Least Squares, Null space, Row space, Projectors

Computational Intelligence, Lecture 2

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Content

Least squares at a glance (1)

Consider the following problem: find the smallest 2-norm $\mathbf{x}$ for which the equality $\mathbf{Ax} = \mathbf{y}$ has least residual. This is the *least squares problem.*

- Residual is defined as $\mathbf{e} = \mathbf{Ax} - \mathbf{y}$
- The idea that we need to find the smallest 2-norm $\mathbf{x}$ and, at the same time, least residual $\mathbf{e}$ seems to call for compromise. However, we will find that there exist a linear subspace of solutions with the exact same residual, and on that subspace we can find $\mathbf{x}$ with the smallest norm.

Least squares at a glance (2)

Minimum of $||\mathbf{e}||_2 = ||\mathbf{A}\mathbf{x} - \mathbf{y}||_2$ is achieved at the same $\mathbf{x}$ as minimum of $(\mathbf{A}\mathbf{x} - \mathbf{y})^\top(\mathbf{A}\mathbf{x} - \mathbf{y})$. With that in mind, let us find its extremum:

$$2\mathbf{A}^\top(\mathbf{A}\mathbf{x} - \mathbf{y}) = 0 \tag{1}$$

$$\mathbf{A}^\top\mathbf{A}\mathbf{x} = \mathbf{A}^\top\mathbf{y} \tag{2}$$

$$\mathbf{x} = (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top\mathbf{y} \tag{3}$$

Thus we can define a *pseudoinverse*:

$$\mathbf{A}^+ = (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top \tag{4}$$

Least squares at a glance (3)

Thus the least residual solution to $\mathbf{Ax} = \mathbf{y}$ is written as:

$$\mathbf{x} = \mathbf{A}^{+}\mathbf{y} \tag{5}$$

We proved that this is the least-residual solution, we will prove that the solution is smallest norm (out of all solutions with the same residual) in the following lectures.

You are given an equation $\mathbf{A}\mathbf{x} = \mathbf{y}$. You want to find an $\mathbf{x}$ that gets the value of $\mathbf{y}$ as close as possible to $\mathbf{y}^*$ in terms of the 2-norm.

We know that $\mathbf{x} = \mathbf{A}^+\mathbf{y}^*$ gives us the least residual solution. Multiplying it by $\mathbf{A}$ we get:

$$\mathbf{y} = \mathbf{A}\mathbf{A}^+\mathbf{y}^* \tag{6}$$

This is the value of $\mathbf{y}$ that we can achieve, which is closest to $\mathbf{y}^*$.

One of the key ideas in Linear Algebra is that every linear operator has four fundamental subspaces:

- Null space
- Row space
- Column space
- Left null space

Our goal is to understand them. The usefulness of this concept is enormous.

Consider the following task: find all solutions to the system of equations $\mathbf{A}\mathbf{x} = \mathbf{0}$.

It can be re-formulated as follows: find all elements of the *null space* of $\mathbf{A}$.

Definition 1

Null space of $\mathbf{A}$ is the set of all vectors $\mathbf{x}$ that $\mathbf{A}$ maps to $\mathbf{0}$

We will denote null space as $\mathcal{N}(\mathbf{A})$. In the literature, it is often denoted as $\ker(\mathbf{A})$ or $\text{null}(\mathbf{A})$.

Now we can find all solutions to the system of equations $\mathbf{A}\mathbf{x} = \mathbf{0}$ by using functions that generate an orthonormal *basis* in the null space of $\mathbf{A}$. In MATLAB it is function `null`, in Python/Scipy - `null_space`:

- `N = null(A).`
- `N = scipy.linalg.null_space(A).`

That is it! Space of solutions of $\mathbf{A}\mathbf{x} = \mathbf{0}$ is the span of the columns of $\mathbf{N}$, and all solutions $\mathbf{x}^*$ can be represented as $\mathbf{x}^* = \mathbf{N}\mathbf{z}$; for any $\mathbf{z}$ we get a unique solution, and for any solution - a unique $\mathbf{z}$.

Let $\mathbf{N}$ be the orthonormal basis in the null space of matrix $\mathbf{A}$. Then, if a vector $\mathbf{x}$ lies in the null space of $\mathbf{A}$, it can be represented as:

$$\mathbf{x} = \mathbf{N}\mathbf{z} \tag{7}$$

where $\mathbf{z}$ are coordinates of $\mathbf{x}$ in the basis $\mathbf{N}$.

However, there are vectors which not only are not lying in the null space of $\mathbf{A}$, but the closest vector to them in the null space is the zero vector.

Let $\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$. Its null space has orthonormal basis $\mathbf{N} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$.

- $\begin{bmatrix} -2 \\ 0 \end{bmatrix} = -2\mathbf{N}$, $\begin{bmatrix} 10 \\ 0 \end{bmatrix} = 10\mathbf{N}$, - both are in the null space.
- for $\mathbf{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ the closest vector in the null space is $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$.
- for $\mathbf{y} = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$ the closest vector in the null space is $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

Orthogonality, definition (1)

Definition

Any two vectors, $\mathbf{x}$ and $\mathbf{y}$, whose dot product is zero are said to be *orthogonal* to each other.

Definition

Vector $\mathbf{x}$, whose dot product with any $\mathbf{y} \in \mathcal{L}$ is orthogonal to the subspace $\mathcal{L}$

Definition (equivalent)

If for a vector $\mathbf{x}$, the closest vector to it from a linear subspace $\mathcal{L}$ is zero vector, $\mathbf{x}$ is called orthogonal to the subspace $\mathcal{L}$.

Orthogonality, definition (2)

Definition

The space of all vectors $\mathbf{y}$, orthogonal to a linear subspace $\mathcal{L}$ is called *orthogonal complement* of $\mathcal{L}$ and is denoted as $\mathcal{L}^{\perp}$.

Definition (equivalent)

The space of all vectors $\mathbf{y}$, such that $\mathrm{dot}(\mathbf{y}, \mathbf{x}) = 0$, $\forall \mathbf{x} \in \mathcal{L}$ is called *orthogonal complement* of $\mathcal{L}$.

Therefore $\mathbf{x} \in \mathcal{L}$ and $\mathbf{y} \in \mathcal{L}^{\perp}$ implies $\mathrm{dot}(\mathbf{y}, \mathbf{x}) = 0$.

Let $\mathbf{L}$ be an orthonormal basis in a linear subspace $\mathcal{L}$. Take vector $\mathbf{a} = \mathbf{x} + \mathbf{y}$, where $\mathbf{x}$ lies in the subspace $\mathcal{L}$, and $\mathbf{y}$ lies in the subspace $\mathcal{L}^{\perp}$.

Definition

We call such vector $\mathbf{x}$ a *projection* of $\mathbf{a}$ onto subspace $\mathcal{L}$, and such vector $\mathbf{y}$ a projection of $\mathbf{a}$ onto subspace $\mathcal{L}^{\perp}$

Projection is the closest element in the subspace to a given vector. Projection of $\mathbf{a}$ onto $\mathcal{L}$ can be found as:

$$\mathbf{x} = \mathbf{L}\mathbf{L}^{+}\mathbf{a} \tag{8}$$

Since $\mathbf{L}$ is orthonormal, this is the same as $\mathbf{x} = \mathbf{L}\mathbf{L}^{\top}\mathbf{a}$

Since $\mathbf{a} = \mathbf{x} + \mathbf{y}$, and $\mathbf{x} = \mathbf{L}\mathbf{L}^\top \mathbf{a}$, we can write:

$$\mathbf{a} = \mathbf{L}\mathbf{L}^\top \mathbf{a} + \mathbf{y} \tag{9}$$

from which it follows that the projection of $\mathbf{a}$ onto $\mathcal{L}^\perp$ can be found as:

$$\mathbf{y} = (\mathbf{I} - \mathbf{L}\mathbf{L}^\top)\mathbf{a} \tag{10}$$

where $\mathbf{I}$ is an identity matrix. Since $\mathbf{L}$ is orthonormal, this is the same as $\mathbf{y} = (\mathbf{I} - \mathbf{L}\mathbf{L}^\top)\mathbf{a}$

Definition

Let $\mathcal{N}$ be null space of $\mathbf{A}$. Then orthogonal subspace $\mathcal{N}^{\perp}$ is called *row space* of $\mathbf{A}$.

Definition

Row space of $\mathbf{A}$ is the space of all smallest-norm solutions of $\mathbf{A}\mathbf{x} = \mathbf{y}$, for $\forall \mathbf{y}$.

We will denote row space as $\mathcal{R}$.

Vectors in Null space, Row space

Given vector $\mathbf{x}$, matrix $\mathbf{A}$ and its nulls space basis $\mathbf{N}$, and we check if $\mathbf{x}$ is in the null space of $\mathbf{A}$. The simplest way is to check if $\mathbf{A}\mathbf{x} = 0$. But sometimes we may want to avoid computing $\mathbf{A}\mathbf{x}$, for example if the number of elements of $\mathbf{A}$ is much larger than the number of elements of $\mathbf{N}$.

If $\mathbf{x}$ is in the null space of $\mathbf{A}$, it will have zero projection onto the row space of $\mathbf{A}$. This gives us the condition we can check:

$$(\mathbf{I} - \mathbf{N}\mathbf{N}^\top)\mathbf{x} = 0 \tag{11}$$

By the same logic, condition for being in the row space is as follows:

$$\mathbf{N}\mathbf{N}^\top\mathbf{x} = 0 \tag{12}$$

Consider another task: find all solutions to the system of equations $\mathbf{A}\mathbf{x} = \mathbf{y}$.

Assume we have two solutions to the system: $\mathbf{x}_1$ and $\mathbf{x}_2$. We know that $\mathbf{A}\mathbf{x}_1 = \mathbf{A}\mathbf{x}_2 = \mathbf{y}$, hence $\mathbf{A}(\mathbf{x}_1 - \mathbf{x}_2) = \mathbf{0}$. In other words, the difference between any two solutions lies in the null space of $\mathbf{A}$.

On the other hand, let $\mathbf{x}^*$ be a solution, and $\mathbf{x}^N \in \mathcal{N}(\mathbf{A})$ be a vector in the null space of $\mathbf{A}$. Then $\mathbf{x}^* + \mathbf{x}^N$ is also a solution, since $\mathbf{A}(\mathbf{x}^* + \mathbf{x}^N) = \mathbf{A}\mathbf{x}^* + \mathbf{A}\mathbf{x}^N = \mathbf{A}\mathbf{x}^* = \mathbf{y}$.

Therefore, the solution space is given by a single partial solution $\mathbf{x}^p \notin \mathcal{N}(\mathbf{A})$ and the whole null space of $\mathbf{A}$.

There are infinitely many ways to chose $\mathbf{x}^p$, since if $\mathbf{x}^p \notin \mathcal{N}(\mathbf{A})$, then $(\mathbf{x}^p + \mathbf{x}^N) \notin \mathcal{N}(\mathbf{A})$, if $\mathbf{x}^N \in \mathcal{N}(\mathbf{A})$. However:

Statement 1

The smallest-norm $\mathbf{x}^p$ will lie in the row space of $\mathbf{A}$.

We can prove it by observing that there can be only one $\mathbf{x}^p \in \mathcal{R}(\mathbf{A})$ and adding to it any vector $\mathbf{x}^N \in \mathcal{N}(\mathbf{A})$ can only increase its magnitude, as $\mathbf{x}^p$ and $\mathbf{x}^N$ are orthogonal.

If we have $\mathbf{x}^*$, which is a solution to $\mathbf{A}\mathbf{x} = \mathbf{y}$, we can find the particular solution $\mathbf{x}^p \in \mathcal{R}(\mathbf{A})$ as a projection:

$$\mathbf{x}^p = (\mathbf{I} - \mathbf{N}\mathbf{N}^\top)\mathbf{x}^* \tag{13}$$

where $\mathbf{N}$ is the null space basis for $\mathbf{A}$. Alternatively, we can simply find it as:

$$\mathbf{x}^p = \mathbf{A}^+\mathbf{y} \tag{14}$$

All solutions to $\mathbf{A}\mathbf{x} = \mathbf{y}$ are then given as:

$$\mathbf{x}^* = \mathbf{A}^+\mathbf{y} + \mathbf{N}\mathbf{z}, \ \forall \mathbf{z} \tag{15}$$

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