Linear Least-Squares Problems

1. Linear Least-Squares as an Optimization Problem

Let $A \in \mathrm{R}^{m\times n}$ and $b \in \mathrm{R}^m$ and assume that $m >> n$, i.e., m is much greater that n. In this setting it is highly unlikely that there exists a vector $x \in \mathrm{R}^n$ such that $Ax = b$. As an alternative goal, we try to find the x that is as *close* to solving $Ax = b$ as possible. But first we must define a notion of *close*. One way is to try to find the vector x that minimizes the norm of the residual error $\|Ax - b\|_2$. That is, we wish to find a vector $\bar{x}$ such that

$$\|A\bar{x} - b\|_2 \le \|Ax - b\|_2 \quad \forall\, x \in \mathrm{R}^n.$$

Equivalently, we wish to solve the optimization problem

$$\mathcal{LLS} \qquad \min_{x\in\mathrm{R}^n} \tfrac{1}{2}\sum_{i=1}^{n}(\sum_{j=1}^{n} A_{ij}x_j - b_i)^2 \ = \ \tfrac{1}{2}\|Ax - b\|_2^2 .$$

If we set

$$f(x) = \tfrac{1}{2}\|Ax - b\|_2^2 ,$$

then the first-order necessary conditions for a point x to solve $\mathcal{LLS}$ is that $\nabla f(x) = 0$. In order to use this fact, we need to compute an expression for the gradient of f.

For $i = 1, 2, \ldots, m$, set $\phi_i(x) = (\sum_{j=1}^n A_{ij}x_j - b_i)^2$, then $f(x) = \frac{1}{2}\sum_{i=1}^m \phi_i(x)$ Observe that for $i \in \{1, 2, \ldots, m\}$ and a given $j_0 \in \{1, 2, \ldots, n\}$

$$\frac{\partial}{\partial x_{j_0}}\phi_i(x) = \frac{\partial}{\partial x_{j_0}}(\sum_{j=1}^{n} A_{ij}x_j - b_i)^2 = 2A_{ij_0}(\sum_{j=1}^{n} A_{ij}x_j - b_i).$$

Consequently,

$$\frac{\partial}{\partial x_{j_0}} f(x) = \sum_{i=1}^{m} A_{ij_0}(\sum_{j=1}^{n} A_{ij}x_j - b_i) = A_{\cdot j_0}^T(Ax - b),$$

and so

$$\nabla f(x) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(x) \\ \frac{\partial}{\partial x_2} f(x) \\ \vdots \\ \frac{\partial}{\partial x_n} f(x) \end{bmatrix} = \begin{bmatrix} A_{\cdot 1}^T(Ax - b) \\ A_{\cdot 2}^T(Ax - b) \\ \vdots \\ A_{\cdot n}^T(Ax - b) \end{bmatrix} = A^T(Ax - b) \ .$$

Therefore, if $x \in \mathrm{R}^n$ solves $\mathcal{LLS}$, then it must be the case that $0 = \nabla f(x) = A^T(Ax - b)$ or equivalently

$$A^TAx = A^Tb \ .$$

This system of equations are called the *normal equations* for the linear least-squares problem $\mathcal{LLS}$.

We must now address the question of whether the exists a solution to the normal equations. For this we make use of the following lemma.

Lemma 1. *For every matrix $A \in \mathrm{R}^{m\times n}$ we have*

$$\mathit{Null}(A^TA) = \mathit{Null}(A) \quad \mathit{and} \quad \mathit{Ran}(A^TA) = \mathit{Ran}(A^T) \ .$$

Proof. Note that if $x \in \mathrm{Null}(A)$, then $Ax = 0$ and so $A^TAx = 0$, that is, $x \in \mathrm{Null}(A^TA)$. Therefore, $\mathrm{Null}(A) \subset \mathrm{Null}(A^TA)$. Conversely, if $x \in \mathrm{Null}(A^TA)$, then

$$A^TAx = 0 \implies x^TA^TAx = 0 \implies (Ax)^T(Ax) = 0 \implies \|Ax\|_2^2 = 0 \implies Ax = 0,$$

or equivalently, $x \in \mathrm{Null}(A)$. Therefore, $\mathrm{Null}(A^TA) \subset \mathrm{Null}(A)$, and so $\mathrm{Null}(A^TA) = \mathrm{Null}(A)$.

Since $\mathrm{Null}\,(A^TA) = \mathrm{Null}\,(A)$, the Fundamental Theorem of the Alternative tells us that

$$\mathrm{Ran}\,(A^TA) = \mathrm{Ran}\,((A^TA)^T) = \mathrm{Null}\,(A^TA)^\perp = \mathrm{Null}\,(A)^\perp = \mathrm{Ran}\,(A^T),$$

which proves the lemma. □

Let us now examine the existence of solutions to the the normal equations in light of this lemma. The normal equations are $A^TAx = A^Tb$. By definition, $A^Tb \in \mathrm{Ran}\,(A^T)$. The lemma tells us that $\mathrm{Ran}\,(A^T) = \mathrm{Ran}\,(A^TA)$. Hence, the must exist and x such that $A^TAx = A^Tb$, that is, the normal equations are always consistent regardless of the choice of matrix $A \in \mathrm{R}^{m\times n}$ and vector $b \in \mathrm{R}^m$.

Theorem 2. *The normal equations are consistent for all $A \in \mathrm{R}^{m\times n}$ and $b \in \mathrm{R}^m$.*

This tells us that the linear least-squares problem $\mathcal{LLS}$ always has a critical point. But it does not tells us when these critical points for $\mathcal{LLS}$ are global solutions to $\mathcal{LLS}$. In this regard, we have the following surprising result.

Theorem 3. *Let $A \in \mathrm{R}^{m\times n}$ and $b \in \mathrm{R}^m$. Then every solution $\bar{x}$ to $A^TAx = A^Tb$ satisfies*

$$\|A\bar{x} - b\|_2 \le \|Ax - b\|_2 \quad \forall\ x \in \mathrm{R}^n, \tag{1}$$

that is $\bar{x}$ is a global solution to $\mathcal{LLS}$.

Proof. Given $u, v \in \mathrm{R}^m$, we have

$$\|u + v\|_2^2 = (u+v)^T(u+v) = u^Tu + 2u^Tv + v^Tv = \|u\|_2^2 + 2u^Tv + \|v\|_2^2\,. \tag{2}$$

Consequently, for every $x \in \mathrm{R}^n$,

$$\begin{aligned}
\|Ax - b\|_2^2 &= \|(Ax - A\bar{x}) + (A\bar{x} - b)\|_2^2 \\
&= \|A(x-\bar{x})\|_2^2 + 2(A(x-\bar{x}))^T(A\bar{x} - b) + \|A\bar{x} - b\|_2^2 && \text{(by (2))} \\
&\ge 2(x-\bar{x})^TA^T(A\bar{x} - b) + \|A\bar{x} - b\|_2^2 && (\text{since } \|A(x-\bar{x})\|_2^2 \ge 0) \\
&= \|A\bar{x} - b\|_2^2 && (\text{since } A^T(A\bar{x} - b) = 0),
\end{aligned}$$

or equivalently, (1) holds. □

So far we know that the normal equations are consistent and that every solution to the normal equations solves the linear least-squares problem. That is, a solution to the linear least-squares problem always exists. We now address the question of when the solution is unique. This is equivalent to asking when the normal equations have a unique solution. From our study nonsingular matrices, we know this occurs precisely when the matrix A^TA is nonsingular or equivalently, invertable, in which case the unique solution is given by $\bar{x} = (A^TA)^{-1}A^Tb$. Note that A^TA is invertible if and only if $\mathrm{Null}\,(A^TA) = \{0\}$. But, by Lemma 1, this is equivalent to $\mathrm{Null}\,(A) = \{0\}$.

Theorem 4. *The linear least-squares problem $\mathcal{LLS}$ has a unique solution if and only if Null$\,(A) = \{0\}$.*

2. Orthogonal Projection onto a Subspace

In the previous section we stated the linear least-squares problem as the optimization problem $\mathcal{LLS}$. We can view this problem in a somewhat different light as a least distance problem to a subspace, or equivalently, as a projection problem for a subspace. Suppose $S \subset \mathrm{R}^m$ is a given subspace and $b \notin S$. The least distance problem for S and b is to find that element of S that is as close to b as possible. That is we wish to solve the problem

$$\min_{z\in S} \tfrac{1}{2}\|z - y\|_2^2\,. \tag{3}$$

The solution is the point $\bar{z} \in S$ such that

$$\|\bar{z} - b\|_2 \leq \|z - b\|_2 \qquad \forall\ z \in S.$$

If we now take the subspace to be the range of A, $S = \mathrm{Ran}\,(A)$, then the problem (3) is closely related to the problem $\mathcal{LLS}$ since

$$\text{if } \bar{z} \text{ solves (3) and } \bar{x} \text{ solves } \mathcal{LLS}, \text{ then } \bar{z} = A\bar{x} \text{ (why?).} \tag{4}$$

Below we discuss the connection between the notion of a projection matrix and solutions to (3). Since the norm $\|\cdot\|_2$ is generated by the dot product, $\|w\|_2 = \sqrt{w \bullet w}$, least norm problems of this type are solved using the notion of *orthogonal projection onto a subspace*.

To understand orthogonal projections, we must first introduce the notion of projection. A matrix $P \in \mathrm{R}^{m\times m}$ is said to be a projection if $P^2 = P$. In this case we say that P is a projection onto the range of P, $S = \mathrm{Ran}\,(P)$. Note that if $x \in \mathrm{Ran}\,(P)$, then there is a $w \in \mathrm{R}^m$ such that $x = Pw$, therefore, $Px = P(Pw) = P^2w = Pw = x$. That is, P leaves all elements of $\mathrm{Ran}\,(P)$ fixed. Also, note that, if P is a projection, then

$$(I - P)^2 = I - P - P + P^2 = I - P,$$

and so $(I - P)$ is also a projection. Since for all $w \in \mathrm{R}^m$,

$$w = Pw + (I - P)w,$$

we have

$$\mathrm{R}^m = \mathrm{Ran}\,(P) + \mathrm{Ran}\,((I - P)).$$

In this case we say that the subspaces $\mathrm{Ran}\,(P)$ and $\mathrm{Ran}\,((I - P))$ are *complementary* since their sum is the whole space and their intersection is the origin, i.e., $\mathrm{Ran}\,(P) \cap \mathrm{Ran}\,((I - P)) = \{0\}$ (why?).

Conversely, given any two subspaces S_1 and S_2 such that $S_1 \cap S_2 = \{0\}$ and $S_1 + S_2 = \mathrm{R}^m$, there is a projection P such that $S_1 = \mathrm{Ran}\,(P)$ and $S_2 = \mathrm{Ran}\,((I-P))$. We do not show how to construct these projections here, but note that they can be generated with the aid of bases for S_1 and S_2.

This relationship between projections and complementary subspaces allows us to define a notion of *orthogonal projection*. For every subspace $S \subset \mathrm{R}^m$, we know that

$$S \cap S^\perp = \{0\} \qquad \text{and} \qquad S + S^\perp = \mathrm{R}^m \qquad \text{(why?).}$$

Therefore, there is a projection P such that $\mathrm{Ran}\,(P) = S$ and $\mathrm{Ran}\,((I - P)) = S^\perp$, or equivalently,

$$((I - P)y)^T(Pw) = 0 \qquad \forall\ y, w \in \mathrm{R}^m. \tag{5}$$

The orthogonal projection plays a very special role among all possible projections onto a subspace. For this reason, we denote the orthogonal projection onto the subspace S by P_S.

We now use the condition (5) to derive a simple test of whether a projection is an orthogonal projection. For brevity, we write $P := P_S$ and set $M = (I - P)^TP$. Then, by (5),

$$M_{ij} = e_i^T M e_j = 0 \qquad \forall\ i, j = 1, \ldots, n,$$

i.e., M is the zero matrix. But then,

$$P = P^TP = (P^TP)^T = P^T.$$

Conversely, if $P = P^T$ and $P^2 = P$, then $(I - P)^TP = 0$. Therefore, a matrix P is an orthogonal projection if and only if $P^2 = P$ and $P = P^T$. An orthogonal projection for a given subspace S can be constructed from any orthonormal basis for that subspace. Indeed, if the columns of the matrix Q form an orthonormal basis for S, then the matrix $P = QQ^T$ satisfies

$$P^2 = QQ^TQQ^T \overset{\text{why}}{=} QI_kQ^T = QQ^T = P \qquad \text{and} \qquad P^T = (QQ^T)^T = QQ^T = P,$$

so that P is an orthogonal projection. Moreover, since we know that $\mathrm{Ran}\,(QQ^T) = \mathrm{Ran}\,(Q) = S$, P is necessarily the orthogonal projector onto S.

Let us now return to the problem (5). We show that $\bar{z}$ solves this problem if and only if $\bar{z} = P_S b$ where P_S is the orthogonal projection onto S. To see this, let $P := P_S$ and $z \in S$ so that $z = Pz$. Then

$$\begin{aligned}
\|z - b\|_2^2 &= \|Pz - Pb - (I-P)b\|_2^2 \\
&= \|P(z-b) + (I-P)b\|_2^2 \\
&= \|P(z-b)\|_2^2 + 2(z-b)^T P(I-P)b + \|(I-P)b\|_2^2 \\
&= \|P(z-b)\|_2^2 + \|(I-P)b\|_2^2 \\
&\geq \|(P-I)b\|_2^2 \\
&= \|\bar{z} - b\|_2^2 ,
\end{aligned}$$

which shows that $\|\bar{z} - b\|_2 \leq \|z - b\|_2$ for all $z \in S$.

Let us now consider the linear least-squares problem $\mathcal{LLS}$ when $m >> n$ and $\mathrm{Null}\,(A) = \{0\}$. In this case, we have shown that $\bar{x} = (A^TA)^{-1}A^Tb$ solves $\mathcal{LLS}$, and $\bar{z} = P_S b$ solves (5) where P_S is the orthogonal projector onto $S = \mathrm{Ran}\,(A)$. Hence, by (4),

$$P_S b = \bar{z} = A\bar{x} = A(A^TA)^{-1}A^Tb.$$

Since this is true for all possible choices of the vector b, we have

$$P_S = A(A^TA)^{-1}A^T \ ! \tag{6}$$

That is, the matrix $A(A^TA)^{-1}A^T$ is the orthogonal projector onto the range of A. One can also check this directly by showing that the matrix $M = A(A^TA)^{-1}A^T$ satisfies $M^2 = M$, $M^T = M$, and $\mathrm{Ran}\,(M) = \mathrm{Ran}\,(A)$.

3. Minimal Norm Solutions to $Ax = b$

Again let $A \in \mathrm{R}^{m\times n}$, but now we suppose that $m << n$. In this case A is short and fat so the matrix A most likely has rank m, or equivalently,

$$\mathrm{Ran}\,(A) = \mathrm{R}^m \ . \tag{7}$$

In this case, regardless of the choice of the vector $b \in \mathrm{R}^m$, the set of solutions to $Ax = b$ will be infinite since the nullity of A is $n - m$. Indeed, if x^0 is any particular solution to $Ax = b$, then the set of solutions is given by $\{x^0 + z \,|\, z \in \mathrm{Null}\,(A)\}$. In this setting, one might prefer the solution to the system having least norm. This solution is found by solving the problem

$$\min_{z\in S} \tfrac{1}{2}\left\|z + x^0\right\|_2^2 \ , \tag{8}$$

where S is the null-space of A. This problem is of the form (3). Consequently, the solution is given by $\bar{z} = -P_S x^0$ where P_S is now the orthogonal projection onto $S := \mathrm{Null}\,(A)$.

In this context, note that $(I - P_S)$ is the orthogonal projector onto $\mathrm{Null}\,(A)^\perp = \mathrm{Ran}\,(A^T)$.Recall that the formula (6) shows that if $M \in \mathrm{R}^{k\times s}$ is such that $\mathrm{Null}\,(M) = \{0\}$, then the orthogonal projector onto $R := \mathrm{Ran}\,(M)$ is given by

$$P_R = M(M^TM)^{-1}M^T \ . \tag{9}$$

In our case, $M = A^T$ and $M^TM = AA^T$. Our working assumption (7) implies that

$$\mathrm{Null}\,(M) = \mathrm{Null}\,(A^T) = \mathrm{Ran}\,(A)^\perp = (\mathrm{R}^m)^\perp = \{0\}$$

and consequently, by (9), the orthogonal projector onto $R = \mathrm{Ran}\,(A^T) = S^\perp$ is given by

$$P_{S^\perp} = A^T(AA^T)^{-1}A \ .$$

Therefore, the orthogonal projector onto S is

$$P_S = I - P_{S^\perp} = I - A^T(AA^T)^{-1}A \ .$$

Putting this all together, we find that the solution to (8) is

$$\bar{z} = -P_S x^0 = (A^T(AA^T)^{-1}A - I)x^0 \ ,$$

and the solution to $Ax = b$ of least norm is

$$\bar{x} = x^0 + \bar{z} = A^T(AA^T)^{-1}Ax^0,$$

where x^0 is any particular solution to $Ax = b$, i.e., $Ax^0 = b$. Plugging $\bar{x}$ into $Ax = b$ gives

$$A\bar{x} = AA^T(AA^T)^{-1}Ax^0 = Ax^0 = b.$$