finite arithmetic it utilizes and due to the limitations of how it stores numbers. This error is called round-off.
and you cannot escape it. As $h$ appears in the denominator in equation (1.28), it amplifies the error made by the computer in evaluating $T(x_o + h) - T(x_o)$, and this begins to manifest itself around $h \sim 10^{-9}$ where the absolute error begins to increase with decreasing $h$. Finally, around $h \sim 10^{-16}$, the computer cannot recognize that it added $h$ to $x_o$ and it computes $T(x_o + h) - T(x_o) = 0$. Therefore, we have wonderful tools in computers, however, we need to be careful how we utilize them, and we need to always remember that what we saw with our example will always occur: we cannot compute the limit that $h \to 0$ exactly. We can only approximate this limit, and, we must do so carefully.

**Conclusions**

We have applied limits to define the base of the natural logarithms $e$ and also to problems in heat transfer. In particular, we have applied limits to the evaluation of the behavior of a general solution for the temperature in a cooling fin. We also applied the concept of limits to evaluate the instantaneous rate of change of the temperature with position in the process of determining the heat flow rate from the fin. In the process, we found an amazing property of the exponential function, namely, that the instantaneous slope of the exponential function is the exponential function itself. This is the only function for which this statement is true. We have seen that we cannot compute the limit $h \to 0$, however, we can see a trend and we can approximate it numerically. You will next learn that the instantaneous rate of change of a function is called the derivative, and you will learn many rules and methods to compute the derivative of functions.
Chapter 2

Chemical Kinetics

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Department of Chemistry

Weeks
February 4 and 11, Spring 2009.
The Derivative as a Function

Example Problem 1. Section 3.2, Exercise 33

The unemployment rate $U(t)$ varies with time. The table (from the Bureau of Labor Statistics) gives the percentage of unemployed in the U.S. labor force from 1991 to 2000.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$U(t)$</td>
<td>6.8</td>
<td>7.5</td>
<td>6.9</td>
<td>6.1</td>
<td>5.6</td>
<td>5.4</td>
<td>4.9</td>
<td>4.5</td>
<td>4.2</td>
<td>4.0</td>
</tr>
</tbody>
</table>

a) What is the meaning of $U'(t)$? What are the units?
b) Construct a table of values for $U'(t)$.

Solution:
a) The rate at which the unemployment rate is changing, in percent unemployed per year.
b) Example:

\[
U'(1991) \approx \frac{U(1992) - U(1991)}{1 \text{ yr.}} = 7.5 - 6.8 = 0.70
\]

\[
U'(1992) \approx \frac{U(1993) - U(1992)}{1 \text{ yr.}} = 6.9 - 7.5 = -0.60
\]

A more accurate value for $U'(1992)$ is to take the average between $U(1992) - U(1991)$ and $U(1993) - U(1992)$

\[
U'(1992) \approx \frac{0.70 - 0.60}{2} = 0.05
\]

Courses in which this topic will be used:

CHM 2046 Chemistry Fundamentals II

In this chapter, we will discuss how derivatives are used in Chemistry to calculate how fast a reaction is occurring.

Background/Motivation

Chemical kinetics is concerned with the measurement of rates of reaction. What is meant by the term 'rates of reaction' is the rate at which a reactant is disappearing (or being consumed) or the rate at which a product is being produced. This, in turn, enables comparisons of reactions to be made and can afford a kinetic classification of reactions. The sort of information used is summarized in terms of:
• The factors influencing rates of reaction,

• The dependence of the rate of reaction on concentration, called the order of the reaction,

• The rate expression, which is an equation which summarizes the dependence of the rate on the concentrations of substances which affect the rate of reaction,

• The rate constant, which is a constant of proportionality linking the rate with the various concentration terms,

• This rate constant collects in one quantity all the information needed to calculate the rate under specific conditions,

• The effect of temperature on the rate of reaction. Increase in temperature generally increases the rate of reaction. Knowledge of just exactly how temperature affects the rate constant can give information leading to a deeper understanding of how reactions occur.

However, the science of kinetics does not end here. The next task is to look at the chemical steps involved in a chemical reaction, and to develop a mechanism which summarizes this information. The final task is to develop theories as to why and how reactions occur, and to examine the physical and chemical requirements for the reaction. But it all begins with collecting concentration versus time data and analyzing it with techniques that you have just covered in your calculus class.

**Interpreting chemical kinetic data and calculating the average rate.**

In any chemical reaction we have reactants being converted to products. This is represented as:

\[
\text{Reactants} \Rightarrow \text{Products}
\]

There may be more than one type of reactant (i.e. different types of molecules) and more than one type of product formed. Examples of three different types of reactions are as follows:

• \(\text{HCl} + \text{NaOH} \Rightarrow \text{H}_2\text{O} + \text{NaCl}\)
  
  This is an acid/base neutralization reaction where hydrochloric acid (HCl) reacts with sodium hydroxide (NaOH, a base) to produce water and sodium chloride (NaCl, table salt).

• \(\text{HCl} + \text{NH}_3 \Rightarrow \text{NH}_4\text{Cl}\)
  
  This is another acid base neutralization reaction. This involves reactants hydrochloric acid and ammonia (NH3, a base) reacting to yield the salt ammonium chloride, NH4Cl.
CaCO₃ ⇌ CaO + CO₂

This is another type of reaction, decomposition reaction of calcium carbonate (CaCO₃) decomposing to form calcium oxide (CaO) and carbon dioxide (CO₂).

The first step in determining how fast the reaction is occurring (i.e. the rate) is to measure either the change in concentration of the reactant with time, or the change in concentration of the product with time. Sometime, the concentration of both are measured. After measuring the concentrations, the next step in analysis is to convert the experimental observations to plots of the [reactants] versus time. The use of brackets, [ ], is the notation meaning ”concentration,” usually in the units moles/liter (known as molarity, M). A mole is a SI unit for a quantity of things and is equal to 6.02 × 10²³ (Avogadro’s number). Thus, for example, a mole of H₂ gas would be equal to 6.02 × 10²³ molecules of H₂. Figure 2.1 illustrates some typical data for a reaction of the type A ⇌ B.

![Figure 2.1: The progress of the reaction A ⇌ B over a 1-minute period.](image)

Note that in Figure 1, the mixture initially contains only A molecules (purple). With increasing time the number of A molecules decreases and the number of B molecules (green) increases.

It should be noted that the plot of concentration of reactants and products is not linear with time. What this means is that the rate at which a reactant is decreasing and product is increasing is not constant but rather changing as the reaction progresses with time.
The more precise meaning of the term *rate of reaction*, defined as how fast the [reactant] changes with time, can be illustrated on graphs of concentration vs. time. One way of doing this is shown in Figure 2.2.

![Graph of concentration verses time, illustrating the meaning of average rate.](image)

The average rate over the time interval $t_1$ to $t_2$ when the concentration decreases from $c_1$ to $c_2$ is specified by:

$$\text{Average rate} = \frac{c_2 - c_1}{t_2 - t_1} = \text{slope of line AB} = \frac{\Delta c}{\Delta t}$$

Notice that the slope of the line AB is negative and this will be true for the change in concentration of any reactant because the reactant is always being *consumed* in any reaction. However, the rate is always expressed as a positive number so the rate when calculated from the change in concentration of a reactant is given as $| -\Delta c/\Delta t |$. Note that if we were tracking a *product formation*, the slope of the secant line would be positive. Because we were plotting *disappearance of a reactant*, the slope is negative.
An example of an average rate calculation is determining the rate of hydrolysis of aspirin. We can use equation 1 to determine the rate of hydrolysis of Aspirin, probably the most commonly used drug in the world. (More than 25 million kilograms are produced annually worldwide.) Aspirin (acetylsalicylic acid) reacts with water (such as water in body fluids) to give salicylic acid and acetic acid. This is called a hydrolysis reaction and is illustrated in the following reaction (Figure 2.3).

![Figure 2.3: An example of a hydrolysis reaction.](image)

Because salicylic acid is the actual substance that relieves pain and reduces fever and inflammation, a great deal of research has focused on understanding this reaction and the factors that affect its rate. Data from the hydrolysis of a sample of aspirin are listed in Table 2.1 and are shown in Figure 2.4. These data were obtained by removing samples of the reaction mixture at the indicated times and analyzing them for the concentration of reactant (aspirin) and one of the products (salicylic acid).

<table>
<thead>
<tr>
<th>Time (h)</th>
<th>[aspirin]</th>
<th>[Salicylic acid]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$5.55 \times 10^{-3}$</td>
<td>$0.00 \times 10^{-3}$</td>
</tr>
<tr>
<td>20</td>
<td>$5.15 \times 10^{-3}$</td>
<td>$0.40 \times 10^{-3}$</td>
</tr>
<tr>
<td>50</td>
<td>$4.61 \times 10^{-3}$</td>
<td>$0.94 \times 10^{-3}$</td>
</tr>
<tr>
<td>100</td>
<td>$3.83 \times 10^{-3}$</td>
<td>$1.72 \times 10^{-3}$</td>
</tr>
<tr>
<td>200</td>
<td>$2.64 \times 10^{-3}$</td>
<td>$2.91 \times 10^{-3}$</td>
</tr>
<tr>
<td>300</td>
<td>$1.82 \times 10^{-3}$</td>
<td>$3.73 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 2.1: Data for the Hydrolysis of Aspirin in aqueous solution at pH 7.0 and 37°C.

We can calculate the average reaction rate for a given time interval from the concentrations of either the reactant or one of the products at the beginning of the interval (time = $t_0$) and at the end of the interval ($t_1$). Using salicylic acid, for example, we find that the rate of the reaction for the interval between $t = 0$ h and $t = 2.0$ h (recall that $\Delta$ is always calculated as "final minus initial"):

$$
\text{Rate}_{(t=0-2.0h)} = \frac{[\text{salicylic acid}]_2 - [\text{salicylic acid}]_0}{2.0 \ h - 0.0 \ h} = \frac{0.04 \times 10^{-3} \ M - 0.00 \ M}{2 \ h} = 2 \times 10^{-5} M/h.
$$
Figure 2.4: The hydrolysis of aspirin graph showing the consumption of aspirin and the production of salicylic acid. Data is given in Table 2.1. The purple line and shading represents consumption of aspirin. The green line and shading represents the production of salicylic acid. The magnitude of the legs of the shaded triangles are the values used to calculate the tangent lines that would represent the average reaction rates over those time periods.

We can also calculate the rate of the reaction from the concentration of aspirin at the beginning and the end of the same interval, remembering to insert a negative sign, because its concentration decreases:

\[
\text{Rate}_{(t=0-2.0h)} = -\frac{\text{[aspirin]}_2 - \text{[aspirin]}_0}{2.0 \text{h} - 0.0 \text{h}} = - \left( \frac{5.51 \times 10^{-3} \text{ M} - 5.55 \text{ M}}{2 \text{h}} \right) = 2 \times 10^{-5} \text{M/h}.
\]

If we now calculate the rate during the last interval given in Table 2.1 (the interval between 200 h and 300 h after the start of the reaction), we find the rate of the reaction is significantly
slower than it was during the first interval \((t = 0 - 2.0 \text{ h})\):

\[
\text{Rate}_{(t=200-300 \text{ h})} = -\frac{[\text{salicylic acid}]_{300} - [\text{salicylic acid}]_{200}}{300 \text{ h} - 200 \text{ h}} = -\left(\frac{3.73 \times 10^{-3} \text{ M} - 2.91 \text{ M}}{100 \text{ h}}\right) = 8.2 \times 10^{-6} \text{M/h}.
\]

(You should verify from the data in Table 2.1 that you get the same rate using the concentrations of aspirin measured at 200 h and 300 h.)

**Determining the instantaneous rate of a reaction**

The average rate gives limited information about how fast a reaction rate is changing with concentration. What is needed is the actual rate at a particular reactant concentration, called the 'instantaneous rate.' This is also the rate at any given point in time. As the period of time used to calculate an average rate of a reaction becomes shorter and shorter, the average rate approaches the instantaneous rate. This corresponds to situations where \(c_2 - c_1 \to 0\) and \(t_2 - t_1 \to 0\), and describes the slope of a tangent to the curve at the particular concentration or time. For example, the slope of line EF, Figure 2.5, gives the instantaneous rate at \(c_1\) and \(t_1\). The slope of EF is negative, but the rate of reaction is defined to be the absolute value which is positive. The initial rate is a very important quantity in kinetics, especially for complex reactions involving many steps where secondary reactions and products of reaction may affect the rate. The initial rate is the rate at the very start of the reaction, Figure 2.6, and, with the exception of chain reactions, is the line of steepest slope giving the maximum rate. The units of rate are given in terms of concentration per unit time. Example: M/s, M/min, mol·L\(^{-1}\)·s\(^{-1}\). An illustration showing how the rate of a reaction depends on concentration of a reactant is given in Figure 2.7. In Figure 2.7, three tangents have been drawn. The magnitudes of the slopes (denoted as \(m\)) lie in the order \(|m_{AB}| > |m_{CD}| > |m_{EF}|\) and these data points are \((t_1, c_1), (t_2, c_2)\) and \((t_3, c_3)\) respectively, i.e. as concentration of reactant decreases, so does the rate. Think of the distinction between the instantaneous and average rates of a reaction as being similar to the distinction between the actual speed of a car at any given time on a trip and the average speed of the car for the entire trip. Although you may travel for a long time at 65 mi/h on an interstate during a long trip, there may be times when you travel only 25 mi/h in construction zones, or 0 mi/h if you stop for meals or gas. Thus, your average speed on the trip may be only 50 mi/h, whereas your instantaneous speed on the interstate at a given moment may be 65 mi/h as measured by the speedometer reading. Whether you are able to stop the car in time to avoid an accident depends on your instantaneous speed, not on your average speed.

There are important differences between the speed of a car during a trip and the speed of a chemical reaction, however. The speed of a car may vary unpredictably over the length of the trip, and the initial part of the trip is often one of the slowest. In a chemical reaction, the initial interval normally has the fastest rate (though this is not always the case) and the rate generally changes smoothly over time. In chemical kinetics, the focus is usually on one particular instantaneous rate, \(t = 0\), which is the initial rate of the reaction.
Figure 2.5: Graph of concentration verses time illustrates the meaning of instantaneous rate at time $t_1$.

**Calculating the rate constant for a reaction**

In the preceding section, you learned that reaction rates generally decrease with time because reactant concentrations decrease as reactants are converted to products. The conclusion follows that the rate is proportional to the concentration of reactants remaining, i.e.

$$\text{Rate} \propto [\text{reactant}]^n,$$

where $n$ is a number which states exactly how the rate depends on the [reactant]. It is called the order. From this,

$$\text{Rate} = k[\text{reactant}]^n,$$

where $k$ is a constant of proportionality called the rate constant.

- If $n = 1$, the reaction is first order; if $n = 2$ the reaction is second order.
- If $n = 3/2$, the reaction is three-halves order; if $n = 0$, it is zero order.

If the order of a reaction is known, then the rate constant can be calculated from rate and concentration data. The units of the rate constant will depend upon the order of the reaction.
Simultaneously determining the order and rate constant from experimental data.

In the preceding sections you learned that reaction rates generally decrease with the time because reactant concentrations decrease as reactants are converted to products. You also learned that reaction rates generally increase when reactant concentrations are increased. We now examine the mathematical expression called rate laws, which describe the relationships between reactant rates and reactant concentrations. Rate laws are mathematical descriptions of experimentally verifiable data. A different rate law expresses the rate of a reaction in terms of changes in the concentration of one or more reactants, that is, $\Delta[R]$, over a specific time interval, $\Delta t$. Or in the limit of small changes, $d[R]$, over a small time interval, $dt$.

For a reaction with the general equation

$$aA + bB \Rightarrow cC + dD$$  \hspace{1cm} (2.1)
the experimentally determined rate law usually has the form

\[ \text{rate} = k[A]^m[B]^n. \]  

(2.2)

The proportionality constant, \( k \), is called the rate constant, and its value is characteristic of the reaction and reaction conditions. A given reaction has a particular value of the rate constant under a given set of conditions, such as temperature, pressure, and solvent; varying the temperature or the solvent usually changes the value of the rate constant. The numerical value of \( k \), however, does not change as the reaction progresses under a given set of conditions. Thus, the rate of a reaction depends on the rate constant for the given set of reactions conditions and on the concentration of each reactant, raised to powers \( m \) and \( n \), respectively. The values of \( m \) and \( n \) are derived from experimental measurements of the changes in reactant concentrations over time and indicate the reaction order, the degree to which the rate of the reaction depends on the concentration of each reactant; \( m \) and \( n \) need not to be integers. For example, Equation (2.2) tells us the Reaction (2.1) is \( m \)th order in
reactant A and \( n \)th order in reactant B. It is important to remember that \( n \) and \( m \) are not related to the stoichiometric coefficients \( a \) and \( b \) in the balanced chemical equation but must be determined experimentally. The overall reaction order is the sum of all the exponents in the rate law, or \( m + n \). Remember that \( m \) and \( n \) can only be determined from experimental data.

Let’s look at one method for determining \( m \) and \( n \). The method calls for taking the quotient of the rate laws for two different experiments. For example rate data for a hypothetical reaction of the type \( A + B \rightarrow \text{products} \) are given in Table 2.2. The general rate law for the reaction is given in Equation 2.2. We can obtain the value of \( m \) or \( n \) directly by finding the ratio of the rate laws for two experiments in which the concentration of one of the reactants is the same, such as Experiments 1, and 3 in Table 2.2.

\[
\frac{\text{rate}_1}{\text{rate}_3} = \frac{k[A_1]^m[B_1]^n}{k[A_3]^m[B_3]^n}.
\]

Inserting the appropriate values from Table 2.2 gives:

\[
\frac{8.3 \times 10^{-3} \text{ M/min}}{33 \times 10^{-3} \text{ M/min}} = \frac{k(0.50 \text{ M})^m(0.50 \text{ M})^n}{k(1.00 \text{ M})^m(0.50 \text{ M})^n}.
\]

By rounding all calculations to two significant figures and noting that 1.00 to any power is 1, we can cancel like terms to give 0.25 = (0.50)^m, which can also be written as 1/4 = (1/2)^m. Thus, we can conclude \( m = 2 \) and that the reaction is second order in A. Note that by selecting two experiments in which the concentration of B is the same, we were able to solve for the value of \( m \).

Conversely, by selecting two experiments in which the concentration of A is the same (for example, Experiments 5 and 1), we can solve for the value of \( n \).

\[
\frac{\text{rate}_1}{\text{rate}_5} = \frac{k[A_1]^m[B_1]^n}{k[A_3]^m[B_3]^n}.
\]

Substituting the appropriate values from Table 2 gives:

\[
\frac{8.3 \times 10^{-3} \text{ M/min}}{8.3 \times 10^{-3} \text{ M/min}} = \frac{k(0.50 \text{ M})^m(0.50 \text{ M})^n}{k(0.50 \text{ M})^m(1.00 \text{ M})^n}.
\]
Canceling leaves $1.0 = (0.50)^n$, which gives $n = 0$; that is, the reaction is zero order in $B$. The experimentally determined rate law is therefore

$$\text{rate} = k[A]^2[B]^0 = k[A]^2$$

We can now calculate the rate constant by inserting the data from any line of Table 2.2 into the experimentally determined rate law and solving for $k$. Using Experiment 2, we obtain:

$$19 \times 10^{-3} \text{ M/min} = k(0.75 \text{ M})^2$$
$$3.4 \times 10^{-2} \text{ M}^{-1} \cdot \text{min}^{-1} = k$$

You should verify that using data from any other line of Table 2.2 gives the same rate constant. This must be true as long as the experimental conditions, such as temperature and solvent, are the same.

The following is a test question from Chemistry 2046 combining the use of calculus with chemical kinetics.

Carbon Monoxide (CO) reacts with nitrogen dioxide (NO$_2$) according to the following equation:

$$CO(g) + NO_2(g) \rightarrow CO_2(g) + NO(g).$$

The rate equation for this reaction at 400$^\circ$K is

$$\text{Rate} = k[CO][NO_2] \quad (k = 1.9 \text{ L/mol} \cdot \text{h}).$$

Determine the initial rate of the reaction when $[CO] = 3.8 \times 10^{-4} \text{ mol/L}$ and $[NO_2] = 0.650 \times 10^{-4} \text{ mol/L}$.

Strategy: A rate equation consists of three parts: a rate, a rate constant ($k$) and the concentration terms. If two of these parts are known (here $k$ and the concentrations), the third can be calculated.

$$\text{Rate} = k[CO][NO_2] = (1.9 \text{ L/mol} \cdot \text{h})(3.8 \times 10^{-4})(0.65 \times 10^{-4} \text{ mol/L})$$

$$\text{Rate} = 4.7 \times 10^{-8} \text{ mol/L} \cdot \text{h}$$
Chapter 3

Detecting Edges in Images

Faculty Contributor
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School of Electrical Engineering and Computer Science

Weeks
February 18 and 25, Spring 2009.
Estimating Derivatives

**Example Problem 1.** Section 3.1, Example 6

Let $D(t)$ be the U.S. national debt at time $t$. The table gives approximate values of this function by providing end of year estimates, in billions of dollars, from 1980 to 2000. Interpret and estimate the value of $D'(1990)$.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$D(t)$</td>
<td>930.2</td>
<td>1945.9</td>
<td>3233.3</td>
<td>4974.0</td>
<td>5674.2</td>
</tr>
</tbody>
</table>

**Solution:**

The derivative $D'(1990)$ means the rate of change of $D$ with respect to $t$ when $t = 1990$, that is, the rate of increase of the national debt in 1990.

According to Equation 3 in section 3.1,

$$D'(1990) = \lim_{t \to 1990} \frac{D(t) - D(1990)}{t - 1990}.$$

So we compute and tabulate values of the difference quotient as follows (the difference quotient records the average rate of change):

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{D(t) - D(1990)}{t - 1990}$</td>
<td>230.31</td>
<td>257.48</td>
<td>348.14</td>
<td>244.09</td>
</tr>
</tbody>
</table>

From this table we see that $D'(1990)$ lies somewhere between 257.48 and 348.14 billion dollars per year. (Here we are making the reasonable assumption that the debt didn’t fluctuate wildly between 1980 and 2000.) We estimate that the rate of increase of the national debt of the United States in 1990 was the average of these two numbers, namely 303 billion dollars per year.

**Example Problem 2.** Section 3.1, Exercise 31

Let $T(t)$ be the temperature (in °F) in Dallas $t$ hours after midnight on June 2, 2001. The table shows values of this function recorded every two hours. What is the meaning of $T'(10)$? Estimate its value.

<table>
<thead>
<tr>
<th>$t$</th>
<th>0</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>73</td>
<td>73</td>
<td>70</td>
<td>69</td>
<td>72</td>
<td>81</td>
<td>88</td>
<td>91</td>
</tr>
</tbody>
</table>

**Solution:**

$T'(10)$ means the way the temperature is changing in Dallas at 10 am. To estimate its value, first we calculate the difference quotient values $\frac{T(t) - T(10)}{t - 10}$.

<table>
<thead>
<tr>
<th>$t$</th>
<th>0</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{T(t) - T(10)}{t - 10}$</td>
<td>0.8</td>
<td>1.0</td>
<td>1.8</td>
<td>3.0</td>
<td>4.5</td>
<td>3.5</td>
<td>2.5</td>
</tr>
</tbody>
</table>
To estimate $T'(10)$, given by $\lim_{t \to 10} \frac{T(t) - T(10)}{t - 10}$, we take the average of the difference quotient values at $t = 8$, and $t = 12$, to get the result $(4.5 + 3.5)/2$, i.e., $4° F/h$.

**Example Problem 3.** Section 3.1, Exercise 32

Life expectancy improved dramatically in the 20th century. The table gives values of $E(t)$, the life expectancy at birth (in years) of a male born in the year $t$ in the United States. Interpret and estimate the values of $E'(1910)$ and $E'(1950)$.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$E(t)$</td>
<td>48.3</td>
<td>51.1</td>
<td>55.2</td>
<td>57.4</td>
<td>62.5</td>
<td>65.6</td>
<td>66.6</td>
<td>67.1</td>
<td>70.0</td>
<td>71.8</td>
<td>74.1</td>
</tr>
</tbody>
</table>

**Solution:**

$E'(1910)$ and $E'(1950)$ refer to the gain or drop (in this case, gain) in life expectancy at birth for males born in 1910 and 1950 respectively. To estimate these quantities, we calculate the difference quotients for each of the require years

$$\frac{E(1900) - E(1910)}{1900 - 1910} = 0.28 \quad \text{and} \quad \frac{E(1920) - E(1910)}{1920 - 1910} = 0.41$$

and take their average for an answer of 0.35.

Similarly, for $E'(1950)$ we calculate the two difference quotients

$$\frac{E(1940) - E(1950)}{1940 - 1950} = 0.31 \quad \text{and} \quad \frac{E(1960) - E(1950)}{1960 - 1950} = 0.1$$

and take their average for an answer of 0.21.

**Images and their edges**

Another important example of using derivatives on lists of data is in the area of image processing and computer vision. We will now discuss the application area of computer vision, and indicate how the ideas from Calculus help the field to conduct the analysis of images.

**Background/Motivation**

Computer Vision is the field that is interested in building systems to understand the contents of digital images and videos. An important step in any image processing system is to detect edges. These edges highlight regions of interest, or can be used to described shapes in images.

Consider the image (picture). In this representation, a picture is made up of a table of dots, called pixels (for picture elements), and the pixel values range from 0 to 256. The pixel values are proportional to the brightness at that location in the picture.

So, the actual numbers in the picture are
Figure 3.1: 20 × 20 pixel image of black box on square white background

```
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
255 255 0 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
```

Consider taking a strip of values along a row, say the 6-th row.

```
255 255 0 0 0 0 0 0 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255 255
```
Then, this is similar to the other tables we have seen so far, and can be written as:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>...</th>
<th>19</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I$</td>
<td>255</td>
<td>255</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>255</td>
<td>255</td>
<td>...</td>
<td>255</td>
<td>255</td>
<td></td>
</tr>
</tbody>
</table>

where $I$ is the pixel value at $x$. Plotting these values, the graph looks like

![Graph](image)

In this case, $I$ is a function of $x$, where $x$ is the distance along the horizontal side of the picture. We use the letter $I$ for the function to stand for (to tell us that it’s meaning is) the word Image and sometimes for the word Intensity (which in turn means the level of brightness). To find the edge here, we would want to detect where the graph drops and where it rises. We can find where $I(x)$ drops and rises by computing the derivative $\frac{dI(x)}{dx}$, or $I'(x)$.

To estimate the derivative $I'(x)$ we use the familiar process of writing the table of difference quotients so that it varies with position $x$. We get

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>...</th>
<th>19</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{I(x)-I(x-1)}{x-(x-1)}$</td>
<td></td>
<td>-</td>
<td>0</td>
<td>-255</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>255</td>
<td>0</td>
<td>...</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Which when graphed, looks like the left picture and taking the absolute value of this expression (right picture), we would get 255 at the two edges, and zero everywhere else.

Similarly, this calculation is done for a column (instead of a row) of numbers from the picture. Note we could “cut” this plot to show which values are high enough. So, we have $I(y)$ and
can estimate $I'(y) = I(y) - I(y-1)$. This would give us the edges going in the vertical direction along the picture. The question at this point is how to get a sensible way to combine the two estimates $I'(x)$ and $I'(y)$. It turns out the correct way given by thinking mathematically is to view the picture as $I(x, y)$, that is as a function of two directions, or as a function of two variables, formally called a function of two-dimensions. In this two dimensional case, when we take a derivative, the derivatives are now called Partial Derivatives, and are denoted by $\frac{\partial I}{\partial x}$ and $\frac{\partial I}{\partial y}$. The two quantities combine to give the Gradient Vector. This is a physical descriptor of two dimensional functions; its magnitude can be obtained by squaring the individual parts, adding them, and taking the square root, to get one scalar number. Its graph would be a surface. This concept is introduced in your Calculus textbook on page 1095, Chapter 17. The symbol for the gradient vector is $\nabla I = \left( \frac{\partial I}{\partial x}, \frac{\partial I}{\partial y} \right)$, and to repeat, it has two parts, the partial derivatives mentioned above.

If we plot the magnitude of the gradient for the picture shown on the left, we would get the output shown on the right (rather than having a surface it is more convenient to plot level curves, the curves where the function is equal to a fix value, so only the edges are represented).

In typical edge detection processing, one then applies a threshold to this output as in the
following picture on the left. In this picture, the horse’s head is not showing up as an edge, because the magnitude of the derivative is small near the area of the head. If we employ a lower threshold (this is like lowering the bar for what it means to get an ’A’ in class), one can get all the edges, as shown in the right picture.

To examine why the output edges are broad, rather than thin, let us look at the twenty pixels and their plots, in a row from the interior of the image, around the rook.

<table>
<thead>
<tr>
<th>$x$</th>
<th>88</th>
<th>89</th>
<th>90</th>
<th>91</th>
<th>92</th>
<th>93</th>
<th>94</th>
<th>95</th>
<th>96</th>
<th>97</th>
<th>98</th>
<th>99</th>
<th>100</th>
<th>101</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I(x)$</td>
<td>11</td>
<td>10</td>
<td>11</td>
<td>11</td>
<td>18</td>
<td>53</td>
<td>95</td>
<td>110</td>
<td>116</td>
<td>122</td>
<td>126</td>
<td>129</td>
<td>130</td>
<td>132</td>
</tr>
<tr>
<td>$\frac{I(x) - I(x-1)}{x - (x-1)}$</td>
<td>$-1$</td>
<td>1</td>
<td>0</td>
<td>7</td>
<td>35</td>
<td>42</td>
<td>15</td>
<td>4</td>
<td>6</td>
<td>4</td>
<td>3</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

A scheme that is based on choosing a threshold is seen to produce too wide an edge (such as with the lowered threshold in the figure earlier). If the threshold is 30, we would get two pixels as outputs; if it were 10, we would get three pixels as edges; this is what makes the results in the pictures earlier be quite wide. Instead, our goal has to be to find the sole point (single point) at the very top of this curve.

One strategy is to compute one additional derivative after the initial derivative, and to use that output for subsequent inspections. This brings us to the topic of Higher Derivatives,
which is Section 3.8 of the textbook. In our case, we are only restricting ourselves to the second derivative. So, suppose we took the values in the chart above, and computed the difference quotient again (the act of doing it again causes it to be called the second derivative), we would get

<table>
<thead>
<tr>
<th>x</th>
<th>88</th>
<th>89</th>
<th>90</th>
<th>91</th>
<th>92</th>
<th>93</th>
<th>94</th>
<th>95</th>
<th>96</th>
<th>97</th>
<th>98</th>
<th>99</th>
<th>100</th>
<th>101</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{I'(x) - I'(x-1)}{x - (x-1)}$</td>
<td>-</td>
<td>-</td>
<td>2</td>
<td>-1</td>
<td>7</td>
<td>28</td>
<td>7</td>
<td>-27</td>
<td>-11</td>
<td>2</td>
<td>-2</td>
<td>-1</td>
<td>-2</td>
<td>1</td>
</tr>
</tbody>
</table>

whose plot is

![Plot of the second derivative](image)

Then, the final step is to look for adjacent pixels that have a transition from one sign to the other sign (i.e., from a large positive to a large negative, or from a large negative to a large positive.) Places where these transitions occur are to be marked as edges. Here is the output (left picture) of employing the difference quotient for a second time. (Observe that using the difference quotient for a second time, is the same as computing the second derivative on an incoming picture.) In this figure, grey means zero; white means positive, and black means negative. Observe the double bands that occur adjacently wherever there is an edge. Then, the final output from this transition detection is shown on the picture on the right, which is what was desired.
Examples

Here are some other examples (shown in pairs) of running edge detectors, and then having an algorithm that straightens out the found edges, producing an artist-like sketch.
Driverless car application

A less artsy application and more artificial intelligence oriented example, is that of road detection for the driver-less car project at UCF. The task is to have the car drive itself based on images it sees through its cameras.

In this domain, here is a sample image before processing (left) and after processing (right).

Further edge detection and processing finds the lanes in the road. Many other interesting applications exist for computer vision, and even more so for Calculus, and now you are familiar with one application. A related but important healthcare example of an application is the area of processing medical imagery for diagnosis and treatment.
Chapter 4

Real Life Derivatives in a Quantum Star.

Faculty Contributor
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Department of Physics

Weeks
March 4 and 18, Spring 2009.
Example Problem 1

Section 4.1, exercise 66 (b), p. 231

(b) Find a model for the acceleration of the shuttle and use it to estimate the maximum and minimum values of the acceleration during the first 125 seconds.

One of several methods one can use is the backwards average: at time $t_2$, compute average acceleration by looking backwards in time to the previous speed measurement, $v_1$ at time $t - 1$. Combine with the speed measurement $v_2$ at time $t_2$, viz.

$$a = \frac{v_2 - v_1}{t_2 - t_1}$$

The elapsed time between the two speed measurements is $\Delta t = t_2 - t_1$. Therefore this method is similar to the derivative definitions of chapter 2.

Now look at the table of data.

<table>
<thead>
<tr>
<th>Event</th>
<th>Time (s)</th>
<th>Velocity (ft/s)</th>
<th>Avg. Acceleration (ft/s²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Launch</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>Begin roll maneuver</td>
<td>10</td>
<td>185</td>
<td>18.5</td>
</tr>
<tr>
<td>End roll maneuver</td>
<td>15</td>
<td>319</td>
<td>26.8</td>
</tr>
<tr>
<td>Throttle to 89%</td>
<td>20</td>
<td>447</td>
<td>25.6</td>
</tr>
<tr>
<td>Throttle to 67%</td>
<td>32</td>
<td>742</td>
<td>24.6</td>
</tr>
<tr>
<td>Throttle to 104%</td>
<td>59</td>
<td>1325</td>
<td>21.5</td>
</tr>
<tr>
<td>Maximum dynamic pressure</td>
<td>62</td>
<td>1445</td>
<td>40.0</td>
</tr>
<tr>
<td>Solid rocket booster separation</td>
<td>125</td>
<td>4151</td>
<td>43.9</td>
</tr>
</tbody>
</table>

Now we can look at the table’s fourth column and decide where the maxima and minima are. The global minimum is at time $t = 0$, and the global maximum is at time $t = 125$. Close inspection of the table shows that there is a local maximum at time $t = 15$ and a local minimum at time $t = 59$. Based upon these maxima and minima, one can see why the astronauts train so carefully: the precise throttle settings and attendant accelerations vary significantly but not in a regular manner of constant accelerations that a falling apple experiences here on the surface of Terra Firma.

This data and computational method yield a very rough set of estimates. When one plots the average acceleration at each of the eight times and then connects the dots with line segments, as in Fig. 4.1, one can more easily see the maxima and minima.

Although this set of estimates is rough, the space flight controllers at NASA are loaded with radars and cameras of top quality. They will have many thousands of time-and-speed data points, instead of the paltry set of eight data points in this exercise. With a new speed measurement every thousandth of a second, instead of every 5 seconds, the line segments will be quite small. The plot of data points will appear very smooth and the location of maxima and minima can be estimated with greater precision. The local minimum, for instance, might actually be at time $t = 57.832$. 
Figure 4.1: Exercise 66, page 231, accelerations as backwards-differenced derivative, plotted as line segments between data points.

There are numerous methods to generate smoother plots, as seen in Fig. 4.2. This figure is the output of Microsoft Excel’s data graphing function, with smoothed curves connecting the data points. NASA’s plot of many thousands of small line segments might look more like Fig. 4.2. The smaller the time increments, the closer one can be to the idealized infinitesimal limit, $\Delta t \to 0$.

This preliminary exercise leads logically to the following question: what can one do when one has all the laws of motion but no measurements? Can one work backwards from forces and accelerations to compute speeds and positions?
Background and motivation

*If we knew what we were doing, it would not be called research.*
- attributed to Albert Einstein

Sometimes, it’s true: you are clueless. You have laws of motion but no initial position or speed. You have all the laws of electromagnetism, but they are expressed in the language of derivative: the spatial derivative of the electric field coupled to the time derivative of the magnetic field, and so forth. You have all the wave equations of quantum mechanics, but they involve the wave function and its derivatives, and sometimes the wave function cannot be derived with paper and pencil. This is a pervasive problem for a scientist or engineer working on something new.

Here is a simple, famous example of this trouble: an apple falling out of Sir Isaac Newton’s apple tree. The acceleration due to gravity, $g$, is $9.8 \text{ m/s}^2$ downward, nearly everywhere on the surface of Earth, from the top of Mt. Everest to the bottom of the Mariana Trench. How can one “back up” from knowledge of acceleration to speed and position? The table technique works nicely. In Table 4.1, we will use $g = -9.8 \text{ m/sec}^2$ with the understanding that the minus sign means *downward*.

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Distance (m)</th>
<th>Velocity (m/s)</th>
<th>Acceleration (m/s$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-9.8</td>
</tr>
<tr>
<td>1</td>
<td>?</td>
<td>?</td>
<td>-9.8</td>
</tr>
<tr>
<td>2</td>
<td>?</td>
<td>?</td>
<td>-9.8</td>
</tr>
</tbody>
</table>

If you reverse the problem solving method from exercise 66, then you’ll be working to the left on this table. This set of accelerations would hold true if the apple’s downward speed increased by another $9.8 \text{ m/s}$ for every second of free fall. E.g., $v_1 = -9.8 \text{ m/s}$ and $v_2 = -19.6 \text{ m/s}$. Note: This is consistent with the function, $v(t) = gt$, as you might recall from high school physics.

When doing real life physics research, sometimes you don’t already know the formula for your function from high school physics class, and you frequently have to work with derivatives as your starting point. Calculating derivatives in real life is a definite skill for all researchers. Let’s look at a few streamlined examples from my astrophysics research program.

**Learning objective 1: Will the quantum star tunnel or not?**

Engineering students get to learn about destructive testing. I can go one better: In my astrophysics research, I get to study ways to detonate exotic astrophysical objects, quantum stars and black holes. Ordinary hydrogen stars, like our star, the Sun, frequently detonate
in a supernova if they are large enough. Those are excellent to study, and many physicists set up elaborate models of supernova detonation. But hydrogen stars are not exotic – they are all over the cosmos. The quantum stars I study were numerous, we think, during the first few milliseconds after the Big Bang, the hot, dense compact beginning of our universe.

A quantum star can be defined as a self-gravitating quantum system, a quantum field with sufficient density and energy that it curves spacetime enough to hold together gravitationally. The “equations of motion” of this quantum field, however, are not Newton’s three laws of motion. If only they were that simple! Instead there are wave equations of quantum mechanics coupled to the Einstein field equations of relativity. Tricky derivatives are everywhere and usually cannot be dodged, so very few solutions come from pencil and paper. A real quantum star, with the mass of a naval destroyer or of a thousand suns, lives in its differential equations, and one must hunt amongst those derivatives, using methods similar to those of exercise 66.

![Quantum field energy function](image)

**Figure 4.3:** A typical early universe potential energy $V(s)$ for quantum field $s$. There are two minima and one local maximum, all of which are important to the physics of the quantum star.

A quantum star holds together because of the energy in the quantum field. Fig. 4.3, shows the shape of a typical quantum energy profile that, we think, must have occurred during the “early universe,” the first few seconds after the Big Bang. To be more precise, this is a temperature-dependent potential energy, a function of quantum field $s$. Its shape determines how the quantum field behaves and what values $s$ can take. One can interpret this curve with the analogy of a hill: the quantum field $s$ is like a ball rolling down the hill whose shape is $V(s)$. Several points on this “hill” are critical for figuring out the detonation process.
a. The top of the bump in the potential is the local maximum at approximately $s = 0.0388$, where $V(s) = 0.0003863$. This is the energy barrier.

b. The bottom of the dip in the potential is the global minimum at approximately $s = 0.0863$, where $V(s) = -0.0002876$. This is called the true vacuum.

c. The potential has its “false vacuum” at local minimum $s = 0$.

Note: Just like in exercise 66, I looked up the values of items a. and b. on the Excel spreadsheet from which I generated the plot. See Appendix. Table 4.2 is a table of backwards derivatives from the spreadsheet. Notice that the backwards derivative changes sign just past $s = 0.0388$, the estimated location of the local maximum; therefore, the true location is somewhere on the interval $(0.0388, 0.0397)$. Similarly, the global minimum is located somewhere on the interval $(0.0863, 0.0871)$. In practice, on real life research, you would try to narrow down your search in these intervals, and perhaps introduce other methods, like a forward derivative. Finding the best, most accurate, most efficient method of finding the maximum or minimum can be a big job.

Table 4.2: Backwards derivatives of potential $V(s)$.

<table>
<thead>
<tr>
<th>$s$</th>
<th>$V(s)$</th>
<th>Backwards derivative of $V$</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0380</td>
<td>0.000386033</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0388</td>
<td>0.000386282</td>
<td>0.000288331</td>
<td>local maximum</td>
</tr>
<tr>
<td>0.0397</td>
<td>0.000385708</td>
<td>-0.000665194</td>
<td>slightly downhill</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0854</td>
<td>-0.000286731</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0863</td>
<td>-0.000287631</td>
<td>-0.001042805</td>
<td>global minimum</td>
</tr>
<tr>
<td>0.0871</td>
<td>-0.000286697</td>
<td>0.001082642</td>
<td>slightly uphill</td>
</tr>
</tbody>
</table>

Back to physics! If a ball starts to the left of the bump, it will roll down the hill toward the bottom. The quantum field $s$, however, can either roll down the hill toward $s = 0$ or it can tunnel through the hill, come out to the right of the bump, and roll down into the true vacuum. Quantum tunneling is one of the most unusual aspects of quantum physics.

One kind of detonation process begins with a tunneling event, from the left side of the bump to the true vacuum on the right. The tunneling event becomes more likely if the bump is lower or narrower, less probable if it is taller or wider. So if you want to detonate some nice quantum stars, you have to know your derivatives and calculate carefully!

Learning objective 2: Quantum star central density and redshift.

The quantum tunneling also depends on where the ball starts on the left side of the barrier. Is its initial value close to the top? If so, tunneling will be more probable. Is its initial value near $s = 0$? If so, tunneling will be less probable.
In addition, when taking gravity into account with the Einstein field equations, starting values of the field $s$ control stability. That is, will the star must have sufficient density and energy to curve spacetime and hold itself together gravitationally?

The starting point for the real life computation is a set of “laws of motion” for the quantum field and the curvature of four-dimensional spacetime. These laws are loaded with derivatives. We can compare the quantum star detonation problem to the backwards table method mentioned at the end of Example Problem 1: *what can one do when one has all the laws of motion but no measurements?*

Figure 4.4 shows a pair of sample quantum field solutions. You can think of them as the plot of a set of data points from a large table like the table in exercise 66.

![Figure 4.4: Two field strength functions, $s_1(r)$ and $s_2(r)$, computed by analyzing derivatives in the wave equation and Einstein field equations. They represent two quantum stars of different diameters and masses.](image)

Field solution $s_1(r)$ shows the strength of the field varying with distance $r$. Most of the field is inside $r = 2$. One could say this quantum star’s surface is at about $r = 2$. Notice that its starting value is $s = 0.035042508$ at $r = 0$. This corresponds to a point about 90% of the way up the hill in Fig. 4.3.

Another field solution, $s_2(r)$, starts at $s_2(0) = 0.0164$. It starts lower, about 42% of the way up the hill, and it pokes along slowly before asymptotically reaching zero out past $r = 6$.

The first solution will trigger detonations more readily, the second solution less readily.

The way for computing the exact field profiles $s_1$ and $s_2$ is complex, requiring great amounts of work, but all the same, it is remarkably similar to exercise 66 and working leftward across
the table, from derivatives to original function \( s(r) \). And it is the function \( s(r) \) which tells us most of the physical properties of a star.

But what do the derivative data look like? What kind of table must one set up? Most of the quantum stars that I work on are quite complex, but there is a fairly simple model we can look at. It is called the Klein-Gordon geon. [1]

\[
s'' - \frac{1}{c^2} \ddot{s} = \left( \frac{mc}{\hbar} \right)^2 s(r)
\]

This is the Klein-Gordon equation, the relation between field \( s \) and two kinds of derivatives: second spatial derivative, \( s'' \) and second time derivative denoted by overdots, with mass of the field denoted \( m \), speed of light \( c \) and the fundamental quantum scale factor, Planck’s constant, \( \hbar \).

The table method for the Klein-Gordon equation here would be fairly complicated, compared to exercise 66. But you can do a reasonable job, starting at the top of the table, working to the left, then down to later and later times. It would take a few Excel spreadsheets linked together, or you could make a custom program in C or MatLab or Maple or Mathematica. In any method, you must work very carefully with these real life derivatives, especially if you like detonating quantum stars!

**Bonus learning objective: Black holes, spacetime curvature and calculating Calculus I derivatives.**

The textbook authors have connected the geometric ideas of tangency and velocity with the concept of a derivative. This is not accidental. Mathematicians tangle with derivatives because they like studying tangents and velocity vectors. In the theory of relativity, we think of spacetime as a four dimensional curved manifold, like the surface of a bowling ball. Think of calculus that must be computed on curvy graph paper. Tangent vectors are key. As one author states, “It is this notion of...tangent vectors that lies at the foundation of calculus on manifolds.” [2]

Another part of my research program involves black holes and how they can detonate various early universe objects. Black holes are objects so dense that even light does not have sufficient escape velocity. Even light is trapped, without escape, inside the event horizon of a black hole.

If we have time during the second lecture, we will take a look at the powerful notion of derivative as applied to an ordinary, everyday curved surface: the spherical surface of a bowling ball! Just as the behavior of tangent vectors quantify the curvature of a bowling ball, so tangent vectors also find frequent use for understanding the curvature of spacetime around a black hole.
Appendix A: The potential $V(s)$

The potential $V(s)$ in section 4 is with $\eta = 12.49$, $\Lambda = 300$ and $\Delta s = 0.00086255$.

$$V(s) = s^2 - 2 \eta s^3 + \frac{1}{2} \Lambda s^4$$

CHAPTER 4. REAL LIFE DERIVATIVES IN A QUANTUM STAR.
Chapter 5

Optimization to Engineering Problems

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Department of Civil and Environmental Engineering

Weeks
March 25 and April 1, Spring 2009.
Graphing a function and finding the maximum and/or minimum values

Example Problem 1. Section 4.1, Exercise 66

On May 7, 1992, the space shuttle Endeavor was launched on mission STS-49, the purpose of which was to install a new perigee kick motor in an Intelsat communications satellite. The table gives the velocity data for the shuttle between liftoff and the jettisoning of the solid rocket boosters.

<table>
<thead>
<tr>
<th>Event</th>
<th>Time (s)</th>
<th>Velocity (ft/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Launch</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Begin roll maneuver</td>
<td>10</td>
<td>185</td>
</tr>
<tr>
<td>End roll maneuver</td>
<td>15</td>
<td>319</td>
</tr>
<tr>
<td>Throttle to 89%</td>
<td>20</td>
<td>447</td>
</tr>
<tr>
<td>Throttle to 67%</td>
<td>32</td>
<td>742</td>
</tr>
<tr>
<td>Throttle to 104%</td>
<td>59</td>
<td>1325</td>
</tr>
<tr>
<td>Maximum dynamic pressure</td>
<td>62</td>
<td>1445</td>
</tr>
<tr>
<td>Solid rocket booster separation</td>
<td>125</td>
<td>4151</td>
</tr>
</tbody>
</table>

(a) Use a graphing calculator or computer to find the cubic polynomial that best models the velocity of the shuttle for the time interval 0 \leq t \leq 125. Then graph this polynomial.

(b) Find a model for the acceleration of the shuttle and use it to estimate the maximum and minimum values of acceleration during the first 125 seconds.

Strategy:

Let us use a computer program (MS-EXCEL) to graph the variation of velocity with time for the first 125 seconds of flight after liftoff. The graph is first created as a scatter plot and then a trendline is added. The trendline menu allows for the selection of a polynomial fit and a cubic polynomial is picked as required in the problem description above.

Solution:

(a) The final curve and the corresponding cubic polynomial function that best models the data are shown in the figure below. From the graph, the function \( y(x) \) or \( v(t) \) can be expressed as

\[
v(t) = 0.0015 t^3 - 0.1155 t^2 + 24.982 t - 21.269.
\]

(b) From physics, we know that acceleration is defined as the derivative of velocity with time. Thus, differentiating the expression for velocity above provides us with a model for the acceleration \( a(t) \):

\[
a(t) = \frac{dv(t)}{dt} = 0.0045 t^2 - 0.231 t + 24.982.
\]
In order to estimate the maximum and minimum values of acceleration during the first 125 seconds of flight, that is in the interval \(0 \leq t \leq 125\), we now apply the Closed Interval Method to the continuous function \(a(t)\) on this interval. The derivative is

\[
a'(t) = \frac{da(t)}{dt} = 0.009 t - 0.231.
\]

The critical number occurs when \(a'(t) = 0\); which gives us

\[
t_1 = \frac{0.231}{0.009} \approx 25.67 \text{ seconds}.
\]

Evaluating the acceleration at the critical number and at the endpoints, we get

\[
a(25.67) = 22.0 \text{ ft/s}^2; \ a(0) = 24.982 \text{ ft/s}^2; \ \text{and} \ a(125) = 66.42 \text{ ft/s}^2.
\]

Thus, the maximum acceleration is \(66.42 \text{ ft/s}^2\) and the minimum is \(22.0 \text{ ft/s}^2\).

**Optimization Problem**

**Example Problem 2.** Section 4.7, Exercise 34

A fence is 8 feet tall and runs parallel to a tall building at a distance of 4 feet from the building. What is the length of the shortest ladder that will reach from the ground over the fence to the wall of the building?
Strategy:
Draw a sketch of the problem to understand the geometry.

Solution:
From the figure using trigonometry, the length of the ladder can be expressed as

\[ L = AB + BC = \frac{H}{\sin \theta} + \frac{D}{\cos \theta}. \]

Next, we need to find the critical number for \( \theta \) for which the length \( L \) of the ladder is minimum. This is done by differentiating \( L \) with respect to \( \theta \) and setting it equal to zero. Thus,

\[ \frac{dL(\theta)}{d\theta} = -H \csc \theta \cot \theta + D \sec \theta \tan \theta = 0 \quad \Rightarrow \quad \frac{H \cos \theta}{\sin^2 \theta} = \frac{D \sin \theta}{\cos^2 \theta} \quad \Rightarrow \quad \tan^3 \theta = \frac{H}{D}. \]

The critical number for \( \theta \) becomes

\[ \theta = \tan^{-1} \left( \frac{H}{D} \right)^{1/3} = \tan^{-1} \left( \frac{8}{4} \right)^{1/3} = 51.56^\circ. \]

The corresponding length of the ladder is \( L = 16.65 \text{ ft} \).

Introductory remarks

In this section, we will discuss the application of these concepts of Calculus to different engineering disciplines. Some of the future courses (that you may take) that this will be relevant for are:
EGN3310  Engineering Mechanics - Statics
EGN3321  Engineering Mechanics - Dynamics
EGN 3331  Mechanics of Materials
EML 3601  Solid Mechanics

and several of your engineering major courses.

Background/Motivation

There are cases of real-world engineering problems in the various areas of engineering practice where the topics that you are learning in Calculus on the use of derivatives are applied. The concepts dealing with finding the global and local extreme values and its application to optimization are very commonly used in engineering. It could be the optimization of the shape of a structure, a transportation system, shape of a component or machinery or a process that moves humans and goods. The diverse applications discussed in this section provide an insight into the world of engineering design and practice.

In this section, we will apply the methods you have learned in Chapter 4 of your Calculus I class to determine the critical number and the global and local maxima/minima of a function. This technique is then applied to solving optimization problems. This section will give you a preview of some of the advanced concepts you are likely to see in later courses.

Calculus Concepts to be covered in this section - reinforcement

- Global and local extreme values
- Critical Number
- Closed Interval Method
- Optimization Problems using application of the concepts above

Applications to engineering to be covered in this section - introductory exercises

- Maximum range of a projectile - (Mechanical and Aerospace Engineering)
- Optimization of Dam location on a river - (Civil Engineering)
- Potential Energy and stability of equilibrium - (Mechanical, Civil, Aerospace, Electrical Engineering)
• Optimal shape of an irrigation channel - (Civil Engineering)

• Overcoming friction and other forces to move an object - (Mechanical, Civil, Aerospace, Electrical Engineering)

These concepts will build upon concepts that you learn in college-level physics courses, in particular Physics I. Calculus is the basis for a large number of engineering analysis that leads up to safe and economical design. The Calculus of extreme values and optimization are used in all disciplines of engineering. Mechanical and civil engineers use it for the optimal design of components and structural systems. They also use the concept of minimization of energy and analysis of the stability of systems. Industrial engineers are involved extensively in optimization of systems that may deal with management of manufactured goods or movement of humans such as theme-park management. Electrical and computer engineers require these principles to analyze the energy and power requirements and an optimal system for miniaturization of components.

I am a faculty member in the civil and environmental engineering department at UCF since 1993 and specialize in geotechnical engineering. This field deals with study of soils and design of foundations. It is also related to the analysis of slopes, earthquake waves in soils and rocks, sinkholes and the design of pavement systems. It is a field with a great degree of uncertainty due to the non-homogeneous and complex nature of soils and rocks. It makes for an exciting and challenging career.

We will try our best to emphasize the importance of these key tools that you are learning in Calculus to application to real world problems in engineering.

Applying Calculus to projectile dynamics problems in Engineering

This introductory exercise is related to mechanical and aerospace application involving projectiles such as missiles.

Maximizing the Range of a Projectile (example, a forward pass in football)

The range \( R \) of a projectile whose velocity out of the muzzle is \( v \) meters per second is given by the expression

\[
R = \frac{v^2 \sin 2\theta}{g}
\]

where \( \theta \) is the angle of elevation in radians and \( g = 9.8 \text{m/s}^2 \) is the acceleration due to gravity. The figure shows the range and angle of elevation. The actual problem is more complex dealing with the vertical height as accelerated motion but we will simplify the
problem to study only the range as a function of, for a constant velocity. What initial angle of elevation provides the maximum range or distance traveled for the projectile?

\[ \theta \]

**Strategy:**

Find the maximum value of the range \( R \) with respect to different angles of elevation. Next, we must differentiate \( R \) with respect to \( \theta \) and set it to zero to find the global maxima. Note that in this case, \( v \) and \( g \) are constants. The end points for the interval for forward motion are \( 0 \leq \theta \leq \pi/2 \).

**Solution:**

Since the range is given by

\[ R = \frac{v^2 \sin 2\theta}{g} \]

\[ \Rightarrow \]

\[ \frac{dR}{d\theta} = \frac{v^2 \sin 2\theta}{g} = 0 \]

As \( v \) and \( g \) are both non-zero,

\[ \cos 2\theta = 0 \]

Using trigonometric double angle formula:

\[ \cos 2\theta = 2 \cos^2 \theta - 1 = 0 \]

\[ \Rightarrow \]

\[ \cos \theta = \frac{1}{\sqrt{2}} \]

\[ \Rightarrow \]

\[ \theta = \frac{\pi}{4} \]

Evaluating the range at the critical value gives \( R(\pi/4) = \frac{v^2}{2} \) and at the two endpoints provides \( R(0) = 0 \) and \( R(\pi/2) = 0 \). Thus, the maximum range for the projectile is reached if the angle of elevation is \( \pi/4 \) or \( 45^\circ \). In general, any projectile travels the longest range when the initial angle of elevation or launch is \( 45^\circ \).

It must be noted that it was not necessary to differentiate in this problem if you were able to recognize the fact that if the function \( \sin 2\theta \) is plotted for different values of \( \theta \), it reaches
Learning the optimization of the shape of a structure under given constraints

This example is related to the courses in Fluid Mechanics and Hydraulics in the Civil Engineering field. Civil Engineers often design hydraulic systems at an optimal location along the river and will also have to optimize the size of the dam to perform its function correctly.

Optimizing the Location of a Dam on a River

The depth of the water in the St. Johns River measured \( x \) miles downstream from Rock Springs is \( D(x) = 20x + 10 \) feet, and the width of the river along \( x \) is given by \( W(x) = 10(x^2 - 8x + 22) \) feet. To create a new lake, it is necessary to place a dam downstream from Rock Springs as shown in the figure below.

\[ \text{(a) If the dam cannot be more than 310 feet wide and 130 feet above the riverbed, and the top of the dam must be 20 feet above the present river water surface, what is a range of locations that the dam can be placed?} \]
(b) What are the dimensions of the widest and narrowest dam that can be constructed in accordance with the above constraints?

(c) If the cost is proportional to the product of the width and the height of the dam, where should the most economical dam be located?

**Strategy:**

Use the Closed Interval Method to find the widest and narrowest dam in the range of acceptable locations of the dam. Define the cost function as proportional to the product of width and height and minimize it with respect to the location $x$ measured from Rock Springs.

**Solution:**

(a) Based on the constraints stated in the problem description, we can state the following relationships

$$D(x) = 20x + 10 \leq 110 \quad \Rightarrow \quad x \leq 5,$$

and

$$W(x) = 10 \left(x^2 - 8x + 22\right) \leq 310 \quad \Rightarrow \quad -1 \leq x \leq 9.$$

Therefore, the range for the location of the dam along the river measured from Rock Springs is given by: $0 \leq x \leq 5$ feet.

(b) In order to obtain the widest (maximum $W$) and narrowest (minimum $W$) for the dam, we will apply the Closed Interval Method for the function $W(x)$ in the interval $0 \leq x \leq 5$.

Given the expression for the width of the dam: $W(x) = 10 \left(x^2 - 8x + 22\right)$

$$\frac{dW(x)}{dx} = 20x - 80 = 0.$$

So, $x = 4$ feet is the critical value and the corresponding width $W(4) = 60$ feet is the minimum width. Next, checking the endpoints of the interval, we obtain the following values: $W(0) = 220$ feet and $W(5) = 70$ feet. Thus, the maximum width of the dam is 220 feet at Rock Spring ($x = 0$).

(c) Since the cost function is proportional to the product of the width and height of the dam, we multiply the expressions for $W(x)$ and $H(x)$. The height of the total dam must be 20 feet more than its depth and can be expressed as $H(x) = D(x) + 20 = 20x + 30 = 10(2x + 3)$. If we incorporate the constant 10 into the constant of proportionality $F$, we can then define the cost function as

$$C(x) = F \left(x^2 - 8x + 22\right)(2x + 3) = F \left(2x^3 - 13x^2 + 20x + 66\right),$$

where $F$ is a positive constant.
Differentiating the cost function to find the critical number for \( x \):

\[
\frac{dC(x)}{dx} = F(6x^2 - 26x + 20) = 2F(3x - 10)(x - 1) = 0.
\]

Solving for the two values of \( x \), which are \( x = 1 \) and \( 10/3 \) and substituting them into the cost function equation, we find that the cheaper dam occurs at \( x = 10/3 \). The cost of the dam at this location is $62.30F. The cost of the dam built at the Rock Springs location \( (x = 0) \) is $66F. Checking the other endpoint of the interval, we get the cost of the dam at \( x = 5 \) is $91F. Therefore, the location with the minimum cost is at \( x = 10/3 \).

**Understanding how to optimize the shape of a water transport channel**

This is an application related to land development and surface hydrology. You will encounter such engineering applications in Water Resources and Geotechnical Engineering fields within Civil Engineering. The related courses in civil engineering are Fluid Mechanics, Hydrology and Hydraulics.

**Optimization the Shape of an Irrigation Channel**

A trapezoidal channel of uniform depth \( d \) is shown in the figure below. To maintain a certain volume of flow in the channel, its cross-sectional area \( A \) is fixed at say 100 square feet. The objective is to minimize the amount of concrete that must be used to construct the lining of the channel.

**Strategy:**

The dimension \( b \) is the base width of the channel, \( \theta \) is the angle of inclination of each side. The other relevant dimensions are labeled on the figure. We must minimize the length \( L \) of
the channel perimeter excluding the top. To simplify this example for our introductory level exercise, let us assume

\[ \theta_1 = \theta_2 = \theta \quad \text{and} \quad e_1 = e_2 = e. \]

**Solution:**

Using the geometry of the channel, we can express the length \( L \) as:

\[ L = h_1 + b + h_2, \]

where \( h_1 \) and \( h_2 \) are the two inclined sides of the channel and are equal to \( d / \sin \theta \) each. Using the given information that the area \( A \) of the channel is exactly 100 square feet,

\[ A = 100 = bd + 2 \left( \frac{1}{2} cd \right) \Rightarrow b = \frac{100}{d} - e = \frac{100}{d} - \frac{d}{\tan \theta}. \]

Therefore, the wetted \( L \), which is the length of the channel cross-section in contact with the water when flowing full, as a function of both \( \theta \) and \( d \) can be written as follows

\[ L = \frac{100}{d} - \frac{d}{\tan \theta} + \frac{2d}{\sin \theta}. \]

Minimizing \( L \) as a function of both variables \( \theta \) and \( d \) requires Advanced Multivariable Calculus which you have not learned as yet. So, we simplify the problem further by specifying one of the variables (or design parameters) and select \( \theta = \pi / 3 \). Thus, the expression for \( L \) reduces to the following

\[ L = f(d) = \frac{100}{d} - \sqrt{3}d. \]

We want to obtain the global minimum of \( L \) for \( 0 < d < \infty \). Differentiating \( L \) with respect to \( d \) and setting it equal to zero yields

\[ \frac{dL}{dd} = f'(d) = -100d^{-2} + \sqrt{3} = 0 \quad \Rightarrow \quad d^2 = \frac{100}{\sqrt{3}} \quad \Rightarrow \quad d = \frac{10}{\sqrt{3}} = 7.5984. \]

Since \( f''(d) = \frac{200}{d^3} > 0 \) on the interval \((0, \infty)\), the length of the channel with \( d = 7.5984 \), i.e. \( f(7.5984) \approx 26.322 \) is the global minimum.
Understanding how to minimize potential energy to build a stable system

This is an application from Mechanical and Civil Engineering. You will first encounter such examples in introductory courses in engineering such as Statics and Dynamics. Following these, such applications will be found in courses in Component and Machine Design and Structural Analysis.

Potential Energy and Stability of Equilibrium

The pinned bars are held in place by a linear spring are parts of a machine. Each bar has a weight of \( W \) and length \( L \). The spring is unstretched when the angle of displacement of the bar, \( \alpha = 0 \), and the bars are in equilibrium when \( \alpha = 60^\circ \). Determine the spring constant \( k \), and also determine if this equilibrium position is stable or unstable.

Note that from an engineering perspective, the minimization of potential energy in this system will help in the stability of the system and maintain it in its equilibrium state.

Strategy:

The only forces that do work on the bars are their weights and the force exerted by the spring. By expressing the total potential energy \( U \) in terms of \( \alpha \) and using the equation \( U'(\alpha) = 0 \), we can solve for the spring constant \( k \).

Solution:

If we use the datum or reference state as shown in figure below, the potential energy associated with the weight of the two bars is equal to the sum of the weights of each bar times the translations of each bar measured at the centers of gravity as shown. Datum is defined as the state from which all changes are measured. Therefore, the potential energy due to the two bars is:

\[
U_1 = W \left(-\frac{1}{2}L \sin \alpha \right) + W \left(-\frac{1}{2}L \sin \alpha \right) = -WL \sin \alpha.
\]
The spring is unstretched when \( \alpha = 0 \) and the distance between the points A and B is \( 2L \cos \alpha \). Thus, the stretch of the spring (\( \delta \)) is

\[
\delta = 2L - 2L \cos \alpha.
\]

The potential energy associated with the spring is

\[
U_2 = \frac{1}{2}k(2L - 2L \cos \alpha)^2.
\]

The total potential energy is given by

\[
U = U_1 + U_2 = -WL \sin \alpha + 2kL^2(1 - \cos \alpha)^2.
\]

When the system is equilibrium, the total potential energy is in a minimum state with respect to the rotation from its rest state. Thus,

\[
\frac{dU}{d\alpha} = -WL \cos \alpha + 4kL^2 \sin \alpha(1 - \cos \alpha) = 0.
\]

Since we are told in this example that the angle at the time of equilibrium is \( \alpha = 60^\circ \), we can solve for the spring constant \( k \), as follows

\[
k = \frac{W \cos \alpha}{4L \sin \alpha(1 - \cos \alpha)} = \frac{W \cos 60}{4L \sin 60(1 - \cos 60)} = \frac{0.289W}{L}.
\]

**Stability Check:**

The second derivative of the potential energy is an indicator of the stability of the equilibrium position. If the second derivative is a positive number, the position is stable.

\[
\frac{d^2 U}{d\alpha^2} = WL \sin \alpha + 4kL^2 \left[ \cos \alpha(1 - \cos \alpha) + \sin^2 \alpha \right] = WL \sin 60 + 4kL^2 \left[ \cos 60(1 - \cos 60) + \sin^2 60 \right].
\]

This is a positive number since \( \cos 60 < 1 \) and \( W, L \) and \( k \) are positive constants. Thus, the equilibrium position is indeed stable.
Understanding how to apply extreme value concepts in Calculus to a friction and static equilibrium problem

Friction is an important topic in many different areas of engineering including mechanical, aerospace, civil and industrial engineering. This application deals with concepts you will see in the Engineering Mechanics class (such as free body diagrams, equilibrium of forces and friction.

Overcoming Forces to Move a Car Stuck in Snow

The man in the figure below exerts a force $P$ on the car at an angle $\alpha$. The car has a mass
of 17.27 kN and is a front wheel drive vehicle. The driver in the car is able to spin the front wheels and the coefficient of kinetic friction there is $\mu_k = 0.02$. The snow behind the rear tires has accumulated and exerts a horizontal resisting force of $S$. Getting the car to get unstuck and move requires overcoming the resistance force of $S = 420$ N. What value of the angle $\alpha$ minimizes the magnitude of the force $P$ needed to push by the man to overcome the resistance on the rear tires due to the snow?

**Strategy**

Draw a pictorial representation of all the forces acting on the car. This is known as the Free Body Diagram (FBD) of the car and is shown in the figure below. Label all the dimensions on the FBD. Then apply equations of equilibrium on this FBD. This is something you will learn in Physics I and then apply it in the Engineering Mechanics - Statics (EGN 3310) class. Express $P$ as a function of the angle of push $\alpha$. Next, find the global minimum for $P$ for different values of $\alpha$ in the range $0 < \alpha < 90^\circ$.

**Solution:**

Referring to the Free-body Diagram shown in the figure, the equations of equilibrium in two-dimensions for the balance of forces and moments (rotations) give us the following three equations:

$$S - \mu_k N_F - P \cos \alpha = 0 \quad (5.1)$$

$$N_R + N_F - W - P \sin \alpha = 0 \quad (5.2)$$

$$-W(1.62) + N_F(2.55) + P \cos \alpha(0.90) - P \sin \alpha(3.40) = 0 \quad (5.3)$$

From Equation 5.1 we can write

$$N_F = \frac{1}{\mu_k} (S - P \cos \alpha) \quad (5.4)$$
and from Equation (5.2),
\[ N_R = -N_F + W + P \sin \alpha. \] (5.5)
Substituting equation (5.4) into equation (5.3) gives us an expression for \( P \) as a function of \( \alpha \) as follows:
\[-1.62W + 2.55 \frac{1}{\mu_k}(S - P \cos \alpha) + 0.90P \cos \alpha - 3.40P \sin \alpha = 0.\]

Differentiating this equation, using the chain rule, to find \( \frac{dP}{d\alpha} \) and setting it equal to zero will provide us with the minimum value of \( \alpha \).

Thus,
\[ \frac{2.55}{\mu_k} \left[ -\frac{dP}{d\alpha} \cos \alpha + P \sin \alpha \right] + 0.90 \frac{dP}{d\alpha} \cos \alpha - 0.90P \sin \alpha - 3.40 \frac{dP}{d\alpha} \sin \alpha - 3.40P \cos \alpha.\]

Solving for \( \frac{dP}{d\alpha} \) yields
\[ \frac{dP}{d\alpha} = -P \left[ \left( \frac{2.55}{\mu_k} - 0.90 \right) \sin \alpha - 3.40 \cos \alpha \right] \frac{2.55}{\mu_k} \cos \alpha = 0 \]

Simplifying this expression we get,
\[ \tan \alpha = \frac{3.40}{\frac{2.55}{\mu_k} - 0.90} \quad \Rightarrow \quad \alpha = 1.54^\circ \]

I hope these real world engineering applications have made you aware of some interesting situations where we use Calculus in engineering.

**References**


Chapter 6

Applications of Integration in Biomedical Science

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Weeks
April 8 and 15, Spring 2009.
Defining area under the curve

Approximating rectangles

Example Problem 1. Section 5.1, Exercise 1

By reading values from the given graph of $f$, use five rectangles to find a lower estimate and an upper estimate for the area under the given graph of $f$ from $x = 0$ to $x = 10$. In each case sketch the rectangles that you use.

![Graph of $y = f(x)$](image)

In this chapter, we will discuss the importance of integration in calculating the quantity of metabolites, proteins, or chemicals from mixtures as it applies to the concept of chromatography. This 'real world' application of calculus is pervasive throughout chemistry, molecular biology, biochemistry and biomedical science in general.

Some of the future courses (that you may take) that this will be relevant for are:

- **MCB 3020** General Microbiology
- **BSC 3403C** Quantitative Biological Methods
- **MCB 4414** Microbial Metabolism
- **BCH 4053** Biochemistry I
- **BCH 4054** Biochemistry II
Background/Motivation

The ability to quantify a given amount of any biological molecule is critical in analysis of biology and the fundamental study of living systems. Calculus is needed to best approximate the concentration of a substance after separation by chromatography in order to gain information on the amount of that substance in a given sample. **Chromatography** is defined as techniques used to separate the components of mixtures. In this section we will apply several methods to determine ‘area under the curve’ and show how this is needed for biomedical applications. This section will then integrate (sorry for the pun) the mathematics of calculus to real world applications, and give you a sneak peak on concepts you are likely to see in later courses. Terms that may be unfamiliar to you are in bold and are defined in a glossary at the end of this chapter.

**Calculus Concepts to be covered in this section - reinforcement**

- Approximating rectangles to determine area under the curve.
- Limits of approximating rectangles.
- Fundamental theorem of calculus - how it applies to ‘area under the curve’.

![Graph of a function y = f(x) with area under the curve shaded.](image)
Applied Concepts to be covered in this section - real world applications

- Use of chromatography to separate mixtures.
- Types and uses of chromatography.
- Brief introduction into methods used to detect target compounds such as proteins.
- Patterning analysis for diagnosis of cancer - cutting edge proteomics.

We will try our best to truly ’integrate’ these concepts to emphasize the importance of these key tools of Calculus on the outside world.

Use of chromatography to separate mixtures

Why are mixtures a part of the study of biology?

Biological cells are made up primarily of Carbon, Hydrogen, Nitrogen, Oxygen, Phosphorus and Sulfur (CHNOPS!), as well as a few choice trace minerals such as Zinc, Magnesium, Manganese, Iron, Selenium, Molybdenum, etc. All living cells, whether they are bacteria, archaeabacteria, or eukaryotes (like us humans) are made up primarily of proteins, nucleic acids and lipids.

Based on studies in the commonly studied bacterium Escherchia coli, there are at least 2000 proteins present under nearly any growth condition. In addition there are hundreds, if not thousands, of small molecules metabolites present in the cytosol. To study proteins (enzymes) we must first isolate them away from other proteins so that we can determine what their particular role is in biology. We also would like to determine changes in the level of certain compounds (e.g. metabolites such as ATP or amino acids) upon varying the growth conditions of the organism. To do this, methods have been devised to separate mixtures by their characteristics.

Separation of proteins will be our best example. Proteins are made up of amino acids that each have a different 'functional group'. These functional groups impart the specific chemical properties that each unique protein exhibits, i.e. no two proteins are alike because they are all made from a unique set of amino acid combinations. This 'signature' characteristic allows biochemists to separate and therefore to study proteins individually. Without the development of chromatography for this purpose the current state of biomedical research would not be nearly as advanced as it is today. Proteins are separated from one another on the basis of:

1. **Net charge** (ion exchange chromatography),
2. **Hydrophobicity** (hydrophobic affinity),
3. **Size** (gel filtration) or
4. **Direct affinity** to a ligand (affinity chromatography).

The figure below shows an example of separation of mixtures using ion exchange chromatography:

![Figure 6.1: Elution of a sample mixture from a chromatographic column.](image)

You may already notice one of the reasons why we have chosen this concept to match with the study of integrals (Hint: look closely at part B of the above figure!). By combining **chromatography** with **spectroscopy** (identifying proteins by their ability to absorb ultraviolet (UV) light as they pass out of a column), we can separate mixtures into purified components. This technique is critical to nearly all aspects of biochemistry.
Limitations of approximating rectangles

Example Problem 2. Section 5.1, Exercise 2

Use six rectangles to find estimates of each type for the area under the given graph of \( f \) from \( x = 0 \) to \( x = 12 \).

(i) \( L_6 \) (sample points are left endpoints)
(ii) \( R_6 \) (sample points are right endpoints)
(iii) \( M_6 \) (sample points are midpoints)

Are left endpoints an overestimate or an underestimate of the true area?
Are right endpoints an overestimate or an underestimate of the true area?
Which gives the best area approximation and why?

Types and uses of chromatography

In addition to its relevance in separating proteins from living cells, there are many different forms of chromatography that are use everyday by researchers in disciplines such as chemistry, forensic science, biology, biochemistry, microbiology and cell biology. Each has an important role in many disciplines, and each also can be quantitative. The primary method for
determining the identity and estimating the quantity of a protein (for example) that is eluting from a column is by determining the area under the curve of a "peak" that is recorded during elution of that protein. Let’s look at some examples of chromatography first, and then further discuss the role that integration plays in data analysis.

Most common types of chromatography used in biomedical research

Liquid chromatography (LC)

Liquid chromatography is a general term to describe the separation of molecules via a liquid phase, or mobile phase as it passes through a column, also known as the solid phase. The solid phase is the the material present in the column. Solid phases can have a variety of functional groups attached so that molecules will be separated out based on charge, size, hydrophobicity, etc. as discussed in the previous section. LC is generally used to purify proteins from cell extracts. Note: you will actually carry out LC experiments in a course called Quantitative Biological Methods if you are a Molecular Biology and Microbiology major.

Figure 6.2: A nineteen fifties era liquid chromatography experiment. Large scale separations are still done using similar columns in the biotech industry today to initially separate proteins such as antibodies and protein-based therapies that have been expressed in bacteria or yeast model systems.
High performance liquid chromatography (HPLC)

HPLC is the workhorse for separations and analysis of small metabolites. This is important since we need to know how changes in the character of cells are produced based on changes in the small molecules present in the cell. For example we know that caffeine can affect a person’s heart rate, but when adding caffeine to a cell in culture we must determine just how much caffeine actually gets inside a cell or tissue. HPLC analysis of the small molecules can help us to identify and quantify the amount of caffeine that actually permeated the cell membrane. Essentially the same as LC, HPLC incorporates a higher pressure on the liquid phase that allows for better separation of molecules while passing through, or binding and eluting to the solid phase support.

An overview of a typical HPLC setup is shown below. This overview shows the components found in a typical HPLC system. The solvent, also known as the mobile phase, is pumped into the column under high pressure (typically 10-20 bar). Samples are injected upstream of the column using an injector loop or an automated sample injector (robot). Based on the properties of the sample, the solvent, and the stationary phase the components of the sample can be separated. A detector is used to identify and/or quantify the compounds as they elute from the column. The resulting chromatogram is needed to quantify the amount of a given compound, and this is where integration is needed. The trace that is recorded is essentially a differentiable, continuous function that is defined by the time of elution during the separation.

Below you see an image of a typical HPLC system in 2007.

Gas chromatography (GC)

Gas chromatography is very similar to HPLC, with the exception that the mobile phase is a gas and the sample is either a gas or is modified chemically by a process known as
derivatization to a volatile form to allow for separation by GC. The column has a liquid stationary phase which is bound to an inert support phase that is solid. This form of chromatography is most common in analytical analysis of drugs (drug testing), pesticides and lipid analysis. This makes GC the workhorse of the chemical and petroleum industry. Various types of detectors are used to identify and quantify samples as they elute from the column, again using integration (area under the curve measurements) to enable this analytical measurement.

Figure 6.3 shows a typical GC chromatogram, used in this case for analysis of chemical weapons at the Lawrence Livermore National Laboratory.

Fundamental theorem of calculus

We have looked at examples of using rectangles to approximate area, but as you have just learned a much simpler way to determine area under the curve is possible if the function you are given is continuous. All chromatography outputs are simple $x$-$y$ plots that are always continuous (unless you turn off the detector!).

The fundamental theorem of calculus states:

Part 1: If $g(x) = \int_a^x f(t) \, dt$, then $g'(x) = f(x)$, where $f$ is a continuous function on $[a, b]$ and $x$ varies between $a$ and $b$. 
Figure 6.3: (a) This chromatograph of a sample was produced by a gas chromatograph-mass spectrometer. Hydrocarbons could be masking trace amounts of chemical weapon agents. (b) Once the hydrocarbons are removed, the analysis reveals the presence of a compound that is a precursor to a chemical warfare agent. This figure is courtesy of the Lawrence Livermore National Laboratory Chemical Weapons testing lab. Note the term red herring refers to a substance that is present in a sample to mask or throw off the analysis so that hidden compounds are not detected.

**Part 2:** If \( f \) is continuous on \([a, b]\), and \( F(x) \) is any antiderivative of \( f(x) \), then:

\[
\int_{a}^{b} f(x) \, dx = F(b) - F(a)
\]
Essentially, for purposes of defining area under the curve \( f \), the difference in the antiderivative \( F \) between two points \([a, b]\) on the curve (assuming a continuous function) is equal to the area between that curve and the \( x \)-axis.

This is the most critical application (in biological sciences) of the fundamental theorem. Say you have a power function. Then another way of stating the above mathematical principle is to simply use the power rule for integration and find the integral of the function at two points \( a \) and \( b \). You can plug in the values given for \( a \) and \( b \) for this integral and the resulting value is the area under the curve! The error that was seen in the use of rectangles to ‘estimate’ the area under the curve is no longer present.

For clarity see the following example from your textbook

**Example Problem 3.** Example 6 (page 346)

Find the area under the parabola \( y = x^2 \) from 0 to 1.

**Solution:**

An antiderivative of \( f(x) = x^2 \) is \( F(x) = 1/3x^3 \). The required area \( A \) is found using Part 2 of the Fundamental Theorem:

\[
A = \int_{0}^{1} x^2 \, dx = \frac{1}{3} x^3 \Big|_{0}^{1} = \frac{1}{3} 1^3 - \frac{1}{3} 0^3 = \frac{1}{3}.
\]

When using modern chromatography systems a computer will evaluate the output function,
then determine (given parameters that you set) where a given peak begins and ends, then integrates those two points to determine the 'peak area under the curve'. The output data is usually given as 'peak area units' and as such is essentially arbitrary. To actually determine the amount of a compound (e.g. ATP), one must inject a series of purified ATP samples over a range of concentrations. This gives one the ability to define a relationship (usually linear) between peak area units and the concentration. This is the so-called 'standard curve'.

Methods of detection in chromatography

For each separation one must be able to detect the sample of interest. This varies based on the chemistry of the compound being detected. For example, nucleotides (the components of the cell that make up deoxyribonucleic acid (DNA) and ribonucleic acid (RNA)) absorb light in the ultraviolet (UV) range.

Once you determine that your sample is detectable by a given technique (such as UV-visible spectrophotometry), you can use chromatography to separate and quantify the molecules of interest. Figure 6.4 shows an example of UV-visible detection for four different purines (precursors of ATP or DNA) separated by HPLC.

You can see that each purine is detected by UV-visible spectrophotometry, and this resulting 'trace' is a fully continuous function over a set time interval - perfect for a good example to apply 'area under the curve'. To determine which purines are present in a sample a standard purified mixture was applied to the column (panel A). Panels B, C and D are experimental samples: The question asked was - what happened to these purines in the presence of an enzyme that adds hydroxyl groups to purines? This is an experimental approach that used HPLC to identify and quantify the purines present in a mixture. The point to made here is that you must first know how to identify your sample of interest (outside of chromatography), and then use this as a method of detection to quantify your compound.

Patterning of analysis for diagnosis of cancer - cutting edge proteomics

Up until now you have seen relative simple chromatography examples, and ones used in basic research. Just for fun we are now going to look at a use for HPLC for cutting edge research related to detection of cancer. Hopefully this cutting edge application will help you to appreciate the need for mathematics, modeling and indeed computers to aid in biomedical science - all still fundamentally looking at two dimensional data!

The basic science:

As many as 100,000 different proteins may be made from 25,000 to 30,000 genes in the human genome. Since not every human is identical, the proteins that each of us produce from each
Figure 6.4: HPLC analysis of purine and hydroxylated derivatives. Retention time is plotted versus absorbance at 263nm, at which all of the tested purine derivatives have significant absorbance. Peaks that represent each compound from the standard are marked in A. (A) Standard mixture of purine, 2OH-purine, hypoxanthine, and xanthine. (B) PH incubated with 2OH-purine. (C) PH incubated with hypoxanthine. (D) PH incubated with purine. See Materials and Methods for further details. Reproduced for Proceedings of the National Academy of Science, June 20, 2000, vol. 97, no. 13, pp. 7208-7213.
cell and tissue are not all made at the same level in every cell. All of the proteins present in a cell, tissue or organism is known as the proteome. We can use HPLC coupled with various detection techniques (UV-visible spectrophotometry, mass spectrometry) to separate these proteins from a human sample such as blood. This separation can give each of us a ‘signature’ based on the proteins present. Of course the vast majority of proteins are the same and do not differ between individuals, otherwise we would not be human. Therefore if you were to compare the ‘profile’ of proteins eluting from a column between hundreds or even thousands of individuals, you would get a basal pattern that is not changing.

In disease states (when you have cancer) the proteins that are made are sometimes different or made in different amounts. Exactly which ones that are upregulated and downregulated (increased or decreased) differs with each disease (each type of cancer or degenerative disease). Recent research first developed by Dr. Lance Liotta (formerly of NIH but now at George Mason University in Virginia) has asked a very basic question. Do the proteins present in a patient’s blood with cancer form a unique pattern, based on HPLC-MS separation and detection, versus the ‘normal’ proteome profiles. The resounding answer is yes - and reveals a powerful tool in cancer diagnosis.

Figure 6.5: The figure above is a chromatogram of the proteins present in the blood of an ovarian cancer patient (General Keynote: Proteomic Patterns in Sera Serve as Biomarkers of Ovarian Cancer, Gynecologic Oncology 88, S25-S28 (2003) doi:10.1006/gyno.2002.6679).

Although a much more complex pattern is shown in this chromatogram, the peaks that are identified are put into a supercomputer to yield a pattern when compared to thousands of other patients. After ‘training’ the computer to find a particular pattern, the function that is derived can be used to match a new patient’s information (separation of proteins by HPLC). The success rate of this technique has generally been found to be effective more than 95%

The possibilities for this use as a screening tool are tremendous, and many other labs are now working to test this technique and similar ones to allow for earlier screening for diseases so that better treatment can be made early on.

I hope this real world and cutting edge application helps to bring to life the
somewhat boring analysis of simple continuous functions of x that may not seem to have a real impact when in Calculus I.

Glossary

Affinity in terms of chromatography, a specific binding of a protein or other ligand to a small molecule that is attached to the stationary phase of the column. For example, if a protein binds to a metal such as nickel one can purify that protein from a mixture of proteins using a column with nickel in the stationary phase.

Analyte a chemical or compound of interest separated during chromatography

Amino acid building blocks for proteins; amino acids contain both an amine and a carboxyl group and this portion makes up the peptide chain in proteins

Archaebacteria one of the three domains of life, the oldest one made up of single-cell microorganisms. Many thrive in extreme environments such as hot springs or deep sea thermal vents, however most are present in soil and the gut of mammals.

Adenosine triphosphate (ATP) nucleotide that functions to supply energy for synthetic reactions in cells. ATP is made by different mechanisms but required by all living cells for survival.

Bacteria another of the three domains of life, representing microorganisms that evolved from archaebacteria but did not further progress to higher life forms (such as mammals).

Biotechnology any technological application that uses biological systems, living organisms, or derivatives thereof, to make or modify products or processes for specific use.

Chromatography laboratory techniques used to separate mixtures into their individual parts; a sample is passed through a column in a mobile phase over a stationary phase that enables separation of components of the mixture.

Deoxyribonucleic acid (DNA) a nucleotide component of cells that contains the information needed to make the ribonucleotide and protein components of the cell. DNA is the 'memory molecule' that enables life to be recreated upon cell division.

Derivatization the process of chemically modifying a compound to produce a new compound which has properties that are suitable for analysis using a GC.

Eluent liquid or gas mobile phase that is passed through a chromatography column to facilitate the elution, or removal, of an analyte from a column.

Elution the process of removal of an analyte from the stationary phase of a chromatography column.
Enzyme proteins that catalyze chemical reactions inside a biological cell. These chemical reactions are the key reactions that allow for energy metabolism and the building of the macromolecules inside the cell.

Eucarya one of the three domains of life. Eucarya includes higher mammals, insects, plants and essentially all life forms that are not in bacteria or archaeabacteria.

Lipids these are the hydrophobic long chain fatty acids that generally comprise the cell membranes of biological cells

Mass spectrometry a technique used to determine the mass of a compound by determining its mass to charge ratio; essentially a molecule is charged and then the mass to charge ratio is determined, and thus the mass is predicted giving valuable information on the chemical makeup a molecule

Metabolite small molecule intermediates of metabolism; these are the small molecules that are found in biological cells that are involved in the synthesis and breakdown of molecules to allow life to function

Nucleic acids these are the small molecules that comprise both RNA and DNA as well as some enzyme cofactors in the cell. Most are found in the nucleus in eukaryotes and thus the name nucleic acid.

Protein linear chain of amino acids that together form a larger macromolecule; the sequence of the protein (linear sequence) is determined by the sequence of the DNA that encodes that particular protein; some proteins that catalyze chemical reactions are enzymes, but not all proteins are enzymes

Proteome collection of all the proteins present in a particular cell, or in a sample derived from a biological cell or animal (e.g. serum from a patients blood)

Red herring a diversion or distraction from the actual question; essentially a red herring can be something inserted in a sample to distract one from determining a smaller component that is of interest

Ribonucleic acid (RNA) nucleic acid polymer that is primarily used to allow for synthesis of proteins based on a copy of the DNA sequence of a gene; RNA also plays other roles in the cell in regulation of protein synthesis and in stability of messenger RNA that encode proteins

Spectroscopy study of the interaction between light (generally in the ultraviolet or visible range) and matter; This interaction gives a scientist valuable information on the properties of a substance or compound, for example DNA absorbs light in the UV range (a peak at 260 nm)