13. The Singular-Value Decomposition (SVD) and applications

Last time

- Least-squares problems
- Minimise $\|\mathbf{A} \mathbf{x} \mathbf{b}\|^2$
- Optimization
- Solution via normal equations and QR
- Action of a matrix

Goals for today

- Action of a matrix A
- Eigen-factorisation (eigen-decomposition) for symmetric, square matrix

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- Action of a matrix A
- Eigen-factorisation (eigen-decomposition) for symmetric, square matrix

- Singular-Value Decomposition (SVD)
 - $\hspace{3.5cm} \hbox{\bf Factorisation} \hspace{3.5cm} \hbox{\bf A} = \hbox{\bf U} \Sigma \hbox{\bf V}^{\rm T} \hspace{3.5cm} \hbox{for any } (m \times n) \hbox{ matrix}$
- Applications to understanding and compressing data

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■ What about in higher dimensions?

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- Idea: Look for different special directions: Those associated with different amounts of stretching
- E.g. Which is the direction x with maximal stretching?

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- Equivalently: $\operatorname{argmax}_{\|x\|=1}\|\mathbf{A}\mathbf{x}\|$
- Another optimisation problem
- Also solvable using linear algebra

- Let's study its action on the unit sphere \mathbb{S}^{n-1} in \mathbb{R}^n
- $\blacksquare \ \mathbb{S}^{n-1} := \{ \mathbf{x} \in \mathbb{R}^n : \| \mathbf{x} \|^2 = 1 \}$

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- Key quantities:
 - Lengths σ_i of semi-axes stretches
 - \blacksquare Directions \mathbf{u}_i of stretches

Collaboration I

Understanding the action of a matrix

Assume for now that A is square and invertible.

- Suppose that **y** lies in the *image* of the sphere under A. What can you say about **y**?
- Can you expand this equation to get something more useful?

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- \blacksquare Since $\|x\|^2=1$ we have $\|\mathbf{A}^{-1}\mathbf{y}\|^2=1$
- So $\mathbf{y}^{\mathsf{T}}(\mathsf{A}^{-1})^{\mathsf{T}}\mathsf{A}^{-1}\mathbf{y} = 1$
- Hence $\mathbf{y}^\mathsf{T} \mathsf{S} \mathbf{y} = 1$
- Where $S := (A^{-1})^T (A^{-1})$ is symmetric

Spectral theorem for symmetric matrices

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- Recall the **spectral theorem** for symmetric matrices
- It tells us that S has a basis of orthogonal eigenvectors, q_i, for S:

$$\mathrm{Sq}_i = \lambda_i \mathrm{q}_i$$

Collaboration II

Eigen-factorisation

- Use the spectral theorem to find an equation involving S and a certain matrix that you can construct.
- 2 Hence write down a matrix factorisation of S, i.e. S = ...
- Can you use that to say something about the image vector y?

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- With

$$\Lambda := \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots & \\ & & \lambda_m \end{bmatrix}$$

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■ Hence $S = Q \Lambda Q^\mathsf{T}$ – the eigen-factorisation

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- $\bullet \operatorname{So} \lambda_1 z_1^2 + \dots + \lambda_n z_n^2 = 1$
- \blacksquare Can show $(\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}$ has eigenvalues $\lambda_i>0$ (exercise)

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- Hence **z** lies on an **ellipse**, with semi-axis lengths $\sigma_i := \sqrt{\lambda_i}$
- Thus y lies on a rotated ellipse!

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- ${\bf v}_i$ such that ${\bf A}{\bf v}_i=\sigma_i{\bf u}_i$ are the right singular vectors
- We arrange the singular values in decreasing order: $\sigma_1 \geq \sigma_2 \geq \cdots$

Singular-value decomposition (SVD)

Any $(m \times n)$ matrix A has an SVD:

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathsf{T}} = \sum_{i} \sigma_{i} \mathbf{u}_{i} \mathbf{v}_{i}^{\mathsf{T}}$$

- \blacksquare the columns of \cup are \mathbf{u}_i
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- lacksquare Σ is diagonal matrix with σ_i on diagonal

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- But any matrix has an SVD
- The CVD is often more useful then an eigen featerisation

Collaboration III

Calculating the SVD

1 How could you *calculate* the SVD, using what we have seen so far in the course?

- We can calculate the SVD
- There are more efficient algorithms that are beyond the scope of the course

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- Form $B := A^T A$
- Calculate the eigenvalues and eigenvectors of the symmetric matrix B
- Do the same for $C := AA^T$
- Exercise: Relate these to the singular values and singular vectors of A

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- The SVD gives as information about the action of a matrix
- **E**.g. the **rank** of a matrix is the dimension of the *image* of \mathbb{R}^n (i.e. the column rank)
- This is given by the number of non-zero singular values!
- Usually floating-point round-off error will make the singular values non-zero
- So we need to look at the numerical rank
 - the number of "non-zero" singular values above a threshold

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- We first de-mean the data (subtract the mean from each component)
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lacktriangle For a data matrix the SVD gives the best approximation by a k-dimensional subspace

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- This is basically asking for the numerical rank!

La The Singular-Value Decomposition (SVD)

PCAII

■ Calculate the SVD

PCA II

- Calculate the SVD
- Plot the "importance" of each direction

$$\sigma_i$$
 or σ_i^2 or $\frac{\sigma_i^2}{\sum_j \sigma_j^2}$

as a function of i

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 or σ_i^2 or $\frac{\sigma_i^2}{\sum_j \sigma_j^2}$

as a function of i

- Called a "scree plot"
- It often has an "elbow" after which the σ_i are small
- lacktriangle This helps to choose the k for the low-rank approximation

$$\mathsf{A}_k := \sum_{i=1}^k \sigma_i \mathsf{u}_i \mathsf{v}_i^{\mathsf{T}}$$

Summary

- The SVD decomposes the action of a matrix
 - rotation + stretch + rotation
- lacksquare Any (m imes n) matrix A has an SVD

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^\mathsf{T} = \sum_i \sigma_i \mathbf{u}_i \mathbf{v}_i^\mathsf{T}$$

■ The SVD is closely related to the eigen-factorisation of the symmetric matrices A^TA and AA^T

Applications to analysing and compressing data