

Supplementary Material

APPENDIX A: GRAMIAN SPACE OF RANDOM VARIABLES

The meaning of Gramian and its role in the joint inversion can be better explained using a probabilistic approach to inverse problem solution. In the framework of this approach, one can treat the observed data and the model parameters as the realizations of some random variables.

We can introduce a Hilbert space of random variables with the metric defined by the covariance between random variables, representing different model parameters. Indeed, let us consider a set, $\Gamma^{(n)}$, of random variables, φ, ψ, \dots , representing different model parameters.

For any two random variables, $\varphi, \psi \in \Gamma^{(n)}$, we can define an inner product operation, $(\varphi, \psi)_{\Gamma^{(n)}}$, as the determinant of the following covariance matrix:

$$(\varphi, \psi)_{\Gamma^{(n)}} = \begin{vmatrix} \text{cov} \left(\gamma^{(1)}, \gamma^{(1)} \right) & \text{cov} \left(\gamma^{(1)}, \gamma^{(2)} \right) & \dots & \text{cov} \left(\gamma^{(1)}, \gamma^{(n-1)} \right) & \text{cov} \left(\gamma^{(1)}, \psi \right) \\ \text{cov} \left(\gamma^{(2)}, \gamma^{(1)} \right) & \text{cov} \left(\gamma^{(2)}, \gamma^{(2)} \right) & \dots & \text{cov} \left(\gamma^{(2)}, \gamma^{(n-1)} \right) & \text{cov} \left(\gamma^{(2)}, \psi \right) \\ \dots & \dots & \dots & \dots & \dots \\ \text{cov} \left(\gamma^{(n-1)}, \gamma^{(1)} \right) & \text{cov} \left(\gamma^{(n-1)}, \gamma^{(2)} \right) & \dots & \text{cov} \left(\gamma^{(n-1)}, \gamma^{(n-1)} \right) & \text{cov} \left(\gamma^{(n-1)}, \psi \right) \\ \text{cov} \left(\varphi, \gamma^{(1)} \right) & \text{cov} \left(\varphi, \gamma^{(2)} \right) & \dots & \text{cov} \left(\varphi, \gamma^{(n-1)} \right) & \text{cov} \left(\varphi, \psi \right) \end{vmatrix}, \quad (\text{S1})$$

where $\gamma^{(1)}, \gamma^{(2)}, \dots, \gamma^{(n-1)}$ are some random variables representing a subset of $(n - 1)$ known model parameters from $\Gamma^{(n)}$. We will call this set a *core* of the set $\Gamma^{(n)}$.

One can check that the operation defined by formula (S1) satisfies all the properties of the inner product in the Hilbert space.

1. The symmetry of operation (S1):

$$(\varphi, \psi)_{\Gamma^{(n)}} = (\psi, \varphi)_{\Gamma^{(n)}}. \quad (\text{S2})$$

2. The linearity of operation (S1):

$$(c_1 \varphi_1 + c_2 \varphi_2, \psi)_{\Gamma^{(n)}} = c_1 (\varphi_1, \psi)_{\Gamma^{(n)}} + c_2 (\varphi_2, \psi)_{\Gamma^{(n)}}. \quad (\text{S3})$$

Equality (S3) comes immediately from the linearity of the covariance:

$$\text{cov} (c_1 \varphi_1 + c_2 \varphi_2, \psi) = c_1 \text{cov} (\varphi_1, \psi) + c_2 \text{cov} (\varphi_2, \psi) \quad (\text{S4})$$

$$= c_1 (\varphi_1, \psi)_{\Gamma(n)} + c_2 (\varphi_2, \psi)_{\Gamma(n)}.$$

3. The functional (S1) defining the inner product operation, $(\varphi, \psi)_{\Gamma(n)}$, is positive definite:

$$(\varphi, \varphi)_{\Gamma(n)} \geq 0, \quad (S5)$$

and

$$(\varphi, \varphi)_{\Gamma(n)} = 0, \text{ if and only if } \varphi \doteq 0. \quad (S6)$$

The symbol "dot" above the equality sign in formula (S6) means that random variable φ is a linear combination of the random variables $\gamma^{(1)}, \gamma^{(2)}, \gamma^{(3)}, \dots, \gamma^{(n-1)}$, forming the core of set $\Gamma^{(n)}$:

$$\varphi = \sum_{i=1}^{n-1} b_i^{(i)} \gamma + c, \quad (S7)$$

where b_i ($i = 1, 2, \dots, n-1$) and c are some constant coefficients.

Inequality (S5) holds because the determinant of the covariance matrix is always positive for independent random variables. This determinant is equal to zero if and only if the random variables, $\gamma^{(1)}, \gamma^{(2)}, \gamma^{(3)}, \dots, \gamma^{(n-1)}$, and φ are linearly dependent

According to the theory of Hilbert spaces, the inner product of some element φ by itself defines the norm square of this element:

$$(\varphi, \varphi)_{\Gamma(n)} = \|\varphi\|_{\Gamma(n)}^2. \quad (S8)$$

Thus, we can see that the zero value of the norm of some random variable φ means that this variable is linearly related to the elements of the core, $\gamma^{(1)}, \gamma^{(2)}, \gamma^{(3)}, \dots, \gamma^{(n-1)}$. In other words, any linear combination of the elements of the core of the set $\Gamma^{(n)}$ has a zero norm.

We will call the set $\Gamma^{(n)}$ of random variables with the metric (inner product) defined by formula (S1), the Gramian space of random variables.

This property of the introduced metric allows us to use this metric to find the solutions to the inverse problem, which would correlate the best with the preselected model parameters forming the core of Gramian space $\Gamma^{(n)}$.

We can now introduce the Gramian space of random variables, $\Gamma^{(j)}$, with inner product defined by the following operation:

$$(\varphi, \psi)_{\Gamma(j)} = \begin{vmatrix} cov(\gamma^{(1)}, \gamma^{(1)}) & cov(\gamma^{(1)}, \gamma^{(2)}) & \dots & cov(\gamma^{(1)}, \psi) & \dots cov(\gamma^{(1)}, \gamma^{(n)}) \\ \dots & \dots & \dots & \dots & \dots \\ cov(\varphi, \gamma^{(1)}) & cov(\varphi, \gamma^{(2)}) & \dots & cov(\varphi, \psi) & cov(\varphi, \gamma^{(n)}) \\ \dots & \dots & \dots & \dots & \dots \\ cov(\gamma^{(n)}, \gamma^{(1)}) & cov(\gamma^{(n)}, \gamma^{(2)}) & \dots & cov(\gamma^{(n)}, \psi) & cov(\gamma^{(n)}, \gamma^{(n)}) \end{vmatrix}, \quad (S9)$$

where random variables φ and ψ are located within the row and column with number j , respectively.

In the Gramian space of random variables, $\Gamma^{(j)}$, the norm square of a variable, $\|\varphi\|_{\Gamma^{(j)}}^2$, is equal to the Gramian of a set of random variables, $(m^{(1)}, m^{(2)}, \dots, m^{(j-1)}, \varphi, m^{(j+1)}, \dots, m^{(n)})$:

$$\|\varphi\|_{\Gamma^{(j)}}^2 = (\varphi, \varphi)_{\Gamma^{(j)}} = G(\gamma^{(1)}, \gamma^{(2)}, \dots, \gamma^{(j-1)}, \varphi, \gamma^{(j+1)}, \dots, \gamma^{(n)}). \quad (\text{S10})$$

Therefore, the norm of variable, φ , in the Gramian space $\Gamma^{(j)}$ provides a measure of correlation between this variable and all other random variables, with the exception of $\gamma^{(j)}$: $\gamma^{(1)}, \gamma^{(2)}, \dots, \gamma^{(j-1)}, \gamma^{(j+1)}, \dots, \gamma^{(n)}$.

The Gramian norm of random variables has the following properties:

$$\left\| \gamma^{(i)} \right\|_{\Gamma^{(i)}}^2 = \left\| \gamma^{(j)} \right\|_{\Gamma^{(j)}}^2, \text{ for } i = 1, 2, \dots, n; j = 1, 2, \dots, n. \quad (\text{S11})$$

The last formula demonstrates that all the random variables, $\gamma^{(1)}, \gamma^{(2)}, \dots, \gamma^{(n)}$, have the same norm in the corresponding Gramian spaces $\Gamma^{(j)}$, $j = 1, 2, \dots, n$.

In conclusion of this section, we should note that in Gramian space $\Gamma^{(1)}$, the inner product of two random variables is equal to their covariance:

$$(\varphi, \psi)_{\Gamma^{(1)}} = \text{cov}(\varphi, \psi), \quad (\text{S12})$$

and the norm square of φ is simply its variance:

$$\|(\varphi, \psi)\|_{\Gamma^{(1)}}^2 = \sigma^2(\varphi). \quad (\text{S13})$$