Math 411 Preliminaries

Objective
- Provide a list of preliminary vocabulary and concepts

Preliminary Vocabulary
Basic Netwon's method, Taylor series expansion (for single and multiple variables), Eigenvalue, Eigenvector, Vector norms, 2-norm, infinite norm, Matrix norms, Condition number, Gauss Elimination

Preliminary Concepts
- Use of Absolute error and Relative error and their relation to number of significant digits
- Solution of linear system of equations via Gauss elimination
- Stopping criteria in iterations
- Rounding error and truncation error
- Floating point system
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***Extra*:**
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Correction to Misconceptions

Floating Point System

Objective
- Understand and handle error from floating point calculation
- Role of stability in numerical calculation

Vocabulary
Base, Sign bit, Exponent, Mantissa, underflow, overflow, rounding, chopping, roundoff error, absolute error, relative error, significant digits, truncation error, machine epsilon.

Concepts
- Distribution of floating point numbers
- Addition of floating point numbers
- Loss of associativity and distributivity
- Catastrophic cancellation
- Prevention of catastrophic cancellation
- Forward error analysis
- Backward error analysis

***Extra*:**
- IEEE standard

Some External Links:

Basic Issues in Floating Point Arithmetic and Error Analysis, Supplementary Lecture Notes of J. Demmel on Floating Point System, University of California at Berkeley, September 1995. (local copy)

Miscalculating Area and Angles of a Needle-like Triangle, Notes of W. Kahan on common misconceptions of floating point calculations, University of California at Berkeley, September 1997. (local copy)

IEEE Floating Point Arithmetic, More advanced Lecture Notes of W. Kahan on the Status of *IEEE Standard 754 for Binary Floating-Point Arithmetic*, University of California at Berkeley, September 1995. (local copy)

Goldberg, David, What every computer scientist should know about floating-point arithmetic,
ACM Computing Surveys, Vol.23, No. 1 (March 1991), pp. 5-48 (Electronic version not available.)

Correction to Misconceptions

Newton's method for several variables vector functions

- Newton's method derivations
- strength and weaknesses of the method
- interpretation of quadratic convergence

Vocabulary
Local convergence, Quadratic rate of convergence, Function Iteration, Jacobian matrix

Concepts
- Newton's method derivations via
  - Generalization of Newton's method for single variable functions
  - Taylor series
- Quadratic rate of convergence and number of significant digits
- "Derivative" appears as a matrix
  - Requires solution of a "totally new" linear system at *each* iteration step
- Non-convergence and slow convergence of Newton's method:
  - Jacobian matrix may become singular
  - Oscillation similar to one dimensional case
  - Flat surface
  - Multiple root

Method properties:

Strength	*Weaknesses*
Derivation of method may be obtained from Taylor series	Determination of starting guess may not be trivial
Local convergence when approximation is close to root	Convergence or rate of convergence is not guaranteed when not close to the root
Quadratic rate of convergence when approximation is close to root	Method may not converge or may converge very slowly
Reasonably easy to implement if Jacobian matrix can be symbolically calculated	Method requires evaluation of the Jacobian matrix as well as solution of a linear system at ***each*** iteration
	Stopping criteria choice not obvious
May be used to find complex roots	Requires initial guess to be complex in order to find a complex root

***Extra*:**
- Can still view Newton's method as a fixed point iteration
  - Quadratic convergence follows from general theory of fixed point iteration
- Theory for system of non-linear equations is still incomplete
- In implementation, some approximates Jacobian matrix via finite differencing (naïve) or "automatic differencing" (sophisticated)

Correction to Misconceptions

Fixed point iteration in higher dimension

Objective
- Contraction mapping and Function iteration method
- Seidel's method to speed convergence

Vocabulary
Functional iteration, Seidel method

Concepts
- Brouwer fixed point theorem (Review)
- Uniqueness of fixed point and derivative bounds
- Functional iteration and contraction mapping
- Use of Seidel's method to accelerate convergence
- Theoretical and Computable (though often pessimistic) error bounds
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***Extra*:**
- Choice of initial guess not obvious
- Often used as a brute force approach or method of last resort even if derivative bounds are not satisfied
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Correction to Misconceptions

Quasi-Newton method- Broyden's method

Objective

- Broyden's method as an efficient way to apply concept from Newton's method
- Efficient computation of inverse of a matrix with a rank-1 update

Vocabulary

Rank 1 update, Sherman-Morrison formula

Concepts

- Entries in Jacobian matrix may be approximated by finite differences
- Deteriotion of rate of convergence from quadratic to superlinear
- Initial computation of inverse requires $O(n^3)$ operations using Gauss Elimination
- Sherman-Morrison implies subsequent calculation requires $O(n^2)$ operations
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***Extra*:**

- Hessian

Correction to Misconceptions

- Broyden's method is implemented by explicitly calculating the inverse using Sherman Morrison formula. Gauss elimination is used only for constructing the inverse of the initial (exact or approximate) Jacobian matrix.
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Steepest Descent method

Objective

- General solution of nonlinear equations
- Special case of solution of linear equations with a symmetric matrix

Vocabulary

Steepest descent direction, Quadratic form, Line search, Quadratic Interpolation

Concepts

- Conversion of nonlinear system of equations to minimization problem
- Use of gradient direction as steepest descent direction
- Slow rate of convergence near minimum point
- Use of steepest descent method to generate initial guess for Newton or quasi-Newton method
- For quadratic forms, performance deteriorates as condition number increases
- Line search has exact value for quadratic form
- Line search for general nonlinear problems is approximated by a quadratic minimization problem

***Extra*:**

- Conjugate direction methods

Correction to Misconceptions

- Even if the original set of nonlinear equations do not admit a solution, a solution to the minimization problem can always be found using the steepest descent method.
- A theoretically optimal method (such as steepest descent method) is not necessarily the best numerical method

Conjugate Gradient method

Objective

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Vocabulary
Conjugate direction, A-conjugate,

Concepts

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- (Theoretical) Finite termination
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***Extra*:**

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Some External Links:

Jonathan R. Shewchuk, *An Introduction to the Conjugate Gradient Method Without the Agonizing Pain*: http://www.cs.cmu.edu/~jrs/jrspapers.html#cg

Correction to Misconceptions

Eigenvalue Problems

Objective
- Application giving rise to eigenvalue problems
- Properties of eigenvalues/ eigenvectors

Vocabulary
Eigenvalue Problem, Shift, Similarity transform

Concepts
- Eigenvalues of diagonal and triangular matrices
- Eigenvalues of inverse matrix
- Gauss elimination does not preserve eigenvalues
- Similarity transformation preserves eigenvalues
- Change to eigenvalues through shifting, scalar product, matrix product
- Determinant as product of eigenvalues
- Gerschgorin theorem- location of eigenvalues
- Eigenvalues of real symmetric matrices are real

***Extra*:**
- Positive definite matrices

Correction to Misconceptions

Power method

Objective

- Power method, Rayleigh quotient and inverse iteration
- Wielandt deflation

Vocabulary

Infinite norm, 2-norm and inner product, deflation

Concepts

- Convergence of power method relies on existence of a dominant eigenvalue
- Normalization is needed within iteration to keep the entries of the eigenvector meaningful
- Eigenvector is obtained along with the eigenvalue
- Rayleigh quotient (for symmteric matrices) converges at twice the rate as regular power method
- LU factorization on A may be performed prior to applying the inverse power method or inverse iteration in order to speed up the calculation
- If the matrix is tridiagonal, each inverse iteration step is only O(n).
- Existence of multiple dominant eigenvalues of the same magnitude lead to either slow convergence or oscillation in the numerical result
- A matrix with the same set of eigenvalues as A, except the dominant eigenvalue is zeroed out, may be constructed using Wielandt deflation

Power method	x(new) = c A x(old)	Largest (in mag.) eigenvalue
Inverse power method	A x(new) = c x(old)	Smallest (in mag.) eigenvalue
Shifted power method	x(new) = c (A-s I) x(old)	Eigenvalue farthest from shift s
Inverse iteration	(A-s I) x(new) = c x(old)	Eigenvalue closest to shift s

Here c denote a normalizing factor

***Extra*:**

- G. Peters and J.H. Wilkinson, *Inverse Iteration, Ill-Conditioned Equations and Newton's Method*, SIAM Review 21. No. 1 (1979), 339-360.   (accessible through JSTOR)
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Some External Links:

Correction to Misconceptions

- Even if the initial random vector does not have a component in the dominant direction, the presence of rounding error will eventually reintroduce a component in the dominant direction, and thus ensuring the success of the power method.
- If the shift s is close to an eigenvalue, the matrix A-sI is near singular and some care must be taken in the inverse iteration. However, even with poor conditioning, the inverse iteration performs well.

Householder Transformation

Objective

- Householder transformation to upper Hessenberg form
- QR factorization

Vocabulary

Orthogonal matrix, Upper Hessenberg form, QR factorization, catastrophic cancellation

Concepts

- Orthogonal matrices have nice stability property: $||Qx|| = ||x||$ in 2-norm, thus condition number is 1
- Product of orthogonal matrices is orthogonal
- Each Householder matrix is constructed from the column vector that it needs to zero out
- Householder transformation is symmetric and orthogonal
- Pre- and post multiplication by a Householder transformation is a similarity transformation
- Construction of Householder transformations for a matrix
- The first component of the vector in the Householder transformation should be constructed with a sign chosen to avoid catastrophic cancellation
- QR factorization is closely related to Gram-Schmidt orthogonalization
- A symmetric matrix in upper Hessengberg form is tridiagonal
- In QR factorization, the matrix Q is the transpose of product of Householder transformations

***Extra*:**

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Correction to Misconceptions

- It is usually not necessary to compute the Householder transformation matrix explicitly, instead, use the normalized vector u or the unnormalized vector x associated with the Householder transformation.
- In QR factorization, the upper triangular matrix R obtained by premultiplication of Householder transformations does not possess the same set of eigenvalues as the original matrix.
- The QR factorization is not unique: by appropiately changing the signs of the entries in the matrices we can get many “different” factorizations
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QR algorithm

Objective

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Vocabulary

Rotation matrix,

Concepts

- Real symmetric matrices have real eigenvalues
- QR algorithm produces similarity transforms even though QR factorization does not preserve eigenvalues
- QR algorithm applied to a matrix with real eigenvalues gives a diagonal matrix in the limit.
- QR algorithm is usually performed after a matrix is converted to an upper Hessenberg form
- Jacobi rotation matrix is orthogonal but usually non-symmetric
- The QR factorization process may be performed using Jacobi rotation (or fast Given's method)
- Construction of rotation matrices
- QR algorithm is closely related to the power method and hence shift may be employed to enhance performance- often convergence rate is cubic
- Choice of shifts

***Extra*:**

Some External Links:

A discussion of the QR algorithm implementation in matlab:
http://www.mathworks.com/publications/newsletter/pdf/sum95cleve.pdf

Correction to Misconceptions