

Lecture 4: Householder reflector, Givens rotation, Least squares problem



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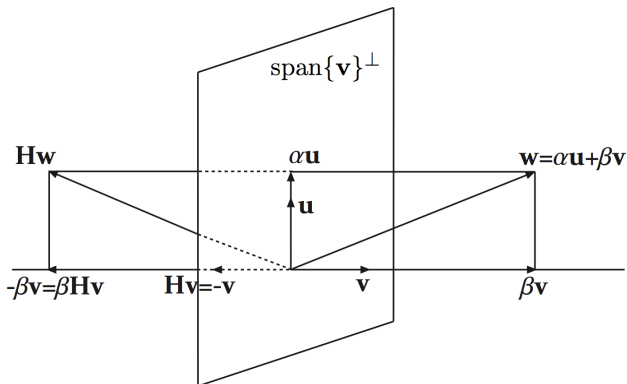
1. Householder reflector

- Let $\mathbf{v} \in \mathbb{C}^m$ and $\mathbf{v} \neq \mathbf{0}$. Then the matrix

$$\mathbf{H} = \mathbf{I} - 2 \frac{\mathbf{v}\mathbf{v}^*}{\mathbf{v}^*\mathbf{v}},$$

is called a *Householder reflector*.

- Geometric interpretation



Exercise: Householder reflector \mathbf{H} satisfies the following properties:

- (1) It is *Hermitian*: $\mathbf{H} = \mathbf{H}^*$
- (2) It is *unitary*: $\mathbf{H}^* = \mathbf{H}^{-1}$
- (3) It is *involutary*: $\mathbf{H}^2 = \mathbf{I}$

Exercise: What are the eigenvalues, the determinant, and the singular values of a Householder reflector \mathbf{H} ?

Hint: eigenvalues 1 with multiplicity $m - 1$ and -1 with multiplicity 1.

Exercise: Prove that $\mathbf{I} - \frac{\mathbf{v}\mathbf{v}^*}{\mathbf{v}^*\mathbf{v}}$ is the orthogonal projector which projects \mathbb{C}^m onto the *hyperplane* $\text{span}\{\mathbf{v}\}^\perp$ along $\text{span}\{\mathbf{v}\}$.

Theorem 1

For all $\mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ with $\mathbf{x} \neq \mathbf{y}$, there exists a Householder reflector \mathbf{H} such that $\mathbf{H}\mathbf{x} = \mathbf{y}$ if and only if $\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2$ and $\mathbf{x}^\mathbf{y} \in \mathbb{R}$.*

Proof.

“ \Rightarrow ” is easy. “ \Leftarrow ”: let $\mathbf{v} = \mathbf{y} - \mathbf{x}$, verify $\mathbf{H}\mathbf{x} = \mathbf{y}$. □

Corollary 2

For all nonzero $\mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ with $\mathbf{x} \neq \mathbf{y}$, there exists a Householder reflector \mathbf{H} and $z \in \mathbb{C}$ such that $\mathbf{H}\mathbf{x} = z\mathbf{y}$.

Proof.

Let

$$z = \frac{\|\mathbf{x}\|_2}{\|\mathbf{y}\|_2} \cdot c, \quad c = \begin{cases} \pm \mathbf{y}^*\mathbf{x}/|\mathbf{x}^*\mathbf{y}|, & \text{if } \mathbf{x}^*\mathbf{y} \neq 0, \\ e^{i\theta}, \theta \in [0, 2\pi), & \text{if } \mathbf{x}^*\mathbf{y} = 0, \end{cases}$$

and $\mathbf{v} = z\mathbf{y} - \mathbf{x}$. Verify $\mathbf{H}\mathbf{x} = z\mathbf{y}$. □

2. QR factorization via Householder reflectors

- Householder method: $\mathbf{Q}_n \cdots \mathbf{Q}_2 \mathbf{Q}_1 \mathbf{A} = \mathbf{R}$ is upper-triangular.

$$\begin{array}{ccccc}
 \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} & \xrightarrow{\mathbf{Q}_1} & \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix} & \xrightarrow{\mathbf{Q}_2} & \begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & 0 & \times \\ & 0 & \times \\ & 0 & \times \end{bmatrix} & \xrightarrow{\mathbf{Q}_3} & \begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ & & 0 \\ & & 0 \end{bmatrix} \\
 \mathbf{A} & & \mathbf{Q}_1 \mathbf{A} & & \mathbf{Q}_2 \mathbf{Q}_1 \mathbf{A} & & \mathbf{Q}_3 \mathbf{Q}_2 \mathbf{Q}_1 \mathbf{A}
 \end{array}$$

\times denotes an entry not necessarily zero; “blank” are zeros

- At the k th step, the unitary matrix \mathbf{Q}_k has the form

$$\mathbf{Q}_k = \begin{bmatrix} \mathbf{I}_{k-1} & \\ & \mathbf{H}_k \end{bmatrix}.$$

Here \mathbf{H}_k is an $(m - k + 1) \times (m - k + 1)$ Householder reflector, which maps an $m - k + 1$ -vector to a scalar multiple of \mathbf{e}_1 .

- The full QR factorization: $\mathbf{A} = \mathbf{Q}_1^* \mathbf{Q}_2^* \cdots \mathbf{Q}_n^* \mathbf{R} = \mathbf{Q} \mathbf{R}$

- QR factorization with column pivoting: $\mathbf{A}\mathbf{P} = \mathbf{Q}\mathbf{R}$. Consider “qr”

2.1. Two possible Householder reflections in real case



- Choose the one that moves \mathbf{x} the larger distance, i.e., $\mathbf{v} = -\text{sign}(x_1)\|\mathbf{x}\|_2 \mathbf{e}_1 - \mathbf{x}$, or $\mathbf{v} = \text{sign}(x_1)\|\mathbf{x}\|_2 \mathbf{e}_1 + \mathbf{x}$
- Convention: $\text{sign}(x_1) = 1$ if $x_1 = 0$

2.2. Algorithms

Algorithm: Householder QR factorization

```
for  $k = 1$  to  $n$ 
     $\mathbf{x} = \mathbf{A}_{k:m,k}$ 
     $\mathbf{v}_k = \text{sign}(x_1) \|\mathbf{x}\|_2 \mathbf{e}_1 + \mathbf{x}$ 
     $\mathbf{v}_k = \mathbf{v}_k / \|\mathbf{v}_k\|_2$ 
     $\mathbf{A}_{k:m,k:n} = \mathbf{A}_{k:m,k:n} - 2\mathbf{v}_k(\mathbf{v}_k^* \mathbf{A}_{k:m,k:n})$ 
end
```

Algorithm: Implicit calculations of $\mathbf{Q}^* \mathbf{b}$ or $\mathbf{Q} \mathbf{x}$

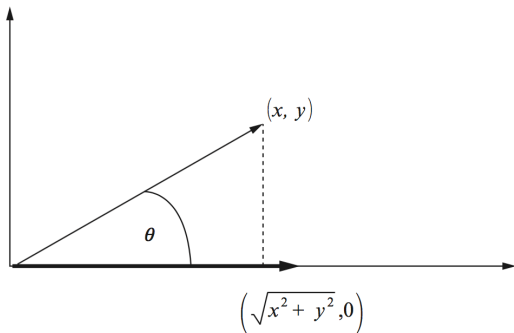
```
for  $k = 1$  to  $n$ 
     $\mathbf{b}_{k:m} = \mathbf{b}_{k:m} - 2\mathbf{v}_k(\mathbf{v}_k^* \mathbf{b}_{k:m})$ 
end
for  $k = n$  downto  $1$ 
     $\mathbf{x}_{k:m} = \mathbf{x}_{k:m} - 2\mathbf{v}_k(\mathbf{v}_k^* \mathbf{x}_{k:m})$ 
end
```

3. Givens rotation (We mainly consider the real case).

- The 2×2 Givens rotation

$$\mathbf{G} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}, \quad \cos \theta = \frac{x}{\sqrt{x^2 + y^2}}, \quad \sin \theta = \frac{y}{\sqrt{x^2 + y^2}}$$

rotates vector $\begin{bmatrix} x \\ y \end{bmatrix}$ in \mathbb{R}^2 onto the x -axis.



- Givens rotation for $\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \sqrt{x^2 + y^2} \\ 0 \end{bmatrix}$

Algorithm: Givens rotation zeroing the 2nd entry

```
function [c, s] =givens(x, y)
    if y = 0
        c = 1,    s = 0
    else
        if |y| > |x|
             $\tau = x/y, \quad s = 1/\sqrt{1 + \tau^2}, \quad c = s\tau$ 
        else
             $\tau = y/x, \quad c = 1/\sqrt{1 + \tau^2}, \quad s = c\tau$ 
        end
    end
```

Exercise: Design a similar algorithm for a Givens rotation zeroing the 1st entry.

- Zeroing a particular entry in a vector using a Givens rotation.

Define the $m \times m$ Givens rotation $\mathbf{G}(i, j; \theta)$,

$$\begin{aligned} \mathbf{G}(i, j; \theta) &= \mathbf{I} + [\mathbf{e}_i \quad \mathbf{e}_j] \begin{bmatrix} \cos \theta - 1 & \sin \theta \\ -\sin \theta & \cos \theta - 1 \end{bmatrix} \begin{bmatrix} \mathbf{e}_i^\top \\ \mathbf{e}_j^\top \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{I} & & & \\ & \cos \theta & \sin \theta & \\ & & \mathbf{I} & \\ & -\sin \theta & \cos \theta & \\ & & & \mathbf{I} \end{bmatrix} \begin{matrix} \text{row } i \\ \text{row } j \end{matrix} . \end{aligned}$$

Exercise: Prove that the matrix $\mathbf{G}(i, j; \theta)$ is orthogonal.

- Creating a sequence of zeros in a vector using Givens rotations

$$\mathbf{G}_n \mathbf{G}_{n-1} \cdots \mathbf{G}_1 \mathbf{x}$$

- QR factorization via Givens rotations?

Exercise: Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be given as

$$\mathbf{A} = \begin{bmatrix} \alpha_1 & \beta_2 & \beta_3 & \cdots & \beta_n \\ \gamma_2 & \alpha_2 & 0 & \cdots & 0 \\ \gamma_3 & 0 & \alpha_3 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \gamma_n & 0 & \cdots & 0 & \alpha_n \end{bmatrix}, \quad \begin{array}{ll} \alpha_i \neq 0, & i = 1:n, \\ \beta_i \neq 0, & i = 2:n, \\ \gamma_i \neq 0, & i = 2:n. \end{array}$$

Describe an algorithm for QR factorization of \mathbf{A} based on as few Givens rotations as possible.

- Complex case:

$$\mathbf{G} = \begin{bmatrix} c & \bar{s} \\ -s & c \end{bmatrix}, \quad c \in \mathbb{R}, \quad c^2 + |s|^2 = 1.$$

4. The least squares problem (LSP)

- LSP: Given $\mathbf{A} \in \mathbb{C}^{m \times n}$, $\mathbf{b} \in \mathbb{C}^m$; find $\mathbf{x}_{\text{ls}} \in \mathbb{C}^n$ such that

$$\|\mathbf{b} - \mathbf{A}\mathbf{x}_{\text{ls}}\|_2 = \min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2.$$

The *least squares solution*, \mathbf{x}_{ls} , maybe *not* unique. Why?

- Note that the 2-norm corresponds to Euclidean distance.

LSP means we seek a vector $\mathbf{x}_{\text{ls}} \in \mathbb{C}^n$ such that the vector $\mathbf{A}\mathbf{x}_{\text{ls}}$ is the closest point in $\text{range}(\mathbf{A})$ to \mathbf{b} .

The *residual*, $\mathbf{r}_{\text{ls}} = \mathbf{b} - \mathbf{A}\mathbf{x}_{\text{ls}}$, is unique. Why?

- Assume that \mathbf{A} and \mathbf{b} are real. Define

$$f(\mathbf{x}) := \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 = \mathbf{b}^\top \mathbf{b} - \mathbf{x}^\top \mathbf{A}^\top \mathbf{b} - \mathbf{b}^\top \mathbf{A}\mathbf{x} + \mathbf{x}^\top \mathbf{A}^\top \mathbf{A}\mathbf{x}.$$

Then the gradient of $f(\mathbf{x})$ is

$$\nabla f(\mathbf{x}) = 2\mathbf{A}^\top \mathbf{A}\mathbf{x} - 2\mathbf{A}^\top \mathbf{b}.$$

4.1. Example: Polynomial least squares fitting

- Given m distinct $x_1, \dots, x_m \in \mathbb{C}$ and data $y_1, \dots, y_m \in \mathbb{C}$ at these points. Consider a polynomial of degree $n - 1$,

$$p(x) = c_0 + c_1x + \cdots + c_{n-1}x^{n-1},$$

s.t., $p(x)$ minimizes

$$\sum_{i=1}^m |p(x_i) - y_i|^2 = \|\mathbf{y} - \mathbf{A}\mathbf{c}\|_2^2,$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} 1 & x_1 & \cdots & x_1^{n-1} \\ 1 & x_2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_m & \cdots & x_m^{n-1} \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_{n-1} \end{bmatrix}.$$

4.2. Solving the least squares problem

Theorem 3

Let \mathbf{P} be the orthogonal projector onto $\text{range}(\mathbf{A})$. A vector \mathbf{x} is a least squares solution if and only if \mathbf{x} satisfies $\mathbf{Ax} = \mathbf{Pb}$.

Proof.

$$\|\mathbf{b} - \mathbf{Ax}\|_2^2 = \|\mathbf{Pb} - \mathbf{Ax} + \mathbf{b} - \mathbf{Pb}\|_2^2 = \|\mathbf{Pb} - \mathbf{Ax}\|_2^2 + \|\mathbf{b} - \mathbf{Pb}\|_2^2. \quad \square$$

Corollary 4

A vector \mathbf{x} is a least squares solution if and only if \mathbf{x} satisfies $\mathbf{A}^*\mathbf{Ax} = \mathbf{A}^*\mathbf{b}$, i.e., $\mathbf{A}^*\mathbf{r} = \mathbf{0}$, or $\mathbf{r} \perp \text{range}(\mathbf{A})$, where $\mathbf{r} := \mathbf{b} - \mathbf{Ax}$.

Proof.

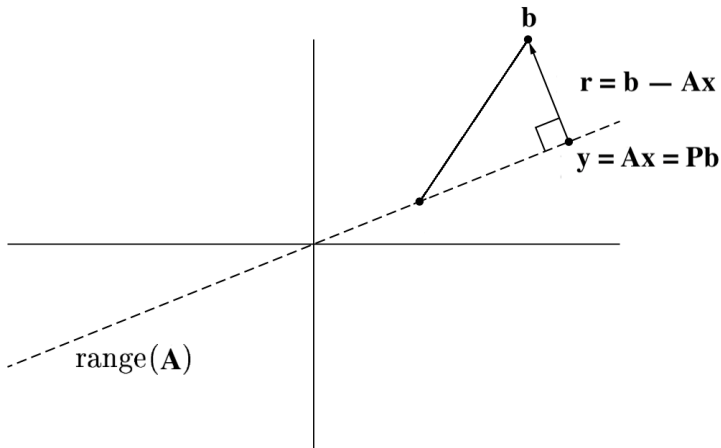
$$\because \mathbf{A}^* = \mathbf{A}^*\mathbf{P}, \therefore \mathbf{A}^*\mathbf{r} = \mathbf{0} \Leftrightarrow \mathbf{A}^*(\mathbf{Pb} - \mathbf{Ax}) = \mathbf{0} \Leftrightarrow \mathbf{Ax} = \mathbf{Pb}. \quad \square$$

- The system $\mathbf{A}^*\mathbf{Ax} = \mathbf{A}^*\mathbf{b}$ is called the *normal equations*.

Corollary 5

The least squares solution \mathbf{x} is unique if and only if $\mathbf{A}^ \mathbf{A}$ has full rank.*

4.3. Geometric interpretation



4.4. Moore–Penrose pseudoinverse solution $\mathbf{A}^\dagger \mathbf{b}$

- Let $\mathbf{A} \in \mathbb{C}^{m \times n}$ have an SVD $\mathbf{A} = \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^*$. The matrix

$$\mathbf{A}^\dagger = \mathbf{V}_r \mathbf{\Sigma}_r^{-1} \mathbf{U}_r^* = \sum_{j=1}^r \frac{1}{\sigma_j} \mathbf{v}_j \mathbf{u}_j^* \in \mathbb{C}^{n \times m},$$

is called the *Moore–Penrose pseudoinverse* of \mathbf{A} . If \mathbf{A} has full column rank, then $\mathbf{A}^\dagger = (\mathbf{A}^* \mathbf{A})^{-1} \mathbf{A}^*$. (Full row rank case?)

Theorem 6

Let $\mathbf{A} \in \mathbb{C}^{m \times n}$ have rank $r < n$ and $\mathbf{b} \in \mathbb{C}^m$. Then the vector $\mathbf{A}^\dagger \mathbf{b}$ is the unique least squares solution with minimal 2-norm.

Proof.

By SVD of \mathbf{A} , the least squares solutions can be expressed as

$$\mathbf{x}_{\text{ls}} = \mathbf{A}^\dagger \mathbf{b} + \mathbf{V}_c \mathbf{z}, \quad \mathbf{z} \in \mathbb{C}^{n-r}.$$

Then the statement follows from $\mathbf{A}^\dagger \mathbf{b} \perp \mathbf{V}_c \mathbf{z}$. □

4.5. Full column rank LSP solvers: $\text{rank}(\mathbf{A}) = n$

- Normal equations: classical way to solve LSP, best for speed
- QR factorization: “modern classical” method to solve LSP, numerically stable. By

$$\mathbf{A} = \mathbf{Q}\mathbf{R} = [\mathbf{Q}_n \quad \mathbf{Q}_c] \begin{bmatrix} \mathbf{R}_n \\ \mathbf{0} \end{bmatrix},$$

we have

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 &= \min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{Q}\mathbf{R}\mathbf{x}\|_2 = \min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{Q}^*\mathbf{b} - \mathbf{R}\mathbf{x}\|_2 \\ &= \min_{\mathbf{x} \in \mathbb{C}^n} \left\| \begin{bmatrix} \mathbf{Q}_n^*\mathbf{b} - \mathbf{R}_n\mathbf{x} \\ \mathbf{Q}_c^*\mathbf{b} \end{bmatrix} \right\|_2 \end{aligned}$$

- SVD, numerically stable, for problems close to rank-deficient. By

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^* = \mathbf{U}_n\mathbf{\Sigma}_n\mathbf{V}^* = [\mathbf{U}_n \quad \mathbf{U}_c] \begin{bmatrix} \mathbf{\Sigma}_n \\ \mathbf{0} \end{bmatrix} \mathbf{V}^*,$$

we have

$$\begin{aligned}\min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 &= \min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{U}\Sigma\mathbf{V}^*\mathbf{x}\|_2 \\ &= \min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{U}^*\mathbf{b} - \Sigma\mathbf{V}^*\mathbf{x}\|_2 \\ &= \min_{\mathbf{x} \in \mathbb{C}^n} \left\| \begin{bmatrix} \mathbf{U}_n^*\mathbf{b} - \Sigma_n\mathbf{V}^*\mathbf{x} \\ \mathbf{U}_c^*\mathbf{b} \end{bmatrix} \right\|_2.\end{aligned}$$

Exercise: Given $\mathbf{A} \in \mathbb{C}^{m \times n}$ of full column rank, $m > n$, $\mathbf{b} \in \mathbb{C}^m$, $\mathbf{b} \notin \text{range}(\mathbf{A})$ and $\mathbf{QR} = [\mathbf{A} \ \mathbf{b}]$ (i.e., full QR factorization of $[\mathbf{A} \ \mathbf{b}]$). Show that

$$\min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 = |\mathbf{R}(n+1, n+1)|,$$

and the least squares solution is given by

$$\mathbf{x} = \mathbf{R}(1:n, 1:n) \backslash \mathbf{R}(1:n, n+1).$$

4.6. Rank-deficient LSP solvers: $\text{rank}(\mathbf{A}) = r < n$

- QR factorization with column pivoting:

$$\mathbf{AP} = \mathbf{QR} = \mathbf{Q} \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{0} & \mathbf{0} \end{bmatrix},$$

where \mathbf{P} is a permutation matrix, $\mathbf{Q} \in \mathbb{C}^{m \times m}$ is unitary, and $\mathbf{R}_{11} \in \mathbb{R}^{r \times r}$ is nonsingular upper triangular. Introduce the auxiliary vectors

$$\mathbf{Q}^* \mathbf{b} = \begin{bmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \end{bmatrix} \quad \text{and} \quad \mathbf{P}^* \mathbf{x} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}.$$

The general least squares solution is

$$\mathbf{x}_{\text{ls}} = \mathbf{P} \begin{bmatrix} \mathbf{R}_{11}^{-1}(\mathbf{d}_1 - \mathbf{R}_{12}\mathbf{y}_2) \\ \mathbf{y}_2 \end{bmatrix}, \quad \mathbf{y}_2 = \text{arbitrary}.$$

The case $\mathbf{y}_2 = \mathbf{0}$ yields the least squares solution with at least $n - r$ zero components. Consider “\” in MATLAB.

- Complete orthogonal factorization (also called UTV factorization)

$$\mathbf{A} = \mathbf{U} \begin{bmatrix} \mathbf{R}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}^*,$$

where $\mathbf{U} \in \mathbb{C}^{m \times m}$ is unitary, $\mathbf{V} \in \mathbb{C}^{n \times n}$ is unitary, and $\mathbf{R}_{11} \in \mathbb{R}^{r \times r}$ is nonsingular upper triangular. Introduce the auxiliary vectors

$$\mathbf{U}^* \mathbf{b} = \begin{bmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \end{bmatrix} \quad \text{and} \quad \mathbf{V}^* \mathbf{x} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}.$$

The general least squares solution is

$$\mathbf{x}_{\text{ls}} = \mathbf{V} \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} = \mathbf{V} \begin{bmatrix} \mathbf{R}_{11}^{-1} \mathbf{g}_1 \\ \mathbf{y}_2 \end{bmatrix}, \quad \mathbf{y}_2 = \text{arbitrary}.$$

The case $\mathbf{y}_2 = \mathbf{0}$ yields the minimum norm least squares solution.

<http://www.netlib.org/numeralgo/>

Consider `lsqminnorm` in MATLAB.

5. Least squares solution flowchart

