Linear Algebra Summary

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Contents

1 Preliminaries

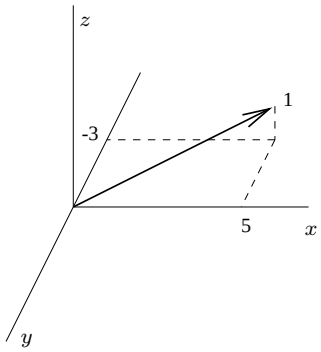
In this section we review our basic algebraic concepts and notation, in order to establish a common vocabulary and harmonize our ways of thinking. For more information on specifics, look up a basic textbook in linear algebra [1].

1.1 Vector Spaces

A vector space $\mathcal{X}$ over $\mathbf{R}$ or over $\mathbf{C}$ as 'base spaces' is a set of elements called 'vectors on which 'addition' is defined with its normal properties (the inverse exists as well as a neutral element called zero), and on which also 'multiplication with a scalar' (element of the base space is defined as well, with a slew of additional properties.

Concrete examples are common:

in $\mathbf{R}^3$: $\begin{bmatrix} 5 \\ -3 \\ 1 \end{bmatrix}$



in $\mathbf{C}^3$: $\begin{bmatrix} 5+j \\ -3-6j \\ 2+2j \end{bmatrix}$ $\approx \mathbf{R}^6$

The addition of vectors belonging to the same $\mathbf{C}^n$ ($\mathbf{R}^n$) space is defined as:

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{bmatrix}$$

and the scalar multiplication:

$a \in \mathbf{R}$ or $a \in \mathbf{C}$:

$$a \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} a$$

Example

The most interesting case for our purposes is where a vector is actually a discrete time sequence $\{x(k) : k = 1 \cdots N\}$. The space that surrounds us and in which electromagnetic waves propagate is mostly linear. Signals reaching an antenna are added to each other.

Composition Rules:

The following (logical) consistency rules must hold as well:

$\mathbf{x} + \mathbf{y}$	$=$	$\mathbf{y} + \mathbf{x}$	commutativity
$(\mathbf{x} + \mathbf{y}) + \mathbf{z}$	$=$	$\mathbf{x} + (\mathbf{y} + \mathbf{z})$	associativity
	0		neutral element
$\mathbf{x} + (-\mathbf{x})$	$=$	0	inverse
$a(\mathbf{x} + \mathbf{y})$	$=$	$a\mathbf{x} + a\mathbf{y}$	distributivity of $*$ w.r. $+$
$0 * \mathbf{x}$	$=$	$a * 0 = 0$	consistencies
$1.\mathbf{x}$	$=$	$\mathbf{x}$	
$a(bx)$	$=$	$(ab)x$	

Vector space of functions

Let $\mathcal{X}$ be a set and $\mathcal{Y}$ a vectorspace and consider the set of functions

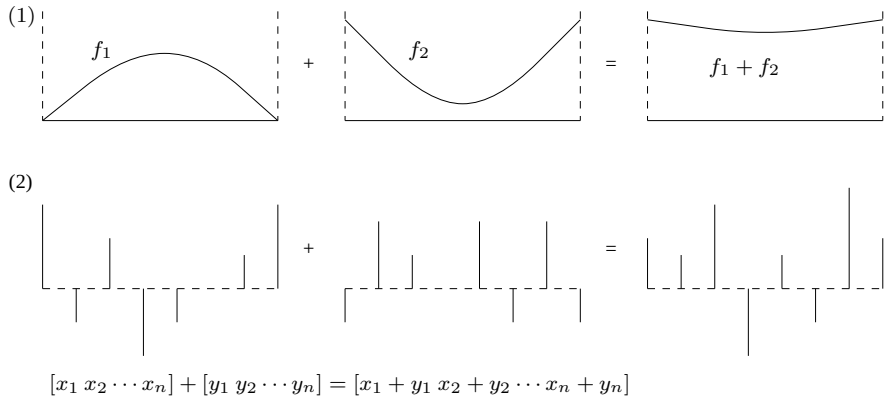
$$\mathcal{X} \to \mathcal{Y}.$$

We can define a new vectorspace on this set derived from the vectorspace structure of $\mathcal{Y}$:

$$(\mathbf{f}_1 + \mathbf{f}_2)(x) = \mathbf{f}_1(x) + \mathbf{f}_2(x)$$

$$(a\mathbf{f})(x) = a\mathbf{f}(x).$$

Examples:



As already mentioned, most vectors we consider can indeed be interpreted either as continous time or discrete time signals.

Linear maps

Assume now that both X **and** Y are vector spaces, then we can give a meaning to the notion 'linear map' as one that preserves the structure of vector space:

$$\mathbf{f}(x_1 + x_2) = \mathbf{f}(x_1) + \mathbf{f}(x_2)$$

$$\mathbf{f}(ax) = a\mathbf{f}(x)$$

we say that $\mathbf{f}$ defines a 'homomorphism of vector spaces'.

1.2 Bases

We say that a set of vectors $\{\mathbf{e}_k\}$ in a vectorspace form a *basis*, if all its vectors can be expressed as a unique linear combination of its elements. It turns out that a basis always exists, and that all the bases of a given vector space have exactly the same number of elements. In $\mathbf{R}^n$ or $\mathbf{C}^n$ the *natural basis* is given by the elements

$$\mathbf{e}_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where the '1' is in the k^{th} position.

If

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

then

$$\mathbf{x} = \sum_{k=1\cdots n} x_k \mathbf{e}_k$$

As further related definitions and properties we mention the notion of *span* of a set $\{\mathbf{v}_k\}$ of vectors in a vectorspace $\mathcal{V}$: it is the set of linear combinations $\{\mathbf{x} : \mathbf{x} = \sum_k \alpha_k \mathbf{v}_k\}$ for some scalars $\{\alpha_k\}$ - it is a subspace of $\mathcal{V}$. We say that the set $\{\mathbf{v}_k\}$ is linearly independent if it forms a basis for its span.

1.3 Matrices

A matrix (over $\mathbf{R}$ or $\mathbf{C}$) is 'a row vector of column vectors over the same vectorspace'

$$\mathbf{A} = [\mathbf{a}_{\cdot 1}\mathbf{a}_{\cdot 2}\cdots\mathbf{a}_{\cdot n}]$$

where

$$\mathbf{a}_{\cdot k} = \begin{bmatrix} a_{1k} \\ \vdots \\ a_{mk} \end{bmatrix}.$$

and each a_{ik} is an element of the base space. We say that such a matrix has dimensions $m \times n$. (Dually the same matrix can be viewed as a column vector of row matrices.)

Given a $m \times n$ matrix $\mathbf{A}$ and an n-vector $\mathbf{x}$, then we define the matrix vector-multiplication $\mathbf{Ax}$ as follows:

$$[a_{\cdot 1}\cdots a_{\cdot n}] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = a_{\cdot 1}x_1 + \cdots + a_{\cdot n}x_n$$

- the vector $\mathbf{x}$ gives the composition recipe on the columns of $\mathbf{A}$ to produce the result.

Matrix-matrix multiplication

can now be derived from the matrix-vector multiplication by stacking columns, in a fashion that is compatible with previous definitions:

$$[a_{\cdot 1}\, a_{\cdot 2}\cdots a_{\cdot n}] \begin{bmatrix} x_1 & y_1 & \cdots & z_1 \\ x_2 & y_2 & \cdots & z_2 \\ \vdots & \vdots & & \vdots \\ x_n & y_n & \cdots & z_n \end{bmatrix}$$

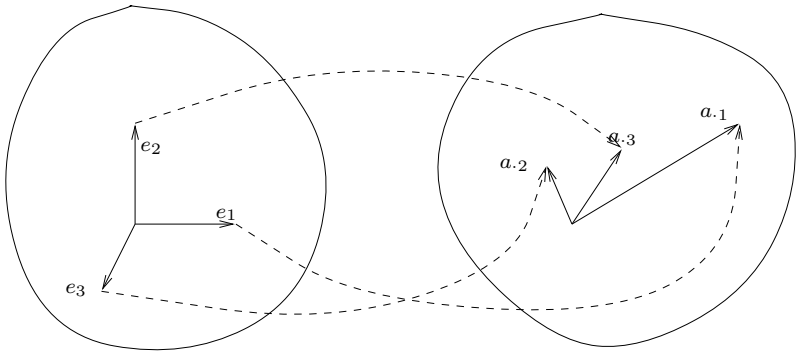
$$= [\mathbf{Ax}\ \mathbf{Ay}\ \cdots\ \mathbf{Az}]$$

where each column is manufactured according to the recipe.

The dual viewpoint works equally well: define row recipes in a dual way. Remarkably, the result is numerically the same! The product $\mathbf{AB}$ can be viewed as 'column recipe $\mathbf{B}$' acting on the columns of $\mathbf{A}$, or, alternatively, 'row recipe $\mathbf{A}$' acting on the rows of $\mathbf{B}$.

1.4 Linear maps represented as matrices

Linear maps $\mathbf{C}^n \to \mathbf{C}^m$ are represented by matrix-vector multiplications:



The way it works: map each natural basis vector $\mathbf{e}_k \in \mathbf{C}^n$ to a column $\mathbf{a}_{\cdot k}$. The matrix $\mathbf{A}$ build from these columns will map a general $\mathbf{x}$ maps to $\mathbf{Ax}$, where $\mathbf{A} = [\mathbf{a}_{\cdot 1} \cdots \mathbf{a}_{\cdot n}]$.

The procedure works equally well with more abstract spaces. Suppose that $\mathcal{X}$ and $\mathcal{Y}$ are such and $\mathbf{a}$ is a linear map between them. Choose bases in each space, then each vector can be represented by a 'concrete' vector of coefficients for the given basis, and we are back to the previous case. In particular, after the choice of bases, $\mathbf{a}$ will be represented by a 'concrete' matrix $\mathbf{A}$ mapping coefficients to coefficients.

Operations on matrices

Important operations on matrices are:

Transpose:	$[A^T]_{ij} = A_{ji}$
Hermitian conjugate:	$[A^H]_{ij} = \bar{A}_{ji}$
Addition:	$[A + B]_{ij} = A_{ij} + B_{ij}$
Scalar multiplication:	$[aA]_{ij} = aA_{ij}$
Matrix multiplication:	$[AB]_{ij} = \sum_k A_{ik}B_{kj}$

Special matrices

We distinguish the following special matrices:

Zero matrix:	$0_{m\times n}$
Unit matrix:	I_n

Working on blocks

Up to now we restricted the elements of matrices to scalars. The matrix calculus works equally well on more general elements, like matrices themselves, provided multiplication makes sense, e.g. provided dimensions match (but other cases of multiplication can work equally well).

Operators

Operators are linear maps which correspond to square matrices, e.g. a map between $\mathbf{C}^n$ and itself or between an 'abstract' space $\mathcal{X}$ and itself represented by an $n \times n$ matrix:

$$\mathbf{A} \in \mathbf{C}^n \to \mathbf{C}^n.$$

An interesting case is a basis transformation:

$$[\mathbf{e}_1\, \mathbf{e}_2 \cdots \mathbf{e}_n] \mapsto [\mathbf{f}_1\, \mathbf{f}_2 \cdots \mathbf{f}_n]$$

such that $\mathbf{f}_k = \mathbf{e}_1 s_{1k} + \mathbf{e}_2 s_{2k} + \cdots \mathbf{e}_n s_{nk}$ produces a matrix $\mathbf{S}$ for which holds (using 'formal' multiplication):

$$[\mathbf{f}_1 \cdots \mathbf{f}_n] = [\mathbf{e}_1 \cdots \mathbf{e}_n]\mathbf{S}$$

If this is a genuine basistransformation, then there must exist an inverse matrix $\mathbf{S}^{-1}$ s.t.

$$[\mathbf{e}_1 \cdots \mathbf{e}_n] = [\mathbf{f}_1 \cdots \mathbf{f}_n]\mathbf{S}^{-1}$$

Basis transformation of an operator

Suppose that a is an abstract operator, $\eta = a\xi$, while for a concrete representation in a given basis $[\mathbf{e}_1 \cdots \mathbf{e}_n]$ we have

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \mathbf{A} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

(abreviated as $\mathbf{y} = \mathbf{A}\mathbf{x}$) with

$$\xi = [e_1 \cdots e_n] \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \eta = [e_1 \cdots e_n] \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

then in the new basis:

$$\xi = [f_1 \cdots f_n] \begin{bmatrix} x'_1 \\ \vdots \\ x'_n \end{bmatrix}, \eta = [f_1 \cdots f_n] \begin{bmatrix} y'_1 \\ \vdots \\ y'_n \end{bmatrix}$$

and consequently

$$\begin{bmatrix} x'_1 \\ \vdots \\ x'_n \end{bmatrix} = \mathbf{S}^{-1} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$\begin{bmatrix} y'_1 \\ \vdots \\ y'_n \end{bmatrix} = \mathbf{S}^{-1} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$\mathbf{y}' = \mathbf{S}^{-1}\mathbf{y} = \mathbf{S}^{-1}\mathbf{A}\mathbf{x} = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}\mathbf{x}' = \mathbf{A}'\mathbf{x}'$$

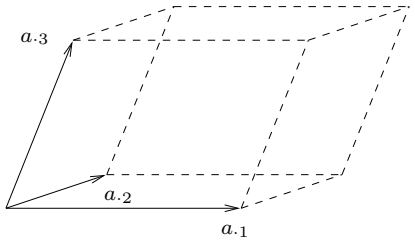
with

$$\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$$

by definition a *similarity transformation*.

Determinant of a square matrix

The determinant of a real $n \times n$ square matrix is *the signed volume of the n-dimensional parallellipeped which has as its edges the columns of the matrix.* (One has to be a little careful with the definition of the sign, for complex matrices one must use an extension of the definition - we skip these details).



The determinant of a matrix has interesting properties:

- $\det\mathbf{A} \in \mathbf{R}(\text{or } \mathbf{C})$
- $\det(\mathbf{S}^{-1}\mathbf{AS}) = \det\mathbf{A}$
- $\det \begin{bmatrix} a_{11} & * & \cdots & * \\ 0 & a_{22} & \cdots & * \\ & & \ddots & * \\ 0 & & & a_{nn} \end{bmatrix} = \prod_{i=1}^{n} a_{ii}$
- $\det[a_{\cdot 1} \cdots a_{\cdot i} \cdots a_{\cdot k} \cdots a_{\cdot n}] = -\det[a_{\cdot 1} \cdots a_{\cdot k} \cdots a_{\cdot i} \cdots a_{\cdot n}]$
- $\det\mathbf{AB} = \det\mathbf{A} \cdot \det\mathbf{B}$
- The matrix $\mathbf{A}$ is invertible iff $\det\mathbf{A} \neq 0$. We call such a matrix *non-singular.*

Minors of a square matrix M

For each entry i, j of a square matrix $\mathbf{M}$ there is a minor $m_{i,j}$:

$$m_{ij} = \det \left[\begin{array}{ccc|cc} * & * & * & * & * \\ * & * & * & * & * \\ \hline & & & & \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{array} \right] * (-1)^{i+j}$$

(ith row, jth column)

(cross out i$^{\text{th}}$ row and j$^{\text{th}}$ column, multiply with sign)

This leads to the famous Cramer's rule for the inverse:
$\mathbf{M}^{-1}$ exists iff $\det\mathbf{M} \neq 0$ and then:

$$\mathbf{M}^{-1} = \frac{1}{\det\mathbf{M}}[m_{ji}]$$

(Note change of order of indices!)

Example:

$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}^{-1} = \frac{1}{-2}\begin{bmatrix} 4 & -3 \\ -2 & 1 \end{bmatrix}$$

The characteristic polynomial of a matrix

Let: λ be a variable over $\mathbf{C}$ then the *characteristic polynomial* of a square matrix $\mathbf{A}$ is

$$\chi_A(\lambda) = \det(\lambda \mathbf{I}_n - \mathbf{A}).$$

Example:

$$\begin{aligned} \chi_{\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}}(\lambda) &= \det \begin{bmatrix} \lambda - 1 & -2 \\ -3 & \lambda - 4 \end{bmatrix} \\ &= (\lambda - 1)(\lambda - 4) - 6 \\ &= \lambda^2 - 5\lambda - 2 \end{aligned}$$

The characteristic polynomial is monic, the constant coefficient is $(-1)^n$ times the determinant, the coefficient of the n-1$^{\text{th}}$ power of λ is minus the *trace* - $\text{trace}(\mathbf{A}) = \sum_i a_{ii}$, the sum of the diagonal entries of the matrix.

Sylvester identity:
The matrix $\mathbf{A}$ satisfies the following remarkable identity:

$$\chi_A(\mathbf{A}) = 0$$

i.e. $\mathbf{A}^n$ depends linearly on $\mathbf{I}, \mathbf{A}, \mathbf{A}^2, \cdots, \mathbf{A}^{n-1}$.

Matrices and composition of functions

Let:

$$f : \mathcal{X} \to \mathcal{Y},\ g : \mathcal{Y} \to \mathcal{Z}$$

then:

$$g \circ f : \mathcal{X} \to \mathcal{Z} : (g \circ f)(x) = g(f(x)).$$

As we already know, linear maps f and g are represented by matrices $\mathbf{F}$ and $\mathbf{G}$ after a choice of a basis. The representation of the composition becomes matrix multiplication:

$$(g \circ f)(x) = \mathbf{GFx}.$$

1.5 Norms on vector spaces

Let $\mathcal{X}$ be a linear space. A norm $\|\cdot\|$ on $\mathcal{X}$ is a map $\|\cdot\| : \mathcal{X} \to \mathbf{R}^+$ which satisfies the following properties:

a. $\|\mathbf{x}\| \geq 0$

b. $\|\mathbf{x}\| = 0 \Leftrightarrow \mathbf{x} = 0$

c. $\|a\mathbf{x}\| = |a| \cdot \|\mathbf{x}\|$

d. $\|\mathbf{x} - \mathbf{z}\| \leq \|\mathbf{x} - \mathbf{y}\| + \|\mathbf{y} - \mathbf{z}\|$
(triangle inequality)

The purpose of the norm is to measure the 'size' or 'length' of a vector according to some measuring rule. There are many norms possible, e.g. in $\mathbf{C}^n$: The '1' norm:

$$\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|$$

The quadratic norm:

$$\|\mathbf{x}\|_2 = \left[\sum_{i=1}^{n} |x_i|^2\right]^{\frac{1}{2}}$$

The 'sup' norm:

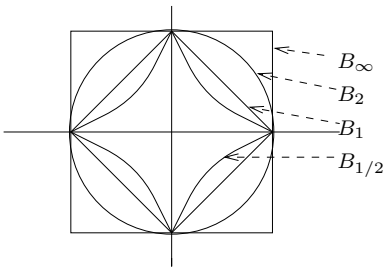
$$\|\mathbf{x}\|_\infty = \sup_{i=1\cdots n} (|x_i|)$$

Not a norm is:

$$\|\mathbf{x}\|_{\frac{1}{2}} = \left[\sum_{i=1}^{n} |x_i|^{\frac{1}{2}}\right]^2$$

(it does not satisfy the triangle inequality).

Unit ball in the different norms: shown is the set $\{\mathbf{x} : \|\mathbf{x}\|_? = 1\}$.



An interesting question is: which norm is the strongest?

The general p-norm has the form:

$$\|\mathbf{x}\|_p = \left[\sum |x_i|^p\right]^{\frac{1}{p}} \ (p \geq 1)$$

P-norms satisfy the following important 'Hölder inequality':
Let $p \geq 1$, $q = p/(p-1)$, then

$$\left|\sum_{i=1}^{n} x_i y_i\right| \leq \|x\|_p \|y\|_q$$

1.6 Inner products

Inner products put even more structure on a vector space and allow us to deal with 'orthogonality' or even more general angles!

Let: $\mathcal{X}$ be a vector space (over $\mathbf{C}$).

An inner product is a map $\mathcal{X} \times \mathcal{X} \to \mathbf{C}$ such that:

a. $(\mathbf{y}, \mathbf{x}) = \overline{(\mathbf{x}, \mathbf{y})}$

b. $(a\mathbf{x} + b\mathbf{y}, \mathbf{z}) = a(\mathbf{x}, \mathbf{z}) + b(\mathbf{y}, \mathbf{z})$

c. $(\mathbf{x}, \mathbf{x}) \geq 0$

d. $(\mathbf{x}, \mathbf{x}) = 0 \Leftrightarrow \mathbf{x} = 0$

Hence: $\|\mathbf{x}\| = (\mathbf{x}, \mathbf{x})^{\frac{1}{2}}$ is a norm

Question: when is a normed space also an inner product space compatible with the norm?

The answer is known: when the parallelogram rule is satisfied. For real vector spaces this means that the following equality must hold for all $\mathbf{x}$ and $\mathbf{y}$ (there is a comparable formula for complex spaces):

$$\|\mathbf{x} + \mathbf{y}\|^2 + \|\mathbf{x} - \mathbf{y}\|^2 = 2\left(\|\mathbf{x}\|^2 + \| \mathbf{y} \|^2\right)$$

(Exercise: define the appropriate inner product in term of the norm!)

The *natural inner product* on $\mathbf{C}^n$ is given by:

$$(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} x_i \bar{y}_i = \mathbf{y}^H \mathbf{x} = [\bar{y}_1 \cdots \bar{y}_n] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

The 'Gramian' of a basis:
Let: $\{f_i\}_{i=1\cdots n}$ be a basis for $\mathbf{C}^n$, then the Gramian $\mathbf{G}$ is given by:

$$\begin{aligned} \mathbf{G} &= [(\mathbf{f}_j, \mathbf{f}_i)] \\ &= \begin{bmatrix} \mathbf{f}_1^H \\ \vdots \\ \mathbf{f}_n^H \end{bmatrix} [\mathbf{f}_1 \cdots \mathbf{f}_n] \end{aligned}$$

A basis is orthonormal when its Gramian is a unit matrix:

$$\mathbf{G} = \mathbf{I}_n$$

Hermitian matrix: a matrix $\mathbf{A}$ is hermitian if

$$\mathbf{A} = \mathbf{A}^H$$

1.7 Definite matrices

Definitions: let $\mathbf{A}$ be hermitian,

$\mathbf{A}$ is *positive (semi)definite* if

$$\forall \mathbf{x} : (\mathbf{Ax}, \mathbf{x}) \geq 0$$

$\mathbf{A}$ is *strictly positive definite* if

$$\forall \mathbf{x} \neq 0 : (\mathbf{Ax}, \mathbf{x}) > 0$$

The Gramian of a basis is strictly positive definite!

1.8 Norms for linear maps

Let $\mathcal{X}$ and $\mathcal{Y}$ be normed spaces, and

$$f : \mathcal{X} \to \mathcal{Y}$$

a linear map, then

$$\|f\| = \sup_{\|\mathbf{x}\| \neq 0} \frac{\|f(x)\|_Y}{\|x\|_X} = \sup_{\|x\|_X = 1} \|f(x)\|_Y$$

is a valid norm on the space $\mathcal{X} \to \mathcal{Y}$. It measures the longest elongation of any vector on the unit ball of $\mathcal{X}$ under f.

1.9 Linear maps on an inner product space

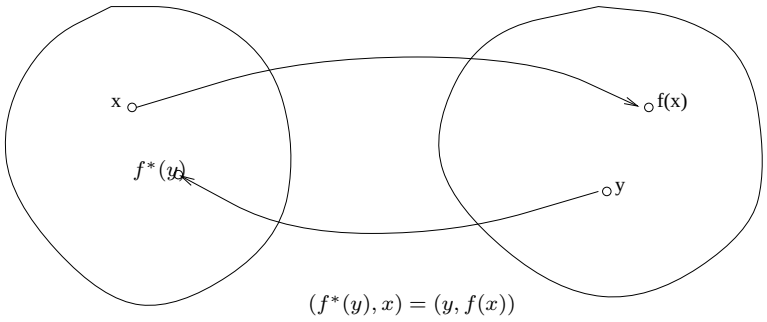
Let

$$f : \mathcal{X} \to \mathcal{Y}$$

where $\mathcal{X}$ and $\mathcal{Y}$ have inproducts $(\cdot, \cdot)_X$ and $(\cdot, \cdot)_Y$.

The adjoint map f^* is defined as:

$$f^* : \mathcal{Y} \to \mathcal{X} : \forall \mathbf{x} \forall \mathbf{y} [(f^*(y), x)_X = (y, f(x))_Y]$$



On matrices which represent an operator in a natural basis there is a simple expression for the adjoint: if f is $\mathbf{y} = \mathbf{Ax}$, and $(y, f(x)) = \mathbf{y}^H \mathbf{Ax}$, then $\mathbf{y}^H \mathbf{Ax} = (\mathbf{A}^H \mathbf{y})^H \mathbf{x}$ so that $f^*(y) = \mathbf{A}^H \mathbf{y}$. (This also shows quite simply that the adjoint always exist and is unique).

The adjoint map is very much like the original, it is in a sense its 'complex conjugate', and the composition with f^* is a 'square' or a 'covariance'.

We say that a map is *self-adjoint* if $\mathcal{X} = \mathcal{Y}$ and $f = f^*$ and that it is *isometric* if

$$\forall \mathbf{x} : \|f(x)\| = \|\mathbf{x}\|$$

in that case:

$$f^* f = \mathbf{I}_X$$

1.10 Unitary (Orthogonal) maps

A linear map f is *unitary* if both f and f^* are isometric:

$$f^* \circ f = \mathbf{I}_X$$

and

$$f \circ f^* = \mathbf{I}_Y$$

In that case $\mathcal{X}$ and $\mathcal{Y}$ must have the same dimension, they are isomorphic: $\mathcal{X} \approx \mathcal{Y}$.

Example:

- $\mathbf{A} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ is isometric with adjoint

$$\mathbf{A}^H = [\frac{1}{\sqrt{2}} \; \frac{1}{\sqrt{2}}]$$

- The adjoint of

$$\mathbf{A} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

  is

$$\mathbf{A}^H = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Both these maps are isometric and hence $\mathbf{A}$ is unitary, it rotates a vector over an angle of $-45°$, while $\mathbf{A}^H$ is a rotation over $+45°$.

1.11 Norms for matrices

We have seen that the measurement of lengths of vectors can be bootstrapped to maps and hence to matrices. Let $\mathbf{A}$ be a matrix.

Definition: the *operator norm* or *Euclidean norm* for $\mathbf{A}$ is:

$$\|\mathbf{A}\|_E = \sup_{\mathbf{x} \neq 0} \frac{\|\mathbf{A}\mathbf{x}\|_2}{\|\mathbf{x}\|_2}$$

It measures the greatest relative elongation of a vector $\mathbf{x}$ subjected to the action of $\mathbf{A}$ (in the natural basis and using the quadratic norm).

Properties:

- $\|\mathbf{A}\|_E = \sup_{\|\mathbf{x}\|=1} \|\mathbf{A}\mathbf{x}\|_2$
- $\mathbf{A}$ is isometric if $\mathbf{A}^H\mathbf{A} = \mathbf{I}$, then $\|\mathbf{A}\|_E = 1$, (the converse is *not* true!).
- Product rule: $\|\mathbf{F}\mathbf{G}\|_E \leq \|\mathbf{F}\|_\mathbf{E}\|\mathbf{G}\|_E$.

Contractive matrices: $\mathbf{A}$ is contractive if $\|\mathbf{A}\|_E \leq 1$.

Positive real matrices: $\mathbf{A}$ is positive real if it is square and if

$$\forall \mathbf{x} : ((\mathbf{A} + \mathbf{A}^H)\mathbf{x}, \mathbf{x}) \geq 0.$$

This property is abbreviated to: $\mathbf{A} + \mathbf{A}^H \geq 0$. We say that a matrix is strictly positive real if $\mathbf{x}^H(\mathbf{A} + \mathbf{A}^H)\mathbf{x} > 0$ for all $\mathbf{x} \neq 0$.

If $\mathbf{A}$ is contractive, then $\mathbf{I} - \mathbf{A}^H\mathbf{A} \geq 0$.

Cayley transform: if $\mathbf{A}$ is positive real, then $\mathbf{S} = (\mathbf{A} - \mathbf{I})(\mathbf{A} + \mathbf{I})^{-1}$ is contractive.

Frobenius norm

The *Frobenius norm* is the quadratic norm of a matrix viewed as a vector, after rows and columns have been stacked:

$$\|\mathbf{A}\|_F = \left[\sum_{i,j=1}^{n,m} |a_{i,j}|^2 \right]^{\frac{1}{2}}$$

Properties:

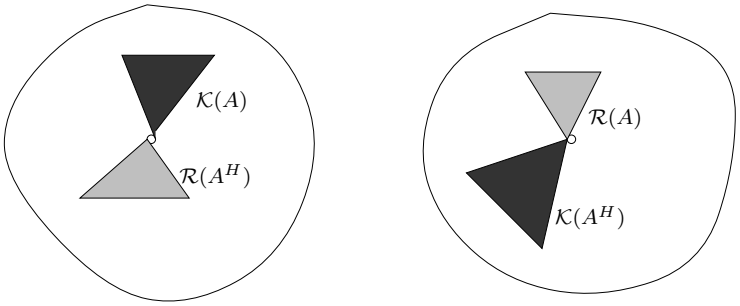
- $\|\mathbf{A}\|_F^2 = \text{trace } \mathbf{A}^H\mathbf{A} = \text{trace } \mathbf{A}\mathbf{A}^H$
- $\|\mathbf{A}\|_2 \leq \|\mathbf{A}\|_F$, the Frobenius norm is in a sense 'stronger' than the Euclidean.

1.12 Kernels and Ranges

Let $\mathbf{A}$ be a matrix $\mathcal{X} \to \mathcal{Y}$.

Definitions:

- Kernel of $\mathbf{A}$: $\mathcal{K}(\mathbf{A}) = \{\mathbf{x} : \mathbf{A}\mathbf{x} = 0\} \subset \mathcal{X}$
- Range of $\mathbf{A}$: $\mathcal{R}(\mathbf{A}) = \{\mathbf{y} : (\exists \mathbf{x} \in \mathcal{X} : \mathbf{y} = \mathbf{A}\mathbf{x})\} \subset \mathcal{Y}$
- Kernel of A^H (cokernel of $\mathbf{A}$): $\{\mathbf{y} : \mathbf{A}^H\mathbf{y} = 0\} \subset \mathcal{Y}$
- Range of $\mathbf{A}^H$ (corange of $\mathbf{A}$): $\{\mathbf{x} : (\exists \mathbf{y} : \mathbf{x} = \mathbf{A}^H\mathbf{y})\} \subset \mathcal{X}$



1.13 Orthogonality

All vectors and subspaces now live in a large innerprod (Euclidean) space.

- vectors: $\mathbf{x} \perp \mathbf{y} \Leftrightarrow (\mathbf{x}, \mathbf{y}) = 0$
- spaces: $\mathcal{X} \perp \mathcal{Y} \Leftrightarrow (\forall \mathbf{x} \in \mathcal{X})(\forall \mathbf{y} \in \mathcal{Y}) : (\mathbf{x}, \mathbf{y}) = 0$
- direct sum: $\mathcal{Z} = \mathcal{X} \oplus \mathcal{Y} \Leftrightarrow (\mathcal{X} \perp \mathcal{Y}) \& (\mathcal{X}, \mathcal{Y} \text{span} \mathcal{Z})$, i.e. $(\forall \mathbf{z} \in \mathcal{Z})(\exists \mathbf{x} \in \mathcal{X})(\exists \mathbf{y} \in \mathcal{Y}) : \mathbf{z} = \mathbf{x} + \mathbf{y}$ (in fact, $\mathbf{x}$ and $\mathbf{y}$ are unique).

Example w.r. kernels and ranges of a map $\mathbf{A} : \mathcal{X} \to \mathcal{Y}$:

$$\mathcal{X} = \mathcal{K}(\mathbf{A}) \oplus \mathcal{R}(\mathbf{A}^H)$$

$$\mathcal{Y} = \mathcal{K}(\mathbf{A}^H) \oplus \mathcal{R}(\mathbf{A})$$

1.14 Projections

Let $\mathcal{X}$ be an Euclidean space.

- $\mathbf{P} : \mathcal{X} \to \mathcal{Y}$ is a projection if $\mathbf{P}^2 = \mathbf{P}$.
- a projection $\mathbf{P}$ is an orthogonal projection if in addition:

$$\forall \mathbf{x} \in \mathcal{X} : \mathbf{P}\mathbf{x} \perp (\mathbf{I} - \mathbf{P})\mathbf{x}$$

- Property: $\mathbf{P}$ is an orthogonal projection if (1) $\mathbf{P}^2 = \mathbf{P}$ and (2) $\mathbf{P} = \mathbf{P}^H$.

Application: projection on the column range of a matrix.
Let

$$\mathbf{A} = [a_{\cdot 1}\, a_{\cdot 2}\, \cdots a_{\cdot m}]$$

such that the columns are linearly independent. Then $\mathbf{A}^H\mathbf{A}$ is non-singular and

$$\mathbf{P} = \mathbf{A}(\mathbf{A}^H\mathbf{A})^{-1}\mathbf{A}^H$$

is the orthogonal projection on the column range of $\mathbf{A}$.

Proof (sketch):

- check: $\mathbf{P}^2 = \mathbf{P}$
- check: $\mathbf{P}^H = \mathbf{P}$
- check: $\mathbf{P}$ project each column of $\mathbf{A}$ onto itself.

1.15 Eigenvalues and Eigenspaces

Let $\mathbf{A}$ be a square $n \times n$ matrix. Then $\lambda \in \mathbf{C}$ is an eigenvalue of $\mathbf{A}$ and $\mathbf{x}$ an eigenvector, if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}.$$

The eigenvalues are the roots of the characteristic polynomial $\det(z\mathbf{I} - \mathbf{A})$.

Schur's eigenvalue theorem: for any $n \times n$ square matrix $\mathbf{A}$ there exists an uppertriangular matrix

$$\mathbf{S} = \begin{bmatrix} s_{11} & \cdots & s_{1n} \\ & \ddots & \vdots \\ 0 & & s_{nn} \end{bmatrix}$$

and a unitary matrix $\mathbf{U}$ such that

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{U}^H.$$

The diagonal entries of $\mathbf{S}$ are the eigenvalues of $\mathbf{A}$ (including multiplicities). Schur's eigenvalue theorem is easy to prove by recursive computation of a single eigenvalue and deflation of the space.

Ill conditioning of multiple or clusters of eigenvalues

Look e.g. at a 'companion matrix':

$$\mathbf{A} = \begin{bmatrix} 0 & & & -p_0 \\ 1 & \ddots & & \vdots \\ & \ddots & 0 & \vdots \\ 0 & & 1 & -p_{n-1} \end{bmatrix}$$

its characteristic polynomial is:

$$\chi_A(z) = z^n + p_{n-1}z^{n-1} + \cdots + p_0.$$

Assume now that $p(z) = (z-a)^n$ and assume a permutation $p_\epsilon(z) = (z-a)^n - \epsilon$. The new roots of the polonymial and hence the new eigenvalues of $\mathbf{A}$ are:

$$a + \epsilon^{\frac{1}{n}} e^{j\pi k/n}$$

Hence: an ϵ error in the data produces $\epsilon^{\frac{1}{n}}$ in the result (take e.g. $n = 10$ and $\epsilon = 10^{-5}$, then the error is ≈ 1!)

2 Systems of Equations, QR algorithm

Let be given: an $n \times m$ matrix $\mathbf{T}$ and an n-vector $\mathbf{b}$.
Asked: an m-vector x such that:

$$\mathbf{Tx} = \mathbf{b}$$

Distinguish the following cases: $\begin{cases} n > m & \text{overdetermined} \\ n = m & \text{square} \\ n < m & \text{underdetermined} \end{cases}$ For ease of discussion we shall look only at the case $n \geq m$.

The general strategy for solution is an orthogonal transformations on rows. Let a and b be two rows in a matrix, then we can generate linear combinations of these rows by applying a transformation matrix to the left (row recipe):

$$\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} \longleftarrow & a & \longrightarrow \\ \longleftarrow & \mathbf{b} & \longrightarrow \end{bmatrix} = \begin{bmatrix} t_{11}\mathbf{a} + t_{12}\mathbf{b} \\ t_{21}\mathbf{a} + t_{22}\mathbf{b} \end{bmatrix}$$

or embedded:

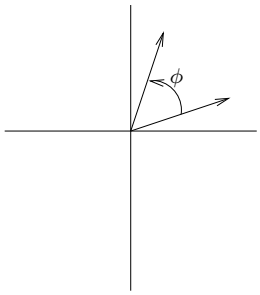
$$\begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & t_{11} & & t_{12} & \\ & & & 1 & & \\ & & t_{21} & & t_{22} & \\ & & & & & 1 \end{bmatrix} \begin{bmatrix} \longleftarrow & \cdot & \longrightarrow \\ \longleftarrow & \cdot & \longrightarrow \\ \longleftarrow & \mathbf{a} & \longrightarrow \\ \longleftarrow & \cdot & \longrightarrow \\ \longleftarrow & \mathbf{b} & \longrightarrow \\ \longleftarrow & \cdot & \longrightarrow \end{bmatrix} = \begin{bmatrix} \longleftarrow & \cdot & \longrightarrow \\ \longleftarrow & \cdot & \longrightarrow \\ t_{11}\mathbf{a} + t_{12}\mathbf{b} & & \\ \longleftarrow & \cdot & \longrightarrow \\ t_{21}\mathbf{a} + t_{22}\mathbf{b} & & \\ \longleftarrow & \cdot & \longrightarrow \end{bmatrix}$$

2.1 Jacobi Transformations

The Jacobi elementary transformation is:

$$\begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}$$

It represents an elementary rotation over an angle ϕ:



A Jacobi transformation can be used to annihilate an element in a row (with $c \doteq \cos\phi$ and $s \doteq \sin\phi$):

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a_1 & a_2 & \cdots & a_m \\ b_1 & b_2 & \cdots & b_m \end{bmatrix} = \begin{bmatrix} ca_1 - sb_1 & ca_2 - sb_2 & \cdots \\ sa_1 + cb_1 & sa_2 + cb_2 & \cdots \end{bmatrix}$$

$$\doteq \begin{bmatrix} \sqrt{|a_1|^2+|b_1|^2} & \star & \cdots & \star \\ 0 & \star & \cdots & \star \end{bmatrix}$$

when $sa_1 + cb_1 = 0$ or

$$\tan\phi = -\frac{b_1}{a_1}$$

which can always be done.

2.2 Householder Reflection

We consider the Householder matrix $\mathbf{H}$, which is defined as

$$\mathbf{H} = \mathbf{I} - 2\mathbf{P}_u, \quad \mathbf{P}_u = \mathbf{u}(\mathbf{u}^T\mathbf{u})^{-1}\mathbf{u}^T,$$

i.e. the matrix $\mathbf{P}_u$ is a projection matrix, which projects along the direction of the vector $\mathbf{u}$. The Householder matrix $\mathbf{H}$ satisfies the orthogonality property $\mathbf{H}^T\mathbf{H} = \mathbf{I}$ and has the property that $\det\mathbf{H} = -1$, which indicates that $\mathbf{H}$ is a reflection which reverses orientation ($\mathbf{Hu} = -\mathbf{u}$). We search for an orthogonal transformation $\mathbf{H}$ which transforms a given vector $\mathbf{x}$ onto a given vector $\mathbf{y} = \mathbf{Hx}$, where $\|\mathbf{x}\| = \|\mathbf{y}\|$ holds. We compute the vector $\mathbf{u}$ specifying the projection direction for $\mathbf{P}_u$ as $\mathbf{u} = \mathbf{y} - \mathbf{x}$.

2.3 QR Factorization

2.3.1 Elimination Scheme based on Jacobi Transformations

A cascade of unitary transformations is still a unitary transformation: let Q_{ij} be a transformation on *rows* i and j which annihilates an appropriate element (as indicated further in the example). Successive eliminations on a 4×3 matrix (in which the $\cdot$ indicates a relevant element of the matrix):

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} (\mathbf{Q}_{12}) \mapsto \begin{bmatrix} \star & \star & \star \\ 0 & \star & \star \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} (\mathbf{Q}_{13}) \mapsto \begin{bmatrix} \star & \star & \star \\ 0 & \cdot & \cdot \\ 0 & \star & \star \\ \cdot & \cdot & \cdot \end{bmatrix} (\mathbf{Q}_{14})$$

$$\mapsto \begin{bmatrix} \star & \star & \star \\ 0 & \cdot & \cdot \\ 0 & \cdot & \cdot \\ 0 & \star & \star \end{bmatrix} (\mathbf{Q}_{23}) \mapsto \begin{bmatrix} \cdot & \cdot & \cdot \\ 0 & \star & \star \\ 0 & 0 & \star \\ 0 & \cdot & \cdot \end{bmatrix} (\mathbf{Q}_{24}) \mapsto \begin{bmatrix} \cdot & \cdot & \cdot \\ 0 & \star & \star \\ 0 & 0 & \cdot \\ 0 & 0 & \star \end{bmatrix} (\mathbf{Q}_{34})$$

$$\mapsto \begin{bmatrix} \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot \\ 0 & 0 & \star \\ 0 & 0 & 0 \end{bmatrix}$$

(The elements that have changed during the last transformation are denoted by a '$\star$'. There are no fill-ins, a purposeful zero does not get modified lateron.) The end result is:

$$\mathbf{Q}_{34}\mathbf{Q}_{24}\mathbf{Q}_{23}\mathbf{Q}_{14}\mathbf{Q}_{13}\mathbf{Q}_{12}\mathbf{T} = \begin{bmatrix} \mathbf{R} \\ 0 \end{bmatrix}$$

in which $\mathbf{R}$ is upper triangular.

2.3.2 Elimination Scheme based on Householder Reflections

A cascade of unitary transformations is still a unitary transformation: let bH_i be a transformation on the *rows* i until and n which annihilates all appropriate elements in rows $i+1:n$ (as indicated further in the example).

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} \sqrt{\mathbf{x}^T\mathbf{x}} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Successive eliminations on a 4×3 matrix (in which the $\cdot$ indicates a relevant element of the matrix):

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} (\mathbf{H}_{14}) \mapsto \begin{bmatrix} \star & \star & \star \\ 0 & \cdot & \cdot \\ 0 & \cdot & \cdot \\ 0 & \cdot & \cdot \end{bmatrix} (\mathbf{H}_{24}) \mapsto \begin{bmatrix} \star & \star & \star \\ 0 & \star & \star \\ 0 & 0 & \cdot \\ 0 & 0 & \cdot \end{bmatrix} (\mathbf{H}_{34}) \mapsto \begin{bmatrix} \star & \star & \star \\ 0 & \star & \star \\ 0 & 0 & \star \\ 0 & 0 & 0 \end{bmatrix}$$

(The elements that have changed during the last transformation are denoted by a '$\star$'. There are no fill-ins, a purposeful zero does not get modified lateron.) The end result is:

$$\mathbf{H}_{34}\mathbf{H}_{24}\mathbf{H}_{14}\mathbf{T} = \begin{bmatrix} \mathbf{R} \\ 0 \end{bmatrix}$$

in which $\mathbf{R}$ is upper triangular.

2.4 Solving the system $Tx = b$

Let also:

$$\mathbf{Q}_{34}\cdots\mathbf{Q}_{12}b \doteq \beta$$

then $\mathbf{Tx} = \mathbf{b}$ transforms to:

$$\begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{bmatrix}$$

.

The solution, if it exists, can now easily be analyzed:

1. $\mathbf{R}$ is non-singular ($r_{11} \neq 0, \cdots, r_{mm} \neq 0$), then the partial set

   $$\mathbf{Rx} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$$

   can be solved for x by backsubstitution:

   $$\mathbf{x} = \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{bmatrix}^{-1} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \begin{bmatrix} \cdots \\ r_{22}^{-1}(\beta_{22} - r_{23}r_{33}^{-1}\beta_3) \\ r_{33}^{-1}\beta_3 \end{bmatrix}$$

(there are better methods, see further!), and:
1. if $\beta_4 \neq 0$ we have a contradiction,
2. if $\beta_4 = 0$ we have found the unique solution.

2. etcetera when $\mathbf{R}$ is singular (one or more of the diagonal entries will be zero yielding more possibilities for contradictions).

2.5 Least squares solutions

But... there is more, even when $\beta_4 \neq 0$:

$$\mathbf{x} = \mathbf{R}^{-1} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$$

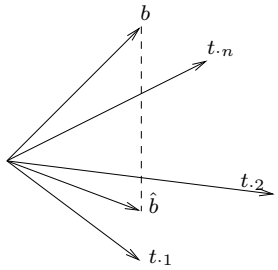
provides for a 'least squares fit' it gives the linear combination of columns of $\mathbf{T}$ closest to $\mathbf{b}$ i.e. it minimizes

$$\|\mathbf{Tx} - \mathbf{b}\|_2.$$

Geometric interpretation: let

$$\mathbf{T} = [\mathbf{t}_{\cdot 1}\, \mathbf{t}_{\cdot 2} \cdots \mathbf{t}_{\cdot m}]$$

then one may wonder whether $\mathbf{b}$ can be written as a linear combination of $\mathbf{t}_{\cdot 1}$ etc.?
Answer: only if $\mathbf{b} \in \text{span}\{\mathbf{t}_{\cdot 1}, \mathbf{t}_{\cdot 2}, \cdots, \mathbf{t}_{\cdot m}\}$!



Otherwise: find the 'least squares fit', the combination of $\mathbf{t}_{\cdot 1}$ etc. which is closest to $\mathbf{b}$, i.e. the projection of $\hat{\mathbf{b}}$ of $\mathbf{b}$ on the span of the columns.

Finding the solution: a QR-transformation rotates all the vectors $t_{\cdot i}$ *and* $\mathbf{b}$ over the same angles, with as result:

$$\mathbf{r}_{\cdot 1} \in \text{span}\{\mathbf{e}_1\},$$

$$\mathbf{r}_{\cdot 2} \in \text{span}\{\mathbf{e}_1, \mathbf{e}_2\}$$

etc., leaving all angles and distances equal. We see that the projection of the vector β on the span of the columns of $\mathbf{R}$ is actually

$$\begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ 0 \end{bmatrix}$$

Hence the combination of columns that produces the least squares fit is:

$$\mathbf{x} = \mathbf{R}^{-1} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$$

Formal proof

Let $\mathbf{Q}$ be a unitary transformation such that

$$\mathbf{T} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ 0 \end{bmatrix}$$

in which $\mathbf{R}$ is upper triangular.

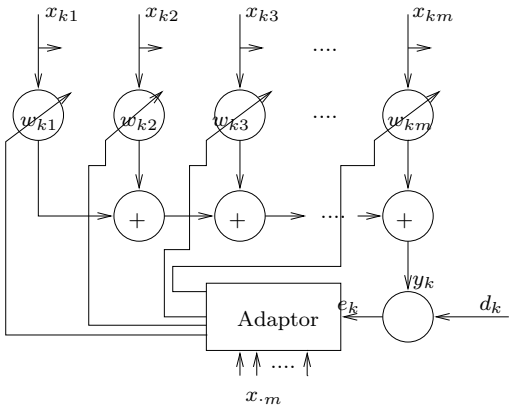
Then: $\mathbf{Q}^H\mathbf{Q} = \mathbf{Q}\mathbf{Q}^H = \mathbf{I}$ and the approximation error becomes, with $\mathbf{Q}^H\mathbf{b} = \begin{bmatrix} \beta' \\ \beta'' \end{bmatrix}$:

$$\|\mathbf{T}\mathbf{x} - \mathbf{b}\|_2^2 = \|\mathbf{Q}^H(\mathbf{T}\mathbf{x} - \mathbf{b})\|_2^2 = \| \begin{bmatrix} \mathbf{R} \\ 0 \end{bmatrix} \mathbf{x} - \beta\|_2^2 = \|\mathbf{R}\mathbf{x} - \beta'\|_2^2 + \|\beta''\|_2^2$$

If $\mathbf{R}$ is invertible a minimum is obtained for $\mathbf{R}\mathbf{x} = \beta'$ and the minimum is $\|\beta''\|_2$.

2.6 Application: adaptive QR

The classical adaptive filter:



At each instant of time k, a data vector $\mathbf{x}(k) = [x_{k1} \cdots x_{km}]$ of dimension m comes in (e.g. from an antenna array or a delay line). We wish to estimate, at each point in time, a signal $\mathbf{y}_k$ as $\mathbf{y}(k) = \sum_i w_{ki}x_{ki}$ - a linear combination of the incoming data. Assume that we dispose of a 'learning phase' in which the exact value $\mathbf{d}_k$ for $\mathbf{y}_k$ is known, so that the error $\mathbf{e}_k = \mathbf{y}_k - \mathbf{d}_k$ is known also - it is due to inaccuracies and undesired signals that have been added in and which we call 'noise'.

The problem is to find the optimal w_{ki}. We choose as optimality criterion: given the data from $t = 1$ to $t = k$, find the w_{ki} for which the total error is minimal if the new weigths w_{ki} had indeed

been used at all available time points $1 \leq i \leq k$ (many variations of the optimization strategy are possible).

For $i \leq k$, let $y_{ki} = \sum_\ell x_{i\ell} w_{i\ell}$ be the output one would have obtained if w_{ki} had been used at that time and let

$$\mathbf{X}_k = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ x_{k1} & x_{k2} & \cdots & x_{km} \end{bmatrix}$$

be the 'data matrix' contained all the data collected in the period $1 \cdots k$. We wish a least squares solution of

$$\mathbf{X}_k \mathbf{w}_{k\cdot} = \mathbf{y}_{k\cdot} \approx \mathbf{d}_{[1:k]}$$

If

$$\mathbf{X}_k = \mathbf{Q}_k \begin{bmatrix} \mathbf{R}_k \\ 0 \end{bmatrix}, \; \mathbf{d}_{[1:k]} = \mathbf{Q}_k \begin{bmatrix} \delta_{k1} \\ \delta_{k2} \end{bmatrix}$$

is a QR-factorization of $\mathbf{X}_k$ with conformal partitioning of $\mathbf{d}$ and $\mathbf{R}_k$ upper-triangular, and assuming $\mathbf{R}_k$ non-singular, we find as solution to our least squares problem:

$$\mathbf{w}_{k\cdot} = \mathbf{R}_k^{-1} \delta_{k1}$$

and for the total error:

$$\sqrt{\sum_{i=1}^{k} [e_{ki}]^2} = \|\delta_{k2}\|_2$$

Note: the QR-factorization will be done *directly* on the data matrix, no covariance is computed. This is the correct numerical way of doing things.

2.7 Recursive (adaptive) computation

Suppose you know $\mathbf{R}_{k-1}, \delta_{k-1}$, how to find $\mathbf{R}_k, \delta_k$ with a minimum number of computations?

We have:

$$X_k = \left[\begin{array}{c} X_{k-1} \\ \hline x_{k1} \quad \cdots \quad x_{km} \end{array}\right], \; d_{[1:k]} = \left[\begin{array}{c} d_{[1:k-1]} \\ \hline d_k \end{array}\right],$$

and let us consider

$$\left[\begin{array}{c|c} Q_{k-1} & 0 \\ \hline 0 & 1 \end{array}\right]$$

as the first candidate for $\mathbf{Q}_k$.

Then

$$\left[\begin{array}{c|c} Q_{k-1}^H & 0 \\ \hline 0 & 1 \end{array}\right] \left[\begin{array}{c} X_{k-1} \\ \hline x_{k\cdot} \end{array}\right] = \left[\begin{array}{c} R_{k-1} \\ \hline 0 \\ \hline x_{k\cdot} \end{array}\right]$$

and

$$\left[\begin{array}{c|c} Q_{k-1}^H & 0 \\ \hline 0 & 1 \end{array}\right] \left[\begin{array}{c} d_{[1:k-1]} \\ \hline d_k \end{array}\right] = \left[\begin{array}{c} \delta_{k-1,\cdot} \\ \hline d_k \end{array}\right]$$

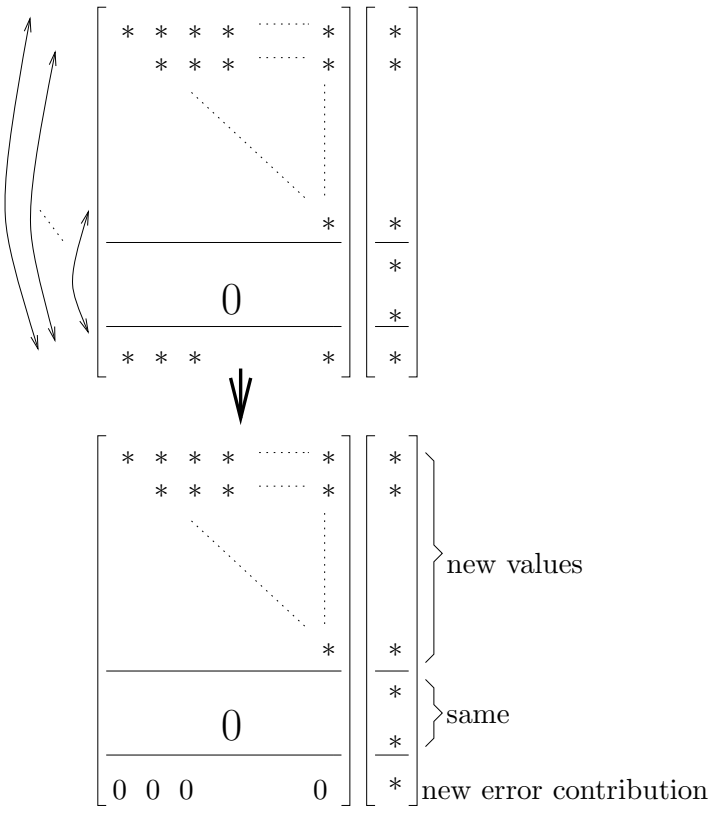
Hence we do not need $\mathbf{Q}_{k-1}$ anymore, the new system to be solved after the previous transformations becomes:

$$\left[\begin{array}{c} R_{k-1} \\ \hline 0 \\ \hline x_{k\cdot} \end{array}\right] \begin{bmatrix} w_{k1} \\ \vdots \\ w_{km} \end{bmatrix} = \left[\begin{array}{c} \delta_{k-1,\cdot} \\ \hline d_k \end{array}\right],$$

i.e.

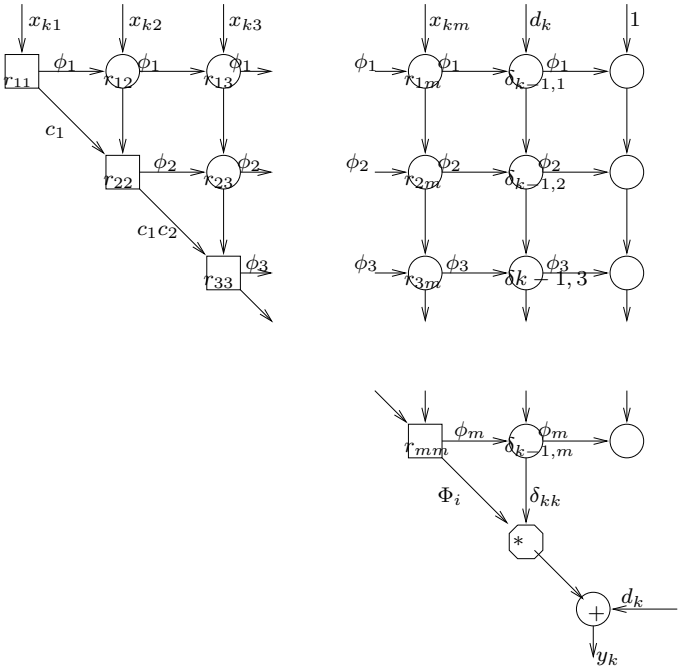
$$\left[\begin{array}{cccc} \star & \star & \cdots & \star \\ 0 & \star & \cdots & \star \\ & & \ddots & \vdots \\ 0 & \cdots & \cdots & \star \\ \hline \multicolumn{4}{c}{0} \\ \hline x_{k1} & x_{k2} & \cdots & x_{km} \end{array}\right] \begin{bmatrix} w_{k1} \\ \vdots \\ w_{km} \end{bmatrix} = \left[\begin{array}{c} \delta_{k-1,\cdot} \\ \hline d_k \end{array}\right],$$

only m row transformations are needed to the find the new R_k, δ_k:

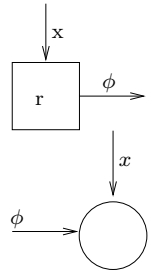


Question: how to do this computationally?

A dataflow graph in which each r_{ij} is resident in a separate node would look as follows:



Initially, before step 1, $r_{ij} = 1$ if $i = j$ otherwise zero. Just before step k the r_{ij}^{k-1} are resident in the nodes. There are two types of nodes:



vectorizing node: computes the angle ϕ from x and r

rotating node: rotates the vector $\begin{bmatrix} r \\ x \end{bmatrix}$ over ϕ.

The scheme produces $\mathbf{R}_k, \delta_{kk}$ and the new error:

$$\|e_k\|_2 = \sqrt{\|\mathbf{e}_{k-1}\|_2^2 + |\delta_{kk}|^2}$$

2.8 Reverse QR

In many applications, not the update of $\mathbf{R}_k$ is desired, but of $\mathbf{w}_k = \mathbf{R}_k^{-1}\delta_{k,1:m}$. A clever manipulation of matrices, most likely due to E. Deprettere and inspired by the old Faddeev algorithm gives a nice solution.

Observation 1: let $\mathbf{R}$ be an $m \times m$ invertible matrix and $\mathbf{u}$ an m-vector, then

$$\begin{bmatrix} \mathbf{R} & \mathbf{u} \\ 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{R}^{-1} & -\mathbf{R}^{-1}\mathbf{u} \\ 0 & 1 \end{bmatrix},$$

hence, $\mathbf{R}^{-1}u$ is implicit in the inverse shown.

Observation 2: let $\mathbf{Q}^H$ be a unitary update which performs the following transformation (for some

new, given vector $\mathbf{x}$ and value $\mathbf{d}$):

$$\mathbf{Q}^H \begin{bmatrix} \mathbf{R} & \mathbf{u} \\ 0 & 1 \\ \mathbf{x} & \mathbf{d} \end{bmatrix} \doteq \begin{bmatrix} \mathbf{R}' & \mathbf{u}'\delta \\ 0 & \delta \\ 0 & 0 \end{bmatrix}$$

($\mathbf{Q}$is thus almost like before, the embedding is slightly different - δ is a normalizing scalar which we must discount).

Let us call $\mathcal{R} \doteq \begin{bmatrix} \mathbf{R} & \mathbf{u} \\ 0 & 1 \end{bmatrix}$, similarly for $\mathcal{R}'$, and $\xi^H = [\mathbf{x}\,\mathbf{d}]$, then we have

$$\mathbf{Q}^H \begin{bmatrix} \mathcal{R} & 0 \\ \xi^H & 1 \end{bmatrix} = \begin{bmatrix} \mathcal{R}' & q_{21}^H \\ 0 & q_{22}^H \end{bmatrix} \begin{bmatrix} I & & \\ & \delta & \\ & & 1 \end{bmatrix}$$

Taking inverses we find (for some a_{12} and a_{22} which originate in the process):

$$\begin{bmatrix} \mathcal{R}^{-1} & 0 \\ -\xi^H\mathcal{R}^{-1} & 1 \end{bmatrix} Q \doteq \begin{bmatrix} \mathbf{I} & & \\ & \delta^{-1} & \\ & & 1 \end{bmatrix} \begin{bmatrix} \mathcal{R}'^{-1} & a_{12} \\ 0 & a_{22} \end{bmatrix}.$$

Hence, an RQ-factorization of the known matrix on the left hand side yields an update of $\mathcal{R}^{-1}$, exclusively using new data. A data flow scheme very much like the previous one can be used.

2.9 Francis' QR algorithm to compute the Schur eigenvalue form

A primitive version of an iterative QR algorithm to compute the Schur eigenvalue form goes as follows. Suppose that the square $n \times n$ matrix $\mathbf{A}$ is given. First we look for a similarity transformation with unitary matrices $\mathbf{U} \cdot \mathbf{U}^H$ which puts $\mathbf{A}$ in a so called 'Hessenberg form', i.e. uppertriangular with only one additional subdiagonal, for a 4×4 matrix:

$$\begin{bmatrix} \star & \star & \star & \star \\ \star & \star & \star & \star \\ 0 & \star & \star & \star \\ 0 & 0 & \star & \star \end{bmatrix},$$

(the purpose of this step is to simplify the following procedure, it also allows refinements that enhance convergence - we skip its details except for to say that it is always possible in $(n-1)(n-2)/2$ Jacobi steps).

Assume thus that $\mathbf{A}$ is already in Hessenberg form, and we set $\mathbf{A}_0 \doteq \mathbf{A}$. A first QR factorization gives:

$$\mathbf{A}_0 \doteq \mathbf{Q}_0\mathbf{R}_0$$

and we set $\mathbf{A}_1 \doteq \mathbf{R}_0\mathbf{Q}_0$. This procedure is then repeated a number of times until $\mathbf{A}_k$ is nearly upper triangular (this does indeed happen sometimes - see the discussion further).

The iterative step goes as follows: assume $\mathbf{A}_{k-1} \doteq \mathbf{Q}_{k-1}\mathbf{R}_{k-1}$, then

$$\mathbf{A}_k \doteq \mathbf{R}_{k-1}\mathbf{Q}_{k-1}.$$

Let's analyze what we have done. A slight rewrite gives:

$$\begin{aligned} \mathbf{Q}_0\mathbf{R}_0 &= \mathbf{A} \\ \mathbf{Q}_0\mathbf{Q}_1\mathbf{R}_1 &= \mathbf{A}\mathbf{Q}_0 \\ \mathbf{Q}_0\mathbf{Q}_1\mathbf{Q}_2\mathbf{R}_2 &= \mathbf{A}\mathbf{Q}_0\mathbf{Q}_1 \\ &\cdots \end{aligned}$$

This can be seen as a fixed point algorithm on the equation:

$$\mathbf{U}\Sigma = \mathbf{A}\mathbf{U}$$

with $\mathbf{U}_0 \doteq \mathbf{I}$, we find successively:

$$\begin{aligned} \mathbf{U}_1\Sigma_1 &= \mathbf{A} \\ \mathbf{U}_2\Sigma_2 &= \mathbf{A}\mathbf{U}_1 \\ &\cdots \end{aligned}$$

the algorithm detailed above produces in fact $\mathbf{U}_k \doteq \mathbf{Q}_0 \cdots \mathbf{Q}_k$. If the algorithm converges, after a while we shall find that $\mathbf{U}_k \approx \mathbf{U}_{k+1}$ and the 'fixed point' is more or less reached.

Convergence of a fixed point algorithm is by no means assured, and even so, it is just linear. Hence, the algorithm must be improved. This is done by using at each step a clever constant diagonal 'offset' of the matrix. We refer to the literature for further information [2], where it is also shown that the improved version has quadratic convergence. Given the fact that a general matrix may have complex eigenvalues, we can already see that in that case the simple version given above cannot converge, and a complex version will have to be used, based on a well-choosen complex offset. It is interesting to see that the method is related to the classical 'power method' to compute eigenvalues of a matrix. For example, if we indicate by $[\cdot]_1$ the first column of a matrix, the previous recursion gives, with

$$\mathbf{Q}_n \doteq Q_0 Q_1 \cdots Q_n$$

and $\lambda_{n+1} \doteq [\mathbf{R}_{n+1}]_{11}$,

$$\lambda_{n+1}[\mathbf{Q}_{n+1}]_1 = \mathbf{A}[\mathbf{Q}_n]_1.$$

Hence, if there is an eigenvalue which is much larger in magnitude than the others, $[\mathbf{Q}_{n+1}]_1$ will converge to the corresponding eigenvector.

QZ-iterations

A further extension of the previous concerns the computation of eigenvalues of the (non singular) *pencil*

$$\mathbf{A} - \lambda\mathbf{B}$$

where we assume that $\mathbf{B}$ is invertible. The eigenvalues are actually values for λ and the eigenvectors are vectors $\mathbf{x}$ such that $(\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = 0$. This actually amounts to computing the eigenvalues of $\mathbf{A}\mathbf{B}^{-1}$, but the algorithm will do so without inverting $\mathbf{B}$. In a similar vein as before, we may assume that $\mathbf{A}$ is in Hessenberg form and $\mathbf{B}$ is upper triangular. The QZ iteration will determine unitary matrices $\mathbf{Q}$ and $\mathbf{Z}$ such that $\mathbf{A}_1 \doteq \mathbf{Q}\mathbf{A}\mathbf{Z}$ and $\mathbf{B}_1 \doteq \mathbf{Q}\mathbf{B}\mathbf{Z}$, whereby $\mathbf{A}_1$ is again Hessenberg, $\mathbf{B}_1$ upper triangular and $\mathbf{A}_1$ is actually closer to diagonal. After a number of steps $\mathbf{A}_k$ will almost be triangular, and the eigenvalues of the pencil will be the ratios of the diagonal elements of $\mathbf{A}_k$ and $\mathbf{B}_k$. We can find the eigenvectors as well if we keep track of the transformation, just as before.

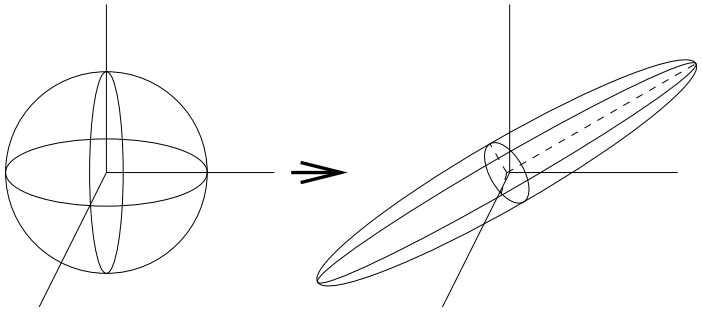
3 The singular value decomposition - SVD

3.1 Construction of the SVD

The all important 'singular value decomposition' or SVD results from a study of the geometry of a linear transformation.

Let $\mathbf{A}$ be a matrix of dimensions $n \times m$, for definiteness assume $n \geq m$ (a 'tall' matrix). Consider the length of the vector $\mathbf{Ax}$, $\|\mathbf{Ax}\| = \sqrt{\mathbf{x}^H \mathbf{A}^H \mathbf{Ax}}$, for $\|\mathbf{x}\| = 1$.

When $\mathbf{A}$ is non singular it can easily be seen that $\mathbf{Ax}$ moves on an ellipsoid when $\mathbf{x}$ moves on the unit ball. Indeed, we then have $\mathbf{x} = \mathbf{A}^{-1}\mathbf{y}$ and the locus is given by $\mathbf{y}^H \mathbf{A}^{-H} \mathbf{A}^{-1} \mathbf{y} = 1$, which is a bounded quadratic form in the entries of y. In general, the locus will be bounded by an ellipsoid, but the proof is more elaborate.



The ellipsoid has a longest elongation, by definition the operator norm for $\mathbf{A}$: $\sigma_1 = \|\mathbf{A}\|$. Assume $\sigma_1 \neq 0$ (otherwise $\mathbf{A} \equiv 0$), and take $\mathbf{v}_1 \in \mathbf{C}^m$ a unit vector producing a longest elongation, so that $\mathbf{Av}_1 = \sigma_1 \mathbf{u}_1$ for some unit vector $\mathbf{u}_1 \in \mathbf{C}^n$. It is now not too hard to show that:

$$\begin{aligned} \mathbf{Av}_1 &= \sigma_1 \mathbf{u}_1 \\ \mathbf{A}^H \mathbf{u}_1 &= \sigma_1 \mathbf{v}_1, \end{aligned}$$

and that $\mathbf{v}_1$ is an eigenvector of $\mathbf{A}^H \mathbf{A}$ with eigenvalue σ_1^2.

Proof: by construction we have $\mathbf{Av}_1 = \sigma_1 \mathbf{u}_1$ maximum elongation. Take any $\mathbf{w} \perp \mathbf{v}_1$ and look at the effect of $\mathbf{A}$ on $(\mathbf{v}_1 + \lambda \mathbf{w})/\sqrt{1 + |\lambda|^2}$. For very small λ the latter is $\approx (\mathbf{v}_1 + \lambda \mathbf{w})(1 - \frac{1}{2}|\lambda|^2) \approx \mathbf{v}_1 + \lambda \mathbf{w}$, and $\mathbf{A}(\mathbf{v}_1 + \lambda \mathbf{w}) = \sigma_1 \mathbf{u}_1 + \lambda \mathbf{Aw}$. The norm square becomes: $\mathbf{v}_1^H \mathbf{A}^H \mathbf{A} \mathbf{v}_1 + \lambda \mathbf{v}_1^H \mathbf{A}^H \mathbf{Aw} + \bar{\lambda} \mathbf{w}^H \mathbf{A}^H \mathbf{A} \mathbf{v}_1 + O(|\lambda|^2)$ which can only be a maximum if for all $\mathbf{w} \perp \mathbf{v}_1$, $\mathbf{w}^H \mathbf{A}^H \mathbf{A} \mathbf{v}_1 = 0$. It follows that $\mathbf{A}^H \mathbf{u}_1$ must be in the direction of $\mathbf{v}_1$, easily evaluated as $\mathbf{A}^H \mathbf{u}_1 = \sigma_1 \mathbf{v}_1$, that σ_1^2 is an eigenvalue of $\mathbf{A}^H \mathbf{A}$ with eigenvector $\mathbf{v}_1$ and that $\mathbf{w} \perp \mathbf{v}_1 \Leftrightarrow \mathbf{Aw} \perp \mathbf{Av}_1$.

The problem can now be deflated one unit of dimension. Consider the orthogonal complement of $\mathbf{C}^m \ominus \text{span}\{\mathbf{v}_1\}$ - it is a space of dimension $m - 1$, and consider the original map defined by $\mathbf{A}$ but now restricted to this subspace. Again, it is a linear map, and it turns out that the image is orthogonal on $\text{span}(\mathbf{u}_1)$.

Let $\mathbf{u}_2$ be the unit vector in that domain for which the longest elongation σ_2 is obtained (clearly $\sigma_1 \geq \sigma_2$), and again we obtain (after some more proof) that

$$\begin{aligned} \mathbf{Av}_2 &= \sigma_2 \mathbf{u}_2 \\ \mathbf{A}^H \mathbf{u}_2 &= \sigma_2 \mathbf{v}_2 \end{aligned}$$

(unless of course $\sigma_2 = 0$ and the map is henceforth zero! We already know that $\mathbf{v}_2 \perp \mathbf{v}_1$ and $\mathbf{u}_2 \perp \mathbf{u}_1$.)

The decomposition continues until an orthonormal basis for $\mathcal{R}(\mathbf{A}^H)$ as $\text{span}(\mathbf{v}_1, \mathbf{v}_2 \cdots \mathbf{v}_k)$ (assume the rank of $\mathbf{A}$ to be k) is obtained, as well as a basis for $\mathcal{R}(\mathbf{A})$ as $\text{span}(\mathbf{u}_1, \mathbf{u}_2 \cdots \mathbf{u}_k)$.

These spaces can be augmented with orthonormal bases for the kernels: $\mathbf{v}_{k+1} \cdots \mathbf{v}_m$ for $\mathcal{K}(\mathbf{A})$ and $\mathbf{u}_{k+1} \cdots \mathbf{u}_n$ for $\mathcal{K}(\mathbf{A}^H)$. Stacking all these results produces:

$$\mathbf{A}[\mathbf{v}_1\ \mathbf{v}_2 \cdots \mathbf{v}_k\ \mathbf{v}_{k+1} \cdots \mathbf{v}_m] = [\mathbf{u}_1\ \mathbf{u}_2 \cdots \mathbf{u}_k\ \mathbf{u}_{k+1} \cdots \mathbf{u}_n] \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix}$$

where Σ is the $k \times k$ diagonal matrix of *singular values*:

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_k \end{bmatrix}$$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_k > 0$. Alternatively:

$$\mathbf{A} = \mathbf{U} \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \mathbf{V}^H$$

where:

$$\mathbf{U} = [\mathbf{u}_1\ \mathbf{u}_2 \cdots \mathbf{u}_k\ \mathbf{u}_{k+1} \cdots \mathbf{u}_n], \mathbf{V} = [\mathbf{v}_1\ \mathbf{v}_2 \cdots \mathbf{v}_k\ \mathbf{v}_{k+1} \cdots \mathbf{v}_m]$$

are unitary matrices.

3.2 Singular Value Decomposition: proof

The *canonical svd form* can more easily (but with less insight) be obtained directly from an eigenvalue decomposition of the Hermitean matrix $\mathbf{A}^H\mathbf{A}$ (we skip the proof: exercise!). From the form it is easy to see that

$$\mathbf{A}^H\mathbf{A} = \mathbf{V} \begin{bmatrix} \Sigma^2 & 0 \\ 0 & 0 \end{bmatrix} \mathbf{V}^H$$

and

$$\mathbf{A}\mathbf{A}^H = \mathbf{U} \begin{bmatrix} \Sigma^2 & 0 \\ 0 & 0 \end{bmatrix} \mathbf{U}^H$$

are eigenvalue decompositions of the respective (quadratic) matrices.

The σ_i's are called singular values, and the corresponding vectors $\mathbf{u}_i, \mathbf{v}_i$ are called pairs of singular vectors or Schmidt-pairs. They correspond to principal axes of appropriate ellipsoids. The collection of singular values is 'canonical' (i.e. unique), when there are multiple singular values then there are many choices possible.

3.3 Properties of the SVD

Since the SVD is absolutely fundamental to the geometry of a linear transformation, it has a long list of important properties.

- $\|\mathbf{A}\|_E = \sigma_1$, $\|\mathbf{A}\|_F = \sqrt{\sum_{i=1\cdots k} \sigma_i^2}$.
- If $\mathbf{A}$ is square and $\mathbf{A}^{-1}$ exists, then $\|\mathbf{A}^{-1}\|_E = \sigma_k^{-1}$.
- Matrix approximation: suppose you wish to approximate $\mathbf{A}$ by a matrix $\mathbf{B}$ of rank at most ℓ. Consider:

$$\mathbf{B} = [\mathbf{u}_1 \cdots \mathbf{u}_\ell] \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_\ell \end{bmatrix} [\mathbf{v}_1 \cdots \mathbf{v}_\ell]^H .$$

  Then

$$\|\mathbf{A} - \mathbf{B}\|_E = \sigma_{\ell+1}$$

  and

$$\|\mathbf{A} - \mathbf{B}\|_F = \sqrt{\sum_{i=\ell+1\cdots k} \sigma_i^2}.$$

  One shows that these are the smallest possible errors when $\mathbf{B}$ is varied over the matrices of rank ℓ. Moreover, the $\mathbf{B}$ that minimizes the Frobenius norm is unique.

- System conditioning: let A be a non-singular square $n \times n$ matrix, and consider the system of equations $\mathbf{Ax} = \mathbf{b}$. The condition number C gives an upper bound on $\|\delta\mathbf{x}\|_2/\|\mathbf{x}\|_2$ when $\mathbf{A}$ and $\mathbf{b}$ are subjected to variations $\delta\mathbf{A}$ and $\delta\mathbf{b}$. We have:

$$(\mathbf{A} + \delta\mathbf{A})(\mathbf{x} + \delta\mathbf{x}) = (\mathbf{b} + \delta\mathbf{b})$$

  Assume the variations small enough (say $O(\epsilon)$) so that $\mathbf{A} + \delta\mathbf{A}$ is invertible, we find:

$$\mathbf{Ax} + \delta\mathbf{A}\ \mathbf{x} + \mathbf{A}\ \delta\mathbf{x} \approx \mathbf{b} + \delta\mathbf{b} + O(\epsilon^2)$$

  and since $\mathbf{Ax} = \mathbf{b}$,

$$\delta\mathbf{x} \approx \mathbf{A}^{-1}\delta\mathbf{b} - \mathbf{A}^{-1}\ \delta\mathbf{A}\ \mathbf{x}.$$

  Hence (using the operator or $\|\cdot\|_2$ norm):

$$\begin{aligned} \|\delta\mathbf{x}\| &\leq \|\mathbf{A}^{-1}\|\|\delta\mathbf{b}\| + \|\mathbf{A}^{-1}\|\|\delta\mathbf{A}\|\|\mathbf{x}\| \\ &\leq \|\mathbf{A}^{-1}\|\tfrac{\|\mathbf{Ax}\|}{\|\mathbf{b}\|}\|\delta\mathbf{b}\| + \|\mathbf{A}^{-1}\|\|\mathbf{A}\|\tfrac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|}\|\mathbf{x}\| \end{aligned}$$

  and finally, since $\|\mathbf{Ax}\| \leq \|\mathbf{A}\|\|\mathbf{x}\|$,

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \|\mathbf{A}^{-1}\|\|\mathbf{A}\| \left\{ \frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|} + \frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|} \right\}.$$

  Hence the condition number $C = \|\mathbf{A}^{-1}\|\|\mathbf{A}\| = \frac{\sigma_1}{\sigma_n}$.

  A note on the strictness of the bounds: C is in the true sense an 'attainable worst case'. To attain the bound, e.g. when $\|\delta b\| = 0$, one must choose $\mathbf{x}$ so that $\|\mathbf{Ax}\| = \|\mathbf{A}\|\|\mathbf{x}\|$ (which is the case for the first singular vector $\mathbf{v}_1$), and $\delta\mathbf{A}$ so that $\|\mathbf{A}^{-1}\delta\mathbf{A}\ \mathbf{x}\| = \|\mathbf{A}^{-1}\|\|\delta\mathbf{A}\|\|\mathbf{x}\|$ which will be the case if $\|\delta\mathbf{A}\ \mathbf{x}\|$ is in the direction of the smallest singular vector of $\mathbf{A}$, with an appropriate choice for $\|\delta\mathbf{A}\|$ so that $\|\delta\mathbf{A}\ \mathbf{x}\| = \|\delta\mathbf{A}\|\|\mathbf{x}\|$. Since all this is possible, the bounds are attainable. However, it is highly unlikely that they will be attained in practical situations. Therefore, signal processing engineers prefer statistical estimates which give a better rendering of the situation, see further.

  Example: given a large number K in $\mathbf{A} = \begin{bmatrix} 1 & K \\ 0 & 1 \end{bmatrix}$, then $\sigma_1 \approx K$ and $\sigma_2 \approx K^{-1}$ so that $C \approx K^2$.

- Generalized inverses and pseudo-inverses: let's restrict the representation for A to its non-zero singular vectors, assuming its rank to be k:

$$\mathbf{A} = [\mathbf{u}_1 \cdots \mathbf{u}_k] \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{bmatrix} [\mathbf{v}_1 \cdots \mathbf{v}_k]^H = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^H$$

(the latter being a sum of 'outer' products of vectors).

The *Moore-Penrose* pseudo-inverse of $\mathbf{A}$ is given by:

$$\mathbf{A}^+ = [\mathbf{v}_1 \cdots \mathbf{v}_k] \begin{bmatrix} \sigma_1^{-1} & & \\ & \ddots & \\ & & \sigma_k^{-1} \end{bmatrix} [\mathbf{u}_1 \cdots \mathbf{u}_k]^H .$$

Its corange is the range of $\mathbf{A}$ and its range, the corange of $\mathbf{A}$. Moreover, it satisfies the following properties:

1. $\mathbf{A}\mathbf{A}^+\mathbf{A} = \mathbf{A}$
2. $\mathbf{A}^+\mathbf{A}\mathbf{A}^+ = \mathbf{A}^+$
3. $\mathbf{A}^+\mathbf{A}$ is the orthonormal projection on the corange of $\mathbf{A}$
4. $\mathbf{A}\mathbf{A}^+$ is the orthonormal projection on the range of $\mathbf{A}$.

These properties characterize $\mathbf{A}^+$. Any matrix $\mathbf{B}$ which satisfies (1) and (2) may be called a pseudo-inverse, but $\mathbf{B}$ is not unique with these properties except when $\mathbf{A}$ is square non-singular.

From the theory we see that the solution of the least squares problem

$$\min_{\mathbf{x} \in \mathcal{C}^n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$$

is given by

$$\mathbf{x} = \mathbf{A}^+\mathbf{b}.$$

The QR algorithm gives a way to compute $\mathbf{x}$, at least when the columns of $\mathbf{A}$ are linearly independent, but the latter expression is more generally valid, and since there exist algorithms to compute the SVD in a remarkably stable numerically way, it is also numerically better, however at the cost of higher complexity (the problem with QR is the back substitution.)

3.4 SVD and noise: estimation of signal spaces

Let $\mathbf{X}$ be a measured data matrix, consisting of an unknown signal $\mathbf{S}$ plus noise $\mathbf{N}$ as follows:

$$\mathbf{X} = \mathbf{S} + \mathbf{N}$$

$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ & \vdots & & \\ & \vdots & & \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1m} \\ s_{21} & s_{22} & \cdots & s_{2m} \\ & \vdots & & \\ & \vdots & & \end{bmatrix} + \begin{bmatrix} N_{11} & N_{12} & \cdots & N_{1m} \\ N_{21} & N_{22} & \cdots & N_{2m} \\ & \vdots & & \\ & \vdots & & \end{bmatrix}$$

What is a good estimate of $\mathbf{S}$ given $\mathbf{X}$? The answer is: only partial information (certain subspaces ...) can be well estimated. This can be seen as follows:

Properties of noise: law of large numbers (weak version)

Let

$$\nu = \frac{1}{n}\sum_{i=1}^{n} \mathbf{N}_i$$

for some stationary white noise, stationary process $\{\mathbf{N}_i\}$ with $E(\mathbf{N}_i\mathbf{N}_j) = \sigma^2_{\mathbf{N}}\delta_{ij}$.
The variance is:

$$\begin{aligned} \sigma^2_\nu &= E(\tfrac{1}{n}\textstyle\sum \mathbf{N}_i)^2 \\ &= \tfrac{1}{n^2}\textstyle\sum_{i,j} E(\mathbf{N}_i\mathbf{N}_j) \\ &= \tfrac{\sigma^2_{\mathbf{N}}}{n} \end{aligned}$$

and hence

$$\sigma_\nu = \frac{\sigma_N}{\sqrt{n}},$$

the accuracy improves with $\sqrt{n}$ through averaging. More generally, we have:

$$\frac{1}{n}\mathbf{N}^H\mathbf{N} = \sigma^2_N(\mathbf{I} + O(\frac{1}{\sqrt{n}}))$$

(this result is a little harder to establish because of the different statistics involved, see textbooks on probability theory.)

Assume now $\mathbf{S}$ and $\mathbf{N}$ independent, and take a large number of samples. Then:

$$\begin{aligned} \tfrac{1}{n}\mathbf{X}^H\mathbf{X} &= \tfrac{1}{n}(\mathbf{S}^H + \mathbf{N}^H)(\mathbf{S} + \mathbf{N}) \\ &= \tfrac{1}{n}(\mathbf{S}^H\mathbf{S} + \mathbf{N}^H\mathbf{N} + \mathbf{N}^H\mathbf{S} + \mathbf{S}^H\mathbf{N}) \end{aligned}$$

(in the *long* direction), and suppose that $s_i, i = 1, m$ are the singular values of $\mathbf{S}$, then $\frac{1}{n}\mathbf{X}^H\mathbf{X}$ equals

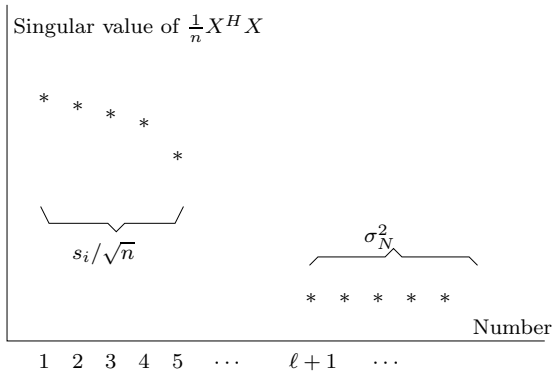
$$\left\{ \mathbf{V}_S \begin{bmatrix} \frac{s_1^2}{n} & & \\ & \ddots & \\ & & \frac{s_m^2}{n} \end{bmatrix} \mathbf{V}_S^H + \begin{bmatrix} \sigma_N^2 & & \\ & \ddots & \\ & & \sigma_N^2 \end{bmatrix} \right\} \cdot \left\{ \mathbf{I} + O(\frac{1}{\sqrt{n}}) \right\}.$$

A numerical error analysis of the SVD gives: $\mathrm{SVD}(\mathbf{A} + O(\epsilon)) = \mathrm{SVD}(\mathbf{A}) + O(\epsilon)$, and hence:

$$\frac{1}{n}\mathbf{X}^H\mathbf{X} = \mathbf{V}_S \begin{bmatrix} \frac{s_1^2}{n} + \sigma_N^2 & & \\ & \ddots & \\ & & \frac{s_m^2}{n} + \sigma_N^2 \end{bmatrix} \mathbf{V}_S^H + O(\frac{1}{\sqrt{n}}).$$

Pisarenko discrimination

Suppose that the original system is of rank ℓ, and we set the singular values of $\mathbf{X}$ out against their order, then we'll find:



We may conclude the following:

1. there is a bias σ_N^2 on the estimates of $\frac{s_i^2}{n}$
2. the error on these estimates *and* on V_S is $O(\frac{\sigma_N}{\sqrt{n}})$.

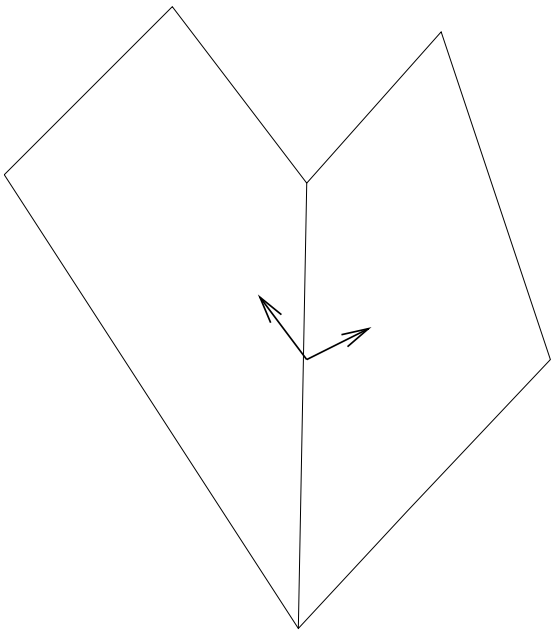
hence it benefits from the statistical averaging. This is however not true for $\mathbf{U}_S$ - the signal subspace - which can only be estimated $O\sigma_N$, since no averaging takes place in its estimate.

3.5 Angles between subspaces

Let

$$\mathbf{U} = [\mathbf{u}_1\, \mathbf{u}_2 \cdots \mathbf{u}_k]$$
$$\mathbf{V} = [\mathbf{v}_1\, \mathbf{v}_2 \cdots \mathbf{v}_\ell]$$

isometric matrices whose columns form bases for two spaces $\mathcal{H}_U$ and $\mathcal{H}_V$. What are the angles between these spaces?



The answer is given by the SVD of an appropriate matrix, $\mathbf{U}^H\mathbf{V}$. Let

$$\mathbf{U}^H\mathbf{V} = \mathbf{A} \left[\begin{array}{ccc|c} \sigma_1 & & & \\ & \ddots & & 0 \\ & & \sigma_k & \\ \hline & 0 & & 0 \end{array}\right] \mathbf{B}^H$$

be that (complete) SVD - in which $\mathbf{A}$ and $\mathbf{B}$ are unitary. The angle cosines are then given by $\cos\phi_i = \sigma_i$ and the principal vectors are given by $\mathbf{UA}$ and $\mathbf{VB}$ ($\cos\phi_i$ is the angle between the ith column of $\mathbf{UA}$ and $\mathbf{VB}$). These are called the *principal vectors* of the intersection.

3.6 Total Least Square - TLS

Going back to our overdetermined system of equations:

$$\mathbf{Ax} = \mathbf{b},$$

we have been looking for solutions of the least squares problem: an $\mathbf{x}$ such that $\|\mathbf{Ax} - \mathbf{b}\|_2$ is minimal. If the columns of $\mathbf{A}$ are linearly independent, then $\mathbf{A}$ has a left inverse (the pseudo-inverse defined earlier), the solution is unique, and is given by that $\mathbf{x}$ for which $\hat{\mathbf{b}} \doteq \mathbf{Ax}$ is the orthogonal projection of $\mathbf{b}$ on space spanned by the columns of $\mathbf{A}$.

An alternative, sometimes preferable approach, is to find a modified system of equations

$$\hat{\mathbf{A}}\mathbf{x} = \hat{\mathbf{b}}$$

which is as close as possible to the original, and such that $\hat{\mathbf{b}}$ is actually in $\mathcal{R}(\hat{\mathbf{A}})$ - the span of the columns of $\hat{\mathbf{A}}$.

What are $\hat{\mathbf{A}}$ and $\hat{\mathbf{b}}$? If the original $\mathbf{A}$ has m columns, then the second condition forces $\text{rank}[\hat{\mathbf{A}}\ \hat{\mathbf{b}}] = m$, and $[\hat{\mathbf{A}}\ \hat{\mathbf{b}}]$ has to be a rank m approximant to the augmented matrix $[\mathbf{A}\ \mathbf{b}]$. The minimal approximation in Frobenius norm is found by the SVD, now of $[\mathbf{A}\ \mathbf{b}]$. Let:

$$\begin{aligned}
[\mathbf{A}\ \mathbf{b}] &= [\mathbf{a}_{\cdot 1} \cdots \mathbf{a}_{\cdot m}\ \mathbf{b}] \\
&= [\mathbf{u}_{\cdot 1} \cdots \mathbf{u}_{\cdot m}\ \mathbf{u}_{\cdot m+1}] \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_m & & \\ & & & \sigma_{m+1} & \end{bmatrix} [\mathbf{v}_{\cdot 1} \cdots \mathbf{v}_{\cdot m} \mathbf{v}_{\cdot m+1}]^H
\end{aligned}$$

be the desired SVD, then we define

$$\begin{aligned}
[\hat{\mathbf{A}}\ \hat{\mathbf{b}}] &= [\hat{\mathbf{a}}_{\cdot 1} \cdots \hat{\mathbf{a}}_{\cdot m}\ \hat{\mathbf{b}}] \\
&= [\mathbf{u}_{\cdot 1} \cdots \mathbf{u}_{\cdot m}] \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_m & \end{bmatrix} [\mathbf{v}_{\cdot 1} \cdots \mathbf{v}_{\cdot m}]^H.
\end{aligned}$$

What is the value of this approximation? We know from the previous theory that the choice is such that $\|[\mathbf{A} - \hat{\mathbf{A}}\ \mathbf{b} - \hat{\mathbf{b}}]\|_F$ is minimal over all possible approximants of reduced rank m. This means actually that

$$\sum_{i=1}^{m} \|\mathbf{a}_{\cdot i} - \hat{\mathbf{a}}_{\cdot i}\|_2^2 + \|\mathbf{b} - \hat{\mathbf{b}}\|_2^2$$

is minimal, by definition of the Frobenius norm, and this can be interpreted as follows:

The span$(\mathbf{a}_{\cdot i}, \mathbf{b})$ *defines a hyperplane, such that the projections of* $\mathbf{a}_{\cdot i}$ *and* b *on it are given by* $\hat{\mathbf{a}}_{\cdot i}$, $\hat{b}$ *and the total quadratic projection error is minimal.*

Acknowledgement

Thanks to many contributions from Patrick Dewilde who initiated to project to create such a summary of basic mathematical prelimenaries.

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