Unsupervised Learning

ACTL3142 & ACTL5110 Statistical Machine Learning for Risk Applications

Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

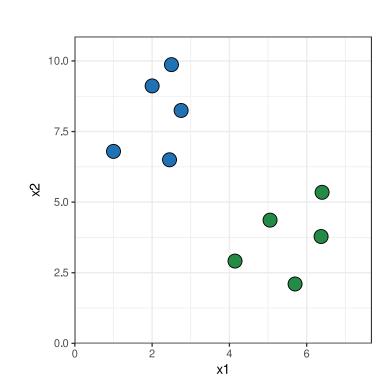


Lecture Outline

- Unsupervised Learning
- *K*-Means Clustering
- Demo: MNIST
- Hierarchical Clustering
- Dimension Reduction
- Demo: PCA on MNIST

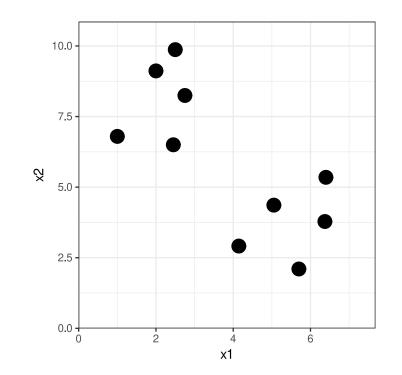


Supervised vs Unsupervised Learning



Supervised

Unsupervised



- Data: X_1, X_2, \ldots, X_p, Y
- Goal: Predict Y using X_1, X_2, \ldots, X_p
- Data: $X_1, X_2, ..., X_p$
- Goal: Discover interesting things using X_1, X_2, \ldots, X_p



Challenge of Unsupervised Learning

- Typical questions
 - Is there an informative way to visualize the data?
 - Can we discover subgroups among the variables?
- More subjective than supervised learning
 - There's no simple goal for the analysis
- Hard to assess the results obtained from unsupervised learning methods
 - There's no way to validate your results on an independent data set

Clustering vs. PCA

- Both seek to simplify the data via a small number of summaries
- Different mechanisms
 - Clustering: find homogeneous subgroups among the observations
 - PCA: find a low-dimensional representation of the observations that explain a good fraction of the variance
- Both useful for visualisation



Clustering Methods

- A very broad set of techniques for finding subgroups, or clusters, in a data set
- The observations within each group are quite similar to each other
- Need to specify what it means for two or more observations to be similar or different (often domain-specific)
- Two clustering methods
 - *K*-means clustering
 - partition the observations into a pre-specified number of clusters
 - Hierarchical clustering
 - do not know in advance how many clusters we want
 - creates a *dendrogram*, a tree representation of clusters (for K = 1, 2, 3, ..., n)



Applications of Clustering

- Market segmentation
- Fraud detection
- Group patients by medical condition (e.g types of diabetes)
- Clustering of documents by type
- Compression of information (e.g. representative policies in a portfolio)

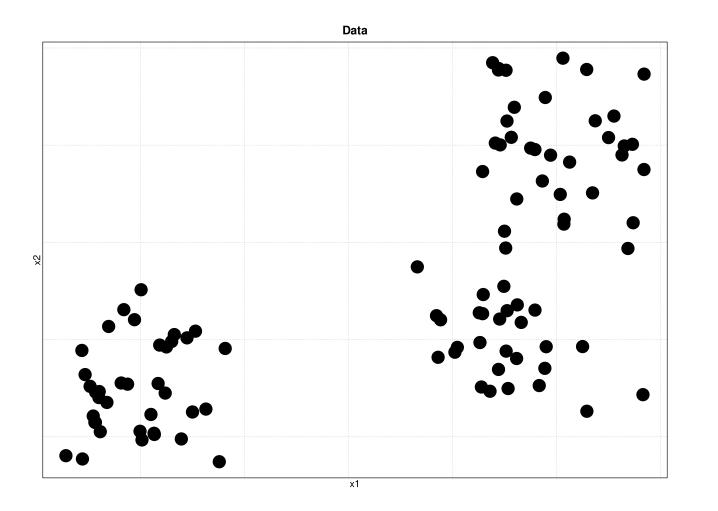


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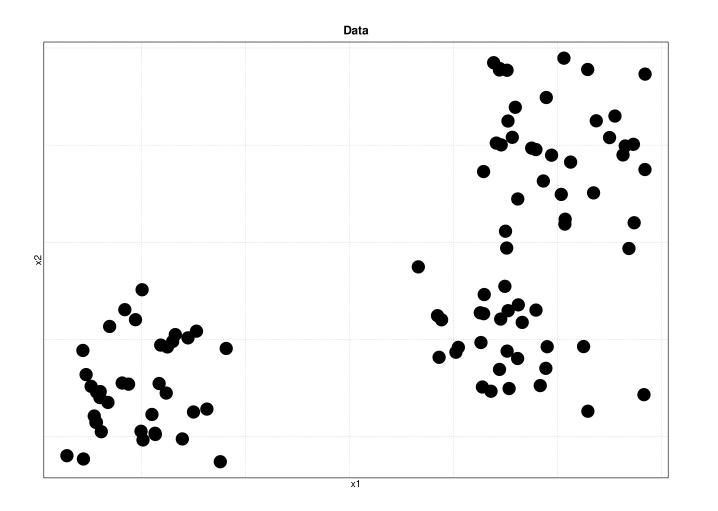
K-means clustering: Demonstration I







K-means clustering: Demonstration II

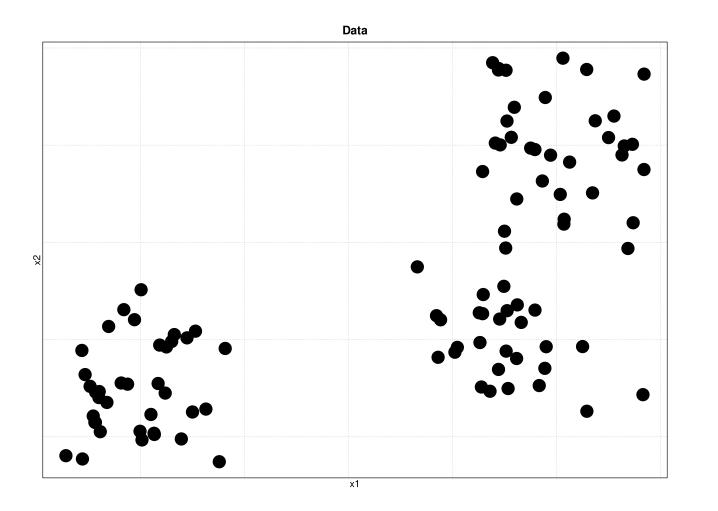






7 / 56

K-means clustering: Demonstration III







K-Means Clustering

Denote C_1, \ldots, C_K as the sets containing the indices of the observations in each cluster. Each observation belongs to at least one of the *K* clusters

```
C_1 \cup C_2 \cup \cdots \cup C_K = \{1, \ldots, n\}.
```

The clusters are non-overlapping; no observation belongs to more than one cluster

 $C_k\cap C_{k'}=\emptyset \ ext{ for all } k
eq k'.$



Mathematical formulation: Clustering

A good clustering is one for which the within-cluster variation is as small as possible

$$\min_{C_1,\ldots,C_K}\sum_{k=1}^K W(C_k).$$

The most common choice of $W(\cdot)$

$$W(C_k) = rac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^p (x_{ij} - x_{i'j})^2$$

where $|C_k|$ is the number of observations in the *k*th cluster.

It turns out that

$$W(C_k) = 2\sum_{i \in C_k} \sum_{j=1}^p (x_{ij} - ar{x}_{kj})^2$$

where \bar{x}_k is the mean of the observations in the kth cluster, a.k.a. the *centroid*.



9/56

K-Means algorithm

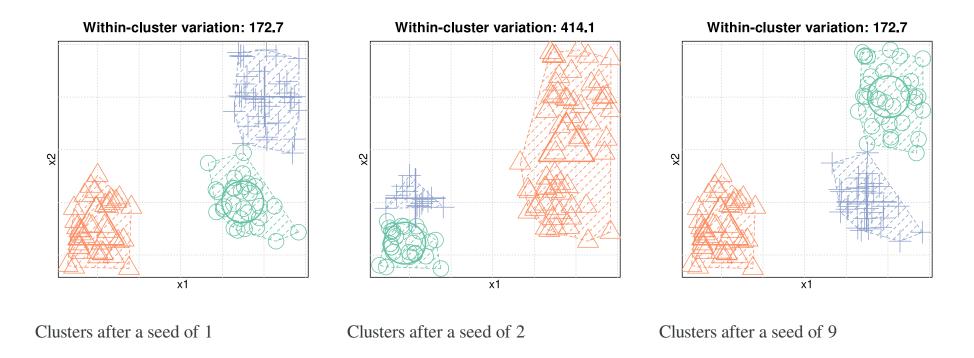
The optimisation problem that defines K-means clustering is

$$\min_{C_1,\ldots,C_k}\sum_{k=1}^K rac{1}{|C_k|}\sum_{i,i'\in C_k}\sum_{j=1}^p (x_{ij}-x_{i'j})^2.$$

It's a difficult problem to solve precisely, but we have a very simple algorithm that provides a local optimum:

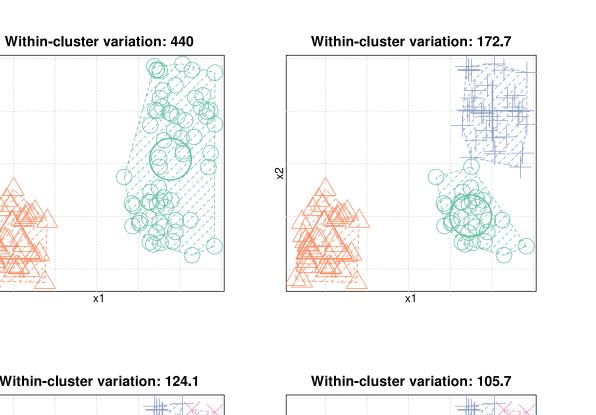
- 1. Randomly initialise K cluster centres/centroids
- 2. Assign each observation to the cluster whose centroid is closest
 - "Closest" is defined using Euclidean distance
- 3. For each of the K clusters, compute the cluster centroid
 - The "centroid" is the vector of the means for the observations in the kth cluster
- 4. Repeat 2 & 3 until convergence

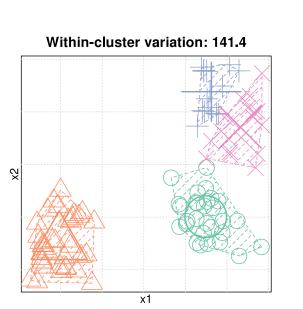
K-means clustering: Local Optima



- The algorithm finds a local rather than a global optimum
- Results depend on initial centroids used
- Important to run the algorithm multiple times and select the best solution (minimum within-cluster variation)



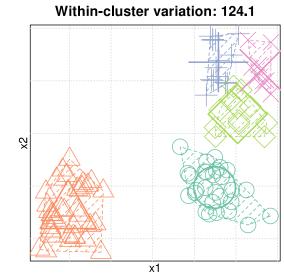




x1

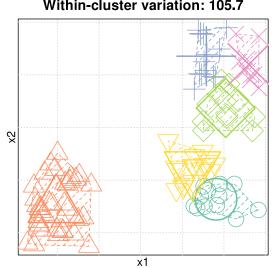
Within-cluster variation: 2022

ХX



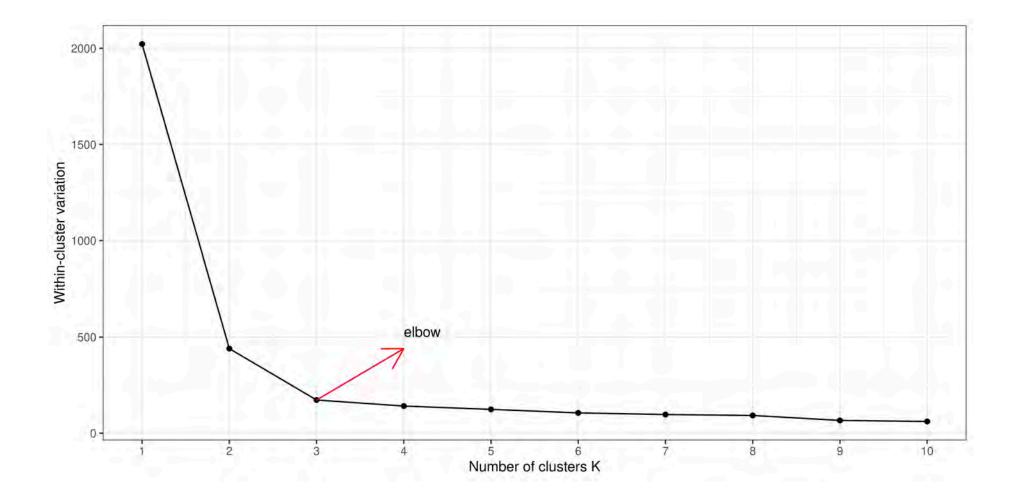
x1

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What is the right value of *K*?



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The data

R Python

- 1 train_df <- read.csv("mnist_train.csv")</pre>
- 2 train_df

A tibble: 60,000 × 785

	X0	X1	X2	ХЗ	X4	X5	X6	X7	X8	X9	X10	X11	X12	
	<dbl></dbl>													
1	0	0	0	0	0	0	0	0	0	0	0	0	0	
2	0	Θ	0	0	0	0	0	0	0	0	0	0	0	
3	0	Θ	0	0	0	Θ	0	0	0	0	0	Θ	0	
4	0	0	0	0	0	0	0	0	0	0	0	0	0	
5	0	0	0	0	0	0	0	0	0	0	0	0	0	
6	0	0	0	0	0	0	0	0	0	0	0	0	0	
7	0	0	0	0	0	0	0	0	0	0	0	0	0	
8	0	Θ	0	Θ	Θ	Θ	Θ	Θ	0	Θ	Θ	Θ	0	
9	0	0	0	0	0	0	0	0	0	0	0	0	0	
10	0	Θ	0	0	0	Θ	0	0	0	0	0	Θ	0	
		o												

i 59,990 more rows

- # i 772 more variables: X13 <dbl>, X14 <dbl>, X15 <dbl>, X16 <dbl>, X17 <dbl>,
- # X18 <dbl>, X19 <dbl>, X20 <dbl>, X21 <dbl>, X22 <dbl>, X23 <dbl>,
- # X24 <dbl>, X25 <dbl>, X26 <dbl>, X27 <dbl>, X28 <dbl>, X29 <dbl>,
- # X30 <dbl>, X31 <dbl>, X32 <dbl>, X33 <dbl>, X34 <dbl>, X35 <dbl>,
- # X36 <dbl>, X37 <dbl>, X38 <dbl>, X39 <dbl>, X40 <dbl>, X41 <dbl>,
- # X42 <dbl>, X43 <dbl>, X44 <dbl>, X45 <dbl>, X46 <dbl>, X47 <dbl>, ...

Only 19% of the data is non-zero.

Which is the odd one out?

X479 X480 X481 X482 X483 X484 X485 X486 X487 0 0 4 7 0 Θ 0 0.01960784 0.5294118 0.9882353 0.9882353 0.7058824 0.0627451 6 0 0 X489 X490 X491 X492 X493 X494 X488 7 0.0000000 0.99215686 0.9882353 0.9882353 0.9882353 0.1647059 0.0000000 6 0.0000000 0.08235294 0.7960784 0.9921569 0.9686274 0.5058824 0.6784314 X495 X496 X497 X498 X499 6 0.9882353 0.9882353 0.7215686 0.2588235 0.1921569

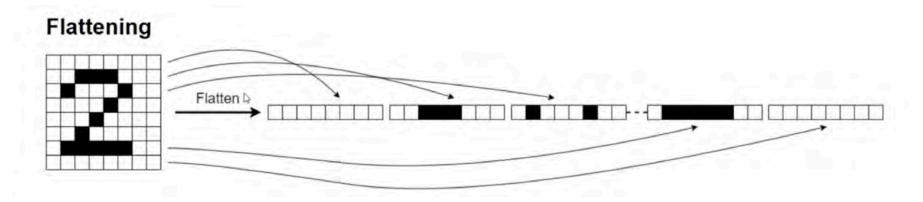


MNIST Dataset



Source: Wikipedia, MNIST database.

The data is flattened



An image turned into a vector.

["]

Preparation

Take just a fraction of the data, and make a plotting function.

R Python 1 # Separate the features and the labels 2 x <- as.matrix(train_df[, -785])</pre> 3 y <- train_df\$label 4 5 # Split the data into train/validation and te 6 set.seed(88) 8 test_indices <- sample(1:nrow(x),</pre> size = 0.2*nrow(x)) 9 10 x_test <- x[test_indices,]</pre>

11 y_test <- y[test_indices]</pre> 12 x_train_val <- x[-test_indices,]</pre> 13 y_train_val <- y[-test_indices]</pre> 14 15 train_indices <- sample(1:nrow(x_train_val),</pre> size = 0.75*nrow(x_train_val)) 16 17 x_train <- x_train_val[train_indices,]</pre> 18 y_train <- y_train_val[train_indices]</pre>

- 19 x_val <- x_train_val[-train_indices,]</pre>
- 20 y_val <- y_train_val[-train_indices]</pre>

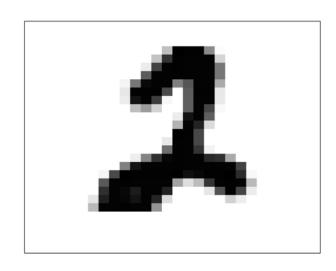
plot_digit(x_train[1,]) 1

Python

R

1:28

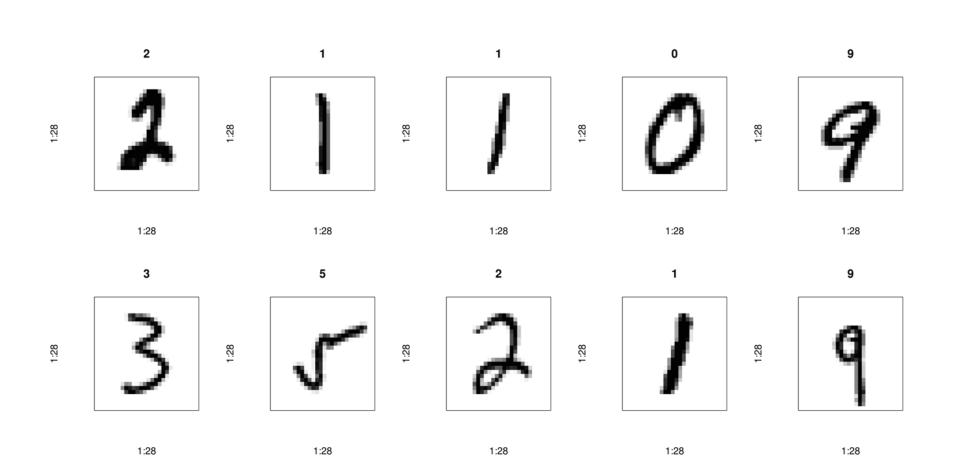
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Plotting the data

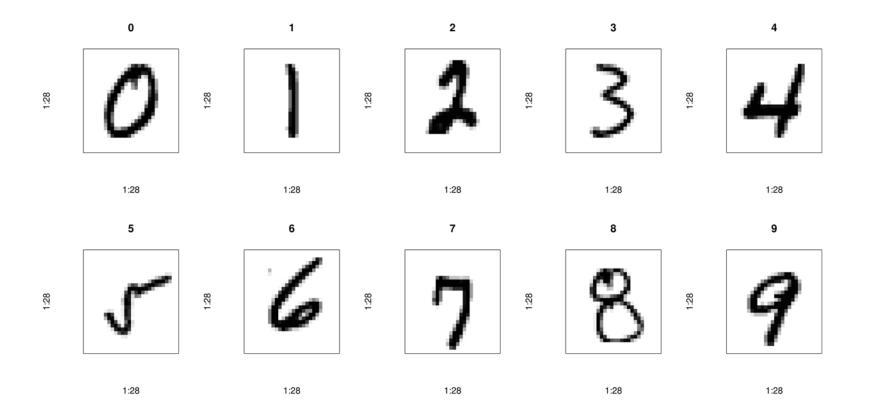
R Python





There are 10 natural clusters

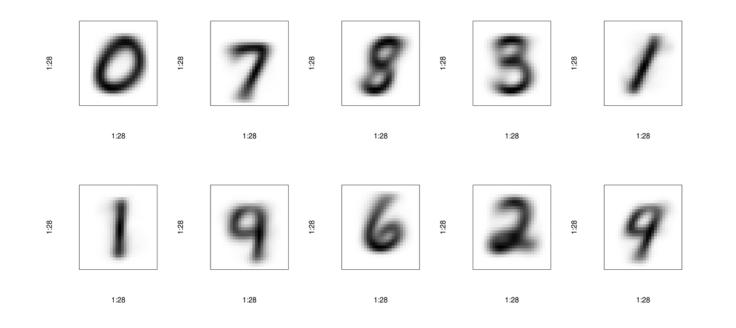
```
1 # Plot one of each digit
2 par(mfrow = c(2,5))
3 for (i in 0:9) {
4     plot_digit(x_train[y_train == i,][1,])
5     title(i)
6 }
```



K-means Clustering on MNIST I

1 set.seed(1)

2 kmeans_out <- kmeans(x_train, centers = 10)</pre>



The within-cluster variation is

1 kmeans_out\$tot.withinss

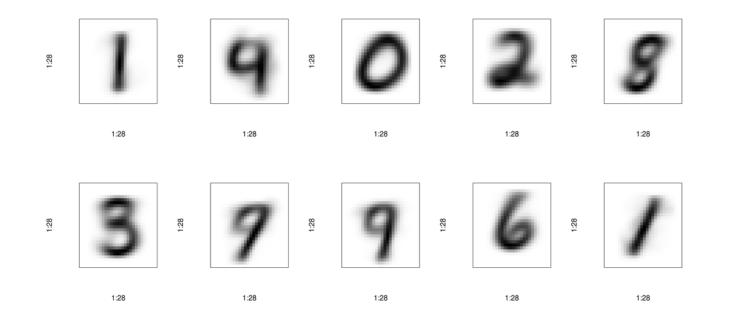


[1] 1413762

K-means Clustering on MNIST II

1 set.seed(2)

2 kmeans_out <- kmeans(x_train, centers = 10)</pre>



The within-cluster variation is

1 kmeans_out\$tot.withinss

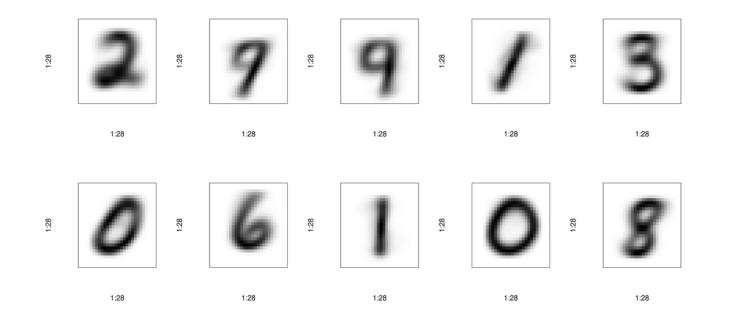


[1] 1410923

K-means Clustering on MNIST III

1 set.seed(3)

2 kmeans_out <- kmeans(x_train, centers = 10)</pre>



The within-cluster variation is

1 kmeans_out\$tot.withinss

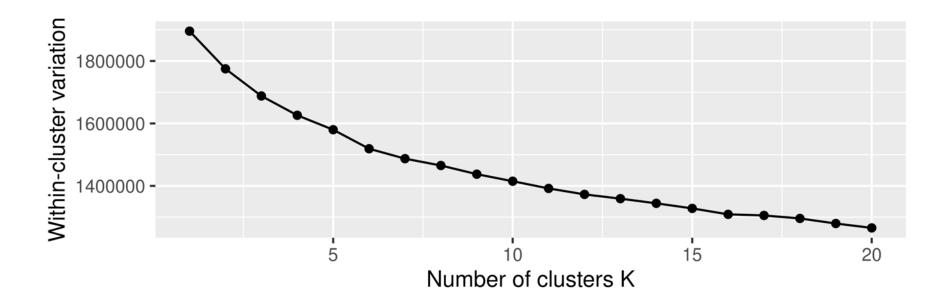


[1] 1410441

Elbow method MNIST I

R Python

1 wss <- rep(0, 20)
2 for (k in 1:20) {
3 kmeans_out <- kmeans(x_train, centers = k)
4 wss[k] <- kmeans_out\$tot.withinss
5 }</pre>

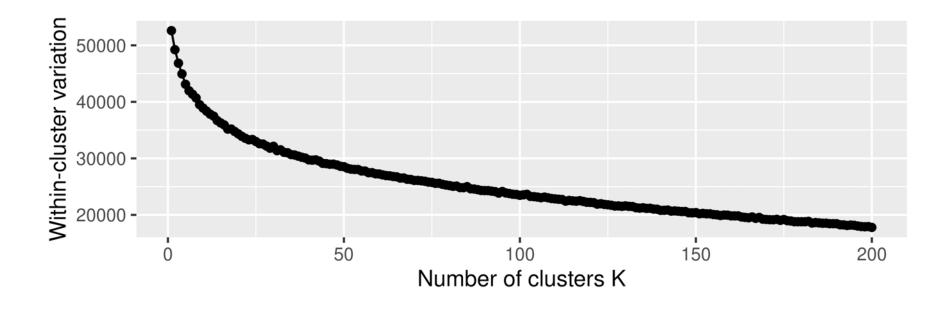




Elbow method MNIST II

R Python

1 wss <- rep(0, 200)
2 x_tiny_subset <- x_train[1:1000,]
3 for (k in 1:200) {
4 kmeans_out <- kmeans(x_tiny_subset, centers = k)
5 wss[k] <- kmeans_out\$tot.withinss
6 }</pre>





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Hierarchical Clustering

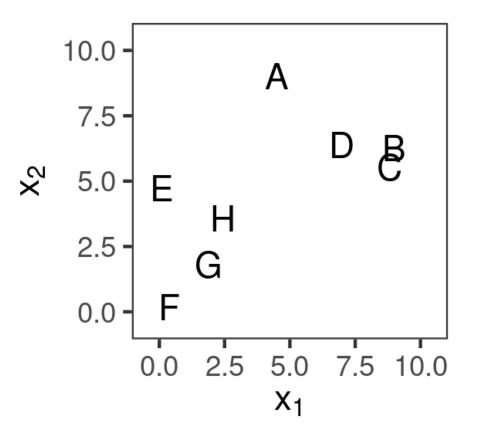
- No need to specify the number of clusters K
- Result is a tree-based representation, called a dendrogram
- Allows user to choose any distance metric
 - *K*-means restricted us to Euclidean distance
- Focus on bottom-up or agglomerative clustering
 - start from the leaves
 - combine the clusters up to the trunk

Algorithm:

- 1. Treat each of the n observations as its own cluster
- 2. For $i = n, n 1, \dots, 2$:
 - 1. Compute the pairwise inter-cluster dissimilarities among the i clusters
 - 2. Identify the pair of clusters that are least dissimilar and merge them



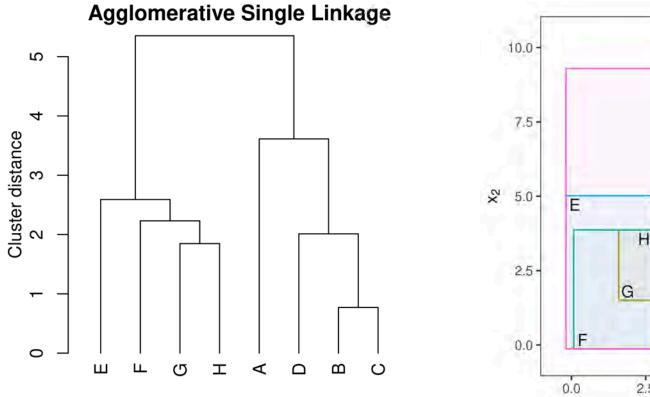
Hierarchical Agglomerative Clustering

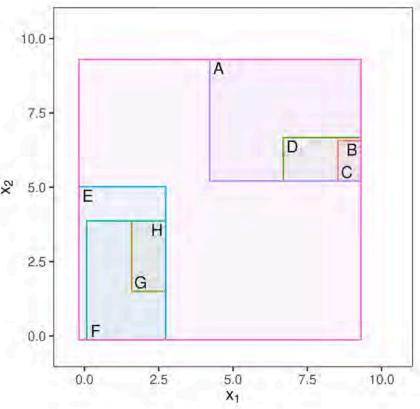


Example of agglomerative clustering (with single linkage).



Hierarchical Clustering: The dendogram



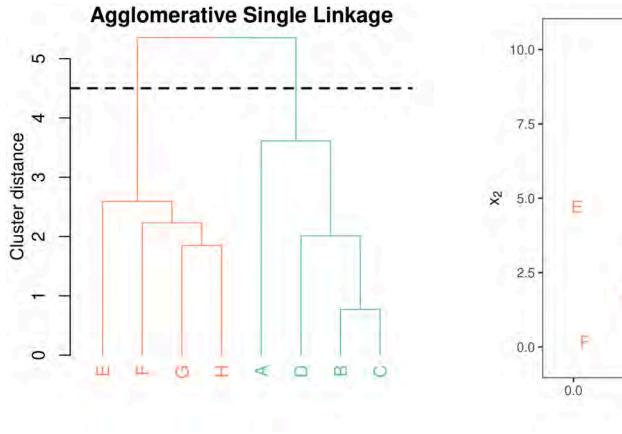


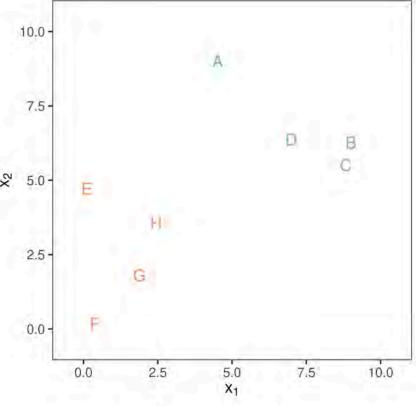
Dendogram

Clusters



Choose a max distance I

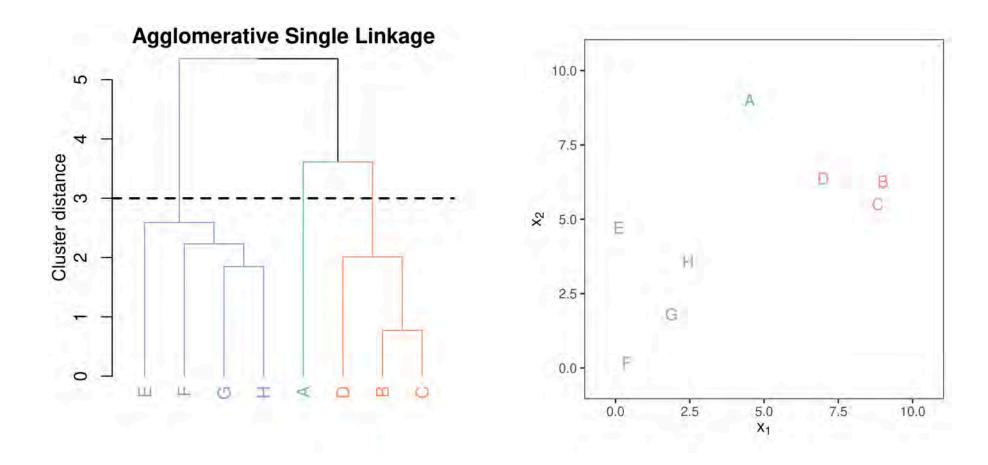




K = 2 clusters



Choose a max distance II



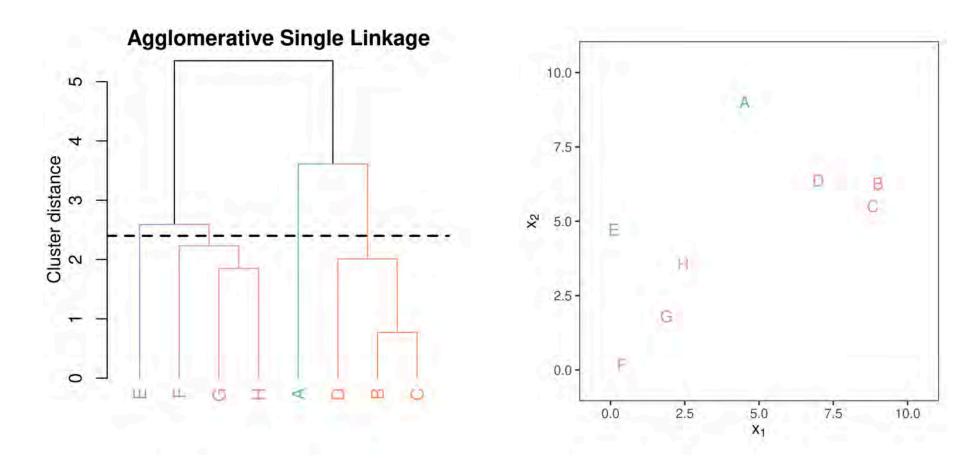


K = 3 clusters





Choose a max distance III





K = 4 clusters



Choice of Dissimilarity Measure

• Euclidean distance

$$\sqrt{\sum_{j=1}^p (x_{ij}-x_{i'j})^2}$$

• Simple matching

$$rac{1}{p}\sum_{j=1}^p I(x_{ij}
eq x_{i'j})$$

• Manhattan distance

$$\sum_{j=1}^p |x_{ij}-x_{i'j}|$$

• Combination of numerical and categorical?

Note that we need to consider how to compare groups as well.



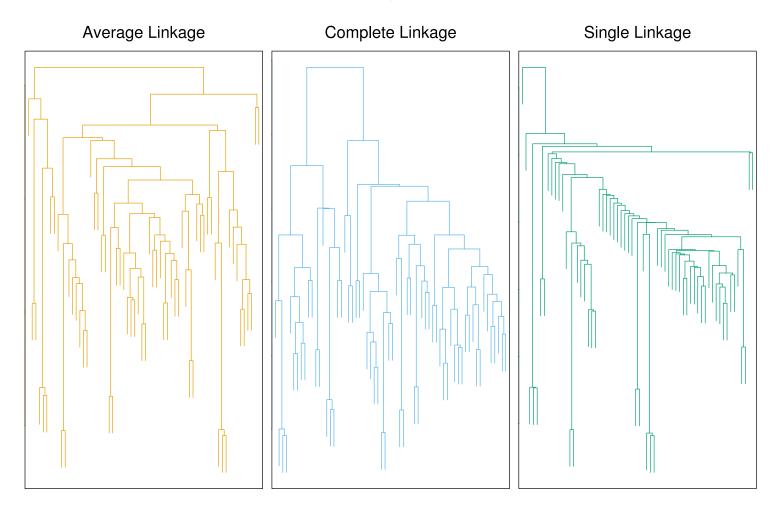
Distance between clusters (linkage)

- Complete
 - maximal inter-cluster dissimilarity
 - compute all pairwise dissimilarities between clusters A and B and take largest.
- Single
 - minimal inter-cluster dissimilarity
 - compute all pairwise dissimilarities between clusters A and B and take smallest.

- Average
 - mean inter-cluster dissimilarity
 - compute all pairwise dissimilarities between clusters A and B and take average.
- Centroid
 - dissimilarity between the centroid for cluster A (a mean vector of length *p*) and the centroid for cluster B
 - an inversion can occur



Same Data, Different Linkage



Average, complete, and single linkage applied to an example data set. Average and complete linkage tend to yield more balanced clusters.

Source: James et al. (2021), An Introduction to Statistical Learning, Figure 12.14.



Practical Issues

- Should the observations / features be standardised in some way?
- Hierarchical clustering
 - dissimilarity measure?
 - type of linkage?
 - where to cut the dendrogram?
- *K*-means clustering
 - how many clusters?
- Validate the clusters obtained
 - does the clusters represent true subgroups in the data?
- Robustness
 - Don't rely on one single answer
 - Try different assumptions/data and check consistency of message



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Can you memorise these in 30 secs?

112358132134

248163264128

203048154248



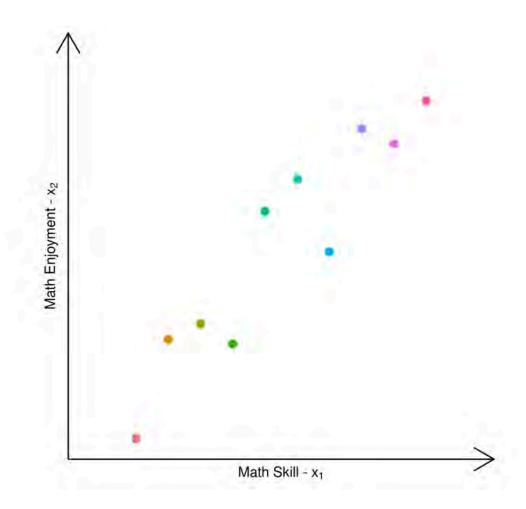
Principal Components Analysis

- Produce derived variables for supervised learning
 - of smaller size than the original data set (i.e. dimension reduction)
 - explain most of the variability in the original set
 - mutually uncorrelated
- A tool for data visualisation

"... our brains are sort of bad at looking at columns of numbers, but absolutely ace at locating patterns and information in a two-dimensional field of vision" Jordan Ellenberg

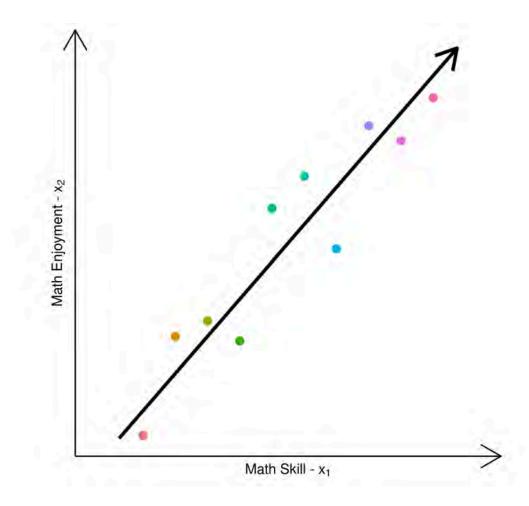


PCA Motivation: Data compression I



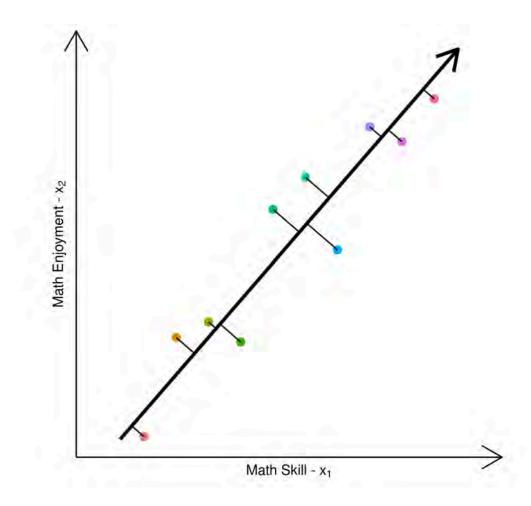


PCA Motivation: Data compression II



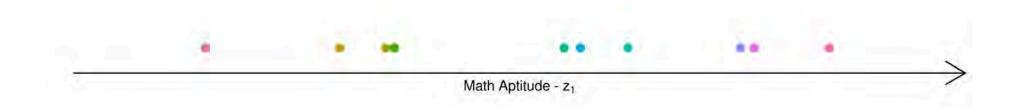


PCA Motivation: Data compression III





PCA Motivation: Data compression IV





38 / 56

PCA Motivation: Data compression V

Reduce data from 2D to 1D

$$egin{aligned} x^{(1)} \in \mathcal{R}^2 & o z^{(1)} \in \mathcal{R} \ x^{(2)} \in \mathcal{R}^2 & o z^{(2)} \in \mathcal{R} \ dots \ dots \ x^{(n)} \in \mathcal{R}^2 & o z^{(n)} \in \mathcal{R} \end{aligned}$$



Principal Components

The first principal component of a set of features X_1, X_2, \ldots, X_p is the normalised linear combination of the features

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \dots + \phi_{p1}X_p, \qquad \sum_{j=1}^p \phi_{j1}^2 = 1$$

that has the largest variance

$\phi_{11},\ldots,\phi_{p1}$	loadings of the first principal component
$\phi_1 = (\phi_{11},\ldots,\phi_{p1})^T$	principal component loading vector
$\sum_{j=1}^p \phi_{j1}^2 = 1$	constraint to prevent an arbitrarily large variance



Further Principal Components

The second principal component is the linear combination of X_1, \ldots, X_p that has maximal variance and are uncorrelated with Z_1

$$z_{i2} = \phi_{12} x_{i1} + \phi_{22} x_{i2} + \dots + \phi_{p2} x_{ip}, \quad i = 1, 2, \dots, n$$

 $\phi_2 = (\phi_{12}, \ldots, \phi_{p2})^T$ is the second principal component loading vector

Geometry of PCA

- The loading vector ϕ_1 defines a direction in feature space along which the data vary the most
- The projection of the *n* data points x_1, \ldots, x_n onto this direction are the principal component scores z_{11}, \ldots, z_{n1}

Is PCA the same as linear regression? Why or why not?

Another Interpretation of PC

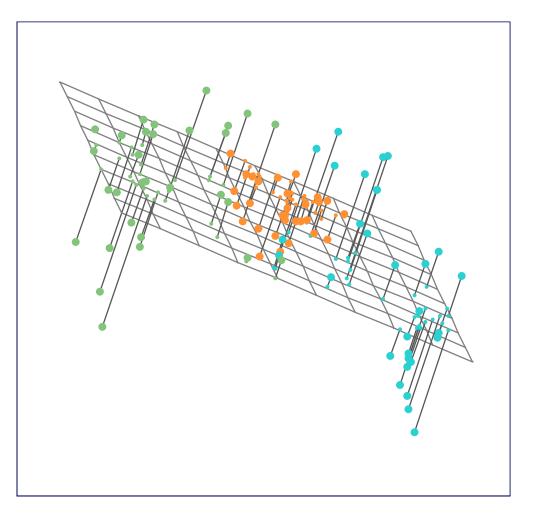
- The first principal component loading vector
 - the line in *p*-dimensional space that is closest to the *n* observations
- Extends beyond the first principal component
 - the first two principal components of a data set span the plane that is closest to the *n* observations
 - the first three principal components of a data set span the hyperplane that is closest to the *n* observations
 - and so forth

In 3 dimensions, first two PCs:

- Plane spans the first two principal component directions.
- Minimises the sum of square distances from each point to the plane.



2 principal component directions I

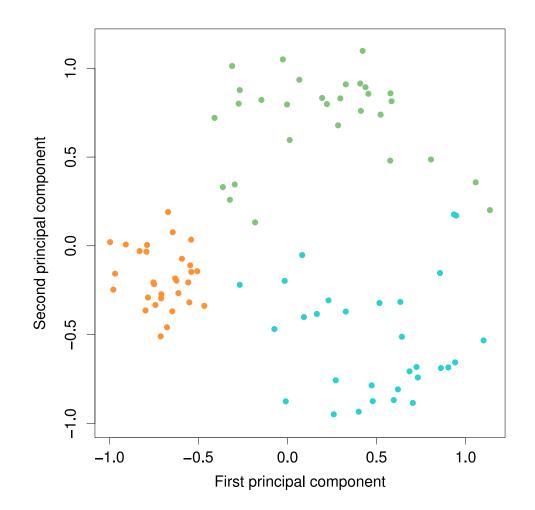


Ninety observations simulated in three dimensions. The observations are displayed in color for ease of visualization. The first two principal component directions span the plane that best fits the data. The plane is positioned to minimize the sum of squared distances to each point.

Source: James et al. (2021), An Introduction to Statistical Learning, Figure 12.2a.

2 principal component directions II

Ļ



The first two principal component score vectors give the coordinates of the projection of the 90 observations onto the plane.

Source: James et al. (2021), An Introduction to Statistical Learning, Figure 12.2b.

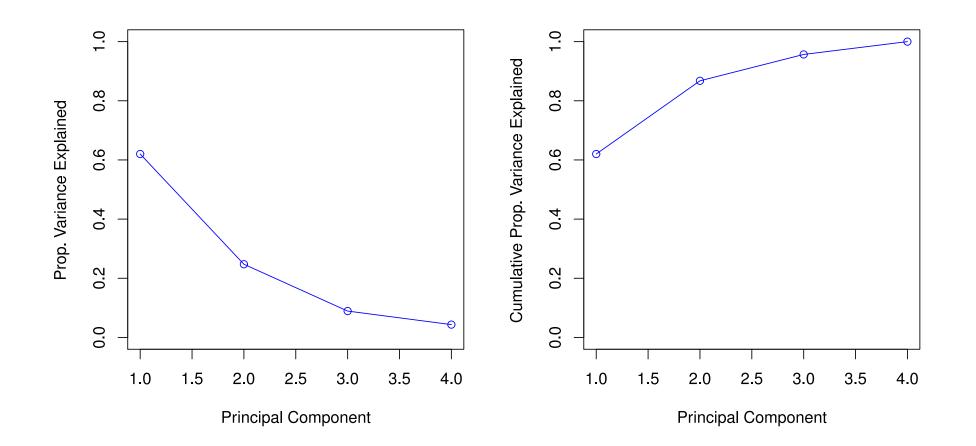
More on PCA

- Scaling the variables
 - typically scale each variable to have standard deviation one before performing PCA
 - may not be necessary if variables are measured in the same units
- Uniqueness of the principal components
 - each principal component loading vector is unique up to a sign flip
- The proportion of variance explained (PVE)
 - the PVE of the *m*th principal component is given by

$$rac{\sum_{i=1}^n \left(\sum_{j=1}^p \phi_{jm} x_{ij}
ight)^2}{\sum_{j=1}^p \sum_{i=1}^n x_{ij}^2}$$



How many principal components to use?



Left: a scree plot depicting the proportion of variance explained by each of the four principal components in the USArrests data. Right: the cumulative proportion of variance explained by the four principal components in the USArrests data.

Source: James et al. (2021), An Introduction to Statistical Learning, Figure 12.3.

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PCA on MNIST (failed attempt)

1 pr_comp_train <- prcomp(x_train, scale = TRUE)</pre>

Error in prcomp.default(x_train, scale = TRUE): cannot rescale a constant/zero column to unit variance

R Python

1 # Calculate the column std devs
2 col_std_devs <- apply(x_train, 2, sd)
3 col_std_devs</pre>

X0	X1	X2	ХЗ	X4	X5
0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
X6	X7	X8	X9	X10	X11
0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
X12	X13	X14	X15	X16	X17
0.0023975438	0.0052497943	0.0000000000	0.0000000000	0.0000000000	0.0000000000
X18	X19	X20	X21	X22	X23
0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
X24	X25	X26	X27	X28	X29
0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
X30	X31	X32	X33	X34	X35
0.0000000000	0.0000000000	0.0000000000	0.0001653479	0.0036899614	0.0073450035
X36	X37	X38	X39	X40	X41
0.0145456588	0.0161569550	0.0211853119	0.0213073459	0.0208507875	0.0195538213
X42	X43	X44	X45	X46	X47
0.0229472506	0.0243856500	0.0230354157	0.0211948495	0.0151041369	0.0109502265
X48	X49	X50	X51	X52	X53
0.0111429515	0.0074043871	0.0041586589	0.0040716909	0.0000000000	0.0000000000
X54	X55	X56	X57	X58	X59
0.0000000000	0.0000000000		0.0000000000	0.0013227829	0.0005993860
X60	X61	X62	X63	X64	X65
0.0015278703	0.0021872664	0.0112660837	0.0184871514	0.0260346078	0.0377863192



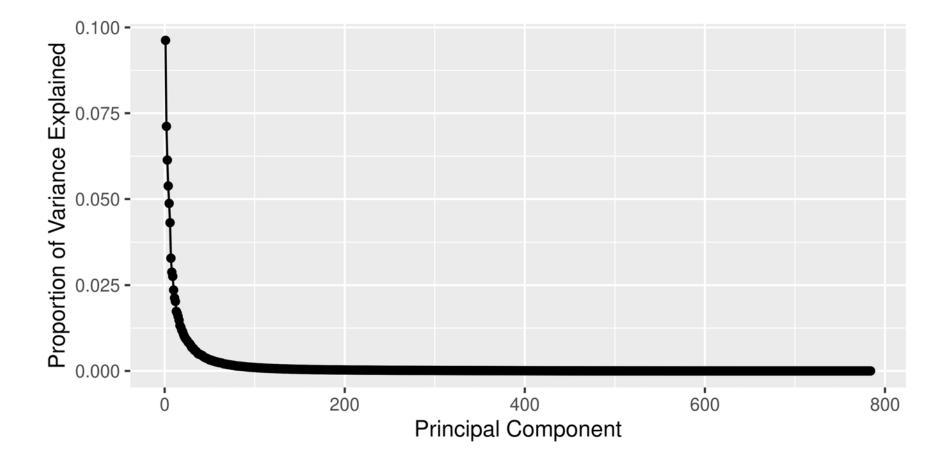
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PCA on MNIST

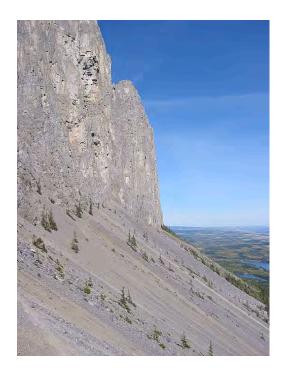
R Python

1 pr_comp_train <- prcomp(x_train)</pre>

2 pve <- pr_comp_train\$sdev^2 / sum(pr_comp_train\$sdev^2)</pre>



Scree plot



A scree plot is a line plot of the eigenvalues of principal components on the y-axis and the factors on the x-axis.

The scree plot is used to determine the number of factors to retain in a principal components analysis.

The point at which the line starts to level off is the number of factors to retain.

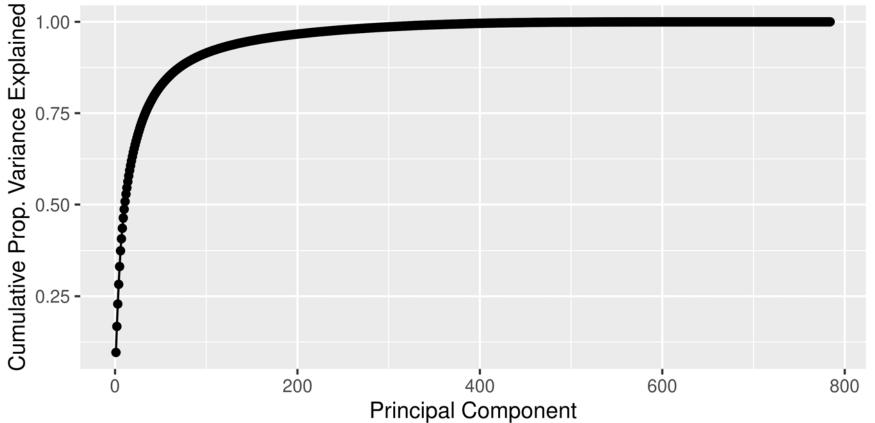
A scree



PCA on MNIST: Cumulative

R Python

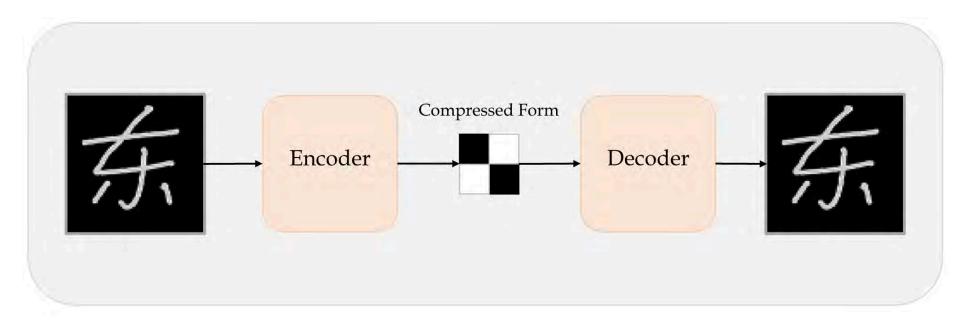
1 cve <- cumsum(pve)</pre>





Autoencoder

An autoencoder takes an observation, maps it to a latent space via an encoder module, then decodes it back to an output with the same dimensions via a decoder module.

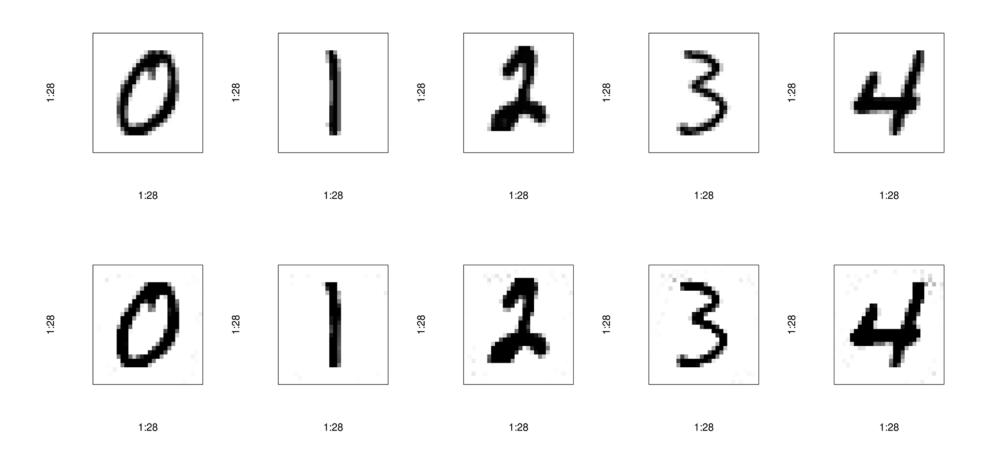


Schematic of an autoencoder.



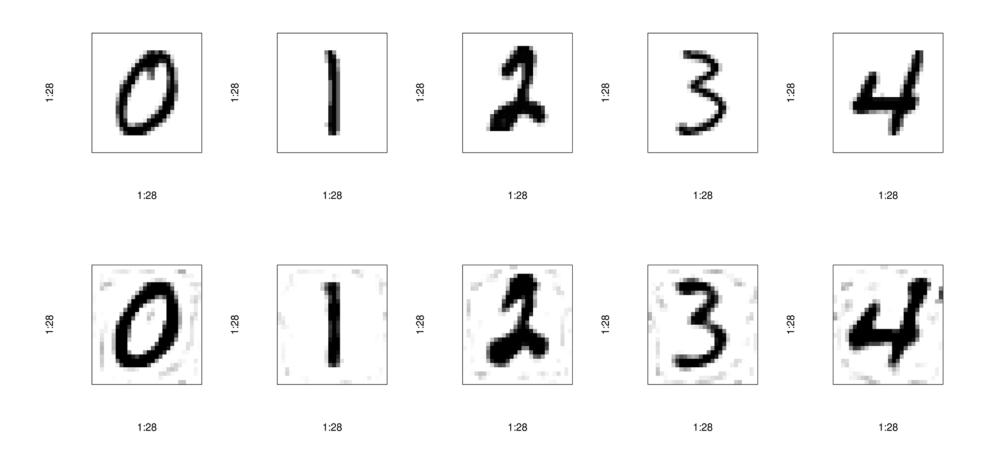
Source: Marcus Lautier (2022).

PCA on MNIST: Reconstructed with 400 PCs



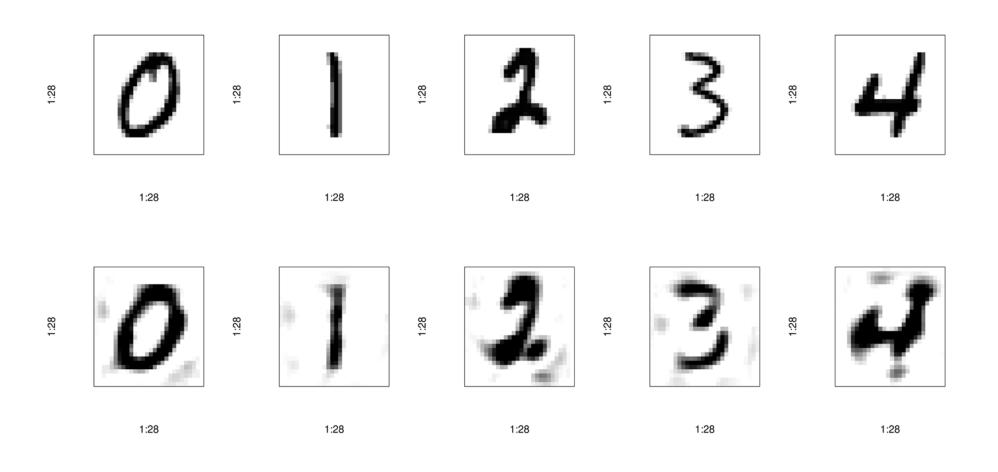


PCA on MNIST: Reconstructed with 100 PCs



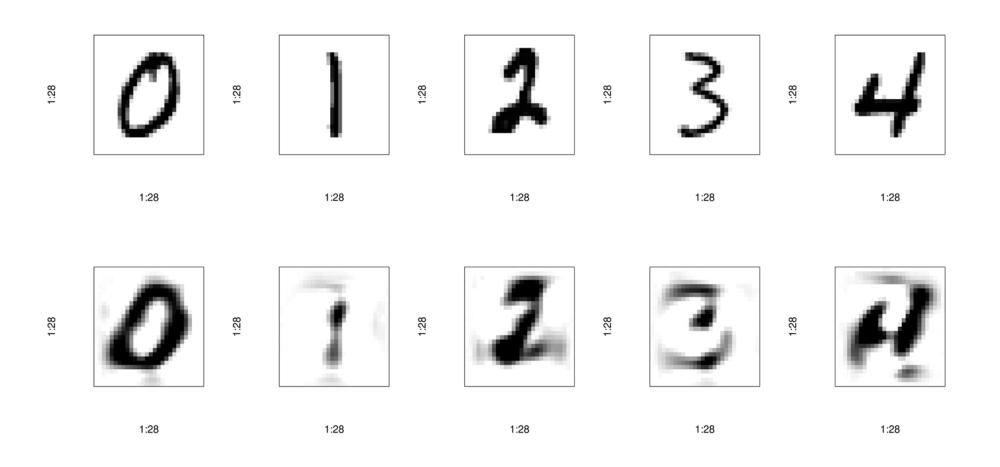


PCA on MNIST: Reconstructed with 25 PCs



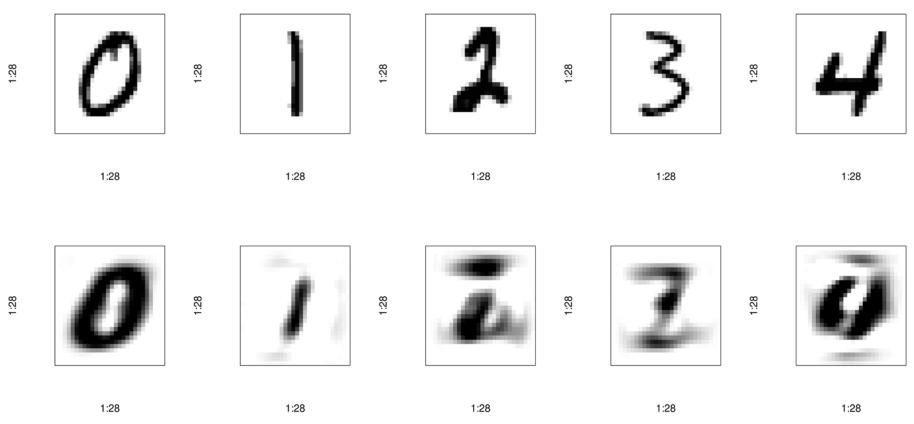


PCA on MNIST: Reconstructed with 10 PCs





PCA on MNIST: Reconstructed with 5 PCs

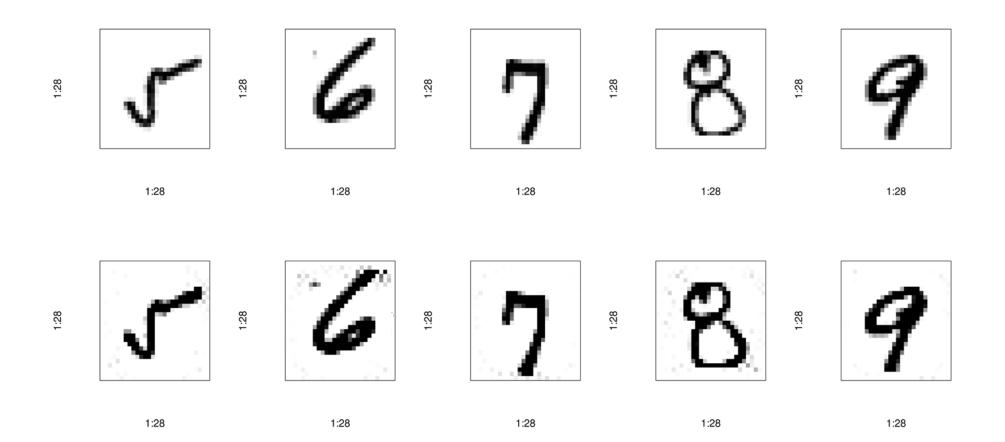






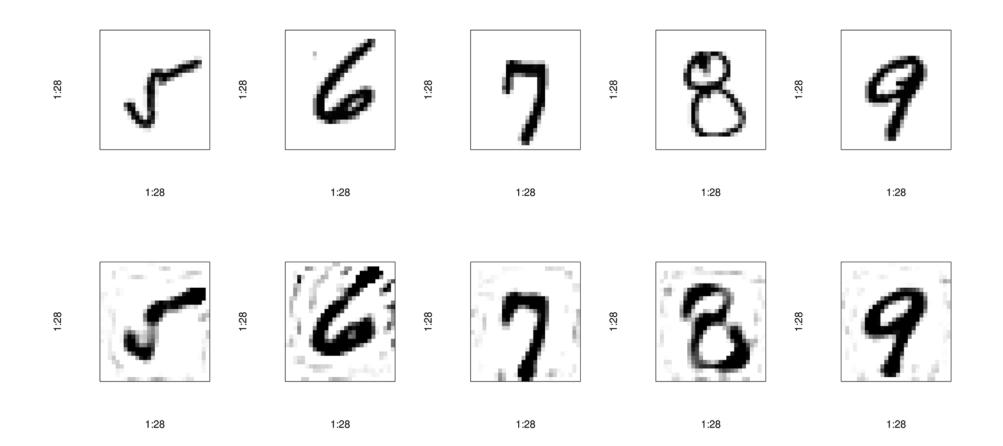
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PCA on MNIST: Reconstructed with 400 PCs II



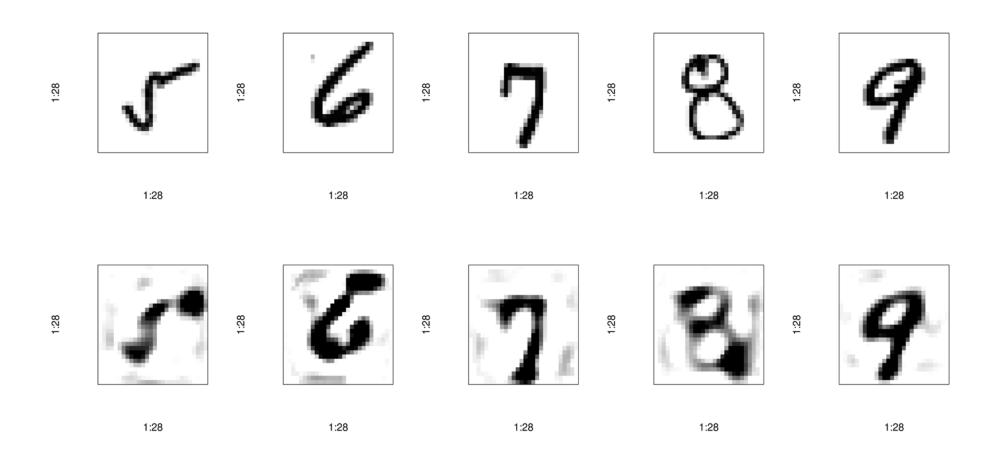


PCA on MNIST: Reconstructed with 100 PCs II

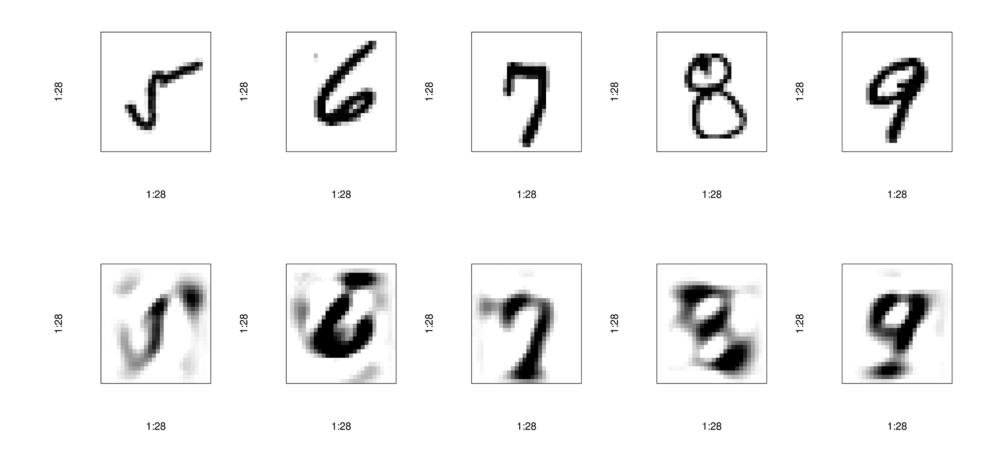




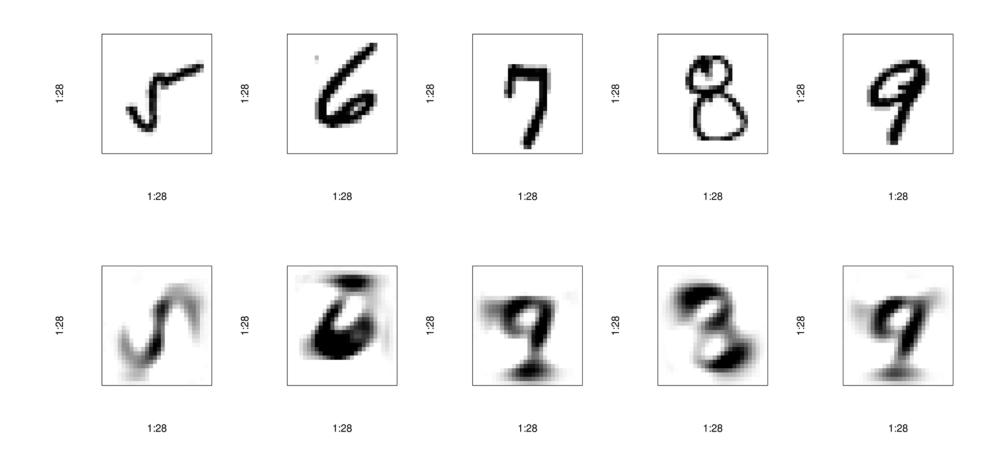
PCA on MNIST: Reconstructed with 25 PCs II



PCA on MNIST: Reconstructed with 10 PCs II



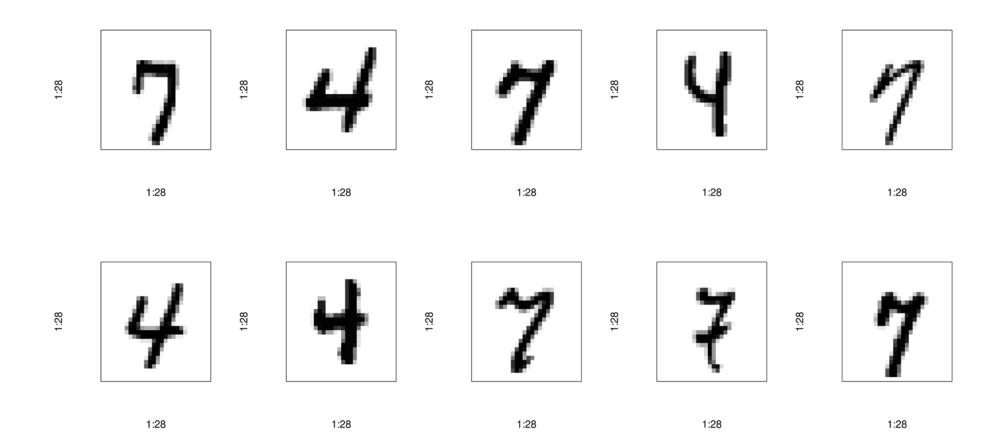
PCA on MNIST: Reconstructed with 5 PCs II





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Just pull out the 4s and the 7s



Logistic regression on 4 vs 7

R Python

```
1 x_train_filtered <- as.data.frame(x_train[, col_std_devs > 0])
2 x_val_filtered <- as.data.frame(x_val[, col_std_devs > 0])
3 x_test_filtered <- as.data.frame(x_test[, col_std_devs > 0])
4
5 logistic_model_varying <- glm(y_train ~ ., data=x_train_filtered, family = binomial)
6 nrow(summary(logistic_model_varying)$coefficients)</pre>
```

[1] 629



["]

Logistic regression on first 50 PCs

R Python

1 pca_train <- as.data.frame(pr_comp_train\$x[, 1:50])</pre>

2 logistic_model_pca <- glm(y_train ~ ., data=pca_train, family = binomial)</pre>

3 summary(logistic_model_pca)\$coefficients

	Estimate	Std. Error	z value	Pr(> z)
(Intercept)	1.198515947	0.21135576		1.422906e-08
PC1	3.647866454	0.19481760	18.72452246	3.124608e-78
PC2	2.851327556	0.17512018	16.28211881	1.322109e-59
PC3	0.677184850	0.09516631	7.11580437	1.112620e-12
PC4	-1.637208408	0.12421894	-13.18002196	1.143575e-39
PC5	-0.077537401	0.12214106	-0.63481847	5.255468e-01
PC6	0.502354456	0.11548195	4.35006906	1.360947e-05
PC7	-0.792560391	0.11826262	-6.70169838	2.060109e-11
PC8	-0.351994691	0.11458539	-3.07189847	2.127021e-03
PC9	0.075791383	0.12492815	0.60667978	5.440634e-01
PC10	0.008328826	0.14043146	0.05930884	9.527061e-01
PC11	0.128684822	0.14642117	0.87886762	3.794731e-01
PC12	-0.717080199	0.15831254	-4.52952237	5.911718e-06
PC13	0.278289184	0.16411883	1.69565667	8.995092e-02
PC14	-0.326632889	0.13879100	-2.35341547	1.860184e-02
PC15	1.260314977	0.22677140	5.55764509	2.734387e-08
PC16	0.517611645	0.19579969	2.64357748	8.203499e-03
PC17	0.203745210	0.17867643	1.14030267	2.541602e-01
PC18	-0.462318412	0.19603068	-2.35839822	1.835399e-02
PC19	1.687111767	0.21417667	7.87719665	3.348078e-15
PC20	0.464271371	0.19228580	2.41448599	1.575743e-02



Compare models on validation accuracy

R Python

```
1 # Perform PCA on the validation set using the same rotation from the training set
2 pca_val <- as.data.frame(predict(pr_comp_train, newdata = x_val)[, 1:50])
3
4 # Calculate accuracy on validation data
5 y_pred <- predict(logistic_model_varying, x_val_filtered, type = "response") > 0.5
6 accuracy_varying <- mean(y_pred == y_val)
7 y_pred <- predict(logistic_model_pca, pca_val, type = "response") > 0.5
8 accuracy_pca <- mean(y_pred == y_val)
9
10 c(accuracy_varying, accuracy_pca)
```

[1] 0.9641089 0.9847360



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Compression

"A photograph, which used to be a pattern of pigment on a sheet of chemically coated paper, is now a string of numbers, each one representing the brightness and color of a pixel. An image captured on a 4-megapixel camera is a list of 4 million numbers-no small commitment of memory for the device shooting the picture. But these numbers are highly correlated with each other. If one pixel is bright green, the next one over is likely to be as well. The actual information contained in the image is much less than 4 million numbers' worth-and it's precisely this fact that makes it possible to have compression, the critical mathematical technology that allows images, videos, music, and text to be stored in much smaller spaces than you'd think." Jordan Ellenberg

