Understanding the Singular Value Decomposition Rigorously

Let X be a real $n \times p$ matrix. I'll assume that $n \geq p$ for simplicity. It's natural to ask in which direction v does multiplication by the matrix A have the most impact (or the most explosiveness, or the most amplifying power). The answer is

$$v_1 \;=\; \arg\max_{w \in \mathbb{R}^p} \| \, Xw \, \|_2 \quad \text{subject to} \quad \|w\|_2 = 1, \tag{1}$$

where $\| \cdot \|_2$ denotes the L^2-norm. A natural follow-up question is, after v_1, what is the next most explosive direction for X? The answer is

$$v_2 \;=\; \arg\max_{w \in \mathbb{R}^n} \| \, Xw \, \|_2 \quad \text{subject to} \quad \langle v_1, w \rangle = 0, \;\; \|w\|_2 = 1.$$

Continuing like this, we obtain an orthonormal basis $v_1, \ldots, v_n$ of $\mathbb{R}^n$. This special basis of $\mathbb{R}^p$ tells us the directions that are, in some sense, most important for understanding X.

Let $\delta_j = \| \, Xv_j \|_2$ (so δ_i quantifies the explosive power of X in the direction v_j). Suppose that unit vectors u_i are defined so that

$$Xv_j = \delta_i \, u_j \quad \text{for} \quad j = 1, \ldots, p. \tag{2}$$

The equations (2) can be expressed concisely using matrix notation as

$$XV \;=\; UD, \tag{3}$$

where V is the $p \times p$ matrix whose jth row is v_j, U is the $n \times p$ matrix whose jth column is u_j, and D is the $n \times n$ diagonal matrix whose jth diagonal entry is δ_j. The matrix V is orthogonal by construction, so we can multiply both sides of (3) by V^T to obtain

$$X \;=\; UDV^T.$$

It might appear that we have now derived the SVD of A with almost zero effort. None of the steps so far have been difficult. However, a crucial piece of the picture is missing — we do not yet know that the columns of U are pairwise orthogonal.

Here is the crucial fact, the missing piece: it turns out that Xv_1 is orthogonal to Xv_2:

$$\langle Xv_1, \, Xv_2 \rangle \;=\; 0. \tag{4}$$

The argument goes that *if this were not true*, then v_1 would not be optimal for problem (1). Indeed, if (4) were not satisfied, then it would be possible to *improve* the choice of v_1 in terms of explosiveness by perturbing it a bit in the direction v_2.

Here's the idea behind the argument:
Suppose (for sake of contradiction) that (4) is not satisfied. If v_1 is perturbed slightly in the orthogonal direction v_2, the norm of v_1 does not change (or at least, the change in the norm of v_1 is negligible). *When I walk on the surface of the earth, my distance from the center of the earth does not change.* However, when v_1 is perturbed in the direction v_2, the vector Xv_1 is perturbed in the *non-orthogonal* direction Xv_2, and so the change in the norm of Xv_1 is non-negligible. The norm of Xv_1 can be increased by a non-negligible amount. This means that v_1 is not optimal for problem (1), which is a contradiction.

A similar argument shows that Xv_3 is orthogonal to both Xv_1 and Xv_2, and so on. The vectors $Xv_1, \ldots, Xv_n$ are pairwise orthogonal. This means that the unit vectors $u_1, \ldots, u_n$ can be shown to be pairwise orthogonal, since $Xv_j = \delta_j u_j$, whose direction is entirely dictated by u_j. This completes our discovery of the SVD.

Making the argument rigorous.

To convert the above intuitive argument into a rigorous proof, we must confront the fact that if v_1 is perturbed in the direction v_2, the perturbed vector

$$\tilde{v}_1 = v_1 + \epsilon\, v_2$$

is not truly a unit vector. Its norm is $\sqrt{1+\epsilon^2}$. To obtain a rigorous proof, define

$$\tilde{v}_1(\epsilon) \;=\; (\sqrt{1-\epsilon^2})\; v_1 \;+\; \epsilon\, v_2.$$

Then the vector $\tilde{v}_1(\epsilon)$ is truly a unit vector. But as you can easily show, if (4) is not satisfied, then for sufficiently small values of ϵ we have

$$f(\epsilon) \;=\; \|\, A\, \tilde{v}_1(\epsilon)\|_2^2 \;>\; \|\, A\, v_1\|_2^2$$

(assuming that the sign of ϵ is chosen correctly). To show this, just check that $f'(0) \neq 0$. This means that v_1 is not optimal for problem (1), which is a contradiction.

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Thanks go to Daniel O'Connor from the Math dept. for this cool argument!