Gram-Schmidt Orthogonalization: 100 Years and More

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Outline of Paper

- Early History
- CGS and MGS and QR
- Elimination Methods and MGS
- Reorthogonalization
- Rank Revealing factorizations
- Gram-Schmidt in Iterative Methods
- Implementing Gram-Schmidt Algorithms

Outline of Talk

- Early History (1795–1907)
- Middle History
  1. The work of Åke Björck
     Least squares, Stability, Loss of orthogonality
  2. The work of Heinz Rutishauser
     Selective reorthogonalization and
     Superorthogonalization

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Early History

- Least Squares - Gauss and Legendre
- Laplace 1812, Analytic Theory of Probabilities (1814, 1820)
- Cauchy 1837, 1847 (Interpolation) and Bienaymé 1853
- J. P. Gram, 1879(Danish), 1883(German)
- Erhard Schmidt 1907

Gauss and least squares

- Priority dispute:
  A. M. Legendre -first publication 1805;

  Gauss claimed discovery in 1795
- G. Piazzi, January 1801 discovered asteroid Ceres. Tracked it for 6 weeks.

The Gauss derivation of the normal equations

Let $\hat{x}$ be the solution $A^T Ax = A^T b$.
For any x we have

$$r = (b - A\hat{x}) + A(\hat{x} - x) \equiv \hat{r} + Ae,$$

and since $A^T \hat{r} = A^T b - A^T A\hat{x} = 0$

$$r^T r = (\hat{r} + Ae)^T (\hat{r} + Ae) = \hat{r}^T \hat{r} + (Ae)^T (Ae).$$

Hence $r^T r$ is minimized when $x = \hat{x}$.

Pierre-Simon Laplace (1749–1827)

- Mathematical Astronomy
- Celestial Mechanics
- Laplace's Equation
- Laplace Transforms
- Probability Theory and Least Squares

Théorie Analytique des Probabilités - Laplace 1812

- Problem: Compute masses of Saturn and Jupiter from systems of normal equations (Bouvart) and to compute the distribution of error in the solutions.
- Method: Laplace successively projects the system of equations orthogonally to a column of the observation matrix to eliminate all variables but the one of interest.
- Basically Laplace uses MGS to prove that, given an overdetermined system with a normal perturbation on the right-hand side, its solution has a centered normal distribution with variance independent from the parameters of the noise.

Laplace 1812 - Linear Algebra

- Laplace uses MGS to derive the Cholesky form of the normal equations, $R^T R\mathbf{x} = A^T\mathbf{x}$
- Laplace does not seem to realize that the vectors generated are mutually orthogonal.
- He does observe that the generated vectors are each orthogonal to the residual vector.

Cauchy and Bienaymé

Figure: A. Cauchy

Figure: I. J. Bienaymé

Cauchy and Bienaymé

- Cauchy (1837) and (1847)- interpolation method leading to systems of the form $Z^T A\mathbf{x} = Z^T\mathbf{b}$, where $Z = (\mathbf{z}_1, \dots, \mathbf{z}_n)$ and $z_{ij} = \pm 1$.
- Bienaymé (1853) new derivation of Cauchy's algorithm based on Gaussian elimination.
- Bienaymé noted that the Cauchy's choice of Z was not optimal in the least squares sense. Least squares solution if $Z = A$ (normal equations) or more generally if $R(Z) = R(A)$. The matrix Z can be determined a column at a time as the elimination steps are carried out.

3×3 example

$$\begin{pmatrix} z_1^T a_1 & z_1^T a_2 & z_1^T a_3 \\ z_2^T a_1 & z_2^T a_2 & z_2^T a_3 \\ z_3^T a_1 & z_3^T a_2 & z_3^T a_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} z_1^T b \\ z_2^T b \\ z_3^T b \end{pmatrix}$$

Transform i, jth element $(2 \le i, j \le 3)$

$$z_i^T a_j - \frac{z_i^T a_1}{z_1^T a_1} z_1^T a_j = z_i^T \left(a_j - \frac{z_1^T a_j}{z_1^T a_1} a_1 \right) \equiv z_i^T a_j^{(2)},$$

Bienaymé Reduction

The reduced system has the form

$$\begin{pmatrix} z_2^T a_2^{(2)} & z_2^T a_3^{(2)} \\ z_3^T a_2^{(2)} & z_3^T a_3^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} z_2^T b^{(2)} \\ z_3^T b^{(2)} \end{pmatrix}$$

where we have defined

$$a_j^{(2)} = a_j - \frac{z_1^T a_j}{z_1^T a_1} a_1, \qquad b^{(2)} = b - \frac{z_1^T b}{z_1^T b} a_1.$$

Finally z_3 is chosen and used to form the single equation

$$z_3^T a_3^{(3)} x_3 = z_3^T b^{(3)}.$$

Taking the first equation from each step gives a triangular system defining the solution.

An interesting choice of Z

Since we want $R(Z) = R(A)$, if we choose $Z = Q$ where

$$q_1 = a_1, \quad q_2 = a_2^{(2)}, \quad q_3 = a_3^{(3)}, \ldots$$

Then we have

$$q_2 = a_2 - \frac{q_1^T a_2}{q_1^T q_1} q_1, \quad q_3 = a_3^{(2)} - \frac{q_2^T a_3^{(2)}}{q_2^T q_2} q_2, \ldots,$$

which is exactly the **modified Gram-Schmidt** procedure!

Jørgen Pedersen Gram (1850–1916)

- Dual career: Mathematics (1873) and Insurance (1875, 1884)
- Research in modern algebra, number theory, models for forest management, integral equations, probability, numerical analysis.
- Active in Danish Math Society, edited Tidsskrift journal (1883–89).
- Best known for his orthogonalization process

J. P. Gram: 1879 Thesis and 1883 paper

- Series expansions of real functions using least squares
- Orthogonalization process applied to generate orthogonal polynomials
- Data approximation using discrete inner product
- Determinantal representation for resulting orthogonal functions
- Continuous inner products
- Application to integral equations

Erhard Schmidt (1876–1959)

- Ph.D. on integral equations, Gottengin 1905
- Student of David Hilbert
- 1917 University of Berlin, set up Inst for Applied Math
- Director of Math Res Inst of German Acad of Sci
- Known for his work in Hilbert Spaces
- Played important role in the development of modern functional analysis

Schmidt 1907 paper

- p 442 CGS for sequence of functions $\phi_1, \ldots, \phi_n$ with respect to inner product

$$\langle f, g \rangle = \int_a^b f(x)g(x)dx$$

- p 473 CGS for an infinite sequence of functions
- In footnote (p 442) Schmidt claims that in essence the formulas are due to J. P. Gram.
- 1935 Y. K. Wong paper refers to "Gram-Schmidt Orthogonalization Process" (First such linkage?)

Original algorithm of Schmidt for CGS

$$\psi_1(x) = \frac{\phi_1(x)}{\sqrt{\int_a^b \phi_1(y)^2 dy}}$$

$$\psi_2(x) = \frac{\phi_2(x) - \psi_1(x)\int_a^b \phi_2(z)\psi_1(z))dz}{\sqrt{\int_a^b (\phi_2(y) - \psi_1(y)\int_a^b \phi_2(z)\psi_1(z))dz)^2 dy}}$$

$$\vdots$$

$$\psi_n(x) = \frac{\phi_n(x) - \sum_{\rho=1}^{\rho=n-1} \psi_\rho(x)\int_a^b \phi_n(z)\psi_\rho(z)dz}{\sqrt{\int_a^b (\phi_n(x) - \sum_{\rho=1}^{\rho=n-1} \psi_\rho(x)\int_a^b \phi_n(z)\psi_\rho(z)dz)^2 dy}}$$

Åke Björck

- Specialist in Numerical Least Squares
- 1967 Solving Least Squares Problems by Gram-Schmidt Orthogonalization
- 1992 Björck and Paige: Loss and recapture of orthogonality in MGS
- 1994 Numerics of Gram-Schmidt Orthogonalization
- 1996 SIAM: Numerical Methods for Least Squares

Stability of MGS for Least Squares

- Forward Stability (Björck, 1967) and Backward Stability (Björck and Paige, 1992)
- If A has computed MGS factorization $\tilde{Q}\tilde{R}$
  - Loss of orthogonality in MGS

$$\|I - \tilde{Q}^T\tilde{Q}\|_2 \leq \frac{c_1(m,n)}{1 - c_2(m,n)\kappa u}\kappa u$$

  - Stability

$$A + E = Q\tilde{R} \text{ where } \|E\| \leq c(m,n)u\|A\|_2 \text{ and } Q^TQ = I$$

  - **b** must be modified as if it were an $n+1$st column of A

Björck and Paige 1992

$$\tilde{A} = \begin{pmatrix} O \\ A \end{pmatrix} = \tilde{Q}\tilde{R} = \begin{pmatrix} \tilde{Q}_{11} & \tilde{Q}_{12} \\ \tilde{Q}_{21} & \tilde{Q}_{22} \end{pmatrix} \begin{pmatrix} \tilde{R}_1 \\ O \end{pmatrix}$$

where $\tilde{Q} = H_1 H_2 \cdots H_n$ (a product of Householder matrices)

$$\tilde{Q}_{11} = O \text{ and } A = \tilde{Q}_{21}\tilde{R}_1$$

(C. Sheffield) $\tilde{Q}_{21}\tilde{R}_1$ and $A = QR$ (MGS) *numerically* equivalent
In fact if $Q = (\mathbf{q}_1, \ldots, \mathbf{q}_n)$ then

$$H_k = I - \mathbf{v}_k\mathbf{v}_k^T, \quad k = 1, \ldots, n$$

where

$$\mathbf{v}_k = \begin{pmatrix} -\mathbf{e}_k \\ \mathbf{q}_k \end{pmatrix}, \quad k = 1, \ldots, n$$

Loss of Orthogonality in CGS

- With CGS you could have catastrophic cancellation.
- Gander 1980 - Better to compute Cholesky factorization of $A^T A$ and then set $Q = AR^{-1}$
- Smoktunowicz, Barlow, and Langou, 2006
  If $A^T A$ is numerically nonsingular and "the Pythagorean version of CGS" is used then the loss of orthogonality is proportional to κ^2

Pythagorean version of CGS

Computation of diagonal entry r_{kk} at step k.

- CGS: $r_{kk} = \|\mathbf{w}_k\|_2$ where $\mathbf{w}_k = \mathbf{a}_k - \sum_{i=1}^{k-1} r_{ik}\mathbf{q}_i$
- CGSP: If

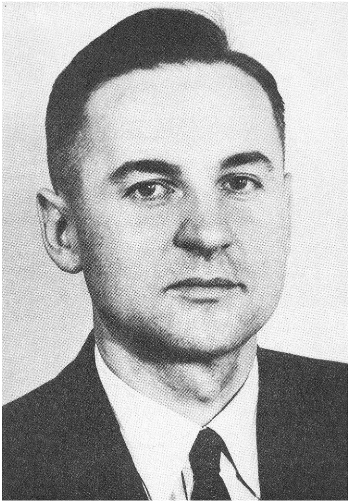
$$s_k = \|\mathbf{a}_k\| \text{ and } p_k = \left(\sum_{i=1}^{k-1} r_{ik}^2\right)^{1/2}$$

then $r_{kk}^2 + p_k^2 = s_k^2$ and hence

$$r_{kk} = (s_k - p_k)^{1/2}(s_k + p_k)^{1/2}$$

Heinz Rutishauser (1918–1970)

- Pioneer in Computer Science and Computational Mathematics
- Long history with ETH as both student and distinguished faculty
- Selective Reorthogonalization for MGS
- Superorthogonalization



Classic Gram-Schmidt

CGS Algorithm

$Q = A$;
for $k = 1 : n$
    for $i = 1 : k - 1$;
        $R(i, k) = Q(:, i)' * Q(:, k)$;
    end (Omit this line for CMGS)
    for $i = 1 : k - 1$, (Omit this line for CMGS)
        $Q(:, k) = Q(:, k) - R(i, k) * Q(:, i)$;
    end
    $R(k, k) = \mathrm{norm}(Q(:, k))$;
    $Q(:, k) = Q(:, k)/R(k, k)$;
end

Columnwise MGS

CMGS Algorithm

$$
\begin{array}{l}
Q = A; \\
\text{for } k = 1 : n \\
\quad \text{for } i = 1 : k-1 \\
\qquad R(i,k) = Q(:,i)' * Q(:,k); \\
\qquad Q(:,k) = Q(:,k) - R(i,k) * Q(:,i); \\
\quad \text{end} \\
\quad R(k,k) = \mathrm{norm}(Q(:,k)); \\
\quad Q(:,k) = Q(:,k)/R(k,k); \\
\text{end}
\end{array}
$$

Reorthogonalization

- Iterative orthogonalization - As each $\mathbf{q}_k$ is generated reorthogonalize with respect to $\mathbf{q}_1, \ldots, \mathbf{q}_{k-1}$
- Twice is enough (W. Kahan), (Giraud, Langou, and Rozložnik, 2002)
- The algorithms MGS2, CGS2
- Selective reorthogonalization

To reorthogonalize or not to reorthogonalize

- For most applications it is not necessary to reorthogonalize if MGS is used
- Both MGS least squares and MGS GMRES are backward stable
- In many applications it is important that the residual vector $\mathbf{r}$ be orthogonal to the column vectors of Q.
- In these cases if MGS is used, $\mathbf{r}$ should be reorthogonalized with respect to $\mathbf{q}_n, \mathbf{q}_{n-1}, \ldots, \mathbf{q}_1$ (note the reverse order)

Selective reorthogonalization

- Reorthogonalize when loss of orthogonality is detected.

$$\mathbf{b} = \mathbf{a}_k - \sum_{i=1}^{k-1} r_{ik}\mathbf{q}_i$$

Indication of cancellation if $\|\mathbf{b}\| << \|\mathbf{a}_k\|$

- (1967) Rutishauser test: Reorthogonalize if $\|\mathbf{b}\| \leq \frac{1}{10}\|\mathbf{a}_k\|$

Selective reorthogonalization

- The Rutishauser reorthogonalization condition can be rewritten as

$$\frac{\|\mathbf{a}_k\|}{\|\mathbf{b}\|} \geq 10 \quad \text{or more generally} \quad \frac{\|\mathbf{a}_k\|}{\|\mathbf{b}\|} \geq K$$

- There are many papers using different values of K. Generally $1 \leq K \leq \kappa_2(A)$; popular choice is $K = \sqrt{2}$. Hoffman, 1989, investigates a range of K values.

- Giraud and Langou, 2003
  - Loss of orthogonality possible for any choice of K
  - Alternate condition

$$\frac{\sum_{i=1}^{k-1} |r_{ik}|}{r_{kk}} > L$$

Rutishauser Superorthogonalization

The vectors $\mathbf{x}$ and $\mathbf{y}$ are *numerically orthogonal* if

$$|fl(\mathbf{x}^T\mathbf{y})| \leq \epsilon \|\mathbf{x}\|\|\mathbf{y}\| \tag{1}$$

In general

$$|\mathbf{x}^T\mathbf{y} - fl(\mathbf{x}^T\mathbf{y})| \leq \gamma_n |\mathbf{x}|^T|\mathbf{y}| \tag{2}$$

$\gamma_n = n\varepsilon/(1 - n\varepsilon)$, $|\mathbf{x}|$ is the vector with elements $|x_i|$

If $\mathbf{x}$ and $\mathbf{y}$ are orthogonal, then (2) becomes

$$|fl(\mathbf{x}^T\mathbf{y})| \leq \gamma_n |\mathbf{x}|^T|\mathbf{y}| \tag{3}$$

We say that $\mathbf{x}$ and $\mathbf{y}$ are *numerically superorthogonal* if (3) is satisfied.

Rutishauser Orthno algorithm

Rutishauer's Orthno algorithm contains a routine for superothogonalizing vectors.

The basic idea is to keep orthogonalizing $\mathbf{x}$ and $\mathbf{y}$ until (3) is satisfied.

The actual stopping condition used is:
While

$$|\mathbf{x}|^T|\mathbf{y}| + \frac{|\mathbf{x}^T\mathbf{y}|}{10} > |\mathbf{x}|^T|\mathbf{y}|$$

reorthogonalize $\mathbf{x}$ and $\mathbf{y}$

Superorthogonalization Example

$$\mathbf{x} = \begin{pmatrix} 1 \\ 10^{-40} \\ 10^{-20} \\ 10^{-10} \\ 10^{-15} \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 10^{-20} \\ 1 \\ 10^{-10} \\ 10^{-20} \\ 10^{-10} \end{pmatrix}$$

are numerically orthogonal, however

$$|\mathbf{x}^T \mathbf{y}| \approx 10^{-20} \text{ and } |\mathbf{x}|^T |\mathbf{y}| \approx 10^{-20}$$

Perform two reorthogonalizations: $\mathbf{y} \to \mathbf{y}^{(2)} \to \mathbf{y}^{(3)}$

Superorthogonalization Calculations

$\mathbf{x}$	$\mathbf{y}$	$\mathbf{y}^{(2)}$	$\mathbf{y}^{(3)}$
$1e{+}00$	$1e{-}20$	$-1.000019999996365e{-}25$	$-1.000020000000000e{-}25$
$1e{-}40$	$1e{+}00$	$1.000000000000000e{+}00$	$1.000000000000000e{+}00$
$1e{-}20$	$1e{-}10$	$1.000000000000000e{-}10$	$1.000000000000000e{-}10$
$1e{-}10$	$1e{-}20$	$9.999999998999989e{-}21$	$9.999999998999989e{-}21$
$1e{-}15$	$1e{-}10$	$1.000000000000000e{-}10$	$1.000000000000000e{-}10$

Decrease in scalar products

$$
\begin{aligned}
|\mathbf{x}^T\mathbf{y}| &= 1e{-}20 \\
|\mathbf{x}^T\mathbf{y}^{(2)}| &= 3.6351e{-}37 \\
|\mathbf{x}^T\mathbf{y}^{(3)}| &= 0
\end{aligned}
$$

Conclusions

- Orthogonality plays a fundamental role in applied mathematics.
- The Gram-Schmidt algorithms are at the core of much of what we do in computational mathematics.
- Stability of GS is now well understood.
- The GS Process is central to solving least squares problems and to Krylov subspace methods.
- The QR factorization paved the way for modern rank revealing factorizations.
- What will the future bring?