The Gram-Schmidt Process

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Theorem (Gram-Schmidt)

If $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r\}$ is an independent set in an inner product space V then there exists and orthonormal set $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r\}$ such that $\operatorname{Span}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r) = \operatorname{Span}(\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r).$

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The process takes r steps, and at the end of step j the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_j$ have the same span as $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_j$.

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The process takes r steps, and at the end of step j the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_j$ have the same span as $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_j$. So, by the last step the set is found. If $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_r\}$ is a basis for a subspace S of V, then $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ is an orthonormal basis for S. When computing by hand, it is quite a bit easier to first create an orthogonal set $\mathbf{v}_1, \ldots, \mathbf{v}_r$ and then normalize them at the end by $\mathbf{u}_j = (1/\|\mathbf{v}_j\|)\mathbf{v}_j$.

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Then step r + 1: set $\mathbf{u}_j = (1/ \|\mathbf{v}_j\|)\mathbf{v}_j$ for each j.

Example: find an orthonormal basis for the span of $\mathbf{x}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}$, $\mathbf{x}_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$, $\mathbf{x}_3 = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$.

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$$\mathbf{v}_{1} = \mathbf{x}_{1} = \begin{pmatrix} 1\\1\\0\\1 \end{pmatrix}, \ \mathbf{v}_{2} = \mathbf{x}_{2} - \mathbf{p}_{1} = \begin{pmatrix} 1\\0\\1\\1 \end{pmatrix} - \frac{2}{3} \begin{pmatrix} 1\\1\\0\\1 \end{pmatrix} = \begin{pmatrix} 1/3\\-2/3\\1\\1/3 \end{pmatrix}.$$

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Since $\|\mathbf{v}_1\| = \sqrt{3}$, $\|\mathbf{v}_2\| = \sqrt{15}/3$ and $\|\mathbf{v}_3\| = (\sqrt{35})/5$ we get the orthonormal basis

$$\mathbf{u}_{1} = \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 0 \\ 1/\sqrt{3} \end{pmatrix}, \quad \mathbf{u}_{2} = \begin{pmatrix} 1/\sqrt{15} \\ -2/\sqrt{15} \\ 3/\sqrt{15} \\ 1/\sqrt{15} \end{pmatrix}, \quad \mathbf{u}_{3} = \begin{pmatrix} -4/\sqrt{35} \\ 3/\sqrt{35} \\ 3/\sqrt{35} \\ 1/\sqrt{35} \end{pmatrix}$$

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A further simplification: since the vs don't have to have norm equal to 1, we can replace \mathbf{v}_2 by any multiple of it. So taking $\mathbf{v}_2 = \begin{pmatrix} 1 \\ -2 \\ 3 \\ 1 \end{pmatrix}$ instead of what we used, the next step simplifies to:

$$\mathbf{v}_3 = \mathbf{x}_3 - \mathbf{p}_2 = \begin{pmatrix} 0\\1\\1\\1 \end{pmatrix} - \frac{2}{3} \begin{pmatrix} 1\\1\\0\\1 \end{pmatrix} - \frac{2}{15} \begin{pmatrix} 1\\-2\\3\\1 \end{pmatrix} = \begin{pmatrix} -4/5\\3/5\\3/5\\1/5 \end{pmatrix}$$

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Because the norms are, respectively, $\sqrt{3}$, $\sqrt{15}$, and $\sqrt{35}$, we will end up with the same orthonormal basis.

The Gram-Schmidt process can be applied to a dependent set, but it will sometimes produce $\mathbf{v}_j = \mathbf{0}$. In that case we discard \mathbf{x}_j and continue with the rest.

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So,
$$\mathbf{u}_1 = \begin{pmatrix} 1\\0\\0 \end{pmatrix}$$
, $\mathbf{u}_2 = \begin{pmatrix} 0\\1/\sqrt{2}\\1/\sqrt{2} \end{pmatrix}$, $\mathbf{u}_3 = \begin{pmatrix} 0\\-1/\sqrt{2}\\1/\sqrt{2} \end{pmatrix}$.

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So the transition matrix from \mathcal{B} to the standard basis \mathcal{C} is $Q^T A = (\mathbf{u}_i^T \mathbf{x}_j)$. But if i > j we know that \mathbf{u}_i is orthogonal to $\operatorname{Span}(\mathbf{u}_1, \ldots, \mathbf{u}_{i-1}) = \operatorname{Span}(\mathbf{x}_1, \ldots, \mathbf{x}_{i-1})$.

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The transition matrix from the basis $\mathcal{B} = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3]$ to the basis $\mathcal{C} = [\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3]$ has a particularly nice form.

The transition matrix from \mathcal{B} to the standard basis \mathcal{E} is $A = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 \end{pmatrix}$. The transition matrix from \mathcal{C} to the standard basis \mathcal{E} is $Q = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{pmatrix}$.

So the transition matrix from \mathcal{B} to the standard basis \mathcal{C} is $Q^T A = (\mathbf{u}_i^T \mathbf{x}_j)$. But if i > j we know that \mathbf{u}_i is orthogonal to $\operatorname{Span}(\mathbf{u}_1, \ldots, \mathbf{u}_{i-1}) = \operatorname{Span}(\mathbf{x}_1, \ldots, \mathbf{x}_{i-1})$. That is, $\mathbf{u}_i^T \mathbf{x}_j = 0$ when i > j. This means that $Q^T A$ is upper triangular. Something like this happens in every Gram-Scmidt process. Start with an $n \times k$ matrix A, whose columns are independent vectors $\mathbf{x}_1, \ldots, \mathbf{x}_k$ in \mathbb{R}^n . Apply Gram-Schmidt to them to get orthonormal vectors $\mathbf{q}_1, \ldots, \mathbf{q}_k$. If we let $Q = \begin{pmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_k \end{pmatrix}$ then $R = Q^T A$ is an upper triangular $k \times k$ matrix and A = QR where Q is an $n \times k$ with orthonormal columns. This is called the QR-factorization of A. If we let $Q = \begin{pmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_k \end{pmatrix}$ then $R = Q^T A$ is an upper triangular $k \times k$ matrix and A = QR where Q is an $n \times k$ with orthonormal columns. This is called the QR-factorization of A.

Note that R is a square matrix. Also its diagonals are $\mathbf{q}_j^T \mathbf{x}_j$. These are not zero because $\mathbf{q}_j = (1/\|\mathbf{v}_j\|)\mathbf{v}_j$ where \mathbf{v}_j has the form

 $\mathbf{v}_j = \mathbf{x}_j - (a \text{ linear combination of } \mathbf{v}_i, i < j)$

If we let $Q = \begin{pmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_k \end{pmatrix}$ then $R = Q^T A$ is an upper triangular $k \times k$ matrix and A = QR where Q is an $n \times k$ with orthonormal columns. This is called the QR-factorization of A.

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$$\mathbf{v}_j = \mathbf{x}_j - (a \text{ linear combination of } \mathbf{v}_i, i < j)$$

which means

 $\mathbf{x}_j = \mathbf{v}_j + (\text{a linear combination of } \mathbf{v}_i, i < j)$ and that says that $\mathbf{q}_j^T \mathbf{x}_j = (1/\|\mathbf{v}_j\|) \mathbf{v}_j^T \mathbf{v}_j = \|\mathbf{v}_j\| \neq 0.$ Examples: our first Gram-Schmidt example gives us

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad Q = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{15} & -4/\sqrt{35} \\ 1/\sqrt{3} & -2/\sqrt{15} & 3/\sqrt{35} \\ 0 & 3/\sqrt{15} & 3/\sqrt{35} \\ 1/\sqrt{3} & 1/\sqrt{15} & 1/\sqrt{35} \end{pmatrix}$$

and

$$Q^{T}A = R = \left(\begin{array}{ccc} 3/\sqrt{3} & 2/\sqrt{3} & 2/\sqrt{3} \\ 0 & 5/\sqrt{15} & 2/\sqrt{15} \\ 0 & 0 & 7/\sqrt{35} \end{array}\right)$$

Our second Gram-Schmidt example gives us:

$$A = \left(\begin{array}{rrr} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{array}\right), \quad Q = \left(\begin{array}{rrr} 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \end{array}\right)$$

Our second Gram-Schmidt example gives us:

$$A = \left(\begin{array}{rrr} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{array}\right), \quad Q = \left(\begin{array}{rrr} 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \end{array}\right)$$

and

$$Q^{T}A = R = \left(\begin{array}{rrr} 1 & 0 & 1\\ 0 & 2/\sqrt{2} & 1/\sqrt{2}\\ 0 & 0 & 1/\sqrt{2} \end{array}\right)$$

The QR factorization of A allows a simplified calculation of least squares problems.

The QR factorization of A allows a simplified calculation of least squares problems. Solving $A\mathbf{x} = \mathbf{b}$ with least squares would normally require solving $A^T A \mathbf{x} = A^T \mathbf{b}$.

But the columns of Q have the same span as the columns of A, and therefore $\mathcal{N}(A^T) = \mathcal{R}(A)^{\perp} = \mathcal{R}(Q)^{\perp} = \mathcal{N}(Q^T).$

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It is also particularly easy to solve because $Q^T A = R$ is upper triangular and $R\mathbf{x} = Q^T \mathbf{b}$ allows a relatively quick solution via back substitution.

$$\left(\begin{array}{rrrr} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{array}\right) \mathbf{x} = \left(\begin{array}{r} 1 \\ 2 \\ 3 \end{array}\right)$$

$$\left(\begin{array}{rrrr} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{array}\right) \mathbf{x} = \left(\begin{array}{r} 1 \\ 2 \\ 3 \end{array}\right)$$

Multiplying by Q^T gives

$$\left(\begin{array}{rrr} 1 & 0 & 1\\ 0 & 2/\sqrt{2} & 1/\sqrt{2}\\ 0 & 0 & 1/\sqrt{2} \end{array}\right) \mathbf{x} = \left(\begin{array}{r} 1\\ 5/\sqrt{2}\\ 1/\sqrt{2} \end{array}\right)$$

$$\left(\begin{array}{rrr}1 & 0 & 1\\0 & 1 & 0\\0 & 1 & 1\end{array}\right)\mathbf{x} = \left(\begin{array}{r}1\\2\\3\end{array}\right)$$

Multiplying by Q^T gives

$$\left(\begin{array}{rrr}1 & 0 & 1\\0 & 2/\sqrt{2} & 1/\sqrt{2}\\0 & 0 & 1/\sqrt{2}\end{array}\right)\mathbf{x} = \left(\begin{array}{r}1\\5/\sqrt{2}\\1/\sqrt{2}\end{array}\right)$$

This is a little easier to handle if we multiply the second and third rows (equations) by $\sqrt{2}$:

$$\left(\begin{array}{rrrr} 1 & 0 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{array}\right) \mathbf{x} = \left(\begin{array}{r} 1 \\ 5 \\ 1 \end{array}\right)$$

$$\left(\begin{array}{rrr}1 & 0 & 1\\0 & 1 & 0\\0 & 1 & 1\end{array}\right)\mathbf{x} = \left(\begin{array}{r}1\\2\\3\end{array}\right)$$

Multiplying by Q^T gives

$$\left(\begin{array}{ccc} 1 & 0 & 1\\ 0 & 2/\sqrt{2} & 1/\sqrt{2}\\ 0 & 0 & 1/\sqrt{2} \end{array}\right) \mathbf{x} = \left(\begin{array}{c} 1\\ 5/\sqrt{2}\\ 1/\sqrt{2} \end{array}\right)$$

This is a little easier to handle if we multiply the second and third rows (equations) by $\sqrt{2}$:

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{x} = \begin{pmatrix} 1 \\ 5 \\ 1 \end{pmatrix}$$

This has solution $\mathbf{x} = \begin{pmatrix} 0 & 2 & 1 \end{pmatrix}^T$.