Geometric Modeling

Summer Semester 2010

Mathematical Tools (1)

Recap: Linear Algebra

UNIVERSITÄT DES SAARLANDES

CLUSTER OF EXCELLENCE

max planck institut informatik

Today...

Topics:

- Mathematical Background
  - Linear algebra
  - Analysis & differential geometry
  - Numerical techniques

Mathematical Tools

Linear Algebra

Overview

Linear algebra

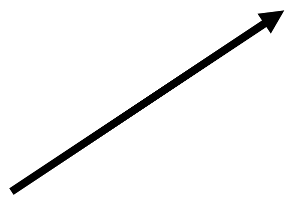
- Vector spaces
- Linear maps
- Quadrics

Vectors

Vector spaces

- Vectors, Coordinates & Points
- Formal definition of a vector space
- Vector algebra
- Generalizations:
  - Infinite dimensional vector spaces
  - Function spaces
  - Approximation with finite dimensional spaces
- More Tools:
  - Dot product and norms
  - The cross product

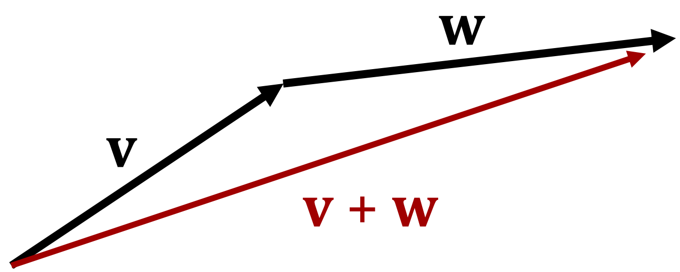
Vectors



vectors are arrows in space

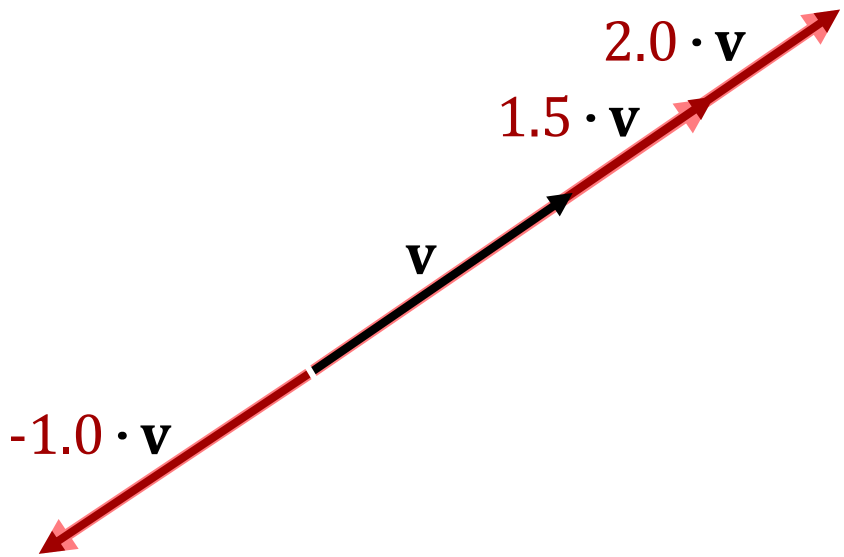
classically: 2 or 3 dim. Euclidian space

Vector Operations



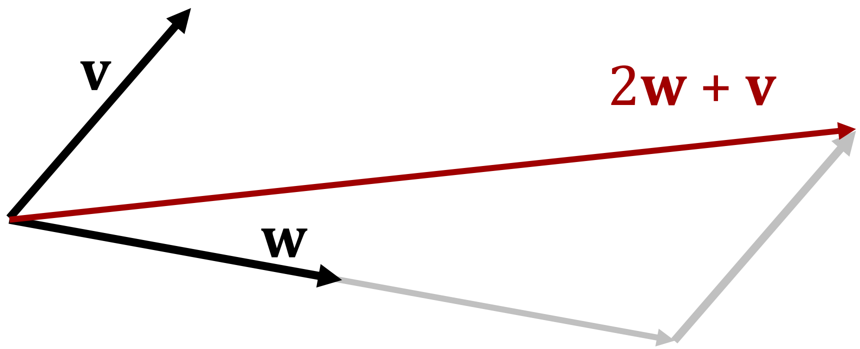
“Adding” Vectors:
Concatenation

Vector Operations



Scalar Multiplication:
Scaling vectors (incl. mirroring)

You can combine it...



Linear Combinations:

This is basically all you can do.

$$\mathbf{r} = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i$$

Vector Spaces

Many classes of objects share the same *structure*:

- Geometric Objects
  - 1,2,3,4... dimensional Euclidian vectors
- But also a lot of other mathematical objects
  - Vectors with complex numbers, or finite fields
  - Certain sets of functions
  - Polynomials
  - ...
- Approach the problem from a more abstract level
  - More general: Saves time, reduces number of proofs
  - Can still resort to geometric vectors to get an intuition about what's going on

Vector Spaces

Definition: *Vector Space V over a Field F*

- Consists of a set of vectors V
- F is a field (usually: Real numbers, $F = \mathbb{R}$)
- Provides two operations:
  - Adding vectors $\mathbf{u} = \mathbf{v} + \mathbf{w}$ ($\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$)
  - Scaling vectors $w = \lambda v$ ($\mathbf{u} \in V, \lambda \in F$)
- The two operations are *closed*, i.e.: operations on any elements of the vector space will yields elements of the vector space itself.
- ...and finally: A number of *properties* that have to hold:

Vector Spaces

Definition: *Vector Space V over a Field F* (cont.)

(a1) $\forall \mathbf{u},\mathbf{v},\mathbf{w} \in \mathrm{V}:\ (\mathbf{u}+\mathbf{v})+\mathbf{w} = \mathbf{u}+(\mathbf{v}+\mathbf{w})$

(a2) $\forall \mathbf{u},\mathbf{v} \in \mathrm{V}:\ \mathbf{u}+\mathbf{v} = \mathbf{v}+\mathbf{u}$

(a3) $\exists \mathbf{0}_{\mathrm{V}} \in \mathrm{V} : \forall \mathbf{v} \in \mathrm{V}:\ \mathbf{v}+\mathbf{0}_{\mathrm{V}} = \mathbf{v}$

(a4) $\forall \mathbf{v} \in \mathrm{V} :\ \exists \mathbf{w} \in \mathrm{V}:\ \mathbf{v}+\mathbf{w} = \mathbf{0}_{\mathrm{V}}$

(s1) $\forall \mathbf{v} \in \mathrm{V}, \lambda, \mu \in \mathrm{F}:\ \lambda(\mu\mathbf{v}) = (\lambda\mu)\mathbf{v}$

(s2) $\text{for } 1_{\mathrm{F}} \in \mathrm{F} : \forall \mathbf{v} \in \mathrm{V}:\ 1_{\mathrm{F}}\mathbf{v} = \mathbf{v}$

(s3) $\forall \lambda \in \mathrm{F} : \forall \mathbf{v},\mathbf{w} \in \mathrm{V}:\ \lambda(\mathbf{v}+\mathbf{w}) = \lambda\mathbf{v}+\lambda\mathbf{w}$

(s4) $\forall \lambda, \mu \in \mathrm{F}, \mathbf{v} \in \mathrm{V}:\ (\lambda+\mu)\mathbf{v} = \lambda\mathbf{v}+\mu\mathbf{v}$

Vector Spaces

Vector spaces

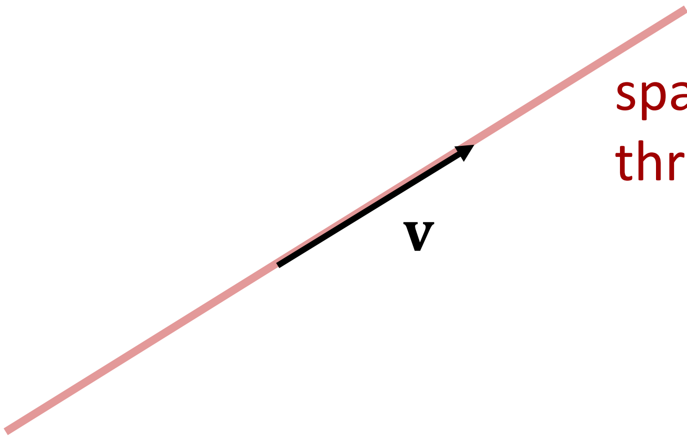
- Out of these formal assumptions, a long list of derivative properties (theorems) can be deduced.
- Will hold for any vector space.
- In particular, we will see that the assumptions are sufficient to obtain the columns with coordinates, we started with (in the finite dimensional case).

Properties

Some properties you can easily prove:

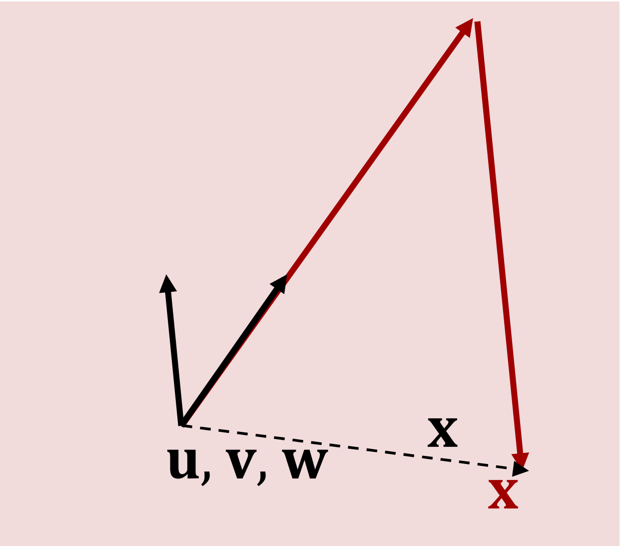
- The zero vector $\mathbf{0}_V$ is unique. For 2D vectors: $\mathbf{0}_V = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- Multiplication with the scalar 0_F yields the zero vector.
- The additive inverse $-\mathbf{v}$ is unique given $\mathbf{v}$.
- Multiplication by -1 yields the inverse vector.
- And so on...

Span and Basis

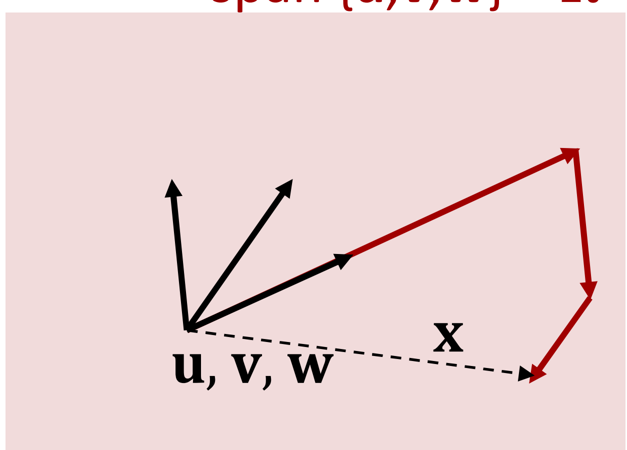


span {**v**} – line through the origin

$\{\mathbf{u},\mathbf{v}\} \subseteq \{\mathbf{u},\mathbf{v},\mathbf{w}\}$
form a basis of $\mathbb{R}^2$



span {**u**,**v**,**w**} = $\mathbb{R}^2$



Example Spaces

Examples of finite-dimensional vector spaces:

- Of course: $\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \mathbb{R}^4 \ldots$
- Standard basis of $\mathbb{R}^3$: $\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$
- Coordinates: $\begin{pmatrix} x \\ y \\ z \end{pmatrix} \hat{=}\, x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} =: x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$

Example Spaces

Examples of finite-dimensional vector spaces:

- Polynomials of fixed degree
  - For example, all polynomials of 2nd order:

    general form: $ax^2 + bx + c$

    addition: $(a_1x^2 + b_1x + c_1) + (a_2x^2 + b_2x + c_2)$
    $= (a_1 + a_2)x^2 + (b_1 + b_2)x + (c_1 + c_2)$

    scalar multiplication: $\lambda(ax^2 + bx + c) = (\lambda a)x^2 + (\lambda b)x + (\lambda c)$
  - Might be confusing: Evaluation of polynomials at x is non-linear, does not relate to the vector space structure
  - Coordinates: $[a, b, c]^T$
  - Basis for these coordinates: $\{x^2, x, 1\}$

Example Spaces

Infinite-dimensional vector spaces:

- Polynomials (of any degree)
- Need to represent coefficients of arbitrary degree
- Coordinate vectors can potentially become arbitrarily long

- General form: $poly(x) = \sum_{i=0}^{\infty} a_i x^i$ (only a finite subset of the a_i nonzero)

- Basis: $\{x^i \mid i = 0,1,2,\ldots\}$

- Coordinate vectors: $(a_0, a_1, a_2, a_3, \ldots)$

Spaces of Sequences

First generalization:

- Make vectors infinitely long
- Spaces of sequences

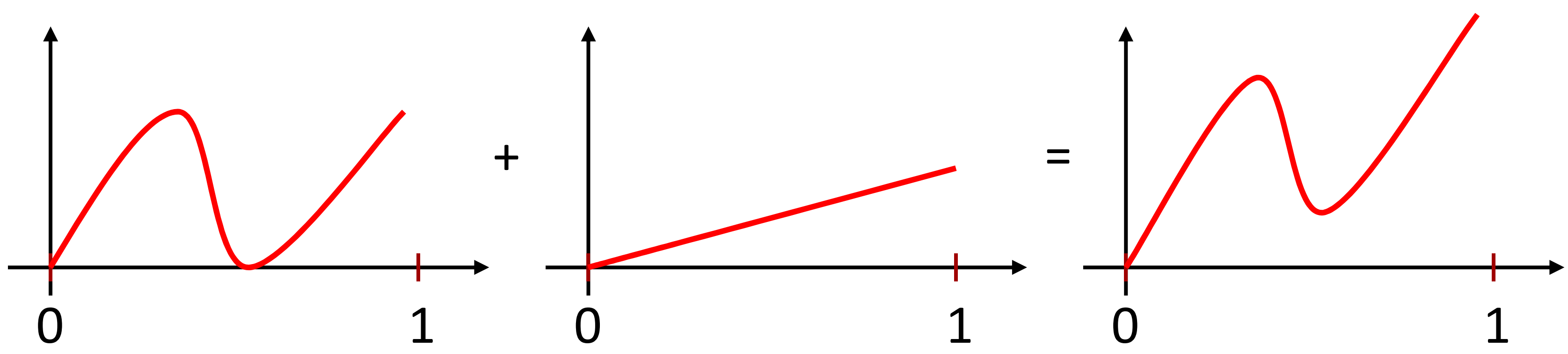
$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_i \\ \vdots \end{pmatrix}$$

- Dimension = ∞, countable

Example Spaces

More infinite-dimensional vector spaces:

- Function spaces
  - Space of all functions $f: \mathbb{R} \to \mathbb{R}$
  - Space of all smooth C^k functions $f: \mathbb{R} \to \mathbb{R}$
  - Space of all functions $f: [0..1] \to \mathbb{R}$
  - Not a vector space: $f: [0..1] \to [0..1]$



Function Spaces

Vector operations

For $f: \Omega \to \mathbb{R}$, define:

- $(f + g)(x) := f(x) + g(x) \; (\forall x \in \Omega)$
- $(\lambda f)(x) := \lambda(f(x)) \; (\forall x \in \Omega)$

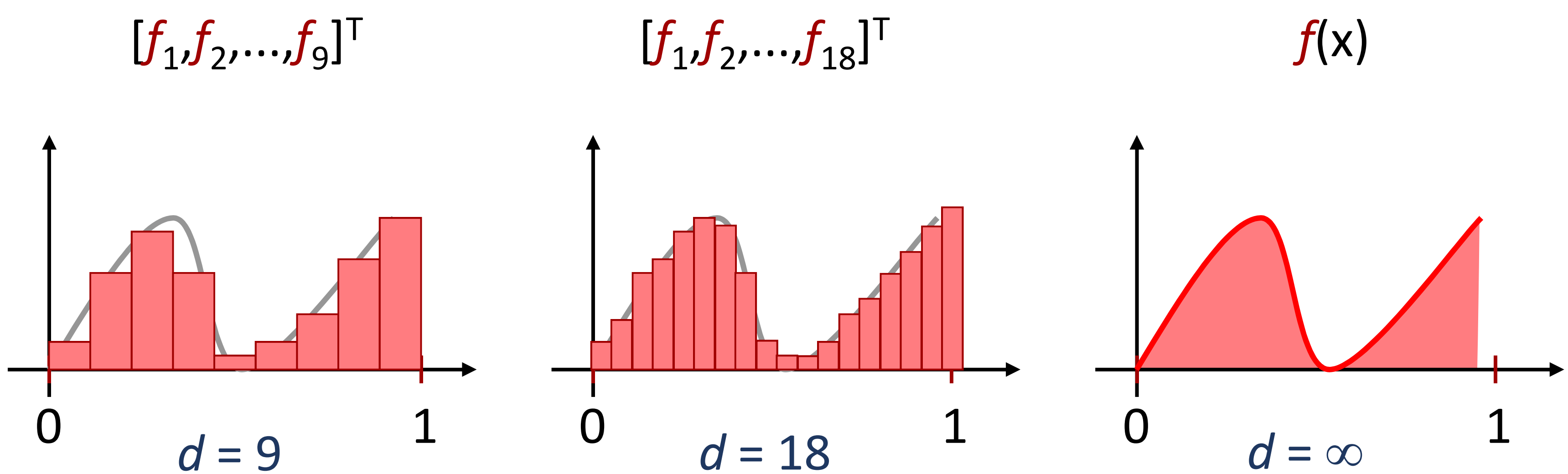
The zero vector is:

- $0_V = (f: f(x) \equiv 0)$

Function Spaces

Intuition:

- Start with a finite dimensional vector
- Increase sampling density towards infinity
- Real numbers: uncountable amount of dimensions



Approximation of Function Spaces

Finite dimensional subspaces:

- Function spaces with infinite dimension are hard to represented on a computer
- For numerical purpose, finite-dimensional subspaces are used to approximate the larger space
- Two basic approaches:

Approximation of Function Spaces

Here is the "recipe":

- We are given an infinite-dimensional function space V.
- We are looking for $f \in V$ with a certain property.
- From a function space V we choose linearly independent functions $f_1,\dots,f_d \in V$ to form the d-dimensional subspace $\mathrm{span}\{f_1,\dots,f_d\}$.
- Instead of looking for the $f \in V$, we look only among the $\tilde{f} := \sum_{i=1}^{d} \lambda_i f_i$ for a function that best-matches the desired property (might be just an approximation, though).
- The good thing: $\tilde{f}$ is described by $(\lambda_1,\dots,\lambda_d)$. Good for the computer...

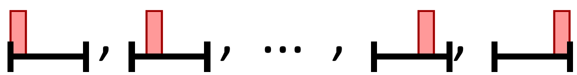
Approximation of Function Spaces

Two Approaches:

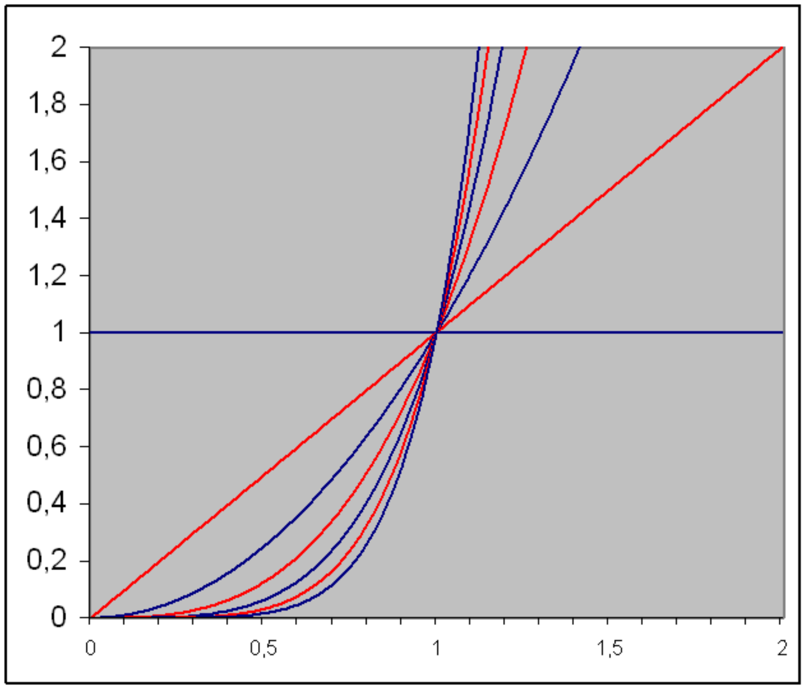
- Construct a basis, that already provides a subspace containing the functions you want
  - Typically, the coefficients will have an intuitive meaning then
  - Bezier Splines, B-Splines, NURBS are all about that
- Choose a basis that can approximate the functions you might want, then pick the closest
  - Standard approach in numerical solutions to *partial differential equations* and *integral equations*
  - Basic idea: Define a measure of correctness $C(f)$, then try to maximize $C(\tilde{f})$

Finite-Dimensional Function Spaces

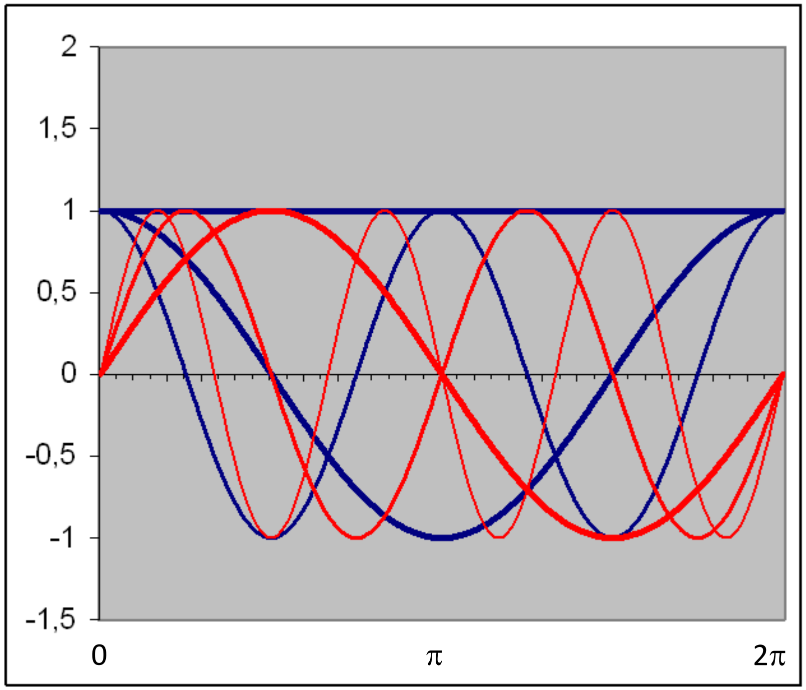
Typical Basis Sets:

- Consider the space of functions f: $[a, b] \rightarrow \mathbb{R}$.
- Some d-dimensional subspaces:
  - span {  } (piecewise constant basis)
  - span $\{ 1, x, x^2, \ldots, x^{d\text{-}1} \}$ (Monomial basis of degree d-1)
  - span $\{ 1, \sin x, \cos x, \sin 2x, \cos 2x, \ldots, \sin (d\text{-}1)x/2, \cos (d\text{-}1)x/2 \}$ (Fourier basis of order $(d$-1$)/2$, usually $a = 0$, $b = 2\pi$)
- It depends all on the application, of course...

Examples



Monomial basis



Fourier basis

More Tools for Vectors

More operations:

- Dot product / scalar product / inner product (measures distances, angles)
- Cross product (only $\mathbb{R}^3$)

The Standard Scalar Product

The *standard dot product* for vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^d$ is defined as:

$$\mathbf{v} \cdot \mathbf{w} = \langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^{\mathrm{T}} \mathbf{w} := \sum_{i=1}^{d} v_i w_i$$

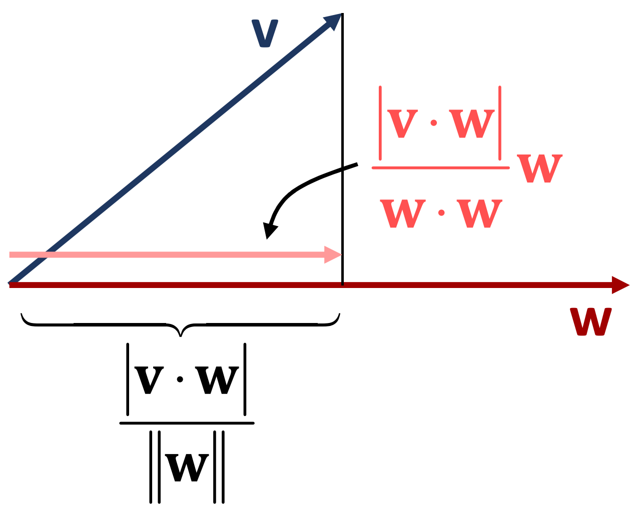
For $\mathbf{v}, \mathbf{w} \in \mathbb{R}^3$:

$$\mathbf{v} \cdot \mathbf{w} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \cdot \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix} = v_x w_x + v_y w_y + v_z w_z$$

Properties

Geometric properties:

- $length(\mathbf{v}) := \|\mathbf{v}\|_2 = \sqrt{\mathbf{v} \cdot \mathbf{v}}$ (Pythagoras)
- $|\mathbf{v} \cdot \mathbf{w}| = \|\mathbf{v}\| \cdot \|\mathbf{w}\| \cdot \cos \angle(\mathbf{v}, \mathbf{w})$ (projection property)



Properties

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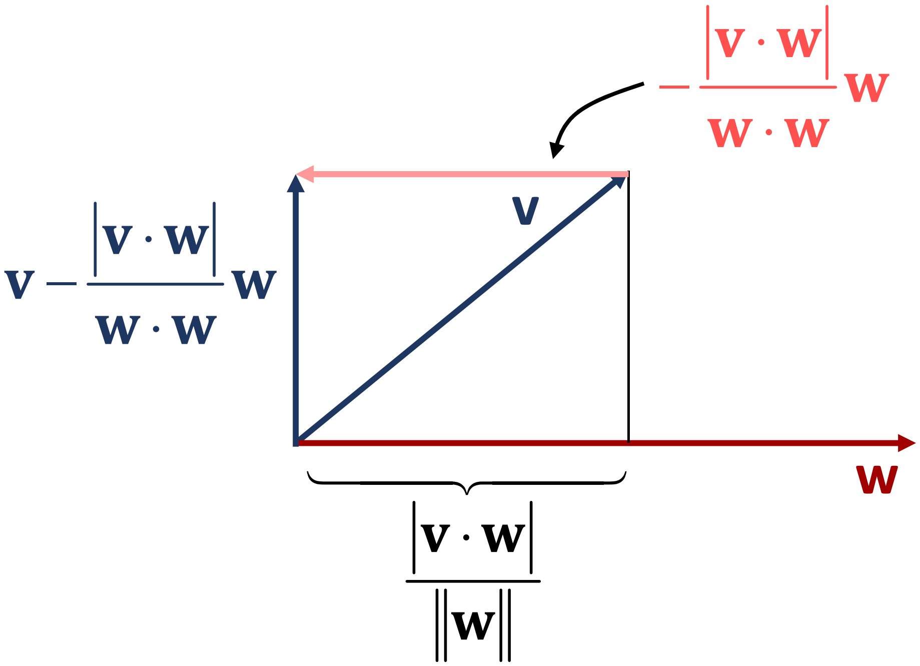
In particular:

- **v** orthogonal to **w** $\Leftrightarrow$ $\mathbf{v} \cdot \mathbf{w} = 0$

Properties

Gram-Schmidt Orthogonalization:



- Repeat for multiple vectors to create orthogonal set of vectors $\{\mathbf{v}'_1, \ldots, \mathbf{v}'_n\}$ from set $\{\mathbf{v}_1,\ldots,\mathbf{v}_n\}$

Properties

Scalar product properties:

$$\left.\begin{array}{ll} \bullet\ \text{Symmetric:} & \mathbf{v}\cdot\mathbf{w}=\mathbf{w}\cdot\mathbf{v} \\ \bullet\ \text{Bi-linear:} & \mathbf{u}\cdot\left(\lambda\mathbf{v}+\mathbf{w}\right)=\mathbf{u}\cdot\lambda\mathbf{v}+\mathbf{u}\cdot\mathbf{w} \\ \bullet\ \text{Positive:} & \mathbf{v}\cdot\mathbf{v}=0\Leftrightarrow\mathbf{v}=\mathbf{0} \end{array}\right\}\ \text{abstract definition}$$

Dot Product on Function Spaces

We need dot products on function spaces...

- For square-integrable functions *f*, *g*: $\Omega \subseteq \mathbb{R}^n \to \mathbb{R}$, the *standard scalar product* is defined as:

$$f \cdot g := \int_{\Omega} f(x) g(x) dx$$

- It measures an abstract normal and angle between function (not in a geometric sense)
- **Orthogonal functions:** Don't influence each other in linear combinations. Adding one to the other does not change the value in the other ones direction.

Linear Maps

Linear maps

- Linear maps and matrices
- Inverting and linear systems of equations
- Eigenvectors and eigenvalues
- Ill-posed problems

Linear Maps

A function f: V $\rightarrow$ W between vector spaces V, W over a field F is a *linear map*, if and only if:

- $\forall v_1, v_2 \in V$: $f(v_1+v_2) = f(v_1) + f(v_2)$
- $\forall v \in V, \lambda \in F$: $f(\lambda v) = \lambda f(v)$

Theorem:

A linear map is uniquely determined if we specify a mapping value for each basis vector of V.

Matrix Representation

Any linear map *f* between finite dimensional spaces can be represented as a matrix:

- We fix a basis (usually the standard basis)
- For each basis vector $\mathbf{v}_i$ of V, we specify the mapped vector $\mathbf{w}_i$.
- Then, the map *f* is given by:

$$f(\mathbf{v}) = f\left(\begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}\right) = v_1\mathbf{w}_1 + \ldots + v_n\mathbf{w}_n$$

Matrix Representation

This can be written as matrix-vector product:

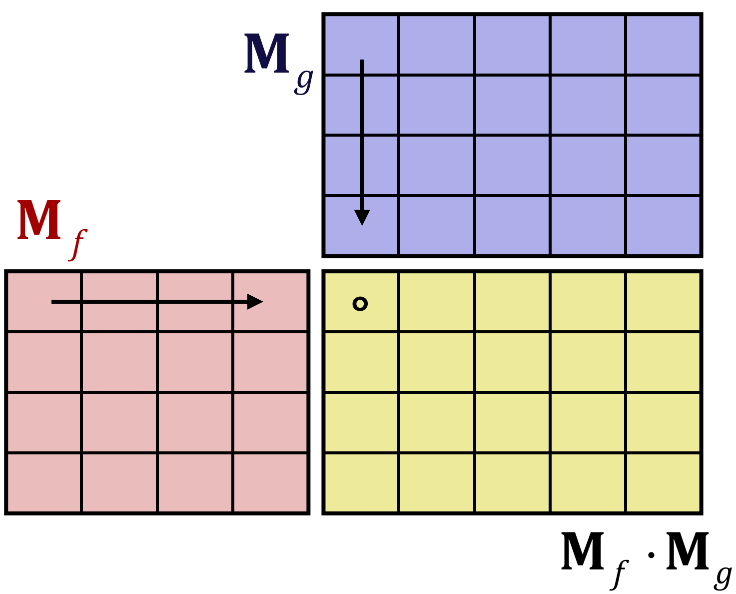
$$f(v) = \begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_n \\ | & & | \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$

The columns are the images of the basis vectors (for which the coordinates of **v** are given)

Matrix Multiplication

Composition of linear maps corresponds to matrix products:

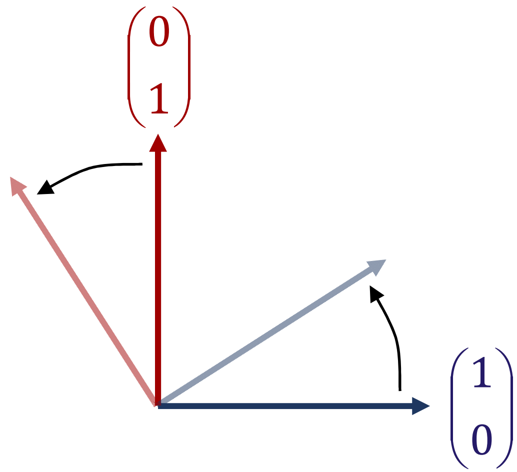
- $f(g) = f \circ g = \mathbf{M}_f \cdot \mathbf{M}_g$
- Matrix product calculation:



The (x,y)-th entry is the dot product of row x of $\mathbf{M}_f$ and column y of $\mathbf{M}_g$

Example

Example: rotation matrix



$$\mathbf{M}_{rot} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$$

Example: identity matrix

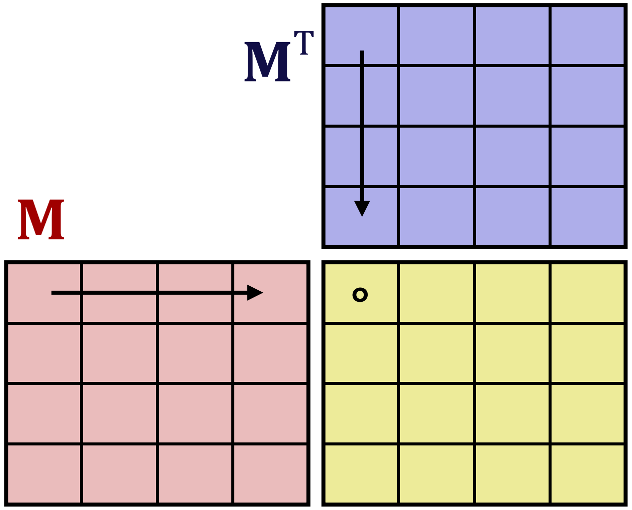
$$\mathbf{I} := \begin{pmatrix} 1 & 0 & & 0 \\ 0 & 1 & & 0 \\ & & \ddots & \\ 0 & 0 & & 1 \end{pmatrix}$$

Orthogonal Matrices

Orthogonal Matrix

- A matrix is called *orthogonal* if all of its columns (rows) are *orthonormal, i.e.* $\mathbf{c}_i \cdot \mathbf{c}_i = 1, \ \mathbf{c}_i \cdot \mathbf{c}_j = 0 \ \text{for} \ i \neq j$
- The inverse of an orthogonal matrix is its transpose:

$$\mathbf{M}\mathbf{M}^{-1} = \mathbf{M}\mathbf{M}^{\mathrm{T}} = \mathbf{I}$$



Affine Maps

Affine Maps

- Translations are not linear (except for zero translation)
- A combination of a linear map and a translation can be described by:

$$f(\mathbf{x}) = \mathbf{M}\mathbf{x} + \mathbf{t}$$

- This is called an affine map
- Composition of affine maps are affine:

$$\begin{aligned} f(g(x)) &= \mathbf{M}_f(\mathbf{M}_g\mathbf{x} + \mathbf{t}_g)\mathbf{x} + \mathbf{t}_f \\ &= (\mathbf{M}_f\mathbf{M}_g)\mathbf{x} + (\mathbf{M}_f\mathbf{t}_g + \mathbf{t}_f) \end{aligned}$$

- For a vector space V, a subspace $S \subseteq V$ and a point $\mathbf{p} \in V$, the set {**x** | **x** = **p** + **v**, $\mathbf{v} \in V$} is called an affine subspace of V. If $\mathbf{p} \neq \mathbf{0}$, this is not a vector space.

Linear Systems of Equations

Problem: Invert an affine map

- Given: **Mx** = **b**
- We know **M**, **b**
- Looking for **x**

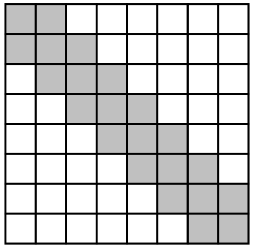
Solution

- The set of solution is always an affine subspace of $\mathbb{R}^n$ (i.e., a point, a line, a plane...), or the empty set.
- There are innumerous algorithms for solving linear systems, here is a brief summary...

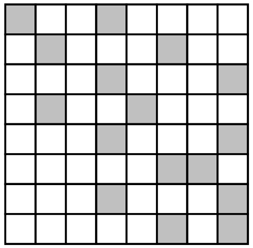
Solvers for Linear Systems

Algorithms for solving linear systems of equations:

- Gaussian elimination: O(n^3) operations for $n \times n$ matrices
- We can do better, in particular for special cases:
  - **Band matrices:**
    constant bandwidth



  - **Sparse matrices:**
    constant number of non-zero entries per row
    – Store only non-zero entries
    – Instead of (3.5, 0, 0, 0, 7, 0, 0), store [(1:3.5), (5:7)]



Solvers for Linear Systems

Algorithms for solving linear systems of equations:

- Band matrices, constant bandwidth: modified elimination algorithm with O(n) operations.
- Iterative Gauss-Seidel solver: converges for diagonally dominant matrices. Typically: O(n) iterations, each costs O(n) for a sparse matrix.
- Conjugate Gradient solver: works for symmetric, positive definite matrices in O(n) iterations, but typically we get a good solution already after O($\sqrt{n}$) iterations.

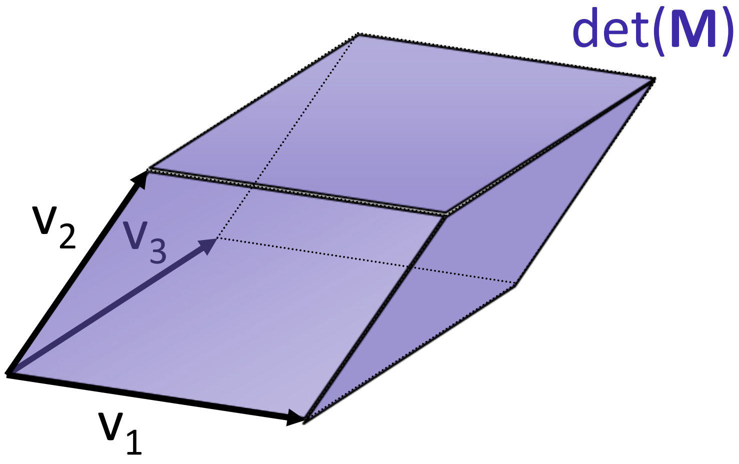
More details on iterative solvers: *J. R. Shewchuk: An Introduction to the Conjugate Gradient Method Without the Agonizing Pain, 1994.*

Determinants

Determinants

- Assign a scalar det(**M**) to square matrices **M**
- The scalar measures the volume of the *parallelepiped* formed by the column vectors:

$$\mathbf{M} = \begin{pmatrix} | & | & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \\ | & | & | \end{pmatrix}$$



Properties

A few properties:

- $\det(\mathbf{A})\det(\mathbf{B}) = \det(\mathbf{AB})$
- $\det(\lambda\mathbf{A}) = \lambda^n\det(\mathbf{A})$ ($n \times n$ matrix $\mathbf{A}$)
- $\det(\mathbf{A}^{-1}) = \det(\mathbf{A})^{-1}$
- $\det(\mathbf{A}^{\mathrm{T}}) = \det(\mathbf{A})$

- Can be computed efficiently using Gaussian elimination

Eigenvectors & Eigenvalues

Definition:

If for a linear map M and a non-zero vector $\mathbf{x}$ we have

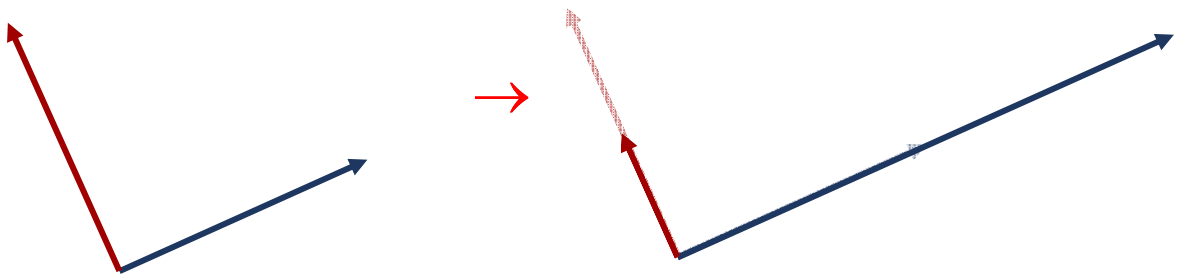
$$\mathbf{Mx} = \lambda\mathbf{x}$$

we call λ an *eigenvalue* of **M** and **x** the corresponding *eigenvector*.

Example

Intuition:

- In the direction of an eigenvector, the linear map acts like a scaling



- Example: two eigenvalues (0.5 and 2)
- Two eigenvectors
- Standard basis contains no eigenvectors

Eigenvectors & Eigenvalues

Diagonalization:

In case an $n \times n$ matrix **M** has n linear independent eigenvectors, we can *diagonalize* **M** by transforming to this coordinate system: $\mathbf{M} = \mathbf{TDT}^{-1}$.

Spectral Theorem

Spectral Theorem:

If $\mathbf{M}$ is a symmetric $n \times n$ matrix of real numbers (i.e. $\mathbf{M} = \mathbf{M}^T$), there exists an *orthogonal* set of n eigenvectors.

This means, every (real) symmetric matrix can be *diagonalized*:

$\mathbf{M} = \mathbf{T}\mathbf{D}\mathbf{T}^T$ with an orthogonal matrix $\mathbf{T}$.

Computation

Simple algorithm

- "Power iteration" for symmetric matrices
- Computes largest eigenvalue even for large matrices
- Algorithm:
  - Start with a random vector (maybe multiple tries)
  - Repeatedly multiply with matrix
  - Normalize vector after each step
  - Repeat until ration before / after normalization converges (this is the eigenvalue)
- Important intuition: Largest eigenvalue is the "dominant" component of the linear map.

Powers of Matrices

What happens:

- A symmetric matrix can be written as:

$$\mathbf{M} = \mathbf{TDT}^{\mathrm{T}} = \mathbf{T}\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}\mathbf{T}^{\mathrm{T}}$$

- Taking it to the *k*-th power yields:

$$\mathbf{M}^k = \mathbf{TDT}^{\mathrm{T}}\mathbf{TDT}^{\mathrm{T}}\ldots\mathbf{TDT}^{\mathrm{T}} = \mathbf{TD}^k\mathbf{T}^{\mathrm{T}} = \mathbf{T}\begin{pmatrix} {\lambda_1}^k & & \\ & \ddots & \\ & & {\lambda_n}^k \end{pmatrix}\mathbf{T}^{\mathrm{T}}$$

- Bottom line: Eigenvalue analysis is the key to understanding powers of matrices.

Improvements

Improvements to the power method:

- Find smallest? – use inverse matrix.
- Find all (for a symmetric matrix)? – run repeatedly, orthogonalize current estimate to already known eigenvectors in each iteration (Gram Schmidt)
- How long does it take? – ratio to next smaller eigenvalue, gap increases exponentially.

There are more sophisticated algorithms based on this idea.

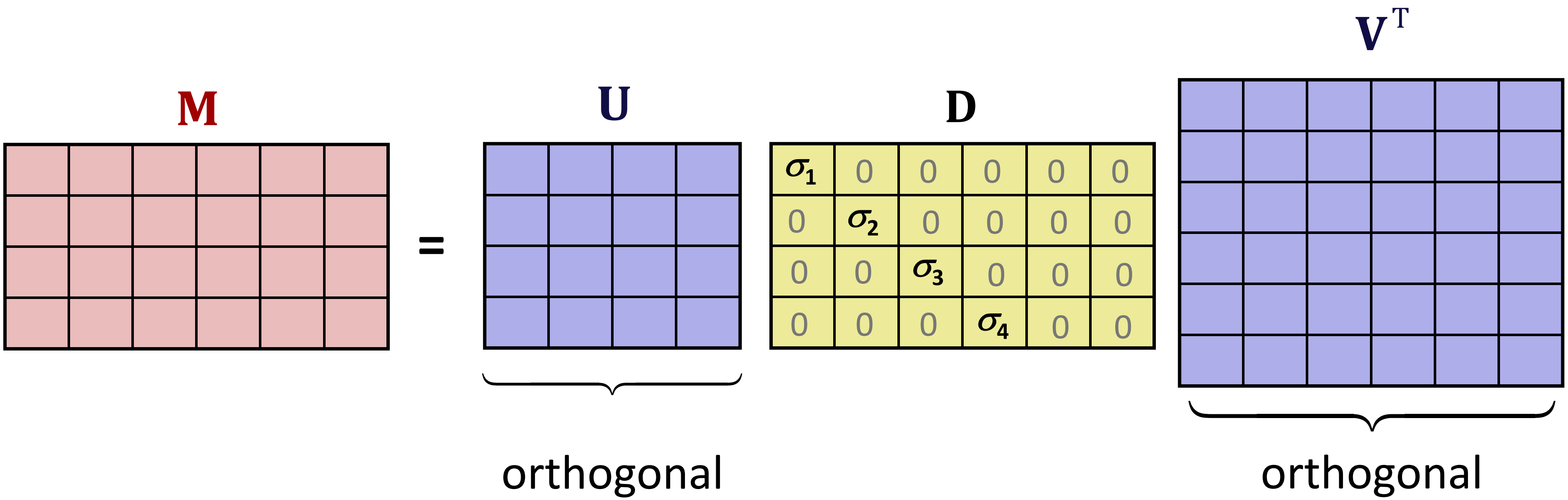
Generalization: SVD

Singular value decomposition:

- Let **M** be an arbitrary real matrix (may be rectangular)
- Then **M** can be written as:
  - $\mathbf{M} = \mathbf{U}\,\mathbf{D}\,\mathbf{V}^{T}$
  - The matrices **U**, **V** are orthogonal
  - **D** is a diagonal matrix (might contain zeros)
  - The diagonal entries are called *singular values.*
- **U** and **V** are different in general. For diagonalizable matrices, they are the same, and the singular values are the eigenvalues.

Singular Value Decomposition

Singular value decomposition



Singular Value Decomposition

Singular value decomposition

- Can be used to solve linear systems of equations
- For full rank, square **M**:

$$\mathbf{M} = \mathbf{U}\,\mathbf{D}\,\mathbf{V}^T$$

$$\Rightarrow \mathbf{M}^{-1} = (\mathbf{U}\,\mathbf{D}\,\mathbf{V}^T)^{-1} = (\mathbf{V}^T)^{-1}\,\mathbf{D}^{-1}\,(\mathbf{U}^{-1}) = \mathbf{V}\,\mathbf{D}^{-1}\,\mathbf{U}^T$$

- Good numerical properties (numerically stable), but expensive
- The OpenCV library provides a very good implementation of the SVD

Inverse Problems

Settings

- A (physical) process f takes place
- It transforms the original input **x** into an output **b**
- Task: recover **x** from **b**

Examples:

- 3D structure from photographs
- Tomography: values from line integrals
- 3D geometry from a noisy 3D scan

Linear Inverse Problems

Assumption: f is linear and finite dimensional

$$f(\mathbf{x}) = \mathbf{b} \;\Rightarrow\; \mathbf{M}_f\mathbf{x} = \mathbf{b}$$

Inversion of f is said to be an ill-posed problem, if one of the following three conditions hold:

- There is no solution
- There is more than one solution
- There is exactly one solution, but the SVD contains very small singular values.

Ill posed Problems

Ratio: Small singular values amplify errors

- Assume our input is inexact (e.g. measurement noise)
- Reminder: $\mathbf{M}^{-1} = \mathbf{V}\,\mathbf{D}^{-1}\,\mathbf{U}^{T}$

does not hurt (orthogonal)

does not hurt (orthogonal)

this one is decisive

- Orthogonal transforms preserve the norm of **x**, so **V** and **U** do not cause problems

Ill posed Problems

Ratio: Small singular values amplify errors

- Reminder: $\mathbf{x} = \mathbf{M}^{-1}\mathbf{b} = (\mathbf{V}\,\mathbf{D}^{-1}\,\mathbf{U}^{T})\mathbf{b}$
- Say **D** looks like that:

$$\mathbf{D} := \begin{pmatrix} 2.5 & 0 & 0 & 0 \\ 0 & 1.1 & 0 & 0 \\ 0 & 0 & 0.9 & 0 \\ 0 & 0 & 0 & 0.000000001 \end{pmatrix}$$

- Any input noise in **b** in the direction of the fourth right singular vector will be amplified by 10^9.
- If our measurement precision is less than that, the result will be unusable.
- Does *not* depend on *how* we invert the matrix.
- Condition number: $\sigma_{max} / \sigma_{min}$

Regularization

Regularization

- Aims at avoiding the inversion problems
- Various techniques; in general the goal is to ignore the misleading information
  - Subspace inversion: do not use directions with small singular values (needs an SVD)
  - Additional assumptions: Assume smoothness (or something similar) in case of unclear or missing information so that compound problem (f + assumptions) is well posed

Quadrics

Quadrics

- Multivariate polynomials
- Quadratic optimization
- Quadrics & eigenvalue problems

Multivariate Polynomials

A *multi-variate* polynomial of total degree *d*:

- A function $f: \mathbb{R}^n \to \mathbb{R}$, $\mathbf{x} \to f(\mathbf{x})$
- f is a polynomial in the components of $\mathbf{x}$
- In any direction $f(\mathbf{s}+t\mathbf{r})$, we obtain a one-dimensional polynomial of maximum degree d in t.

Examples:

- $f([x,y]^T) := x + xy + y$ is of total degree 2. In diagonal direction, we obtain $f(t[1/\sqrt{2}, 1/\sqrt{2}]^T) = t^2$.
- $f([x,y]^T) := c_{20}x^2 + c_{02}y^2 + c_{11}xy + c_{10}x + c_{01}y + c_{00}$ is a quadratic polynomial in two variables

Quadratic Polynomials

In general, any quadratic polynomial in *n* variables can be written as:

- $\mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + c$
- A is an $n \times n$ matrix, **b** is an n-dim. vector, c is a number
- Matrix **A** can always be chosen to be symmetric
- If it isn't, we can substitute by $0.5 \cdot (\mathbf{A} + \mathbf{A}^T)$, not changing the polynomial

Example

Example:

$$f\left(\begin{pmatrix} x \\ y \end{pmatrix}\right) = f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}} \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \mathbf{x}$$

$$= [x\ y] \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = [x\ y] \begin{pmatrix} 1x & 2y \\ 3x & 4y \end{pmatrix}$$

$$= x1x + x2y + y3x + y4y$$

$$= 1x^2 + (2+3)xy + 4y^2$$

$$= 1x^2 + (2.5+2.5)xy + 4y^2$$

$$= \mathbf{x}^{\mathrm{T}} \frac{1}{2} \left[\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} + \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} \right] \mathbf{x} = \mathbf{x}^{\mathrm{T}} \begin{pmatrix} 1 & 2.5 \\ 2.5 & 4 \end{pmatrix} \mathbf{x}$$

Quadratic Polynomials

Specifying quadratic polynomials:

- $\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} + \mathbf{b}^{\mathrm{T}}\mathbf{x} + c$
- **b** shifts the function in space (if **A** has full rank):

$$\begin{aligned}
&(x-\mu)^{\mathrm{T}}\mathbf{A}(x-\mu)+c \\
&= x^{\mathrm{T}}\mathbf{A}x - \mu^{\mathrm{T}}\mathbf{A}x - x^{\mathrm{T}}\mathbf{A}\mu + \mu\cdot\mu + c \\
&\overset{(\text{A sym.})}{=} x^{\mathrm{T}}\mathbf{A}x - \underbrace{(2\mathbf{A}\mu)\mathbf{x}}_{=\,\mathbf{b}} + \mu\cdot\mu + c
\end{aligned}$$

- c is an additive constant

Some Properties

Important properties

- Multivariate polynomials form a vector space
- We can add them component-wise:

$$\begin{array}{rl} & 2x^2 + 3y^2 + 4xy + 2x + 2y + 4 \\ + & 3x^2 + 2y^2 + 1xy + 5x + 5y + 5 \\ \hline\hline = & 5x^2 + 5y^2 + 5xy + 7x + 7y + 9 \end{array}$$

- In vector notation:

$$\begin{aligned} & \mathbf{x}^T \mathbf{A}_1 \mathbf{x} + \mathbf{b}_1^T \mathbf{x} + \mathbf{c}_1 \\ + \; & \lambda(\mathbf{x}^T \mathbf{A}_2 \mathbf{x} + \mathbf{b}_2^T \mathbf{x} + \mathbf{c}_2) \\ = \; & \mathbf{x}^T(\mathbf{A}_1 + \lambda \mathbf{A}_2)\mathbf{x} + (\mathbf{b}_1 + \lambda \mathbf{b}_2)^T \mathbf{x} + (\mathbf{c}_1 + \lambda \mathbf{c}_2) \end{aligned}$$

Quadratic Polynomials

Quadrics

- The zero level set of such a quadratic polynomial is called a “quadric”
- Shape depends on eigenvalues of **A**
- **b** shifts the object in space
- **c** sets the level

Shapes of Quadrics

Shape analysis:

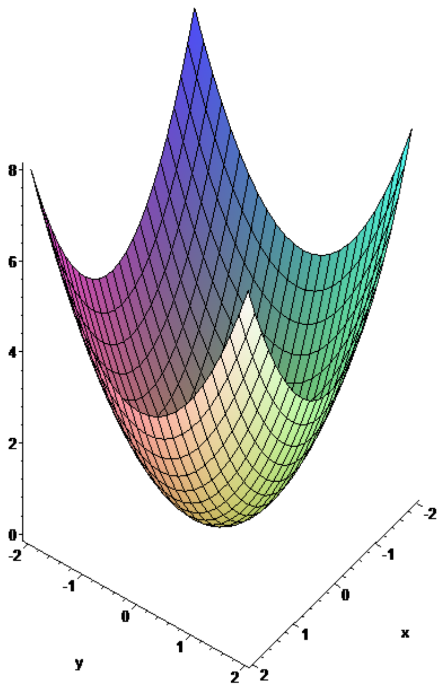
- **A** is symmetric
- A can be *diagonalized* with orthogonal *eigenvectors*

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = x^{\mathrm{T}}\left[\mathbf{Q}^{\mathrm{T}}\begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{pmatrix}\mathbf{Q}\right]x$$

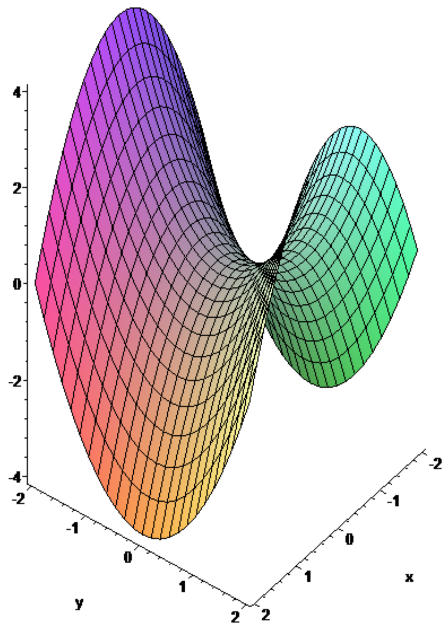
$$= (\mathbf{Q}x)^{\mathrm{T}}\begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{pmatrix}(\mathbf{Q}x)$$

- **Q** contains the principal axis of the quadric
- The eigenvalues determine the quadratic growth (up, down, speed of growth)

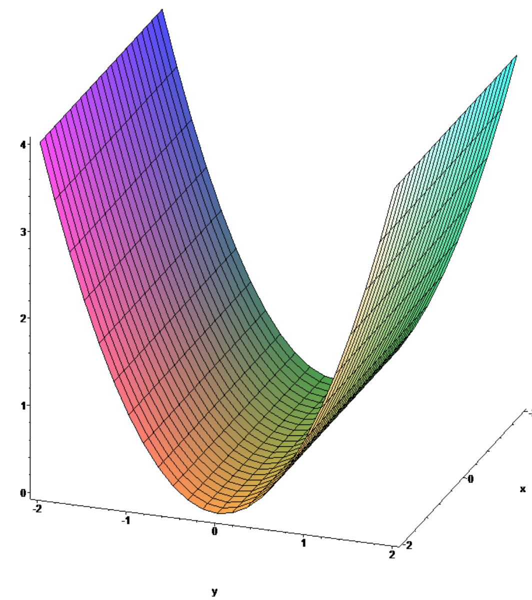
Shapes of Quadratic Polynomials



$\lambda_1 = 1, \lambda_2 = 1$



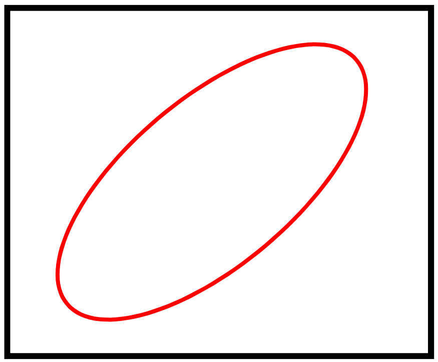
$\lambda_1 = 1, \lambda_2 = -1$



$\lambda_1 = 1, \lambda_2 = 0$

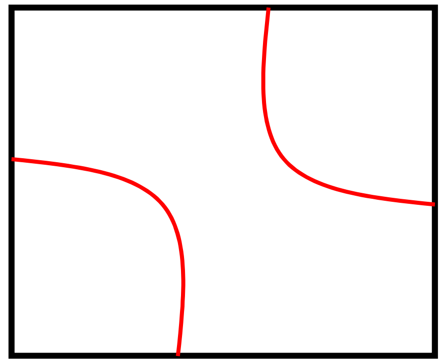
The Iso-Lines: Quadrics

elliptic



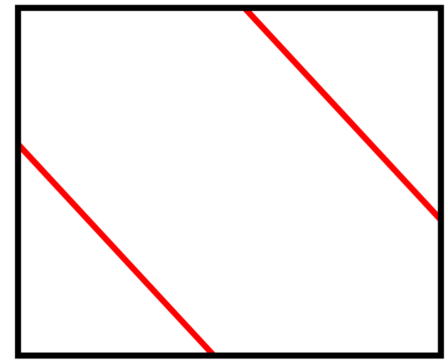
$\lambda_1 > 0, \lambda_2 > 0$

hyperbolic



$\lambda_1 < 0, \lambda_2 > 0$

degenerate case



$\lambda_1 = 0, \lambda_2 \neq 0$

Quadratic Optimization

Quadratic Optimization

- Assume we want to minimize a quadratic objective function $\mathbf{x}^T\mathbf{A}\mathbf{x} + \mathbf{b}^T\mathbf{x} + c$
- $\mathbf{A}$ has only positive eigenvalues.
- Means: It's a paraboloid with a unique minimum
- The vertex (critical point) of the paraboloid can be determined by simply solving a linear system
- More on this later (need some more analysis first)

Rayleigh Quotient

Relation to eigenvalues:

- The minimum and maximum eigenvalues of a symmetric matrix **A** can be expressed as constraint quadratic optimization problem:

$$\lambda_{\min} = \min \frac{\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}}{\mathbf{x}^{\mathrm{T}}\mathbf{x}} = \min_{\|x\|=1} \left(\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}\right) \qquad \lambda_{\max} = \max \frac{\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}}{\mathbf{x}^{\mathrm{T}}\mathbf{x}} = \max_{\|x\|=1} \left(\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}\right)$$

- The other way round – eigenvalues solve a certain type of constrained, (non-convex) optimization problem.

Coordinate Transformations

One more interesting property:

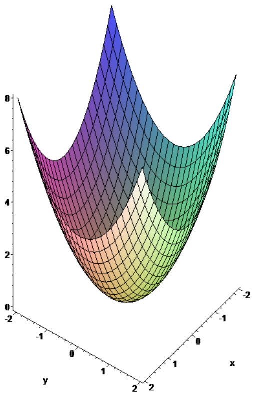
- Given a positive definite symmetric (“SPD”) matrix **M** (all eigenvalues positive)
- Such a matrix can always be written as square of another matrix:

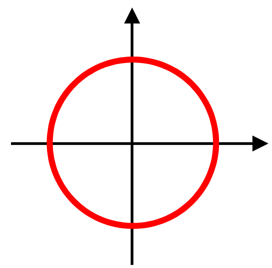
$$\mathbf{M} = \mathbf{TDT}^{\mathrm{T}} = \left(T\sqrt{D}\right)\left(\sqrt{D}^{T} T^{T}\right) = \left(T\sqrt{D}\right)\left(T\sqrt{D}\right)^{T} = \left(T\sqrt{D}\right)^{2}$$

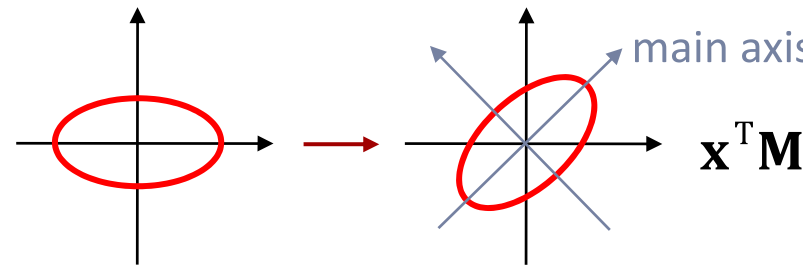
$$\sqrt{D} = \begin{pmatrix} \sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n} \end{pmatrix}$$

SPD Quadrics

$\mathbf{x}^{\mathrm{T}}\mathbf{x}$







$\mathbf{x}^{\mathrm{T}}\mathbf{M}\mathbf{x}$

Identity $\mathbf{I}$

$$\mathbf{M} = \mathbf{T}\mathbf{D}\mathbf{T}^{\mathrm{T}} = \left(T\sqrt{D}\right)^2$$

Interpretation:

- Start with a unit positive quadric $\mathbf{x}^{\mathrm{T}}\mathbf{x}$.
- Scale the main axis (diagonal of D)
- Rotate to a different coordinate system (columns of **T**)
- Recovering main axis from **M**: Compute eigensystem ("principal component analysis")

Software

GeoX

GeoX comes with several linear algebra libraries:

- 2D, 3D, 4D vectors and matrices: *LinearAlgebra.h*
- Large (dense) vectors and matrices: *DynamicLinearAlgebra.h*
- Gaussian elimination: *invertMatrix()*
- Sparse matrices: *SparseLinearAlgebra.h*
- Iterative solvers (Gauss-Seidel, conjugate gradients, power iteration): *IterativeSolvers.h*