Evaluations of the 1997 Spend a Summer with a Scientist Program

1997 SaS Participants

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Spend A Summer With A Scientist

Paola Argaez

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This summer program was a valuable experience for me as an undergraduate student. I learned a lot from graduate students as well as other undergraduate students involved in this program. Their experiences have helped me to look beyond an undergraduate career. Because of their different backgrounds, their excellence ideas and view of the future, I can now understand and appreciate how important diversity is in this country.

As part of the Spend a Summer with a Scientist program, I had a project to complete. My main goal was to learn to use Latex. Latex is a software program that scientists, engineers, and graduate students use to write their technical reports and presentations. My goal was to use Latex to format and edit a book consisting of some notes for an optimization course taught at Rice University. These notes which were written by Dr. Tapia, will be use as the class course textbook for the fall 1997 eventually will be formally published as a book.

The process of learning Latex was totally new for me because I had no experience with such a computer language. I had previously written papers for my classes, but in this case a regular editor would not do it, since editors do not deal with such symbols as integral, matrices or even other complex mathematical expressions. In the process of writing in Latex I also learned Unix which is the operating system I worked with. I could not completed my project without learning both Unix and Latex. In the end after so many mistakes and frustrations, I finished the project. Besides doing the project I also learned some Linear Algebra and Vector Calculus in order to prepare for the next semester. An important issue that I learned in Linear Algebra was a classical problem for Algebra and Geometry:

$$\begin{aligned} a_1 x + b_1 y &= C_1; l_1 \\ a_2 x + b_2 y &= C_2; l_2 \end{aligned} \tag{1}$$

for this system of linear equations we can have any of the following three solutions:

1. A Unique Solution: which is when the lines intersect.

2. An Infinite Number of Solutions: when both lines represent only one line.

3. No Solution: when the lines are parallel or have the same slope.

Equation (1) can be expressed as a product in the following way

$$AX = b$$

where

$$A = [a_1, b_1; a_2, b_2]$$

$$X = [x, y]^T, b = [c_1, c_2]^T.$$

Using Linear Algebra the solution of the system is given by:

$$X = A^+ b$$

where A^+ is the pseudo-inverse of the matrix A.

The pseudo-inverse has the following properties: Any Matrix has a unique pseudo-inverse A^+ such that satisfies:

(i) $AA^+A = A$

(ii) $A^+AA^+ = A^+$

(iii) $(AA^+)^T = (AA^+)$

(iv) $(A^+A)^T = A^+A$.

The solution is interpreted in the following way:

1. A Unique Solution

$$X =^{-1} X$$

where

$$A^{-1} = A^+.$$

2. An Infinite Number of Solutions:

$$\begin{aligned} &\text{minimize} && \|X\|_2 \\ &\text{subject to} && AX = b. \end{aligned} \tag{2}$$

3. No Solution:

$$\begin{aligned} \text{minimize} \quad & \|X\|_2 \\ \text{subject to} \quad & \|AX - b\|_2. \end{aligned} \tag{3}$$

Overall it has been a great summer for me. The people in the program were very friendly and helped me tremendously when I needed it. But most important, I learned a lot about Linear Algebra, Latex and the axe editor.

William Christian Jr.
Spend a Summer with a Scientist - 1997
CRPC
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Consider the standard Integer Programming problem (IP)

$$\begin{array}{lrcl} minimize & c^T x & & \\ subjectto & Ax & \leq & b \\ & x & \geq & 0 \\ & x & \in & Z_+^n. \end{array}$$

A typical approach to solving these problems is to generate inequalities which successively "cut off" infeasible regions of the polytope $P = \left\{x \in R_+^n : Ax \leq b\right\}$.

With the support of the Spend a Summer with a Scientist program I independently surveyed several classic and more recent texts of Integer Programming and Operations Research. The subjects included Linear Programming, Integer Programming, Probability and Data Structures.

In addition, I began to code a Branch and Bound code to solve general Integer Programming problems. After completing this code, I shall begin to implement different classes of cutting plane algorithms.

Although this research with the Spend a Summer with a Scientist program was preliminary, it is the foundation for my future work.

On the Use of the Multivariate Skew-Normal Distribution for Directly Modeling Ambient Ozone Levels*

Nancy L. Glenn**

August 8, 1997

Abstract

There are several models that predict ambient (ground level) ozone pollution by transforming the data. However, transformations sometime increase prediction error. Our goal is to directly model ambient ozone levels in regions located away from monitoring stations. Our objective is not to predict future ozone levels.

Some Key Words: Multivariate skew-normal distribution; Bivariate skew-normal distribution; Ambient ozone.

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Introduction

Ambient ozone (O_3) pollution is a major environmental problem in many metropolitan areas in this country. In particular, the Houston, Texas area is second to Los Angeles in nationwide ambient air quality (Carroll, Chen, George, Li, Newton, Schmiediche and Wang, 1997). There are several models for estimating O_3, however, many modeling strategies use transformed data. Our objective is to use the multivariate skew-normal (MSN) distribution to directly model data in an attempt to reduce prediction error. The data, provided by the Texas Natural Resources Conservation Commission, are hourly ozone measurements of the Houston-Galveston area for 1980 - 1993.

The Multivariate Skew-Normal Distribution

The MSN distribution, a parametric distribution which has an extra parameter to regulate skewness, includes the normal as a special case. Its density is given by

$$f(z;\lambda)=2\phi(z)\Phi(\lambda z), z\in\Re. \quad (1)$$

$$\phi(z),\Phi(z)$$

denote the N(0,1) density and distribution function, respectively (Azzalini and Valle, 1996). O'Hagan and Leonard (1976) introduced the MSN density as a prior density for estimating normal location parameters.

The MSN distribution is seldom used in practice, however, Azzalini and Valle (1996) superimposed contours of the bivariate skew-normal

distribution onto Australian athletes' data since observed points and the fitted density indicated skewness. One advantage of using this distribution is that it allows one to retain variables on their original scale, making them more interpretable.

Ambient Ozone Levels

The recombination of oxygen after ionization by photochemical reactions form O_3 (Guttorp, Meiring and Simpson, 1997). Various species of Nitrogen Oxide (NO_x) are primary precursors to O_3 (Cox and Ensor, 1995). Temperature, as sunlight, is another contributor to the formation of O_3. We will consider the pairs of variables (temperature, ozone) and (NO_x,ozone) and use the bivariate case to model O_3.

Preliminary Results

Figures 1 and 2 are scatter-plots of (temperature, ozone) and (NO_x,ozone), respectively. Observed points display skewness in each of the components. We use the conditional mean, given by Azzalini and Valle (1996), to predict O_3.

$$E(Y\_Z=z)=\omega z+(\Delta-\omega\delta)\sqrt{(}2/\pi)H(\lambda z),\quad H(x)=\phi(x)/\Phi(\sqrt{\lambda}x),\quad (2)$$

where H(x) denotes the hazard function of the standard normal density.

Further Research

Some components of pollution modeling are not incorporated into equation (2). For example, emission and deposition of precursors, diffusion and turbulent motion, and chemical reactions involved in the creation and destruction of O_3 (Cox and Ensor, 1995) are not accounted for. In future research, we will incorporate these and other features into the model, specifically define parameters of the distribution and access the quality of the model.

We will also address the topic of missing data since this is an issue with the NO_x data.

The data set that covers through 1996 will soon be available, so we will compare this with the present data.

Acknowledgments

I thank my mentor, Dr. Kathy Ensor. I thank Dr. Richard Tapia for his leadership in the Spend the Summer With A Scientist Program. I also thank my undergraduate advisor, Dr. Todd Ogden.

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Figure 1: -1 = missing value

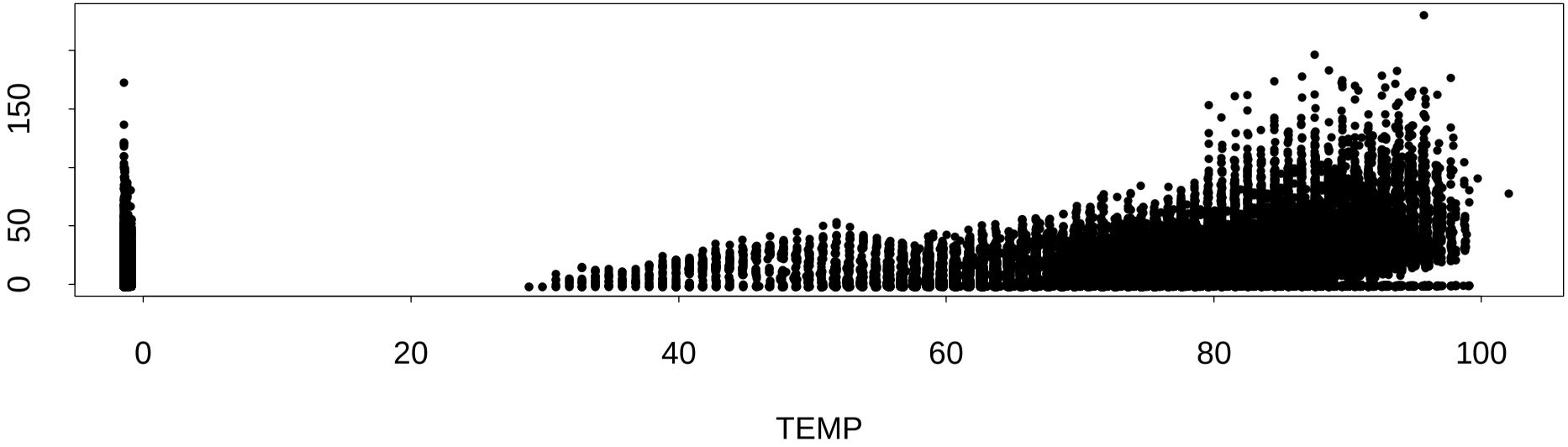
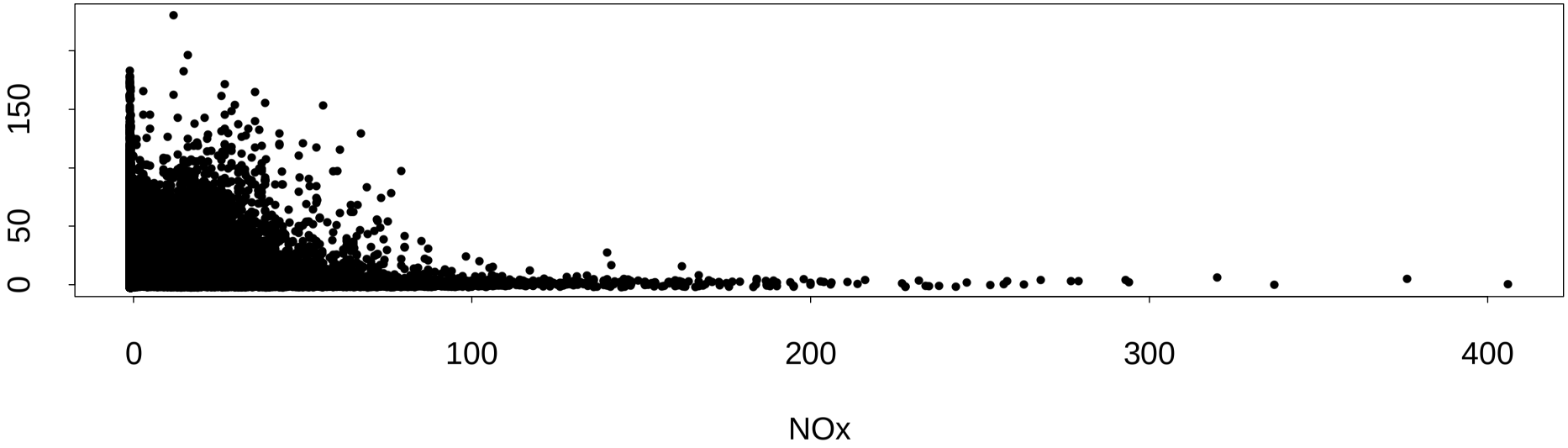


Figure 2: -1 = missing value



Regina Hill
Spend a Summer With a Scientist Final Report
Summer 1997

This summer I worked on formulating the Galerkin finite element method for the wave equation in one-dimension with my mentor, Dr. William Symes in the department of Computational and Applied Math at Rice University. The wave equation is a partial differential equation that gets its name because its solutions take on wave-like forms. An example of the wave equation is

$$u_{tt} - u_{xx} = 0.$$

This is the simplest form of the wave equation. We will use this form until we are comfortable with the fintie element method. The first step in formulating the Galerkin FEM, is to choose a basis of trial functions. The trial functions form a polynomial approximation to the solution of the differential equation. The higher the degree of your trial function the better the approximation to the true solution and the harder the formulation of the FEM (finite element method). So, we start off with a simple first order (or linear) trial function. We will call the trial functions ϕ_k.

Now that we have our trial functions we can find the weak form of the FEM by multiplying by ϕ_k and integrating by parts. The weak form is

$$\int_0^1 (u_{tt}\phi_k + u_x\phi_k)dx$$

The Galerkin FEM means we let some function u^h be an approximate solution to the wave equation.

$$u^h(x,t) = \sum_{j=1}^{N} Q_j(t)\phi_j(x)$$

where $Q_j(t)$ are weights on the approximating functions $\phi_j(x)$. Next, we perform numerical integration on the weak form with our approximate solution $u^h(x,t)$ substituted for u. The system of equation obtained from numerical integration is

$$\sum_{j=1}^{N} \int_0^1 \left(\frac{\partial^2 Q_j}{\partial t^2}\phi_j\phi_k + Q_j \frac{\partial \phi_j}{\partial x}\frac{\partial \phi_k}{\partial x} \right) dx$$

where $k = 1 \ldots N$

In vector form our equation is

$$MQ'' + KQ = 0.$$

where

$$M = \begin{pmatrix} 4 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 4 \end{pmatrix}$$

and

$$K = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}$$

We then solve this system using finite differences.

The solution to our system can be expensive to compute, so we want to somehow decrease the expense of solving our system, without losing much accuracy. We want to use Mass Lumping, which is a process by which we approximate the tridiagonal matrix M by a diagonal matrix. We would expect that the accuracy of the finite element method would decrease significantly by such an approximation. Interestingly enough it turns out that when using linear trial functions and a nodal quadrature rule for numerical integration, the mass matrix is diagonal and the diagonal elements are the sum of the terms in the tridiagonal mass matrix. Future work will be to determine what happens to the accuracy of the method when you use higher order elements, or move to higher dimensions.

Comparison of Coleman-Li and Perturbed KKT Formulations for Nonlinear Optimization with Simple Bounds

Diane Jamrog

August 8, 1997

1 The Minimization Problem.

The minimization problem is to compute a local minimizer, x_*, of a smooth nonlinear objective function, $f(x)$, subject to simple bounds on the variables.

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & l \leq x \leq u \end{array}$$

where $x,\ l,\ u \in \Re^n,\ l < u,\ f : \Re^n \to \Re$.

There are many algorithms to solve constrained optimization problems. My research this summer was to compare two formulations for such a minimization problem and determine which formulation performs better when Newton's Method is applied to each formulation. The two formulations compared are the Coleman-Li formulation and the perturbed KKT formulation.

1.1 The Coleman-Li Formulation.

In the Coleman-Li paper, *An Interior Trust Region Approach for Nonlinear Minimization Subject to Bounds*, T. Coleman and Y. Li propose a strictly feasible trust region method for the problem given above, defining the feasible region as $\mathcal{F} \stackrel{\text{def}}{=} \{x : l \leq x \leq u\}$. Their method involves choosing a scaling matrix D_k and a quadratic model ψ_k. They choose D_k by examining the optimality conditions.

Let $g(x) \stackrel{\text{def}}{=} \nabla f(x)$. Define $v(x) : \Re^n \to \Re^n$, for each component $1 \leq i \leq n$, as follows:

$$\begin{cases} \text{if } g_i < 0 & \text{and } u_i < \infty & \text{then } v_i = x_i - u_i \\ \text{if } g_i \geq 0 & \text{and } l_i > -\infty & \text{then } v_i = x_i - l_i \\ \text{if } g_i < 0 & \text{and } u_i = \infty & \text{then } v_i = -1 \\ \text{if } g_i \geq 0 & \text{and } l_i = -\infty & \text{then } v_i = 1 \end{cases}$$

Now define $D(x) \stackrel{\text{def}}{=} diag(|v(x)|^{-1/2})$, so that D^{-2} is the diagonal matrix with the ith diagonal component equal to $|v_i|$. Note that $diag(x)$ denotes an $(n \times n)$ diagonal matrix with the vector x defining the diagonal entries, (as in Matlab).

Let $g_* \stackrel{\text{def}}{=} g(x_*)$. Now the first order necessary conditions for x_* to be a local minimizer, as stated in the Coleman-Li paper, are:

$$\begin{cases} g_{*i} = 0 & \text{if } l_i < x_{*i} < u_i \\ g_{*i} \leq 0 & \text{if } x_{*i} = u_i \\ g_{*i} \geq 0 & \text{if } x_{*i} = l_i \end{cases}$$

With the scaling matrix D defined as above they consider the following system of nonlinear equations:

$$D(x)^{-2} g(x) = 0,$$

which is an equivalent statement of first order necessary conditions. This is essentially their formulation of the problem.

The system is continuous but not everywhere differentiable, particularly when $v_i = 0$. This is avoided by the strict feasibility of the iterates which force $|v_i| > 0$. Assume $x_k \in \text{int}(\mathcal{F}) \stackrel{\text{def}}{=} \{x : l < x < u\}$, that is, the iterates are strictly feasible. Then a Newton step, d_k, satisfies the following system of equations:

$$(D_k^{-2} \nabla^2 f_k + diag(g_k) J_k^v) d_k = -D_k^{-2} g_k$$

where $J^v(x) \in \Re^{n \times n}$ is the Jacobian matrix of $|v(x)|$ whenever $|v(x)|$ is differentiable.

1.2 The Perturbed Karush-Kuhn-Tucker Formulation.

The Perturbed KKT formulation for this particular minimization problem was derived through my understanding of Rice University's Technical Report 92-40, *On the Formulation and Theory of the Newton Interior-Point Method for Nonlinear Programming*, co-authored by A. El-Bakry, R. Tapia, T. Tsuchiya, and Y. Zhang. The problem can be equivalently stated as:

$$\begin{array}{lll} \min & f(x) & \\ \text{s.t.} & g(x) \geq 0 & \text{where } g(x) = x - l \\ & h(x) \geq 0 & h(x) = u - x \end{array}$$

Thus, $g(x) \geq 0$, $h(x) \geq 0$ imply $x \in \mathcal{F}$.

The Lagrangian for the above problem is

$$L(x, y, z) = f(x) - y^T g(x) - z^T h(x).$$

Thus, $\nabla_x L(x, y, z) = \nabla f(x) - \nabla g(x) y - \nabla h(x) z$, with $\nabla g(x) = I$ and $\nabla h(x) = -I$, so

$$\nabla_x L(x, y, z) = \nabla f(x) - y + z.$$

The KKT conditions are:

$$\begin{aligned} \nabla_x L(x, y, z) &= 0 \\ g(x) &\geq 0 \\ h(x) &\geq 0 \\ Y g(x) &= 0 \\ Z h(x) &= 0 \\ (y, z) &\geq 0 \end{aligned}$$

where Y denotes a diagonal matrix with diagonal y.

Thus the Perturbed KKT conditions are:

$$\begin{aligned} \nabla_x L(x, y, z) &= 0 \\ g(x) &\geq 0 \\ h(x) &\geq 0 \\ Y g(x) &= \mu e \\ Z h(x) &= \mu e \\ (y, z) &\geq 0 \end{aligned}$$

where e is a vector of ones whose dimension will vary with the context.

Thus we are finding a Newton step for this system of equations:

$$\begin{aligned} \nabla f(x) - y + z &= 0 \\ Y g(x) - \mu e &= 0 \\ Z h(x) - \mu e &= 0 \end{aligned}$$

The above system may also be denoted as $F(x, y, z) = 0$. Consequently, a Newton step, d, satisfies $F'(x, y, z)\, d = -F(x, y, z)$, or

$$\begin{bmatrix} \nabla^2 f(x) & -I & I \\ Y & X - L & 0 \\ -Z & 0 & U - X \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} = - \begin{bmatrix} \nabla f(x) - y + z \\ Y g(x) - \mu e \\ Z h(x) - \mu e \end{bmatrix}$$

where $d = (\Delta x, \Delta y, \Delta z)$.

2 Numerical Experimentation.

I wrote Matlab code to implement the Coleman-Li, KKT and Perturbed KKT formulations in conjunction with Newton's Method. I performed many experiments, in the end, varying only the parameter, γ, which determines the position of the initial point, x_0.

To simplify matters we design a convex quadratic nonlinear function $f(x)$. As a result there will be only one optimal solution, a global minimum. We generate a random $(n \times n)$ matrix, A, and a random $(n \times 1)$ vector, b, and define our function as

$$f(x) = .5(Ax)^T(Ax) - b^T x.$$

We choose $n = 10$, that is, $f : \Re^{10} \to \Re$, $u = (.5, .5, .5, .5, .5, .5, .5, .5, .5, .5)^T$ and $l = -u$.

We generate 100 random initial points x_{0i}, including γu and γl where $0 < \gamma < 1$. To do so we generate 100 random (10×1) vectors, v_i, $i = 1 \ldots 100$, with entries of 1, 0 or -1. These vectors are then multiplied both by .5 and the scaling factor γ, where again $0 < \gamma < 1$, so that they become strictly feasible points. Thus,

$$x_{0i} = .5\gamma v_i.$$

If γ is close to 1, then the initial point will be close to the boundary. If γ is close to 0, then the initial point will be close to the origin. Since the entries of the vectors v_i consist of 1, 0 or -1 these vectors represent points on the center of the faces or points of the edges of the faces of this 10-dimensional "cube". For instance in 3 dimensions, that is, $n = 3$, the point $(0, 1, 0)$ lies in the interior of a face of the cube, while $(1, 0, 1)$ lies on the edge of two faces of the cube.

We apply Newton's method to the three formulations. Step lengths are chosen so that all iterates x_k remain in the interior of the feasible region. The algorithm is said to have failed if a stopping criterion is not satisfied after 100 iterations or an iterate lands on the boundary. For Coleman-Li, the stopping criterion is $\| D(x_k)^{-2} g(x_k) \| < 10^{-6}$, for KKT and Perturbed KKT it is

$$\left\| \begin{array}{c} \nabla f(x) - y + z \\ Yg(x) \\ Zh(x) \end{array} \right\| < 10^{-6}.$$

The following table shows the number failures, out of the 100 initial points, for each of the three formulations.

γ	.5	.6	.7	.9	.99999
PKKT	0	0	0	0	0
KKT	0	0	0	0	6
Coleman-Li	1	4	13	30	50

As we can see the Coleman-Li formulation does not do well when the initial points are close to the boundary of the feasible region, while the KKT formulation does quite well except under the extreme case of $\gamma = .99999.$, In all cases, the Perturbed KKT formulation is quite robust with zero failures.

Implementing Computational Mathematics in K-12 Education

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Spend a Summer With a Scientist

Rice University

August 15, 1997

A strongly held belief by professors and students participating in the 1997 Spend a Summer with a Scientist program is that high school mathematics education is not what it should be. Students are not motivated to pursue high-level mathematical problems or specializations by continuing their math education, and most cannot answer the typical question "Where is math used in everyday life?" There is great potential for improvement with an infusion of applied math and computational science in the high school math curriculum. Such an introduction of this non-traditional math subject matter requires two efforts: teacher training and the publication of texts on applied math and computational science. CRPC's GirlTECH program is making great strides in teacher education by training teachers in computer technology and informing them of the vast resources available on the web. We spent our summer working on the much-needed high school textbooks.

The first project of the summer consisted of reviewing and making recommendations on a proposed linear algebra text for high school seniors. This text was originally a thesis entitled *An Introduction to Linear Algebra: A Curricular Unit for Pre-Calculus Students*, and was written by Tamara Anthony Carter in pursuit of her master's degree at Rice University. In preparation for a meeting with Tamara, we composed a chapter by chapter assessment of strengths and suggestions. A more general list outlining the need for a high school linear algebra textbook and the "selling points" of Tamara's particular text was also given to Tamara and is included in this report.

In addition to presenting Tamara with suggestions for her text, we coordinated a trial case for the textbook to gather student input. A linear algebra workshop was organized for students from Milby Science Institute, a magnet school in Houston, who were participating in the Howard Hughes summer programs. We compiled a mini-text on linear algebra using

certain chapters and sections from Tamara's text. Only minor alterations to Tamara's explanations, examples, and problems were made so that student comments would apply to Tamara's text as a whole. The workshop lasted four days, and included two hours of formal instruction each night as well as homework assignments. All of the Spend a Summer with a Scientist students participated as teachers. A schedule of objectives and homework problems for each night is included in this report. The students answered evaluation questions on the last night, and we prepared a summary of these responses. Copies of the mini-text and summary of evaluations were given to Tamara for her use in preparing the final textbook for potential publication.

The next project began as a summer project, but will actually be continued by us next school year in an independent study course. This project also involves a thesis that is actually a high school textbook. This thesis, *Introduction to Computational Science: A High School Curriculum*, was written by Sarah Benkendorf who was also pursuing a master's degree at Rice University. Unlike Tamara, Sarah has no plans for editing and publishing her text. There is currently no textbook on this subject for senior high school students. Furthermore, computational science is of great importance to young students for understanding real-world problems and being exposed to problems that are so interesting they may motivate further study in mathematics. For these reasons, we, along with Dr. Tapia and Dr. El-Bakry, are editing and making additions to Sarah's original text in hopes of publishing a textbook that will serve as an introduction to computational science. This text is being written for high school seniors, but is appropriate for and could easily be used by college freshmen or professionals who desire an introduction to computational science. The plans for this textbook as of July 30, 1997, are included in this report. One unique quality in its design is

that it is being written so that is may be used in modules. In other words, an understanding of each chapter does not depend on the material presented in the previous chapters. This approach may attract a wider audience including those who wish to study or teach one particular topic in computational science that fits well into another course. For example, the chapters on solving linear systems and linear regression could be used in an algebra course or a chemistry course with lab work. We have spent the second half of the summer designing the text and editing and rewriting Chapter Two. We also attended the Conference for the Advancement of Mathematics Teaching to examine current high school mathematics textbooks and speak with publishers about the computational science text. We expect to complete the rewriting and editing of the text by May of 1998.

Erin Kellam
Samitra Seales
June 6, 1997

Review of **An Introduction to Linear Algebra: A Curricular Unit for Pre-Calculus Students** written by Tamara Anthony Carter

Selling Points: Why We Support the Unit

- Allows students to recognize that challenging concepts in mathematics exist and are still in need of research.
- Sets a foundation on which students can build for college linear algebra.
- Since it can be argued that linear algebra is as important as calculus to scientists and engineers, it is important that students are introduced to linear algebra prior to advanced studies in science and engineering.
- It has useful cross-disciplinary applications such as curve-fitting, which students will find beneficial in other areas of study.
- Teaches concepts rather than procedures, so students will be able to expand beyond examples in the book.
- Flows coherently from chapter to chapter.
- Allows students to develop computer programming skills.
- Satisfies all but one of the essential elements that the state of Texas requires in order for a pre-college textbook to be adopted.

Schedule for
Milby Science Institute Math Workshop
June 16 - 19, 1997

Monday

- **Objectives/Goals:**

  Cover Chapters One and Two- introduction to matrices, and addition and subtraction of matrices. More specifically, the introduction to matrices includes determining matrix dimensions, the transpose of a matrix, and symmetric and square matrices.

- **Recommended Group Problems:**

  Chapter One Problems: 1a,b,c, 2a, 3a,b

  Chapter Two Problems: 1a,d,j, 3a,b,c

- **Recommended Take-Home Problems:**

  Chapter One: 2d, 4, 5

  Chapter Two: 1e,h,i, 2, 4

Tuesday

- **Objectives/Goals:**

  Cover Chapter Three on matrix multiplication and Section 4.1 on coding. Topics include inner/dot product, scalar multiplication of matrices, multiplication of matrices, and the identity matrix.

- **Recommended Group Problems:**

  Chapter Three Questions: 2, 3, 4, 5, 7

  Chapter Three Problems: 2b,i, 3

- **Recommended Take-Home Problems:**

  Chapter Three Problems: 1, 2f,k,l,m

  Chapter Four Problems: 5a,c

Wednesday

- **Objectives/Goals:**

  Cover Sections One and Two of Chapter Five. For the primary method of determining the determinant, use expansion by minors and focus on 2 x 2 and 3 x 3 matrices. For determining the determinant of larger matrices, use Gaussian elimination (teacher may want to provide more examples).

- **Recommended Group Problems:**

  Chapter Five Questions: 1, 2

  Chapter Five Problems: 1a,c,f

- **Recommended Take-Home Problems:**

  Chapter Five Problems: the remaining exercises in problem #1

Thursday

- **Objectives/Goals:**

  Cover Chapter Eight (with the exception of Section One) on least squares and [1]Chapter Nine on eigenvalues. Least squares includes interpolation/extrapolation, best least squares fit, minimization, and normal equations.

- **Recommended Group Problems:**

  Chapter Eight Problems: 1c, 2, 4

  Chapter Nine Problems: 5

- **Recommended Take-Home Problems:**

  Chapter Eight Problems: 3, 5

  Chapter Nine Problems: 6, 7

[1] If time allows.

Plans for
Introduction to Computational Science text
as of July 30, 1997

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Vision

We will design the Introduction to Computational Science text so that it may be used in two ways. It may be used as *the* text for a high school or college freshman course in computational science, or individual chapters may be used as supplementary material for the "standard" math and science courses. For example, the chapters on solving linear systems and linear regression could be used in an algebra course or a chemistry course with lab work. The chapter on solving nonlinear equations would fit into a geometry or calculus course, and the chapter on differential equations could supplement a calculus course. In order for the text to be used in this way, each chapter will be written so that it is independent from the others. Writing the text with these alternate uses should attract the largest audience, give as many students as possible an exposure to computational science, and appeal to teachers. Finally, our Introduction to Computational Science text is a transition stage between an educational system with no computational science courses and one with a stand-alone computational science course.

Proposed List of Chapters (in order)

1. *Introduction*
   - What is computational science?
   - Why do we need computational science? (include careers)
   - History of relationship between mathematical theory and applications (Theory and applications were combined historically, then separated in mid-twentieth century, now combining again)
   - Numerical errors (Can computers make mistakes?)
   - Representation of numbers (base 2 to base 10)

2. *The Solution of Linear Equations*
   - Direct computational methods (Gaussian elimination, Gauss-Jordan elimination, Inverse, Cramer's Rule)
   - Operation counts and a comparison of methods (cost)
   - Conjugate gradient method

3. *Linear Regression*
   - The line of best fit
   - Least squares regression

4. *Solutions of Nonlinear Equations*
   - The method of bisection
   - Newton's method
   - The secant method
   - The method of false position
   - A comparison of methods

5. *Differential Equations*

   This chapter is not in the original text (thesis copy). We will search for the "standard" calculus text to use as a tool in writing this chapter so the transition to differential equations will be as smooth as possible. This chapter will include no equations with second derivatives.

6. *Optimization*

   This chapter is not in the original text (thesis copy). This chapter will serve

to introduce students to a very important, interesting, and hopefully inspirational class of problems. Since the math involved is very advanced, there will be a focus on the different problems and their purposes with a careful treatment of the appropriate computations.

7. *Linear Programming*
   - History
   - Graphical solutions with contour lines (and the limitations of this method)
   - Linear programs in standard form
   - The simplex method
   - Parallel programming

Additional Comments

- Since high school math students frequently solve problems on graphing calculators, we will discuss the methods various calculators use to solve problems. For example, does a calculator use Newton's Method to find the square root of 2?
- We want to include some computer programs, written by us, for the students to vary the input and run. These programs may be written in Matlab.
- We also will include many real-world examples in the text that are interesting to the students, easy for them to relate to, and will broaden their experience and exposure to scientific problems.

SAS Project Description 1997

Cassandra Moore McZeal

1 Introduction

This summer I investigated the use of a primal-dual interior-point method in a branch-and-bound algorithm to solve a class of 0/1 mixed integer programming problems. These problems originate from Consolidated Rail Corporation (Conrail). The model attempts to choose the departure times for 998 trains over 559 yards such that the trains depart at some point during the correct day, and the number of trains used to power the schedule is minimized. For each schedule that is generated, we have a different 0/1 mixed integer programming problem. These problems range in size from 17,442 variables and 6118 constraints to 538,800 variables and 144,595 constraints.

1.1 Preliminary Numerical Tests

There are 41 problems in the Conrail test set. The trains run according to a weekly schedule, and there is an adjustable parameter that controls the number of departure time periods each day. When this parameter is set to three the trains leave every eight hours, when set to twelve they leave hourly, and when set to the maximum, 96, trains leave every fifteen minutes. There is a time period parameter for each of the two types of trains in the model. For regular trains the time period parameter is called TP. For ENS (exchange) trains the parameter is called EnsTP, and must divide TP evenly. Due to the size and the computational effort expended, we report preliminary results for only 14 of the problems.

In our numerical test we used CPLEX 4.0 on four SGI Power Challenge-L multiprocessors. We limited the time for finding a solution to each of the 14 problems to 10,000 secs. The initial node (parent subproblem) was solved with CPLEX's interior-point code, and the child subproblems were

solved by either the interior-point code or the dual simplex method. We used default settings for the interior-point code used by CPLEX to solve the subproblems. For the dual simplex method implemented by CPLEX, we used steepest edge pricing. All other parameters are at default settings. We also did not change the mixed integer programming strategies used by CPLEX.

As can be seen in the following table, CPLEX's branch-and-bound algorithm using an interior-point method does not generate and solve as many nodes as it does using the dual simplex method for most of the smaller problems. This trend changes, however, when NumTP is 12 and NumEnsTP is 3. At this point, the interior-point based algorithm generates and solves more nodes than the simplex based algorithm. Interestingly, the best integer solution generated by the interior-point based algorithm is strictly less than the best integer solution generated by the simplex based algorithm in all but one case.

Name	Time Periods		Interior-Point		Dual Simplex	
	TP	Ens TP	Nodes	Best Solution	Nodes	Best Solution
con33	3	3	237	732.20847689	21895	740.21218707
con42	4	2	237	741.02028929	8704	772.97597399
con44		4	152	739.4346237	12684	756.67890073
con62	6	2	166	752.13986307	5194	750.77552675
con63		3	191	746.24917505	11353	754.55165118
con66		6	84	731.54857074	6029	744.62647646
con82	8	2	257	741.81485425	10073	754.63084237
con84		4	115	714.78230402	3896	737.54665082
con88		8	53	707.4105	879	722.77691535
con122	12	2	281	744.81368653	2578	769.81717300
con123		3	148	751.39205827	26	n/a
con124		4	112	740.94480932	0	n/a
con126		6	63	721.97262339	0	n/a
con1212		12	21	n/a	0	n/a

2 Our Current Implementation

Heuristic algorithms are designed to find good integer feasible solutions quickly. These solutions are not necessarily optimal. We designed an heuristic rounding algorithm for the generation of integer feasible solutions based upon the structure of the constraints in the problem. We also modified our search tree based upon this algorithm. We summarize our preliminary results in the following table.

NAME	TP	EnsTP	NODES	INT SOLN	LP SOLN
con33	3	3	221	745.293278	659.695861
con42	4	2	140	781.143485	648.165406
con44		4	62	758.369945	634.557275
con62	6	2	92	780.052713	630.337850
con63		3	61	779.944154	621.350284
con66		6	29	770.240096	609.545147
con82	8	2	50	780.419443	616.993064
con84		4	23	764.033574	605.152821
con88		8	7	760.279625	597.927929
con122	12	2	18	783.714431	605.431433
con123		3	12	737.344716	599.151543
con124		4	8	753.505517	593.081605
con126		6	5	755.585682	588.265380
con1212		12	2	739.494864	583.338884

A Mathematical Model of Respiratory Muscle Micromechanics

Luis A. Melara *

Mentors:
Dr. Petr Klouček, CAAM, Rice University
Dr. Aladin Boriek, Baylor College of Medicine

August 8, 1997

1 The mathematical formulation of the fiber micromechanics

The diaphragm is the major muscle of respiration in mammals. The diaphragm is a composite structure that consists of muscle fibers and connective tissue. Understanding the micromechanics of the diaphragmatic muscle is fundamental to any explanation to its physiological or pathological behavior. Mathematical modeling of the micromechanincs of the diaphragm will improve our understanding to the ability of this muscle to perform without local muscle injury. There is an extensive research on the mechanics of the diaphragm [1]-[8] but there is no significant research on the micromechanics of this vital muscle.

Anatomically, the diaphragmatic muscle is a relatively thin sheet of muscle bundles that extend radially from the central tendon (CT) to the chest wall (CW), see Fig. 3 and Fig. 4. Recent work from Dr. Boriek laboratory demonstrated that fiber architecture in the diaphragmatic muscle of the dog is discontinuous, and therefore muscle fibers do not necessarily span the entire length of the muscle from chest wall insertion to the origin on the central tendon. The majority of the fibers are shorter than the length of the muscle from CT to CW. These fibers do taper along 30% of their length and taper down to a very fine thread with a taper angle of about 1 degree, see Fig. 5. The tapered portion of the fiber generates an interface between muscle fibers and connective tissue that is essentially loaded in shear.

During inspiration and expiration the diaphragm contracts and expands, respectively. During the contraction process, muscle fibers shorten, while maintaining their volume and surface area. Therefore, fiber cross-sectional shape changes to minimize the change in volume and surface area of the muscle fiber, see Fig. 6. Because the muscle are mostly water, muscle fibers are incompressible and therefore isovolumic. Maintaining the surface area of the fibers is crucial during muscle contraction because the surface area of the fiber is the interface between the fibers and the connective tissue, through which contractible forces are transmitted. The deformation of the fibers should satisfy the nonlinear stress-strain law of single muscle fibers during muscle contraction.

In this project, we mathematically model active shortening of single muscle fiber under physical, mechanical, and geometric constraints provided above. This mathematical model is described by the formulation

$$\inf_{u \in W^{1,2}(\Omega, R^2)} \left\{ \Phi(u) + \left| \frac{1}{|\Omega|} \int_\Omega ||E(x) - E_0|| dx \right|^2 + \left| \left(\int_0^1 w'(t) dt \right)^2 - (meas(\partial\Omega))^2 \right|^2 \right\} \qquad (1.1)$$

*Participant in Spend A Summer With A Scientist. Project funded by Center for Research on Parallel Computation.

Here, $\Phi(u)$ represents the elastic energy, $u : R^2 \to R^2$ is the continuous deformation, the domain Ω refers to the fiber, $E(x)$ is the strain tensor and E_0 is the perscribed strain value that is equivalent to the magnitude of muscle shortening during the inspiratory effort and $W^{1,2}$ is the space of functions whose derivative is square integrable.

Moreover, $\int_0^1 w'(t)dt$ represents the measure of the boundary of the fiber which is parametrized by w, $meas(\partial\Omega)$ relates to the measure of the boundary of fiber at funcitonal residual capacity.

2 The preliminary model of a micromechanics

We studied the one-dimensional counterpart of (1.1) which reads

(2.3)

$$E(u) = \int_0^1 (u'(x)^2 - 1)^2 + u(x)^2 dx.$$

This example is linked with the general problem (1.1) via the lack of convexity of the total stored energy. This indicates that there is no continuous deformation yielding the minimum. This can be demostrated in the above one-dimensional example (??) as follows. First, note that

$$\inf(\int_0^1 (u'(x)^2 - 1)^2 + u(x)^2 dx) = 0$$

hence if there would be a minimizer then

$$(u'(x)^2 - 1)^2 = 0 \text{ and } u(x)^2 = 0.$$

But these two condition cannot be satisfied simultaneously. Therefore, there is no continuous function u at which the stored energy E would attain its minimum value.

Using the Matlab Optimization Toolbox, we minimize this energy for number of different initial guesses and number of partitions. The Figs.1-2 indicate what we have seen from the proof. The minimization procedure is forcing the minimizer to produce more and more oscillations as the values of the function get smaller and smaller. It seems that the we can get $O(h)$ oscillations of the minimizer which is dictated by imposing the condition on the derivative. We have used P_1 finite elements to discretize the deformation u and midpoint qudrature formula to approximate the integral in the definition of E.

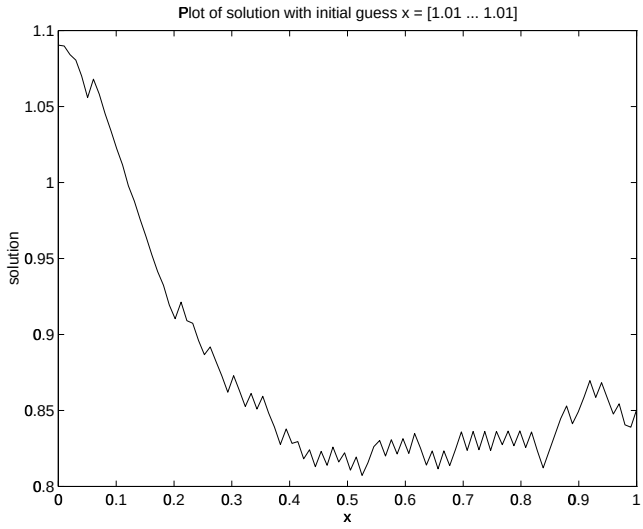

Figure 1: The result of calculations using piece-wise linear finite element with $h = 1/100$. The computed function has derivatives close to ± 1.

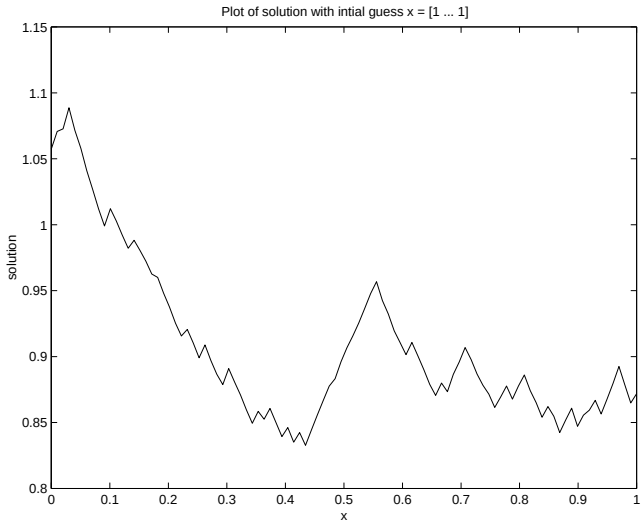

Figure 2: The result of calculations using piece-wise linear finite element with $h = 1/100$. Though the computed function has derivatives close to ± 1 the function itself is different from the one plotted on Fig 1. due to the slightly different initial guess.

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[10pt]report

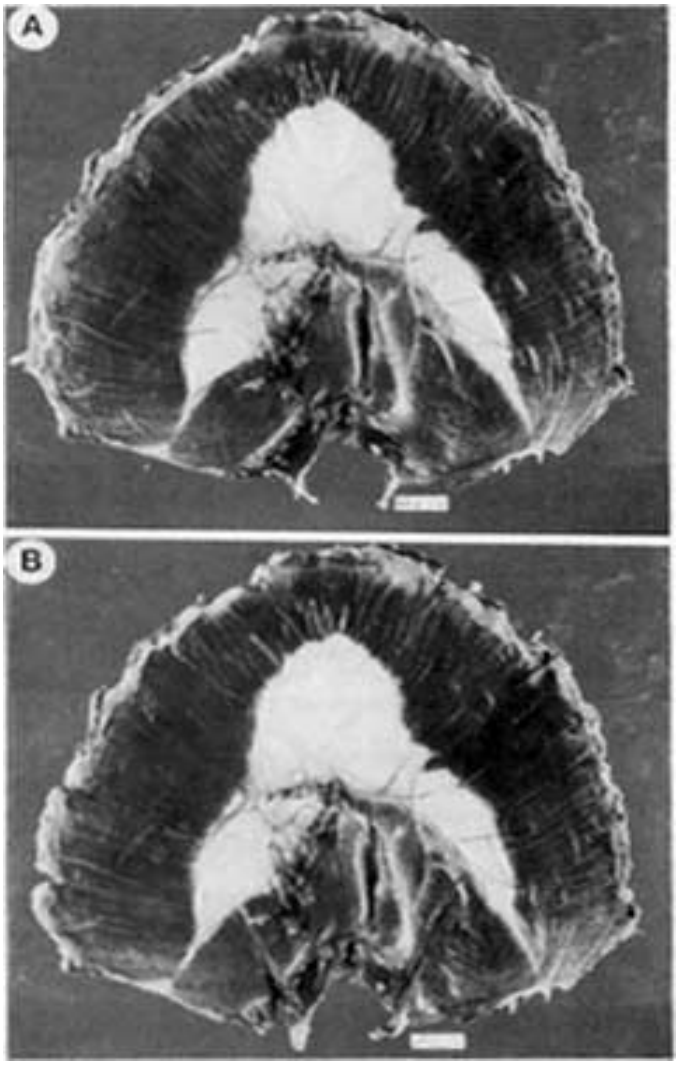

Fig. 3 Photographs of dog diaphragm, laid flat on transparency, viewed from abdominal surface. A: intact diaphragm. B: same diaphragm cut into 13 wedge regions. Note there is minimal gross wrinkling of intact diaphragm and virtuall y no distortion of escised diaphragm. Most of muscle bundles are approximately perpendicular to their insertions. From Journal of Applied Physiology, 77(5):206 5-2074 (1994) A.M. Boriek and J.R. Rodarte.

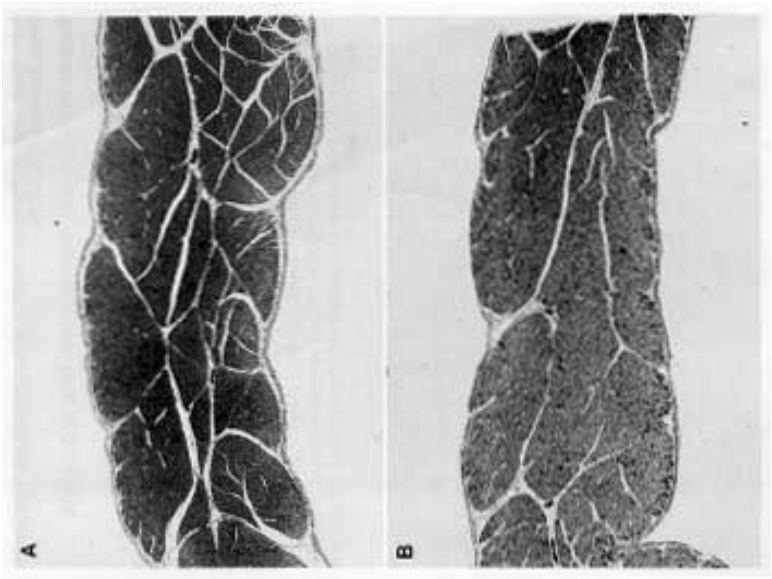

Fig. 4 Light photomicrographs of transverse sections of midcostal diaphragm along course of muscle near CT (A) and near CW (B). Sections show muscle fibers, connective tissue, diaphragmatic ligament from thoraic side, and peritoneum attached to abdominal surface of diaphragm. Total magnification, X22 .8. From Journal of Applied Physiology, 77(5):2065-2074 (1994), A.M. Boriek and J.R. Rodarte.

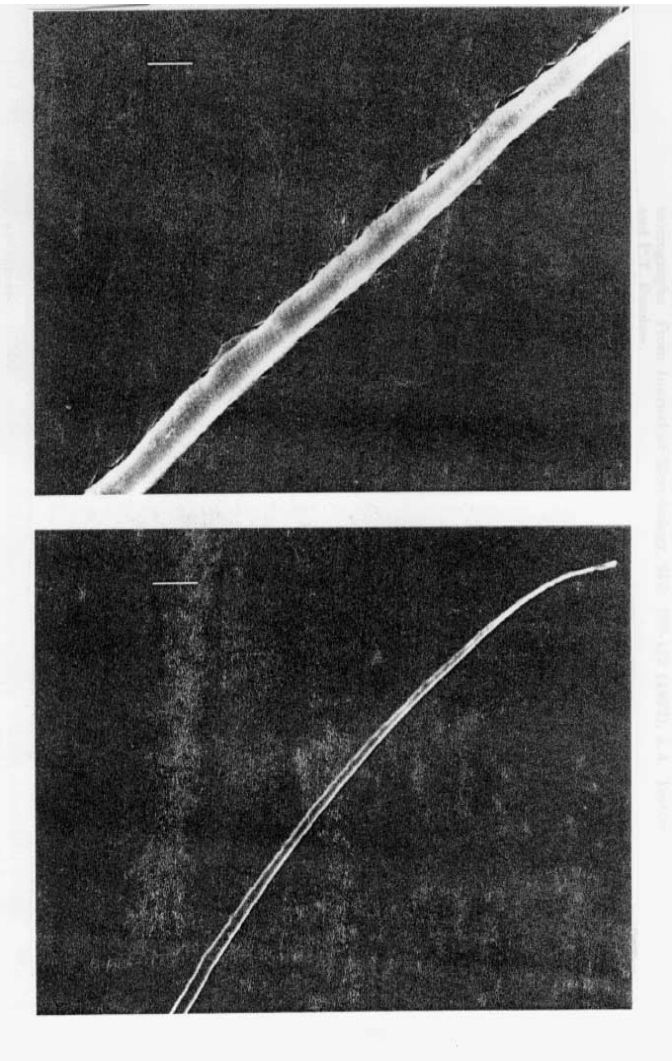

Fig. 5 Scanning electron micrographs of the tapered end of an isolated biceps femoris muscle fiber. Note the abscence of surface specializations and the grad ual taper toward the end. Bar = 50 μm in upper panel and 10 μm in lower pan el. From Journal of Applied Physiology, 207: 211-223 (1991), J.A. Trotter.

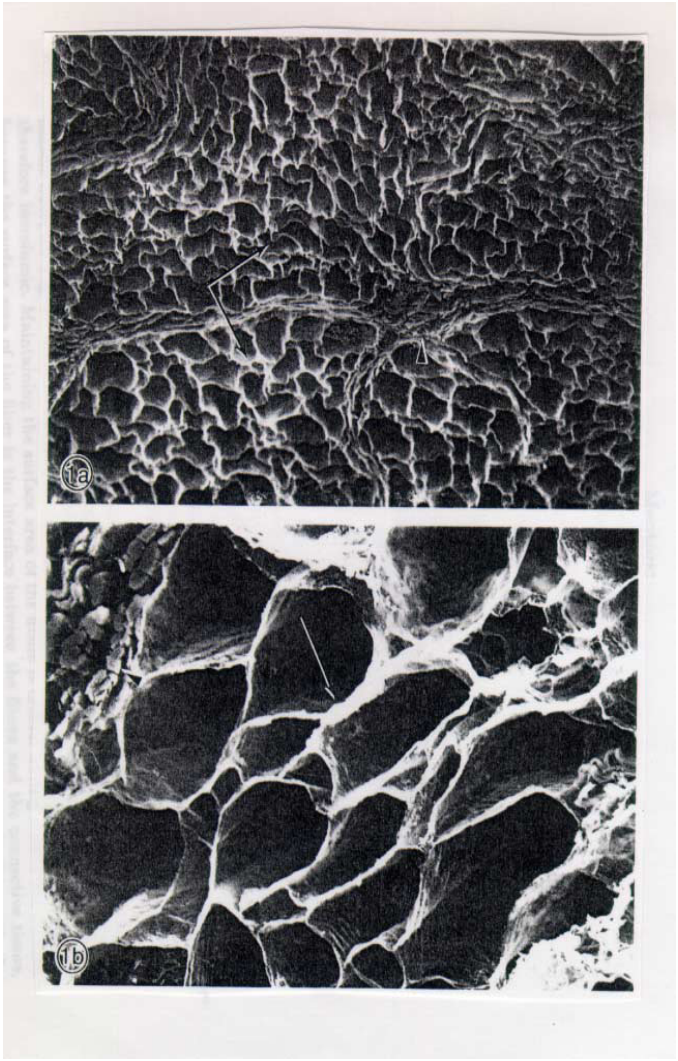

Fig. 6 Scanning electron micrographs of collagenous stroma from which muscle fi bers were removed by treatment with NzOH. a: X200. b: X700. The endomysium (arrows) is a continuous network surrounding tubular cavities. The perimysium (arrowhead s), consisting of thick collagen fibers, is also seen in these micrographs. From Journal of Morphology, 212: 109-122 (1992), J.A. Trotter and P.T. Purslow.

Phytoremediation of 2,4,6-Trinitrotoluene using *Catharanthus roseus*

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Angélica Diana Rodríguez

Abstract

Soils contaminated with 2,4,6-trinitrotoluene (TNT) from former munitions facilities are present world wide. Using hairy root cultures of the periwinkle, *Catharanthus roseus*, TNT is effectively and inexpensively transformed into less harmful substances. The effects of TNT on *C. roseus* in its exponential and stationary growth phases will be examined with this experiment.

Introduction

Hairy root cultures used in this experiment are derivative root structures of *Catharanthus roseus*, commonly known as the periwinkle, and contain intrinsic abilities to phytoremediate TNT at various life stages. The four main life phases of hairy roots are: lag (inoculation), exponential growth, stationary, and death. The inoculation phase is the stage right after roots have been subcultured and added to a new flask environment (50 mL medium) to begin growth. Roots experience a lag phase during inoculation where no growth or increase in mass is observed. This occurs for a short while until the exponential growth phase begins. Hairy roots grow exponentially until stationary phase is reached, that is, the stage where the roots will not grow any longer and eventually die, entering the death phase in which an exponential decay occurs (Bailey & Ollis). The exponential growth and stationary phases are the two life stages in which TNT phytoremediation will be examined.

Phytoremediation is an intracellular (inside the root) process which benefits the extracellular (outside the root) environment. During phytoremediation, the hairy roots take up metals and toxic chemicals, and then transform them into less harmful substances. This method of rejuvenating the toxic soil is preferred to expensive incineration and composting

which produces recalcitrant reduction products (Lauritzen, et. al 1996). Effects of TNT on *C. roseus* have been studied using growth kinetics to model its life cycle by adding various TNT concentrations to all growth phases of the hairy roots and measuring its concentration at different time intervals.

Methods and Materials

C. roseus hairy root clone LBE-6-1, grown in Gamborg B5/2 salts and 30g/L sucrose in constant stirrer and bacteria free environment with no light was maintained prior to experimentation (Bhadra, et. al). For exponential growth phase tests, 20, 30, and 40(mg/L) concentrations of TNT were added to the flasks containing 5g fresh weight (FW) roots at 19 days per 50mL medium. Stationary phase tests were performed by adding TNT concentrations of 15.97, 28.00, 42.34, and 55.44 (mg/L) to roots in stationary phase. Samples of medium were withdrawn at specified intervals and later analyzed by using a High Performance Liquid Chromatography (HPLC).

Results

Exponential Growth Phase

During exponential growth, the hairy root and TNT concentrations are simultaneously changing as displayed in Figure 1 and Figure 2.

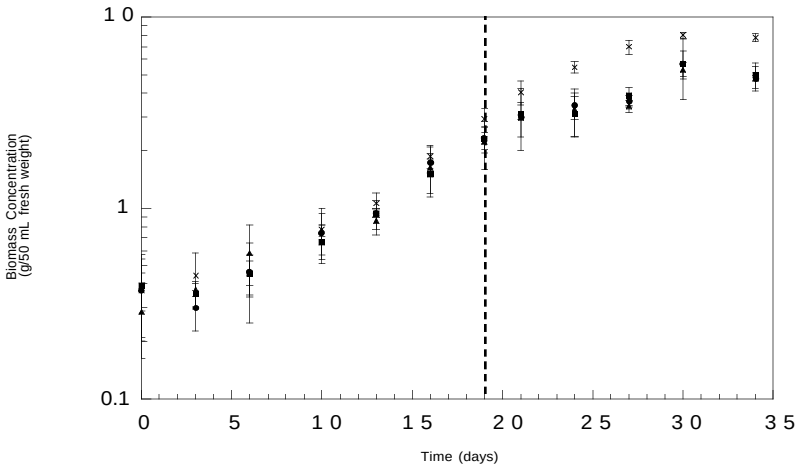

Figure 1 Exponential phase biomass growth. (l 20 mg/L, n 30 mg/L, s 40 mg/L, X control - no TNT)

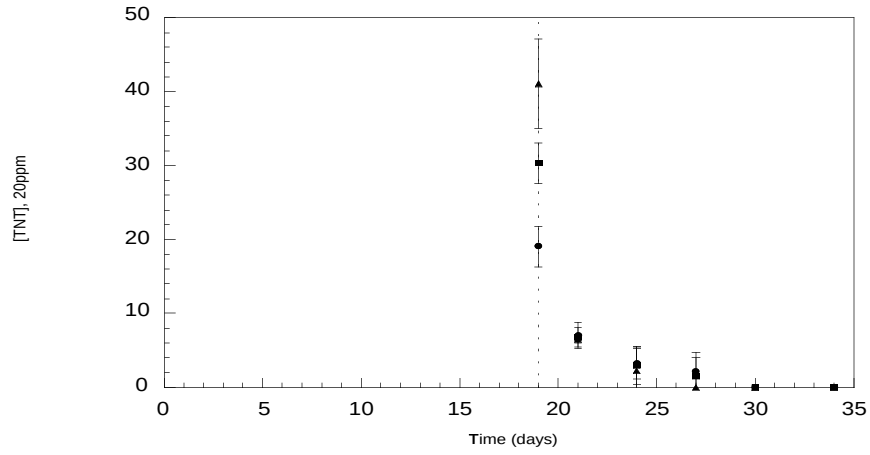

Figure 2 Exponential phase TNT disappearance. (l 20 mg/L, n 30 mg/L, s 40 mg/L, X control - no TNT)

These systems can be modeled according to equation 1, the second order reaction rate law (Hill) :

$$r = -k * [X] * [TNT] \quad \textbf{(1)}$$

r = reaction rate (L/g-day)

k = reaction rate constant

[X] = Plant concentration (g FW/L)

[TNT] = TNT concentration (mg/L)

The second order rate law is implemented in a Matlab routine which loops through matrices of plant mass and TNT concentrations then uses the 'fmin' function to determine the least squared error values and calculates the kinetic constants for each system. Table 1 displays the kinetic constants for the three different batches of flasks.

Table 1 TNT Reaction Rate Constants in Exponential Phase, 34 day cycle

TNT Concentration (mg/L)	Kinetic Rate Constant (L/g-hr)
20	0.0075 ± 0.0032
30	0.0126 ± 0.0051
40	0.0156 ± 0.0030

As the TNT concentration increases, the reaction rate constant also increases. These rate constants are helpful in modeling the growth of hairy roots by modeling their growth according to the specific growth rate equation (equation 2) which is only valid for exponential growth phase (Blanch & Clark):

$$r = \mu * [X] \quad \textbf{(2)}$$

r = reaction rate (L/g-day)

μ = specific growth rate constant (day^{-1})

[X] = plant concentration (DW)

Using [X]=100 g/L and the reaction rates from Table 1, μ can be backed out of equation 2 which will yield the specific growth rate and the doubling time of the hairy roots, shown in Table 2.

Table 2 TNT effects on *C. roseus* growth in Exponential Phase, 34 day cycle

[TNT] (mg/L)	DW Specific Growth Rate (day^{-1})	DW Doubling Time (day)	FW Specific Growth Rate (day^{-1})	FW Doubling Time (day)
Control	0.185	3.74	0.0503	13.8
20	0.0125 ± 0.00704	89.4 ± 58.0	0.145 ± 0.0331	4.79 ± 0.685
30	0.0134 ± 0.00523	59.3 ± 29.8	0.140 ± 0.0479	5.16 ± 1.22
40	0.0130 ± 0.0035	55.5 ± 14.9	0.126 ± 0.0389	5.76 ± 1.77

These values for the specific growth rate show that as the TNT concentration increases, the rate of growth decreases slightly. It is important to notice that specific growth rates can only be determined using dry weight (DW) values (Blanch & Clark). These dry weight values are measured after the hairy roots have been freeze dried and all water has been removed from their roots and vary from the fresh weight growth rates by one order of magnitude.

Stationary Phase

The stationary life cycle phase of hairy roots occurs approximately 21-24 days after inoculation. At this phase, hairy roots have passed their peak growth period and are no longer growing. However, TNT degradation in this phase is phenomenal. As shown from Figure 4, a rapid disappearance of TNT occurs within the first 48 hours of addition; 25.6% to 32.2% of the initial TNT concentration was degraded during the first time interval.

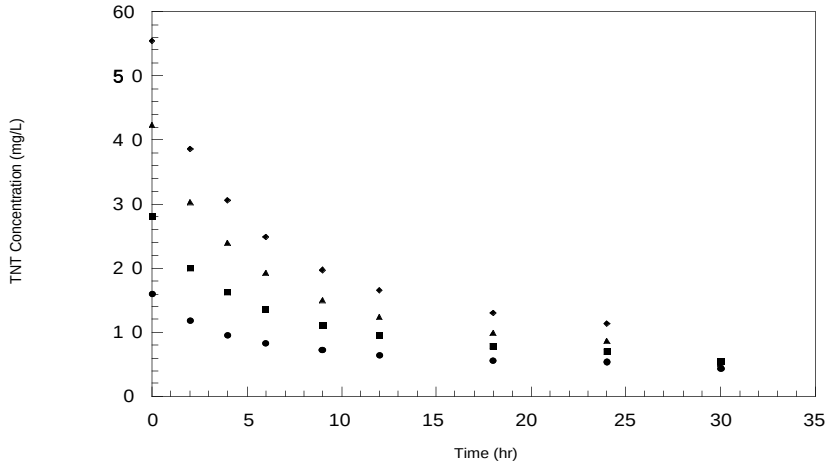

Figure 3 Stationary phase TNT disappearance in four batches. (l A, n B, s C, u D)

Plant concentration [X] where will have a constant concentration [X] = 100g/L as TNT concentrations are changing with time, therefore it is assumed that stationary phase is modeled according to the pseudo-first order reaction rate law, similar to equation 1. The kinetic reaction rate constants for stationary phase are listed in Table 3. They have been determined analytically by graphing the rate of [TNT] change versus [TNT]. These values are should be relatively similar to the kinetic rate constants of the exponential phase.

Table 3 TNT effects on *C. roseus* in Stationary Phase, 30 hour cycle

TNT Concentration (mg/L)	Kinetic Rate Constant (L/g-hr)
15.97	0.0184 ± 0.00237
28.00	0.0566 ± 0.0255
42.34	0.0892 ± 0.0344
55.44	0.139 ± 0.0819

Conclusion

TNT disappearance was only observed in the presence of live *C. roseus* hairy roots in 50mL of medium. As the TNT disappeared in the medium, traces of 2-monoamino-4,6-dinitrotoluene (ADNT) and 4-monoamino-2,6-dinitrotoluene began to appear. These two isomers of ADNT are the only byproducts detected of TNT's transformation so far and were the byproducts were formed in both phases. Hairy roots in exponential growth transformed the TNT slower than those in stationary phase. However, both sets of roots effectively transformed TNT with final concentrations ranging from 0 ppm to 4 ppm. *C. roseus* has abilities to transform low concentrations of TNT at a rapid and efficient pace. The reproducibility and upscaling of these results promises a future for biodegradation and environmental clean-ups using natural catalysts.

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Spend a Summer with a Scientist 1997
Final Report

Carlos G. Uribe

August 20, 1997

Abstract

In the past, medical procedures as related to disease diagnosis have basically involved trial and error methods. Many medical examinations, such as an electromyography (EMG) examination which is used to diagnose muscle disease, involve direct observation and crude measurements making it difficult for the untrained eye to arrive at an accurate diagnosis. Diagnosis is based on historical medical findings which require much clinical experience and is prone to human error. The computer, as opposed to special hardwired devices, is extremely flexible and can be used to assist medical and health care professionals at arriving at fast and accurate diagnosis. The advantages are limitless and could result in saving a life to treating an incurable disease. Although the involvement of Computer Scientists in medical and health care science is relatively recent, I believe that medical science can benefit from a quantitative analysis of medical data which is reduced and interpreted on a computer system. My summer project involved understanding methods used in conducting research of this nature, specifically an analysis of the electromyographic signal.

1 EMG Defined

Electromyography is the study of muscle response to nervous stimulation measuring electrical patterns in muscle fiber. When neural impulses, transmitted from the brain, reach the muscle fiber, a wave of De-polarization spreads over the muscle fiber resulting in a twitch followed by complete relaxation. Electrical signals produced by the potential difference of the electrode and neural impulses are then recorded and analyzed.

The exam involves inserting a needle electrode through the skin and into the muscle. The electrical impulse is amplified and transferred to a digital signal processor where it undergoes a process of mathematical transformation into its wave representation which is then displayed onto a computer screen. It may also be displayed audibly through external speakers.

During muscle contraction the presence, amplitude and shape of the wave form is then used to provide information about the muscles ability to respond to nervous stimulation. It is a standard medical procedure that is used to reveal nuero-muscular disorders and other medical problems. For example, myopathies such as muscular dystrophy, which cause muscle degeneration, can be accurately assessed by a clinician performing an EMG examination.

2 Study Phase

During my initial phase of this study I was guided by Dr. Richard Tapia to develop and explore a set of questions to determine the direction of this research. He explains that this initial questioning phase is a crucial step in conducting research. These questions are then used as a foundation to precisely quantify a series of well defined manageable sub-problems. The formulation of the questions used in this research is based on the advice of Dr. James Killian, a neurologist at Baylor College of Medicine.

The main use of EMG is to detect and differentiate between the various types of muscle disease. The major concerns at arriving at a diagnosis are:

- Is the wave form present, absent, or modified during voluntary muscle contraction?
- Are the characteristics of the wave form during voluntary contraction normal in duration, shape, and amplitude?
- Are there any spontaneous, irregular signals at rest and what are their characteristics?

Extensive time was spent during this phase of research. There are many different variables that make a problem such as this very difficult to analyze therefore most of my time was spent studying the anatomical and physiological aspects of the examination. Problems such as electrical noise patterns distributed through the recording medium are very difficult to filter. Data reduction and interpretation of real medical data is the next phase of my study.

3 Conclusion

Although I was not able to test and analyze real data, I did however learn how to take the initial and necessary steps needed to conduct research. My experience in SAS is a positive one which will help me in every aspect of my life.

Spend a Summer with a Scientist Program

1997 Progress Report

On Global Optimization Least Squares Techniques with

Application to the Phase Problem in X-Crystallography

Leticia Velázquez

Advisors: Dr. George Phillips Jr., Dr. Richard Tapia, Dr. Yin Zhang

An important activity in X-ray crystallography is to determine effective globalization strategies for solving the semi-local and global stage of the phase problem. This problem occurs when trying to determine the molecular structure of proteins. Scientists are interested in understanding the composition of these molecules and their relevant functions in the human being.

Scientists perform an X-ray crystallography experiment: a beam of X-rays is passed through a crystallized protein, diffracted X-rays emerge from the crystal at different angles and at different intensities. These intensities are recorded on detection film. The phase information cannot be measured from the experiment and the 3-dimensional structure cannot be determined without further computation. This is what is know as the phase problem in X-ray crystallography.

Our project is to formulate the phase problem as a constrained global minimization problem where the objective function is expressed in a least-squares format, i.e, the error between the intensity measurements and the calculated amplitudes of the scattering functions must be driven to zero. This objective function is highly nonlinear implying there exists many local minima which makes it difficult to locate the desired global minimizer. Specifically, we want to address the semi-local refinement stage of the phase problem and present some effective global optimization techniques. We want to compare numerically the advantages of using or not the proposed strategies and their impact over existing techniques available today. The globalization techniques that we are using and developing cannot just only be applied to the phase problem where a zero or small residual is desired, but also to other application areas like seismic problems that can also be modeled as least-squares problems.

During this summer, we have been trying to solve the phase problem of a real known 39 atoms

(117 unknown variables) molecule after successfully solving known structures of about 22 atoms (66 unknown variables). We realize that solving this structure from a random guesses of the position of the atoms is quite challenging, so we have decided to focus in the semi-local stage of the problem, i.e., having a rough idea of how the structure looks like, we want to refine the given position of the atoms that will match more perfectly the observable data.
The framework of interior-point methods consists of minimizing an objective function subject to several constraints. These methods have been proven to work reasonably good when the starting point is feasible with respect to the constraints which can be done for the semi-local refinement problem. In our particular application of the interior-point code for the phase problem, we do not want to obtain any local minimizer, but we are looking for a specific one: the global minimizer. So we have to extend the developed theory on interior-point methods to obtain a global optimization method, or to use the available local codes and add the necessary modifications to our model to help us reach our desired solution.
One goal is to smooth the function to make it less nonlinear. We are trying to do this by controlling the number of intensity measurements involved in the objective function. In other words, smoothing the function will filter out some local minimizers and increase our chances of obtaining the desired global minimizer.
Part of this work was presented recently at the SIAM's 1997 annual meeting at Stanford University and we are in the process in writing a technical report on the work on solving the zero or small residual least squares problems for small to medium size molecules. It will also include some other applications besides the area of Biochemistry.
Also I have been working with Dr. Richard Tapia and Miguel Argaez in determining effective path-following strategies and their implementations using merit function technology for attacking general nonlinear programming problems. We have written a more robust line-search primal–dual interior-point Newton algorithm that presents several options of using different types of merit functions and centrality conditions that can guide the initial point to a local minimizer when the starting guess is not in the neighborhood of the solution. This will be very helpful for us, especially for implementing the for attacking the phase problem. Presently, we are writing a technical report that discusses the numerical experiments obtained by this code entitled: Numerical Comparisons of Path-Following Strategies

for a Basic Interior–Point Method for Nonlinear Programming. Also at the SIAM's Annual Meeting at Stanford University a talk was presented on this work.

The Behavior of Newton's Method on Two Equivalent Systems

Cristina Villalobos

August 6, 1997

Abstract

Newton's method is a fundamental technique for solving optimization problems. In theory, it may give different behavior for two equivalent problems. In this paper, we explore the differences when Newton's method is applied to the perturbed Karush-Kuhn-Tucker conditions of the linear programming problem and when it is applied to the Karush-Kuhn-Tucker conditions of the logarithmic barrier formulation of the linear programming problem. A point we wish to convey is that the perturbed system is more effective at solving the linear programming problem than the barrier system. We will support these results through numerical experiments.

1 Introduction

Newton's method is used to solve a system of nonlinear equations, $F(X) = 0$, where $F : \Re^n \to \Re^n$. It is a local method and has good properties, like quadratic convergence, that allow it to be used in the applied mathematics community to solve optimization problems. The problem of interest lies in solving the following linear programming problem (LP):

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax = b \\ & x \geq 0 \end{array}$$

where $c, x \in \Re^n, b \in \Re^m, A \in \Re^{mxn}$, $m < n$, and A full rank. Two systems of nonlinear equations associated with the LP problem will be considered. Newton's method will then be applied to each system and the differences between the two systems will be discussed.

2 Logarithmic Barrier Formulation

Newton's method is applied to a system of nonlinear equations, i.e. $F(X) = 0$, where $F : \Re^n \to \Re^n$. Thus, the LP problem must be formulated in such a way to extract a system of nonlinear equations. The first approach to take is to formulate the LP problem in the logarithmic barrier framework: for $\mu > 0$

$$\begin{array}{ll} \text{minimize} & c^T x - \mu \sum_{i=1}^{n} \log x_i \\ \text{subject to} & Ax = b \\ & (x > 0). \end{array}$$

Notice that the inequality constraints are part of the objective function, thus reducing the constraint set to a set of equality constraints. The fact that $x > 0$ is taking care of implicitly in the input to the *log* function. The above problem can be solved sequentially for different values of μ and it is well-known that, under mild assumptions, the sequence of iterates x^*_μ obtained from solving the log-barrier problem converges to the solution of the LP problem as μ converges to zero, i.e.

$$\lim_{\mu \to 0} x^*_\mu = x^*$$

where x^* is the solution to the linear programming problem [2].

In order to solve the log-barrier problem using Newton's method, we must derive the optimality conditions. These conditions are obtained by constructing the Lagrangian function, $L(x, y; \mu)$, and taking gradients, $\nabla_x L(x, y; \mu)$ and $\nabla_y L(x, y; \mu)$ to obtain:

$$\begin{array}{rcccl} \nabla_x L(x, y; \mu) & = & c - \mu X^{-1} e + A^T y & = & 0 \\ \nabla_y L(x, y; \mu) & = & Ax - b & = & 0 \end{array}$$

where $\quad L(x, y; \mu) = c^T x - \mu \Sigma \log x_i + y^T (Ax - b).$
This creates the nonlinear system of equations,

$$\hat{F}_\mu(x, y) \equiv \left[\begin{array}{c} Ax - b \\ A^T y + \mu X^{-1} e - c \end{array} \right] = 0$$
$$(x > 0)$$

where $\quad X = diag(x), \quad e = (1, ..., 1)^T.$

3 Perturbed KKT System

Using $\nabla_x L(x, y; \mu)$ of $\hat{F}_\mu(x, y)$ and introducing an auxiliary variable, z and defining $z = \mu X^{-1} e$ we obtain $XZe = \mu e$. Making this substitution of z into $\hat{F}_\mu(x, y)$ we obtain the perturbed Karush-Kuhn-Tucker (PKKT) conditions for the LP problem:

$$F_\mu(x, y, z) \equiv \left[\begin{array}{c} Ax - b \\ A^T y + z - c \\ XZe - \mu e \end{array} \right] = 0,$$
$$x, z > 0$$
$$\mu > 0$$

These conditions can also be viewed as constructing the KKT conditions for the LP problem and perturbing the complementarity equation, $XZe = 0$, by μ.

We remark that both systems $\hat{F}_\mu(x, y)$ and $F_\mu(x, y, z)$ are equivalent, that is, for $\mu > 0$

$$\hat{F}_\mu(x^*, y^*) = 0 \Leftrightarrow F_\mu(x^*, y^*, z^*) = 0$$

.

4 Newton Interior-Point Algorithm

Now that we obtained two systems of nonlinear equations for the LP problem, we are ready to apply Newton's method to each system and compare the differences. A basic Newton interior-point algorithm was constructed for each nonlinear system. The two algorithms are similar and vary in the termination procedure and this is due to the number of equations in the PKKT system. Thus, we present only the algorithm for the perturbed system.

Given $tol > 0$, $\mu tol > 0$, $\tau \in (0,1)$, and $\sigma \in (0,1)$.
For $k = 1 : maxiter$

- Solve $F'_\mu(x,y,z)\Delta v = -F_\mu(x,y,z)$
- Compute steplength
  $\alpha_x = \tau * \frac{-1}{min(\Delta x_i/x_i, -1)}, \quad \alpha_z = \tau * \frac{-1}{min(\Delta z_i/z_i, -1)}$
- New iterates
  $x_+ = x + \alpha_x \Delta x$
  $y_+ = y + \alpha_z \Delta y$
  $z_+ = z + \alpha_z \Delta z$
- Test
  If $\frac{\|Ax-b\|}{1+\|b\|} + \frac{\|A^T y+z-c\|}{1+\|c\|} + \frac{x^T z}{n} < tol$

  break;
- Update μ
  If $\|Ax-b\| + \|A^T y + z - c\| + \|XZe - \mu\| < \mu tol$

  $\mu = \sigma\mu$

end

5 Numerical Results

The Newton interior-point algorithms were applied to the equivalent systems, $F_\mu(x,y,z)$ and $\hat{F}_\mu(x,y)$. The algorithms were written in Matlab code and tested on a set of nine randomly generated problems. The problems varied in the size of the constraint matrix, A from the smallest having a size of 13 rows and 15 columns and the largest having 62 rows and 89 columns. Only the parameter μtol was varied, and tol, τ, σ were kept constant.

Significant differences were observed when we compared the results obtained from applying the Newton interior-point algorithm to both nonlinear systems. Specifically, fewer iterations were required to converge to the solution of the perturbed system compared to the log-barrier system. This is illustrated in Table 1. Also, note that convergence in the barrier system required that the iterates closely follow the central path. However, in the case of the perturbed system, the iterates need not be in a tight neighborhood about the central path to get convergence, especially for $\mu tol = 10^{-1}$. Further, the Jacobian of $F_\mu(x, y, z)$ is better conditioned than the Jacobian of $\hat{F}_\mu(x, y)$. However, having an ill-conditioned Jacobian does not preclude convergence[3]. In all the above test problems, convergence was easily obtained for the perturbed system. It was difficult trying to determine the correct values of μtol to use in order to obtain convergence in the barrier system. Convergence could have been precluded in the barrier system because we are asking the parameter μ to play two roles. That is, μ must be a barrier parameter and it must also function as part of the multiplier, z [1]. This leads us to believe that to solve the LP problem, we must use the perturbed system instead of the barrier system.

6 Conclusion and Future Work

We received good numerical results from the implementation of a basic Newton interior-point algorithm to the two nonlinear systems. Having studied these algorithms, we plan to modify the algorithms to better suit each nonlinear system. For example, we plan to do a linesearch procedure to obtain the steplength, α, in the barrier system. This should lead to a decrease in the number of iterations to converge to the solution. We also will run more numerical tests, primarily those from the Netlib set, to reinforce our hypothesis that the perturbed system should be used in place of the barrier system to solve the linear programming problem.

Table 1: Numerical Results

Numerical Results on Random Problems						
Problem Size m x n	Values of μtol vs. Iterations					
	10^{-6}		10^{-4}		10^{-1}	
	F	$\hat{F}$	F	$\hat{F}$	F	$\hat{F}$
13 x 15	35	118	24	–	14	–
14 X 16	37	142	25	–	17	–
13 x 22	43	140	32	–	21	–
23 x 27	45	144	34	–	32	–
26 x 34	41	122	30	–	18	–
34 x 45	50	142	37	–	26	–
27 x 54	58	140	45	–	33	–
62 x 89	52	140	41	–	28	–

Parameters: $tol = 10^{-8}$, $\tau = 0.95$, $\sigma = 0.2$

Notation:
– maximum number of iterations exceeded (> 500) and Jacobian very ill-conditioned

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7 SAS Program Comments

This summer I believe I accomplished a lot in many areas, especially in my graduate studies. I can definitely say that this summer was productive and I owe it all to my advisors Dr. Richard Tapia and Dr. Yin Zhang, and also to the SAS program. Dr. Tapia expects much from his students and it was reflected this summer. I enjoyed the work because it was research and not just something like "busywork" or an educational experience. I got really excited at writing the algorithms, coding, and obtaining results. Most importantly, I was motivated to work, learn and experiment. Perhaps all of this I felt because I had matured academically within the past years. However, I believe much of the credit also goes to the program and Dr. Tapia.

I advised several first year graduate students in my department to apply to the SAS program. Basically, I told them it would give them an opportunity to do research and also to begin on research projects, which could possibly lead to a publication or to a thesis. I did not follow my own advice at the time that I was beginning graduate school and wish I had, but these things you do not figure out until after the fact. However, I am quite happy that this summer turned out well.

I gave a talk at the Society of Industrial and Applied Mathematics at Stanford University this summer over the research I was doing. At first, I thought the research I was doing was just something of little interest or no value. However, when when my advisors and I looked at the numerical results I obtained, there seemed to be more information in the results than what we expected. Thus, I am continuing the research, and my advisors and I will be writing a technical report on my summer research.

I would like to advice other students to apply to the SAS program also, especially if they have never done research. This program provides one with support to do research. Dr. Tapia pairs his applicants with professors who are willing to spend time with students and who are also motivational.

Application of Interior-Point Optimization Techniques to NonlinearTraveltime Tomography

Donald C. Williams *

28 July 1997

Abstract

Seismic traveltime tomography aims to infer the velocity field from arrival times picked on prestack seismic data. Typically, algorithms employed for traveltime tomography involve the minimization of an unconstrained cost function, Φ, that measures the misfit between the traveltime data and the computed traveltimes. It is believed that the mathematical model for traveltime tomography can be greatly improved by adding rigorous feasibility constraints to the underlying model. In this work, we present a method which uses a primal-dual interior-point optimization algorithm for solving the underlying constrained model, and an upwind finite-difference technique to obtain the computed traveltimes as a solution of the eikonal equations.

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1 Introduction

Seismic traveltime calculations play a central role in many methods of seismic data processing. In this paper we discuss a research direction which involves the application of primal-dual interior-point optimization techniques for accurate and efficient gradient based traveltime tomography computations. Our main problem is to reconstructs a slowness (i.e., reciprocal wave speed) model of a medium, from measured first arrival traveltimes.

Typically, the traveltime tomography problem involves the unconstrained minimization of a functional which characterizes a misfit between computed traveltimes and the traveltime data [SS95a]. In our research, we aim to augment the typical unconstrained traveltime tomography model with rigorous physical feasibility constraints. It is our contention that the addition of feasibility constraints will greatly enhance the behavior of the underlying reconstruction algorithm.

We first discuss the idea of employing rigorous feasibility constraints derived from Fermat's principle within a nonlinear traveltime inversion problem. Next, a canonical unconstrained traveltime model is introduced along with a similar constrained model containing feasibility constraints. We then discuss the idea of using interior-point optimization techniques for the constrained traveltime model followed by some concluding remarks and future goals of this work

2 Fermat's Principle

Typically Fermat's principle has been used extensively in forward modeling. That is, given a slowness model, Fermat's principle determines the ray paths. However, recently it has been proposed, by James Berryman [Ber89], that Fermat's principle be used in an entirely different manner during the reconstruction of the slowness model using first arrival traveltime data. Using Fermat's principle, rigorous feasibility constraints are established for the nonlinear traveltime inversion problem.

The traveltime of a seismic wave is the integral of slowness along a ray path connecting the source and receiver. An expression for the traveltime along an arbitrary path, P, in a continuous slowness distribution, $s(x)$, is given by

$$\tau^P(s) = \int_p s(x)\, dl^P$$

where, dl defines the infinitesimal distance along the path, P. The physical principle of Fermat postulates that the correct ray path between two points is the one of least overall traveltime. Mathematically, we express this principle as

$$\tau^*(s) = \min_{P \in \overline{P}} \tau^P(s)$$

where, $\tau^*(s)$ is the correct traveltime, and $\overline{P}$ defines the set of all continuous paths connecting a given source and receiver pair.

Suppose that P_i is a be a trial ray path connecting the i^{th} source-receiver pair. Let $t_1, ..., t_m$ be the observed first arrival traveltime from m source-receiver pairs in slowness medium, $s(x)$. Then we obtain the following **feasibility constraints** for the traveltime problem.

$$\int_{P_i} s(x)\, dl^{P_i} \geq t_i$$

It can be shown that Fermat's principle yields a definite convex set of feasible slowness models, depending only on the traveltime data, for the fully nonlinear traveltime inversion problem. We take advantage of this fact in developing our reconstruction algorithm. Furthermore, we note that one can employ Fermat's principle to rule out infeasible trail wave-speed models which produce ray paths with traveltime smaller than the measured traveltime (accuracy assumed). Thus, as noted by Berryman [Ber90], non-feasible models can be classified by their total number of "feasibility violations". That is, the number of ray paths with traveltime less than that measured. This information is also useful in developing more efficient algorithms. Augmenting a typical unconstrained nonlinear traveltime inversion model with these ideas yields a constrained model which suggests the need for an effective constrained optimization technique to address the new constrained model.

3 Traveltime Tomography

Seismic tomography, or more generally, the inversion for laterally varying structures using data collected on the boundary surface has become a very important geophysical tool for reconstructing a slowness model from first arrival traveltimes. For the unconstrained traveltime tomography model, one generally minimizes a cost functional, $\Phi(s)$, which is a measure of the misfit between computed traveltimes and the traveltime data. For example,

$$\min_s \Phi(s) = \frac{1}{2} \sum_{r \in \mathcal{R}} \left| \tau(s,r) - t^d(r) \right|^2$$

where

$$\begin{aligned} s(x,z) &\equiv \text{ slowness field, } s(x,z) \in \Omega \subset \mathbf{R}^2 \\ \tau(s,r) &\equiv \text{ computed traveltimes} \\ t^d(r) &\equiv \text{ the traveltime data at receiver } r \\ \mathcal{R} &\equiv \text{ array of receivers} \end{aligned}$$

For a given slowness field, the traveltime τ is determined by solving the eikonal equation

$$\begin{cases} |\nabla \tau|^2 = s^2 & \text{in } \Omega \\ \\ \tau = \phi & \text{on } \Gamma_0. \end{cases}$$

Our current work involves augmenting the above unconstrained traveltime tomography model with constraints on minimum traveltimes derived from Fermat's Principle. We can express our initial constrained traveltime tomography model as

$$\boxed{\begin{array}{ll} & \min\limits_{s} \Phi(s) = \frac{1}{2} \sum\limits_{r \in \mathcal{R}} \left| \tau(s,r) - t^d(r) \right|^2 \\ s.t & \\ & g(s) = \tau(s,r) - t^d(r) \geq 0. \end{array}}$$

where, again, the computed traveltime satisfies the eikonal equation. As a standard form convex programming problem, we rewrite the problem as

$$\boxed{\begin{array}{ll} & \min\limits_{s} \Phi(s) \\ s.t & \\ & g(s) \geq 0 \end{array}} \Leftrightarrow \boxed{\begin{array}{ll} & \min\limits_{s} \Phi(s) \\ s.t & \\ & g(s) + y = 0 \\ & y \geq 0 \end{array}} \tag{1}$$

where, $\Phi(s)$, $\{-g(s)\}$ are convex continuous functions. To make the discussion of the optimization ideas more lucid, we use the notation given in (1).

4 Optimization

4.1 Log-Barrier Formulation

One approach to solving (1) is to use a log-barrier approach. Although this approach effectively reduces the inequality constrained model to an equality[1] constrained problem via the introduction of a penalty term defined by the log function and penalty parameter, μ, the log-barrier method is not without problems. The log-barrier formulation of (1) is given below,

Log Barrier Formulation:

$$\boxed{\begin{array}{ll} & \min\limits_{s} \Phi(s) - \mu \sum\limits_{i=1}^{m} \log\ y_i \\ s.t & \\ & g(s) + y = 0 \end{array}}$$

where $\mu > 0$, $y > 0$.

The Lagrangian for the log-barrier formulation is given by,

$$L(s, y, \lambda, \mu) = \Phi(s) + \lambda^T [g(s) + y] - \mu \sum_{i=1}^{m} \log\ y_i$$

[1]Note, equality constrained optimization problems are inherently easier to solve than inequality constrained problem.

The Karush-Kuhn-Tucker (KKT) conditions for the log-barrier formulation are

$$\widehat{F}_{\mu}(s,y) = \begin{bmatrix} \nabla\Phi(s) + G(s)^T\lambda \\ g(s) + y \\ \lambda - \mu Y^{-1}e \end{bmatrix} = 0, \quad (y,\mu) \geq 0$$

where

$$Y = diag(y_1, y_2, ..., y_m)$$
$$e = (1, 1, ..., 1)^T$$

The KKT conditions are characteristic of a stationary point, given additional constraint qualification hold. For a convex region, the KKT condtions characterize a local minimum. The constraint qualifications basically tell us whether or not a linearized model of $\widehat{F}_{\mu}$ is representative $\widehat{F}_{\mu}$ for a given point of the model space.

It should be noted that we do not use the log-barrier approach for our application, due to the inherent ill-conditioning of the method as $y \rightarrow$ boundary of feasible set. Physically, this is saying that the method is ill-conditioned as the computed traveltime goes to a measured traveltime. There also, exist conditioning problems as $\mu \rightarrow 0$. The reason the log-barrier method is mentioned is to discuss its similarities to the primal-dual interior-point method which we employ for our current application.

4.2 Primal-Dual Interior Point Optimization

The emergence of primal-dual interior point methods, as an effective tool for solving linear programming problems, motivates us to investigate the applicability of these methods in the arena of nonlinear inversion and tomography (problems). In the context of our constrained traveltime tomography problem, characterized by (1), we define KKT conditions, perturbed-KKT conditions, and a primary Newton step for the algorithm.

The Lagrangian for (1) is given by,

$$L(s,y,\lambda,\mu) = \Phi(s) + \lambda^T[g(s) + y] - \mu^T y$$

The corresponding Karush-Kuhn-Tucker (KKT) condition are

$$F(s,y,\lambda) = \begin{bmatrix} \nabla\Phi(s) + G(s)^T\lambda \\ g(s) + y \\ \Lambda Y e \end{bmatrix} = 0, \quad (y,\lambda) \geq 0 \tag{2}$$

and the Perturbed KKT conditions are

$$F_{\mu}(s,y,\lambda) = \begin{bmatrix} \nabla\Phi(s) + G(s)^T\lambda \\ g(s) + y \\ \Lambda Y e - \mu e \end{bmatrix} = 0, \quad (y,\lambda) \geq 0 \tag{3}$$

There is a rub associated with applying Newton's method or a modification thereof to the KKT conditions for a given problem. This rub involves, what is consider in the optimization community as "sticking to the walls". That is, if a variable becomes zero prematurely during the iterations of the algorithm, global convergence may be precluded. We avoid the problem of "sticking to the walls" by applying a modified Newton method to the perturbed-KKT conditions given in (3). The typical primal-dual step is a modified Newton step on the perturbed-KKT. That is,

$$\begin{bmatrix} \nabla_{ss} L(s,\lambda) & G(s)^T & 0 \\ G(s) & 0 & I \\ 0 & Y & \Lambda \end{bmatrix} \begin{bmatrix} \Delta s \\ \Delta\lambda \\ \Delta y \end{bmatrix} = \begin{bmatrix} -\nabla\Phi(s) + G(s)^T\lambda \\ -g(s) + y \\ -\Lambda Y e + \mu e \end{bmatrix}$$

where

$$\mu = \sigma\frac{\lambda^T y}{m}, \text{ defines a duality measure}$$
$$\sigma \in [0,1] \text{ defines a centering parameter}$$

It is our contention that the most effective optimization technique for solving our constrained model, (1), is a primal-dual interior point algorithm. Furthermore, the deficiency of "sticking to the walls" of the feasible region can be avoided, as opposed to the inherent deficiencies of the log-barrier approach. The price we pay for eliminating ill-conditioning with the perturbed-KKT is extra variables and "sticking to the walls" of the feasible region.

It should be noted that under the nonlinear transformation

$$\lambda = \mu Y^{-1} e$$

the perturbed-KKT conditions and the KKT conditions for the log-barrier formulations are "equivalent". That is, equivalent in the sense that they have the same solutions for $\mu > 0$.

$$F_\mu\left(s, y, \mu Y^{-1} e\right) = 0 \Leftrightarrow \widehat{F}_\mu(s,y) = 0$$

This was shown by El-Bakry, Tapia, Zang, and Tsuchiya in [EBTZT92]. It is interesting to note that this equivalence is only valid at a solution. Algorithms based on the two methods actually produce different iterates.

As we continue our research in this area, we will consider the influence of centrality on the behavior of our algorithm.

5 Remarks and Future Work

We have illustrated in our preliminary research that when an inverse problem can be formulated so the data are a minima of one of the variational problems of mathematical physics, feasibility constraints can be found for the nonlinear inversion problem. These feasibility constraints guarantee that optimal solutions

of the inverse problem lie in the convex feasible region of the model space (cf. [Ber91]).

Currently, we are developing a Hilbert Class Library (HCL) based implementation of a convex primal-dual interior-point algorithm for the constrained nonlinear gradient based tomography problem. HCL is a collection of C++ classes designed for implementing numerical optimization algorithms in the context of Hilbert spaces [GS96]. It is our contention that the use of the object-oriented programming paradigm provided by HCL will allow for maximum code reuse with respect to model variations in this and other seismic inversion work. We will eventually develop a general HCL based primal-dual interior-point algorithm class which should prove useful in examining the effects of different constraint models within a given reconstruction algorithm. Furthermore, we will employ an Automatic Differentiation (AD) tool (ADIFOR) to obtain derivatives via an adjoint state method.

There are certainly a couple of mathematical points which we will address with regards to this work. One of the main points being the consistency of the chosen numerical scheme. As shown by Sei and Symes in [SS95b], the consistency of a numerical scheme with a continuous equation does not imply the consistency of the adjoint scheme. This yields the interesting fact, that the adjoint difference scheme is either of lower order than the forward scheme or not adjoint to (discrete) the forward scheme. In choosing the former of these two consequences, it seems clear that the projection onto the smooth velocity space will bring the accuracy back up, but this is something that we will have to prove.

This research is in its infancy and additional model constraints will also be consider in future work. For example, there exist varying degrees of difficulty with regards to using traveltime tomography to infer wave speed distributions in a given media [Ber94]. That is, the velocity contrast within the media is a major factor in the level of difficulty of the problem. If the velocity contrasts are small, seismic waves are weakly refracted and straight ray tomographic algorithms provide suitable results. However, if the velocity contrasts are large, then seismic waves are strongly refracted, implying that nonlinear tomography algorithms are required to invert the data. Instead of employing ad hoc regularization constraints on the range of variation of velocities within a given model for our nonlinear tomography algorithms, it is our contention that it would be more advantageous to use information which can be obtained directly from the data of the given problem. This problem data can be employed to establish rigorous constraints, as we have presented using Fermat's principle in our preliminary work, on the minimum and maximum wave speeds in a propagating medium.

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Finite Termination in Interior-Point Methods for Linear Programs

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Abstract

We investigate finite termination procedures in interior point methods for linear programming. The implementation of finite termination procedures will enable interior point algorithms to generate highly accurate solutions for problems in which the ill-conditioning of the Jacobian in the neighborhood of the solution currently precludes such accuracy. The critical issues of finite termination are activating the procedure, predicting the optimal partition, formulating a simple mathematical model to find a solution and developing computational techniques to solve the model.

1 Introduction

The simplex method and interior-point methods are two fundamentally different approaches for solving linear programming problems. The simplex method travels from vertex to vertex in search of an optimal solution. Interior-point methods generate iteration sequences that travel through the interior of the feasible region and, under the proper assumptions, converge to the solution set. In addition, while the simplex method possesses finite termination, the method has worst case exponential running time complexity. On the other hand, interior-point methods have polynomial complexity but not finite termination.

Finite termination procedures attempt to compute an exact solution in a finite number of steps before the worst-case time bound is reached. For linear programming problems, the duality gap is zero at the exact solution. Obviously, by definition of interior-point methods the exact solution cannot be attained without algorithmic modifications.

The basic idea for finite termination procedures is as follows. Once the iteration sequence gets close enough to the solution set, the interior-point method can be terminated and the zero-nonzero structure of the solution set can be used to obtain a solution through some finite procedure. The arithmetic complexity of the procedure is bounded by a polynomial in the size of the input data. Assuming infinite precision arithmetic, the solution would be exact.

Research in finite termination can be categorized into two areas, optimal facet [12], [13], [18], [19] and optimal basis identification [1], [2], [3], [9],[14], [15], [16], [17]. Optimal facet identification techniques describe the facet upon which the objective function attains its optimal value. The facet is uniquely defined by the set of variables which are zero at the solution. Once the zero variables have been identified, the solution to the linear program can be found by simply calculating a feasible point on the facet.

In 1989, Gay [5] proposed stopping tests that computed optimal solutions for interior-point methods that solved linear programming problems. While these tests do not constitute a finite termination procedure, they are clearly forerunners of current optimal facet identification techniques. Gay's idea was to use the nonzero-zero partition of the variables to find the solution of the linear programs. It was his belief that the solutions could be used as stopping criteria for the algorithm. Furthermore, he thought the early stopping tests could help circumvent numerical difficulties associated with singular limiting Jacobians.

Gay solved two linear feasibility problems to find on point on the primal and dual optimal facets. However, Gay used an iterative, not direct method to find a feasible point. Hence, his technique cannot be categorized as a finite termination procedure. The linear feasibility models were defined to take advantage of the Cholesky factorization which was already implemented in the interior-point algorithm. Therefore, he solved a scaled linear system in the least squares sense, to obtain a normal equations coefficient matrix. His influence can be seen in [13] where the authors solve an linear feasibility problem with Gaussian elimination.

Implementing finite termination procedures within the interior-point framework would lead to definitive stopping criteria, computational savings, and highly accurate solutions. For degenerate problems, the Jacobian is necessarily singular at the solution. Therefore, we expect that the Jacobian will be ill-conditioned close to the solution set. The ill-conditioned Jacobian may produce step directions which prevents the problem from being solved to high accuracy. With a finite termination procedure, we can avoid the

effects of ill-conditioning to some degree.

2 Background and Notation

We consider linear programs in the standard form:

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax = b, \quad x \geq 0, \end{array} \tag{1}$$

where $c, x \in \mathbf{R}^n$, $b \in \mathbf{R}^m$, $A \in \mathbf{R}^{m \times n}$ $(m < n)$ and A has full rank m.

The optimality conditions for (1) are

$$F(x, y, z) = \begin{pmatrix} Ax - b \\ A^T y + z - c \\ XZe \end{pmatrix} = 0, \quad (x, z) \geq 0, \tag{2}$$

where $y \in \mathbf{R}^m$ are the Lagrange multipliers corresponding to the equality constraints, $z \in \mathbf{R}^n$ are the Lagrange multipliers corresponding to the inequality constraints, $X = diag(x)$, $Z = diag(z)$ and e is the n-vector of all ones.

The feasibility set of problem (2) is defined as

$$\mathcal{F} = \{(x, y, z) : Ax = b, A^T y + z = c, (x, z) \geq 0\}.$$

We denote the solution set of (2) as

$$\mathcal{S} = \{(x, y, z) : F(x, y, z) = 0, (x, z) \geq 0\}.$$

If in addition to $XZe = 0$,

$$x + z > 0$$

the solution satisfies strict complementarity. For linear programming problems, Goldman, Tucker [6], proved that among all optimal solutions there exists at least one solution that satisfies strict complementarity. Thus for nondegenerate problems, the unique solution satisfies strict complementarity.

If $\mathcal{S} \neq \emptyset$, then the relative interior of $\mathcal{S}$, $ri(\mathcal{S})$, is nonempty. In this case, the solution set $\mathcal{S}$ has the following structure (see [4] for a proof): (i) all points in the relative interior satisfy strict complementarity; (ii) the zero-nonzero pattern of points in the relative interior is invariant. Therefore, for

any $(x^*, y^*, z^*) \in ri(\mathcal{S})$, we define the support of a vector in the following manner:

$$\mathcal{B} = \{i : x_i^* > 0,\ 1 \leq i \leq n\} \quad \text{and} \quad \mathcal{N} = \{i : z_i^* > 0,\ 1 \leq i \leq n\}.$$

see [7], [10]. Moreover,

$$\mathcal{B} \bigcup \mathcal{N} = \{1, ...n\} \quad \text{and} \quad \mathcal{B} \bigcap \mathcal{N} = \emptyset.$$

The primal optimal facet is defined as

$$\Theta_p = \{x : Ax = b, x \geq 0, x_j = 0\ j \in \mathcal{N}\}.$$

Similarly, the optimal dual facet is

$$\Theta_d = \{(y, z) : A^T y + z = c, z \geq 0, z_j = 0\ j \in \mathcal{B}\}.$$

Thus $\mathcal{N} = \{1, ...n\} \setminus \mathcal{B}$ is the optimal partition of the linear program. The matrix B comprises the columns of A corresponding to the indices of $\mathcal{B}$. The matrix N is formed in an analogous manner. We denote the vector corresponding to matrix B as $x_{\mathcal{B}} := x_{j \in \mathcal{B}}$. Unless otherwise denoted, $\|\cdot\|$ is the Euclidean norm.

The central path is defined as

$$\mathcal{C} = \{(x, z) : (x, z) \geq 0, \quad \min(XZe) = \max(XZe)\}. \tag{3}$$

We define a neighborhood of the central path as

$$\mathcal{N}_{-\infty}(\gamma) = \{(x, z) | \quad \min(X^k Z^k e) \geq \gamma \mu^k\} \tag{4}$$

where $\mu^k = ({x^k}^T z^k)/n,\ \gamma \in (0, 1)$.

3 Algorithm

In this section, we describe a general primal-dual interior point method. The first primal-dual method was suggested by Kojima, Mizuno, and Yoshise [8]. It is well known that this algorithm can be viewed as perturbed and damped Newton's method.

Algorithm 1 (Generic Kojima-Mizuno Yoshise primal-dual algorithm)

Given $(x^0, z^0) > 0$, *for* $k = 0, 1, 2, \ldots$, *do*

(1) *Choose* $\sigma^k \in [0,1)$ *and set* $\mu^k = \sigma^k \frac{(x^k)^T z^k}{n}$.

(2) *Solve for the step* $(\Delta x^k, \Delta y^k, \Delta z^k)$

$$F'(x^k, y^k, z^k) \begin{pmatrix} \Delta x^k \\ \Delta y^k \\ \Delta z^k \end{pmatrix} = -F(x^k, y^k, z^k) + \begin{pmatrix} 0 \\ 0 \\ \mu^k e \end{pmatrix}.$$

(3) *Choose* $\tau^k \in (0,1)$ *and set* $\alpha^k = min(1, \tau^k \hat{\alpha^k})$, *where*

$$\hat{\alpha^k} = \frac{-1}{\min((X^k)^{-1}\Delta x^k, (Z^k)^{-1}\Delta z^k)}.$$

(4) *Let* $(x^{k+1}, y^{k+1}, z^{k+1}) := (x^k, y^k, z^k) + \alpha^k(\Delta x, \Delta y, \Delta z)$.

(5) *Test for convergence.*

Consider a nondegenerate problem (i.e., an unique solution exists). Within the interior-point framework, assume the variables that are zero at the solution are known. Thus for the standard linear programming problem, n-m nonbasic variable candidates (zero at the solution) and m basic variable candidates (positive at the solution) have been identified. After setting the nonbasic variable candidates to zero, the reduced square system can be solved for the basic variables. If optimality and feasibility conditions are satisfied for both the primal and dual problems, the algorithm can be terminated.

However, in practice most problems are degenerate. Consider the problem *scsd1* from the *netlib* test set for linear programming problems. Problem *scsd1* has 77 constraints and 760 variables. At the k-th iteration, indicators predict 31 variables are nonzero at the solution. The problem can then be reduced to one which consists of 77 constraints and 31 variables. Note, this problem is highly degenerate. By removing zero rows, we can further reduce the problem to one which consists of 20 constraints and 31 variables. Since the coefficient matrix is rectangular, there is no straightforward way to compute a nonnegative solution of the reduced system.

We now describe a generic finite termination procedure.

Algorithm 2 (Finite Termination Procedure)

(1) *At some iteration* k, *guess* $(\mathcal{B}, \mathcal{N})$.

(2) *Set* $x_{\mathcal{N}} = 0$ *and* $z_{\mathcal{B}} = 0$.

(3) *Solve a mathematical model as a function of* $(x_{\mathcal{B}}, y, z_{\mathcal{N}})$.

(4) *If* $x_{\mathcal{B}} > 0$ *and* $z_{\mathcal{N}} > 0$, *stop. We have found an exact solution. Else return to interior point algorithm.*

From the outline above, four important questions must be addressed in all finite termination procedures. When do we test for finite termination? How do we determine the partition of variables into their respective zero-nonzero sets? In the presence of degeneracy, what mathematical model should be used to find a solution? Given the model, what is the most computationally efficient way to solve the model? Our research focuses on these issues.

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On Finding the Minimum Cost of a Water Treatment Plant using Membrane Filtration, A Nonlinear Mixed Integer Programming Problem

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1 Introduction

Motivated by optimization problems arising in Environmental Engineering, this problem and formulation is derived from the desire to design the 'optimal' water treatment plant using membrane filtration for a minimum cost. Many water treatment plants today use filtration processes that do not guarantee that certain bacteria and viruses are removed. Membrane filtration does guarantee that certain size particles such as these can be removed. Membrane filtration, however, is not widely used in large scale water treatment plants. This is because it is a relatively new precedure, and so the cost of building such a plant is not known. The goal of my summer research is to begin formulating a model for water treatment plants using membrane filtration which would allow the user to find the minimum cost to build a plant with certain spefications.

2 Problem Formulation

This problem is a nonlinear mixed integer programming problem. An IMSL subroutine implementing of a sequential quadratic programming method is used to solve the nonlinear constrained optimization problem. The problem formulation is as follows.

Objective Function

minimize $operating\ \ cost + capital\ \ cost$

subject to $constraints\ \ of\ \ the\ \ plant$

The operating cost includes costs for the energy required for pumps, membrane replacement, chemical cost, concentrate disposal, and labor costs. The capital costs include costs of the pumps, pipes, valves, and framework, housing, and other miscellaneous costs. The constraints of the plant are redundancy for pumps, banks, and modules, and practical size limitations.

The decision variables which have been incorporated into the model thus far are the number of feed, backflushing, recycle, and fastflushing pumps, the number of modules, and the number of banks.

3 Operating Costs

The operating costs models, which are currently constant in the objective function, come from the Ph.D thesis work of Sandeep Sethi of Rice University and are as follows.

$$C_{energy} = \frac{c_{kw}(E_f + E_r + E_{ff} + E_{bf})}{Q_{des}},$$

where C_{energy} is the total energy costs per unit of treated water for operating the system, c_{kw} is the cost for a unit of energy, E_f is the energy utilized by the feed pump, E_r is the energy consumed by the recycle pump, E_{bf} and E_{ff} are the energies associated with backflushing and fastflushing respectively, and Q_{des} is the design flow.

$$C_{mr} = \frac{c_{mod}N_{mod}(\frac{A}{F})}{Q_{des}},$$

where C_{mr} is the annualized cost associated with replacement of membranes, c_{mod} is the cost per module, N_{mod} is the number of modules, and $\frac{A}{F}$ is the amortization factor.

$$C_{chemical} = \frac{Q_f CH_d CHc}{Q_{des}},$$

where $C_{chemical}$ is the cost of chemical treatment of the water, Q_f is the feed flow rate, and CH_d is the chemical dosage, CH_c is the chemical cost.

$$C_{disposal} = \frac{(c_{kw}\frac{P_f Q_w}{\eta_f}) + (CH_d CH_c Q_w)}{Q_{des}},$$

where $C_{disposal}$ is the disposal costs per unit volume of water treated, P_f is the feed pressure, Q_w is the waste water flow rate, and η_f is the efficiency of the feed pump.

4 Capital Costs

The capital costs models also come from the Ph.D thesis work of Sandeep Sethi and are as follows.

$$C_{pump} = k_p(flowrate \times pressure)^{n_p},$$

where C_{pump} is the cost for the pumps.

$$C_{PV} = k_{PV}(A_{mem})^{n_{PV}},$$

where C_{PV} is the cost for pipes and valves and A_{mem} is the membrane area.

$$C_{IC} = k_{IC}(A_{mem})^{n_{IC}},$$

where C_{IC} is the cost of instruments and controls.

$$C_{TF} = k_{TF}(A_{mem})^{n_{TF}},$$

where C_{TF} is the cost of tanks and frames.

$$C_{MI} = k_{MI}(A_{mem})^{n_{TF}},$$

where C_{MI} is the miscellaneous cost.

5 Future Work

A Future work will include solving the problem using other nonlinear constrained optimiation routines for comparison, including constraints for size limitation, including constraints which incorporate redundancy for banks, and introducing discreteness to decision variables.