

# What is a tensor? (Part I)

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# goals of these tutorials

- very elementary introduction to tensors
- through the lens of linear algebra and numerical linear algebra
- highlight their roles in computations
- trace chronological development through three definitions
  - ① a multi-indexed object that satisfies tensor transformation rules
  - ② a multilinear map
  - ③ an element of a tensor product of vector spaces
- all three definitions remain useful today

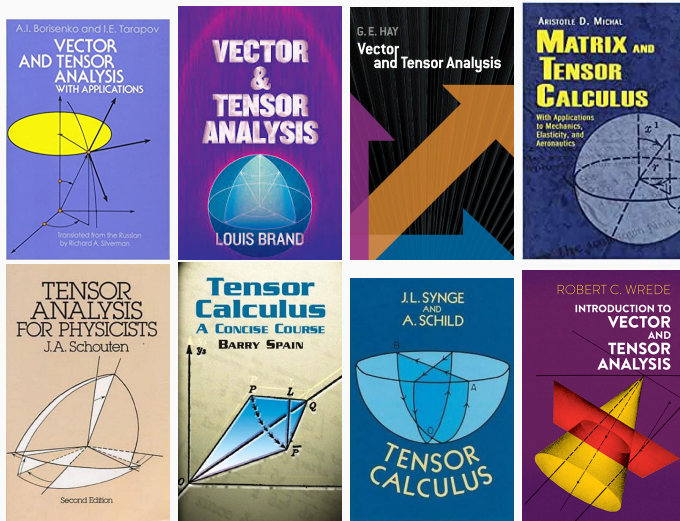
## tensors via transformation rules

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## earliest definition

- trickiest among the three definitions
- first appearance in Woldemar Voigt's 1898 book on crystallography
  - ▶ "An **abstract entity** represented by an array of components that are functions of coordinates such that, under a transformation of coordinates, the new components are related to the transformation and to the original components in a definite way"
- main issue: defines an entity by giving its change-of-bases formulas but without specifying the entity itself
- likely reason for notoriety of tensors as a difficult subject to master
  - ▶ J. Earman, C. Glymour, "Lost in tensors: Einstein's struggles with covariance principles 1912–1916," *Stud. Hist. Phil. Sci.*, **9** (1978), no. 4, pp. 251–278

# definition in Dover books c. 1950s



- “a multi-indexed object that satisfies certain transformation rules”

- linear algebra as we know it today was a subject in its infancy when Einstein was trying to learn tensors
- vector space, linear map, dual space, basis, change-of-basis, matrix, matrix multiplication, etc, were all obscure notions back then
  - ▶ 1858:  $3 \times 3$  matrix product<sup>1</sup> (Cayley)
  - ▶ 1888: vector space and  $n \times n$  matrix product (Peano)
  - ▶ 1898: tensor (Voigt)
- we enjoy the benefit of a hundred years of pedagogical progress
- next slides: look at tensor transformation rules in light of linear algebra and numerical linear algebra

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<sup>1</sup>we still do not know the optimal algorithm for this

# eigen and singular values

- **eigenvalue and vectors:**  $A \in \mathbb{C}^{n \times n}$ ,  $Av = \lambda v$ , for any invertible  $X \in \mathbb{C}^{n \times n}$ ,

$$(XAX^{-1})Xv = \lambda Xv$$

► eigenvalue  $\lambda' = \lambda$ , eigenvector  $v' = Xv$ , and  $A' = XAX^{-1}$

- **singular values and vectors:**  $A \in \mathbb{R}^{m \times n}$ ,

$$\begin{cases} Av = \sigma u, \\ A^T u = \sigma v \end{cases}$$

for any orthogonal  $X \in \mathbb{R}^{m \times m}$ ,  $Y \in \mathbb{R}^{n \times n}$ ,

$$\begin{cases} (XAY^T)Yv = \sigma Xu, \\ (XAY^T)^T Xu = \sigma Yv \end{cases}$$

► singular value  $\sigma' = \sigma$ , left singular vector  $u' = Xu$ , left singular vector  $v' = Yv$ , and  $A' = XAY^T$

- **matrix product:**  $A \in \mathbb{C}^{m \times n}$ ,  $B \in \mathbb{C}^{n \times p}$ ,  $C \in \mathbb{C}^{m \times p}$ ,  $AB = C$ , for any invertible  $X, Y, Z$ ,

$$(XAY^{-1})(YBZ^{-1}) = XCZ^{-1}$$

►  $A' = XAY^{-1}$ ,  $B' = YBZ^{-1}$ ,  $C' = XCZ^{-1}$

- **linear system:**  $A \in \mathbb{C}^{m \times n}$ ,  $b \in \mathbb{C}^m$ ,  $Av = b$ , for any invertible  $X, Y$ ,

$$(XAY^{-1})(Yv) = Xb$$

►  $A' = XAY^{-1}$ ,  $b' = Xb$ ,  $v' = Yv$



# ordinary and total least squares

- **ordinary least squares:**  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$ ,

$$\min_{v \in \mathbb{R}^n} \|Av - b\|^2 = \min_{v \in \mathbb{R}^n} \|(XAY^{-1})Yv - Xb\|^2$$

for any orthogonal  $X \in \mathbb{R}^{m \times m}$  and invertible  $Y \in \mathbb{R}^{n \times n}$

►  $A' = XAY^{-1}$ ,  $b' = Xb$ ,  $v' = Yv$ , minimum value  $\rho' = \rho$

- **total least squares:**  $A \in \mathbb{R}^{m \times n}$  and  $b \in \mathbb{R}^m$ , then

$$\begin{aligned} \min \{ \|E\|^2 + \|r\|^2 : (A + E)v = b + r \} \\ = \min \{ \|XEY^T\|^2 + \|Xr\|^2 : (XAY^T + XEY^T)Yv = Xb + Xr \} \end{aligned}$$

for any orthogonal  $X \in \mathbb{R}^{m \times m}$  and orthogonal  $Y \in \mathbb{R}^{n \times n}$

►  $A' = XAY^T$ ,  $E' = XEY^T$ ,  $b' = Xb$ ,  $r' = Xr$ ,  $v' = Yv$

# rank, norm, determinant, inertia

- **rank, norm, determinant:**  $A \in \mathbb{R}^{m \times n}$

$$\text{rank}(XAY^{-1}) = \text{rank}(A), \quad \det(XAY^{-1}) = \det(A), \quad \|XAY^{-1}\| = \|A\|$$

for  $X$  and  $Y$  invertible, special linear, or orthogonal, respectively

- ▶ determinant identically zero whenever  $m \neq n$
  - ▶  $\|\cdot\|$  either spectral, nuclear, or Frobenius norm
- **positive definiteness:**  $A \in \mathbb{R}^{n \times n}$  positive definite iff

$$XAX^T \quad \text{or} \quad X^{-T}AX^{-1}$$

positive definite for any invertible  $X \in \mathbb{R}^{n \times n}$

- almost everything we study in linear algebra and numerical linear algebra satisfies tensor transformation rules
- different names, same thing:
  - ▶ equivalence of matrices:  $A' = XAY^{-1}$
  - ▶ similarity of matrices:  $A' = XAX^{-1}$
  - ▶ congruence of matrices:  $A' = XAX^T$
- almost everything we study in linear algebra and numerical linear algebra is about 0-, 1-, 2-tensors

- transformation rules may mean different things

$$A' = XAY^{-1}, \quad A' = XAY^T, \quad A' = XAX^{-1}, \quad A' = XAX^T$$

and more

- matrices in transformation rules may have different properties

$$X \in \text{GL}(n), \text{SL}(n), \text{O}(n),$$

$$(X, Y) \in \text{GL}(m) \times \text{GL}(n), \text{SL}(m) \times \text{SL}(n), \text{O}(m) \times \text{O}(n), \text{O}(m) \times \text{GL}(n)$$

and more

- alternative (but equivalent) forms just as common

$$A' = X^{-1}AY, \quad A' = X^{-1}AY^{-T}, \quad A' = X^{-1}AX, \quad A' = X^{-1}AX^{-T}$$

- multi-indexed object  $\lambda \in \mathbb{R}$ ,  $v \in \mathbb{R}^n$ ,  $A \in \mathbb{R}^{m \times n}$ , etc, represents the tensor
- transformation rule  $A' = XAY^{-1}$ ,  $A' = XAY^{-1}$ ,  $A' = XAX^T$ , etc, defines the tensor
- but the tensor has been left unspecified
- easily fixed with modern definitions ② and ③
- need a context in order to use definition ①
- is  $A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{bmatrix}$  a tensor?
- it is a tensor if we are interested in, say, its eigenvalues and eigenvectors, in which case  $A$  transforms as a mixed 2-tensor

- remember definition ① came from physics — they don't ask
  - ▶ what is a tensor?but
  - ▶ is stress a tensor?
  - ▶ is deformation a tensor?
  - ▶ is electromagnetic field strength a tensor?
- unspecified quantity is placeholder for physical quantity like stress, deformation, etc
- it is a tensor if the multi-indexed object satisfies transformation rules under change-of-coordinates, i.e., definition ①
- makes perfect sense in a physics context
- is  $A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{bmatrix}$  a tensor?
- it is a tensor if it represents, say, stress, in which case  $A$  transforms as a contravariant 2-tensor

## 0-, 1-, 2-tensor transformation rules

contravariant 1-tensor:	$a' = X^{-1}a$	$a' = Xa$
covariant 1-tensor:	$a' = X^T a$	$a' = X^{-T} a$
covariant 2-tensor:	$A' = X^T A X$	$A' = X^{-T} A X^{-1}$
contravariant 2-tensor:	$A' = X^{-1} A X^{-T}$	$A' = X A X^T$
mixed 2-tensor:	$A' = X^{-1} A X$	$A' = X A X^{-1}$
contravariant 2-tensor:	$A' = X^{-1} A Y^{-T}$	$A' = X A Y^T$
covariant 2-tensor:	$A' = X^T A Y$	$A' = X^{-T} A Y^{-1}$
mixed 2-tensor:	$A' = X^{-1} A Y$	$A' = X A Y^{-1}$

# multilinear matrix multiplication

- $A \in \mathbb{R}^{n_1 \times \cdots \times n_d}$
- $X \in \mathbb{R}^{m_1 \times n_1}, Y \in \mathbb{R}^{m_2 \times n_2}, \dots, Z \in \mathbb{R}^{m_d \times n_d}$
- define

$$(X, Y, \dots, Z) \cdot A = B$$

where  $B \in \mathbb{R}^{m_1 \times \cdots \times m_d}$  given by

$$b_{i_1 \dots i_d} = \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \cdots \sum_{j_d=1}^{n_d} x_{i_1 j_1} y_{i_2 j_2} \cdots z_{i_d j_d} a_{j_1 \dots j_d}$$

- $d = 1$ : reduces to  $Xa = b$  for  $a \in \mathbb{R}^n, b \in \mathbb{R}^m$
- $d = 2$ : reduces to

$$(X, Y) \cdot A = XAY^T$$



# higher-order transformation rules 1

- $X_1 \in \text{GL}(n_1), X_2 \in \text{GL}(n_2), \dots, X_d \in \text{GL}(n_d)$
- covariant  $d$ -tensor transformation rule:

$$A' = (X_1^\top, X_2^\top, \dots, X_d^\top) \cdot A$$

- contravariant  $d$ -tensor transformation rule:

$$A' = (X_1^{-1}, X_2^{-1}, \dots, X_d^{-1}) \cdot A$$

- mixed  $d$ -tensor transformation rule:

$$A' = (X_1^{-1}, \dots, X_p^{-1}, X_{p+1}^\top, \dots, X_d^\top) \cdot A$$

- contravariant order  $p$ , covariant order  $d - p$ , or **type**  $(p, d - p)$

## higher-order transformation rules 2

- when  $n_1 = n_2 = \dots = n_d = n$ ,  $X \in \text{GL}(n)$
- covariant  $d$ -tensor transformation rule:

$$A' = (X^T, X^T, \dots, X^T) \cdot A$$

- contravariant  $d$ -tensor transformation rule:

$$A' = (X^{-1}, X^{-1}, \dots, X^{-1}) \cdot A$$

- mixed  $d$ -tensor transformation rule:

$$A' = (X^{-1}, \dots, X^{-1}, X^T, \dots, X^T) \cdot A$$

- getting ahead of ourselves, with definition ②, difference is between multilinear

$$f : \mathbb{V}_1 \times \dots \times \mathbb{V}_d \rightarrow \mathbb{R} \quad \text{and} \quad f : \mathbb{V} \times \dots \times \mathbb{V} \rightarrow \mathbb{R}$$

## change-of-coordinates matrices

- $X_1, \dots, X_d$  or  $X$  may belong to:

$$\mathrm{GL}(n) = \{X \in \mathbb{R}^{n \times n} : \det(X) \neq 0\}$$

$$\mathrm{SL}(n) = \{X \in \mathbb{R}^{n \times n} : \det(X) = 1\}$$

$$\mathrm{O}(n) = \{X \in \mathbb{R}^{n \times n} : X^T X = I\},$$

$$\mathrm{SO}(n) = \{X \in \mathbb{R}^{n \times n} : X^T X = I, \det(X) = 1\}$$

$$\mathrm{U}(n) = \{X \in \mathbb{C}^{n \times n} : X^* X = I\}$$

$$\mathrm{SU}(n) = \{X \in \mathbb{C}^{n \times n} : X^* X = I, \det(X) = 1\}$$

$$\mathrm{O}(p, q) = \{X \in \mathbb{R}^{n \times n} : X^T I_{p,q} X = I_{p,q}\}$$

$$\mathrm{SO}(p, q) = \{X \in \mathbb{R}^{n \times n} : X^T I_{p,q} X = I_{p,q}, \det(X) = 1\}$$

$$\mathrm{Sp}(2n, \mathbb{R}) = \{X \in \mathbb{R}^{2n \times 2n} : X^T J X = J\}$$

$$\mathrm{Sp}(2n) = \{X \in \mathbb{C}^{2n \times 2n} : X^T J X = J, X^* X = I\}$$

- $I := I_n$  is  $n \times n$  identity,  $I_{p,q} := \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix} \in \mathbb{R}^{n \times n}$ ,  $J := \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$

## change-of-coordinates matrices

- again getting ahead of ourselves with definitions ② or ③,
  - ▶ if vector spaces involve have no extra structure, then  $GL(n)$
  - ▶ if inner product spaces, then  $O(n)$
  - ▶ if equipped with yet other structures, then whatever group that preserves those structures
- e.g.,  $\mathbb{R}^4$  equipped with Euclidean inner product:

$$\langle x, y \rangle = x_0y_0 + x_1y_1 + x_2y_2 + x_3y_3$$

want  $X \in O(4)$  or  $SO(4)$

- e.g.,  $\mathbb{R}^4$  equipped with Lorentzian scalar product,

$$\langle x, y \rangle = x_0y_0 - x_1y_1 - x_2y_2 - x_3y_3,$$

want  $X \in O(1, 3)$  or  $SO(1, 3)$

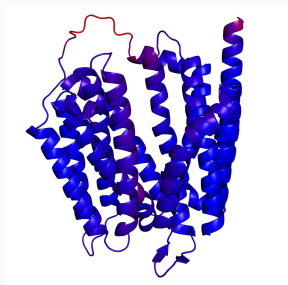
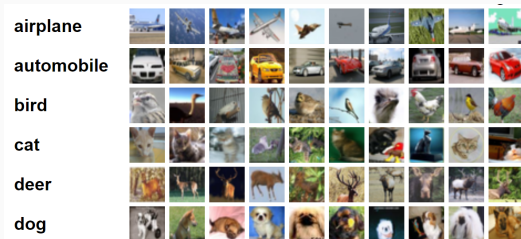
- called **Cartesian tensors** or **Lorentzian tensors** respectively

**transformation rule is the crux**

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# why important (in machine learning)

- tensor transformation rules in modern parlance: **equivariance**
- exact same idea in **equivariant neural network** used by Google's **AlphaFold 2** [Jumper et al, 2020]



## why important (in physics)

- special relativity is essentially the observation that the laws of physics are invariant under Lorentz transformations in  $O(1, 3)$  [Einstein, 1920]
- transformation rules under  $O(1, 3)$ -analogue of Givens rotations:

$$\begin{bmatrix} \cosh \theta & -\sinh \theta & 0 & 0 \\ -\sinh \theta & \cosh \theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} \cosh \theta & 0 & -\sinh \theta & 0 \\ 0 & 1 & 0 & 0 \\ -\sinh \theta & 0 & \cosh \theta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} \cosh \theta & 0 & 0 & -\sinh \theta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh \theta & 0 & 0 & \cosh \theta \end{bmatrix}$$

enough to derive most standard results of special relativity

- “Geometric Principle: The laws of physics must all be expressible as geometric (coordinate independent and reference frame independent) relationships between geometric objects (scalars, vectors, tensors, ...) that represent physical entities.” [Thorne, 1973]

## why important (in mathematics)

- deriving higher-order tensorial analogues not a matter of just adding more indices to

$$\sum_{j=1}^n a_{ij}x_j = b_i, \quad \sum_{j=1}^n a_{ij}x_j = \lambda x_i, \quad \sum_{\sigma \in \mathfrak{S}_n} \text{sgn}(\sigma) \prod_{i=1}^n a_{i\sigma(i)}$$

- need to satisfy tensor transformation rules
- e.g.,  $A \in \mathbb{R}^{2 \times 2 \times 2}$  has hyperdeterminant

$$\begin{aligned} \det(A) = & a_{000}^2 a_{111}^2 + a_{001}^2 a_{110}^2 + a_{010}^2 a_{101}^2 + a_{011}^2 a_{100}^2 \\ & - 2(a_{000} a_{001} a_{110} a_{111} + a_{000} a_{010} a_{101} a_{111} + a_{000} a_{011} a_{100} a_{111} \\ & + a_{001} a_{010} a_{101} a_{110} + a_{001} a_{011} a_{110} a_{100} + a_{010} a_{011} a_{101} a_{100}) \\ & + 4(a_{000} a_{011} a_{101} a_{110} + a_{001} a_{010} a_{100} a_{111}), \end{aligned}$$

- preserved by transformation  $A' = (X, Y, Z) \cdot A$  for  $X, Y, Z \in \text{SL}(2)$
- just as determinant preserved by  $A' = XAY^T$  for  $X, Y \in \text{SL}(n)$



# tensor multiplication?

- Hadamard product:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \circ \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} \\ a_{21}b_{21} & a_{22}b_{22} \end{bmatrix}$$

- seems a lot more obvious than standard matrix product

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{bmatrix}$$

- matrix product satisfies transformation rule for mixed 2-tensors  $(XAY^{-1})(YBZ^{-1}) = X(AB)Z^{-1}$ , i.e., defined on tensors
- Hadamard product undefined on tensors — depends on coordinates
- product on  $\mathbb{R}^{m \times n \times p}$  or  $\mathbb{R}^{n \times n \times n}$  that satisfies 3-tensor transformation rules does not exist

# identity tensor?

- identity matrix  $I \in \mathbb{R}^{3 \times 3}$

$$I = \sum_{i=1}^3 e_i \otimes e_i \in \mathbb{R}^{3 \times 3}$$

with  $e_1, e_2, e_3 \in \mathbb{R}^3$  standard basis vectors

- $(Q, Q) \cdot I = QIQ^T = I$  for any  $Q \in O(3)$ , unique up to scalar multiples
- $I$  is a Cartesian 2-tensor
- analogue in  $\mathbb{R}^{3 \times 3 \times 3}$  is not

$$A = \sum_{i=1}^3 e_i \otimes e_i \otimes e_i \in \mathbb{R}^{3 \times 3 \times 3}$$

as  $(Q, Q, Q) \cdot A \neq A$

# identity tensor?

- analogue is

$$J = \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 \varepsilon_{ijk} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \in \mathbb{R}^{3 \times 3 \times 3}$$

where  $\varepsilon_{ijk}$  is the Levi-Civita symbol

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2), \\ -1 & \text{if } (i, j, k) = (1, 3, 2), (2, 1, 3), (3, 2, 1), \\ 0 & \text{if } i = j, j = k, k = i \end{cases}$$

- $(Q, Q, Q) \cdot J = J$  for any  $Q \in O(3)$ , unique up to scalar multiples
- $J$  is a Cartesian 3-tensor

## why important (in computations)

two simple properties:

- **group:** change-of-coordinates matrices may be multiplied/inverted:
  - ▶ if  $X, Y$  orthogonal or invertible, so is  $XY$
  - ▶ if  $X$  orthogonal or invertible, so is  $X^{-1}$
- **group action:** transformation rules may be composed:
  - ▶ if  $a' = X^{-T}a$  and  $a'' = Y^{-T}a'$ , then  $a'' = (YX)^{-T}a$
  - ▶ if  $A' = XAX^{-1}$  and  $A'' = YA'Y^{-1}$ , then  $A'' = (YX)A(YX)^{-1}$

plus one more fact about the change-of-coordinate matrices (next slides)

## why important (in computations)

- recall Givens rotation, Householder reflector, Gauss transform:

$$G = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & \cos \theta & \cdots & -\sin \theta & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & \sin \theta & \cdots & \cos \theta & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix} \in SO(n),$$

$$H = I - \frac{2vv^T}{v^T v} \in O(n), \quad M = I - ve_i^T \in GL(n)$$

- $a' = Ga$  rotation of  $a$  in  $(i, j)$ -plane by an angle  $\theta$
- $a' = Ha$  reflection of  $a$  in the hyperplane with normal  $v/\|v\|$
- for judiciously chosen  $v$ ,  $a' = Ma \in \text{span}\{e_{i+1}, \dots, e_n\}$ , i.e., has  $(i+1)$ th through  $n$ th coordinates zero

## why important (in computations)

- facts about change-of-coordinate matrices in transformation rules
  - ▶ any  $X \in SO(n)$  is a product of Givens rotations
  - ▶ any  $X \in O(n)$  is a product of Householder reflectors
  - ▶ any  $X \in GL(n)$  is a product of elementary matrices
  - ▶ any unit lower triangular  $X \in GL(n)$  is a product of Gauss transforms
- in group theoretic lingo:
  - ▶ Givens rotations generate  $SO(n)$
  - ▶ Householder reflectors generate  $SO(n)$
  - ▶ elementary matrices generate  $GL(n)$
  - ▶ Gauss transforms generate lower unitriangular subgroup of  $GL(n)$

## why important (in computations)

- algorithms in numerical linear algebra implicitly based on these:
  - apply a sequence of tensor transformation rules

$$A \rightarrow X_1 A \rightarrow X_2 (X_1 A) \rightarrow \cdots \rightarrow B$$

$$A \rightarrow X_1^{-T} A \rightarrow X_2^{-T} (X_1^{-T} A) \rightarrow \cdots \rightarrow B$$

$$A \rightarrow X_1 A X_1^T \rightarrow X_2 (X_1 A X_1^T) X_2^T \rightarrow \cdots \rightarrow B$$

$$A \rightarrow X_1 A X_1^{-1} \rightarrow X_2 (X_1 A X_1^{-1}) X_2^{-1} \rightarrow \cdots \rightarrow B$$

$$A \rightarrow X_1 A Y_1^{-1} \rightarrow X_2 (X_1 A Y_1^{-1}) Y_2^{-1} \rightarrow \cdots \rightarrow B$$

- required  $X$  obtained as either  $X_m X_{m-1} \dots X_1$  or its limit as  $m \rightarrow \infty$
- caveat: in numerical linear algebra, we tend to view these transformation rules as giving **matrix decompositions**

## example: full-rank least squares

- tensor transformation rules for ordinary least squares: mixed 2-tensor  $A' = XAY^{-1}$  with change-of-coordinates  $(X, Y) \in O(m) \times GL(n)$
- method of solution essentially obtains

$$X = Q \in O(m), \quad Y = R^{-1} \in GL(n)$$

by applying a sequence of tensor transformation rules

- suppose  $\text{rank}(A) = n$ , with sequence of tensor transformation rules

$$A \rightarrow Q_1^T A \rightarrow Q_2^T (Q_1^T A) \rightarrow \cdots \rightarrow Q^T A = \begin{bmatrix} R \\ 0 \end{bmatrix}$$

given by **Householder QR algorithm**, get

$$A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$$

- practically Voigt's definition: transform problem into form where solution of transformed problem is related to original solution in a definite way



## example: full-rank least squares

- minimum value is invariant Cartesian 0-tensor

$$\begin{aligned}\min \|Av - b\|^2 &= \min \|Q^T(Av - b)\|^2 = \min \left\| \begin{bmatrix} R \\ 0 \end{bmatrix} v - Q^T b \right\|^2 \\ &= \min \left\| \begin{bmatrix} R \\ 0 \end{bmatrix} v - \begin{bmatrix} c \\ d \end{bmatrix} \right\|^2 = \min \|Rv - c\|^2 + \|d\|^2 = \|d\|^2\end{aligned}$$

where

$$Q^T b = \begin{bmatrix} c \\ d \end{bmatrix}$$

- solution of transformed problem  $Rv = c$  equals original solution, and may be obtained through **back substitution**, i.e., a sequence

$$c \rightarrow Y_1^{-1}c \rightarrow Y_2^{-1}(Y_1^{-1}c) \rightarrow \cdots \rightarrow R^{-1}c = v$$

where  $Y_i$ 's are Gauss transforms

## example: Krylov subspaces

- $A \in \mathbb{R}^{n \times n}$  with all eigenvalues distinct and nonzero, arbitrary  $b \in \mathbb{R}^n$
- change-of-coordinates matrix  $K$  whose columns are

$$b, Ab, A^2b, \dots, A^{n-1}b$$

is invertible, i.e.,  $K \in \text{GL}(n)$

- transformation rule gives

$$A = K \begin{bmatrix} 0 & 0 & \cdots & 0 & -c_0 \\ 1 & 0 & \cdots & 0 & -c_1 \\ 0 & 1 & \cdots & 0 & -c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -c_{n-1} \end{bmatrix} K^{-1}$$

- seemingly trivial but when combined with other techniques, give powerful iterative methods for linear systems, least squares, eigenvalue problems, or evaluating various matrix functions

## example: Krylov subspaces

- why not use more obvious

$$A = X \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_n \end{bmatrix} X^{-1}$$

with change-of-coordinates matrix  $X \in \text{GL}(n)$  given by eigenvectors?

- much more difficult to compute than  $K$
- one way is in fact to implicitly exploit relation between  $K$  and  $X$ :

$$\begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_n \end{bmatrix} = \begin{bmatrix} 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^{n-1} \\ 1 & \lambda_2 & \lambda_2^2 & \cdots & \lambda_2^{n-1} \\ 1 & \lambda_3 & \lambda_3^2 & \cdots & \lambda_3^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_m & \lambda_m^2 & \cdots & \lambda_m^{n-1} \end{bmatrix} \begin{bmatrix} 0 & 0 & \cdots & 0 & -c_0 \\ 1 & 0 & \cdots & 0 & -c_1 \\ 0 & 1 & \cdots & 0 & -c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -c_{n-1} \end{bmatrix} \begin{bmatrix} 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^{n-1} \\ 1 & \lambda_2 & \lambda_2^2 & \cdots & \lambda_2^{n-1} \\ 1 & \lambda_3 & \lambda_3^2 & \cdots & \lambda_3^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_m & \lambda_m^2 & \cdots & \lambda_m^{n-1} \end{bmatrix}^{-1}$$

- primal and dual forms of **cone programming** problem over a symmetric cone  $\mathbb{K} \subseteq \mathbb{V}$  conform to transformation rules for Cartesian 0-, 1-, 2-tensors
- but change-of-coordinates matrices would have to be replaced a linear map from the *orthogonal group of the cone*:

$$O(\mathbb{K}) := \{\varphi : \mathbb{V} \rightarrow \mathbb{V} : \varphi \text{ linear, invertible, and } \varphi^* = \varphi^{-1}\}$$

- special cases include linear programming (LP), convex quadratic programming (QP), second-order cone programming (SOCP), and semidefinite programming (SDP)

- vector space  $\mathbb{V}$  may not be  $\mathbb{R}^n$ , e.g.,  $\mathbb{K} = \mathbb{S}_{++}^n$  and  $\mathbb{V} = \mathbb{S}^n$  for SDP
- numerical linear algebra notations we have been using to describe definition ① awkward and unnatural
- want to work with tensors over arbitrary vector spaces
  - ▶ space of Toeplitz or Hankel or Toeplitz-plus-Hankel matrices
  - ▶ space of polynomials or differential forms or differential operators
  - ▶ space of  $L^2$ -functions on homogeneous spaces
- another impetus for coordinate-free approach in definitions ② and ③ next week

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