Evaluations of the 1993 Spend a Summer with a Scientist Program

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MESH DISPLACEMENT: AN IMPROVED CONTOURING METHOD FOR TRIVARIATE DATA

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BACKGROUND

The demand for the visualization of scalar data has always been prevalent. The need for the visualization of trivariate data arises in a wide range of industrial and medical applications. One of the most popular way to visualize this data, over a cubic grid, is by computing isocontours of the data. The data is usually the result of a continuous function that interpolates the data. An isocontour of the function is simply the set of all points such that the function equals a variable. Displaying several isocontours of the function for appropriate values of the variable is often an effective tool for understanding the behavior of the original trivariate data. In general, the problem of computing an isocontour of the function equated to the variable can be transformed trivially into the simpler problem of computing the isocontour of the variable subtracted from the variable and the difference equated to zero. In other words

F(xyz) - continous function
(xyz) - set of points
c - variable

$$F(xyz) = c$$
$$F = c$$
$$F - c = 0$$

Therefore, we focus on approximating the zero contour of scalar data specified over cubic grid.

The method of creating zero contours entails you processing the data seperately on each cube of the cubic grid, and use linear interpolation along the edges of a cube to compute a collection of points lying on the zero contour. The problem with this method is there are cases that may arise which the data is ambiguous. This method does not guarantee a contour that is continuous, because adjacent cubes that share a face may subdivide differently. An alternative method is to disambiguate the ambiguous data by sampling the function at the center of the ambiguous face. This method is edge-based interpolation methods.

One drawback of these methods is that the surface meshes they produce can be highly irregular, even for simple trivariate data. These irregularities consist of tiny triangles, produced when the contour passes near a vertex of the cubic mesh, and narrow triangles produced when the contour passes near an edge of the mesh. Such triangles can account for up to 50% of the triangles in some surface meshes. These badly shaped elements often degrade the performance of rendering algorithms and finite element analysis applied to the mesh while contributing little to the overall accuracy of the approximation.

All data cited in the background was reported from the technical report by Doug Moore and Joe Warren entitled the same as this paper. The technical report's number is TR91-166.

METHOD

Due to the desire to be rid of those irregular triangles another method was employed. This method, known as mesh displacement, produced an approximation without those badly shaped triangles and the loss of accuracy is minute. This method also results in the number of triangles generated being reduced by up to 50%.

The way this method works is basically the same as the edge-based interpolation methods up to a point. Once you have the data from the continous function, you analyze it. Since we are approximating the zero contour, the boundary is zero. This means that any number less than zero is not a part of the object, and any number greater than or equal to zero is part of the object. What we do first is look at one cube of numbers at a time. The cube of numbers will have eight vertices, and we will evaluate each vertice. When we evaluate each vertices we are trying to see if the number is above or equal to the boundary of if the number is below the boundary. Since we have eight vertices, we will also have lines that connect these vertices known as edges. If all the numbers in that cube is greater than or equal to the boundary then there are no triangles in that cube since the whole cube is part of the object. By the same token, if all the numbers in the cube are less than the boundary then there are no triangles in that cube since the whole cube is not part of the object. If one of the vertices at one end of the edge is less than, or greater than or equal to the boundary and the vertice at the other end is the opposite, then you have to find where zero is between those two numbers, since somewhere between the two numbers is part of the object and somewhere it is not part of the object, and that will be one of the vertices of the triangle. This last operation is where the difference is between edge-based interpolation and mesh displacement differ. At this point by using mesh displacement instead of finding the zero between the two numbers, we would put the point on whichever of the two numbers is closer to zero. This eliminates some of the triangles, but not the accuracy. We keep this process up until all the cubes have been evaluated. At the end of this process the object you desired to make will be produced by several triangles.

STUDENT'S PARTICIPATION

All of the things mentioned before now where already established before I became involved. When I became involved this was a novel concept for me. It took time for me to understand the purpose and process of mesh displacement. I then was assigned the task of writing a small program, using the computer language C, that would generate triangles in the form of a sphere. That was relatively simple. Then I had to generate triangles to form a torus. That was more complicated because I

had to find the formula for a torus. This took me a little while. but I finally finished. The figure at the end of the paper is proof of that.

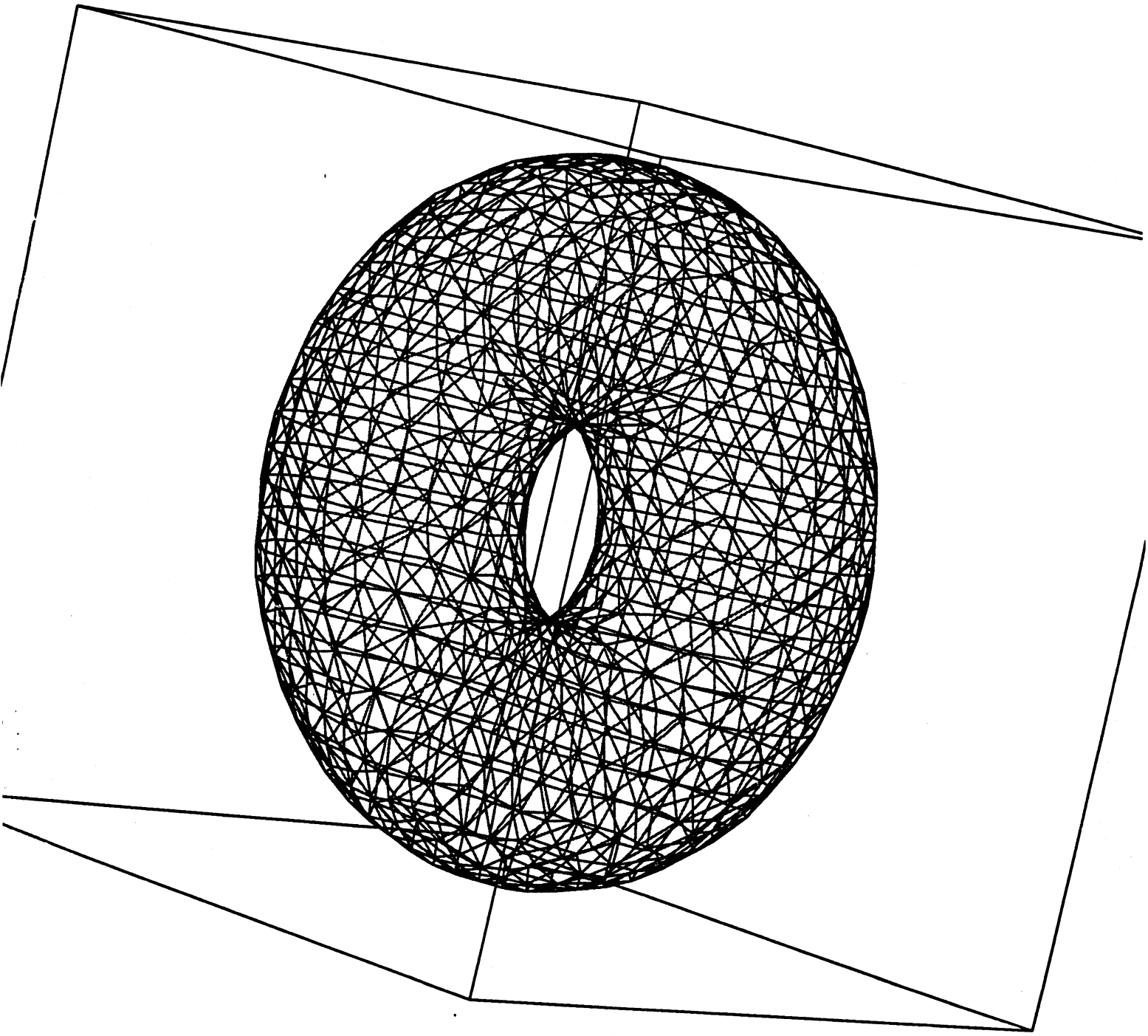
Dr. Moore then felt I was ready to work with the actual program that generated the triangles. Up to that point the output of the programs I wrote was put into the program that generated the triangles and the triangles were produced. The main program was somewhat overwhelming when I first saw it. I had only had one semester of the language C, so I only knew the basics of the language. The code in this program was much more advanced than that. I tried to plow my way through it line by line so I could understand it. It got to the point that I understood what each line of code was supposed to do, but I could not understand the logic of what it was doing. Dr. Moore then decided that maybe if I rewrote the code using my own logic. I would better understand what it was doing and why. He told me to do this. but in two-dimesions instead of three. The only difference is that lines were being generated instead of triangles. The program came, but slowly. I had to use concepts of C I had not encountered before, and I was unsure. Dr. Moore guided me, and the program began to flow. At the time this paper was printed, the program was basically finished and working correctly. The whole point of me trying to understand the code that generated the triangles. was because Dr. Moore wanted me to make modifications to the program. I do not know if I will get the chance to do that considering the time limitations. but I would at least like to start on it.

PROGRAM ASSESMENT

It has been my good fortune to be allowed to participate in the Spend a Summer with a Scientist program a second time this summer. Before I participated in the program, I had no idea what I wanted to do once I graduated. I was scared and I felt dumb because I didn't know what I wanted. This program gave me some direction. The summer of 1992 in this program exposed me to the concept of graduate school. It also made me realize that my interest was no longer in hardware, but in software. This summer I was given the opportunity to work extensively with C. It strengthend my belief that software was the route I wanted to take. Also, that graduate school would be the best thing for me to do once I graduated. I have become more interested in computer science because of this summer and that would be my field of interest in graduate school. I have also become interested in computer graphics.

This program has had such an impact on my life that I could not begin to describe it. The program literally changed my life. I was able to be around graduate students and hear from a students point of view what graduate school is like. The other participants in the program have become, in a sense, my mentors. Seeing them working toward their goals, makes me want to work more and more toward mine. The exposure to the professor's knowledge and their willingness to help was a wonderful

experience for me. The experince I have obtained due to this program will stay with me forever.



AN APPROXIMATION OF A TORUS

AIRFOIL OPTIMIZATION

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Spend a Summer With a Scientist 1993

INTRODUCTION

Airfoil Optimization is to structure the aircraft wing to produce optimal factors that determine the durability of the aircraft during flight. The ability of the aircraft wing is important in many ways. It must withstand pressures far greater than we experience in normal everyday life and in most cases under extreme turbulence such as stall and drag, the wing must perform with optimal ability. Realizing that the wing is 95% of the aircraft, designing becomes very precise and complex in structure.

PROJECT DESCRIPTION

Coming into the summer with my project in mind, I wanted to design a aircraft so during flight it could fly with optimal performance in lift over drag. I also wanted to design a wing that had maximum resistance not only to drag but to have the best performance in stalling citations. In the beginning of the program I had to get a basic knowledge in the area of aerodynamics. In understanding how aircrafts generally fly you have to look at factors such as fluid mechanics. In the idea of fluid mechanics you realize that during flow, when a fluid passes through a tube that is thinner than the rest of the tube the fluid inside of the tube moves much faster. So in a sense the compressed portion of the tube is where the lower pressure is. In the part of the tube that is not compressed, a higher pressure is therefore enforced. In thinking about an aircraft wing we

see that the wing has a curvature portion on top of the wing and is more straight at the bottom of the aircraft wing. In flight when the air passes over the top of the wing you see that the air streams become compressed together. At the bottom of the wing the air streams go straight pass the wing to form a higher pressure on the bottom verses a lower pressure on the top. In thinking in more simpler terms the pressure on the bottom has a greater force pushing upward than pressure pushing downward. In this case the aircraft is "sucked" in a sense or forced into the air. I studied further into the project and learned that the angle of attack of the aircraft is not solely dependent on the angle of the wing on the aircraft. The major factor in deciding the angle of attack is the amount of force the engine can exert while the aircraft is in flight. Any aircraft such as the cessena 170 and 175 can only have an angle of attack of no more than 60 degrees because of the engine, whereas a f-14 Navy Tomcat can turn upward and downward in a full 360 degrees. The reason for this is because the engine is powerful enough to force the airplane in all directions. When the aircraft proceeds its maximum angle of attack, the aircraft goes into what we call a "stall." Also during the length of my project I was given certain data on different aircrafts such as cessenas which fly in subsonic air speed and the Airforce SR-71 blackbird, which fly's at excessive hypersonic speeds. In doing so, I was to examine the durability and the overall performance of the wing at

high speeds. I acknowledged that at high speeds the wing of the aircraft gets to enormous temperatures and at low speeds the temperature of the wing barely changes. Also at high speeds the shape and structure of the wing at its leading edge is more V-shaped to produce a large amount of resistance over drag. At slower speeds the drag isn't all that important so the leading edge of the wing is more of a curvature shape, in such the wing has greater strength during flight.

In future research I wish to design a wing physically under certain restrictions for maximum durability during space flight. In doing so I wish to produce maximum lift to save fuel in flight. Also I wish to find out other materials for aircraft wings that are less heavy but more stronger.

INTERNSHIP EVALUATION

The summer research program here at Rice University has given me many opportunities to learn different computer systems that many Universities don't have. It made me more aware of what research is all about in graduate school. One of the most important advantages about the program is it gave me many opportunities to network, which is most important in the economy today. I will use the knowledge and skills I've learned from the program to better prepare me for the world I'm about to face. I also highly recommend that the program continue for many years to come. It gives

many minorities the chance to see what the world beyond undergraduate school is all about.

"SPEND A SUMMER WITH A SCIENTIST"
END-OF-SUMMER REPORT

DOES INCREASED LOW-COST VOTER REGISTRATION LEAD TO INCREASED VOTER TURNOUT?

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ABSTRACT

The debate over recent legislation to increase voter turnout has focused attention on ways to reduce the costs of voting, particularly the costs associated with voter registration. Underlying these proposed reforms in voter registration laws is an unexamined relationship between registration and voting.In this report -- which summarizes the research and consequent paper completed during the Spend a Summer with a Scientist program -- it is argued that efforts to reverse declining rates of voter turnout with low cost voter registration may fall short of expectations. This is due to the fact that low cost registration does not have a uniform effect on voting across all registrants. The findings show that relative to all other registrants, voter turnout is diminished among first time registrants.

I. Introduction

Turnout has been on the decline in the U.S. steadily since the 1950's. Consequently, many political advocates and policy-makers have concentrated their efforts in finding means to reverse the declining pattern. To this end, recent legislation focused on increasing turnout has been based on reducing the cost of voting, particularly the cost of voter registration (ie., the motor-voter bill). However, although there are many advocates of low-cost voter registration, the true relationship between low-cost registration and its effects on voter turnout has yet to be examined.

II. Theory

Literature on voting behavior is lead by three dominant behavioral theories: instrumental, institutional, and social-psychological. The instrumental theory of voting behavior stems from Down's Economic Theory of Voting and is based on the premise that an individual's expected utility must outweigh the costs of voting in order for a vote to be cast. Also utilizing the concepts of costs and benefits to voting, the institutional model of voting states that the legal political structure may present costs which decrease voter turnout (i.e., the process of registering to vote). The social-psychological model of voting states that socialization has an effect of political behavior; social interaction may decrease the costs and/or increase the benefits of voting.

III. Data, Methodology and Hypotheses

Two important historical trends lead to the hypothesis that voter turnout among new voter registrants will be significantly lower than those who reregister due to recent mobility and continuing registrants. Relaxation of the costs associated with voter registration (c.f. Teixeira,1992; Mitchell and Wlezien,1989) and the predominance of targeted registration drives both operate to reduce the costs of voter registration. Absent an investment by new registrants, it is expected that their probability of voting will be diminished.

in the 1980s. The tests are quite simple. Our dependent variable is the percentage of registered voters voting for president in each state.[3]

The principal independent variable is percentage change in registered voters, or the change in the number of registered voters from the previous presidential election year to the current year divided by the number of registrants in the previous year. So, if state X had 50 registered voters in YEARt and 55 in YEARt+1, then the percent change would be 10. An institutional perspective would suggest no significant effect for this variable. Borrowing from the social context perspective, however, we hypothesize that increased registration will suppress turnout rates, in light of recent efforts to reduce the cost of registration. In order to test for the attenuating effects of higher cost registration, we include a dummy variable for closing date of registrationan and an interaction between the registration change variable and the closing date dummy. Those states that require registration 30 days or more prior to the election are coded 1, others are coded 0. The coefficient for the interaction is hypothesized to be positive for the reasons noted above.

Finally, we include a lagged measure of the dependent variable which effectively controls for the effect that prior levels of turnout have on current levels. In those instances where turnout has been historically high and/or low, we cannot be certain that a change in either the level of registration or the costs imposed by early closing dates for registration will have a uniform (i.e., linear) impact on turnout.[4]

Results of OLS estimation are presented in Table 1. As hypothesized, for each year, increases in registration result in lower levels of turnout; however, this effect is weakened in states with high cost registration, indicated by positive and significant coefficients for X3. Table 2 provides an interpretation of the results for several alternative hypothetical cases. A "high" level in the "change in registration" category indicates one standard deviation above the mean on that measure, and a "low" indicates one standard deviation below. A "high" in the restriction category is given to those states ending registration 30 days or more before election day, "low" otherwise. The mean of the lagged dependent variable is used for each year. As such, our results

(i.e., exclusive of 1980) presidential elections in which the respondent voted . With these two pieces of information we identified new voter registrants as those individuals who had registered between 1976 and 1980 and did not vote in any previous presidential elections (circa 1960).[6] Those individuals who also registered to vote between 1976 and 1980, but who claimed to have voted in one or more previous presidential elections we identified as reregistrants. Finally, individuals whose registration at their current address predates 1976, and who claimed to have voted in at least one previous presidential election were identified as continual registrants.

As expected and consistent with estimates generated by others (Piven and Cloward,1989:261-263), the proportion of new voter registrants is small. Only 4.2 (N=37) percent of the NES sample registered between 1976 and 1980 and claimed not to have voted in any previous presidential election.[7] Squire, Wolfinger and Glass (1987) observed that a significant portion of the American electorate changes residences within a single year and must reregister in order to be eligible to vote. We have identified 331 respondents (37.9%) who registered between 1976 and 1980, but had voted in at least one previous presidential election. This population is thought to be comprised of individuals who changed residences during the interpresidential period and were required to reregister in order to vote in the 1980 election. The majority of respondents for which a valid registration record was found (57.4%) have remained registered at their current address for at least four years.

Table 3 reports the distribution of selected demographic and attitudinal characteristics by voter registration experience. As expected, registrants are demographically and attitudinally differentiated by their registration history. New registrants are significantly younger, and personally poorer,[8] than reregistrants and those with uninterrupted registration. Consistent with the youth of new registrants, these individuals have slightly higher educational levels than either reregistrants or those with uninterrupted registration. New registrants and reregistants are significantly more mobile, and as a result significantly less likely to be home owners. The racial make-up of registrants is skewed. New registrants are twice as likely to be black or Hispanic than all other registrants. Partisan preferences are largely invariant across different populations

A final means of assessing the differences in turnout among different types of registered voters is to estimate turnout for each population of registered voters. Our previous review of the literature identified three dominate explanations for voter turnout: socioeconomic status, which linked turnout to the voter's ability to bear the costs of voting; statutory barriers to voting, including restrictive registration laws; and a political interest measure that links voting to the individual's socio-psycholoigical motivations. Table 4 reports the logit regression of validated 1980 voting behavior (0=did not vote, 1=voted) on the responent's educational level, his/her interest in the presidential election, and closing date for voter registration in the state (1=less than thirty days before an election, 0= more than thirty days before an election). [10] We have reported the change in the probability of voting across the range of each independent variable, controlling other independent variables at their mean value.

For all registrants the model peforms well. As expected, turnout is higher among better educated voters, those who express significant interest in the presidential election, and among voters residing in states where the closing date for registration is less than thirty days before the election. The probability that a respondent voted in the 1980 election increases 21 percent between those expressing "not much" to "very much" interest in the presidential campaign. There is an 11 percent increase in the probability of voting between those with less than 12 years education and those with a post-college education. Liberal closing dates have a modest effect on turnout for all registrants. The probability of voting increases three percent among respondents residing in states which allow voter registration 30 or fewer days before an election. The performance of this model varies significantly with different registration experiences.

Voter turnout among newly registered voters is not significantly related to any of the hypothesized determinants of voter turnout. Among reregistrants, turnout is significantly related in the expected direction to interest in the campaign, education, and the closing date for voter registration. Only interest in the campaign and education are significantly related to turnout among individuals with uninterrupted voter registration. The closing date for registration does not have a significant independent effect on turnout for these voters. Among reregistrants the

additional incentive/ assistance (ie., similarly low cost voting opportunities) to stimulate their decision to vote.

The significance of the findings reported in this paper extend beyond the debate over how to increase voter turnout. There is little doubt that low cost voting will enhance turnout -- particularly among new registrants. The political consequences of this finding, however, are not altogether obvious. DeNardo suggests that the vote choices of peripheral voters (i.e., those with a low probability of voting) are random and not subject to the same influences of more likely voters. Our own findings suggest that among new registants, interest in and attentiveness to politics in general and specific campaigns is minimal. This might suggest that the consequence of reform toward low cost voting is to expand the electorate to individuals who make largely uninformed and disinterested vote choices. There is another possibility -- one which identifies a dynamic property to low cost voting: new registrants who are induced to voting by low cost voting procedures (i.e., early voting as now practiced in Colorado and Texas) may acquire an interest in politics which more experienced voters have already acquired. Viewed dynamically, low cost/early voting may serve as a "loan" on the sunken costs in politics and individual campaigns that new registrants often lack. Both explanations are worthy of more serious study.

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ENDNOTES

1 The validated voter sample is preferred to the Current Population Survey (Census, 1984, 1984,1988) because it validates (i.e., by checking individual voter registration records) registration status, length of registration and voting histories, all critical variables in our analysis. The NES surveys provide extensive attitudinal and demographic information not available in from CPS. The weaknesses of NES include a smaller sample, and the potential skewness of the sample in terms of demographic representation (e.g., under representation of blacks and other minorities). The strengths and weaknesses of NES and CPS data bases are discussed in Teixeira (1992). Unfortunately two key pieces of information (i.e., year in which respondent registered and the number of presidential elections the respondent voted in) are omitted from the 1984 and 1988 NES surveys making it impossible test our hypotheses in elections subsequent to 1980.

2 We focus on turnout among registered rather than eligible voters because it is trivial (statistically, not civicly) to say that increasing the number of registrants will increase the number of voters. A problem arises with the use of registration figures reported by individual states. These figures necessarily over report the number registered voters because of the lack of timely purging of names of deceased individuals or those who have moved. Squire, Wolfinger and Glass (1987) report that a third of population in the United States changes residence in course of a two year period. Piven and Cloward (1989:266) estimate that because of incomplete purging registration figures reported by individual states over state registration figures by an average of 20 percent. We recognize this problem, however, given the nature of our research question there is no viable alternative to the use of registration data as reported by individual states. Confirmation of our thesis at both the state and behavioral levels of analysis provides further confidence that this measurement problem is not significant rival explanation for our findings.

3 North Dakota and Wisconsin do not require registration and so they are excluded from our analysis. Mississippi did not require registration in 1976, so a lagged dependent variable could not be created for the 1980 model, requiring its exclusion in that year.

4 See Shrodt and Ward (1981) for a further discussion of this issue.

5 The 1980 NES interviewed 1,463 persons, 872 respondents were interviewed in both the pre- and post-election survey and were validated as registered and eligible to vote in the 1980 presidential elections. Missing data reduce our effective sample to 841 respondents.

6 Respondents were specifically asked "in how many previous presidential elections have you voted?" New registrants were those who responded as not having voted in any previous presidential election (i.e., answered "none").

7 New registrants may have been motivated to register after their NES pre-election interview. The 1980 NES includes information on the month and day on which the respondent registered to vote from their current address and the date of their pre-election interview. These data allow us to test the hypothesis that the pre-election survey had an independent effect on decision to register. Twenty-one of our 37 new registrants registered to vote in 1980. Only two of these 21 respondents registered after their pre-election interview. We assess the influence the NES interview on the likelihood of the respondent to register as insignificant.

8 It is note worthy that personal income is significantly lower among new registrants but, family income is slightly higher for this group. This suggests that new registrants, who are mostly under the age of 24, still reside at home with parents who have higher than average incomes. It might be inferred from this finding that new registrants are encouraged to register by family

Table 1
OLS Estimates for State-Level Turnout of Registered Voters

	1980		1984		1988	
Variable	Estimate	t-stat.	Estimate	t-stat.	Estimate	t-stat.
Intercept	34.6913	7.33	13.3200	2.17	-0.8111	-0.42
X_1	-0.4072	-5.57	-0.3443	-4.46	-0.3717	-6.27
X_2	-1.8157	-1.62	0.0602	0.05	-0.7259	-1.04
X_3	0.2367	2.61	0.1688	1.62	0.2438	2.83
X_4	0.5760	9.15	0.8352	10.29	0.9983	16.75
	N = 47		N = 48		N = 48	
	R^2 = .72		R^2 = .76		R^2 = .89	

where, X_1 = Δ in registration from previous election year;
X_2 = dummy variable coded 1 for filing deadline 30 days or more, 0 otherwise;
$X_3 = X_1 * X_2$;
X_4 = dependent variable lagged for one presidential election.

Table 2
The Effect of Registration on Turnout

	1980			1984			1988		
	Δ in Registration			Δ in Registration			Δ in Registration		
Restriction	High	Mean	Low	High	Mean	Low	High	Mean	Low
High	73.1%	74.4%	75.7%	72.6%	73.9%	75.3%	70.4%	71.4%	72.4%
Low	70.9%	74.0%	77.1%	69.9%	72.5%	75.1%	68.6%	71.5%	74.5%

Table 3: Demographic and Attitudinal Characteristics by Voter Registration Experience

	New Registrants (n=37)	Re-registrants (n=331)	Continual Registrants (n=491)
Party Identification			
Democrat	45.9	38.4	44.2
Independent	27	27.2	23.4
No Preference	10.8	8.2	6.5
Other	0	0.9	0
Republican	16.2	25.4	25.8
Age			
18-24	43.2	15.1	1.8
25-34	37.9	29	11.3
35-64	18.9	44.7	58.9
Over 64	0	11.2	28
Family income			
$0-$9,999	8.3	10.5	14.3
$10-$14,999	12.5	15.4	13.4
$15-$24,999	41.7	29.1	26
$25-34,999	29.2	21.1	27.8
$35,000 or more	8.3	23.9	18.5
Personal income			
$0-$9,999	64.7	51.5	51.8
$10-$14,999	17.6	14.6	15.8
$15-$24,999	14.7	21.7	20.8
$25-34,999	2.9	6.8	8.4
$35,000 or more	0	5.5	3.2
Race			
White	73	87.3	87.3
Black	24.3	10.9	12.3
Other	2.7	1.8	0.2
			0.2
Homeowners			
Own	62.2	69.2	84.9
Renter	35.1	29	12.1
Other	2.7	1.8	3

Table 3: Continued

	New Voters (n=37)	Re-registrants (n=331)	Continual Registrants (n=491)
Education			
0-8 years	27	17.5	29.7
9-12 years	48.5	35.6	33.1
1-4 years college	21.6	39	32.3
5 or more yrs colle	2.7	7.9	4.8
Interest in campaign			
Very much	37.8	14.7	22
Somewhat	43.2	50.2	40.5
Not much	18.9	35.1	37.5
Voted in 1980 election			
Yes	70.3	86.1	83.1
No	29.7	13.9	16.9
Vote Choice			
Did not vote	27	16.6	19.6
Reagan	35.1	43.5	40.9
Carter	24.3	28.1	31.7
Clark	5.4	1.2	0.2
Anderson	2.7	9.1	4.6
Other	5.5	1.5	3
Have say			
Yes	34.3	32.4	39
No	65.7	67.6	61
Interest in politics			
Most of the time	11.4	29.4	30.6
Some of the time	22.9	39.9	38.3
Only now and then	40	20.9	19.2
Hardly at all	25.7	9.8	11.8
Length of Residence			
One year or less	29.7	25.7	4.6
1-2 years	10.8	18.7	3.6
2-3 years	13.5	13.6	2.8
3-4 years	8.1	7.3	5
More than 4 years	37.8	34.7	84

Table 4

Logit Estimates for Voter Turnout by Registration Experience

	All Registrants		New Registrants		Reregistrants		Continuing Registrants	
Variable	Estimate (S.E.)	Prob. Δ[a]	Estimate (S.E.)	Prob. Δ	Estimate (S.E.)	Prob. Δ	Estimate (S.E.)	Prob. Δ
Intercept	.668* (.32)		1.15 (1.33)		1.23* (.62)		.324 (.39)	
Education	.306** (.11)	.109	.299 (.53)	.196	.352* (.21)	.105	.273* (.15)	.102
Interest	.762** (.13)	.208	.719 (.56)	.310	1.01** (.26)	.247	.167* (.17)	.181
Closing Date	-.304* (.20)	.038	.613 (.83)	.138	.469* (.35)	.047	.267 (.27)	.022
-2 log	754.1		45.0		254.1		449.3	
% Correctly Predicted	64.7		63.6		70.3		63.7	
N	841		37		313		491	

Note: * = P<.05; ** = P<.01.

See Appendix A for variable description.

[a] Change in the probability of voting across the range of the independent variable, holding constant all other independent variables at their mean value.

TELRC

(Texas Environmental Learning Resource Center)

By

Steven Harris

Advisors:
Joel Castellanos
Dr. Leslie Miller

Center for Research in Parallel Computation
SASWS participant
Summer 1993

TELRC

by
Steven Harris

Abstract

Rice University and the Texas Environmental Commission have joined in a partnership in order to create an electronic resource library. This resource library is to be accessed by high schools, libraries, and various other organizations throughout the state.
The Texas Environmental Resource Library Contains:

a) A collection of articles and maps.
b) Reviews and references to books and other publications.
c) Ongoing and dynamic collaborative student, teacher projects.
d) Automated connections to networked environmental resource servers.
e) A repository for climatology and water quality data collected throughout Texas.
f) Data entry and analysis software.

Supported by Center for Research on Parallel Computation
Supported in part by Compac Computers and Exxon

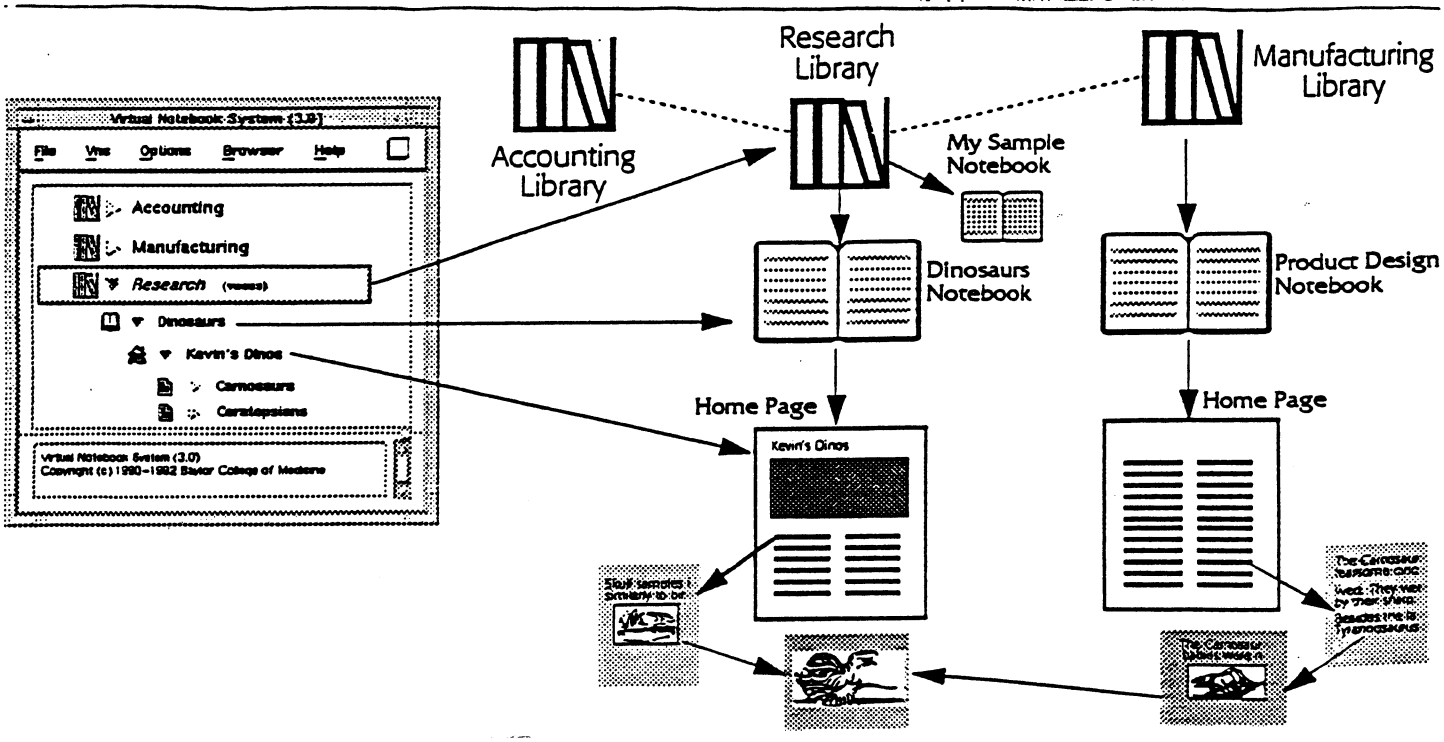
Introduction

In the common model for high school assignments, students work towards the same objectives with little or no contact with each other. A model which is contrary to the methods commonly employed by professional research and development groups, in which collaboration is encouraged and is benificial to the whole. The TELRC is made possible through a software known as VNS, which is a multi-user, distributed software that fosters communication.

Overview of VNS

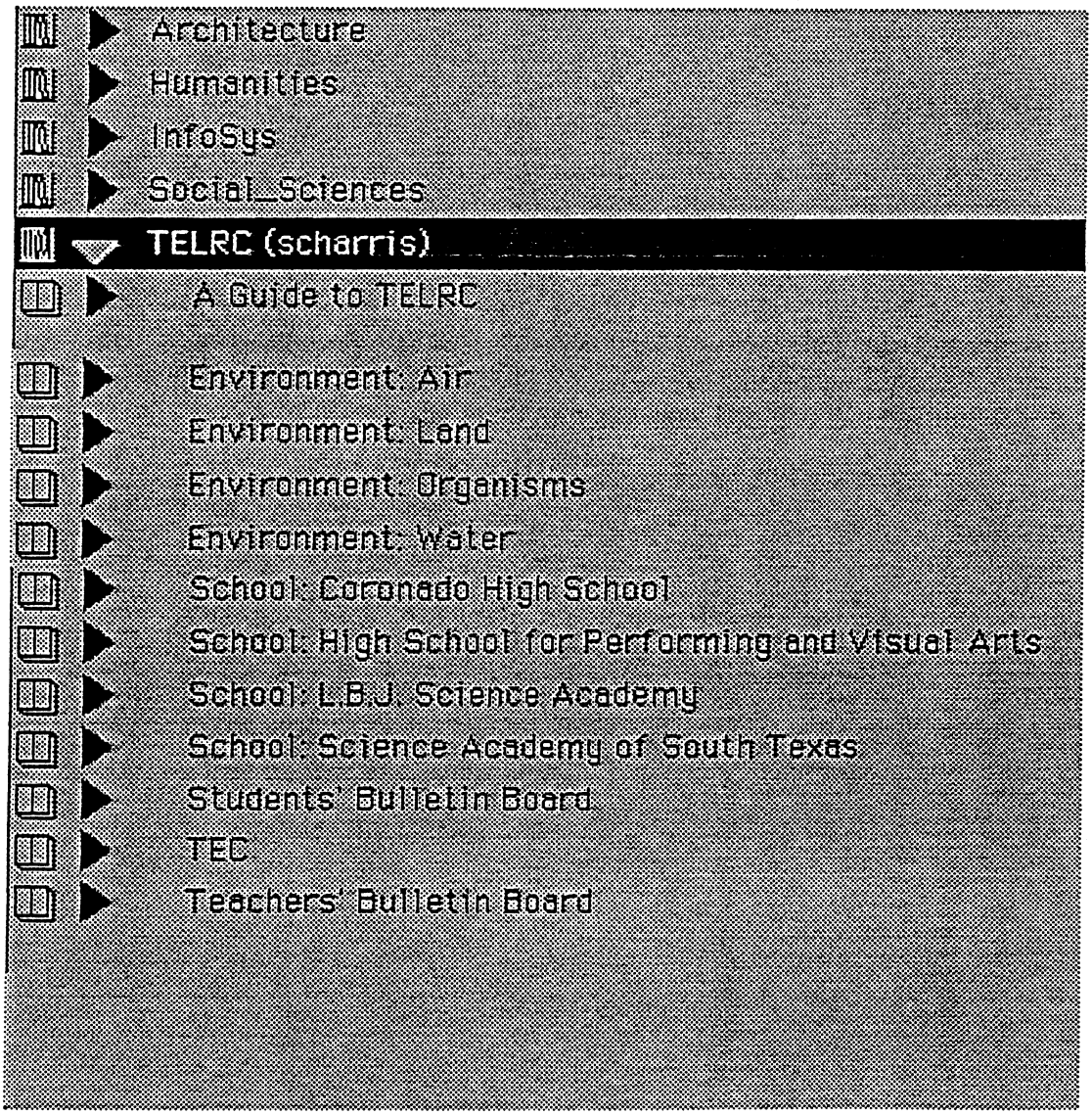
The Virtual Notebook System is designed to be used as an electronic notebook. Like a paper notebook, a VNS notebook is a series of pages containing information. However, information on a VNS page in organized into objects. These objectes can be color text and drawings just as on a paper notebook. There can also be links to other programs external to VNS, audio and vedio segments, animated images, and real-time telecommunication links. VNS has hypertext capabilities wich allow pages to be cross-refferenced among the pages of one or more notebooks.

VNS also offers security options for controlled access. When a user creates a notebook,he or she has ownership of that notebook and can specify who has no access, read access, or read-write access.



The TELRC

The TELRC library is made up of several notebooks. There is a notebook relating to all environmental topics. Each notebook on an environmental topics contains example lessons that a teacher may choose to fallow. There are also links to various external programs designed to supplement each lesson. Student accessing the library from anywhere in Texas can collaborate through the student clipboard, a notebook designed especially for student communication; or they can communicate directly through the objects on a page. There is a teacher clipboard for teacher communication as well.



Evaluation

The SASWS program has given me the opportunity to enhance my knowledge of computer programming, as well as gaining knowledge through being in a professional environment that I would not have gotten otherwise. I was exposed to several new programming languages that I was not familiar with. In today's market, being competitive means being on top of technology. I believe that the TELRC is a step in the rite direction in building a better model for high school learning. The TELRC project gave the exposure to working with a group of people, all working towards the same goal. Something I believe every graduate, if they are to be competitive, should have.

Acknowledgments

First, I would like to thank Dr. Tapia for the opportunity to participate in the program and for his constant outreach to the community. I would like to thank Joel Castellanos for his guidance through out the course of the summer. Also, I would like to thank Dr. Kennan for his guidance and the insite that I gained through working with him this summer. Finally I would like to thank Dr. Miller and all the other participants in the program, I enjoyed meeting and working with them all.

Spend a Summer with a Scientist

Project Description

Nina C. Hernandez

Summer 1993

Spend A Summer With A Scientist

Project Description

Many algorithms for solving linear programming problems are currently available. However, most algorithms require that the data necessary to describe the problem, the initial dictionary, be made available in a specific format, usually some form of tableau. This makes comparison of the algorithms difficult since the data files are not portable to other algorithms. In addition industry uses it's own format, MPS, in representing linear programming problems. Many algorithms now have available a program to convert MPS formatted problems to the data format necessary to the specific algorithm. Considering the fact that there are many ways to store the tableau format and only one for MPS it is often convenient to convert a linear programming problem to MPS format and then use that format to solve the problems. This conversion process can be tedious and time consuming when dealing with larger problems emphasizing the need to standardize a data format for the academic environment.

During my participation with the Spend a Summer program in 1992 my project entailed writing a program entitled ToMPS. ToMps was implemented in FORTRAN which I also learned that summer. ToMPS is a program that places the data for a linear programming problem into MPS format. The program is currently limited to problems of the standard form:

minimize $c^T x$

subject to:

$$Ax = b$$

Where A is a matrix, b,c, and x are vectors.

This summer has entailed the fine tuning of the program ToMPS. Ensuring that the code is sufficiently commented so that others may use it and understand it. Amending the code so that it may be easily adjusted to handle larger problems. Restructuring the code so that all related code is in the same subroutine. Since a technical report on the project was the next step some time had to be spent learning the laTEX environment. A technical report is now in the finishing stages. It should be noted that ToMPS was developed strictly for research purposes. It is not intended as a commercial code. During both summers I have worked with Dr. Amr El-Bakry and Dr. R. A. Tapia.

Summer With a Scientist: Summer Project Final Report

Tony Kearsley *

August 6, 1993

Participation from May 11, 1993 to August 13, 1993

The primary component of my summer project has concerned itself with a very simple optimization problem arising from a data fitting least squares problem motivated by applications is molecular dynamics. This problem can be thought of as: given a set of initial estimates of distances, find a set of solution distances that are 'close' to the given set of approximate distances *and* represent a configuration of points. In order to justify the use of the Euclidean distance formula i.e.

$$dist[(\hat{x},\hat{y},\hat{z}),(x,y,z)] = \sqrt{(x_i-\hat{x}_i)^2+(y_i-\hat{y}_i)^2+(z_i-\hat{z}_i)^2} \quad \forall x,y,z \in \Re^3 \qquad (1)$$

the configuration must be a configuration in $\Re^3$. Let Δ denote the square matrix of approximate inter-point distances. So $\Delta = [\delta_{i,j}]$, and $\delta_{i,j}$ denotes the inter-point distance between the ith point and the jth point of some configuration of n points not necessarily in $\Re^3$ (if the there is a configuration in $\Re^3$ associated with the approximate set of inter-point distances, then there is nothing to solve). The mathematical problem of finding this set of inter-point distances can be solved by a minimizing the following nonlinear function,

$$\min F_\kappa(X) = \sum_{i=1}^n \sum_{j=i+1}^n (\delta_{i,j}^{2\kappa} - [\sum_k^3 (x(i,k)-x(j,k))^2]^\kappa)^2$$

where (P)

$$X = [x_{i,l}] \in \Re^{n\times p},$$

$$\Delta = [\delta_{i,j}] \in \Re^{n\times n}.$$

This smooth nonlinear unconstrained minimization problem (P) is well defined and easy to solve in the event that Δ is or is close to being a matrix whose entries correspond to the inter-point distances of some configuration in $\Re^3$. The κ is included in the objective function $F_\kappa(X)$ for convenience so that the two related problems of fitting distances and

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fitting squared distances are incorporated into one problem formulation (typically we will have $\kappa = 1$ or $\kappa = \frac{1}{2}$). Given the solution to (P), say X^*, it is obvious how to construct a matrix $D(X^*)$, where $D(X^*)$ is our set of distances that are closest to Δ and correspond to the configuration X^*.

One issue that that was examined is that of missing data, or what to do if an off diagonal of Δ, is zero. Clearly the diagonal of Δ and $D(X)$ must be identically zero for all $X \in \Re^{n\times p}$. It is my opinion that a subproblem must be solved to approximate the missing elements of Δ, before the unconstrained minimization algorithm is employed. If no more than one element of each row and column is missing, then we substitute for the missing distance $d_{I,J}$ some value $\hat{d}_{I,J}$ that satisfies

$$\hat{d}_{I,J} = \max_{i,j}[\max(d(I,j)^2 - d(i,J)^2), \max(d(i,J)^2 - d(I,j)^2)]. \tag{2}$$

The motivation for choosing this approximation to a missing datum is obvious (simply examine the triangle inequality). It is worth noting that in limited numerical experimentations, deviation from (2) has almost always resulted in a deterioration of convergence speed (here we abuse the use of the phrase *speed of convergence* to mean total number of iterations i.e. convergence close to the solution will still be rapid). In some cases a larger objective function value at the solution for problem (P) resulted. Moreover, after (2) has been administered, various smoothing techniques can be employed to massage the matrix Δ (e.g. Newton divided difference smoothing, Kalman filters, and even Fourier Transformations). A preliminary investigation of the applicability of these smoothing techniques has been conducted this summer. While this investigation was far from exhaustive it was conclusive in so far as it demonstrated that the numerical smoothing of given data was very effective if one had any notion at at all about the type and/or size of the error present in the given initial data.

Another issue addressed successfully this summer was the generating of a starting point. It turns out that one can write down a simple linear least squares problem and and associated analytic solution that generates a very effective starting point. Details of this starting point will follow in a forthcoming paper.

Numerical experimentation continues, and it appears that the most naive method of solving our distance problem (via solutions of (P)) is fruitful. In particular, I have started investigating various numerical methods of dynamically updating the given initial approximate distances, and using smoothing techniques mentioned above to solve a sequence of problems, whose solutions are monotone decreasing. In other words we diagonalize; first smoothing the given data, then solving problem (P) with associated smoothed data. Preliminary numerical results appear promising.

Numerical effectiveness is demonstrated with the following test problem: The following problem begins with data given to us by Prof. Gary King who was visiting Department of Chemistry at Rice University briefly this summer. We begin with initial data of the exact inter-point distances between the atoms of a *Cranbin* molecule. We then added randomly distributed error to the every element of the matrix of exact distances (in this case error was approximately %15) and then try to recover the original inter-point distances as accurately as possible. The molecule has 394 particles or atoms the associated optimization problem had to approximate 1182 ($= 3 \times 394$) scalar components. These, in turn, were used to generate the

desired 77421 ($= (394^2 - 394)/2$) approximations to the inter-point distances. The following are some interesting values involving the norms of differences between the formula generated initial guess matrix, a randomly generated initial guess matrix, our computed approximation matrix, and the true matrix of inter-point distances.

Matrix	Norm - 1	Norm - 2	Norm - Frob.
solutions: computed - real	1.5743E+03	477.6585	725.9819
computed: solution-initial matrix	1.5199e+07	6.8876E+06	9.7282E+06
computed: solution-random matrix	3.3280E+19	6.1470E+10	1.2529E+12

TABLE 1: **Some interesting norms involving our solution**

In addition to the primary research, I have consulted with Paul Boggs of the National Institutes of Standards and Technology, Roland Glowinski of the University of Houston, and Jon Tolle of the University of North Carolina on research topics of mutual interest and collaborations. I have also consulted with Donald Jones of General Motors who described a class of problems that his division attempts to solve regularly. I have provided him with software I wrote that implements an algorithm for constrained non-smooth optimization. I also began work with Mark Gockenbach of Rice University on developing an algorithm for the minimization of the Leonard-Jones potential using ideas developed by the Geophysics research group here at Rice.

On the Use of Direct Seach Methods for the Molecular Conformation Problem

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ABSTRACT

An important area of research in computational biochemistry is the design of molecules for specific applications. The design of these molecules, which depends on the accurate determination of their three-dimensional structure, can be formulated as a global optimization problem. In this study, we present results from the application of a new conformation searching method based on direct search methods. We compare these results to some earlier results using genetic algorithms and simulated annealing.

Keywords: global optimization, molecular conformation, nonlinear programming.

1. Introduction

An important area of research in computational biochemistry is the design of molecules for specific applications. Examples of these types of applications occur in the development of enzymes for the removal of toxic wastes, the development of new catalysts for material processing, and the design of new anti-cancer agents. The design of these drugs depends on the accurate determination of the structure of biological macro-molecules. This problem, known as the molecular conformation problem, consists of finding the configuration of a molecule that yields its lowest free energy.

Under the assumption that the native structure of a molecule corresponds to a conformation for which the energy is at or near the global minimum, the molecular conformation problem can be formulated as an optimization problem. In general, one can decompose the search for a global minimum into two phases. In the first phase, we are interested in generating conformations that will be used as starting guesses for a second energy minimization phase. Using standard optimization techniques, each starting structure can be minimized to yield a final low-energy configuration. Unfortunately, because the total energy of a molecule depends on atom-atom interactions, the number of possible low-energy configurations can grow exponentially with the number of atoms and has been estimated by Hoare to be on the order of $O(e^{N^2})$ for an N-atom molecule [1].

There have been many attempts at developing efficient methods for the solution of this optimization problem. For a review of conformational searching methods see [2, 3]. Other recent attempts at conformational searching involve parallel stochastic methods as in [4, 5], and direct optimization methods as in [6, 7]. To address the multiple minimum problem, several people have attempted to use new search algorithms based on genetic algorithms [8] and simulated annealing [9]. Genetic algorithms (GA) [10] belong to a class of stochastic optimization methods based on analogies to natural selection strategies from evolution. Simulated annealing (SA) [11] is another stochastic optimization method that is based on a thermodynamic process called annealing. Both GA and SA have the property that they allow uphill directions and the iterates will therefore not necessarily decrease monotonically. This

property can be exploited to allow the search methods to jump out of local wells by moving uphill. However, both of these approaches can be time consuming and depend heavily on certain carefully chosen parameters.

As has been previously pointed out [3] the generation of the starting geometries will have the greatest effect on the final configurations found. The purpose of this study is to suggest an alternative methodology to genetic algorithms and simulated annealing for conformational searching. The new approach is based on the use of a particular instance of a class of methods known as pattern search methods. The new approach which uses a method known as the parallel direct search method [12] is robust, depends on only one parameter, and is easily parallelized.

2. Numerical Methods

2.1 Model Problem

For the purpose of this study, it was helpful to develop a model problem for which we could easily estimate the global minimum and which could easily be scaled while still retaining the same functional characteristics. We used a two-dimensional polymer consisting of N atoms connected by rigid rods of unit length. The function used to describe the energy of this system is given by a pairwise additive function consisting of Lennard-Jones potentials, that is,

$$V(\Theta[r]) = \sum_{i,j>i}^{N} \left[\left(\frac{\alpha}{r_{ij}} \right)^{12} - 2 \left(\frac{\alpha}{r_{ij}} \right)^{6} \right], \tag{1}$$

where r_{ij} is the distance between the atoms x_i and x_j, Θ is the bond angle between any three consecutive atoms, and α is a constant. In this study, we have conducted the conformational search in internal coordinates which has the advantage of implicitly enforcing the bond length constraints. If we set $\alpha = 1$, the minimum for a given pair of atoms will correspond to a unit distance, and the global minimum corresponds to closed hexagonal packs with unit spacing. This test problem has two nice features: 1) the dimension of the problem can be easily adjusted, and 2) the minimum energy can be easily deduced for any given dimension.

For this model problem, the parameter space can be visualized as having two easily distinguished regions. The first region is characterized by high energies and corresponds to configurations that are knotted. The second region is characterized by energies less than zero and corresponds to un-knotted configurations. The probability that a random configuration will have at least one knot (and therefore fall into the first region) is a function of the number of atoms in a molecule with that probability approaching one for even moderately sized molecules. As an example, for a molecule with 61 atoms, of 10,000 randomly generated conformations, only one conformation had an energy less than 0.0.

2.2 Direct Search Methods

Direct search methods belong to a class of optimization methods that do not compute derivatives. Examples of direct search methods are the Nelder-Mead Simplex method [13], Hooke and Jeeves' pattern search [14], the box method [15], and Dennis and Torczon's parallel direct search algorithm (PDS). The PDS algorithm can be viewed as an intelligent adaptive grid search algorithm employing a multi-sided simplex.

Starting from an initial simplex S_o, the function value at each of the vertices in S_o is computed and the vertex corresponding to the lowest function value, v_o, is determined. Using the underlying grid structure, the simplex S_o is rotated 180° about v_o and the function values at the vertices of this rotation simplex, S_r, are compared against v_o. If one of the vertices in the simplex S_r has a function value less than the function value corresponding to v_o, then an expansion step to form a new simplex, S_e, is attempted in which the size of S_r is expanded by some multiple, usually 2. The function values at the vertices of S_e are compared against the lowest function value found in S_r. If a lower function value is encountered, then S_e is accepted as the starting simplex for the next iteration; otherwise S_r is accepted for the next iteration. If no function value lower than the one corresponding to v_o is found in S_r, then a contraction simplex is created by reducing the size of S_o by some multiple, usually 1/2, and is accepted for the next iteration.

Because PDS only uses function comparisons it is easy to implement and use. Since the

rotation, expansion, and contraction steps are all well-determined it is possible to determine ahead of time a set of grid points corresponding to the vertices of the simplices constructed from various combinations of rotations, expansions, and contractions. Given this set of grid points, called a search scheme, the PDS algorithm can compute the function values at all of these vertices in parallel and take the vertex corresponding to the lowest function value. An interesting consequence of this approach is that the PDS algorithm can jump out of local wells by using a large enough search scheme size. By varying the size of the search scheme one can therefore use the PDS algorithm as a means of efficiently generating conformations in a manner similar to GA and SA.

It is also worthwhile to contrast PDS with grid search methods. In a grid search method the grids are generated by starting with a fixed molecule and systematically varying one of the parameters. This method works well for small molecules but becomes computationally prohibitive for larger molecules. The grid in PDS however is adaptive and will automatically change in response to the contours of the energy surface.

3. Numerical Results

In an earlier study [8], it was noted that both genetic algorithms and simulated annealing outperform random search for large molecules. However, both approaches were computationally expensive and depended heavily on carefully chosen certain parameters. In this study, we performed numerical experiments to compare direct search methods against both genetic algorithms and simulated annealing. The PDS code we used is a slight modification to a code developed by Torczon and obtained from the Center for Research on Parallel Computation at Rice University. For the energy minimization phase we used several well-known optimization methods, including a conjugate gradient method, a limited memory BFGS (LBFGS) method, and a quasi-Newton method, SUMSL, developed by D. Gay. Details of these methods can be found in [16, 17, 18]. All numerical tests were run on SGI workstations using IEEE double precision arithmetic with a machine precision, $\mu \approx 1.1 \cdot 10^{-16}$.

Using the model problem (1) we tested various combinations of methods for molecules

with different numbers of atoms. We studied molecules of 19, 37, and 61 atoms because the minima correspond to configurations that are hexagonal closed packs of radii 2, 3, and 4. Each test case consisted of running a set of trials starting from a set of randomly chosen starting points. To provide consistency across all of the test cases a set of 1000 configurations was generated from a uniform random distribution and stored in a file. This file was then used as the set of initial guesses for all of the test cases.

Because of the different methods used there were three different stopping criteria used. The PDS method uses a step tolerance, that is, the method terminates whenever the following condition is met:

$$\frac{1}{\Delta}\left(\max_{i,j}||v_i - v_j||_2\right) \leq \text{XTOL},$$

where $\Delta = \max(1, ||v_0||_2)$, and v_0 is the initial guess. The conjugate gradient method from [19] used a convergence criteria based on the function values:

$$2\frac{|f_{k+1} - f_k|}{|f_{k+1}| + |f_k| + \epsilon} \leq \text{FTOL},$$

where ϵ is equal to the machine precision. For the LBFGS method, the convergence test used consists of a test on the gradient, that is,

$$||g_k|| \leq \text{GTOL}\,(\max(1, ||x_k||))\,.$$

Unless otherwise indicated, all of our tests used the following tolerances: XTOL $= 10^{-3}$, FTOL $= 10^{-5}$, and GTOL $= 10^{-5}$.

3.1 Search Scheme Size

The first question we wished to address is whether the size of the search scheme has an effect on the geometries generated by PDS. Clearly the larger the scheme size the larger the sampling of the parameter space, at the expense of each iteration being more costly. In the first set of test cases, we chose the simplex shape to be regular, allowing PDS to construct the entire initial simplex from the initial random configuration. We considered search scheme sizes (SSS) of $2m$, $5m$, $10m$, $20m$, and $40m$ where $m = N - 2$ for a molecule of N-atoms and ran 100 trials for each test case. Table I contains the results for the 61 atom case.

Table I: Comparison of different PDS search size schemes (SSS) for 61 atom case.

Method	Trials	Minimum	% Negative
PDS(118)	200	-92.63	0.5
PDS(295)	200	-115.95	45.0
PDS(590)	200	-113.94	78.0
PDS(1180)	100	-115.02	83.0
PDS(2360)	100	-117.47	85.0

As Table I shows, all of the test cases yielded configurations with negative energies. For the first three tests, we ran 200 trials while the last two test cases used 100 trials. Each trial typically converged in about 50 iterations and took about 1-3 minutes of CPU time per trial. The fourth column of Table I also displays the percentage of all trials that yielded a negative energy. In a sense, this is an indication of how robust the method is. We note that with a search scheme size of $10m$ approximately 80% of the trials had configurations with negative energies. As the search scheme size increases we get a higher percentage of trials with negative energies but at the cost of substantially more CPU time per trial. Figure 1 contains a representative configuration for the 61 atom test case computed by PDS using a search scheme size of 2360 points.

3.2 Energy Minimization

The next step in our numerical experiments was to test the combination of PDS with an energy minimization phase. For the purposes of a direct comparison with GA and SA, we ran a test case using PDS with the same CG routine used in [8]. The lowest energies found are given in Table II and compared against the best known global minimum energy.

For the 19 and 37 atom test cases, the results for all three methods are similar in terms of the final energies. In the 61-atom case, the various methods start to exhibit greater

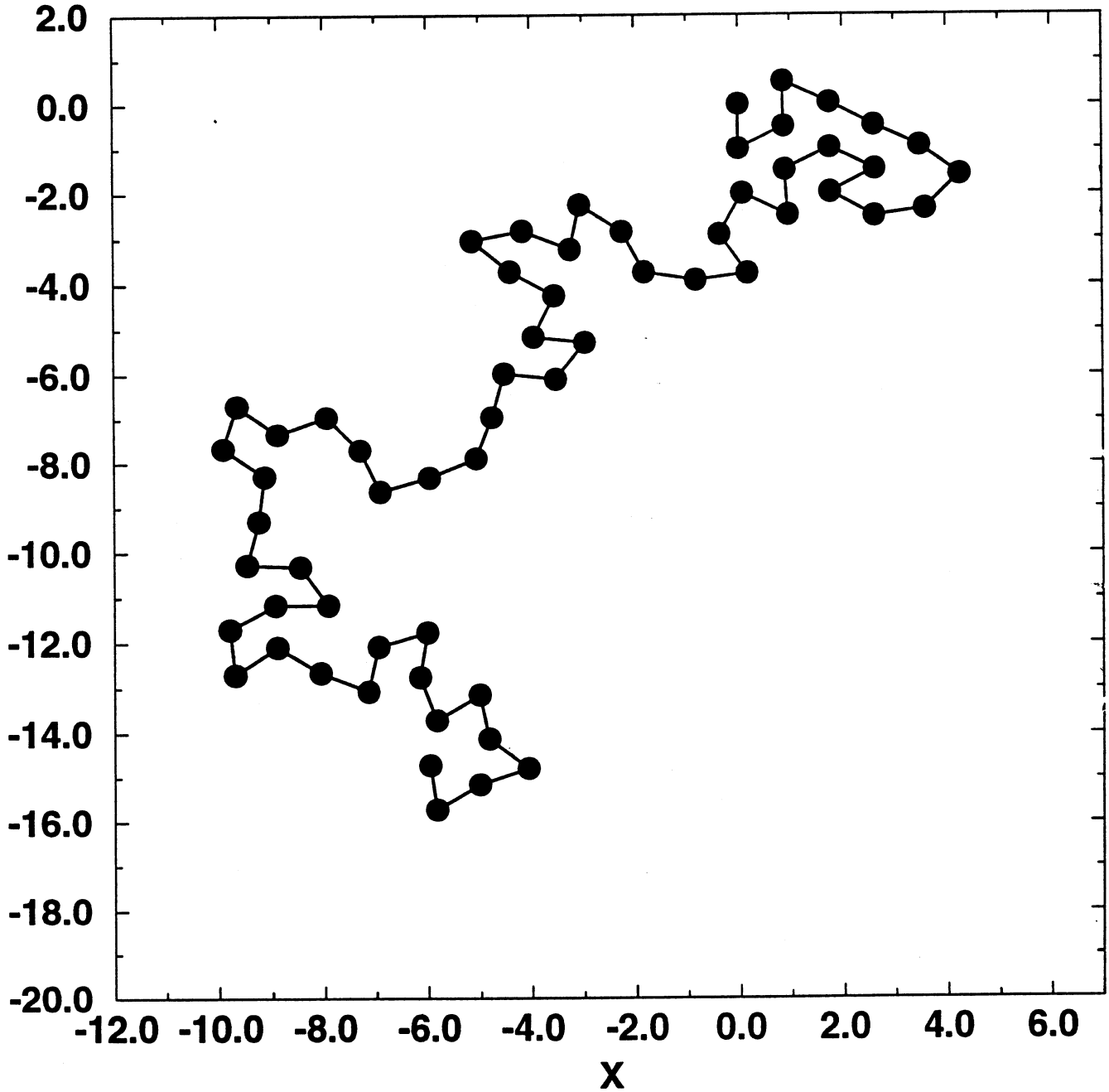

Figure 1: Conformation computed for a 61 atom test case using PDS(2360).

Table II: Comparison of PDS versus GA and SA for 19, 37, and 61 atom test cases.

Method		Minimum		
		19 atoms	37 atoms	61 atoms
GA	CG	-44.3	-97.3	-166.6
SA	CG	-44.2	-94.8	-164.4
PDS	CG	-45.3	-95.3	-142.6
Best Known		-45.3	-98.3	-170.5

differences. In this case, the lowest energies computed by GA with CG and SA with CG are much closer to the best known global minimum than PDS with CG. Table II however does indicate that PDS can be used in a similar manner to GA or SA to generate good starting conformations for the energy minimization phase.

The next set of tests combine PDS with gradient methods. All of these tests use PDS with a value of SSS of $40m = 2360$. From tests using random search we can predict that it would not be useful to do an energy minimization starting from a configuration that has a high energy. We therefore modified our algorithm to set a user-defined energy tolerance such that if the value returned from the PDS algorithm is higher than this energy tolerance, the minimization phase is skipped.

We also note that PDS was modified so that it would restart after it had converged using the best vertex as its initial guess for the restart. To allow for greater flexibility, we allowed the user to set the maximum number of restarts. In these tests we set the number of restarts equal to 5.

The results of these tests are displayed in Table III. The first observation we make is that PDS is not effective as an energy minimization algorithm. Even with restarts, PDS does not get a solution near a minimum. Theoretically PDS should not converge to a non-minimizer so this behavior seemed unusual at first. In fact, if the search scheme size is increased at the

Table III: Minimum energies found using PDS for 61 atom test case.

Method		Energy
PDS(2360)	PDS(2360)	-117.5
PDS(2360)	CG	-142.6
PDS(2360)	LBFGS	-167.2
PDS(2360)	SMSNO	-166.0
PDS(2360)	SUMSL	-163.6

same time that a restart occurs, then PDS will start to progress towards a minimum again, although at an extremely slow rate.

For the gradient based methods, the results are all similar in terms of the final energy. The combination of PDS with LBFGS yielded the lowest energy overall, but not substantially better than the other methods. The difference between SUMSL and SMSNO lies in the availability of first derivatives. The SMSNO method uses finite differences to compute gradients, whereas SUMSL uses analytic gradients. For these test problems, we used ADIFOR to generate analytic derivatives [20]. Figure 2 contains a representative configuration computed by using a combination of PDS(2360) and SUMSL.

3.3 Distribution of Minima

Although our main goal is to find the global minimum it is also important to find any local minima that are close to the global minimum. One way of depicting this result is to generate a distribution of the local minima found for each method. Figure 3 contains the distributions for the test cases corresponding to the 61 atom molecule. The three curves using PDS(2360) all compare favorably with the distribution corresponding to the test results using GA. In fact, all four curves generate distributions with at least 80% of the final configurations having negative energies. Simulated annealing (SA) is the only method that does not do well on this

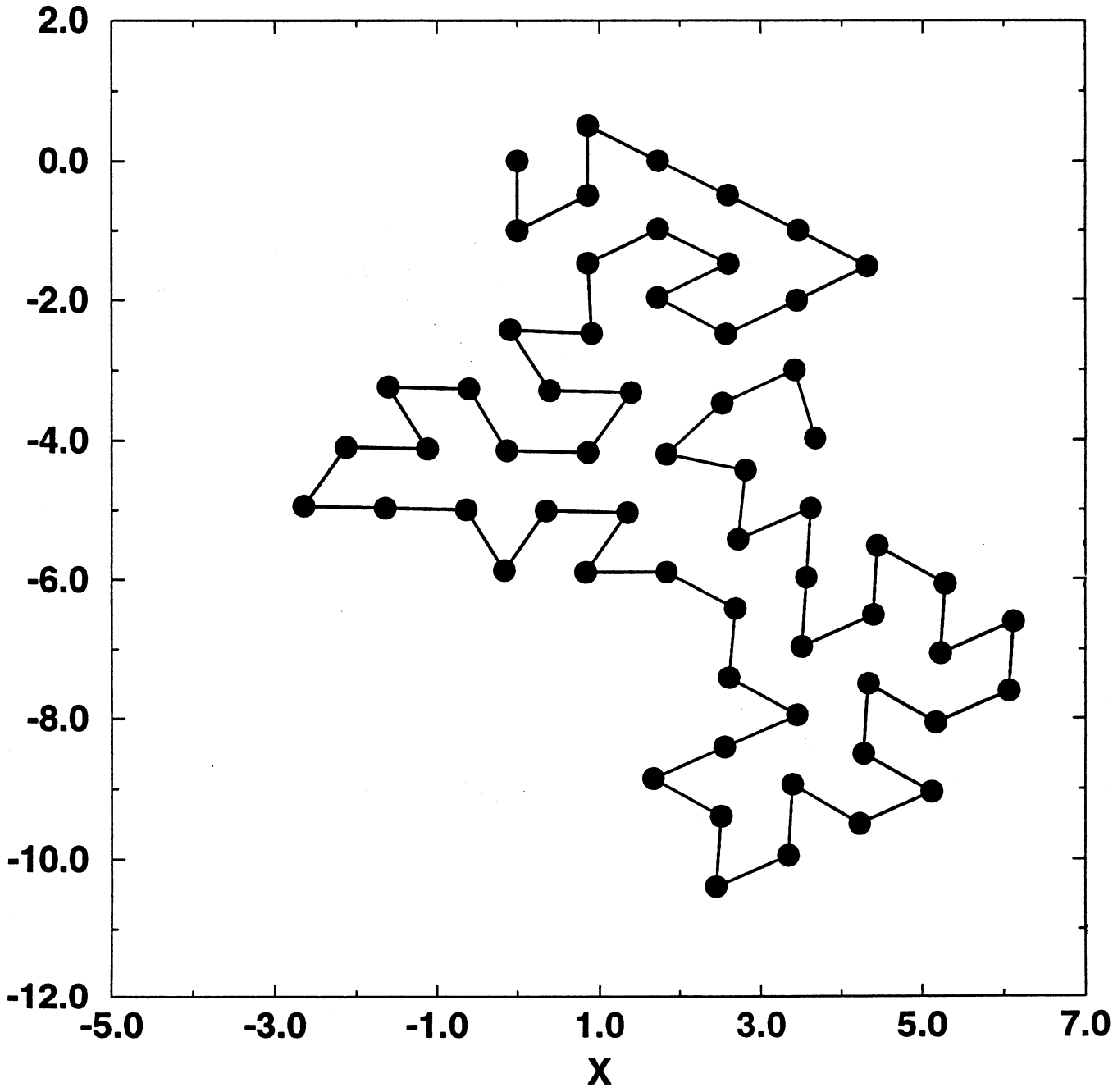

Figure 2: Final configuration computed using PDS(2360) + SUMSL for 61 atom test case.

problem. We also note that of these methods, the combination of PDS(2360) with SUMSL yields the best distribution with approximately 80% of the minima having energies below -144.0.

4. Conclusions

We can make several conclusions from the numerical results. In [8], we studied GA and SA with the conclusion that GA could be used for conformational searching. In this study, we showed that PDS can also be used for conformational searching and performs at least as well as GA and substantially better than SA for larger molecules. One of the advantages of the PDS algorithm is that the user only has to decide on the value of one parameter. This parameter, the search scheme size, has some effect on the convergence rate, but typically the parameter can be chosen to be some small multiple of the dimension of the problem. The PDS algorithm can also be easily parallelized allowing for even greater computational efficiency.

We feel that these results are suggestive of the power of these new optimization methods for conformational searching for large molecules. Further research will concentrate on new experiments using more realistic molecules. In particular, it would be interesting to do a direct comparison with the methods used in [3] for computing the conformations of cycloheptadecane.

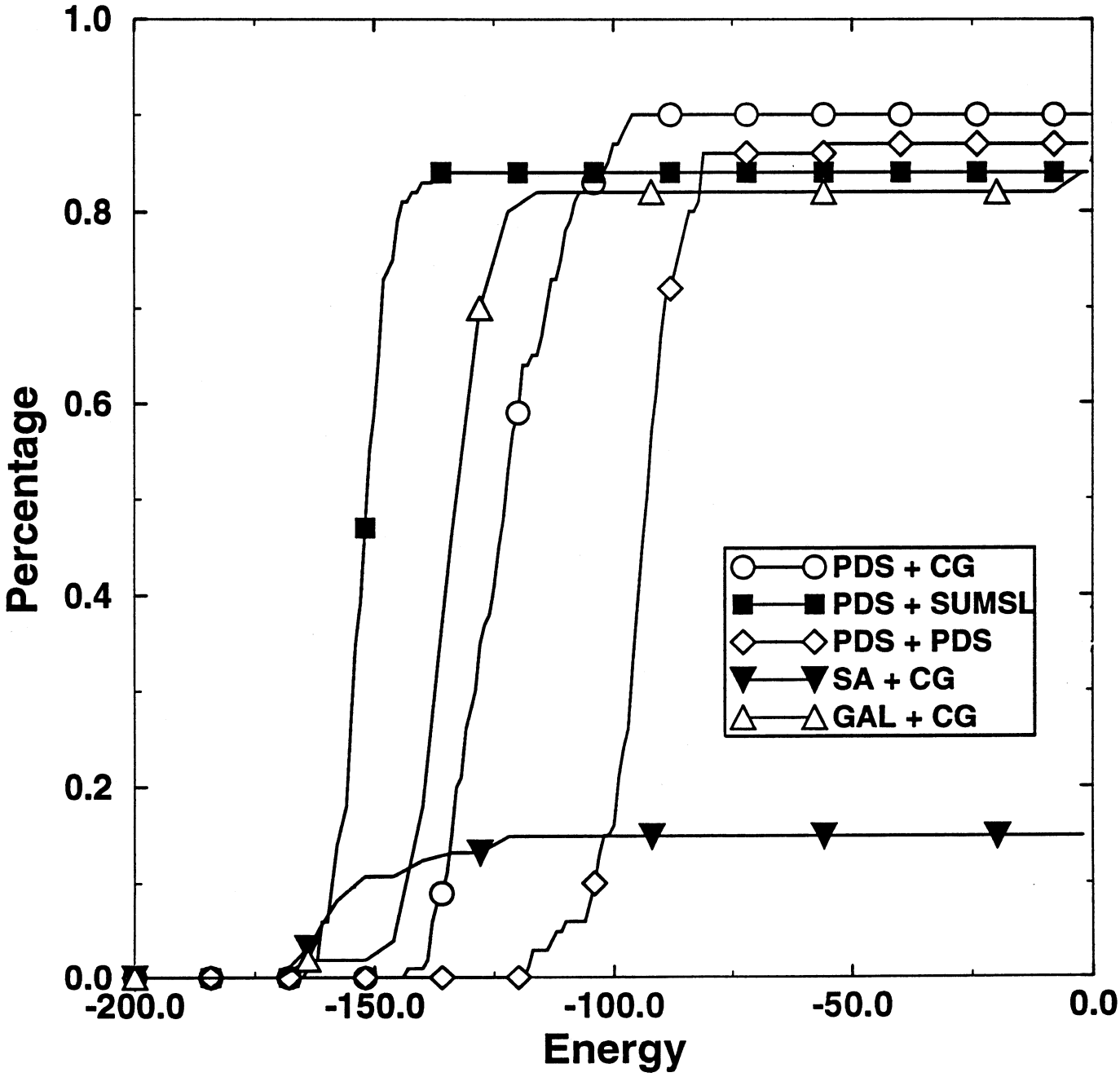

Figure 3: Distribution of minima for 61 atom test case.

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On Crossing Over From Primal-Dual Interior Point Method to Simplex

Casssandra Moore

6 August 1993

Abstract

During the summer of 1993, I worked with Dr. Amr El-Bakry, Dr. Richard Tapia, and Dr. Robert Bixby. I spent much of the summer reading papers and listening to lectures concerning primal-dual interior point methods. I was assigned these tasks in order to prepare me for the project that I was to begin toward the end of the summer. My final project was to generate computational results using a new method for recovering an optimal linear programming basis from a primal-dual interior point solution on the netlib test problem set.

1 Introduction

Consider the linear programming problem in standard form:

$$\begin{aligned} min \quad & c^T x \\ st \quad & Ax = b \\ & x \geq 0 \end{aligned} \tag{1}$$

where $c \in \mathbf{R}^n$, $b \in \mathbf{R}^m$, $A \in \mathbf{R}^{m \times n}$ $(m < n)$ and A has full rank m. This is referred to as the primal problem. The dual of this problem is:

$$\begin{aligned} max \quad & b^T y \\ st \quad & A^T \lambda + y = c \\ & y \geq 0 \end{aligned} \tag{2}$$

where $\lambda \in \mathbf{R}^m$, and $y \in \mathbf{R}^m$ are the Lagrange multiplier vectors corresponding to the equailty and inequality constraints of problem (1) respectively. The multipliers y are also known as the dual variables and z as the dual slack variables. The first-order optimality (or Karush-Kuhn-Tucker) conditions for the problem are:

$$F(x, y, \lambda) = \begin{pmatrix} Ax - b \\ A^T\lambda + y - c \\ XYe \end{pmatrix}$$

where $X = diag(x)$, $Y = diag(y)$ and e is the n-vector of all ones. A point (x, y, λ) is said to be strictly feasible if it satisfies $Ax = b$, $A^T\lambda + y = c$ and $(x, y) > 0$.

Under standard conditions, we know that Newton's Method is a highly effective method for solving $F(x, y, \lambda)$, if it is started close to the solution. Convergence is not assured if Newton's Method is started too far away. Primal-dual interior point methods can be described as a perturbed damped Newton's Method. In solving $F(x, y, \lambda)$, the primal-dual interior point method generates iterates that adhere generally to the central path curve ensuring the global convergence of Newton's method. Currently the state of the art high performance interior point code is OB1 (trademark of XMP, Inc).

Currently the best method for solving (1) is the Simplex Method. Simplex does not involve solving a linear system. The grand strategy of Simplex is that of successive improvements. We find some feasible solution to (1) and systematically find another solution which is better. The Simplex Method naturally terminates with an optimal basic pair of primal and dual solutions. At present the state of the art high performance Simplex code is CPLEX (trademark of CPLEX, Inc.).

2 Problem

The results obtained for many problems solved using OB1 are impressive. There are however some drawbacks. The primary one being that interior point methods do not terminate with an optimal basis. In some cases, if there are multiple optima the interior point solution falls somewhere in the middle. The reason why an optimal basis is so important is that currently post-optimality analysis centers upon the recovery of such a basis. Another

disadvantage of interior point methods is that they depend upon the linear system being solvable, and for most problems the linear system either becomes progressively more ill-conditioned or is singular at the solution.

It is known that for certain problems CPLEX is better that OB1, but the reverse is also true. In fact, there is no clearly superior code. Our best option, therefore, is to attempt to combine the two. As stated before, post-optimality analysis depends upon a optimal basis, so our problem is crossing over from OB1 to CPLEX. In order to start CPLEX, however, we must recover an optimal basis from our interior point solution.

3 Indicators

An indicator is a function that identifies constraints that are active at a solution of a constrained minimization problem, in other words a problem like (1). In order for a component x_i^* of x^* to be a part of the basis it must be nonzero. We use our indicator functions to determine which components are zero (non-basic) and which are nonzero (basic). Also, it has been hypothesized by Dr. Amr El-Bakry that those components that have converged are basic at every basic feasible solution. There are four indicator functions that we will test separately:

1. Variables as Indicator

$$V_P(x^k) = x^k \text{ and } V_D(y^k) = y^k.$$

2. Primal Dual Indicator

$$PD(x^k, y^k) = \frac{x^k}{y^k}.$$

3. Tapia Indicator

$$T_P(x^k) = \frac{x^{k+1}}{x^k} \text{ and } T_D(y^k) = \frac{y^{k+1}}{y^k}.$$

4. Logarithmic Tapia Indicator

$$LOGT_P(x_i^k) = \log \mid 1 - T_P(x_i^k) \mid,$$

and

$$LOGT_D(y_i^k) = \log \mid 1 - T_D(x_i^k) \mid .$$

4 Computational Results

- pending

5 Conclusions

- pending

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Spend A Summer With A Scientist Program

Rice University School Mathematics Project

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Mathematics Education
August 6, 1993

Spend A Summer With A Scientist Program

Rice University School Mathematics Project

Introduction

The Rice University School Mathematics Project (RUSMP) is a partnership between Rice University and Houston area K-12 mathematics teachers. The project began in 1987 in response to the national mathematics reform movement, initiated because traditional teaching methods had failed to produce literate students in mathematics. Such traditional methods consisted of students learning through worksheets, applying math concepts to rudimentary word problems, and teacher demonstrations and lectures. Students were graduating from high school and entering the work force with a very limited knowledge of basic mathematics.

Thus, Rice University took the lead to bring the national reform movement in the teaching of K-12 mathematics to the Houston area. RUSMP reaches out to teachers to help them improve the quality of mathematics classroom instruction by implementing the use of manipulatives, technology, and the *Standards* from the National Council of Teachers in Mathematics in the curriculum. The mathematics reform movement aims for more student classroom involvement, student discovery, and hands-on-activities which will enable the student to develop critical thinking skills and actually work with real-life mathematics applications. To help teachers contribute to the national reform movement, the program also supplies them with classroom set materials, like graphing calculators and manipulatives, and with continued support from the project.

Work Description

As a Research Assistant for the project, I was assigned to read and summarize the participants' journals for use in our yearly evaluation report of the project. But in order to perform this task with good evaluation, I needed insight into the project to understand the journal entry information, so I decided to interact with the participants and observe the classrooms. Further, I wanted to discover if there was any parallel between observations and the journals.

Everyday, I tried to visit each program for approximately two hours. Sometimes, I spent time with one program in the morning and a second program in the afternoon.

Then, the following day, the third program took priority. However, another factor also determined which programs I would be visiting. The Master Teachers, RUSMP instructors and former RUSMP participants, would ask me to observe their classrooms during certain periods, because they felt it would be of interest to me, as I wish to study mathematics education in graduate school.

Conclusions

The observations helped me greatly to record, summarize, and understand journal information. Since I had participated in activities, I was able to relate to the participants' thoughts and learning experiences of the activities. Therefore, I was able to better understand their explanations on the difficulty or easiness of the activities.

In addition, the observations were consistent with the journals. For example, teachers who had difficulty with class material exclaimed this in their journals. Others who were knowledgeable on the material went in depth to expand on the topics. All of these observations and interactions led me to the following conclusions of our present educational system:

1) Elementary teachers require more pre-service mathematics education. The teachers knew only basic mathematics, like arithmetic. Few, if any knew some algebra. I was quite disappointed to discover this, for elementary teachers teach the foundations of mathematics to young children. If a student does not grasp the material, he is caught in a web of confusion, and later becomes disinterested with mathematics.

   I understand teachers do not have to teach algebra in the lower elementary levels, but it can be INTRODUCED in the higher elementary grades so that kids can get a feel for the various branches of mathematics. More importantly, KIDS DO ALGEBRA except they probably are not aware of it. Here is an example of a possible algebra problem:

   If a child has 7 chips and he wants 10 chips, how many more chips does he need?

   $$7 + X = 10.$$

   Further, elementary teachers need to be educated in math, because students pick up on teachers' performance. If the teacher does not know enough or even a little beyond of what he is teaching, the student loses motivation to learn. Teachers are role models, and students look up to teachers; students want to know

as much as their teachers and even more. So, when a teacher is "handicapped" in his area, students' motivation is again driven away.

In addition, students need to be challenged in mathematics. Elementary kids observe and question much; they need to be challenged so their critical thinking skills can develop. But how can we do this, if our elementary teachers do not know more beyond their area of teaching.

2) Manipulatives and technology are important for the development of concepts and skills. Further, technology allows students to apply mathematics to real-life situations. The majority of students need to work with manipulatives in order to understand concepts, for manipulatives give a concrete meaning to the concept; this enables the student to remember and understand the concept better than through chalkboard lectures.

Moreover, students can discover and investigate with manipulatives. Manipulatives also can help to create a collaborative learning environment, since students can investigate with manipulatives and share their ideas with other students. Using technology, such as calculators, graphing calculators, and computers, students can see how technology requires mathematics and how mathematics is applicable in many academic disciplines.

Program Evaluation

RUSMP

The entire aspect of the program is outstanding! The entire staff worked together and shared ideas to improve the quality of the program.

I learned much from talking and working with the teachers in class activities. These teachers were very excited to learn and share their classroom ideas with other people, and this is what we really need if we all wish to help students succeed in math. I was glad to have been given the opportunity to work in this program, because it is quite rare for a student to work in an environment such as this and to work with a group of teachers to discuss mathematics and mathematics education. This program has given me some ideas as to what we, as educators, need to change in education. Most importantly, it has given me more understanding and determination to help students, teachers, and their schools.

SAS

Great! I was thrilled to have worked in my area of interest: mathematics education. I enjoyed the in-depth conversations I had with my professor, Dr. Papakonstantinou, on

issues regarding mathematics education. Many undergraduate students find it difficult to discuss such issues with their university professors for various reasons, primarily because their professors have little time to converse or are involved in research. But, SAS professors spend time with their students and this is accomplished because Dr. Tapia searches for those professors who are interested in working with students.

The presentations and reports we had to do were very beneficial and educational to me. Prior to this program, I had little knowledge of how to give presentations. Once I did it, the students were very helpful with their feedback, which is what someone always needs if they desire to improve.

Finally, I enjoyed having the Friday afternoon meetings. Many times, program coordinators ignore their participants, but Dr. Tapia interacted with us through and outside the meetings. During meetings, he was open to discuss basically anything. This showed his great concern for us in our educational careers, as well as, in our lives.

Newsletter

Cristina Villalobos is a senior mathematics student at the University of Texas-Austin, interested in both mathematics and K-12 mathematics education. At UT, she works as a mathematics grader and a Research Assistant for the UT-Hispanic Mother-Daughter Program (HMDP). HMDP was created to support and encourage the participation of female Hispanic women in higher education in the areas of mathematics and science. Research indicates that female students lose interest in mathematics and science during middle school, thus HMDP targets 7th-grade Hispanic female students and provides them with continued support through college.

This summer, Cristina worked as a Research Assistant for RUSMP. She read and summarized journals for the yearly evaluation report of the program. Further, she observed classrooms to discover if there was any parallel between observations and the journals.

The entire aspect of a program is ~~astounding!~~ outstanding! The entire staff works together and shares ideas to improve the quality of the program. I greatly enjoyed interacting with the Master Teachers and teachers. The Master Teachers are very supportive, mathematically educated, and present material in a clear manner. Several forms are administered to the participants to assess the quality of the prog., then I learned much from talking and working with the teachers in class activities. These teachers are very excited to learn and share their classroom ideas with other people, and this is what we really need if we all wish to help students succeed in math. I was glad to have been given the opportunity to work in this program, because it is quite rare for a student to work in an environment such as this and with a group of teachers to discuss mathematics and mathematics education. This program has given me some ideas as to what we, as educators, need to change in education. Most importantly, it has given me more understanding and determination to help students, teachers, and their schools.

ISOTONIC REGRESSION:
A PARALLEL ASPECT

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PROBLEM

Isotonic Regression is used to fit data that we know should be isotonic. In other words, given some arbitrary data, the result should be monotonous or a steadily increasing graph. In some cases, the ending result is not monotonous and so, this application must be applied. When a case such as this does occur, the results may be difficult to receive because the data set may be too large and would take much time to get an accurate reading. To minimize the time it takes to do such problems, this application was created.

In order to attain the right result, boundaries must be found and set. The upper and lower bounds of the graph or the highest and lowest points in the data set give the graph its shape. If points are plotted outside these boundaries, then we have a result that is not monotonous. The isotonic regression application corrects this.

MATHEMATICS

The mathematical aspect was the minimization of the following objective quadratic function:

$$\text{minimize } x_i \sum_{i=1}^{n} (x_i - d_i)\, w_i\, (x_i - d_i)$$

$$\text{s.t. } x_i <= x_2 <= x_3 <= \ldots x_n$$

Where x_i is the solution we hope to find and d_i is the original data with x_i approximately equal to d_i. For practical purposes later on in this paper, I will refer to this function as P.

BLACK BOX SOLUTION

After minimizing the previous function, a computational solution was sought. This solution was eventually found. This black box solution is attributed to Grotziner-Witzgall '84. The computation involves an averaging of numbers. When it is found that a solution is not monotone or a point is plotted outside the established boundaries, then this solution takes the average of the points before and after the point that is out of bounds and the point. If the new point is still outside of the boundaries, the average is taken again, and so on, until a better result is obtained. This computation is very fast. It is unlike any other solution. With this solution, there are no derivatives computed. It is simply the minimizing of an objective quadratic function subject to linear constraints.

PARALLEL ASPECT

Earlier, a program was written by Anthony Kearsley, a senior graduate student in Computational and Applied Mathematics Department at Rice University, that would solve large and small scale isotonic regression problems. His solution was

accomplished using a sequential processor. This algorithm is very fast and very accurate. However, my assignment was to assist him in finding a way to parallelize this program. That is, to correctly break up the problem in such a way as not to change the original problem and compute these individual problems on a parallel machine. To work on this project, we used the IPSC/i860 located at CalTech and eventually, hoped to incorporate this algorithm on the DELTA, also located at CalTech, as well. To get this algorithm to work on a parallel machine would mean faster results and even better success.

OBSERVATIONS

The program written by Anthony Kearsley did use minimum time. It also produced a monotonous graph. This seems like the perfect result, but can it be improved? This was the objective of our project. This is where Amdahl's Law comes in. We must compare the results of our algorithm with Amdahl's Law. Amdahl's Law determines the maximum speedup with p processors. According to Amdahl's Law, maximum speedup is defined as follows:

$$S_p = T_1 / T_p;$$

Where T_1 is the time taken to run the best algorithm on a single processor and T_p is the time taken to run the best algorithm on more than one processor.

PLAN OF ATTACK

First, we wanted to compute the component-wise squares of elements of a vector in parallel. In other words, compute the following:

$x_1(i)$ <-- x(i) * x(i);

The result of this computation is very close to Amdahl's Law. We could only hope to come close to this result. Second, we wanted to compute our solution to P in parallel which we call xsim or compute the following:

$x_2(i)$ <-- xsim(i).

Third, we would compare the time to compute x_1 vs. x_2 vs. Amdahl's Law on the IPSC/i860 and the DELTA. We would hope that our results are very close.

CONCLUSION

At this time, the project is unfinished, but I hope that eventually it will be complete. This summer I had a chance to work with someone who is closer to my level. It made it easier to work and to learn. It was truly a pleasure working with Anthony Kearsley. He totally changed my way of thinking, as

far as, graduate school is concerned. The knowledge that I have obtained from working with him is invaluable. The knowledge that I have gained from working in this program the past two summers is invaluable, period. I am very grateful to Dr. Richard Tapia for making me a part of this program and enabling me to gain the necessary experience I believe will help me make it in the work force of today. The students that I have come in contact with while in this program, as well as, the visitors we have been introduced to have enriched me with the many diverse topics that have been spoken on. All in all, I think this program will continue to be a success with all future students and activities.