Gramian matrix

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In linear algebra, the Gram matrix (Gramian matrix or Gramian) of a set of vectors $v_1, \dots, v_n$ in an inner product space is the Hermitian matrix of inner products, whose entries are given by $G_{ij} = \langle v_i, v_j \rangle$.[1]

An important application is to compute linear independence: a set of vectors is linearly independent if and only if the Gram determinant (the determinant of the Gram matrix) is non-zero.

It is named after Jørgen Pedersen Gram.

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Examples

For finite-dimensional real vectors with the usual Euclidean dot product, the Gram matrix is simply $G = V^\mathrm{T} V$ (or $G = V^H V$ for complex vectors using the conjugate transpose), where *V* is a matrix whose columns are the vectors v_k.

Most commonly, the vectors are elements of a Euclidean space, or are functions in an L^2 space, such as continuous functions on a compact interval [*a*, *b*] (which are a subspace of $L^2([a, b])$).

Given real-valued functions $\{\ell_i(\cdot),\ i = 1, \dots, n\}$ on the interval $[t_0, t_f]$, the Gram matrix $G = [G_{ij}]$, is given by the standard inner product on functions:

$$G_{ij} = \int_{t_0}^{t_f} \ell_i(\tau)\bar{\ell}_j(\tau)\, d\tau.$$

For a general bilinear form *B* on a finite-dimensional vector space over any field we can define a Gram matrix *G* attached to a set of vectors $v_1, \ldots, v_n$ by $G_{ij} = B(v_i, v_j)$. The matrix will be symmetric if the bilinear form *B* is symmetric.

Applications

- If the vectors are centered random variables, the Gramian is approximately proportional to the covariance matrix, with the scaling determined by the number of elements in the vector.
- In quantum chemistry, the Gram matrix of a set of basis vectors is the overlap matrix.
- In control theory (or more generally systems theory), the controllability Gramian and observability Gramian determine properties of a linear system.
- Gramian matrices arise in covariance structure model fitting (see e.g., Jamshidian and Bentler, 1993, Applied Psychological Measurement, Volume 18, pp. 79–94).
- In the finite element method, the Gram matrix arises from approximating a function from a finite dimensional space; the Gram matrix entries are then the inner products of the basis functions of the finite dimensional subspace.
- In machine learning, kernel functions are often represented as Gram matrices.[2]

Properties

Positive semidefinite

The Gramian matrix is positive semidefinite, and every positive symmetric semidefinite matrix is the Gramian matrix for some set of vectors. Further, in finite-dimensions it determines the vectors up to isomorphism, i.e. any two sets of vectors with the same Gramian matrix must be related by a single unitary matrix. These facts follow from taking the spectral decomposition of any positive semidefinite matrix *P*, so that $P = UDU^H = (U\sqrt{D})(U\sqrt{D})^H$ and so *P* is the Gramian matrix of the columns of $U\sqrt{D}$. The Gramian matrix of any orthonormal basis is the identity matrix. The infinite-dimensional analog of this statement is Mercer's theorem.

Change of basis

Under change of basis represented by an invertible matrix *P*, the Gram matrix will change by a matrix congruence to P^TGP.

Gram determinant

The Gram determinant or Gramian is the determinant of the Gram matrix:

$$G(x_1,\dots,x_n) = \begin{vmatrix} \langle x_1,x_1\rangle & \langle x_1,x_2\rangle & \dots & \langle x_1,x_n\rangle \\ \langle x_2,x_1\rangle & \langle x_2,x_2\rangle & \dots & \langle x_2,x_n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle x_n,x_1\rangle & \langle x_n,x_2\rangle & \dots & \langle x_n,x_n\rangle \end{vmatrix}.$$

Geometrically, the Gram determinant is the square of the volume of the parallelotope formed by the vectors. In particular, the vectors are linearly independent if and only if the Gram determinant is nonzero (if and only if the Gram matrix is nonsingular).

The Gram determinant can also be expressed in terms of the exterior product of vectors by

$$G(x_1,\dots,x_n) = \|x_1 \wedge \cdots \wedge x_n\|^2.$$

See also

- Controllability Gramian
- Observability Gramian

References

1. Horn & Johnson 2013, p. 441
   Theorem 7.2.10 Let $v_1,\dots,v_m$ be vectors in an inner product space V with inner product $\langle\cdot,\cdot\rangle$ and let $G = [\langle v_j,v_i\rangle]_{i,j=1}^m \in M_m$. Then
   (a) G is Hermitian and positive-semidefinite
   (b) G is positive-definite if and only if the vectors $v_1,\dots,v_m$ are linearly-independent.
   (c) rank(G)=dimspan$\{v_1,\dots,v_m\}$
2. Lanckriet, G. R. G.; Cristianini, N.; Bartlett, P.; Ghaoui, L. E.; Jordan, M. I. (2004). "Learning the kernel matrix with semidefinite programming". *Journal of Machine Learning Research*. 5: 27–72 [p. 29].

- Horn, Roger A.; Johnson, Charles R. (2013). "7.2 Characterizations and Properties". *Matrix Analysis (Second Edition)*. Cambridge University Press. ISBN 978-0-521-83940-2.

External links

- Hazewinkel, Michiel, ed. (2001), "Gram matrix", *Encyclopedia of Mathematics*, Springer, ISBN 978-1-55608-010-4
- *Volumes of parallelograms (http://www.owlnet.rice.edu/~fjones/chap8.pdf)* by Frank Jones

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