Lecture 8: The Curse of Dimensionality

Attendance code: 3MQWR9DH

Iain Styles

5 November 2018

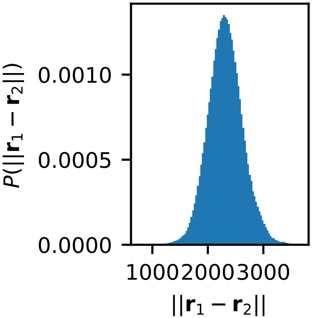
Learning Outcomes

By the end of this lecture you should:

- Understand why the dimensionality of data can be reduced without losing information
- Understand and explain the properties of high dimensional random vectors
- Explain the implications of the Johnson-Lindesnstrauss lemma
- Reduce the dimensionality of a dataset using random projections

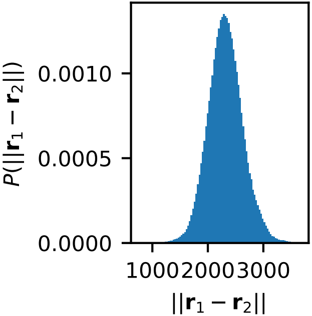
Distances in MNIST

- 1000 points from the test set and 1000 points from the training set



Distances in MNIST

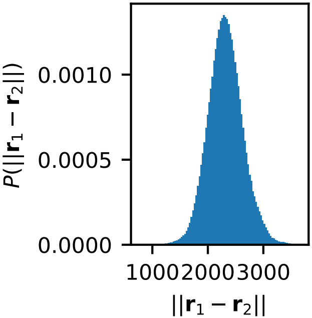
- 1000 points from the test set and 1000 points from the training set



- Mean/median of ≈ 2300 and a standard deviation of ≈ 300.
- 68% of pairwise distances lie between 2000 and 2600, and 95% between 1700 and 2900.

Distances in MNIST

- 1000 points from the test set and 1000 points from the training set



- Mean/median of ≈ 2300 and a standard deviation of ≈ 300.
- 68% of pairwise distances lie between 2000 and 2600, and 95% between 1700 and 2900.
- Not as "bad" as we might expect? Why?

Characteristics of "real" data

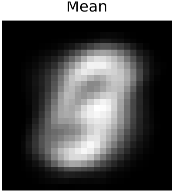
- Data is not uniformly distributed

Characteristics of "real" data

- Data is not uniformly distributed
- Lies on some low-dimensional structure embedded in the high-dimensional space.

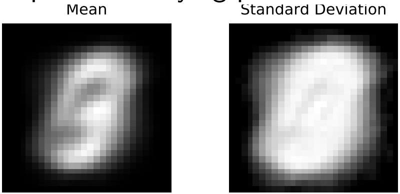
Characteristics of "real" data

- Data is not uniformly distributed
- Lies on some low-dimensional structure embedded in the high-dimensional space.
- Example: non-varying pixels in MNIST



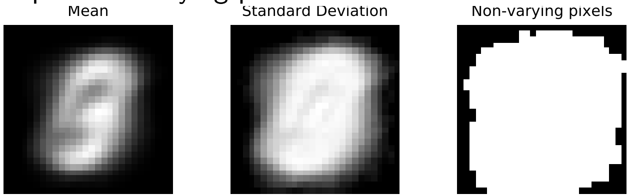
Characteristics of "real" data

- Data is not uniformly distributed
- Lies on some low-dimensional structure embedded in the high-dimensional space.
- Example: non-varying pixels in MNIST



Characteristics of "real" data

- Data is not uniformly distributed
- Lies on some low-dimensional structure embedded in the high-dimensional space.
- Example: non-varying pixels in MNIST



- 175 pixels (22%) do not vary and can be ignored.

Intrinsic Dimensionality

- More generally, low-dimensional structure can be bent into high-dimensional objects

Intrinsic Dimensionality

- More generally, low-dimensional structure can be bent into high-dimensional objects
- A rolled-up poster (intrinsically 2d); cooked spaghetti (1d)

Intrinsic Dimensionality

- More generally, low-dimensional structure can be bent into high-dimensional objects
- A rolled-up poster (intrinsically 2d); cooked spaghetti (1d)
- MNIST digits have intrinsic (underlying) degree of freedom
  - Ten digit class.
  - Width and height
  - Minor shape variation (1 vs 1)
- A few ten's of intrinsic variables
- How do we extract them?

Dimensionality Reduction

- Limit to *linear* methods: single, global linear transformation.
- Aim: find a transformation to a new coordinate system that preserves structure and reduces the dimensionality.
- Hope: that it will mitigate the issues seen in high-dimensional spaces.
- Many methods: PCA, NNMF, LDA
- We will study random projections: simple, low-cost, elegant theory.

Random Projections

- Very simple basic idea
- N samples in M dimensions, arranged as an $M \times N$ matrix $\mathbf{X}$

Random Projections

- Very simple basic idea
- N samples in M dimensions, arranged as an $M \times N$ matrix $\mathbf{X}$
  - Generate K random vectors with M components randomly sampled from $\mathcal{N}(0, 1)$. Arrange these as a matrix $\mathbf{R}$ of size $M \times K$, with one vector per column.

Random Projections

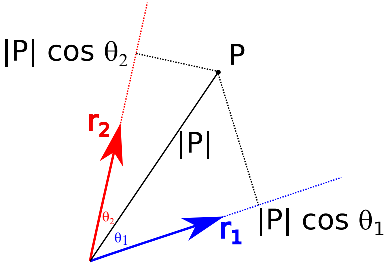
- Very simple basic idea
- N samples in M dimensions, arranged as an $M \times N$ matrix $\mathbf{X}$
  - Generate K random vectors with M components randomly sampled from $\mathcal{N}(0, 1)$. Arrange these as a matrix $\mathbf{R}$ of size $M \times K$, with one vector per column.
  - Normalise the columns of $\mathbf{R}$ so each has unit length.

Random Projections

- Very simple basic idea
- N samples in M dimensions, arranged as an $M \times N$ matrix $\mathbf{X}$
  - Generate K random vectors with M components randomly sampled from $\mathcal{N}(0, 1)$. Arrange these as a matrix $\mathbf{R}$ of size $M \times K$, with one vector per column.
  - Normalise the columns of $\mathbf{R}$ so each has unit length.
  - Compute $\mathbf{X}' = \mathbf{R}^{\mathrm{T}}\mathbf{X}$

Random Projections

- Very simple basic idea
- N samples in M dimensions, arranged as an $M \times N$ matrix $\mathbf{X}$
  - Generate K random vectors with M components randomly sampled from $\mathcal{N}(0, 1)$. Arrange these as a matrix $\mathbf{R}$ of size $M \times K$, with one vector per column.
  - Normalise the columns of $\mathbf{R}$ so each has unit length.
  - Compute $\mathbf{X}' = \mathbf{R}^{\mathrm{T}}\mathbf{X}$
  - The columns of $\mathbf{X}'$ contain the samples projected onto K dimensions



Why does random projection work?

- Distances in large n are of limited use
- Desire to map to a lower-dimensional space to make distances meaningful again
- Map should preserve local structure (nearest-neighbours stay nearest neighbours, etc)

Why does random projection work?

- Distances in large n are of limited use
- Desire to map to a lower-dimensional space to make distances meaningful again
- Map should preserve local structure (nearest-neighbours stay nearest neighbours, etc)
- Key: The **Johnson-Lindenstrauss lemma**
- Given a set X of N data points in $\mathbb{R}^M$...

Why does random projection work?

- Distances in large n are of limited use
- Desire to map to a lower-dimensional space to make distances meaningful again
- Map should preserve local structure (nearest-neighbours stay nearest neighbours, etc)
- Key: The **Johnson-Lindenstrauss lemma**
- Given a set X of N data points in $\mathbb{R}^M$...
- There is a linear map $f : \mathbb{R}^M \mapsto \mathbb{R}^K$ where $K < M$

Why does random projection work?

- Distances in large n are of limited use
- Desire to map to a lower-dimensional space to make distances meaningful again
- Map should preserve local structure (nearest-neighbours stay nearest neighbours, etc)
- Key: The **Johnson-Lindenstrauss lemma**
- Given a set X of N data points in $\mathbb{R}^M$...
- There is a linear map $f : \mathbb{R}^M \mapsto \mathbb{R}^K$ where $K < M$
- The map obeys

$$(1-\varepsilon)\|x_1 - x_2\|^2 \leq \|f(x_1) - f(x_2)\|^2 \leq (1+\varepsilon)\|x_1 - x_2\|^2$$

for all $x_1, x_2 \in X$ and for $0 < \varepsilon < 1$ and $K > 8\ln(N)/\varepsilon^2$.

Interpreting Johnson-Lindenstrauss

- Helpful to rewrite as

$$1 - \varepsilon \leq \frac{\|f(x_1) - f(x_2)\|^2}{\|x_1 - x_2\|} \leq 1 + \varepsilon \tag{1}$$

Interpreting Johnson-Lindenstrauss

- Helpful to rewrite as

$$1 - \varepsilon \leq \frac{\|f(x_1) - f(x_2)\|^2}{\|x_1 - x_2\|} \leq 1 + \varepsilon \tag{1}$$

- Clarifies that J-L is a a statement about *relative* distances.
- The map f preserves relative distances to a range $1 \pm \varepsilon$
- Since $K > 8\ln(N)/\varepsilon^2$, smaller ε requires larger K.

Finding the map f

- J-L states that the linear map $f : \mathbb{R}^M \mapsto \mathbb{R}^K$ is onto a *random subspace*.
- Refinement by Frankl and Maehara (2008) states that J-L holds when "f is a random, orthonormal linear transformation"
- Random? ✓
- Linear? ✓
- Orthonormal?

Finding the map f

- J-L states that the linear map $f : \mathbb{R}^M \mapsto \mathbb{R}^K$ is onto a *random subspace*.
- Refinement by Frankl and Maehara (2008) states that J-L holds when "f is a random, orthonormal linear transformation"
- Random? ✓
- Linear? ✓
- Orthonormal?
- Normalisation ($\mathbf{r}_i \cdot \mathbf{r}_i = 1$) is easy
- Orthogonality ($\mathbf{r}_i \cdot \mathbf{r}_j = 0,\ i \neq j$) is less so - can be costly

Finding the map f

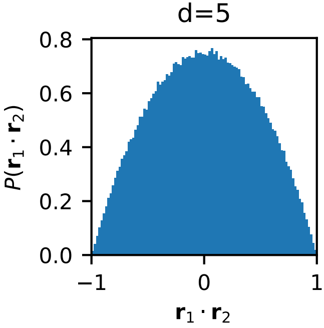
- J-L states that the linear map $f : \mathbb{R}^M \mapsto \mathbb{R}^K$ is onto a *random subspace*.
- Refinement by Frankl and Maehara (2008) states that J-L holds when "f is a random, orthonormal linear transformation"
- Random? ✓
- Linear? ✓
- Orthonormal?
- Normalisation ($\mathbf{r}_i \cdot \mathbf{r}_i = 1$) is easy
- Orthogonality ($\mathbf{r}_i \cdot \mathbf{r}_j = 0$, $i \neq j$) is less so - can be costly
- The curse of dimensionality to the rescue. . . !

Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram

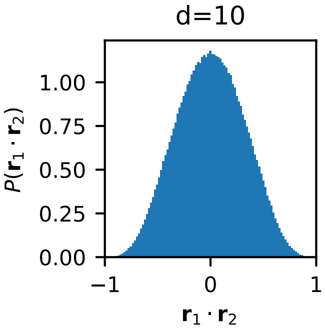
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \to \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



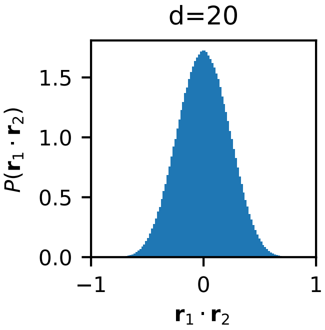
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



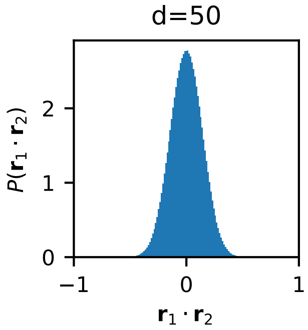
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



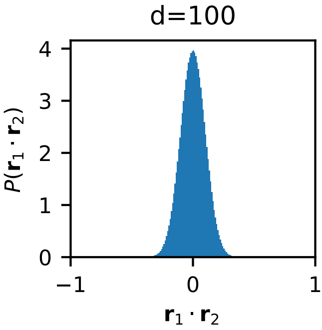
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



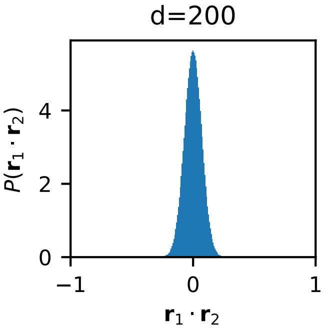
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



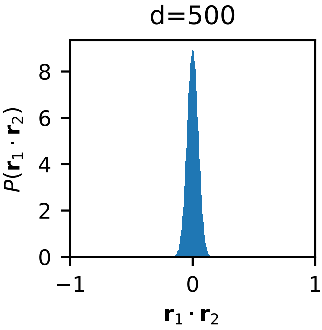
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \to \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



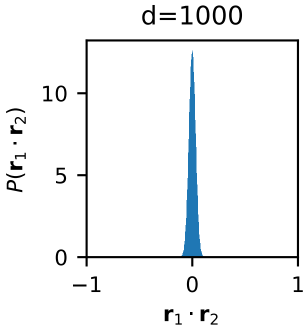
Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



Orthogonality of Random Vectors

- $\mathbf{r}_i \cdot \mathbf{r}_j = 0 \rightarrow \theta = 90^\circ$
- Generate 100,000 normalised random vectors of different dimensionality
- Compute the angle between each pair $(\mathbf{r}_i \cdot \mathbf{r}_j)$, plot histogram



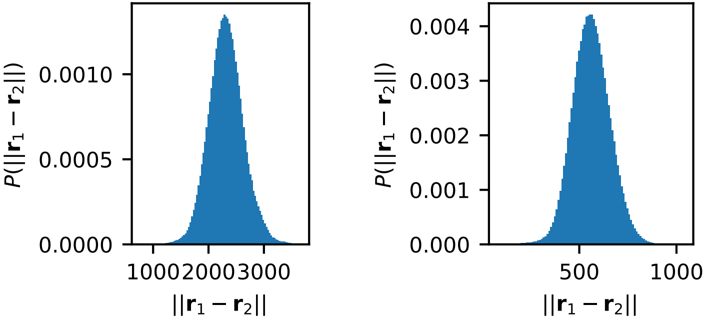
Orthogonality of Random Vectors

- Random vectors in high dimensions are (nearly) orthogonal!

Orthogonality of Random Vectors

- Random vectors in high dimensions are (nearly) orthogonal!
- So no need to explicitly orthogonalise
- Means random projection is very cheap indeed!

Effect on MNIST Data



- Absolute distances reduced
- Relative distances preserved to with factor ≈ 3

Summary

- Problems in high dimensions
- One way for overcoming them

Summary

- Problems in high dimensions
- One way for overcoming them
- Next time: pushing the performance limits
- An alternative generative approach to classification