Distributional Semantic Models

Part 4: Elements of matrix algebra

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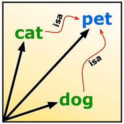

Outline

Outline

Matrices and vectors

- $k \times n$ matrix $\mathbf{M} \in \mathbb{R}^{k \times n}$ is a rectangular array of real numbers

$$\mathbf{M} = \begin{bmatrix} m_{11} & \cdots & m_{1n} \\ \vdots & & \vdots \\ m_{k1} & \cdots & m_{kn} \end{bmatrix}$$

- Each row $\mathbf{m}_i \in \mathbb{R}^n$ is an n-dimensional vector

$$\mathbf{m}_i = (m_{i1}, m_{i2}, \ldots, m_{in})$$

- Similarly, each column is a k-dimensional vector $\in \mathbb{R}^k$

```
> options(digits=3)
> M <- DSM_TermTerm$M
> M[2, ]  # row vector m2 for "dog"
> M[, 5]  # column vector for "important"
```

Matrices and vectors

- Vector $\mathbf{x} \in \mathbb{R}^n$ as single-row or single-column matrix
  - $\mathbf{x} = \mathbf{x}^{TT} = n \times 1$ matrix ("vertical")
  - $\mathbf{x}^T = 1 \times n$ matrix ("horizontal")
  - **transposition** operator $\cdot^T$ swaps rows & columns of matrix

```
> r <- DSM_TermTerm$rows$f
> c <- DSM_TermTerm$cols$f
> N <- DSM_TermTerm$globals$N
> t(r)       # "horizontal" vector
> t(t(r))    # "vertical" vector
```

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  - $\mathbf{x}^T = 1 \times n$ matrix ("horizontal")
  - **transposition** operator $\cdot^T$ swaps rows & columns of matrix
- We need vectors $\mathbf{r} \in \mathbb{R}^k$ and $\mathbf{c} \in \mathbb{R}^n$ of marginal frequencies
- Notation for cell ij of co-occurrence matrix:
  - $m_{ij} = O$ . . . observed co-occurrence frequency
  - $r_i = R$ . . . row marginal (target)
  - $c_j = C$ . . . column marginal (feature)
  - N . . . sample size

```
> r <- DSM_TermTerm$rows$f
> c <- DSM_TermTerm$cols$f
> N <- DSM_TermTerm$globals$N
> t(r)     # ‘‘horizontal’’ vector
> t(t(r))  # ‘‘vertical’’ vector
```

Scalar operations

- **Scalar** operations perform the same transformation on each element of a vector or matrix, e.g.
  - add / subtract fixed shift $\mu \in \mathbb{R}$
  - multiply / divide by fixed factor $\sigma \in \mathbb{R}$
  - apply function ($\log, \sqrt{\cdot}, \ldots$) to each element
- Allows efficient processing of large sets of values

```
> log(M + 1) # discounted log frequency weighting
> (M["cause", ] + M["effect", ]) / 2 # centroid vector
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  - apply function ($\log, \sqrt{\cdot}, \ldots$) to each element
- Allows efficient processing of large sets of values
- Element-wise binary operators on matching vectors / matrices
  - $\mathbf{x} + \mathbf{y}$ = **vector addition**
  - $\mathbf{x} \odot \mathbf{y}$ = element-wise multiplication (**Hadamard product**)

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The outer product

- Compute matrix $\mathbf{E} \in \mathbb{R}^{k \times n}$ of expected frequencies

$$e_{ij} = \frac{r_i c_j}{N}$$

i.e. `r[i] * c[j]` for each cell ij

```
> outer(r, c) / N
```

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- This is the **outer product** of $\mathbf{r}$ and $\mathbf{c}$

$$\begin{bmatrix} r_1 \\ \vdots \\ r_k \end{bmatrix} \cdot \begin{bmatrix} c_1 & c_2 & \cdots & c_n \end{bmatrix} = \begin{bmatrix} r_1 c_1 & r_1 c_2 & \cdots & r_1 c_n \\ \vdots & \vdots & & \vdots \\ r_k c_1 & r_k c_2 & \cdots & r_k c_n \end{bmatrix}$$

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- The **inner product** of $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ is the sum $x_1 y_1 + \ldots + x_n y_n$

```
> outer(r, c) / N
```

Outline

Matrix multiplication

$$\begin{bmatrix} & & \\ & a_{ij} & \\ & & \\ & & \end{bmatrix} = \begin{bmatrix} b_{i1} & \cdots & b_{in} \\ & & \\ & & \end{bmatrix} \cdot \begin{bmatrix} & c_{1j} & \\ & \vdots & \\ & \vdots & \\ & c_{nj} & \end{bmatrix}$$

$$\underset{(k \times m)}{\mathbf{A}} = \underset{(k \times n)}{\mathbf{B}} \cdot \underset{(n \times m)}{\mathbf{C}}$$

- **B** and **C** must be **conformable** (in dimension n)
- Element a_{ij} is the inner product of the i-th row of **B** and the j-th column of **C**

$$a_{ij} = b_{i1}c_{1j} + \ldots + b_{in}c_{nj} = \sum_{t=1}^{n} b_{it}c_{tj}$$

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Some properties of matrix multiplication

Associativity:	$\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C} =: \mathbf{ABC}$
Distributivity:	$\mathbf{A}(\mathbf{B} + \mathbf{B}') = \mathbf{AB} + \mathbf{AB}'$
	$(\mathbf{A} + \mathbf{A}')\mathbf{B} = \mathbf{AB} + \mathbf{A}'\mathbf{B}$
Scalar multiplication:	$(\lambda\mathbf{A})\mathbf{B} = \mathbf{A}(\lambda\mathbf{B}) = \lambda(\mathbf{AB}) =: \lambda\mathbf{AB}$

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- Not commutative in general: $\mathbf{AB} \neq \mathbf{BA}$
- The k-dimensional square-diagonal **identity matrix**

$$\mathbf{I}_k := \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} \quad \text{with} \quad \mathbf{I}_k \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{I}_n = \mathbf{A}$$

is the **neutral element** of matrix multiplication

Transposition and multiplication

- The **transpose** $\mathbf{A}^T$ of a matrix $\mathbf{A}$ swaps rows and columns:

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ a_3 & b_3 \end{bmatrix}^T = \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix}$$

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  - $(\mathbf{A} \cdot \mathbf{B})^T = \mathbf{B}^T \cdot \mathbf{A}^T$ [note the different order of **A** and **B**!]
  - $\mathbf{I}^T = \mathbf{I}$

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  - $(\mathbf{A} \cdot \mathbf{B})^T = \mathbf{B}^T \cdot \mathbf{A}^T$ [note the different order of **A** and **B**!]
  - $\mathbf{I}^T = \mathbf{I}$
- **A** is called **symmetric** iff $\mathbf{A}^T = \mathbf{A}$
  - symmetric matrices have many special properties that will become important later (e.g. eigenvalues)

The outer product as matrix multiplication

- The outer product is a special case of matrix multiplication

$$\mathbf{E} = \frac{1}{N}(\mathbf{r} \cdot \mathbf{c}^T)$$

```
# three ways to compute the matrix of expected frequencies
> E <- outer(r, c) / N
> E <- (r %*% t(c)) / N
> E <- tcrossprod(r, c) / N
> E
```

The outer product as matrix multiplication

- The outer product is a special case of matrix multiplication

$$\mathbf{E} = \frac{1}{N}(\mathbf{r} \cdot \mathbf{c}^T)$$

- The other special case is the **inner product**

$$\mathbf{x}^T\mathbf{y} = \sum_{i=1}^{n} x_i y_i$$

- NB: $\mathbf{x} \cdot \mathbf{x}$ and $\mathbf{x}^T \cdot \mathbf{x}^T$ are not conformable

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Outline

Computing association scores

- Association scores = element-wise combination of **M** and **E**, e.g. for (pointwise) Mutual Information

$$\mathbf{S} = \log_2(\mathbf{M} \oslash \mathbf{E})$$

  - $\oslash$ = element-wise division similar to Hadamard product $\odot$

```
> log2(M / E)
> S <- pmax(log2(M / E), 0) # not max() !
> S
```

Computing association scores

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  - $\oslash$ = element-wise division similar to Hadamard product $\odot$
- For sparse AMs such as PPMI, we need to compute $\max\{s_{ij}, 0\}$ for each element of the scored matrix $\mathbf{S}$

```
> log2(M / E)
> S <- pmax(log2(M / E), 0) # not max() !
> S
```

Normalizing vectors

- Compute Euclidean norm of vector $\mathbf{x} \in \mathbb{R}^n$:

$$\|\mathbf{x}\|_2 = \sqrt{x_1^2 + \ldots + x_n^2}$$

```
> x <- S[2, ]
> b <- sqrt(sum(x ^ 2)) # Euclidean norm of x
> x0 <- x / b           # normalized vector
> sqrt(sum(x0 ^ 2))
```

Normalizing vectors

- Compute Euclidean norm of vector $\mathbf{x} \in \mathbb{R}^n$:

$$\|\mathbf{x}\|_2 = \sqrt{x_1^2 + \ldots + x_n^2}$$

- Normalized vector $\|\mathbf{x}_0\|_2 = 1$ by scalar multiplication:

$$\mathbf{x}_0 = \frac{1}{\|\mathbf{x}\|_2}\mathbf{x}$$

```
> x <- S[2, ]
> b <- sqrt(sum(x ^ 2))  # Euclidean norm of x
> x0 <- x / b            # normalized vector
> sqrt(sum(x0 ^ 2))
```

Normalizing matrix rows

- Compute vector $\mathbf{b} \in \mathbb{R}^k$ of norms of row vectors of $\mathbf{S}$
- Can you find an elegant way to multiply each row of $\mathbf{S}$ with the corresponding normalization factor b_i^{-1}?

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- Multiplication with **diagonal matrix** $\mathbf{D_b}^{-1}$

$$\mathbf{S}_0 = \mathbf{D_b}^{-1} \cdot \mathbf{S}$$

$$\mathbf{S}_0 = \begin{bmatrix} b_1^{-1} & & \\ & \ddots & \\ & & b_k^{-1} \end{bmatrix} \cdot \begin{bmatrix} s_{11} & \cdots & s_{1n} \\ \vdots & & \vdots \\ s_{k1} & \cdots & s_{kn} \end{bmatrix}$$

☞ What about multiplication with diagonal matrix on the right?

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$$\mathbf{S}_0 = \mathbf{D_b}^{-1} \cdot \mathbf{S}$$

```
> b <- sqrt(rowSums(S^2))
> b <- rowNorms(S, method="euclidean") # more efficient

> S0 <- diag(1 / b) %*% S
> S0 <- scaleMargins(S, rows=(1 / b))   # much more efficient

> S0 <- normalize.rows(S, method="euclidean") # the easy way
```

Outline

Metric: a measure of distance

- A **metric** is a general measure of the distance $d(\mathbf{u}, \mathbf{v})$ between points $\mathbf{u}$ and $\mathbf{v}$, which satisfies the following axioms:
  - $d(\mathbf{u}, \mathbf{v}) = d(\mathbf{v}, \mathbf{u})$
  - $d(\mathbf{u}, \mathbf{v}) > 0$ for $\mathbf{u} \neq \mathbf{v}$
  - $d(\mathbf{u}, \mathbf{u}) = 0$
  - $d(\mathbf{u}, \mathbf{w}) \leq d(\mathbf{u}, \mathbf{v}) + d(\mathbf{v}, \mathbf{w})$ (**triangle inequality**)
- Metrics form a very broad class of distance measures, some of which do not fit in well with our geometric intuitions

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- Metrics form a very broad class of distance measures, some of which do not fit in well with our geometric intuitions
- Useful: family of **Minkowski** p-metrics

$$d_p(\mathbf{u}, \mathbf{v}) := \left(|u_1 - v_1|^p + \cdots + |u_n - v_n|^p\right)^{1/p} \qquad p \geq 1$$

$$d_p(\mathbf{u}, \mathbf{v}) := |u_1 - v_1|^p + \cdots + |u_n - v_n|^p \qquad 0 \leq p < 1$$

Norm: a measure of length

- A general **norm** $\|\mathbf{u}\|$ for the length of a vector $\mathbf{u}$ must satisfy the following axioms:
  - $\|\mathbf{u}\| > 0$ for $\mathbf{u} \neq \mathbf{0}$
  - $\|\lambda\mathbf{u}\| = |\lambda| \cdot \|\mathbf{u}\|$ (**homogeneity**)
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- Every norm **induces** a metric

$$d(\mathbf{u}, \mathbf{v}) := \|\mathbf{u} - \mathbf{v}\|$$

with two desirable properties

- **translation-invariant**: $d(\mathbf{u} + \mathbf{x}, \mathbf{v} + \mathbf{x}) = d(\mathbf{u}, \mathbf{v})$
- **scale-invariant**: $d(\lambda\mathbf{u}, \lambda\mathbf{v}) = |\lambda| \cdot d(\mathbf{u}, \mathbf{v})$

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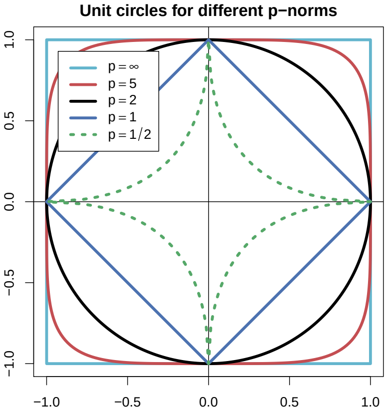
  - **scale-invariant**: $d(\lambda\mathbf{u}, \lambda\mathbf{v}) = |\lambda| \cdot d(\mathbf{u}, \mathbf{v})$
- $d_p(\mathbf{u}, \mathbf{v})$ is induced by the **Minkowski norm** for $p \geq 1$:

$$\|\mathbf{u}\|_p := \left(|u_1|^p + \cdots + |u_n|^p\right)^{1/p}$$

Norm: a measure of length



- Visualisation of norms in $\mathbb{R}^2$ by plotting **unit circle**, i.e. points $\mathbf{u}$ with $\|\mathbf{u}\| = 1$
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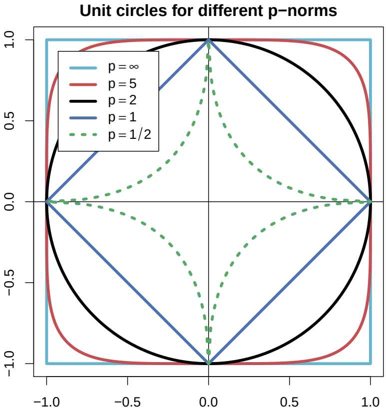

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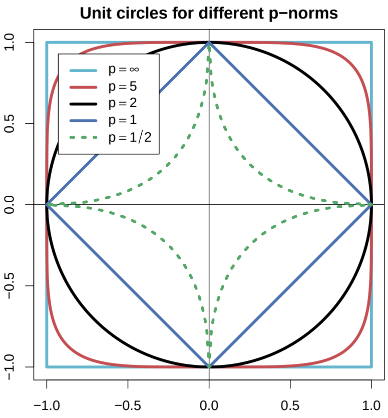

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☞ Consequence for DSM: $p \ll 2$ sensitive to small differences in many coordinates, $p \gg 2$ to larger differences in few coord.

Outline

Euclidean norm & inner product

- The Euclidean norm $\|\mathbf{u}\|_2 = \sqrt{\mathbf{u}^T\mathbf{u}}$ is special because it can be derived from the **inner product**:

$$\mathbf{x}^T\mathbf{y} = x_1 y_1 + \cdots + x_n y_n$$

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- The inner product is a positive definite and symmetric bilinear form with an important geometric interpretation:

$$\cos\phi = \frac{\mathbf{u}^T\mathbf{v}}{\|\mathbf{u}\|_2 \cdot \|\mathbf{v}\|_2}$$

  for the **angle** ϕ between vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$
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  for the **angle** ϕ between vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$
  - the value $\cos\phi$ is known as the **cosine similarity** measure
- In particular, $\mathbf{u}$ and $\mathbf{v}$ are **orthogonal** iff $\mathbf{u}^T\mathbf{v} = 0$

Cosine similarity in R

- Cosine similarities can be computed very efficiently if vectors are pre-normalized, so that $\|\mathbf{u}\|_2 = \|\mathbf{v}\|_2 = 1$

☞ just need all inner products $\mathbf{m}_i^T \mathbf{m}_j$ between row vectors of $\mathbf{M}$

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$$\mathbf{M} \cdot \mathbf{M}^T = \begin{bmatrix} \cdots & \mathbf{m}_1 & \cdots \\ \cdots & \mathbf{m}_2 & \cdots \\ & & \\ \cdots & \mathbf{m}_k & \cdots \end{bmatrix} \cdot \begin{bmatrix} \vdots & \vdots & & \vdots \\ \mathbf{m}_1 & \mathbf{m}_2 & & \mathbf{m}_k \\ \vdots & \vdots & & \vdots \end{bmatrix}$$

$$\hookrightarrow \quad \left(\mathbf{M} \cdot \mathbf{M}^T\right)_{ij} = \mathbf{m}_i^T \mathbf{m}_j$$

```
# cosine similarities for row-normalized matrix:
> sim <- tcrossprod(S0)
> angles <- acos(pmin(sim, 1)) * (180 / pi)
```

Euclidean distance or cosine similarity?

- Proof that Euclidean distance and cosine similarity are equivalent looks much simpler in matrix algebra
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$$
\begin{aligned}
d_2(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\|_2 &= \sqrt{(\mathbf{u} - \mathbf{v})^T (\mathbf{u} - \mathbf{v})} \\
&= \sqrt{\mathbf{u}^T \mathbf{u} + \mathbf{v}^T \mathbf{v} - 2\,\mathbf{u}^T \mathbf{v}} \\
&= \sqrt{\|\mathbf{u}\|_2^2 + \|\mathbf{v}\|_2^2 - 2\,\mathbf{u}^T \mathbf{v}} \\
&= \sqrt{2 - 2\cos\phi}
\end{aligned}
$$

☞ $d_2(\mathbf{u}, \mathbf{v})$ is a monotonically increasing function of ϕ

Outline

Linear subspace & basis

- A linear **subspace** $B \subseteq \mathbb{R}^n$ of rank $r \leq n$ is spanned by a set of r linearly independent basis vectors

$$B = \{\mathbf{b}_1, \ldots, \mathbf{b}_r\}$$

Linear subspace & basis

- A linear **subspace** $B \subseteq \mathbb{R}^n$ of rank $r \leq n$ is spanned by a set of r linearly independent basis vectors

$$B = \{\mathbf{b}_1, \ldots, \mathbf{b}_r\}$$

- Every point $\mathbf{u}$ in the subspace is a unique linear combination of the basis vectors

$$\mathbf{u} = x_1\mathbf{b}_1 + \ldots + x_r\mathbf{b}_r$$

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- Basis matrix $\mathbf{V} \in \mathbb{R}^{n \times r}$ with column vectors $\mathbf{b}_i$:

$$\mathbf{u} = \mathbf{V}\mathbf{x}$$

Linear subspace & basis

- Basis matrix $\mathbf{V} \in \mathbb{R}^{n \times r}$ with column vectors $\mathbf{b}_i$:

$$\mathbf{u} = x_1\mathbf{b}_1 + \ldots + x_r\mathbf{b}_r = \mathbf{V}\mathbf{x}$$

$$\begin{bmatrix} x_1 b_{11} + \ldots + x_r b_{r1} \\ x_1 b_{12} + \ldots + x_r b_{r2} \\ \vdots \\ x_1 b_{1n} + \ldots + x_r b_{rn} \end{bmatrix} = \begin{bmatrix} b_{11} & \cdots & b_{r1} \\ b_{12} & \cdots & b_{r2} \\ \vdots & & \vdots \\ b_{1n} & \cdots & b_{rn} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ \vdots \\ x_r \end{bmatrix}$$

$$\underset{(n \times 1)}{\mathbf{u}} = \underset{(n \times r)}{\mathbf{V}} \cdot \underset{(r \times 1)}{\mathbf{x}}$$

Orthonormal basis

- Particularly convenient with orthonormal basis:

$$
\begin{aligned}
\|\mathbf{b}_i\|_2 &= 1 \\
\mathbf{b}_i^T \mathbf{b}_j &= 0 \qquad \text{for } i \neq j
\end{aligned}
$$

- Corresponding basis matrix $\mathbf{V}$ is (column)-**orthogonal**

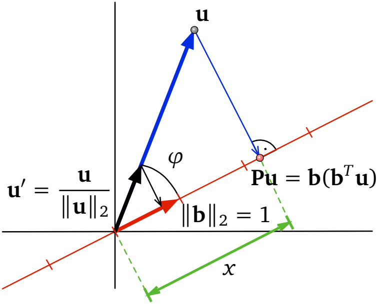
$$\mathbf{V}^T \mathbf{V} = \mathbf{I}_r$$

  and defines a Cartesian coordinate system in the subspace

The mathematics of projections

- 1-d subspace spanned by basis vector $\|\mathbf{b}\|_2 = 1$
- For any point $\mathbf{u}$, we have

$$\cos\varphi = \frac{\mathbf{b}^T\mathbf{u}}{\|\mathbf{b}\|_2 \cdot \|\mathbf{u}\|_2} = \frac{\mathbf{b}^T\mathbf{u}}{\|\mathbf{u}\|_2}$$



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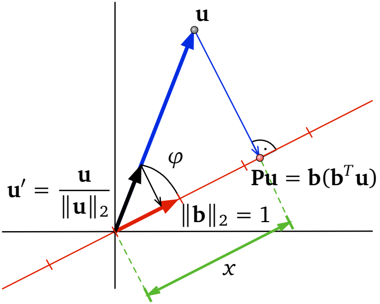

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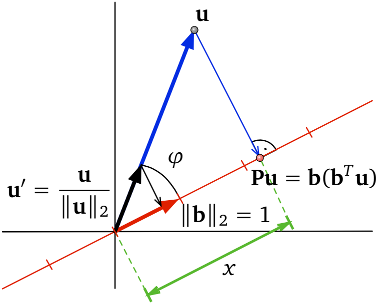

- The projected point in original space is then given by

$$\mathbf{b} \cdot x = \mathbf{b}(\mathbf{b}^T\mathbf{u}) = (\mathbf{b}\mathbf{b}^T)\mathbf{u} = \mathbf{P}\mathbf{u}$$

where $\mathbf{P}$ is a **projection matrix** of rank 1

The mathematics of projections

- For an orthogonal basis matrix $\mathbf{V}$ with columns $\mathbf{b}_1, \ldots, \mathbf{b}_r$, the projection into the rank-r subspace B is given by

$$\mathbf{P}\mathbf{u} = \left(\sum_{i=1}^{r} \mathbf{b}_i \mathbf{b}_i^T \right) \mathbf{u} = \mathbf{V}\mathbf{V}^T \mathbf{u}$$

  and its subspace coordinates are $\mathbf{x} = \mathbf{V}^T \mathbf{u}$

The mathematics of projections

- For an orthogonal basis matrix $\mathbf{V}$ with columns $\mathbf{b}_1, \ldots, \mathbf{b}_r$, the projection into the rank-r subspace B is given by

$$\mathbf{Pu} = \left(\sum_{i=1}^{r} \mathbf{b}_i \mathbf{b}_i^T \right) \mathbf{u} = \mathbf{V}\mathbf{V}^T \mathbf{u}$$

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- Projection can be seen as decomposition into the projected vector and its orthogonal complement

$$\mathbf{u} = \mathbf{Pu} + (\mathbf{u} - \mathbf{Pu}) = \mathbf{Pu} + (\mathbf{I} - \mathbf{P})\mathbf{u} = \mathbf{Pu} + \mathbf{Qu}$$

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- Because of orthogonality, this also applies to the squared Euclidean norm (according to the Pythagorean theorem)

$$\|\mathbf{u}\|^2 = \|\mathbf{Pu}\|^2 + \|\mathbf{Qu}\|^2$$

Aside: the matrix cross-product

- We already know that the (transpose) cross-product $\mathbf{M}\mathbf{M}^T$ computes all inner products between the row vectors of $\mathbf{M}$
- But $\mathbf{V}\mathbf{V}^T$ it can also be unterstood as a superposition of the outer products of the columns of $\mathbf{V}$ with themselves

$$\mathbf{V}\mathbf{V}^T = \begin{bmatrix} b_{11} \\ \vdots \\ b_{1n} \end{bmatrix} \cdot \begin{bmatrix} b_{11} & \cdots & b_{1n} \end{bmatrix} + \ldots + \begin{bmatrix} b_{r1} \\ \vdots \\ b_{rn} \end{bmatrix} \cdot \begin{bmatrix} b_{r1} & \cdots & b_{rn} \end{bmatrix}$$

Projections in R

```
# column basis vector for "animal" subspace
> b <- t(t(c(1, 1, 1, 1, .5, 0, 0)))
> b <- normalize.cols(b)  # basis vectors must be normalized

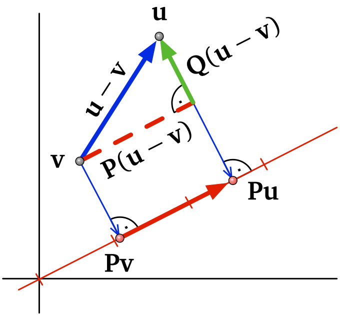
> (x <- M %*% b)  # projection of data points into subspace coordinates
> x %*% t(b)      # projected points in original space
> tcrossprod(x, b)  # outer() only works for plain vectors

> P <- b %*% t(b)   # projection operator
> P - t(P)          # note that P is symmetric
> M %*% P           # projected points in original space
```

Optimal projections and subspaces

- Orthogonal decomposition of squared distances btw vectors

$$\|\mathbf{u}-\mathbf{v}\|^2 = \|\mathbf{Pu}-\mathbf{Pv}\|^2 + \|\mathbf{Qu}-\mathbf{Qv}\|^2$$



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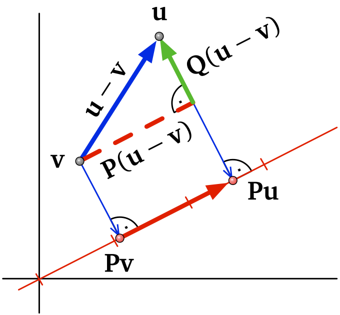
- Define projection **loss** as difference btw squared distances

$$\begin{aligned} &\left|\, \|\mathbf{P}(\mathbf{u}-\mathbf{v})\|^2 - \|\mathbf{u}-\mathbf{v}\|^2 \,\right| \\ &= \|\mathbf{u}-\mathbf{v}\|^2 - \|\mathbf{P}(\mathbf{u}-\mathbf{v})\|^2 \\ &= \|\mathbf{Q}(\mathbf{u}-\mathbf{v})\|^2 \end{aligned}$$



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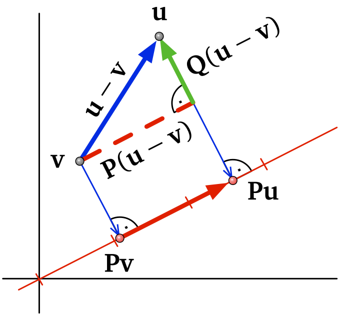
- Projection quality measure:

$$R^2 = \frac{\|\mathbf{P}(\mathbf{u}-\mathbf{v})\|^2}{\|\mathbf{u}-\mathbf{v}\|^2}$$



Optimal projections and subspaces

- Optimal subspace maximises R^2 across a data set $\mathbf{M}$, which is now specified in terms of row vectors $\mathbf{m}_i^T$:

$$\mathbf{x}_i^T = \mathbf{m}_i^T \mathbf{V} \qquad \mathbf{m}_i^T \mathbf{P} = \mathbf{m}_i^T \mathbf{V} \mathbf{V}^T$$

$$\mathbf{X} = \mathbf{M}\mathbf{V} \qquad \mathbf{M}\mathbf{P} = \mathbf{M}\mathbf{V}\mathbf{V}^T$$

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$$\mathbf{X} = \mathbf{M} \mathbf{V} \qquad \mathbf{M} \mathbf{P} = \mathbf{M} \mathbf{V} \mathbf{V}^T$$

- We will now show that the overall projection quality is

$$R^2 = \frac{\sum_{i=1}^k \|\mathbf{m}_i^T \mathbf{P}\|^2}{\sum_{i=1}^k \|\mathbf{m}_i^T\|^2} = \frac{\|\mathbf{M}\mathbf{P}\|_F^2}{\|\mathbf{M}\|_F^2}$$

with the (squared) **Frobenius norm**

$$\|\mathbf{M}\|_F^2 = \sum_{ij} (m_{ij})^2 = \sum_{i=1}^k \|\mathbf{m}_i\|^2$$

Optimal projections and subspaces

- For a centered data set with $\sum_i \mathbf{m}_i = \mathbf{0}$, the Frobenius norm corresponds to the average (squared) distance between points

$\sum_{i,j=1}^{k} \|\mathbf{m}_i - \mathbf{m}_j\|^2$

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$$\sum_{i,j=1}^{k} \|\mathbf{m}_i - \mathbf{m}_j\|^2$$
$$= \sum_{i,j=1}^{k} (\mathbf{m}_i - \mathbf{m}_j)^T (\mathbf{m}_i - \mathbf{m}_j)$$

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Optimal projections and subspaces

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$$
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&\qquad = \sum_{j=1}^{k} \|\mathbf{M}\|_F^2 + \sum_{i=1}^{k} \|\mathbf{M}\|_F^2 - 2 \sum_{i=1}^{k} \mathbf{m}_i^T \Big(\underbrace{\sum_{j=1}^{k} \mathbf{m}_j}_{\mathbf{0}} \Big)
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&= 2k \cdot \|\mathbf{M}\|_F^2
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&= 2k \cdot \|\mathbf{M}\|_F^2
\end{aligned}
$$

- Similarly for the overall projection loss and quality R^2:

$$
R^2 = \frac{\sum_{i,j=1}^{k} \|\mathbf{P}(\mathbf{m}_i - \mathbf{m}_j)\|^2}{\sum_{i,j=1}^{k} \|\mathbf{m}_i - \mathbf{m}_j\|^2} = \frac{2k \cdot \|\mathbf{MP}\|_F^2}{2k \cdot \|\mathbf{M}\|_F^2}
$$

Outline

Singular value decomposition

- Fundamental result of matrix algebra: **singular value decomposition** (**SVD**) factorises any matrix $\mathbf{M}$ into

$$\mathbf{M} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

where $\mathbf{U}$ and $\mathbf{V}$ are orthogonal and $\mathbf{\Sigma}$ is a diagonal matrix of **singular values** $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m > 0$

$$\begin{array}{cc} & n \\ k & \begin{bmatrix} & & \\ & \mathbf{M} & \\ & & \end{bmatrix} \end{array} = \begin{array}{cc} & m \\ k & \begin{bmatrix} & & \\ & \mathbf{U} & \\ & & \end{bmatrix} \end{array} \cdot \begin{array}{cc} & m \\ m & \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & \mathbf{\Sigma} & \sigma_m \end{bmatrix} \end{array} \cdot \begin{array}{cc} & n \\ m & \begin{bmatrix} & & \\ & \mathbf{V}^T & \\ & & \end{bmatrix} \end{array}$$

Singular value decomposition

- $m \leq \min\{k, n\}$ is the inherent dimensionality (**rank**) of $\mathbf{M}$
- Columns $\mathbf{a}_i$ of $\mathbf{U}$ are called left singular vectors,
  columns $\mathbf{b}_i$ of $\mathbf{V}$ ($=$ rows of $\mathbf{V}^T$) are right singular vectors

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- Recall the "outer product" view of matrix multiplication:

$$\mathbf{U}\mathbf{V}^T = \sum_{i=1}^{m} \mathbf{a}_i \mathbf{b}_i^T$$

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- Recall the "outer product" view of matrix multiplication:

$$\mathbf{U}\mathbf{V}^T = \sum_{i=1}^{m} \mathbf{a}_i \mathbf{b}_i^T$$

- Hence the SVD corresponds to a sum of rank-1 components

$$\mathbf{M} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_{i=1}^{m} \sigma_i \mathbf{a}_i \mathbf{b}_i^T$$

Singular value decomposition

- Key property of SVD: the first r components give the best rank-r approximation to $\mathbf{M}$ with respect to the Frobenius norm, i.e. they minimize the loss

$$\|\mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^T - \mathbf{M}\|_F^2 = \|\mathbf{M}_r - \mathbf{M}\|_F^2$$

☞ **Truncated** SVD
  - $\mathbf{U}_r$, $\mathbf{V}_r$ = first r columns of $\mathbf{U}$, $\mathbf{V}$
  - $\mathbf{\Sigma}_r$ = diagonal matrix of first r singular values

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  - $\mathbf{U}_r$, $\mathbf{V}_r$ = first r columns of $\mathbf{U}$, $\mathbf{V}$
  - $\mathbf{\Sigma}_r$ = diagonal matrix of first r singular values
- It can be shown that

$$\|\mathbf{M}\|_F^2 = \sum_{i=1}^{m} \sigma_i^2 \quad \text{and} \quad \|\mathbf{M}_r\|_F^2 = \sum_{i=1}^{r} \sigma_i^2$$

SVD dimensionality reduction

- Columns of $\mathbf{V}_r$ form an orthogonal basis of the optimal rank-r subspace because

$$\mathbf{MP} = \mathbf{M}\mathbf{V}_r\mathbf{V}_r^T = \mathbf{U}\mathbf{\Sigma}\underbrace{\mathbf{V}^T\mathbf{V}_r}_{=\mathbf{I}_r}\mathbf{V}_r^T = \mathbf{U}_r\mathbf{\Sigma}_r\mathbf{V}_r^T = \mathbf{M}_r$$

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- **Dimensionality reduction** uses the subspace coordinates

$$\mathbf{M}\mathbf{V}_r = \mathbf{U}_r\mathbf{\Sigma}_r$$

- If $\mathbf{M}$ is centered, this also gives the best possible preservation of pairwise distances ➜ principal component analysis (**PCA**)
  - ☞ but centering is usally omitted in order to maintain sparseness, so SVD preserves vector lengths rather than distances

Scaling SVD dimensions

- Singular values σ_i can be seen as weighting of the latent dimensions, which determines their contribution to

$$\|\mathbf{MV}_r\|_F = \sigma_1^2 + \ldots + \sigma_r^2$$

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- Weighting adjusted by **power scaling** of the singular values:

$$\mathbf{U}_r \mathbf{\Sigma}_r^p = \begin{bmatrix} \vdots & & \vdots \\ \sigma_1^p \mathbf{a}_1 & \cdots & \sigma_r^p \mathbf{a}_r \\ \vdots & & \vdots \end{bmatrix}$$

  - $p = 1$: normal SVD projection
  - $p = 0$: dimension weights equalized
  - $p = 2$: more weight given to first latent dimensions
- Other weighting schemes possible (e.g. skip first dimensions)

SVD projection in R

```
> fact <- svd(S0)         # SVD decomposition of S0
> round(fact$u, 3)        # left singular vectors (columns) = U
> round(fact$v, 3)        # right singular vectors (columns) = V
> round(fact$d, 3)        # singular values = diagonal of Σ
# note that S0 has effective rank 6 because σ7 ≈ 0
> barplot(fact$d ^ 2)     # R^2 contributions

> r <- 2                  # truncated rank-2 SVD
> (U.r <- fact$u[, 1:r])
> (Sigma.r <- diag(fact$d[1:r], nrow=r))
> (V.r <- fact$v[, 1:r])
```

SVD projection in R

```
> (X.r <- S0 %*% V.r)  # project into latent coordinates
> U.r %*% Sigma.r      # same result
> scaleMargins(U.r, cols=fact$d[1:r]) # the wordspace way

> rownames(X.r) <- rownames(S0)         # NB: keep row labels

> S0r <- U.r %*% Sigma.r %*% t(V.r)     # rank-2 matrix approx.
> round(S0r, 3)
# compare with S0: where are the differences?

> round(X.r %*% t(V.r), 3)              # same result
```

☞ see example code for comparison against PCA with centering