Research Summary
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My **past research** has centered upon several themes, primarily related to computational linear algebra, scientific computing, and optimization. The work has involved a mixture of algorithm development and scientific applications, drawing upon tools in applied mathematics, numerical analysis, and computer science. These themes have led to applications in science and engineering.

This work has been published in computer science and applied mathematics journals as well as journals of physics, aerospace engineering, medicine, and electrical engineering. The references in the following sections are numbered chronologically in three groups: journal publications [J_], conference proceedings [C_], and technical reports[T_].

1 Numerical solution of Markov Chains

Markov Chains are used to model processes such as behavior of queueing networks. Both the short term behavior (e.g., mean first passage times) and the long term behavior (e.g., stationary vector) are of interest, and this work has focused on both of these problems.

The basic computational problem for Markov chains is determining the stationary vector, defining the long-term behavior of the chain. Grassman, Taksar, and Heyman proposed an algorithm that O'Cinneide has shown to compute an approximation to the stationary vector with low relative error in each component. Jason Wu and I developed a block form of the GTH algorithm, more efficient on high performance architectures, and showed that it, too, produces a vector with low relative error. We demonstrated the efficiency of the algorithm on vector processors and on workstations with hierarchical memory [J42]. Iterative methods for finding stationary vectors were studied in [C9].

A great deal of attention has been devoted to computing stationary vectors, but less attention has been given to computational algorithms for other parameters associated with these chains. Daniel Heyman (Bellcore) and I developed and evaluated algorithms for computing the fundamental matrix, the group generalized inverse, and the mean and variance of first passage times for discrete time regular Markov chains [C15] and then studied ill-conditioned problems arising in this area [J44].

[C9] (invited) Dianne P. O'Leary, "Iterative Methods for Finding the Stationary Vector for Markov Chains," *Linear Algebra, Markov Chains, and Queuing Models (IMA, January 1992)*, Carl Meyer and Robert Plemmons, eds., Springer-Verlag, IMA Volumes in Math. and Its Applics. Vol. 48 New York, 1993, 125-136.

[C15] D. P. Heyman and Dianne P. O'Leary, "What is Fundamental for Markov Chains: First Passage Times, Fundamental Matrices, and Group Generalized Inverse s," *Proceedings of the Second International Workshop on Markov Chains*, W. Stewart, ed., Kluwer Academic Publishers, 1995, 151-161.

[J42] Dianne P. O'Leary and Yuan-Jye Jason Wu, "A Block-GTH Algorithm for Finding the Stationary Vector of a Markov Chain," *SIAM Journal on Matrix Applications,* 17 (1996) 470-488.

[J44] Daniel P. Heyman and Dianne P. O'Leary, "Overcoming instability in computing the fundamental matrix for a Markov chain," *SIAM Journal on Matrix Analysis and Applications,* 19 (1998) 534-540.

2 Numerical Solution of Ill-Posed Problems

In ill-posed problems, small changes in the data can cause arbitrarily large changes in the results. Although it would be nice to avoid such problems, they have important applications in medicine (computerized tomography), remote sensing (determining whether a nuclear reactor has a crack), and astronomy (image processing).

Two projects were performed jointly with workers at the National Institute of Standards and Technology (formerly the National Bureau of Standards).

In the first, data related to non-destructive detection of crack formation was analyzed by filtering techniques using a small problem-dependent set of basis functions [J11]. This was the first *hybrid algorithm* for ill-posed problems: the given problem was projected to a subspace and regularization was applied there.

In the second project, confidence intervals for spectroscopy data were computed using a nonnegativity constraint on the solution [J21] [J38].

Other work focused on the choice of optimization criteria for ill-posed problems [J37], studying the characteristics of solutions produced by various regularization methods, including truncated least squares, regularized least squares, regularized total least squares, and truncated total least squares [C12] [C16] [J43] [J51]. Efficient numerical algorithms for computing these solutions in image processing applications were also proposed [J50] [J45] [C18] [J61].

The regularization of discretized problems by iterative methods was studied with Misha Kilmer [J57], demonstrating that regularization could be provided easily if the iterative method was viewed as projecting the continuous problem into a lower dimensional subspace. Choice of the regularization parameter was considered in [J59].

[C12] Richardo Fierro, Gene H. Golub, Per Christian Hansen, and Dianne P. O'Leary, "Regularization by Truncated Total Least Squares," *Proceedings of the Fifth SIAM Conference on Applied Linear Algebra*, J.G. Lewis, ed., SIAM Press, Philadelphia, 1994, 250-254.

[C16] Dianne P. O'Leary, "The SVD in Image Restoration," *SVD and Signal Processing III: Algorithms, Architectures, and Applications,* Marc Moonen and Bart DeMoor, eds., Elsevier, New York, 1995, 315-322.

[C18] James G. Nagy and Dianne P. O'Leary, "Fast Iterative Image Restoration with a Spatially Varying PSF," in *Advanced Signal Processing Algorithms, Architectures, and Implementations VII* F. T. Luk, ed., SPIE, 1997, 388–399.

[J11] Dianne P. O'Leary and John A. Simmons, "A bidiagonalization- regularization procedure for large scale discretizations of ill-posed problems," *SIAM J. on Scientific and Statistical Computing* 2 (1981) 474-489.

[J21] Dianne P. O'Leary and B. W. Rust, "Confidence intervals for inequality-constrained least squares problems, with applications to ill-posed problems," *SIAM Journal on Scientific and Statistical Computing* 7 (1986) 473-489.

[J37] Per Christian Hansen and Dianne P. O'Leary, "The use of the L-curve in the regularization of discrete ill-posed problems," *SIAM Journal on Scientific Computing* 14 (1993) 1487-1503.

[J38] Bert W. Rust and Dianne P. O'Leary, "Confidence intervals for discrete approximations to ill-posed problems ," *The Journal of Computational and Graphical Statistics*, 3 (1994) 67-96.

[J43] Ricardo D. Fierro, Gene H. Golub, and Per Christian Hansen, and Dianne P. O'Leary, "Regularization by Truncated Total Least Squares," *SIAM Journal on Scientific Computing,* 18 (1997) 1223-1241

[J45] James G. Nagy and Dianne P. O'Leary, "Restoring Images Degraded by Spatially-Variant Blur," *SIAM Journal on Scientific Computing,* 19 (1998), 1063-1082.

[J50] Misha E. Kilmer and Dianne P. O'Leary, "Pivoted Cauchy-Like Preconditioners for Regularized Solution of Ill-Posed Problems," *SIAM Journal on Scientific Computations,* 21 (1999) 88-110.

[J51] Gene H. Golub, Per Christian Hansen, Dianne P. O'Leary, "Tikhonov Regularization and Total Least Squares," *SIAM Journal on Matrix Analysis and Applications*, 21 (1999) 185-194.

[J57] Misha E. Kilmer and Dianne P. O'Leary, "Choosing Regularization Parameters in Iterative Methods for Ill-Posed Problems," *SIAM J. on Matrix Analysis and Applications*, 22 (2001) 1204-1221.

[J59] Dianne P. O'Leary, "Near-Optimal Parameters for Tikhonov and Other Regularization Methods," *SIAM J. on Scientific Computing*, 23 (2001) 1161-1171.

[J61] James G. Nagy and Dianne P. O'Leary, "Image Restoration through Subimages and Confidence Images," *Electronic Transactions on Numerical Analysis*, 13 (2002) 22-37.

3 Linear Algebra and Optimization in Image Processing

This work, joint with various experts in image processing, involves the adaptation of techniques in linear algebra and optimization. Projects included using the singular value decomposition for classifying images [J9], applying function minimization methods to noise smoothing and edge reinforcement [J13] [J14], using multi-level iterative methods for function minimization [J15], and analyzing convergence of iterations used in image processing [J17]. An efficient algorithm for image compression was also developed, making use of linear algebra and discrete optimization techniques [J16], and several algorithms were studied for approximating two dimensional convolution operators by a product of convolutions with smaller support [J27].

Recent work has focussed on the solution of the ill-posed problems arising in deblurring. Various optimization criteria have been evaluated [C13], and J. G. Nagy and I have developed algorithms that are efficient when the point spread function (the blurring function) is spatially variant, as in the Hubble Space Telescope [C18],[J45]. We have also worked on computing and displaying confidence intervals for the reconstructed images [J61]. Armin Pruessner and I studied blind deconvolution, in which the blurring function as well as the true image is to be determined [J63],and the structure of the blurring matrix was exploited in [J67] and [J74].

An application to Ladar images was made in [J66].

Some of this work is summarized in a monograph [B1], written at the level of an advanced undergraduate or beginning graduate student, designed to motivate mathematics and computer science students to learn about computational methods.

[B1] Per Christian Hansen, James G. Nagy, and Dianne P. O'Leary, *Deblur-*

ring Images: Matrices, Spectra, and Filtering*, SIAM Press, Philadelphia, 2006.

[**C13**] Dianne P. O'Leary, "Regularization of Ill-Posed Problems in Image Restoration," *Proceedings of the Fifth SIAM Conference on Applied Linear Algebra*, J.G. Lewis, ed., SIAM Press, Philadelphia, 1994, 102-105. [**C18**]] James G. Nagy and Dianne P. O'Leary, "Fast Iterative Image Restoration with a Spatially Varying PSF," in *Advanced Signal Processing Algorithms, Architectures, and Implementations VII* F. T. Luk, ed., SPIE, 1997, 388–399.

[**J9**] Timothy J. O'Leary, Dianne P. O'Leary, Mary C. Habbersett, and Chester J. Herman, "Classification of gynecologic flow cytometry data: a comparison of methods," *J. of Analytical and Quantitative Cytology* 3 (1981) 135-142.

[**J13**] K. A. Narayanan, Dianne P. O'Leary, and Azriel Rosenfeld, "Image smoothing and segmentation by cost minimization," *IEEE Transactions on Systems, Man, and Cybernetics* SMC-12 (1982) 91-96.

[**J14**] K. A. Narayanan, Dianne P. O'Leary, and Azriel Rosenfeld, "An optimization approach to edge reinforcement," *IEEE Transactions on Systems, Man, and Cybernetics* SMC-12 (1982) 551-553.

[**J15**] K. A. Narayanan, Dianne P. O'Leary, and Azriel Rosenfeld, "Multiresolution relaxation," *Pattern Recognition* 16 (1983) 223-230.

[**J16**] Dianne P. O'Leary and Shmuel Peleg, "Digital image compression by outer product expansion," *IEEE Transactions on Communications* COM-31 (1983) 441-444.

[**J17**] Dianne P. O'Leary and Shmuel Peleg, "Analysis of relaxation processes: the two node, two label case," *IEEE Transactions on Systems, Man, and Cybernetics* SMC-13 (1983) 618-623.

[**J27**] Dianne P. O'Leary, "Some algorithms for approximating convolutions," *Computer Vision, Graphics, and Image Processing* 41 (1988) 333-345.

[J45] James G. Nagy and Dianne P. O'Leary, "Restoring Images Degraded by Spatially-Variant Blur," *SIAM Journal on Scientific Computing,* 19 (1998), 1063-1082.

[J61] James G. Nagy and Dianne P. O'Leary, "Image Restoration through Subimages and Confidence Images," *Electronic Transactions on Numerical Analysis*, 13 (2002) 22-37.

[J63] Armin Pruessner and Dianne P. O'Leary, "Blind Deconvolution Using a Regularized Structured Total Least Norm Approach," *SIAM J. on Matrix Analysis and Applications*, 24 (2003) 1018-1037.

[J66] David E. Gilsinn, Geraldine S. Cheok, and Dianne P. O'Leary, "Reconstructing Images of Bar Codes for Construction Site Object Recognition," *Automation in Construction* (Elsevier), 13 (2004) 21-35.

[J67] Nicola Mastronardi, Phillip Lemmerling, Anoop Kalsi, Dianne O'Leary, and Sabine Van Huffel, "Regularized structured total least squares algorithms for blind image deblurring," *Linear Algebra and Its Applications,* 391 (2004) 203-221

[J74] Anoop Kalsi and Dianne P. O'Leary, "Algorithms for Structured Total Least Squares Problems with Applications to Blind Image Deblurring," *Journal of Research of the National Institute of Standards and Technology*, 111, No. 2 (2006) pp. 113-119.

4 Parallel Algorithms

G.W. Stewart and I proposed the use of the data-flow model for developing fine- and medium-grained algorithms for dense matrix problems on message-passing parallel machines; the computational model and several sample algorithms were developed [J19], and a detailed analysis of a parallel Cholesky algorithm was given [J22]. A similar analysis was given for the block conjugate gradient algorithm [J24].

Some "coloring algorithms" were developed which make parallel iterative methods more efficient for certain network problems, including discretizations of elliptic differential equations [J18]. A different class of parallel iterative methods was developed in joint work with R.E. White, which proposed and analyzed the simultaneous use of several matrix splittings [J20]. These *multisplitting algorithms* have since been the subject of considerable work by other researchers and formed the basis for the preconditioning algorithms used in [C7] [J36].

[C7] Chiou-Ming Huang and Dianne P. O'Leary, "Preconditioning Parallel Multisplittings for Solving Linear Systems of Equations," International Conference on Supercomputing (Washington, DC, July 1992) ACM Press, New York, 1992, 478-484.

[J18] Dianne P. O'Leary, "Ordering schemes for parallel processing of certain mesh problems," *SIAM Journal on Scientific and Statistical Computing* 5 (1984) 620-632.

[J19] Dianne P. O'Leary and G. W. Stewart, "Data-flow algorithms for parallel matrix computations," *Communications of the ACM* 28 (1985) 840-853.

[J20] Dianne P. O'Leary and R. E. White, "Multi-splittings of matrices and parallel solution of linear systems," *SIAM Journal on Algebraic and Discrete Methods* 6 (1985) 630-640.

[J22] Dianne P. O'Leary and G. W. Stewart, "Assignment and scheduling in parallel matrix factorization," *Linear Algebra and Its Applications* 77 (1986) 275-300.

[J24] Dianne P. O'Leary, "Parallel implementation of the block conjugate gradient algorithm," *Parallel Computing* 5 (1987) 127-139.

[J36] Chiou-Ming Huang and Dianne P. O'Leary, "A Krylov multisplitting algorithm for solving linear systems of equati ons," *Linear Algebra and Its Applications*, 194 (1993) 9-29.

5 Parallel Architectures and Systems

In the course of collaborative experimental work on parallel algorithms in the early 1980's, deficiencies of existing software systems led to the development of a multi-tasking and portable communication system [C4] and to the proof that its underlying principle led to deterministic computation [J26]. The deficiencies of hardware systems spurred the development of some specialized systolic arrays for matrix data movement [J23] and the design of a hybrid machine, capable of shared-memory interaction for neighboring processors and efficient message passing for more distant processors [T8].

[C4] Dianne P. O'Leary, G.W. Stewart and Robert van de Geijn, "Domino: A Transportable System for Parallel Processing," in *Parallel Processing and Medium-Scale Multiprocessors* (Proceedings of a 1986 Conference), Arthur Wouk (Ed.), SIAM Press, Philadelphia (1989) 25-34.

[J23] Dianne P. O'Leary, "Systolic arrays for matrix transpose and other reorderings," *IEEE Transactions on Computers* C-36 (1987) 117-122.

[J26] Dianne P. O'Leary and G. W. Stewart, "From determinacy to systaltic arrays," *IEEE Transactions on Computers* C-36 (1987) 1355-1359.

[T8] Dianne P. O'Leary, Roger Pierson, G. W. Stewart, and Mark Weiser, "The Maryland Crab: A module for building parallel computers," Computer Science Department Report CS-1660, Institute for Advanced Computer Studies Report UMIACS-86-9, University of Maryland, April, 1986.

6 Krylov Sequence Methods for Linear Systems and Optimization

In my thesis and in subsequent work, the effectiveness of the preconditioned conjugate gradient algorithm was demonstrated for discretizations of linear elliptic partial differential equations [C1], nonlinear elliptic equations [J1], and free boundary problems for linear and nonlinear elliptic equations [J8]

[J3]. Application of the conjugate gradient algorithm to general quadratic programming problems was considered [T4]. This work was applied to the analysis of torsion on an elasto-plastic bar [J2] and water flow in an excavation site [C2].

Polynomial preconditioners for the conjugate gradient algorithm were studied in [J33].

A block form of the conjugate gradient algorithm, useful for solving multiple linear systems and for linear systems with specialized eigenvalue distributions, was developed and analyzed [J6]. The parallel implementation of the algorithm was studied [C3] [J24] [J32].

The quasi-Newton family of algorithm was extended to block form in [J39], and new insights on Broyden's method applied to linear systems were developed [J41]. Efficient use of conjugate gradient algorithms for computing the search directions in interior point methods was studied in [J55].

A literature review of the first 25 years of the conjugate gradient algorithm was published in 1989, jointly with Gene Golub [J28] and a more recent overview is given in [C17].

Stagnation of the GMRES algorithm for solving nonsymmetric systems of equations was studied in [J64].

We reviewed the modified Newton methods based on the Cholesky factorization in [T23], determining the properties of existing methods and deriving new methods that perform better.

Zdeněk Strakoš, Petr Tichý, and I have recently contributed to the understanding of the convergence of Krylov methods when implemented on computers in inexact arithmetic [T24], by exploiting the relation of these methods to Gauss quadrature.

[C1] (Invited paper) Paul Concus, Gene H. Golub, and Dianne P. O'Leary, "A generalized conjugate gradient method for the numerical solution of elliptic partial differential equations,"
in *Sparse Matrix Computations*, James R. Bunch and Donald J. Rose (Eds.) Academic Press, New York (1976) 309-332.
reprinted in *Studies in Numerical Analysis*, Gene H. Golub (Ed.), Vol-

ume 25 of Studies in Mathematics, The Mathematical Association of America (1984) 178-198.

[C2] Dianne P. O'Leary, "Linear programming problems arising from partial differential equations," in *Sparse Matrix Proceedings 1978*, Iain S. Duff and G. W. Stewart (Eds.) SIAM Press, Philadelphia (1979) 25-40.

[C3] (invited, extended abstract) Dianne P. O'Leary, "Fine and Medium Grained Parallel Algorithms for Matrix QR Factorization," *Algorithms and Applications on Vector and Parallel Computers*, H.J.J. te Riele, Th.J. Dekker and H.A. van der Vorst, eds., Elsevier Science Publishers B.V. (North Holland), (1987) 347-349.

[C17] Dianne P. O'Leary, "Conjugate Gradients and Related KMP Algorithms: The Beginnings," in *Linear and Nonlinear Conjugate Gradient-Related Methods,* Loyce Adams and J. L. Nazareth, eds., SIAM, Philadelphia, 1996, 1-8.

[J1] Paul Concus, Gene H. Golub, and Dianne P. O'Leary, "Numerical solution of nonlinear elliptic partial differential equations by a generalized conjugate gradient method," *Computing* 19 (1978) 321-339.

[J2] Dianne P. O'Leary and Wei H. Yang, "Elasto-plastic torsion by quadratic programming," *Computer Methods in Applied Mechanics and Engineering* 16 (1978) 361-368.

[J3] Dianne P. O'Leary, "Conjugate gradient algorithms in the solution of optimization problems for nonlinear elliptic partial differential equations," *Computing* 22 (1979) 59-77.

[J6] Dianne P. O'Leary, "The block conjugate gradient algorithm and related methods," *Linear Algebra and Its Applications* 29 (1980) 293-322.

[J8] Dianne P. O'Leary, "A generalized conjugate gradient algorithm for solving a class of quadratic programming problems," *Linear Algebra and Its Applications* Special Issue on Large Scale Matrix Problems 34 (1980) 371-399. Also in *Large Scale Matrix Problems*, A. Bjorck, R. J. Plemmons and H. Schneider, eds. North Holland Pub. Co. NY (1981) 391-399.

[**J24**] Dianne P. O'Leary, "Parallel implementation of the block conjugate gradient algorithm," *Parallel Computing* 5 (1987) 127-139.

[**J28**] Gene H. Golub and Dianne P. O'Leary, "Some history of the conjugate gradient and Lanczos algorithms: 1948-1976," *SIAM Review* 31 (1989) 50-102.

[**J32**] Dianne P. O'Leary and Peter Whitman, "Parallel QR factorization by Householder and modified Gram-Schmidt algorithms," *Parallel Computing* 16 (1990) 99-112.

[**J33**] Dianne P. O'Leary, "Yet another polynomial preconditioner for the conjugate gradient algorithm," *Linear Algebra and Its Applications,* 154 (1991) 377-388.

[**J39**] Dianne P. O'Leary and A. Yeremin, "The linear algebra of block quasi-Newton algorithms," *Linear Algebra and Its Applications*, 212/213 (1994) 153-168.

[**J41**] Dianne P. O'Leary, "Why Broyden's nonsymmetric method terminates on linear equations," *SIAM Journal on Optimization*, 5 (1995) 231-235.

[**T4**] Dianne P. O'Leary, "Sparse quadratic programming without matrix updating," Computer Science Department Report TR-1200, University of Maryland (1982).

[**J55**] Weichung Wang and Dianne P. O'Leary, "Adaptive Use of Iterative Methods in Predictor-Corrector Interior Point Methods for Linear Programming," *Numerical Algorithms*, (special issue honoring Richard Varga), 25 (2000) 387-406.

[**J64**] Ilya Zavorin, Dianne P. O'Leary, and Howard Elman, "Complete Stagnation of GMRES," *Linear Algebra and Its Applications,* 367 (2003) 165-183.

[**T23**] Daniel M. Dunlavy, Dianne P. O'Leary, John M. Conroy, and Judith D. Schlesinger, "QCS: A System for Querying, Clustering, and Summarizing Documents," SANDIA Technical Report, July 2006.

[**T24**] Dianne P. O'Leary, Zdeněk Strakoš, Petr Tichý, On Sensitivity of Gauss-Christoffel Quadrature, preprint, 2006.

7 Signal Processing and Control

Collaborators in aeronautical engineering were interested in the numerical solution of a constrained Sylvester equation, with applications in control theory, and we developed an efficient algorithm [C5] [C6] [C8] [J34] [J35].

An efficient variant of the ESPRIT algorithm for determining direction of arrival of signals reaching an array of sensors was developed [C11] [J40].

[**C5**] M. Monahemi, J. Barlow, and Dianne P. O'Leary, "The Design of Reduced Order Luenberger Observers with Precise LTR," *Proceedings of the AIAA Meeting on Guidance, Navigation and Control* New Orleans, August 1991, AIAA-91-2731.

[**C6**] M. Monahemi, J. Barlow, and Dianne P. O'Leary, "Considerations on Loop Transfer Recovery for Non-minimum Phase Plants," *Proceedings of the AIAA Aircraft Design Systems and Operations Meeting*, Baltimore, September 1991, AIAA-91-3086.

[**C8**] M. Monahemi, J. Barlow and Dianne P. O'Leary, "On the Precise Loop Transfer Recovery and Transmission Zeroes," First IEEE Conference on Control Applications, Dayton, Ohio, September 1992.

[**C11**] K.J.R. Liu, Dianne P. O'Leary, G.W. Stewart, and Yuan-Jye J. Wu, "An Adaptive ESPRIT Based on URV Decomposition," International Conference on Acoustics, Speech, and Signal Processing (ICASSP-93), Vol. IV, 37-40.

[**J34**] Jewel B. Barlow, Moghen M. Monahemi, and Dianne P. O'Leary, "Constrained matrix Sylvester equations," *SIAM Journal on Matrix Analysis and Applications,* 13 (1992) 1-9.

[**J35**] Moghen M. Monahemi, Jewel B. Barlow and Dianne P. O'Leary, "The design of reduced order observers with precise loop transfer recovery," *AIAA Journal of Guidance, Control, and Dynamics* 15 (1992) 1320-1326

[**J40**] K. J. Ray Liu, Dianne P. O'Leary, G. W. Stewart, and Yuan-Jye J. Wu, "URV ESPRIT for tracking time-varying signals," *IEEE Transactions on Signal Processing*, 42 (1994) 3441-3448.

8 Robust Regression

The development of computational algorithms for iteratively reweighted least square problems [J30] led to an interesting problem concerning the uniform boundedness of scaled projectors [J29].

[J29] Dianne P. O'Leary, "On bounds for scaled projections and pseudoinverses," *Linear Algebra and Its Applications* 132 (1990) 115-117.

[J30] Dianne P. O'Leary, "Robust regression computation using iteratively reweighted least squares," *SIAM Journal of Matrix Analysis and Applications* 11 (1990) 466-480.

9 Optimization

Optimization problems arising from partial differential equations can lead to linear programming [C2], quadratic programming [J2], [J8], or more general optimization problem [J3].

I developed the discrete Newton method [J12], today called the truncated Newton method, for use when derivatives are not easy to calculate.

Other work concerned understanding quasi-Newton methods [J41] and making them more efficient [J47].

[J54] is a survey of the impact of numerical linear algebra on optimization.

Efficient adaptive use of conjugate gradient algorithms for computing the search directions in interior point methods was studied in [J55].

In [T25], Haw-ren Fang and I reviewed modified Newton methods based on the Cholesky factorization [T25], determining the properties of existing methods and deriving new methods that perform better.

Jin Hyuk Jung and I proposed efficient algorithms for solving linear programming problems on inexpensive parallel computers [C37], GPUs.

Simon Schurr, Andre' Tits, and I have posed two problems related to conic convex optimization. First [J75] we studied conditions under which such problems are well posed, in the sense that solutions can be constructed for arbitrary specifications of the data values. Second (in forthcoming work), we studied the accuracy necessary to evaluate the functions in order to preserve polynomial complexity in the solution algorithms.

[**J54**] Dianne P. O'Leary, "Symbiosis between Linear Algebra and Optimization," invited paper, *J. of Computational and Applied Math.* 123 (2000) 447-465; reprinted in a book *Numerical Analysis 2000*.

[**C2**] Dianne P. O'Leary, "Linear programming problems arising from partial differential equations," in *Sparse Matrix Proceedings 1978*, Iain S. Duff and G. W. Stewart (Eds.) SIAM Press, Philadelphia (1979) 25-40.

[**J2**] Dianne P. O'Leary and Wei H. Yang, "Elasto-plastic torsion by quadratic programming," *Computer Methods in Applied Mechanics and Engineering* 16 (1978) 361-368.

[**J3**] Dianne P. O'Leary, "Conjugate gradient algorithms in the solution of optimization problems for nonlinear elliptic partial differential equations," *Computing* 22 (1979) 59-77.

[**J8**] Dianne P. O'Leary, "A generalized conjugate gradient algorithm for solving a class of quadratic programming problems," *Linear Algebra and Its Applications* Special Issue on Large Scale Matrix Problems 34 (1980) 371-399. Also in *Large Scale Matrix Problems*, A. Bjorck, R. J. Plemmons and H. Schneider, eds. North Holland Pub. Co. NY (1981) 391-399.

[**J12**] Dianne P. O'Leary, "A discrete Newton algorithm for minimizing a function of many variables," *Mathematical Programming* 23 (1982) 20-33.

[**J41**] Dianne P. O'Leary, "Why Broyden's nonsymmetric method terminates on linear equations," *SIAM Journal on Optimization*, 5 (1995) 231-235.

[**J47**] Tamara Kolda, Dianne P. O'Leary, and Larry Nazareth, "BFGS with Update Skipping and Varying Memory," *SIAM Journal on Optimization,* 8 (1998) 1060-1083. `http://epubs.siam.org/sam-bin/dbq/article/30645`

[J55] Weichung Wang and Dianne P. O'Leary, "Adaptive Use of Iterative Methods in Predictor-Corrector Interior Point Methods for Linear Programming," *Numerical Algorithms*, (special issue honoring Richard Varga), 25 (2000) 387-406.

[J75] Simon P. Schurr, Andre' L. Tits, and Dianne P. O'Leary, "Universal Duality in Conic Convex Optimization," *Mathematical Programming A*, (2006) DOI: 10.1007/s10107-005-0690-4 http://dx.doi.org/10.1007/s10107-005-0690-4

[T25] Haw-ren Fang* and Dianne P. O'Leary, "Modified Cholesky Algorithms: A Catalog with New Approaches," CS-TR-4807, University of Maryland, August 2006.

[C37] Jin Hyuk Jung* and Dianne P. O'Leary, "Cholesky Decomposition and Linear Programming on a GPU," Workshop on Edge Computing Using New Commodity Architectures (EDGE), Chapel Hill, North Carolina. (May 2006)

[T26] Nicola Mastronardi and Dianne P. O'Leary, "Robust Regression and ℓ_1 Approximations for Toeplitz Problems," preprint, 2006.

10 Information Retrieval

The semi-discrete decomposition, developed with Shmuel Peleg for image compression, has proved quite useful in latent semantic indexing, a method of document retrieval [C20] [J48].

Methods for document summarization based on hidden Markov models and matrix decompositions are studied in [J62]. We demonstrated the success of the methods for summarizing medical documents in [C31]. Our methods have been quite successful in the DUC (Document Understanding Conference) and TREC competitions [C25],[C26],[C27],[C30],[C32],[C33], and recently they performed as well as human summarizers in an evaluation on summarizing multi-lingual document sets [C34]; this shows that our summarizer is quite good, but also that the evaluation metrics are quite primitive!

A full retrieval system that processes a query, clusters the resulting documents, and creates summaries of each cluster is presented in [T22] and available at http://stiefel.cs.umd.edu:8080/qcs/

[**J48**] Tamara G. Kolda and Dianne P. O'Leary, "A Semi-Discrete Matrix Decomposition for Latent Semantic Indexing in Information Retrieval," *ACM Transactions on Information Systems*, 16 (1998) 322-346.

[**J62**] Judith D. Schlesinger, John M. Conroy, Mary Ellen Okurowski, and Dianne P. O'Leary, "Machine and Human Performance for Single- and Multi-Document Summarization," IEEE Intelligent Systems (special issue on Natural Language Processing) 18(1), 2003, 46-54.

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[**C25**] J. M. Conroy, J. D. Schlesinger, D. P. O'Leary, and M. E. Okurowski, "Using HMM and Logistic Regression to Generate Extract Summaries for DUC," *DUC 01 Conference Proceedings*, 2001.

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11 Eigenproblems and Matrix Studies

A discussion during an informal seminar led to a proposal for a quick estimation of the largest eigenvalue of a matrix [J5]. A minor improvement on condition number estimation was given in [J7]. The accurate computation of eigenvalues of arrowhead matrices was considered in [J31]. Pete Stewart and I also studied the use of a modified Rayleigh quotient iteration for finding eigenvalues [J49].

Matrix scaling was studied in [J65], and factorizations of symmetric tridiagonal and triadic matrices were studied in [J78], for later use in modified Newton methods for optimization.

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12 Quantum Computing

Quantum computers may offer a way to solve certain problems that are larger and more complex than any that can be solved on conventional computers. One way to view a quantum computer is as a machine that multiplies a vector by a unitary matrix. The number of possible data values equals the dimension of the vector, and the absolute value of the ith component of the vector represents the probability that the data or the answer is equal to the ith value. The unitary matrix is designed to make the absolute value of the entry corresponding to the correct answer quite close to one.

Stephen Bullock, Gavin Brennen, and I investigated several questions relevant to the decomposition of the unitary matrix into quantum "gates" that can actually be implemented in hardware. In [J69], we used a matrix decomposition to construct these gates. In [J70], [J71] and [J76], we used controlled Householder gates to implement circuits for qudits, quantum variables that can take on $d > 2$ values rather than the traditional 2 values used for qubits.

Some Givens and Householder gates are cheaper than others, depending on the components they access, and we determined a systematic way to determine whether a set of rotation planes is sufficient in [J72]. Then we considered how much such quantum operations might be sped up [J79], for example by using more than one pair of lasers to excite multiple transitions among the hyperfine states of the atomic alkalies.

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[**J76**] Gavin K. Brennen, Stephen S. Bullock, and Dianne P. O'Leary, "Efficient Circuits for Exact-Universal Computation with Qudits," *Quantum Information and Computation*, 6 (2006), 436-454.

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13 Problems from Computational Physics

Helmholtz equations are used to model a variety of important physical systems, ranging from heat distribution to the transmission of sound. Olof Widlund and I developed efficient algorithms for solving the Helmholtz equation on general three dimensional regions with Dirichlet or Neumann boundary conditions, imbedding the region in a cube. Innovations involved the proof of existence of the discrete solution, development of effective scaling strategies, and the choice of effective storage structures [J4] [J10]. Efficient variants of these algorithms for problems with mixed boundary conditions over a union of rectangles were later developed [J25], with application to a National Bureau of Standards (now National Institute of Standards and Technology) model of smoke transport in buildings.

More recently, Howard Elman, Oliver Ernst, and I have considered the difficulties encountered when the Helmholtz parameter is negative, leading to indefinite systems of linear equations. Results are presented in [J46] [J52] [J60]. These problems arise in studying wave phenomena, for example, transmission of sound underwater. In collaboration with post-doc Michael Stewart, we extended our study to problems in which the boundary conditions are stochastic [J68].

A method for solving an important physics problem, approximating the number of monomer-dimer coverings in periodic lattices, was given in [J58]. This model has a variety of uses in solid state physics, ranging from studying spontaneous magnetization to phase transitions in multicomponent liquids and biological membranes.

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[J10] Dianne P. O'Leary and Olof Widlund, "Algorithm 572: Solution of the Helmholtz equation for the Dirichlet problem on general bounded three dimensional regions," *ACM Transactions on Mathematical Software* 7 (1981) 239-246.

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14 Medical, Biological, and Physics Applications

In addition to work in medical informatics, I have worked on medical image processing. Numerical methods for classifying cytology specimens (e.g., pap smears) were compared in [J9]. In collaboration with medical researchers, methods for identifying chromosomes were developed in [J53] and [C28].

The structure of a protein provides critical information in determining its function. A new algorithm for determining the 3-dimensional configuration of proteins was described in [J73], and its use was demonstrated on a backbone model of proteins. In [J77] we proposed a fast screening algorithm for finding proteins whose structure is expected to be similar to one presented for classification.

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O'Leary, and Tamara G. Kolda, "Hidden Markov Models for Chromosome Identification," Proceedings of the 14th IEEE Symposium on Computer-Based Medical Systems (CBMS'01), 2001.

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15 Software

My publicly available software includes an algorithm for solving the Helmholtz equation for the Dirichlet problem on general bounded three dimensional regions [J10], an algorithm to compute the Semidiscrete Matrix Decomposition [J56], and a system for processing queries (as, for example, Google might), cluster the potentially relevant documents, and return a summary of each cluster [T22].

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16 Current work

Current funding from NSF and DOE supports work on ill-posed problems, quantum computing, computational linear algebra, nonlinear programming, and protein folding

As always, research directions are determined by a mixture of planning and serendipity, with motivation from applications problems as well as open questions in applied mathematics and numerical analysis.