▪ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions:

• Matrix factorization:

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdot \end{bmatrix}$$

$\Longleftrightarrow$ $M = QR$

A matrix **M** written as a matrix product **QR**. **M** is a $k \times k$ matrix with columns that are linearly independent; **Q** is a $k \times k$ matrix with columns that are mutually, pairwise orthogonal; **R** is an upper triangular matrix with value 0 below the matrix diagonal.

In our setting, matrix factorization is based on the k sample "histogram functions" $h_i(c)$. The functions define the entries of matrix M. Once M has been established its factors Q and R can be computed and stored.

Future computations involving M can be "simplified" to computations using Q and R instead — leading to more efficiency and stability.

• **Note.** We have discussed orthonormalization in the specific context of representing/expanding a given, new "histogram function" in terms of stored, known "histogram sample functions." We have described a method for ensuring that the number of bins/segments **(B)** of all functions is equal to the number of "histogram sample functions" **(k)**: **B=k.** **The** sample functions $h_i(c)$ are assumed to be linearly independent, defining a function basis for a k-dimensional space, i.e., the space $\left\{ \sum_{i=1}^{k} \alpha_i h_i(c) \right\}$ with coefficients α_i; the new function is $h(c)$ can be expanded in the basis $\{h_i(c)\}_{i=1}^{k}$. THE COMPUTATION OF THE EXPANSION OF $h(c)$ SHOULD BE HIGHLY EFFICIENT, NUMERICALLY STABLE AND **ALGO**RITHMICALLY ELEGANT.

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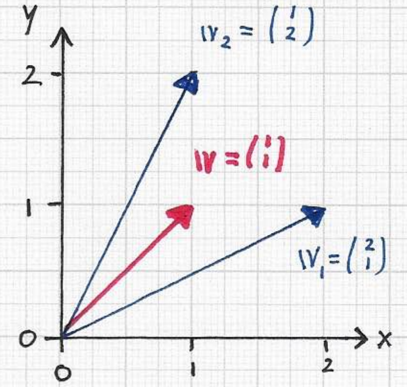
MATRIX FACTORIZATION, QR DECOMPOSITION, ORTHONORMALIZATION, GRAM-SCHMIDT ORTHONORMALIZATION AND THE HOUSEHOLDER TRANSFORMATION SERVE OUR ALGORITHMIC DESIGN GOALS. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... The objective is to compute the expansion of $h(c)$ in the basis $\{h_i(c)\}_{i=1}^{k}$ – i.e., the unknown coefficients α_i in $h(c) = \sum_{i=1}^{k} \alpha_i h_i(c)$ – as efficiently as possible. If one used the given basis in its "native" form, one would have to perform matrix calculations involving the $k \times k$ matrix of all inner products $\langle h_i(c), h_j(c)\rangle$, $i,j = 1...k$. Since this matrix generally has no specific structure, the complexity of computing the expansion of $h(c)$ is of order $\mathcal{O}(k^3)$, which can become prohibitively expensive for large values of k. The linear system to be solved would be

$$\begin{bmatrix} \langle h_1(c), h_1(c)\rangle & \dots & \langle h_1(c), h_k(c)\rangle \\ \vdots & & \vdots \\ \langle h_k(c), h_1(c)\rangle & \dots & \langle h_k(c), h_k(c)\rangle \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_k \end{bmatrix} = \begin{bmatrix} \langle h(c), h_1(c)\rangle \\ \vdots \\ \langle h(c), h_k(c)\rangle \end{bmatrix}.$$

When solving this system – $M\boldsymbol{\alpha} = \mathbf{h}$ – naively, one must compute k^2 inner products for M and k inner products for $\mathbf{h}$; one must invert the $k \times k$ matrix M; and one must multiply M^{-1} and $\mathbf{h}$ to obtain $\boldsymbol{\alpha}$: $\boldsymbol{\alpha} = M^{-1}\mathbf{h}$. ...



Geometrical example. Needed are the values of the coefficients in

$$\mathbf{v} = \sum_{i=1}^{2} \alpha_i \mathbf{v}_i .$$

The solution is defined as follows, when using the basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ directly:

$$\begin{bmatrix} \langle \mathbf{v}_1, \mathbf{v}_1\rangle & \langle \mathbf{v}_1, \mathbf{v}_2\rangle \\ \langle \mathbf{v}_2, \mathbf{v}_1\rangle & \langle \mathbf{v}_2, \mathbf{v}_2\rangle \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} \langle \mathbf{v}, \mathbf{v}_1\rangle \\ \langle \mathbf{v}, \mathbf{v}_2\rangle \end{bmatrix}$$

$$\Leftrightarrow \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$

$$\Rightarrow (\alpha_1, \alpha_2) = (1/3, 1/3)$$

This approach for computing values of coefficients "directly" is inappropriate when calculating the expansion of $h(c)$ with respect to a non-orthogonal basis $\{h_i(c)\}_{i=1}^{k}$. A QR DECOMPOSITION CAN BE USED TO IMPROVE THE CALCULATIONS.

Stratovan

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

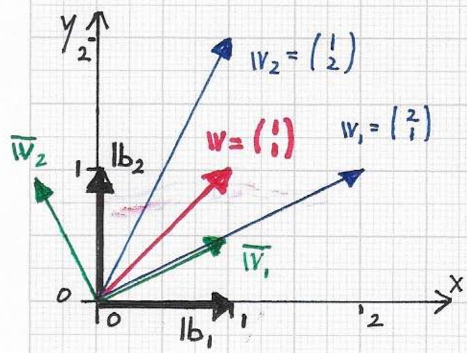
• Laplacian eigenfunctions: ... A QR decomposition of the matrix M represents M as a product $Q \cdot R$, where Q is an orthogonal (or even an orthonormal) matrix and R is an upper triangular matrix. The described and demonstrated Gram–Schmidt orthonormalization method is one of many used techniques to compute $M = QR$.

• QR decomposition of matrix M with column vectors $\mathbb{v}_1$ and $\mathbb{v}_2$:

$$M = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ +1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} \begin{bmatrix} 5/\sqrt{5} & 4/\sqrt{5} \\ 0 & 3/\sqrt{5} \end{bmatrix} = Q \quad R .$$

This QR decomposition results when using the "QR decomposition" function in WolframAlpha.

The column (and row) vectors of Q are mutually orthogonal to each other and have length 1.



WolframAlpha generates the orthonormal matrix Q whose column vectors define the orthonormal basis vectors:

$$\overline{\mathbb{v}}_1 = 1/\sqrt{5}\,(2,1)^T = (2/\sqrt{5}, 1/\sqrt{5})^T$$

$$\overline{\mathbb{v}}_2 = 1/\sqrt{5}\,(-1,2)^T = (-1/\sqrt{5}, 2/\sqrt{5})^T$$

For the simple example presented on the left side one obtains as epansion of $\binom{1}{1}$:

$$\alpha_1 \binom{2}{1} + \alpha_2 \binom{1}{2} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \binom{\alpha_1}{\alpha_2} = \binom{1}{1}$$

$$\Leftrightarrow \quad M \,\boldsymbol{\alpha} = \mathbb{v}$$

$$\Leftrightarrow \quad Q R \,\boldsymbol{\alpha} = \mathbb{v}$$

$$\Leftrightarrow \quad \underbrace{\begin{pmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ 1/\sqrt{5} & 2/\sqrt{5} \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} 5/\sqrt{5} & 4/\sqrt{5} \\ 0 & 3/\sqrt{5} \end{pmatrix}}_{R} \boldsymbol{\alpha} = \mathbb{v}$$

$$\overset{Q^{-1} = Q^T}{\Leftrightarrow} \quad R \,\boldsymbol{\alpha} = Q^T \mathbb{v}$$

$$\Leftrightarrow \quad \boldsymbol{\alpha} = R^{-1} Q^T \mathbb{v}$$

$$\Rightarrow \quad \boldsymbol{\alpha} = \begin{pmatrix} \sqrt{5}/5 & -4/3\sqrt{5} \\ 0 & \sqrt{5}/3 \end{pmatrix} \begin{pmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{pmatrix} \binom{1}{1}$$

$$= \begin{pmatrix} \sqrt{5}/5 & -4/3\sqrt{5} \\ 0 & \sqrt{5}/3 \end{pmatrix} \binom{3/\sqrt{5}}{1/\sqrt{5}} = \binom{3/5 - 4/15}{1/3} = \binom{1/3}{1/3}.$$

This computation of $\boldsymbol{\alpha}$ can also be viewed as a two-step calculation:

(i) compute two inner products, $\langle \mathbb{v}, \overline{\mathbb{v}}_1 \rangle = 3/\sqrt{5}$ and $\langle \mathbb{v}, \overline{\mathbb{v}}_2 \rangle = 1/\sqrt{5}$.

$$\Rightarrow \mathbb{v}_{\{\overline{\mathbb{v}}_1, \overline{\mathbb{v}}_2\}} = (3/\sqrt{5}, 1/\sqrt{5})^T \quad \ldots$$

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... (ii) apply R^{-1} (also an upper triangular matrix) to $\mathbf{v}_{\{\bar{\mathbf{v}}_1, \bar{\mathbf{v}}_2\}}$ to obtain the desired result:

$$\mathbf{v}_{\{\mathbf{v}_1, \mathbf{v}_2\}} = R^{-1}\begin{pmatrix} 3/\sqrt{5} \\ 1/\sqrt{5} \end{pmatrix} = \begin{pmatrix} 5/5\sqrt{5} & -4/3\sqrt{5} \\ 0 & 5/3\sqrt{5} \end{pmatrix}\begin{pmatrix} 3/\sqrt{5} \\ 1/\sqrt{5} \end{pmatrix} = \begin{pmatrix} 3/5 - 4/15 \\ 1/3 \end{pmatrix} = \begin{pmatrix} 1/3 \\ 1/3 \end{pmatrix}$$

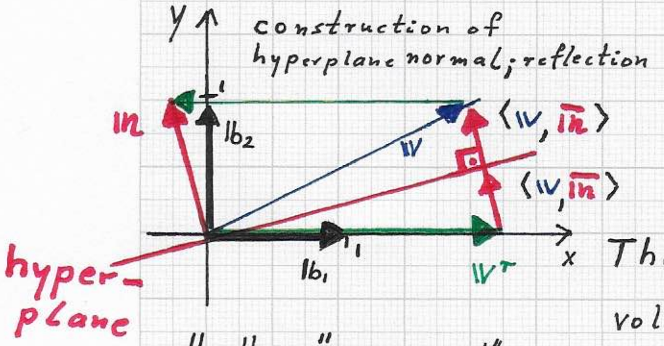
This result – and the calculations involved to perform the necessary basis transformations – agrees with that derived in detail via the Gram-Schmidt orthonormalization method. Thus:

Given a square $k \times k$ matrix M with non-orthogonal but linearly independent column vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$, one can decompose as $M = QR$, where Q is an orthonormal matrix with column vectors $\bar{\mathbf{v}}_1, \ldots, \bar{\mathbf{v}}_k$ and R is an upper triangular matrix. The representation of a given vector $\mathbf{v}$ in the basis $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ is obtained as

$$\boxed{\mathbf{v}_{\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}} = R^{-1} Q^T \mathbf{v}_{\{\mathbf{b}_1, \ldots, \mathbf{b}_k\}}}\,, \quad !$$

where $\{\mathbf{b}_1, \ldots, \mathbf{b}_k\}$ is the underlying "canonical" basis. ...

• Householder transformation:



$\mathbf{b}_1, \mathbf{b}_2$ — "canonical" basis vectors

$\mathbf{v}$ — given vector to be reflected

$\mathbf{n}$ — normal vector of hyperplane used for reflection

$\mathbf{v}^T$ — image of $\mathbf{v}$ obtained via reflection with respect to hyperplane

• **Computations:**

$$\mathbf{n} = \mathbf{v} - \|\mathbf{v}\|\,\mathbf{b}_1$$

$$\bar{\mathbf{n}} = \mathbf{n} / \|\mathbf{n}\|$$

$$\mathbf{v}^T = \mathbf{v} - 2\langle \mathbf{v}, \bar{\mathbf{n}}\rangle \bar{\mathbf{n}}$$

The Householder transformation uses reflections of basis vectors to compute a new orthogonal basis. It is numerically more stable than the projection-based Gram-Schmidt orthonormalization method. Both methods compute $Q \cdot R$.

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ...: **Note.** Numerical libraries compute QR decompositions via different algorithms. Gram-Schmidt orthonormalization is based on repeated projections; the Householder method for computing a QR decomposition uses repeated hyperplane reflections (see figure on previous page). Performing hyperplane reflections repeatedly is the numerically more stable algorithm. Thus, one should use a Householder implementation for QR computations.

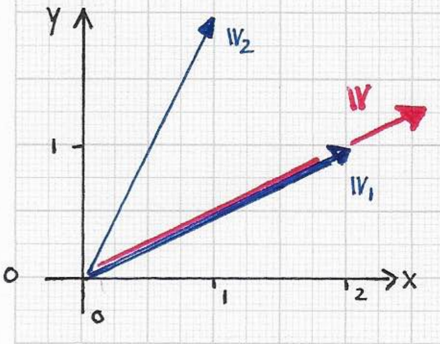
• **Note.** We have described QR decomposition only for a $k \times k$ square matrix M. (We can always "force" this square matrix case by making the number of "histogram function" bins (B) equal to the number of "sample histogram functions" (k), i.e., ensuring that $k = B$ holds; we have discussed a method for achieving this.) **A matrix M with n rows and m columns with $n \geq m$, rank $M = m$, can also be factorized as QR:**

→ **Gram-Schmidt orthonormalization generates Q as a matrix with n rows and m columns and R as an $m \times m$ matrix.**

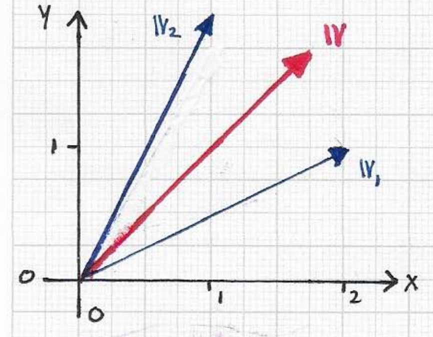
→ **Householder orthogonalization produces an $n \times n$ Q matrix and R with n rows and m columns.**

...

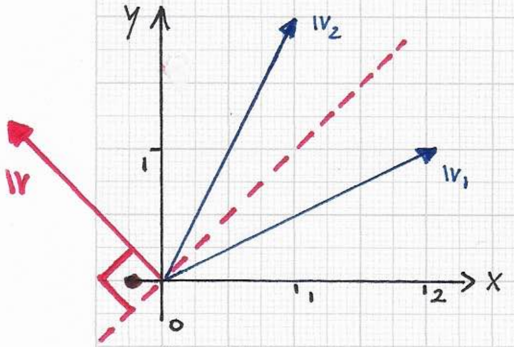
• "Meaning, interpretation" of a vector's (function's) representation with respect to a non-orthogonal basis:



Case 1: $\mathbb{v} = \alpha \mathbb{v}_1 + 0\, \mathbb{v}_2$



Case 2: $\mathbb{v} = \alpha \mathbb{v}_1 + \alpha \mathbb{v}_2$



Case 3: $\mathbb{v} = -\alpha \mathbb{v}_1 + \alpha \mathbb{v}_2$

One must define "similarity" between $\mathbb{v}$ and the basis vectors for "classification."