Derivation of Normal Equations

One of the main topics of this course has been when and how can you solve an equation of the form $A\boldsymbol{x} = \boldsymbol{b}$. For the how we use Gaussian elimination, i.e., reduced row echelon form. The when we've answered by saying the system of equations has a solution if and only if $\boldsymbol{b} \in \mathrm{CS}(A)$. So what do we do if we know the system must have a solution, but it can't because $\boldsymbol{b} \notin \mathrm{CS}(A)$.

One answer to this problem is to find an $\boldsymbol{x}$ such that $A\boldsymbol{x}$ is as close as possible to $\boldsymbol{b}$. The following describes one way to do this. But before getting to this we need a definition and theorem.

Definition 1. *Let $\mathcal{M}$ and $\mathcal{N}$ be two subsets of a vector space $\mathcal{V}$. We say these subsets are orthogonal if*

$$\forall \boldsymbol{m} \in \mathcal{M} \text{ and } \forall \boldsymbol{n} \in \mathcal{N}, \quad \langle \boldsymbol{m}, \boldsymbol{n} \rangle = 0\,.$$

Theorem 1. *Let $\mathcal{M}$ and $\mathcal{N}$ be two orthogonal subspaces of a vector space $\mathcal{V}$, and suppose*

$$\dim(\mathcal{M}) + \dim(\mathcal{N}) = dim(\mathcal{V})\ .$$

Then for every $\boldsymbol{x} \in \mathcal{V}$, there is a unique $\boldsymbol{m} \in \mathcal{M}$ and $\boldsymbol{n} \in \mathcal{N}$ such that

$$\boldsymbol{x} = \boldsymbol{m} + \boldsymbol{n}\,.$$

More over we have $\boldsymbol{m} = Proj_{\mathcal{M}}\boldsymbol{x}$ and $\boldsymbol{n} = Proj_{\mathcal{N}}\boldsymbol{x}$.

Proof: Let $\{\boldsymbol{u}_i\}_{i=1}^n$ be an orthonormal basis of $\mathcal{V}$ such that $\{\boldsymbol{u}_i\}_{i=1}^k$ is an orthonormal basis of $\mathcal{M}$, and $\{\boldsymbol{u}_i\}_{i=k+1}^n$ is an orthonormal basis of $\mathcal{N}$. The facts that these two subspaces are orthogonal to each other, and their dimensions add up to the dimension of $\mathcal{V}$ ensures that there is such a basis. Then for any $\boldsymbol{x} \in \mathcal{V}$ we have

$$\boldsymbol{x} = \sum_{i=1}^{n} < \boldsymbol{x}, \boldsymbol{u}_i > \boldsymbol{u}_i = \sum_{i=1}^{k} < \boldsymbol{x}, \boldsymbol{u}_i > \boldsymbol{u}_i + \sum_{i=k+1}^{n} < \boldsymbol{x}, \boldsymbol{u}_i > \boldsymbol{u}_i = Proj_{\mathcal{M}}\boldsymbol{x} + Proj_{\mathcal{N}}\boldsymbol{x}$$

So we've shown that such a sum is possible. To see that it is unique suppose that we have:

$$\boldsymbol{x} = \boldsymbol{m}_1 + \boldsymbol{n}_1 = \boldsymbol{m}_2 + \boldsymbol{n}_2\,,$$

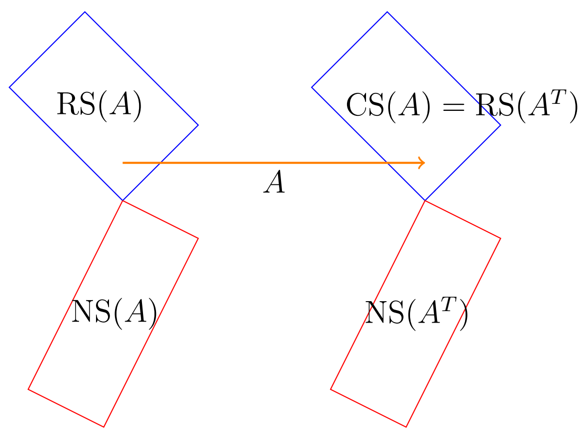
where the $\boldsymbol{m}_i \in \mathcal{M}$ *and* $\boldsymbol{n}_i \in \mathcal{N}$*. This implies*

$$\boldsymbol{m}_1 - \boldsymbol{m}_2 = \boldsymbol{n}_2 - \boldsymbol{n}_1 \,,$$

Thus, $\boldsymbol{m}_1 - \boldsymbol{m}_2 \in \mathcal{M} \cap \mathcal{N}$*. This implies that* $\boldsymbol{m}_1 - \boldsymbol{m}_2$ *is perpendicular to itself, which means that* $\boldsymbol{m}_1 - \boldsymbol{m}_2 = 0$*, and this implies* $\boldsymbol{n}_2 - \boldsymbol{n}_1 = 0$ *too. Thus, there is only one way to write* $\boldsymbol{x}$ *as the sum of a vector in* $\mathcal{M}$ *plus a vector in* $\mathcal{N}$*.*

Theorem 1 can be generalized, but we will not do so here.

The following picture is instructive. Let's assume that A is an $m \times n$ matrix with real entries. Then $\mathbb{R}^n$ and $\mathbb{R}^m$ can be thought of as the sum of two orthogonal subspaces. For $\mathbb{R}^n$ we have the row space of A and the null space of A, while for $\mathbb{R}^m$ we have the row space of A^T, which equals the column space of A, and the null space of A^T.



Since $\boldsymbol{x} \in \mathrm{NS}(A)$ means $A\boldsymbol{x} = \mathbf{0}$, it's clear that $\boldsymbol{x} \in \mathrm{NS}(A)$ if and only if $\boldsymbol{x}$ is perpendicular to each row of A, and hence to the span of those rows, which is the RS(A). We also know that $\dim(\mathrm{RS}(A)) + \dim(\mathrm{NS}(A)) = \dim(\mathbb{R}^n)$. Thus, (cf. Theorem 1) every vector $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{b} \in \mathbb{R}^m$ satisfies

$$\boldsymbol{x} = \mathrm{Proj}_{\mathrm{RS}(A)}\boldsymbol{x} + \mathrm{Proj}_{\mathrm{NS}(A)}\boldsymbol{x}, \quad \boldsymbol{b} = \mathrm{Proj}_{\mathrm{CS}(A)}\boldsymbol{b} + \mathrm{Proj}_{\mathrm{NS}(A^T)}\boldsymbol{b} \qquad (1)$$

We now come to the main result of this note, which is a very simple way to find solutions to the equation $A\boldsymbol{x} = \text{Proj}_{\text{CS}(A)}\boldsymbol{b}$.

Theorem 2. *Let A be an $m \times n$ matrix. Then $\boldsymbol{x} \in \mathbb{R}^n$ satisfies*

$$A\boldsymbol{x} = Proj_{CS(A)}\boldsymbol{b} \tag{2}$$

if and only if $\boldsymbol{x}$ satisfies

$$A^T A\boldsymbol{x} = A^T\boldsymbol{b}\,. \tag{3}$$

Suppose first that $\boldsymbol{x}$ satisfies the equation $A\boldsymbol{x} = \text{Proj}_{\text{CS}(A)}\boldsymbol{b}$. We note that $\boldsymbol{b} - \text{Proj}_{\text{CS}(A)}\boldsymbol{b}$ is in the null space of A^T. ($\boldsymbol{b} = \text{Proj}_{\text{CS}(A)}\boldsymbol{b} + \text{Proj}_{\text{NS}(A^T)}\boldsymbol{b}$). Thus,

$$\begin{aligned} \mathbf{0} \;&=\; A^T\left(\boldsymbol{b} - \text{Proj}_{\text{CS}(A)}\boldsymbol{b}\right) = A^T(\boldsymbol{b} - A\boldsymbol{x}) \\ &\quad \text{or } A^T A\boldsymbol{x} = A^T\boldsymbol{b} \end{aligned}$$

Now suppose that $\boldsymbol{x}$ satisfies the equation $A^T A\boldsymbol{x} = A^T\boldsymbol{b}$. This says that $\boldsymbol{b} - A\boldsymbol{x}$ is in the null space of A^T, and we have

$$\boldsymbol{b} = A\boldsymbol{x} + (\boldsymbol{b} - A\boldsymbol{x})\ . \tag{4}$$

Now from Theorem 1 we know that $\boldsymbol{b} = \text{Proj}_{CS(A)}\boldsymbol{b} + \text{Proj}_{NS(A^T)}\boldsymbol{b}$, and that this is unique. However, Equation 4 already expresses $\boldsymbol{b}$ as sum of such vectors. Thus, we must have

$$A\boldsymbol{x} = \text{Proj}_{CS(A)}\boldsymbol{b}\,.$$