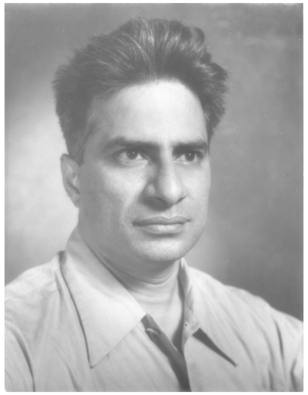
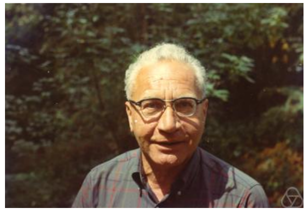
The ‘KLT’: Introduction

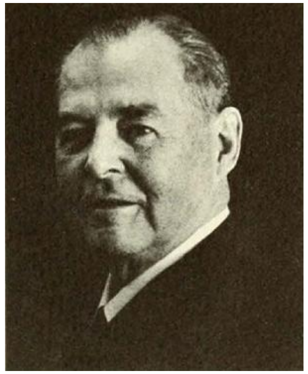


D. D. Kosambi
[1907-1966]
1943

K. Karhunen
[1915-1992]
1945



M. Loève
[1907-1979]
1948



H. Hotelling
[1895-1973]

https://upload.wikimedia.org/wikipedia/commons/0/0f/Kosambi-dd.jpg

https://upload.wikimedia.org/wikipedia/commons/d/d0/Michel_Lo%C3%A8ve.jpg

https://upload.wikimedia.org/wikipedia/en/4/49/Harold_Hotelling.jpg

People call it names!

- Karhunen-Loeve Transform
- Hotelling Transform
- Principal Component Analysis
- Eigenvalue-Eigenvector Transform

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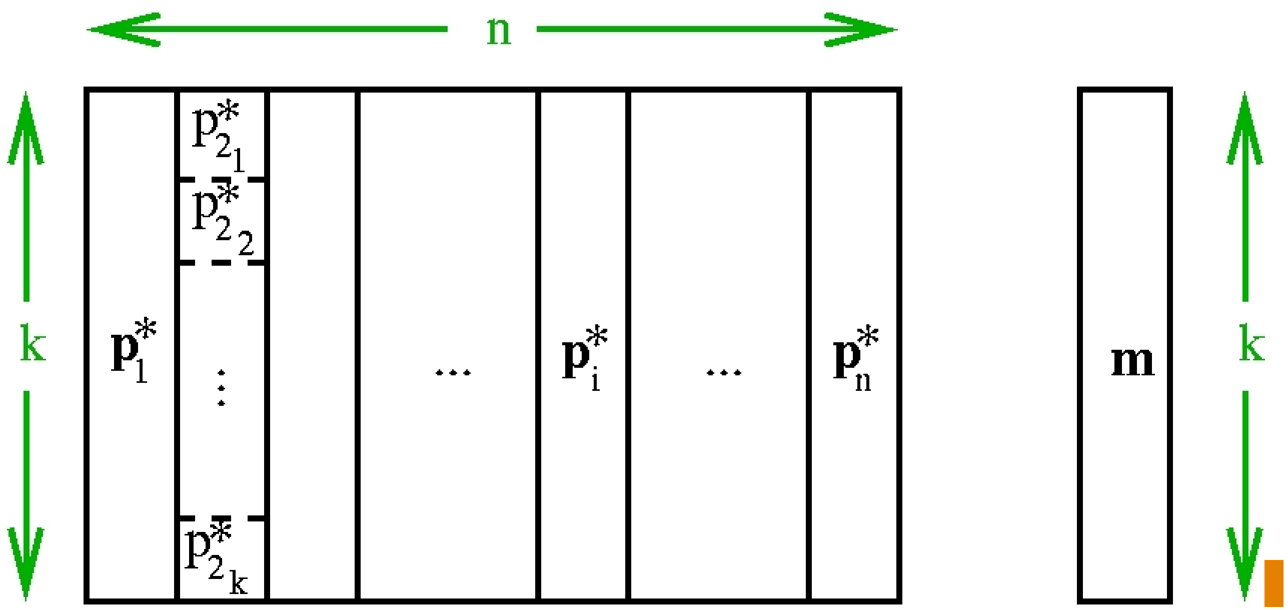
Pattern Recognition Terms

- A 'pattern' is a $k \times 1$ column vector - a 1-D signal can be represented as a 'pattern'. A $k_1 \times k_2$ 2-D signal (an image) can be represented as a 'pattern' by taking all pixels in raster scan order (row major order) to form a $k \times 1$ 'pattern', $k = k_1 \cdot k_2$
- k-dimensional 'patterns' $\mathbf{p}_i^*$, $1 \leq i \leq n$
- Stack them up together (in any order) to form a $k \times n$ Pattern Matrix $\mathbf{P}^*$



- Normalise each pattern: $\mathbf{p}_i \triangleq \mathbf{p}_i^* - \mathbf{m}$
- $\mathbf{A} \triangleq \frac{1}{n}\,\mathbf{P}\,\mathbf{P}^T$: The Covariance Matrix
- Stack together EigenVectors $\mathbf{u}_i$ of $\mathbf{A}$ in decreasing order of the corresponding EigenValues to get the $k \times k$ matrix $\mathbf{U}$

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Linear Algebra Fundamentals

- Phys significance of Eigenvalues & Eigenvectors
- Similar Matrices
- Diagonalisation of a $k \times k$ matrix
- Gram-Schmidt Orthogonalisation
- Eigenvalues of a symmetric real matrix are real
- Eigenvecs of a symmetric matrix: orthonormality

Phys Sig of E'values, E'vectors

- For a $k \times k$ matrix $\mathbf{B}$, if $\mathbf{B}\mathbf{u_i} = \lambda_i \mathbf{u_i}$, λ_i are the eigenvalues, and $\mathbf{u_i}$, the corresponding eigenvectors
- Phys sig: matrix $\times$ vector $\equiv$ scaling it!
- Computing eigenvalues: $\mathbf{B}\mathbf{u} - \lambda\mathbf{u} = \mathbf{0} \Longrightarrow$ $(\mathbf{B} - \lambda\mathbf{I})\mathbf{u} = \mathbf{0} \Longrightarrow$ non-trival solution: $|\mathbf{B} - \lambda\mathbf{I}| = 0$
- E'vecs: not unique! scaled versions also e'vecs

Some Less Important Properties

- Rank($\mathbf{B}$) = # of non-zero eigenvals
- $\sum \lambda_i$ = Trace($\mathbf{B}$) (sum of main diag), $\prod \lambda_i = |\mathbf{B}|$
- A square matrix $\mathbf{A}$ and $\mathbf{A}^T$ have the same eigenvalues (but usually, different eigenvectors)
  $|\mathbf{A}^T - \lambda \mathbf{I}| = |\mathbf{A}^T - \lambda \mathbf{I}^T| = |(\mathbf{A} - \lambda \mathbf{I})^T| = |\mathbf{A} - \lambda \mathbf{I}|$
- The eigenvalues of a diagonal matrix are those!
  eigenvalues: $|\mathbf{B} - \lambda \mathbf{I}| = 0, \prod(b_{ii} - \lambda_i) = 0$
- $\mathbf{B}_{k \times k}$ is invertible iff 0 isn't an eigenvalue. eigenvalue 0 iff $|\mathbf{B} - 0\mathbf{I}| = 0$ iff $|\mathbf{B}| = 0$ i.e., non-invertible
- If $\mathbf{B}$ has an eigenvalue-eigenvector pair $(\lambda, \mathbf{u})$, then $\mathbf{B}^n$ $(n \in \mathcal{N})$ has the pair $(\lambda^n, \mathbf{u})$.
  $\mathbf{B}_{k \times k}\mathbf{u}_{k \times 1} = \lambda \mathbf{u}_{k \times 1}$, $\mathbf{B}\mathbf{B}\mathbf{u} = \lambda \mathbf{B}\mathbf{u}$, $\mathbf{B}^2\mathbf{u} = \lambda^2\mathbf{u}$, etc
- If $\mathbf{B}$ has an eigenvalue-eigenvector pair $(\lambda, \mathbf{u})$, then $\mathbf{B}^{-1}$ has the pair $(\lambda^{-1}, \mathbf{u})$.
  $\mathbf{B}_{k \times k}\mathbf{u}_{k \times 1} = \lambda \mathbf{u}_{k \times 1}$, $\mathbf{B}^{-1}\mathbf{B}\mathbf{u} = \lambda \mathbf{B}^{-1}\mathbf{u}$, $(1/\lambda)\mathbf{u} = \mathbf{B}^{-1}\mathbf{u}$

- Eigenvectors of a matrix with distinct eigenvalues are linearly independent: Can form a basis
  Proof by Contradiction: Suppose not. 'Thin out' this to l indep eigenvectors $\mathbf{u}_1, \ldots \mathbf{u}_l \equiv \lambda_1, \ldots \lambda_l$
  Suppose $\mathbf{u}$ was 'thinned out' $\mathbf{u} = \sum_{j=1}^{l} c_j \mathbf{u_j}$ (1)
  1. Multiply (1) by $\mathbf{B}$: $\mathbf{Bu} = \sum c_j(\mathbf{Bu_j})$, $\lambda \mathbf{u} = \sum c_j \lambda_j \mathbf{u_j}$
  2. Multiply (1) by λ: $\lambda \mathbf{u} = \sum c_j \lambda \mathbf{u}_j$
  Subtract: $\mathbf{0} = \sum c_j(\lambda - \lambda_j)\mathbf{u}_j$. Hence, $\forall j$:
  $c_j = 0$ (no!) or $\mathbf{u}_j = \mathbf{0}$ (no, as eigenvector is a non-trival solution) or $\lambda = \lambda_j$ (no!): Contradiction!

- Eigenvalues of a symmetric real matrix are real
  $\mathbf{Au} = \lambda \mathbf{u}$ and $\mathbf{A}^*\mathbf{u}^* = \lambda^*\mathbf{u}^*$, $\mathbf{A}^* = \mathbf{A}$: real
  Pre-multiply by $\mathbf{u}^{*T}$ and $\mathbf{u}^T$, and subtract:
  $\mathbf{u}^{*T}\mathbf{Au} - \mathbf{u}^T\mathbf{Au}^* = \lambda \mathbf{u}^{*T}\mathbf{u} - \lambda^*\mathbf{u}^T\mathbf{u}^*$ LHS: Consider $(\mathbf{u}^{*T}\mathbf{Au})^T$, scalar's transpose. $= \mathbf{u}^T\mathbf{Au}^*$. LHS = 0
  RHS: $\mathbf{u}^{*T}\mathbf{u}$: sum-of-sq $\neq 0$ unless all 0, e'vec $\neq \mathbf{0}$
  e.g., $[a - jb\ c - jd][a + jb\ c + jd]^T = a^2 + b^2 + c^2 + d^2$
  Hence $\lambda = \lambda^*$, only possible if λ is real. QED

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- Definiteness of a symmetric matrix depends on the sign of its eigenvalues. Quadratic Form: for $\mathbf{B}_{k\times k}$ the scalar $\mathbf{x}^T\mathbf{B}\mathbf{x}$ is a quadratic form $= \sum_{i=1}^{k}\sum_{j=1}^{k} b_{ij}x_ix_j$. $(\mathbf{x}^T\mathbf{B}\mathbf{x})^T = \mathbf{x}^T\mathbf{B}^T\mathbf{x}$: $\mathbf{B}$ is symmetric!

  Quadratic form: defined only for symmetric $\mathbf{B}_{k\times k}$

  Positive Definite: $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0,\ \forall\mathbf{x}$

  Positive Semi-Definite: $\mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0,\ \forall\mathbf{x}$

  $(*)$ PSD matrix has non-negative eigenvalues:

  Let λ be an eigenvalue of $\mathbf{A}_{k\times k}$ with eigenvector $\mathbf{u}$. $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$: $\mathbf{u}^T\mathbf{A}\mathbf{u} = \lambda\mathbf{u}^T\mathbf{u}$. Since $\mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0\ \forall\mathbf{x}$, $\mathbf{u}^T\mathbf{A}\mathbf{u} \geq 0$. $\mathbf{u}^T\mathbf{u} \geq 0 \implies \lambda \geq 0$

  $(*)$ Non-negative eigenvalues $\implies$ PSD:

  Symmetric matrix $\mathbf{A} = \mathbf{U}\Lambda\mathbf{U}^T$. $\mathbf{x}^T\mathbf{A}\mathbf{x} = \mathbf{x}^T\mathbf{U}\Lambda\mathbf{U}^T\mathbf{x} = \mathbf{y}^T\Lambda\mathbf{y} = \sum_{i=1}^{k}\lambda_i y_i^2$. If all $\lambda_i \geq 0$, $\mathbf{x}^T\mathbf{A}\mathbf{x}$ is PSD

- The Quadratic form for Constrained Optimisation of a Symmetric Matrix: $\max / \min_{\mathbf{x}} \mathbf{x}^T \mathbf{A}\mathbf{x}, \; ||\mathbf{x}||^2 = 1$

  Take $f(\mathbf{x}) = \mathbf{x}^T\mathbf{A}\mathbf{x} + \lambda(\mathbf{x}^T\mathbf{x} - 1)$ (or $(1 - \mathbf{x}^T\mathbf{x})$)

  $\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = 0 :$ $2\mathbf{A}\mathbf{x} + \lambda 2\mathbf{x} = \mathbf{0}$: $(\mathbf{A} + \lambda \mathbf{I})\mathbf{x} = \mathbf{0}$

  For this, take $\mu = -\lambda$ (λ suffices for $(1 - \mathbf{x}^T\mathbf{x})$)

  $(\mathbf{A} - \mu \mathbf{I})\mathbf{x} = \mathbf{0}$: Soln: eigenvec $\mathbf{u}$ of $\mathbf{A} \equiv$ eigenval μ

  To optimise: $\mathbf{x}^T\mathbf{A}\mathbf{x}$. At the opt: $\mathbf{x}^T\mathbf{A}\mathbf{x} = \mathbf{u}^T\mathbf{A}\mathbf{u} = \lambda \mathbf{u}^T\mathbf{u} = \lambda \implies$ $\max = \lambda_{\max}, \; \min = \lambda_{\min}$

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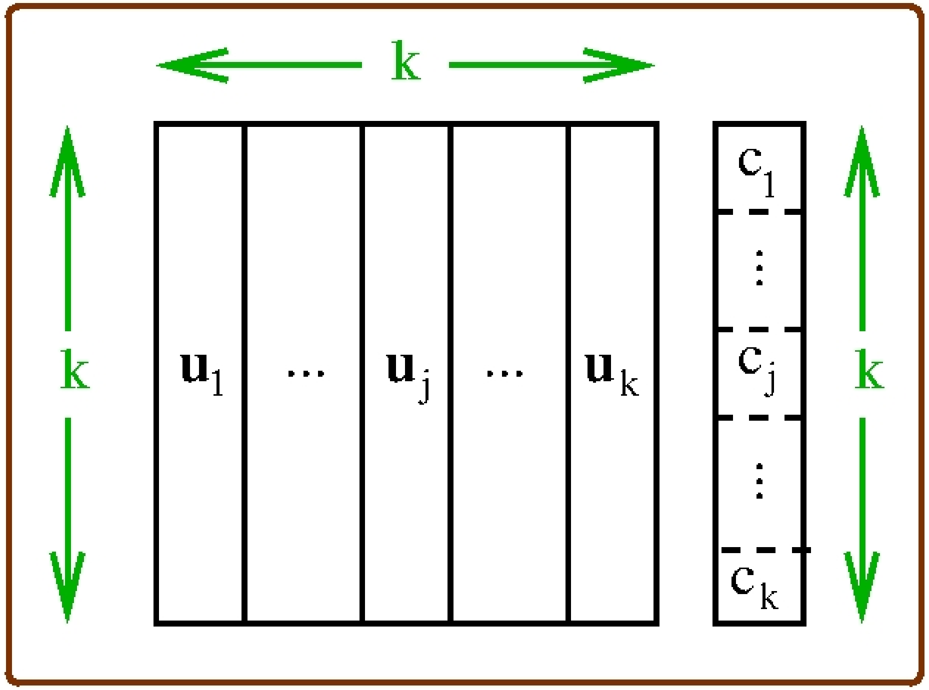
Similar Matrices

- For a $k \times k$ matrix $\mathbf{B}$ and any invertible $k \times k$ matrix $\mathbf{E}$, $\mathbf{EBE}^{-1}$ and $\mathbf{B}$ are Similar Matrices
- $\mathbf{Bu} = \lambda \mathbf{u}, \implies \mathbf{EBu} = \lambda \mathbf{Eu}, \implies \mathbf{EB}\ \mathbf{E}^{-1}\mathbf{E}\ \mathbf{u} = \lambda \mathbf{Eu}$ $\implies \mathbf{EBE}^{-1}\ \mathbf{Eu} = \lambda\ \mathbf{Eu}, \implies \mathbf{EBE}^{-1}\ \mathbf{v} = \lambda\ \mathbf{v}$

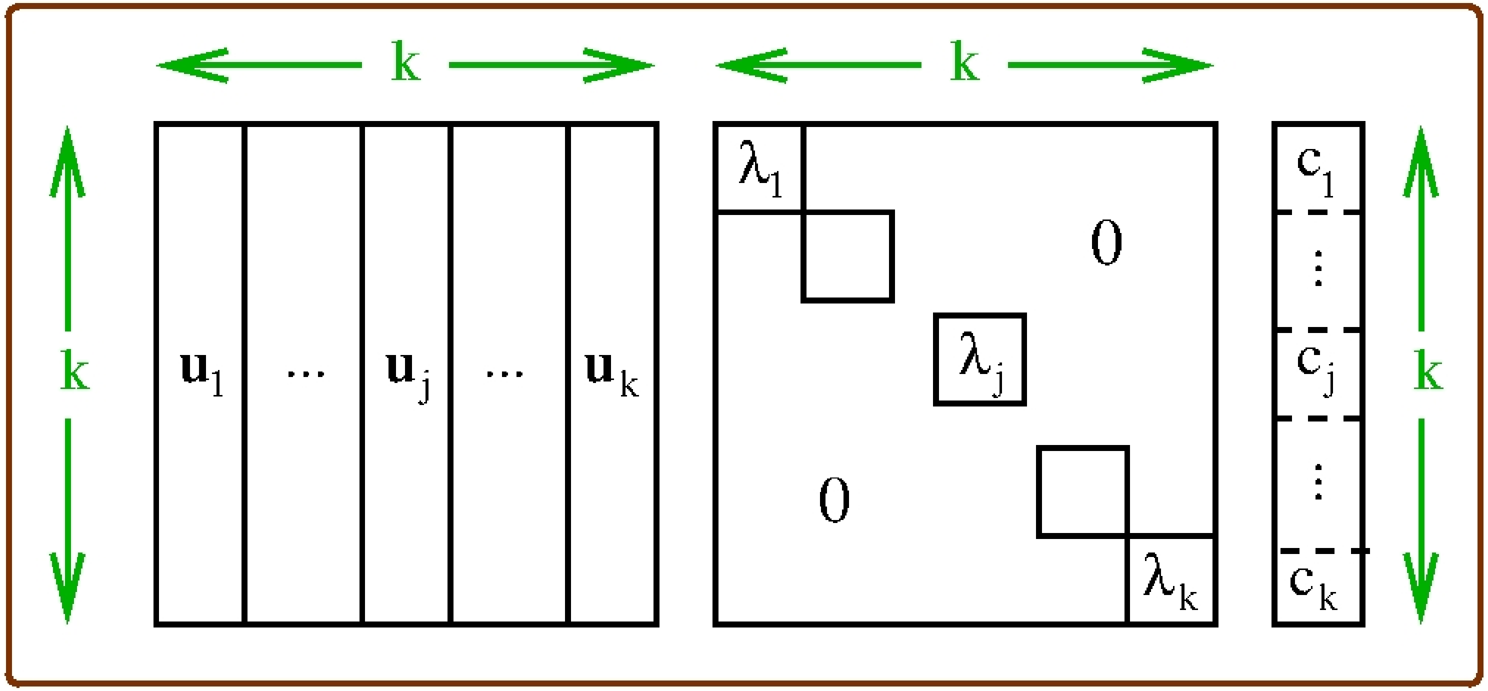
Diagonalisation of a $k \times k$ matrix $\mathbf{B}$

- $\mathbf{B}$: eigenvectors $\mathbf{u_i}$, stacked to get $\mathbf{U}$. $\mathbf{u_i}$'s not necessarily orthonormal, assume lin indep (non-repeated e'vals) $\implies$ basis of $k-$dim space
- What if accidentally end up with repeated eigen-values? SVD always works. Applications: use eigenvectors as an orthonormal basis. Extend with extra orthonormal vectors to span the space
- Any k-dimensional pattern $\mathbf{p_i}$ can be written as a linear combination of these basis vectors
- $\mathbf{p_i} = \sum_{j=1}^{k} c_j \mathbf{u_j}$



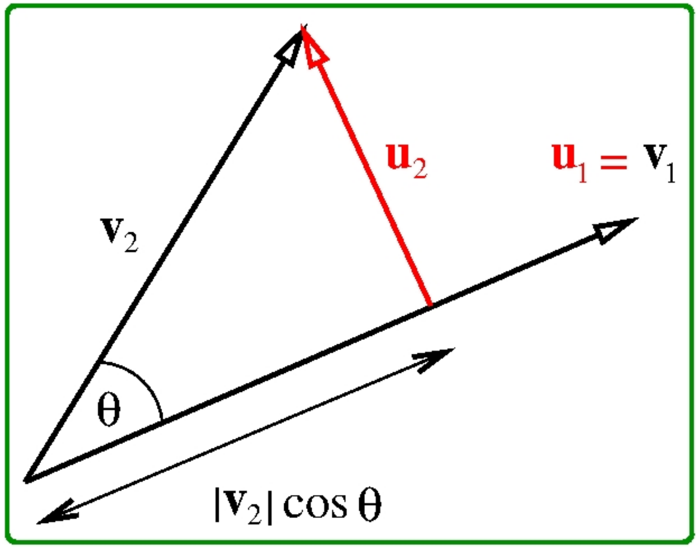
- $\mathbf{p_i} = \sum_{j=1}^{k} c_j \mathbf{u_j} = \mathbf{Uc}$
- $\mathbf{Bp_i} = \sum_{j=1}^{k} c_j \mathbf{Bu_j}$
  $= \sum_{j=1}^{k} c_j \lambda_j \mathbf{u_j} = \mathbf{U\Lambda c}$
- $\mathbf{BUc} = \mathbf{U\Lambda c} \implies$
  $\mathbf{BU} = \mathbf{U\Lambda} \implies$
- $\mathbf{B} = \mathbf{U\Lambda U}^{-1} \iff$
- $\mathbf{U}^{-1}\mathbf{BU} = \mathbf{\Lambda}$

If $\mathbf{U}$ is additionally orthonormal, $\mathbf{U}^{-1} = \mathbf{U}^T$



Gram-Schmidt Orthogonalisation

Orthonormalisation: compute all, then normalise!



- Dot product definition:
  $\mathbf{v_2} \cdot \mathbf{u_1} = |\mathbf{v_2}|\ |\mathbf{u_1}| \cos\theta$
  so $|\mathbf{v_2}| \cos\theta = \mathbf{v_2} \cdot \mathbf{u_1} / |\mathbf{u_1}|$
- This is the magnitude.
- Vector: magnitude $\times$ unit vector in that dirn

- unit vector in that dirn: $\mathbf{u_1}/|\mathbf{u_1}|$
- This vector: $\frac{\mathbf{v_2}\cdot\mathbf{u_1}}{|\mathbf{u_1}|}\frac{\mathbf{u_1}}{|\mathbf{u_1}|} = \frac{\langle \mathbf{v_2},\mathbf{u_1}\rangle}{\langle \mathbf{u_1},\mathbf{u_1}\rangle}\mathbf{u_1}$
- Triangle law: this $+\ \mathbf{u_2} = \mathbf{v_2}$
- Particular expression: $\boxed{\mathbf{u_2} = \mathbf{v_2} - \frac{\langle \mathbf{v_2},\mathbf{u_1}\rangle}{\langle \mathbf{u_1},\mathbf{u_1}\rangle}\mathbf{u_1}}$
- General Expression: $\boxed{\mathbf{u_k} = \mathbf{v_k} - \sum_{j=1}^{k-1} \frac{\langle \mathbf{v_k},\mathbf{u_j}\rangle}{\langle \mathbf{u_j},\mathbf{u_j}\rangle}\mathbf{u_j}}$

- Gram-Schmidt $>$ 2-D: graphical proof clumsy!
- Given $\mathbf{v}_1, \ldots \mathbf{v}_k$ linearly independent vectors (basis), to create an orthogonal set $\mathbf{u}_1, \ldots \mathbf{u}_k$
- Step 1: Start with $\mathbf{u}_1 = \mathbf{v}_1$
- Step 2: ($\perp$) $\mathbf{u}_1$, $\mathbf{u}_2$ span same space as $\mathbf{v}_1, \mathbf{v}_2$
  Take $\mathbf{u_2} = a_1\mathbf{u}_1 + \mathbf{v}_2$ (lin combo, $\mathbf{u_1} = \mathbf{v_1}$)
  To find a_1, take a dot product with $\mathbf{u}_1$: (ortho)
  $a_1 = -\frac{\langle \mathbf{v}_2, \mathbf{u}_1 \rangle}{\langle \mathbf{u}_1, \mathbf{u}_1 \rangle}$: $\boxed{\mathbf{u_2} = \mathbf{v_2} - \frac{\langle \mathbf{v_2}, \mathbf{u_1} \rangle}{\langle \mathbf{u_1}, \mathbf{u_1} \rangle}\mathbf{u_1}}$
- Step 3: ($\perp$) $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ span same space as $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$
  Take $\mathbf{u_3} = a_2\mathbf{u}_2 + a_1\mathbf{u}_1 + \mathbf{v}_3$ (lin combo, $\mathbf{v_1}, \mathbf{v}_2, \mathbf{v}_3$)
  a_1: take a dot product with $\mathbf{u}_1$: $a_1 = -\frac{\langle \mathbf{v}_3, \mathbf{u}_1 \rangle}{\langle \mathbf{u}_1, \mathbf{u}_1 \rangle}$
  a_2: take a dot product with $\mathbf{u}_2$: $a_2 = -\frac{\langle \mathbf{v}_3, \mathbf{u}_2 \rangle}{\langle \mathbf{u}_2, \mathbf{u}_2 \rangle}$
  $$\boxed{\mathbf{u_3} = \mathbf{v_3} - \frac{\langle \mathbf{v_3}, \mathbf{u_1} \rangle}{\langle \mathbf{u_1}, \mathbf{u_1} \rangle}\mathbf{u_1} - \frac{\langle \mathbf{v_3}, \mathbf{u_2} \rangle}{\langle \mathbf{u_2}, \mathbf{u_2} \rangle}\mathbf{u_2}}$$
- General Expression: $\boxed{\mathbf{u_k} = \mathbf{v_k} - \sum_{j=1}^{k-1} \frac{\langle \mathbf{v_k}, \mathbf{u_j} \rangle}{\langle \mathbf{u_j}, \mathbf{u_j} \rangle}\mathbf{u_j}}$

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- Eigenvectors of a symmetric matrix are orthonormal (Assumes no repeated eigenvalues) Actually follows from the diagonalisation result: $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ for symmetric matrices

  Explicit proof: consider $\mathbf{u}_i^T\mathbf{u}_j = (1/\lambda_j)\mathbf{u}_i^T\lambda_j\mathbf{u}_j = (1/\lambda_j)\mathbf{u}_i^T\mathbf{A}\mathbf{u}_j = (1/\lambda_j)(\mathbf{A}^T\mathbf{u}_i)^T\mathbf{u}_j = (1/\lambda_j)(\mathbf{A}\mathbf{u}_i)^T\mathbf{u}_j = (1/\lambda_j)(\lambda_i\mathbf{u}_i)^T\mathbf{u}_j = (\lambda_i/\lambda_j)\mathbf{u}_i^T\mathbf{u}_j \implies$ (as $\mathbf{A}^T = \mathbf{A}$) $(\lambda_i - \lambda_j)\mathbf{u}_i^T\mathbf{u}_j = 0 \implies \mathbf{u}_i \perp \mathbf{u}_j$, as $\lambda_i \neq \lambda_j$