Least square problem

Consider a linear system $\vec{A}\vec{x} = \vec{b}$. if $\vec{b} \notin \operatorname{col}\vec{A}$, this equation has no solutions. However, we can use the method of **least squares** to find the **best solution**.

We define $\vec{A}_{m\times n}, \vec{b} \in \mathbb{R}^n$. A **least squares solution** of $\vec{A}\vec{x} = \vec{b}$ is $\hat{x} \in \mathbb{R}^n$ such that $||\vec{b} - \vec{A}\hat{x}|| \leq ||\vec{b} - \vec{A}\vec{x}|| \ \forall \ \vec{x} \in \mathbb{R}^n$. We can use orthogonal projections to solve this, since we know that the orthogonal projection of a point P to a subspace π is the (not necessarily unique) point in π with the minimal distance to p. This can be seen by substituting $\vec{A}\hat{x} = \hat{b}$ into the above equation. So, we know that the least squares solution is the solution to $\vec{A}\hat{x} = proj_{\operatorname{col}\vec{A}}\vec{b}$. However, this is a very difficult way to compute it.

Alternatively, we know that $\vec{b} - \hat{b} \perp \operatorname{col}\vec{A} \iff \vec{b} - \hat{b} \perp \vec{a}_i, 1 \leq i \leq n$, where $\vec{a}_i$ are the columns of $\vec{A}$. This can also be expressed using the inner product, as $\vec{a}_i^T\left(\vec{b} - \hat{b}\right) = 0, 1 \leq i \leq n \implies \vec{A}^T\left(\vec{b} = \hat{b}\right) = 0 \implies \vec{A}^T\vec{A}\hat{x} = \vec{A}^T\vec{b}$.

Theorem: The system $\vec{A}^T\vec{A}\hat{x} = \vec{A}^T\vec{b}$ will always have solutions, and these solutions are precisely the least square solutions to $\vec{A}\vec{x} = \vec{b}$. If $\vec{A}\vec{x} = \vec{b}$ has solutions, then the solutions for the two systems will be the same.

It is also important to note that if $\vec{A}^T\vec{A}$ is invertible, then $\hat{x} = \left(\vec{A}^T\vec{A}^{-1}\right)\vec{A}^T\vec{b}$. Therefore, we can express $\hat{b} = proj_{\operatorname{col}\vec{A}}\vec{b} = \vec{A}\hat{x} = \vec{A}\left(\vec{A}^T\vec{A}^{-1}\right)\vec{A}^T\vec{b}$. This is a very useful formula to calculate orthogonal projections, since we know that $\forall \ W \subset \mathbb{R}^n \exists \vec{A} : W = \operatorname{col}\vec{A}$.

When is $\vec{A}^T\vec{A}$ invertible? This is the case iff

1. The columns of $\vec{A}$ are linearly independent
2. $\vec{A}\vec{x} = \vec{b}$ has a unique least squares solution

Point (2) is obvious, and point (1) can be easily proven:

Proof. Given that $\vec{A}^T\vec{A}$ is invertible, we know that $\vec{A}^T\vec{A}\vec{x} = \vec{0} \implies \vec{x} = 0$. Therefore, if $\vec{A}\vec{x} = \vec{0}$, we can multiply by $\vec{A}^T$ and show that this implies that $\vec{x} = \vec{0}$, i.e. that the columns of $\vec{A}$ are linearly independent. Now we need to prove the other direction. We know that $\vec{A}\vec{x} = \vec{0}$. Therefore, $\vec{A}^T\vec{A}\vec{x} = \vec{0} \implies \vec{x}^T\vec{A}^T\vec{A}\vec{x} = \vec{0} \implies \left(\vec{A}\vec{x}\right)^T\vec{A}\vec{x} = \vec{0} \implies \left(\vec{A}\vec{x}\right)\cdot\left(\vec{A}\vec{x}\right) = 0 \implies \vec{A}\vec{x} = \vec{0} \implies \vec{x} = 0.$ □