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Vector set orthoormalization method The first two stages of the Gram-Schmidt process in mathematics, in particular linear algebra and numerical analysis, the Gram-Schmidt process is a vector set orthoormalization method in the inner space of the product, usually in the Euclid space Rn with a standard internal product. The Gram-Schmidt process takes a limited, linearly independent set of S = {v1, ..., vk} k ≤ n and generates a set of orthogonal s′ = {u1, ..., uk}, which includes the same k-dimensional subspace Rn as S. Method named Jørgen Pedersen Gram and Erhard Schmidt, but Pierre-Simon Laplace was familiar with it before Gram and Schmidt. [1] In the theory of the cleavage of the melo group, it is summed up by the breakdown of Iwasawa. Applying the Gram-Schmidt process to the entire column rank matrix columns vectors yields qr decomposition (it is split into an orthogonal and triangular matrix). Gram-Schmidt process The modified Gram-Schmidt process is run by three linearly independent, non-orthodox R3-based vectors. For more information, click the image. The modification is explained in the Digital Stability section of this article. We define the projection operator according to p r o j u (v) = ⟨ u , v ⟩ ⟨ u , u ⟩ u , {\displaystyle \mathrm {proj} _{\mathbf {u} }\,(\mathbf {v})={\langle \mathbf {u} ,\mathbf {v } \rangle \over \langle \mathbf {u} ,\mathbf {u} \rangle }{\mathbf {u} },} where ⟨ u , v ⟩ {\displaystyle \langle \mathbf {u} ,\mathbf {v} \rangle } refers to the inner vector product you and v. This operator vector v orthogonically designs on the line , which includes vector u. if = 0, we define p r o j 0 (v) := 0 {\displaystyle \mathrm {proj} _{0}\,(\mathbf {v} :=0} . i.e. the projection map p r o j 0 {\displaystyle \mathrm {proj} _{0}} is a zero map that sends each vector to a zero vector. The Gram-Schmidt process then proceeds as follows: u 1 = v 1 , e 1 = u 1 ‖ u 1 ‖ u 2 = v 2 – p r o j u 1 (v 2) , e 2 = u 2 ‖ u 2 ‖ u 3 = v 3 - p r o j u 1 (v 3) − p r o j u 2 (v 3) , e 3 = u 3 ‖ 3 ‖ 4 = v 4 − p r o j u 1 (v 4) − p r o j u 2 (v 4) – p r o j u 3 (v 4) , e 4 = for 4 ‖ for 4 ‖ ⋮ ⋮ ‖ ⋮ ⋮ ∑ j = 1 k – 1 p r o j u j (v k) , e k = u k ‖ ‖ . {\displaystyle {\begin{aligned}\mathbf {u} _{1}&=\mathbf {v} _{1},&\mathbf {e} _{1}&={\mathbf {u} _{1} {1}_{1}_mathbf {u} _{1} \over \|\mathbf {u} _{1}\|} \\\mathbf {u} _{2}&=mathbf {v} _{2}-_mathrm {proj} _{\mathbf {u} _{1}},(\mathbf {v} _{2}),&\mathbf {e} _{2}&={\mathbf {u} _{2} \over \|mathbf {u} _{2}\|} \\\mathbf {u} _{3}&=mathbf {v} _{3}-\mathrm {proj} _{\mathbf {u} _{1}}\ ,(\mathbf {v} _{3})-\mathrm {proj} _{\mathbf {u} _{2}}\,(\mathbf {v} _{3}),&\mathbf {e} _{3}&A;={\mathbf {u} _{3} \over \|\mathbf {u} _{3}\|} \\\mathbf {u} _{4}&=\mathbf {v} _{4}-\mathrm _{\mathbf {u} _{1}}\,(\mathbf {v} _{4})-\mathrm {proj} _{\mathbf {u} _{2}}\,(\mathbf {v} _{4})-\mathrm {proj } _{\mathbf {u} _{3}}\,(\mathbf {v} _{4}),&\mathbf {e} _{4}&={\mathbf {u} _{4} \over \over \|\mathbf {u} _{4}\|} \\\&{}\ \vdots &&{}\ \\vdots \\\mathbf {u} _{k}&=\mathbf {v} _{k}-\sum _{j=1}^{k-1}\mathrm {proj } _{\mathbf {u} _{j}}\,(\mathbf {v} _{k}),&\mathbf {e} _{k}&={\mathbf {u} _{k} \over \|\mathbf {u} _{k}\|.. \end{aligned}}} Sequence u1, ..., uk requires an orthogonal vector system, and normalized vectors e1, ..., ek form a set of orthoormals. Sequencing u1, ..., uk is known as Gram-Schmidt orthogonalization, and sequencing e1, ..., ek is known as Gram-Schmidt orthoormalization as vectors are normalized. To verify that these formulas give an orthogonal sequence, first calculate the ⟨ u 1 , u 2 ⟩ {\displaystyle \langle \mathbf {u} _{1},\mathbf {u} _{2}\rangle } by confusing the above formula u2: We get zero. Then use this to calculate ⟨ u 1 , u 3 ⟩ {\displaystyle \langle \mathbf {u} _{1},\mathbf {u} _{3}\rangle } by replacing the formula u3 again: We get zero. The general evidence continues with mathematical induction. Geometrically this method proceeds as follows: to calculate ui, it designs vi ortogonally in subspace U generated u1, ..., ui−1, which is the same as the subspace generated by v1, ..., vi−1. The vector is then defined as the difference between vi and this projection, guaranteeing that orthogonals for all vectors in the subspace U. Gram-Schmidt process is also applied in a linearly independent infinite sequence {vi}i. The result is an orthogonal (ortonormali) sequence {ui}i such that for the natural number n: algebraic v1, ..., vn interval is the same as u1, ..., un. If the Gram-Schmidt process is applied linearly depending on the sequence, it outputs 0 vectors on the ith step, assuming that vi is a linear v1, ..., vi−1 combination. If it is necessary to create an orthoormal basis, the algorithm should check the zero vectors in the output and throw them away, since none of the multiples of the zero vector can be 1 length. The number of vector outputs in the algorithm will be the dimension of the space covered by the initial input. The Gram-Schmidt process variant using transfinite recursion applied (possibly unreadable) vector (v α) α < λ {\displaystyle (v_{\alpha })_{alpha <\lambda }} gives the ortonormatic vector set (u α) α < κ {\displaystyle (u_{\alpha })_{alpha <\kappa }} with κ ≤ λ {\displaystyle \kappa \leq \lambda } so that any α ≤ λ {\displaystyle \alpha \leq \lambda } β : β < min (α , κ) } {\displaystyle \lbrace u_{\beta }:\beta <\min(\alpha ,\kappa)\rbrace } is the same as { v β : < α } {\displaystyle \lbrace v_{\beta }:\beta <\alpha \rbrace } . In particular, when applied (algebraic) hilbert on a space basis (or, more generally, on the basis of any dense post-plant area), it gives (functional analysis) ortonormal basis. Please note that in general, in general often have a strict inequality κ < λ {\displaystyle \kappa <\lambda }, even if the original set was linearly independent, and (u α) α < κ {\displaystyle (u_{\alpha })_{alpha <\kappa }} interval does not have to be an interval (v α) α < λ {\displaystyle (v_{\alpha })_{alpha <\lambda }} (rather, this is the finish gap). Example euclid space Consider this vector set R2 (with the usual internal product) S = { v 1 = (3 1) , v 2 = (2 2) } . {\displaystyle S=\left\lbrace \mathbf {v} _{1}={\begin{pmatrix}3\\1\end{pmatrix}},\mathbf {v} _{2}={\begin{pmatrix}2\\2\end{pmatrix}\right\rbrace .} Now, perform Gram-Schmidt, to obtain the orthogonal vector set: u 1 = v 1 = (3 1) {\displaystyle \mathbf {u} _{1}=\mathbf {v} _{1}={\begin{pmatrix}3\\1\end{pmatrix}}} u2 = v 2 − p r o j u 1 (v 2) = (2 2) - p r o j (3 1) (2 2) = (2 2) − 8 10 (3 1) = (- 2 / 5 6 / 5) . {\displaystyle \mathbf {u} _{2}=\mathbf {v} _{2}-\mathrm {proj} _{\mathbf {u} _{1}}\,(\mathbf {v} _{2})= {\begin{pmatrix}2\\2\end{pmatrix}}-\mathrm {proj} _{({{3 \atop 1}},({{3 \atop 1}})},({{3 \atop 1}})},({{3 \atop 1}})},({{\begin{pmatrix}2\\2\end{pmatrix}}})}={\begin{pmatrix}2\\2\end{pmatrix}-{8 \over 1 }{\begin{pmatrix}3\\1\end{pmatrix}}={\begin{pmatrix}-2/5\\6/5\end{pmatrix}}.} We check that vectors u1 and u2 are indeed orthogonal: ⟨ u 1 , u 2 ⟩ = ⟨ (3 1) , (− 2 / 5 6 / 6 /5) ⟩ = 6 5 + 6 5 = 0 , {\displaystyle \langle \mathbf {u} _{1},\mathbf {u} _{2}\rangle =\left\langle {\begin{pmatrix}3\\1\end{pmatrix}},{\begin{pmatrix}-2/5\\6/5\end{pmatrix}}\right\rangle =-{\frac {6}{5}}+{\frac {6}{5}}=0,} that if the point product of the two vectors is 0, they are orthogonal. In the case of zero vectors, we can then normalize the vectors by dividing their as above: e 1 = 1 10 (3 1) {\displaystyle \mathbf {e} _{1}={1 \over {\sqrt {10}}}{\begin{pmatrix}3\\1\end{pmatrix}} e 2 = 1 40 25 (− 2 / 5 6 / 5) = 1 10 (- 1 3) . {\displaystyle \mathbf {e} _{2}={1 \over {\sqrt {40 \over 25}}}{\begin{pmatrix}-2/5\\6/5\end{pmatrix}}=={1 \over {\sqrt {10}}}{\begin{pmatrix}-1\\3 end\{pmatrix}.} Properties specified by GS (v 1 , ... , v k) {\displaystyle \operatorname {GS} (v_{1},\dots ,v_{k})}, the Gram-Schmidt process is applied to vector set v 1 , ... v k {\displaystyle v_{1},\dots v_{k}} . This results in a map GS : (R n) k → (R n) k {\displaystyle \operatorname {GS} \colon (\mathbf {R} ^{n})^{k}\to (\mathbf {R} ^{n})^{k}} . It has the following characteristics: It is a permanent orientation that saves the sense (v 1 , ... , v k = or (GS (v 1 , ... , v k) {\displaystyle \operatorname {or} (v_{1},\dots ,v_{k})=\operatorname {or} (\operatorname {GS} (v_{1},\dots ,v_{k}))}. It commutes orthogonal maps: Let g: R n → R n {\displaystyle g\colon \mathbf {R} ^{n}\to \mathbf {R} ^{n}} to be orthogonal (depending on the internal product given). Then we have GS (g (v 1) , ... , g (v k) = (gs (v 1 , ... , v k) 1) , ... , g (GS (v 11 , ... , v k) {\displaystyle \operatorname {GS} (g(v_{1}),\dots ,g(v_{k}))=(g(\operatorname {GS} (v_{1},\dots ,v_{k})_{1}),\dots ,g(\operatorname {GS} (v_{1},\dots ,v_{k})__{k}))} Further parameterized The Gram-Schmidt process version brings (strong) deflection retraction from the common liner group G L (R n) {\displaystyle GL(\mathbf {R} ^{ n})} to the orthogonal group O (R n) {\ displaystyle O(\mathbf {R} ^{n})} . Numeric stability When this process is implemented on a computer, vectors u k {\displaystyle \mathbf {u} _{k}} are often not fully orthogonal due to rounding errors. In the Gram-Schmidt process, as described above (sometimes referred to as the classic Gram-Schmidt), this loss of orthogonality is particularly bad; therefore it is said that the (classic) Gram-Schmidt process is numerically unstable. The Gram-Schmidt process can be stabilized by a small modification; this version is sometimes called modified Gram-Schmidt or MGS. This method gives the same result as the original formula of precise arithmetic and introduces smaller errors in the arithmetic of finite accuracy. Instead of turning the vectors in the UK as a u k = v k – p r o j u 1 (v k) − p r o j u 2 (v k) − ⋯ − p r o j u k − 1 (v k) , {\displaystyle \mathbf {u} _{k}=\mathbf {v} _{k}_mathrm {proj} _{\mathbf {u} _{1}}\,(\mathbf {v} _{k})-mathrm {proj} _{\mathbf {u} _{2}}\ ,(\mathbf {v} _{k})-\cdots -\mathrm {proj} _{\mathbf {u} _{k-1}}\ ,(\mathbf {v} _{k}),} it is calculated as u k (1) = v k − p r o j u 1 (v k) , u k (2) = u k (1) − p r o u 2 (u k (1) , ⋮ (k − 2) = 2 (3) , u k (k − 1) = u k (k − 2) − p r o j u k − 1 (k (k − 2) , u k = k (k − 1) ‖ u k (k − 1) ‖ {\displaystyle {\begin{aligned}\mathbf {u} _{k}{{(1)}&=mathbf {v} _{k}-\mathrm {proj} _{\mathbf {u} _{1}}\,(\mathbf {v} _{k}),\\mathbf {u} _{k}{{{2)}&=mathbf {u} _{k}^{{(1)}-mathrm {proj} _{\mathbf {2} { ,(\mathbf {u} _{k}^{(1)}),\\\,\,\,\vdots \\\mathbf {u} _{k}^{(k-2)}&=\mathbf {u} _{k}^{(k-2)}&=mathbf {u} _{k}^{(k-2)}&=mathbf {u} _{k}^{(k-2)}3)}-\mathrm {proj} _{\mathbf {u} _{k-2}}\,(\mathbf {u} _{k}^{(k-3)}),\\mathbf {u} _{k}^{{{(k-1)}>>#1 amp;=\mathbf {u} _{k}^{(k-2)}-\mathrm {proj} _{\mathbf {u} _{k-1}}\,(\mathbf {u} _{k}^{(k-2)}),\\\mathbf {u} _{k}&={\mathbf {u} _{k}^{{(k-1)} \over \|\mathbf {u} _{k}{{(k-1)}\|} \end{aligned}}} This method is used in previous animation , intermediate vector v'3 is used for orthogonalization of blue vector v3. Algorithm This MATLAB algorithm implements gram-schmidt ortonormalization for Euclid vectors. Vectors v1, ..., vk (columns V of the matrix to make V(:,j) jth vector) are replaced by orthoormal vectors (U columns) which cover the same space. n = size(V, 1); k = size(V, 2); U = zeros(n, k); U(:, 1) = V(:, 1) / sqrt(V(:, 1)'*V(:,1)); i = 2:k U(:, i) = V(:, i); j = 1:i - 1 U(:, i) = U(:, i) - (U(:, j)'*U(:,i))/(U(:,j)' * U(:, j)) * U(:, j); end U(:, i) = U(:, i) / sqrt(U(:, i)'*U(:,i)); End the cost of this algorithm is asymptomatic O(nk2) floating point operations with n vector dimensions (Golub & Van Loan 1996, §5.2.8). Via Gaussian Elimination If rows {v1, ..., vk} are written as matrix A {\displaystyle A}, then gaussian removal by applying the augmented matrix [A T | A] {\displaystyle [AA^{\mathrm {T} }| A]} will produce orthogonalized vectors instead of A {\displaystyle A}. However, matrix A T {\displaystyle AA^{\mathrm {T} }} must be uploaded to the row each form by using only the row operation by adding a scalar multiple of one row to another. [2] For example, taking v 1 = (3 1) , v 2 = (2 2) {\displaystyle \mathbf {v} _{1}={\begin{pmatrix}3&1\end{pmatrix}},\mathbf {v} _{2}={\begin{pmatrix}2&2\end{pmatrix}}, as indicated above, we have [A T | A] = [10 8 3 1 8 2 2] {\displaystyle [AA^{\mathrm {T} }| A]=\left[{\begin{array}{rr|rr}10&8&3&1\\8&8&8&2&end{array}}\right]} And sum [1.8.3.1 0 1 – .25.75] {\displaystyle \left[{\begin{array}{rr|rr}1&.8&. 3&. 1\\0&1&25&. 75\end{array}}\right]} Normalized vectors are then e 1 = 1 .3 2 + .2 1 2 (.3.1) = 1 10 (3 1) {\displaystyle \mathbf {e} _{1}={1 \over {\sqrt {.3^{2}+.1^{2}}{matrix}.3&.1\end{{pmatrix}}==={1 \over {\sqrt {10}}}{\begin{pmatrix}3&1\end{pmatrix}} e 2 = 1 .25 2 + .75 2 (- .25 .75) = 1 10 (- 1 3) . {\displaystyle \mathbf {e} _{2}={1 \over {\sqrt {.25^{2}+.75^{2}}{_begin{pmatrix}-.25&25 .75\end{pmatrix}}==={1 \over {\sqrt {10}}}{\begin{pmatrix}-1&3\end{pmatrix}}.} as in the example above. The decisive result of the Gram-Schmidt process formula can be expressed in a non-recursive formula using determinants. e j = 1 D j – 1 D j | ⟨ v 1 , v 1 ⟩ ⟨ v 2 , v 1 ⟩ ... ⟨ v 1 ⟩ ⟨ v 1 , v 2 ⟩ ⟨ v 2 , v 2 ⟩ ... ⟨ v 2 ⟩ ⋮ ⋮ ⋱ ⋮ ⟨ v 1 , v j – 1 ⟩ ⟨ v 2 , v j – 1 ⟩ ... ⟨ v j – 1 ⟩ v 1 v 2 ... v j | {\displaystyle \mathbf {e} _{j}={\frac {1}{\sqrt {D_{j-1}D_{j}}}{{{start{vmatrix}\langle \mathbf {v} _{1},\mathbf {v} _{1}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{1}\rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{1}\rangle \\langle \mathbf {v} _{1},\mathbf {v} &\langle \mathbf {v} {v} {v} _{2}\rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{2}\rangle \\vdots &\vdots &\vdots &\ddots &\vdots \\\langle \mathbf {v} _{1},\mathbf {v} _{j-1}\rangle &\langle \mathbf {v} _{2}, \mathbf {v} _{j-1}\rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{j-1}\rangle \\\mathbf {v} _{1}&\mathbf {v} _{2}&\dots &\mathbf {v} _{j}\end{vmatrix}}} u j = 1 D j - 1 | ⟨ v 1 , v 1 ⟩ ⟨ v 2 , v 1 ⟩ ... ⟨ v 1 ⟩ ⟨ v 1 , v 2 ⟩ ⟨ v 2 , v 2 ⟩ ... ⟨ v 2 ⟩ ⋮ ⋮ ⋱ ⋮ ⟨ v 1 , v j – 1 ⟩ ⟨ v 2 , v j – 1 ⟩ ... ⟨ v j – 1 ⟩ v 1 v 2 ... v j | {\displaystyle \mathbf {u} _{j}={\frac {1}{D_{j-1}}} {\begin{vmatrix}\langle \mathbf {v} _{1},\mathbf {v} _{1}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{1} rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{1}\rangle \\\langle \mathbf {v} _{1},\mathbf {v} _{2}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{2}\rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{2}\rangle \\vdots &\vdots &\ddots &\vdots \\\langle \mathbf {v} _{1} ,\mathbf {v} _{j-1}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{j-1}\rangle &\langle \mathbf {v} _{j},\mathbf {v} _{j-1}\rangle \\\mathbf {v} _{1}&\mathbf {v} _{2}&\mathbf {v} _{j}\end{vmatrix}}}} where D 0=1 and j ≥ 1, D j is the determining factor for the gram D j = | ⟨ v 1 , v 1 ⟩ ⟨ v 2 , v 1 ⟩ ... ⟨ v 1 ⟩ ⟨ v 1 , v 2 ⟩ ⟨ v 2 , v 2 ⟩ ... ⟨ v 2 ⟩ ⋮ ⋮ ⋱ ⋮ ⟨ v 1 , v j ⟩ ⟨ v 2 , v j ⟩ ... ⟨ ⟩ | {\displaystyle D_{j}={\begin{vmatrix}\langle \mathbf {v} _{1},\mathbf {v} _{1}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{1}\rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{1}\rangle \\langle \mathbf {v} _{1},\mathbf {v} _{2}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{2}\rangle &\dots &\langle \mathbf {v} _{j},\mathbf {v} _{2}\rangle \\vdots &\vdots &\ddots &\vdots \\\langle \mathbf {v} _{1} ,\mathbf {v} _{j}\rangle &\langle \mathbf {v} _{2},\mathbf {v} _{j}\rangle &\langle \mathbf {v} _{j},\mathbf {v} _{j}\rangle \end{vmatrix}}.} Please note that the uk expression is a formal determining factor, i.e. the matrix contains both scalars and vectors; the meaning of this expression is defined as the result of the expansion of the cofactor in the vector queue. Gram-Schmidt's decisive formula is a calculation slower (exponentially slower) than the recursive algorithms described above; it is mainly theoretically interested. Alternatives Other orthogonalization algorithms use household transformations or given rotations. Algorithms that use household transformations are more stable than the stabilized Gram-Schmidt process. On the other hand, the gram-schmidt process creates j {\displaystyle j} th orthogonalized vector after j {\displaystyle j} th iteration, while orthogonalization using household reflections produces all End. As a result, only the Gram-Schmidt process is applied to itetic methods, such as the iteration of Arnoldi. Another alternative is motivated by the use of Cholesky decomposition to flip the matrix of the usual equations in straight at least squares. Let V {\displaystyle \mathbf {V} } be a full column rank matrix whose columns need to be orthogonalized. Matrix V ∗ V {\displaystyle \mathbf {V} ^{*}\mathbf {V} } is hermitian and positive and can be written as V ∗ V = L L ∗ , {\displaystyle \mathbf {V} ^{*}\mathbf {V} =\mathbf {L} \mathbf {L} ^{*}} using Cholesky decomposition. The lower triangular matrix L {\displaystyle \mathbf {L} } with strictly positive diagonal entries is unreadable. The matrix columns U = V (L - 1) ∗ {\displaystyle \mathbf {U} =\mathbf {V} (\mathbf {L} ^{-1})^{*}} are ortonormal and cover the same space as the columns of the original matrix V {\displaystyle \mathbf {V} . The clear use algorithm for V ∗ V {\displaystyle \mathbf {V} ^{*}\mathbf {V} } becomes unstable, especially if the product status number is high. Nevertheless, this algorithm is used in practice and implemented in some software packages due to its high efficiency and simplicity. Quantum mechanics contains several orthogonalization schemes with characteristics better suited to certain applications than the original Gram-Schmidt. Nevertheless, it remains a popular and effective algorithm even for the largest calculations of the electronic structure. [3] Links

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