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By

Kevin William Sunderland

A DISSERTATION

Submitted in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

In Biomedical Engineering

MICHIGAN TECHNOLOGICAL UNIVERSITY

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This dissertation has been approved in partial fulfillment of the requirements for the Degree of DOCTOR OF PHILOSOPHY in Biomedical Engineering.

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Dedication

To my famliy and friends

who

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Preface

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Acknowledgments

I would like to thank all the members of my committee and my advisor Dr. Jingfeng Jiang. Their leadership, support, knowledge and motivation not only helped me throughout my research, but helped drive me to become a better scientist and to never stop learning.

Special thanks are also needed for Dr. Autumn Schumacher, who was willing to take a gamble on a brand new scientist fresh out of their undergraduate education. Her guidence and expertise (and many hours of manuscript editing) were invaluable in getting me to where I am today.

I would also like to thank my friends for their boundless confidence in me which helped push me through my PhD work. Last but not the least, I would of courselike to thank my family. All of their love and support helped make this thesis possible.

Definitions

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List of Abbreviations

ACA	Anterior Communicating Artery
AFI	Aneurysm Formation Indicator
CFD	Computational Fluid Dynamics
DICOM	Digital Imaging and Communications in Medicine
DVO	Degree of Volume Overlap
IA	Intracranial Aneurysm
ICA	Internal Carotid Artery
MCA	Middle Cerebral Artery
MLR	Multiple Logistic Regression
OSI	Oscillatory Shear Index
PC-MRI	Phase Contrast Magnetic Resonance Imaging
ROC	Receiver Operator Characteristic
STA-WSS	Spatiotemporaly Averaged Wall Shear Stress
TA-WSS	Temporally Averaged Wall Shear Stress
VMTK	Vascular Modeling Toolkit
VTK	Visualization Toolkit
WSS	Wall Shear Stress
WSSG	Wall Shear Stress Gradient

λ_2	Lambda$_2$
ACL	Access Control List
AIB	Add-In Board
ALE	Arbitrary Lagrangian Eulerian
AMANDA	Advanced Maryland Automatic Network Disk Archiver
AMBER	Assisted Model Building with Energy Replacement
AMD	Advanced Micro Devices
AMOLED	Active-Matrix Organic Light Emitting Diode
AMPI	Adaptive Message Passing Interface
ANL	Argonne National Laboratory
API	Application Program Interface
ASCII	American Standard Code for Information Interchange
ATLAS	Automatically Tuned Linear Algebra Software
b_eff	effective bandwidth Benchmark
BIOS	Basic Input/Output Operating System
BLAS	Basic Linear Algebra Subprograms
BOMD	Born-Oppenheimer Molecular Dynamics
BP	Bootstrap Protocol
CCSR	Center for Computer Systems Research
CentOS	Community enterprise Operating System
CFD	Computational Fluid Dynamics

CHARMM	Chemistry at HARvard Macromolecular Mechanics
CHAMBER	CHarmm $\leftrightarrow$ AMBER
CMake	Cross Platform Make
CODINE	Computing in Distributed Networked Environments
CP2K	Car-Parrinello 2000
CPMD	Car-Parrinello Molecular Dynamics
CPU	Central Processing Unit
CSS	Central Security Service
CTM	Chemical Transport Model
CUDA	Compute Unified Device Architecture
CUDPP	CUDA Data-Parallel Primitives Library
DAE	Differential Algebraic Equation
DARPA	Defense Advanced Research Projects Agency
DAE	Delay Differential Equation
DFT	Discrete Fourier Transform
DFT	Density Functional Theory
DGEMM	Double Precision GEneralized Matrix Multiplication
DHCP	Dynamic Host Configuration Protocol
DMCA	Digital Millennial Copyright Act
DOD	Department of Defense
DOE	Department of Energy

DRM	Distributed Resource Manager
DRMAA	Distributed Resource Manager Application API
EFF	Electron Force Field
EVL	Electronic Visualization Laboratory
FCA	Fabric Collectives Accelerator
FEA	Finite Element Analysis
FFT	Fast Fourier Transform
FFTW	Fastest Fourier Transform in the West
FLOPS	Floating Point OPerations per Second
FPU	Floating Point Unit
FSI	Fluid Structure Interaction
FTDT	Finite Difference Time Domain
FTP	File Transfer Protocol

Abstract

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Chapter 1

Introduction

Subarachnoid hemorrhage is a potentially devastating pathologic condition in which bleeding between the brain and the tissues that cover the brain. One of the prevalent pathologic conditions that may result in subarachnoid hemorrhage is the rupture of an intracranial aneurysm (IA)

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Section 1

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Objective

Although there exists a number of studies[14, 108, 117] and methodologies[40, 49] that attempt to assess IAs at a high risk of rupture, inconsistencies between investigations leave the development of an ideal model out of reach. In addition, many of these previous studies assessed the geometric[1, 67, 108] and/or hemodynamic wall stressors[14, 83, 117] as a means to predict IA rupture, with limited quantitative assessment of the hemodynamic flow conditions within the aneurysm. **The primary objective** of this work is to assess the viability of adapting quantitative analysis of hemodynamic flow patterns, specifically the swirling flow pattern(s) (vortex), within IAs to improve upon predictive models for IA rupture. In this work, an overview of recent theories concerning

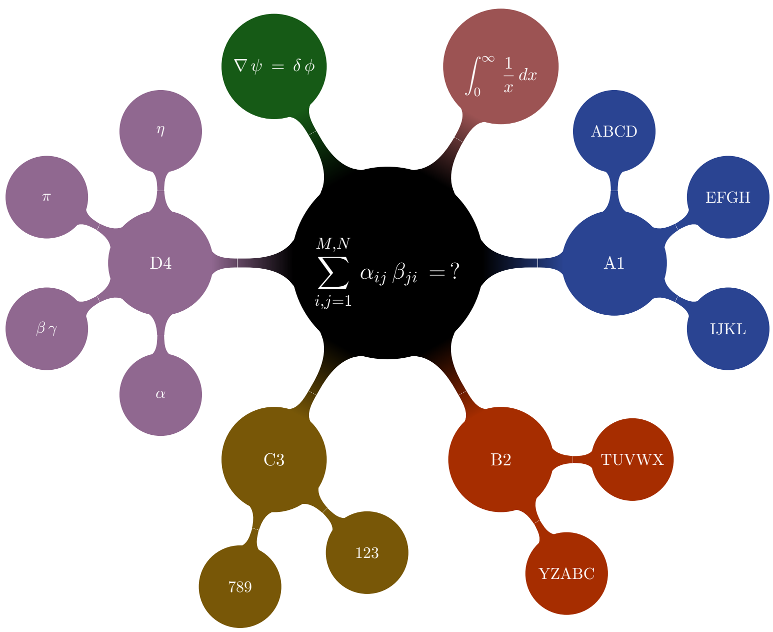

Figure 1.1: Schematic representation of our universe

Methodolgy

For the initial part of this work, image-based computational fluid dynamics models of patient-specific IA geometry will be constructed from 3D phase-contrast magnetic resonance imaging (PCMRI)

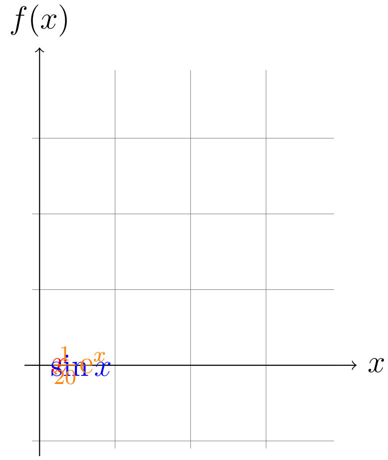

Figure 1.2: Mathematical functions plotted using TikZ package

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Section 2

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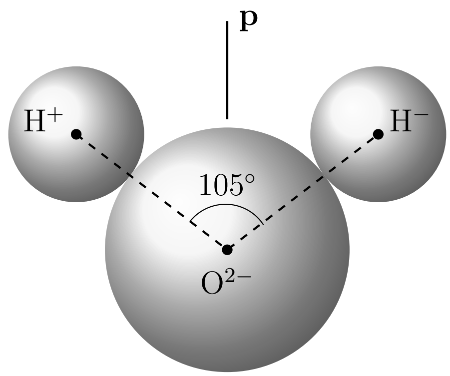

Figure 1.3: Schematic representation of a water molecule

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Chapter 2

Theory and Practice

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$$d\nu = \frac{N}{V} \left(\frac{m}{2\pi\, kT}\right)^{3/2} e^{-mv^2/2kT}\, v^3\, \sin\theta\, \cos\theta\, d\theta\, d\phi\, dv \qquad (2.1)$$

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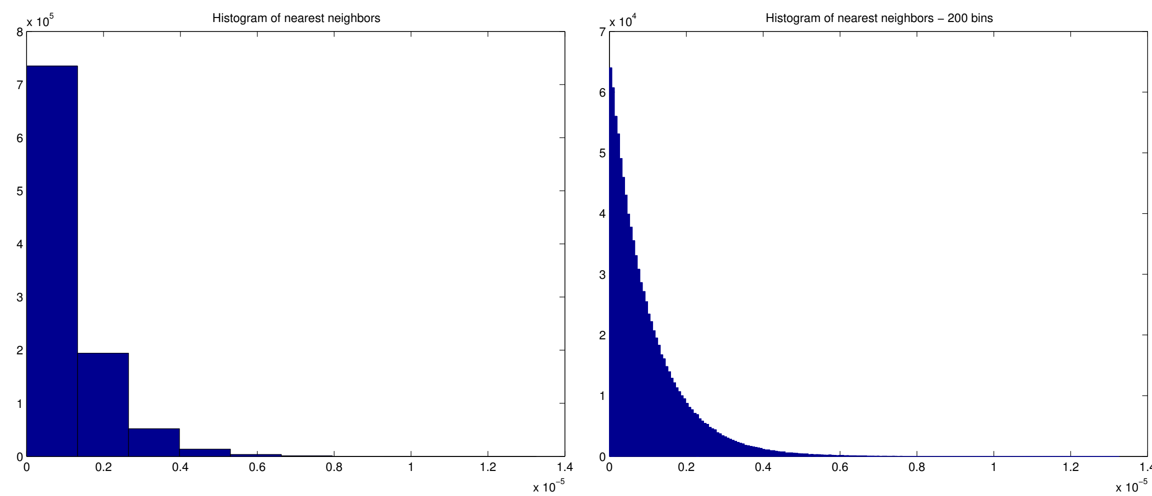

(a) Generic

(b) 200 bins

Figure 2.1: Histogram of nearest neighbors

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Table 2.1

A portrait table: first column represents the year in which the Nobel prize in physics was awarded; second column indicates the name of the scientist and the third column is the work for which the Nobel prize was awareded

Year	**Scientist(s)**	**Nobel Work**
1901	W. C. Röntgen	X-rays
1902	H. A. Lorentz	Influence of magnetism on radiation
	P. Zeeman	Influence of magnetism on radiation
1903	A. H. Becquerel	Spontaneous radioactivity
	M. Curie	Radiation phenomena discovered by Becquerel
	P. Curie	Radiation phenomena discovered by Becquerel
1904	J. W. Strutt	Argon
1905	P. E. A. von Lenard	Cathode rays
1906	J. J. Thomson	Electrical conductivity of gases
1907	A. A. Michelson	Spectroscopic and metrological investigations
1908	G. Lippmann	Photographic reproduction of colours
1909	K. F. Braun	Wireless telegraphy
	G. Marconi	Wireless telegraphy
1910	J. D. van der Waals	Equation of state of gases and liquids
1911	W. Wien	Laws governing heat radiation
1912	N. G. Dalèn	Automatic regulators for lighting coastal beacons and light buoys

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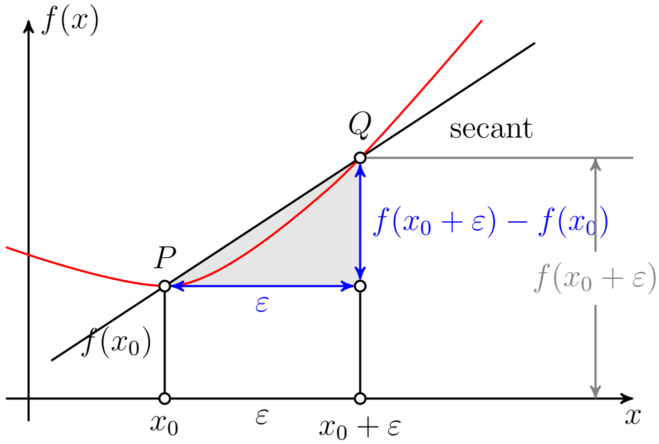

Figure 2.2: Fancy mathematical plots using TikZ package

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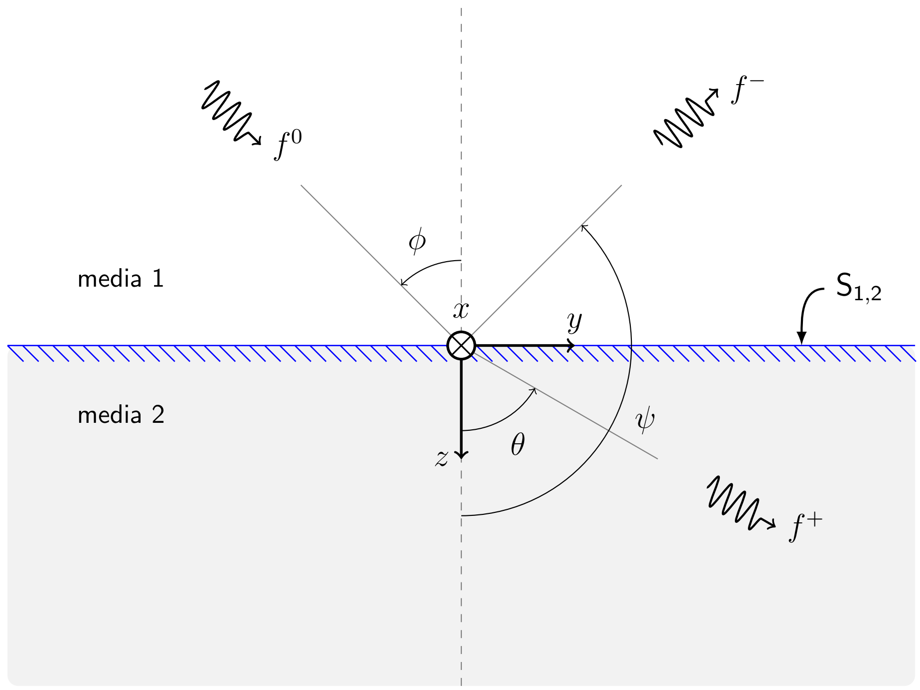

Figure 2.3: Incidence, transmission and reflection

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Chapter 3

Results and Discussion

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$$d\nu_\theta \;=\; \frac{N}{V}\,\left(\frac{m}{2\pi\, kT}\right)^{3/2}\,\left[\int_0^{2\pi}\,\int_0^{\infty}\,v^3\,e^{-mv^2/2kT}\,dv\,d\phi\right]\,\sin\theta\,\cos\theta\,d\theta$$

$$=\;2\,\pi\,\frac{N}{V}\,\left(\frac{m}{2\pi\, kT}\right)^{3/2}\,\left[\int_0^{\infty}\,v^3\,e^{-mv^2/2kT}\,dv\,\right]\,\sin\theta\,\cos\theta\,d\theta$$

At vix indoctum disputando. Eam cu doctus reprimique, quaeque democritum an eos, sit veniam facete dissentias id. Tale volumus eos te, an eum nulla tincidunt. Mea id recteque theophrastus.

$$d\nu_\theta \;=\; \frac{N}{V}\,\left(\frac{2\,k\,T}{m\,\pi}\right)^{1/2}\,\sin\theta\,\cos\theta\,d\theta \tag{3.1}$$

Liber liberavisse nec at, movet albucius principes has at. Ea sed persius accusam, clita sententiae adversarium ne sed. Usu no graecis theophrastus delicatissimi, sint aliquam an eam. Mei elit mnesarchum dissentias te, in essent laboramus per. Affert mucius quidam mel ex, per dicam insolens ad.

Sed altera placerat an, id verterem abhorreant interesset mea. Eum at ceteros efficiantur. Eos id voluptaria efficiendi comprehensam. Continuing from Eqn. (3.1)

$$d\nu_v \;=\; \frac{N}{V}\;\left(\frac{m}{2\pi\, kT}\right)^{3/2}\;\left[\int_0^{2\pi}\;\int_0^{\pi/2}\,\sin\theta\;\cos\theta\;d\theta\;d\phi\right]\;v^3\;e^{-mv^2/2kT}\;dv$$

$$=\;2\;\pi\;\frac{N}{V}\;\left(\frac{m}{2\pi\, kT}\right)^{3/2}\;\left[\int_0^{\pi/2}\,\sin\theta\;\cos\theta\;d\theta\right]\;v^3\;e^{-mv^2/2kT}\;dv$$

In mel modo dicam vocibus, eruditi consectetuer vim no, cu quaestio instructior eum. Justo nostrud fuisset ea mea, eam an libris repudiandae vituperatoribus. Est choro corrumpit definitionem at. Vel sint adhuc vocibus ea, illud epicuri eos no. Sea simul officiis ea, et qui veri invidunt appellantur. Vix et eros ancillae pertinax.

In mel modo dicam vocibus, eruditi consectetuer vim no, cu quaestio instructior eum. Justo nostrud fuisset ea mea, eam an libris repudiandae vituperatoribus. Est choro corrumpit definitionem at. Vel sint adhuc vocibus ea, illud epicuri eos no. Sea simul officiis ea, et qui veri invidunt appellantur. Vix et eros ancillae pertinax.

$$d\nu_v \;=\; \frac{N}{V}\;\pi\;\left(\frac{m}{2\pi\, kT}\right)^{3/2}\;v^3\;e^{-mv^2/2kT}\;dv \tag{3.2}$$

Aliquip lobortis ei est, at error viris graeco sed. Vel te elitr detracto, modo graecis scripserit ex nec. Errem utamur viderer per no, eam ea eripuit referrentur. Pro te dicat disputando.

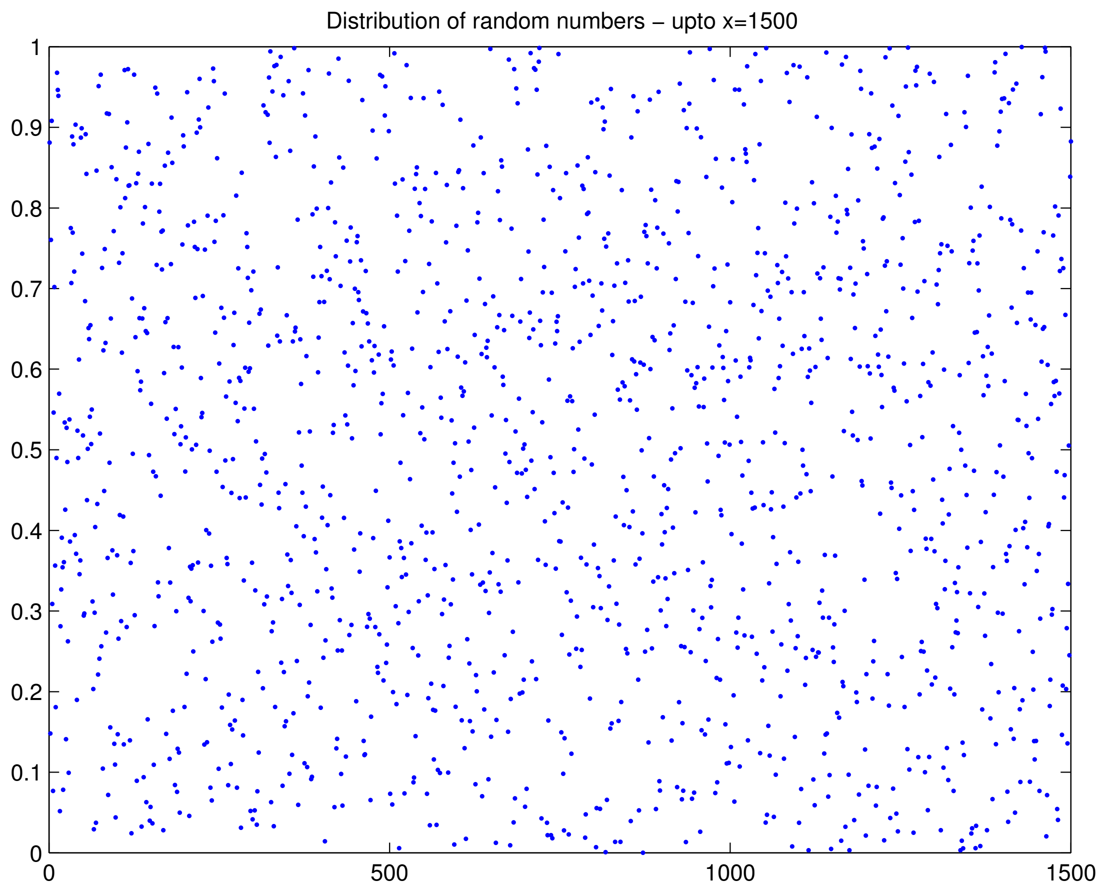

Figure 3.1: Distribution of random numbers

Table 3.1
Measured data points representing the relationship between x and y

x	0	1	2	3	4	5	6	7	8	9	10
y	0	0.94	0.99	-0.52	-1.82	-0.44	3.54	6.69	5.38	0.00	-4.42

Et mei mollis scripta, et vim labores phaedrum, in cum facete saperet. Splendide elaboraret comprehensam qui ne. Putant verterem no vim, mea solum veritus definitiones ei, no labitur propriae deseruisse est. Ius illud everti salutandi id, eu facer pericula principes est.

Table 3.2
A landscape table: first column represents the year in which the Nobel prize in physics was awarded; second column indicates the name of the scientist and the third column is an *as is* Nobel citation

Year	Scientist(s)	Nobel Work
1901	W. C. Röntgen	in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him
1902	H. A. Lorentz and P. Zeeman	in recognition of the extraordinary service they rendered by their researches into the influence of magnetism upon radiation phenomena
1903	A. H. Becquerel	in recognition of the extraordinary services he has rendered by his discovery of spontaneous radioactivity
	M. Curie and P. Curie	in recognition of the extraordinary services they have rendered by their joint researches on the radiation phenomena discovered by Prof. Henri Becquerel
1904	J. W. Strutt	for his investigations of the densities of the most important gases and for his discover argon in connection with these studies
1905	P. E. A. von Lenard	Cathode rays
1906	J. J. Thomson	Electrical conductivity of gases
1907	A. A. Michelson	Spectroscopic and metrological investigations
1908	G. Lippmann	Photographic reproduction of colours
1909	K. F. Braun and G. Marconi	Wireless telegraphy
1910	J. D. van der Waals	Equation of state of gases and liquids
1911	W. Wien	Laws governing heat radiation
1912	N. G. Dalèn	Automatic regulators for lighting coastal beacons and light buoys

Et mei mollis scripta, et vim labores phaedrum, in cum facete saperet. Splendide elaboraret comprehensam qui ne. Putant verterem no vim, mea solum veritus definitiones ei, no labitur propriae deseruisse est. Ius illud everti salutandi id, eu facer pericula principes est.

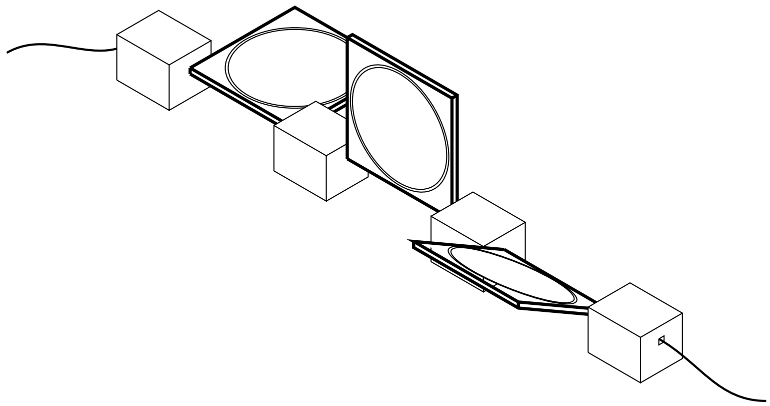

Figure 3.2: Fibre optics

Simul noster voluptaria eam ei, sint regione pri ei. Cum no utinam equidem, falli bonorum prodesset an qui. Alterum dissentiet vituperatoribus te eam, eos ea suas oblique. Per ea utinam facilisi. Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te.

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Adipisci molestiae vim at, eum everti accommodare eu. Duo ex maiorum consetetur. Sea et vivendo concludaturque, rebum conclusionemque pro eu. Mei an everti dolorem. Per id alterum mandamus deseruisse. Copiosae evertitur eum ea, atqui interesset est in. Vim magna munere nostrum an, cu congue equidem est. Mediocrem reformidans ne mel. Et summo nihil mel, an nam postea incorrupte an everti dolorem. Per id alterum mandamus deseruisse. Copiosae evertitur eum ea, atqui interesset est in. Vim magna munere nostrum an, cu congue equidem est. Mediocrem reformidans ne mel. Et summo nihil mel, an nam postea incorrupte. Mediocrem reformidans ne mel. Et summo nihil mel, an nam postea incorrupte an everti dolorem.

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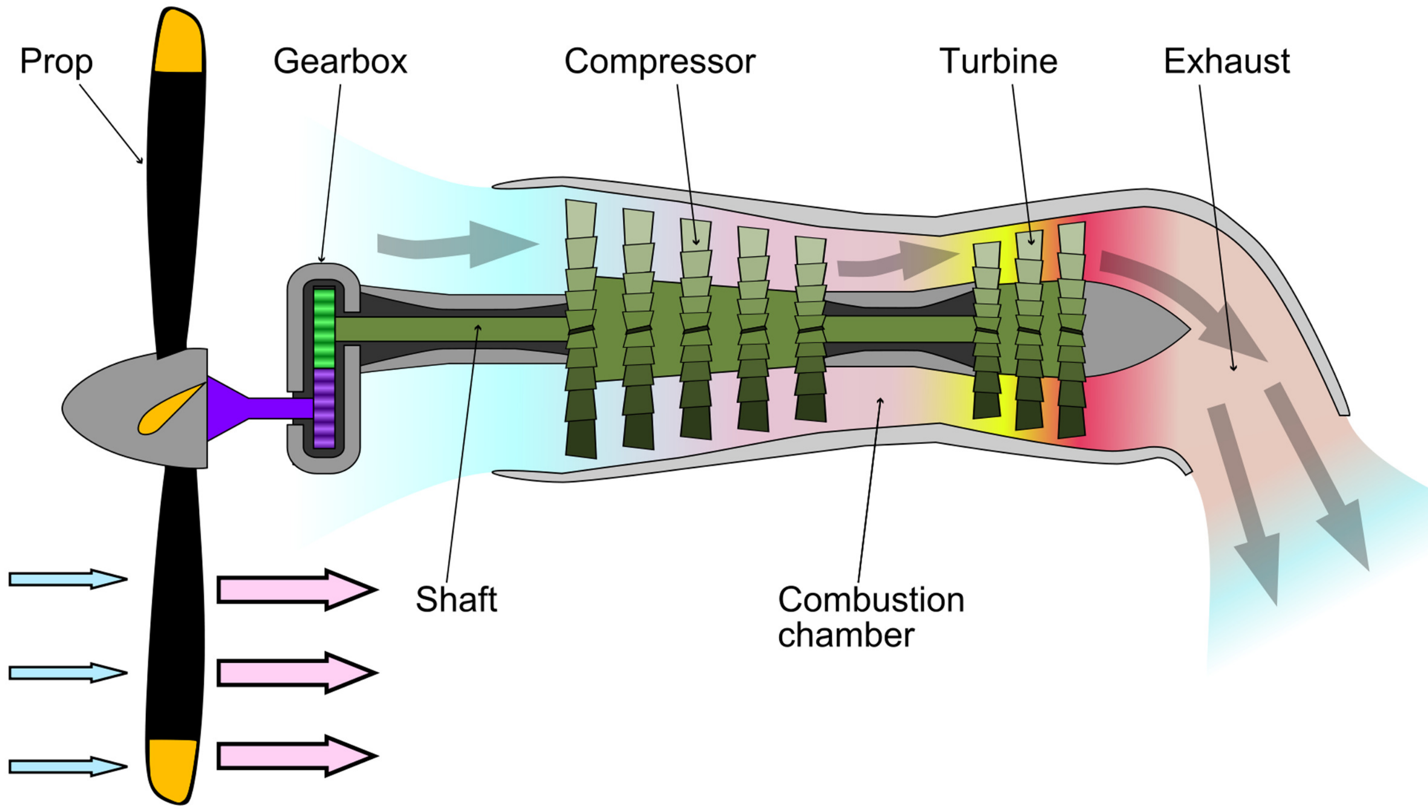

Figure 3.3: A landscape view of a Turboprop engine - these are jet engine derivatives, still gas turbines, that extract work from the hot-exhaust jet to turn a rotating shaft, which is then used to produce thrust by some other means

Id ius soluta semper audiam, ad eos scriptorem concludaturque, id mel rebum volumus deserunt. Mel libris percipit scriptorem te, his an dicat putent menandri, mazim officiis aliquando mei no. Ne clita veniam disputando vim, postea hendrerit maiestatis qui id. Mei te suscipit quaerendum, an aliquando intellegebat ius, ei simul detraxit dissentiet eam. Zril dolor ut usu.

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Appendix A

Statistics

Multiple logistic regression (MLR) analysis looks both to estimate the odds of a dichotomous outcome occurring, and to determine the effects of a specific covariate in relation to the other covariates in a model. The probability of an outcome occuring in MLR can be calculated as such:

$$\hat{p} = \frac{exp(b_0 + b_1X_1 + b_2X_2 + ... + b_pX_p)}{1 + exp(b_0 + b_1X_1 + b_2X_2 + ... + b_pX_p)} \tag{A.1}$$

$\hat{p}$ being the probability of the desired outcome, X_1 through X_p as the individual dependent variables applied to the model, and b_1 to b_p being the regression coefficients. To determine the expected log odds ratios of the model's variables, the logit function of the above equation can be calculated:

$$
\begin{aligned}
logit[\hat{p}] &= ln[\frac{\hat{p}}{1-\hat{p}}] \\
&= ln\left[\frac{\frac{exp(b_0+b_1X_1+b_2X_2+...+b_pX_p)}{1+exp(b_0+b_1X_1+b_2X_2+...+b_pX_p)}}{1-\frac{exp(b_0+b_1X_1+b_2X_2+...+b_pX_p)}{1+exp(b_0+b_1X_1+b_2X_2+...+b_pX_p)}}\right] \\
&= ln\left[\frac{\frac{exp(b_0+b_1X_1+b_2X_2+...+b_pX_p}{1+exp(b_0+b_1X_1+b_2X_2+...+b_pX_p}}{\frac{1}{1+exp(b_0+b_1X_1+b_2X_2+...+b_pX_p}}\right] \\
&= ln[exp(b_0+b_1X_1+b_2X_2+...+b_pX_p] \\
&= b_0+b_1X_1+b_2X_2+...+b_pX_p
\end{aligned}
\tag{A.2}
$$

Taking the logit of the event's (desired outcome) probability, transforms the occurrence of the event given X into a simplified linear function.

For each variable added to a regression model, the resultant R^2 (coefficient of multiple determination) increases, indication an improved fit of the data. However applying an large number of variables to a predictive model may result in overfitting: attempting to estimate too many parameters from too small a sample size. In an overfitted model, the regression coefficients and R^2 values determined may lead to misleading outcomes. To reduce the initial choices of variables to apply to (eventual) predictive models, the correlation between variables were determined. The correlation of data can be determine by:

$$r_{jk} = \frac{s_{jk}}{s_j s_k} = \frac{\sum_{i=1}^{n}(x_{ij} - \overline{x}_j)(x_{ik} - \overline{x}_k)}{\sqrt{\sum_{i=1}^{n}(x_{ij} - \overline{x}_j)^2}\sqrt{\sum_{i=1}^{n}(x_{ik} - \overline{x}_k)^2}} \tag{A.3}$$

with r as the Pearson correlation coefficient between variables x_j and x_k, n as the sample size, and $\overline{x}$ is a variable sample mean. Correlations between multiple variables are often displayed in a correlation table:

$$R = \begin{bmatrix} 1 & r_{12} & r_{13} & \dots & r_{1p} \\ r_{21} & 1 & r_{23} & \dots & r_{2p} \\ r_31 & r_{32} & 1 & \dots & r_{3p} \\ \vdots & \vdots & \vdots & \ddots & \dots \\ r_{p1} & r_{p2} & r_{p3} & \dots & 1 \end{bmatrix}$$

Initial correlation analysis of all available geometric and hemodynamic variables was performed to eliminate highly correlated variables from analysis: i.e aneurysm volume and surface area are highly correlated so surface area was removed from analysis.

From the remaining variables, stepwise MLR was implemented to determine the parsimonious model (ideal model with the fewest number of variables). First a linear regression is perfomred for each variable X one at a time, and the variable with the highest R^2 is kept as the first variable. Next, a multiple regression step is performed with the first variable and each remaining variable, adding the subsequent variable with the largest increase in R_2, if the p value of the R^2 is below a desired cuttoff

(<0.05). The calculation of the p value of an increase in R^2 resulting from the increasing of X variable(s) from a to b is as follows:

$$p_{ab} = \frac{(R_b^2 - R_a^2)/(b-a)}{(1-R_b^2)/(n-b-1)} \tag{A.4}$$

with the total sample size n.

Each time a new variable is added to the model, the impact of removing any of the other variables (already added to the model) on equation outcomes is tested. The chosen (removed) variable is excluded from the model if it does not make R^2 significantly worse. This process is continued till adding any new X variables does not increase R^2 and removing any X variables does not significantly decrease R^2

In the event that all of the independent variables in the model are completely uncorrelated with each other, the interpretation of coefficients are as such:

$$OR = exp(b_1)^z \tag{A.5}$$

Where z is the number of unit changes for a variable X, and OR is the odds ratio resultant from said change. When the variables are not uncorrelated, the $OR = exp^z b_1$ is expressed as the change of unit z for a variable *adjusted in relation to the impacts of the other variables in the model.* This stresses the need to assess collinearity between variables prior to model assessment.

in Section ??.

Section 1

To assess the diagnostic ability of predictive model(s), a receiver operating characteristic curve (ROC) is often deployed (REFERENCES). The ROC curve assesses a model's predictive true positive rate (TPR) against its false positive rate (FPR) as a means to determine overall predictive strength (HANLEY). From a statistical perspective, ROC analysis can be considered as a plot of the power (probability of a test correctly rejecting the null hypothesis when an alternative hypothesis is true)

$$\begin{aligned} TPR &= \frac{\Sigma TruePositive}{\Sigma ConditionPositive} \\ FPR &= \frac{\Sigma FalsePpositive}{\Sigma ConditionNegative} \\ FNR &= \frac{\Sigma FalseNegative}{\Sigma ConditionPositive} \\ Specificity &= \frac{\Sigma TrueNegative}{\Sigma ConditionNegative} \end{aligned} \tag{A.6}$$

When dealing with a binary classification, as per this study, the prediction for each instance is based on a continuous random variable (x), which is the value computed for each instance. Given a desired threshold (T), each instance is positive if x>T (and negative if x<T). As the value of x is akin to a probability density function each instance can be considered positive when $f_1(x)$. Given this, TPR is calculated as:

$$TPR(T) = \int_T^\infty f_1(x)dx \tag{A.7}$$

and the FNR as:

$$FPR(T) = \int_T^\infty f_0(x)dx \tag{A.8}$$

The ROC curve is generated by plotting TPR(T) against FPR(T) parametrically, varying across T.

Comparing the resultant ROC curves across model conditions provides the capability to select a desired model based off of varying predictive accuracies. To quantify the predictive accuracy, the area under the curve (AUC) of the ROC curve is calculated, as it equals the probability of a classifier ranking a positive instance higher than a negative instance (both chosen at random).

$$\begin{aligned} A &= \int_\infty^{-\infty} TPR(T)FPR'(T)dT \\ &= \int_{-\infty}^\infty \int_{-\infty}^\infty I(T' > T)f_1(T')f_0(T)dT'dT = P(X_1 > X_0) \end{aligned} \tag{A.9}$$

The initial integral has reversed boundaries due to larger T values having a lower value on the x-axis.

Section 2

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Appendix B

Sample Code

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HelloWorld.c

```c
// HelloWorld.c
// C program to display 'Hello, World!' in the terminal.
//
// Compilation:
// gcc -g -Wall HelloWorld.c -o HelloWorld.x
//
// Execution:
// ./HelloWorld.x

// Standard headers
#include <stdio.h>

// main() begins
int main() {

  // Print the message
  printf("\n  Hello, World!\n\n");

  // Indicate the termination of main()
  return 0;
}
// main() ends
```

Appendix C

Letters of Permission

Include letters of permission from journal editors and/or other sources from which you may have used materials (images, information, etc.) in this this work.

These materials may also be submitted separately to the Graduate School as a single, well-organized PDF file.