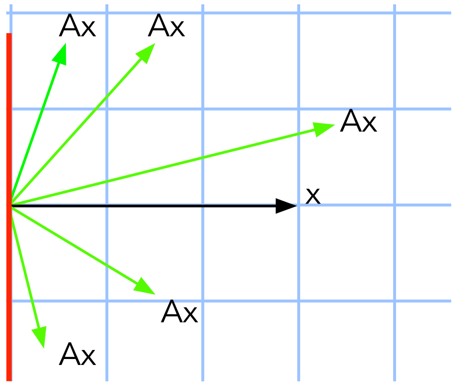

FIGURE 3.1. Positive definite matrix does not change the vector direction too much – no more than 90°.

3. LECTURES 5,6

Plan:
Symmetric and positive definite matrices.
More on norms of matrices. Useful inequalities.
Projectors.
SVD: Eckart-Young theorem.
QR factorization.

3.1. **Symmetric and positive definite matrices.** Here we explain the main properties of symmetric positive definite matrices. Symmetric means $A^T = A$, and transpose means that in the scalar product of two vectors (or functions, more generally), $x \cdot Ay$, if we move the matrix A over to x (transpose it), then we get the same answer: $x \cdot Ay = A^T x \cdot y$. Generally, such a transpose A^T will be different from A, but for symmetric matrices, it's the same.

For a derivative, the transpose will come from integration by parts

$$\int u \frac{d}{dx} v \, dx = uv|_b - \int v \frac{d}{dx} u \, dx = \int v \left(-\frac{d}{dx} \right) u \, dx.$$

So,

$$\left(\frac{d}{dx} \right)^T = -\frac{d}{dx}.$$

Definition. Matrix A is called positive definite if $x^T A x > 0$ for any $x \neq 0$.

Any A can be written as a sum of symmetric and skew-symmetric matrices: $A = \frac{1}{2}\left(A + A^T\right) + \frac{1}{2}\left(A - A^T\right) = A_+ + A_-$. Then $x^T A x = x^T A_+ x + x^T A_- x = x^T A_+ x$ since $x^T A_- x = 0$ for any x. Then A is positive definite if $sym\,(A) = A_+$ is positive definite. The fact $x^T A_- x = 0$ follows from the following. Note that $x^T A_- x = a$ is some number. We can transpose it and should get back the same: $a^T = a$ or, since $\left(x^T A_- x\right)^T = x^T A_-^T x = -x^T A_- x$, we get $a = -a$, that is $a = 0$.

Symmetric matrices enjoy many nice properties. They are also important in applications. For example, the matrix K that represented stiffnesses of springs in the spring-mass oscillator system,

$$\ddot{u} + Ku = 0,$$

was symmetric and also positive definite. This makes sure that its eigenvalues are all real and positive, which physically implies that the system is oscillatory, as the solution will consist of sines and cosines as opposed to exponentially decaying or growing functions. So positive definite K is basically a generalization of positive stiffness k for a single oscillator equation $\ddot{u} + ku = 0$.

Another example of a symmetric matrix came up when discretizing the differential equation

$$\phi'' + k^2(x)\,\phi = 0$$

from the second derivative operator. We have found the discrete version of this problem becomes

$$-Au + \omega^2 K u = 0,$$

with K diagonal with positive numbers on the diagonal, and A symmetric matrix with $(-1, 2, -1)$'s down its main diagonal. So

$$-\underbrace{\frac{d^2}{dx^2}}_{continuous} \to A = \underbrace{\begin{bmatrix} 2 & -1 & 0 & \cdots & \\ -1 & 2 & -1 & 0 & \\ 0 & -1 & 2 & -1 & 0 \\ \vdots & & \ddots & & -1 \\ & & & -1 & 2 \end{bmatrix}}_{discrete}.$$

That A here is positive definite again ensures that the eigenvalues of A give a physically reasonable solution of the spectral problem. More general eigenvalue problems of this sort arise in multiple dimensions with ϕ'' becoming the Laplacian $\Delta\phi = \phi_{xx} + \phi_{yy} + \phi_{zz}$. The operator $-\Delta$ (with proper boundary conditions) can be shown to be positive definite, which we will do later in the course.

One more example is given by the SVD that gives rise to symmetric matrices $A^T A$ and AA^T, which play a very important role in various applications that we will see in the future.

Claim. Symmetric matrices have real e-values.

Indeed, let $As = \lambda s$, then $A\bar{s} = \bar{\lambda}\bar{s}$ (the bar denotes complex conjugation) and

$$s^* A s = \lambda s^* s = \lambda\,|s|^2$$
$$s^T A \bar{s} = \bar{\lambda} s^T \bar{s} = \bar{\lambda}\overline{s^* s} = \bar{\lambda}\,|s|^2$$

(* means conjugate transpose). Now note that in the second line, $s^T A\bar{s} = \bar{s}^T A^T s = s^* A s$, which is the same as on the first line. Therefore, the rhs on both lines above must be the same, and so $\lambda = \bar{\lambda}$ and λ is real.

Claim. Symmetric positive definite matrices have positive e-values.

Clearly, since pos. def. means that $x^T A x > 0$, then this must be true for e-vectors. Then $s^T A s = \lambda s^T s = \lambda\,|s|^2 > 0$ implies $\lambda > 0$.

Claim. E-vectors of a symmetric matrix can be chosen orthogonal.

We prove this only for distinct e-values. Consider e-values λ_1 and $\lambda_2 \neq \lambda_1$: $As_1 = \lambda_1 s_1$ and $As_2 = \lambda_2 s_2$. Then

$$s_2^T A s_1 = \lambda_1 s_2^T s_1,$$
$$s_1^T A s_2 = \lambda_2 s_1^T s_2 = \lambda_2 s_2^T s_1.$$

Subtracting these expressions, we get $(\lambda_1 - \lambda_2)\, s_2^T s_1 = s_2^T A s_1 - s_1^T A s_2 = s_2^T A s_1 - s_2^T A^T s_1 = 0$. Therefore, $s_2^T s_1 = 0$.

Claim. E-vectors of a symmetric matrix are complete.

That is, e-vectors of a symmetric $n \times n$ matrix form a basis for $\mathbb{R}^n$. Skip the proof for now. We will see symmetric positive definite (s.p.d.) matrices many times in the future.

Positive definite matrices are important in solving minimization problems. We will return to it later. For now, let's look at an example.

Example 11. Consider a quadratic form

$$z = x^2 + 2xy + 3y^2 + 4x + 5y + 6$$

and ask a question: does this function z have a minimum? If yes, how do we find it?

This is how we proceed. Notice that $z = u^T A u + 2b^T u + d$, where $u = \begin{bmatrix} x & y \end{bmatrix}^T$, $b = \frac{1}{2}\begin{bmatrix} 4 & 5 \end{bmatrix}^T$, $d = 6$, and matrix A can be figured out from:

$$x^2 + 2xy + 3y^2 = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}, \quad A = \begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix}.$$

This matrix is symmetric and positive definite, as all the leading determinants are positive: 1 and 2. (Leading determinants are all determinants of submatrices of A formed by choosing top-left corners of A).

The minimum is found from

$$\frac{\partial z}{\partial u} = 0, \rightarrow Au + b = 0, \rightarrow u_0 = -A^{-1}b = \begin{bmatrix} 7/4 \\ 1/4 \end{bmatrix}.$$

Now shift the origin to this minimum point: let $v = u - u_0$. Then

$$\begin{aligned} z &= (u_0 + v)^T A (u_0 + v) + 2b^T (u_0 + v) + d = \\ &= u_0^T A u_0 + u_0^T A v + v^T A u_0 + v^T A v + 2b^T u_0 + 2b^T v + d = \\ &= -u_0^T b + 2u_0^T A v + v^T A v + 2b^T u_0 + 2b^T v + d = \\ &= 2v^T A u_0 + v^T A v + 2b^T v + b^T u_0 + d = \\ &= -2v^T b + v^T A v + 2v^T b + b^T u_0 + d = v^T A v + b^T u_0 + d = \\ &= v^T A v + e, \end{aligned}$$

where $e = d + b^T u_0$. Thus, in new variables $v = u - u_0$, the quadratic form has no linear terms. Furthermore, if we use $A = Q\Lambda Q^T$, then

$$z = v^T Q \Lambda Q^T v + e = \left(Q^T v\right)^T \Lambda \left(Q^T v\right) + e = \lambda_1 w_1^2 + \lambda_2 w_2^2 + e,$$

which shows how the quadratic form is positive and that the shape is a paraboloid with elliptic cross section. E-values of A determine the semi-axes of the ellipse.

We have also found the minimum value of z: $z_{min} = e = d + b^T u_0 = 81/8$.

This could also be found much easier simply plugging $Au_0 = -b$ into $z = u_0^T A u_0 + 2b^T u_0 + d = b^T u_0 + d$.

3.2. **More on norms of vectors and matrices.** Suppose, we have a symmetric matrix $A = A^T$, then $A = Q\Lambda Q^T$ where $Q^TQ = I$, and

$$\|A\|_2^2 = \max_{x\in\mathbb{R}^n} \frac{(Ax)^T Ax}{x^Tx} = \max_{x:\, x^Tx=1} x^TA^TAx = \max_{\|x\|=1} x^TQ\Lambda Q^TQ\Lambda Q^Tx =$$
$$= \max_{\|x\|=1} x^TQ\Lambda^2Q^Tx = \max_{\|x\|=1} \left(Q^Tx\right)^T \Lambda^2Q^Tx = \lambda_{max}^2.$$
$$\Rightarrow \|A\|_2 = |\lambda_{max}|\,.$$

Therefore, for a symmetric matrix A, its 2-norm is the magnitude of its largest eigenvalue.

If A is not symmetric or square, we use the SVD, $A = U\Sigma V^T$, and follow similar calculations

$$\|A\|_2^2 = \max_{\|x\|=1} x^TA^TAx = \sigma_{max}^2 = \sigma_1^2$$
$$\Rightarrow \|A\|_2 = \sigma_1.$$

since A^TA is symmetric and its largest e-value is σ_1.

- ⋄ Hölder inequality: for any vectors x, y, their p-norms satisfy

$$\left|x^Ty\right| \le \|x\|_p\|y\|_q,$$

where $1/p + 1/q = 1$.

- ⋄ Cauchy-Schwarz: take $p = q = 2$

$$\left|x^Ty\right| \le \|x\|_2\|y\|_2.$$

- ⋄ Matrix norms induced by the above vector norms simply follow from the definition given above

$$\|A\|_{(m,n)} = \sup_{x\in\mathbb{R}^n, \|x\|=1} \|Ax\|_{(m)},$$

where we are measuring the size of an $m \times n$ matrix A, such that $x \in \mathbb{R}^n$ while $Ax \in \mathbb{R}^m$.

- ⋄ Frobenius norm is not induced by vector norm:

$$\|A\|_F^2 = \sum_{i,j} |a_{ij}|^2 = \sum_j \|a_j\|_2^2 = Tr\left(A^TA\right) = Tr\left(AA^T\right).$$

It is a sum of squares of all the elements of the matrix A. That is, if one makes a long vector by stacking all columns of A, then the Frobenius norm of A is the 2-norm of that long vector. The second summation above states the same – it is the sum of squared norms of all the columns a_j of A.

The trace equality above follows directly if we write out

$$A^TA = \left[A^Ta_1\ A^Ta_2\ \ldots\right] = \begin{bmatrix} a_1^Ta_1 & a_1^Ta_2 & \ldots \\ a_2^Ta_1 & a_2^Ta_2 & \\ \vdots & & \end{bmatrix}.$$

If we use the SVD of A, then using the fact that the trace of a matrix is the sum of its e-values, we get

$$\|A\|_F^2 = Tr\left(A^TA\right) = \sum_i \sigma_i^2.$$

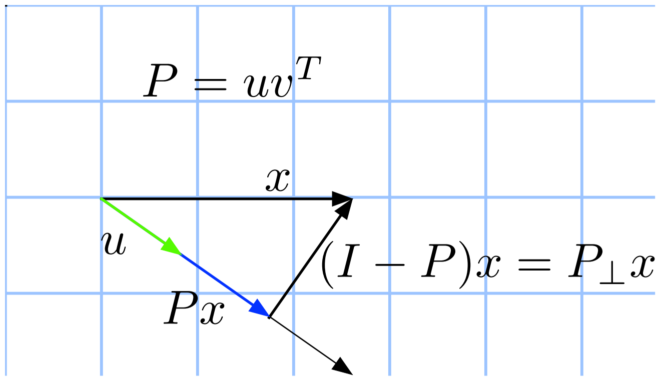

FIGURE 3.2. Orthogonal projections by the rank-one matrix $P = uv^T$.

One can also establish the inequality

$$\|AB\|_F^2 \leq \|A\|_F^2 \|B\|_F^2$$

and invariance of the 2-norm as well as the Frobenius norm under orthogonal transformation. That is A and QA have the same norm with Q orthogonal.

3.3. **Projectors.** Recall that $P = uv^T$ is a matrix that converts any vectors x to a vector pointing in the direction of u: $Px = u\left(v^T x\right) = \alpha u$, where $\alpha = v^T x$ is a scalar.

Generally, uv^T will align vectors with u, but not project them orthogonally. The matrix will be a projection if the difference between x and Px is orthogonal to Px:

$$(Px)^T (x - Px) = 0.$$

(Now P is assumed square, as otherwise x and Px live in different spaces). That is

$$x^T P^T (x - Px) = x^T P^T x - x^T P^T P x = 0.$$

Any symmetric matrix with $P^T P = P^2 = P$ will satisfy this condition.

That is, P^2 should be the same as P, as the double projection should do nothing more than a single projection. For $P = uv^T$, we get $P^2 = uv^T uv^T = u\left(v^T u\right) v^T = \left(v^T u\right) uv^T = P$ provided $v^T u = 1$. For example, if $v = u$ and $u^T u = 1$, then $P = uu^T$ is the true orthogonal projection matrix to the direction of u.

More generally, $P = QQ^T$ with $Q^T Q = I$ is an orthogonal projection to the subspace spanned by the columns of Q. Indeed, both symmetry, $P^T = P$, and $P^2 = QQ^T QQ^T = QQ^T = P$ are satisfied.

Always Px is in the column space of P. If Q is orthogonal, then $P = QQ^T$ projects to the basis $\{q_i\}$ that make Q: $Q = [q_1 q_2 \ldots]$.

If P projects onto subspace S, then $P_\perp = I - P$ is a projector to subspace $\perp S$. That it is a projector follows from

$$(I - P)^2 = I - P - \left(P - P^2\right) = I - 2P + P^2 = I - 2P + P = I - P.$$

3.4. **More SVD:** $A = U\Sigma V^T$ **.** The theorem by Eckart and Young is the main result on SVD allowing for an approximation of A.

Theorem 12. *(Eckart-Young). Let matrix B have rank$(B) = k$ (more generally, rank$(B) \leq k$). Then $\|A - B\| \geq \sigma_{k+1} = \|A - A_k\|$, where the norms are 2-norms. That is, of all matrices of rank k, the matrix closest to A in 2-norm is $A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$.*

Proof. Recall that

$$\|A - B\| = \max \frac{\|(A - B)\, x\|}{\|x\|},$$

and if we can identify such an x that the ratio $\|(A - B)\, x\|/\|x\|$ is at least σ_{k+1}, then the norm $\|A - B\|$ can only get larger for other x.

That x is found from the nullspace of B: $Bx = 0$. How do we know that such an $x \neq 0$ exists?

The nullspace of B has dimension $n - k$. Take $x \neq 0$, $x \in \mathbb{R}^n$ from that nullspace.

Now take subspace S_k of A spanned by $k+1$ right singular vectors $\{v_1, v_2, \ldots, v_{k+1}\}$, $Av_i = \sigma_i u_i$. We claim that the nullvector x can be expanded in the basis of S_k as $x = \sum_{i=1}^{k+1} c_i v_i$. Why? Because the dimensions of the subspace S_k and $N(B)$ add to $n+1$: $n - k + k + 1 = n + 1$, which is bigger than n, and therefore, $N(B)$ and S_k must intersect, i.e. they have to share a vector. That vector is x. Think of two planes in space $\mathbb{R}^3$. They have to either intersect or coincide (subspaces must go through the origin, i.e. they must contain the zero vector 0).

Now, having the vector x that belongs to both $N(B)$ and S_k, we can write

$$\|(A - B)\, x\|^2 = \|Ax\|^2 = \|\sum_{i=1}^{k+1} c_i \sigma_i u_i\|^2 = \sum_{i=1}^{k+1} c_i^2 \sigma_i^2 \geq \sigma_{k+1}^2 \sum_{i=1}^{k+1} c_i^2 = \sigma_{k+1}^2 \|x\|^2.$$

Therefore, for this particular x, we get

$$\frac{\|(A - B)\, x\|}{\|x\|} \geq \sigma_{k+1}.$$

There may be some other x that can give even a larger value for this ratio, but in any case, the norm $\|A - B\|$ will be at least this large. Therefore, we have established the required inequality

$$\|A - B\| \geq \|A - A_k\| = \sigma_{k+1}.$$

□

3.5. **Some consequences of SVD.**

3.5.1. *Basis of matrices.* The representation of $A = U\Sigma V^T$ as

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + ... + \sigma_r u_r v_r^T$$

is an expansion in "orthogonal"[1] basis matrices

$$A = \sigma_1 A_1 + \sigma_2 A_2 + \ldots + \sigma_r A_r$$

like a vector is expanded in the basis vectors

$$x = x_1 s_1 + x_2 s_2 + \ldots + x_r s_r.$$

Except now we have rank-1 matrices instead of the basis vectors. But these matrices share the same nice properties as basis vectors. For example, different basis matrices are "orthogonal" to each other in the sense that

$$A_i^T A_j = v_i u_i^T u_j v_j^T = v_i \left(u_i^T u_j\right) v_j^T = 0, \quad i \neq j$$

[1]Not in the same sense as $Q^T Q = I$

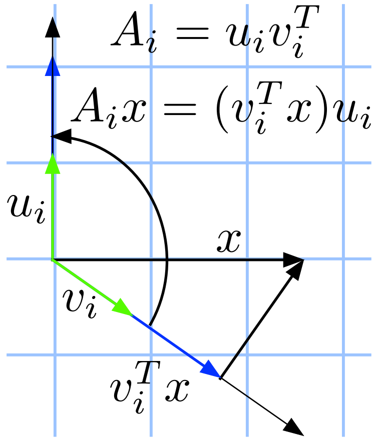

FIGURE 3.3. Action of the rank-one matrix $A_i = u_i v_i^T$ on a vector x: first, find the component $v_i^T x$ of x along v_i, then align that component along u_i.

and

$$A_i^T A_i = v_i v_i^T$$

is a projection to v_i. Its 2-norm is $\max\left\{\|v_i v_i^T x\|/\|x\|\right\} = \max\left\{\|v_i x_i\|/\|x\|\right\} = \max\left\{\|x\|/\|x\|\right\} = 1$.

What does A_i do to a vector x? Look at:

$$A_i x = \left(v_i^T x\right) u_i.$$

It takes the component of x along v_i, $v_i^T x$, and creates a vector with the same component, but along u_i. So it rotates the part of x that was along v_i to point along u_i. Then, what matrix $\sigma_i A_i$ does, it additionally stretches that vector by a factor of σ_i.

The full expansion $A = \sum \sigma_i A_i$ will be a sequence of such rotations and stretches. The largest stretch is made by the first term $\sigma_1 A_1$. All others will do rotations, but with less stretching.

3.5.2. *The first singular vector.* We next look even more carefully at the first singular vector v_1. We want to solve the problem:

Problem 13. Determine the maximum value of $\|Ax\|/\|x\|$.

Solution. We know the solution is σ_1 and it corresponds to $x = v_1$. But we now pretend we do not know SVD and want to get the solution without using it, by direct calculation of the derivative. Consider the function $R(x) = \|Ax\|^2/\|x\|^2$ (Rayleigh quotient) and look for its maximum, that will be the maximum of $\|Ax\|/\|x\|$ squared. Then

$$R(x) = \frac{x^T A^T A x}{x^T x} = \frac{x^T S x}{x^T x},$$

and

$$\begin{aligned}
\frac{\partial R}{\partial x_i} &= \frac{1}{x^T x}\frac{\partial}{\partial x_i}\sum_{k,l} s_{kl}x_k x_l - \frac{x^T S x}{(x^T x)^2}\frac{\partial}{\partial x_i}\sum_k x_k^2 = \\
&= \frac{1}{x^T x}\left(\sum_l s_{il}x_l + \sum_k s_{ki}x_k\right) - \frac{x^T S x}{(x^T x)^2}2x_i = \\
&= \frac{2}{x^T x}\left[(Sx)_i - \frac{x^T S x}{x^T x}x_i\right] = 0.
\end{aligned}$$

Therefore, $Sx = \lambda x$ and $R = \lambda$ is the e-value of S that maximizes the function $R(x)$. The maximum value is λ and it happens at the corresponding e-vector x of S. Since $S = A^T A$, then these e-value and e-vector are the first singular value squared σ_1^2 and its corresponding right e-vector v_1.

We could move on and ask further questions. For example: Find the maximum of $R(x)$, but now only among x that are perpendicular to v_1. Then we get a constrained maximization problem:

Problem 14. Determine the maximum value of $\|Ax\|/\|x\|$ subject to $x^T v_1 = 0$.

Solution. This time the solution is σ_2 and it corresponds to $x = v_2$. It is found using the Lagrange multipliers.

One can proceed in the same way to find out that singular values maximize the Rayleigh quotient subject to orthogonality to all previous singular vectors.

3.6. QR factorization: $A = QR$, Q orthogonal, R upper triangular

3.6.1. *QR factorization.* Let the $m \times n$ matrix

$$A = \begin{bmatrix} \vdots & \vdots & & \vdots \\ a_1 & a_2 & \dots & a_n \\ \vdots & \vdots & & \vdots \end{bmatrix},$$

have independent columns and assume $m \geq n$. Then the columns of A form a basis for the n dimensional subspace of $\mathbb{R}^m$. Using the columns a_k we can construct an orthonormal basis by the Gram-Schmidt process which proceeds as follows.

Take a_1 and normalize it to get $q_1 = a_1/\|a_1\|$. Then take a_2, subtract from it its component along q_1 (projection p of a_2 onto q_1, see Figure), so that the result is orthogonal to q_1: let

$$b_2 = a_2 - cq_1,$$

then require

$$b_2^T q_1 = 0 = a_2^T q_1 - cq_1^T q_1.$$

From here

$$c = \frac{a_2^T q_1}{q_1^T q_1} = a_2^T q_1$$

since the length of q_1 is 1. Then

$$b_2 = a_2 - \left(a_2^T q_1\right) q_1 = a_2 - q_1\left(a_2^T q_1\right) = a_2 - q_1\left(q_1^T a_2\right) = a_2 - \left(q_1 q_1^T\right) a_2.$$

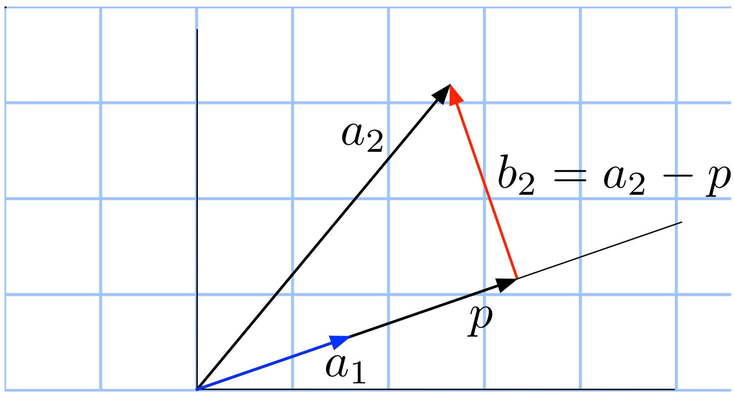

FIGURE 3.4. Orthogonalizing independent vectors a_1 and a_2 by Gram-Schmidt process.

Please notice the motion of parentheses here that lead to the projection $p = \left(a_2^T q_1\right) q_1$ of a_2 onto q_1 to become $p = \left(q_1 q_1^T\right) a_2 = P_1 a_2$, where $P_1 = q_1 q_1^T$ is the rank-one *projection matrix* that, when multiplied by any vector u, takes its projection onto q_1: $P_1 u$ is the projection of u onto q_1.

Now we have orthogonalized two columns of A so that from a_1 and a_2 two orthonormal vectors q_1 and $q_2 = b_2/\|b_2\|$ were constructed.

The next one comes along the same lines: let

$$b_3 = a_3 - c_1 q_1 - c_2 q_2$$

and choose c_1 and c_2 so that b_3 is orthogonal to both q_1 and q_2. These two conditions result in $c_1 = q_1^T a_3$ and $c_2 = q_2^T a_3$ so that

$$b_3 = a_3 - q_1 q_1^T a_3 - q_2 q_2^T a_3 = a_3 - P_2 a_3.$$

Here

$$P_2 = q_1 q_1^T + q_2 q_2^T$$

is the rank-two projection matrix. For any vector u, $P_2 u$ is the projection of u onto the plane formed by the orthonormal vectors q_1 and q_2. Now it is clear how the next q_k's must be constructed. Just take a_k and subtract from it its projection onto the subspace spanned by q_1, q_2, ..., q_{k-1}, to obtain b_k and normalize to get q_k.

Now we have constructed the $m \times n$ matrix

$$Q = \begin{bmatrix} \vdots & \vdots & & \vdots \\ q_1 & q_2 & \dots & q_n \\ \vdots & \vdots & & \vdots \end{bmatrix}$$

which has orthonormal columns:

$$Q^T Q = \begin{bmatrix} \vdots & \vdots & & \vdots \\ Q^T q_1 & Q^T q_2 & \dots & Q^T q_n \\ \vdots & \vdots & & \vdots \end{bmatrix} = I.$$

Indeed,

$$Q^T q_k = \begin{bmatrix} \dots & q_1^T & \dots \\ \dots & q_2^T & \dots \\ \dots & \vdots & \dots \end{bmatrix} q_k = \begin{bmatrix} q_1^T q_k \\ q_2^T q_k \\ \vdots \\ q_k^T q_k \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

has zeros everywhere because of the orthogonality of $q's$, except for 1 in the $k-th$ position because $q's$ are normalized.

The question we ask now is:

What is the matrix R that connects A and Q by the above Gram-Schmidt process?

The answer is found by looking at the product

$$Q^T A = \begin{bmatrix} \vdots & \vdots & & \vdots \\ Q^T a_1 & Q^T a_2 & \dots & Q^T a_n \\ \vdots & \vdots & & \vdots \end{bmatrix} = \begin{bmatrix} q_1^T a_1 & q_1^T a_2 & \dots & q_1^T a_n \\ q_2^T a_1 & q_2^T a_2 & \dots & q_2^T a_n \\ q_3^T a_1 & q_3^T a_2 & \dots & q_3^T a_n \\ \vdots & \vdots & \dots & \vdots \\ q_n^T a_1 & q_n^T a_2 & \dots & q_n^T a_n \end{bmatrix} = \begin{bmatrix} q_1^T a_1 & q_1^T a_2 & \dots & q_1^T a_n \\ 0 & q_2^T a_2 & \dots & q_2^T n \\ 0 & 0 & \dots & q_3^T a_n \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & q_n^T a_n \end{bmatrix} = R.$$

The matrix R is upper triangular because, by Gram-Schmidt construction, q_2 is orthogonal to a_1, q_3 is orthogonal to a_1 and a_2, q_4 is orthogonal to a_1, a_2, and a_3, and so on, so that the components below the main diagonal of $Q^T A$ are all zero. Then

$$A = QR$$

is the sought-for factorization. Q has the same shape $m \times n$ as A, and R is square, $n \times n$.

Thus, *any matrix A with independent columns can be written as a product of an orthogonal matrix and upper triangular matrix.* One problem when this is helpful is that of solving a linear system. Suppose we need to solve $Ax = b$. Then with $A = QR$ we get $QRx = b$ and multiplying from left by Q^T we end up with a triangular system to solve: $Rx = Q^T b$.

Example. Suppose $A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$. Then $q_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$ and

$$b_2 = \left(I - q_1 q_1^T\right) \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ 1 \end{bmatrix}.$$

Then $q_2 = \frac{1}{\sqrt{3/2}} \begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ 1 \end{bmatrix}$ and $Q = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{2}{\sqrt{6}} \end{bmatrix}$. R is found as

$$R = \begin{bmatrix} q_1^T a_1 & q_1^T a_2 \\ 0 & q_2^T a_2 \end{bmatrix} = \begin{bmatrix} \sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & \frac{3}{\sqrt{6}} \end{bmatrix}$$

and

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{2}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} \sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & \frac{3}{\sqrt{6}} \end{bmatrix}.$$

3.7. **Right polar decomposition: $A = QB$, Q orthogonal, B symmetric positive definite.** Question: In a given matrix A, can we somehow separate rotation and stretch?

We know that an orthogonal matrix, Q, represents pure rotation that does not change the lengths of vectors. Then can we find B which is positive definite?

The question stems from the analogy with polar representation of complex numbers: $z = e^{i\vartheta} r$ has rotation $e^{i\vartheta}$, and stretch $r > 0$, so that $e^{i\vartheta} \cdot e^{-i\vartheta} = 1$ and $\sqrt{z^* z} = r$. Complex conjugation plays a role of transpose.

By analogy, we try $B = \sqrt{A^T A}$, which is symmetric positive definite and luckily, find that $Q = AB^{-1}$ is indeed orthogonal:

$$Q^T Q = \left(AB^{-1}\right)^T AB^{-1} = B^{-1}\left(A^T A\right) B^{-1} = B^{-1} B^2 B^{-1} = I.$$

To compute the right polar decomposition, first construct $B = \sqrt{A^T A}$, and then calculate $Q = AB^{-1}$. Note that there is also the *left polar decomposition*, $A = CQ$, with $C = \sqrt{AA^T}$ and $Q = C^{-1} A$.

How does one calculate the square root of a matrix?

For symmetric positive definite matrix A, the positive definite square root is found using the spectral factorization $A = S\Lambda S^{-1}$, where S contains eigenvectors of A and Λ is a diagonal matrix with eigenvalues on the diagonal, as

$$\sqrt{A} = S\sqrt{\Lambda} S^{-1}.$$

Note that for general matrices, the square root may not exist or may not be unique. For example, both

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

are square roots of $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, but only the second one is positive definite, while $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ has no square root at all.

3.8. **General orthogonal projectors.** .... Recall that $P = qq^T$ with an orthonormal q, $m \times 1$, is an orthogonal projector onto q. If orthonormal vectors q_i, $i = 1, 2, \ldots, n$, are put in a matrix $Q = [q_1 q_2 \ldots]$, then Q is $m \times n$ and $P = QQ^T$ is an orthogonal projector onto the *span* $\{q_i\}$. Indeed, $Px = QQ^T x = Qy = y_1 q_1 + y_2 q_2 + \ldots$, where $y = Q^T x$. Note $Q^T Q$ does not exist unless $m = n$.

When a is not of unit length, we let

$$P = \frac{aa^T}{a^T a}$$

to obtain the orthogonal projection matrix.

Now we ask the question: Can we construct an orthogonal projection starting with a basis that is not orthonormal? Suppose we have a subspace spanned by the linearly independent set of vectors $\{a_1, a_2, \ldots, a_n\}$, and would like to build a projector onto that subspace.

Let A, $m \times n$, have columns a_j. We want to project an arbitrary vector b to the range of A.

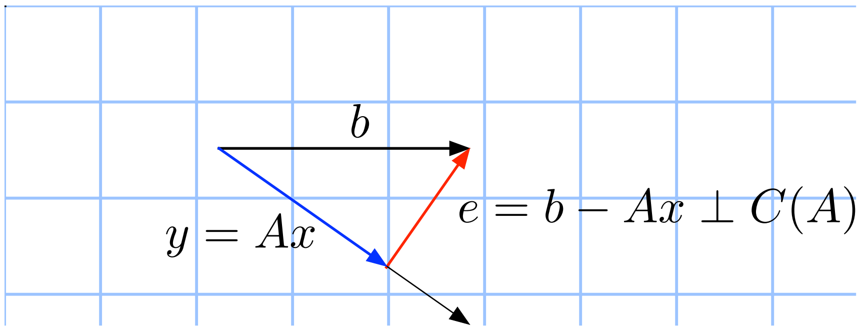

FIGURE 3.5. For any b, we want to project it onto the range of A. If b is not in the range of A, then there will be some error $e = b - Ax$ that is perpendicular to the range of A.

Suppose the projection is $y = Ax$, then the error vector $e = b - Ax$ must be orthogonal to the range of A:

$$\begin{aligned} a_j^T (b - Ax) &= 0 \\ A^T (b - Ax) &= 0 \\ A^T A x &= A^T b. \end{aligned}$$

Therefore, using the fact that $A^T A$ is not singular due to the linear independence of columns of A, we obtain the solution

$$x = \left(A^T A\right)^{-1} A^T b.$$

The projection is then

$$y = Ax = A\left(A^T A\right)^{-1} A^T b = Pb,$$

where the projector is

$$P = A\left(A^T A\right)^{-1} A^T. \tag{3.1}$$

Notice how this generalizes

$$P = \frac{aa^T}{a^T a} = \left(a^T a\right)^{-1} aa^T = a\left(a^T a\right)^{-1} a^T.$$

Thus (3.1) defines the orthogonal projection onto a subspace spanned by arbitrary linearly independent vectors $\{a_j\}$.