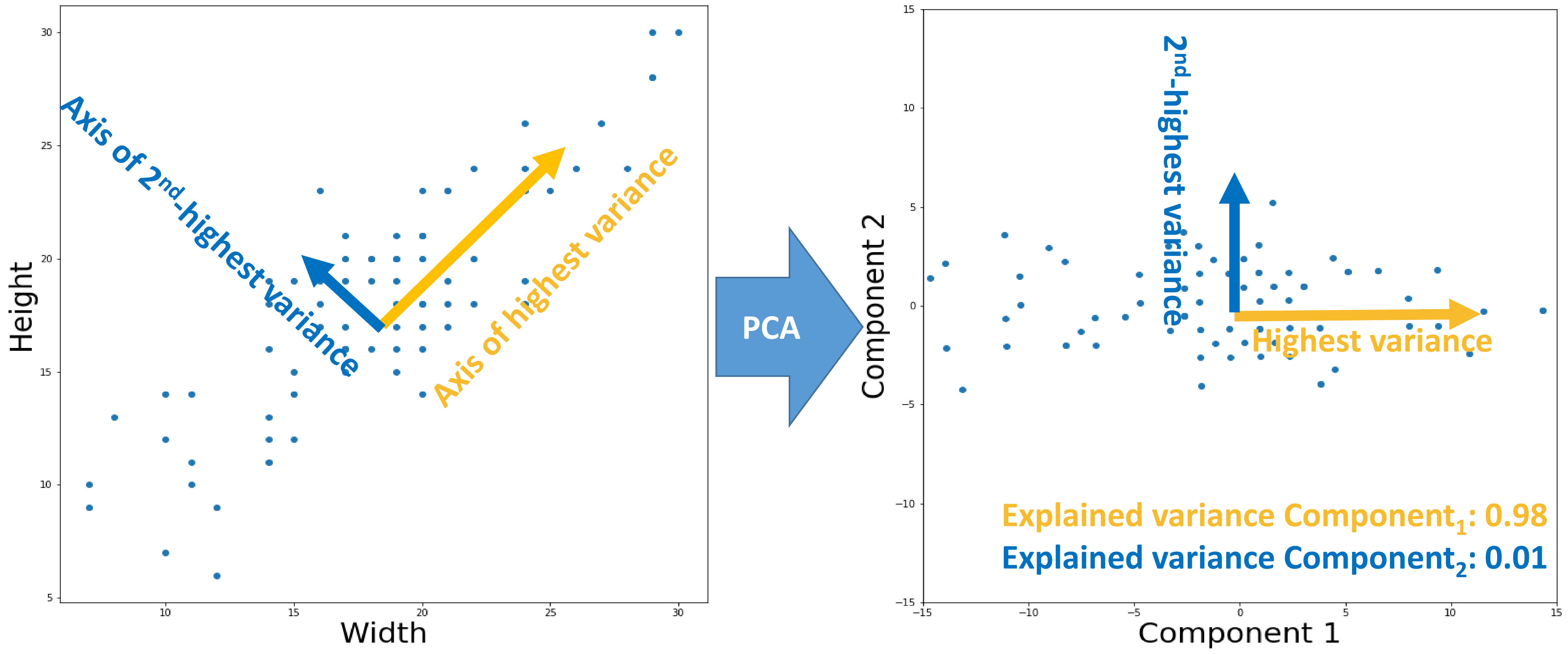
Recap day 4

Robert Haase, Marcelo Zoccoler, Johannes Müller

October 2022

Dimensionality reduction and clustering



Explained variance Component$_1$: 0.98

Explained variance Component$_2$: 0.01

PCA: Linear transformation and identifies axes that explain most of the variance in the data

→ If the explained variances of component$_1$ and component$_2$ are [0.32, 0.2], we…

Need more components	Cry	Will find no groups in the data

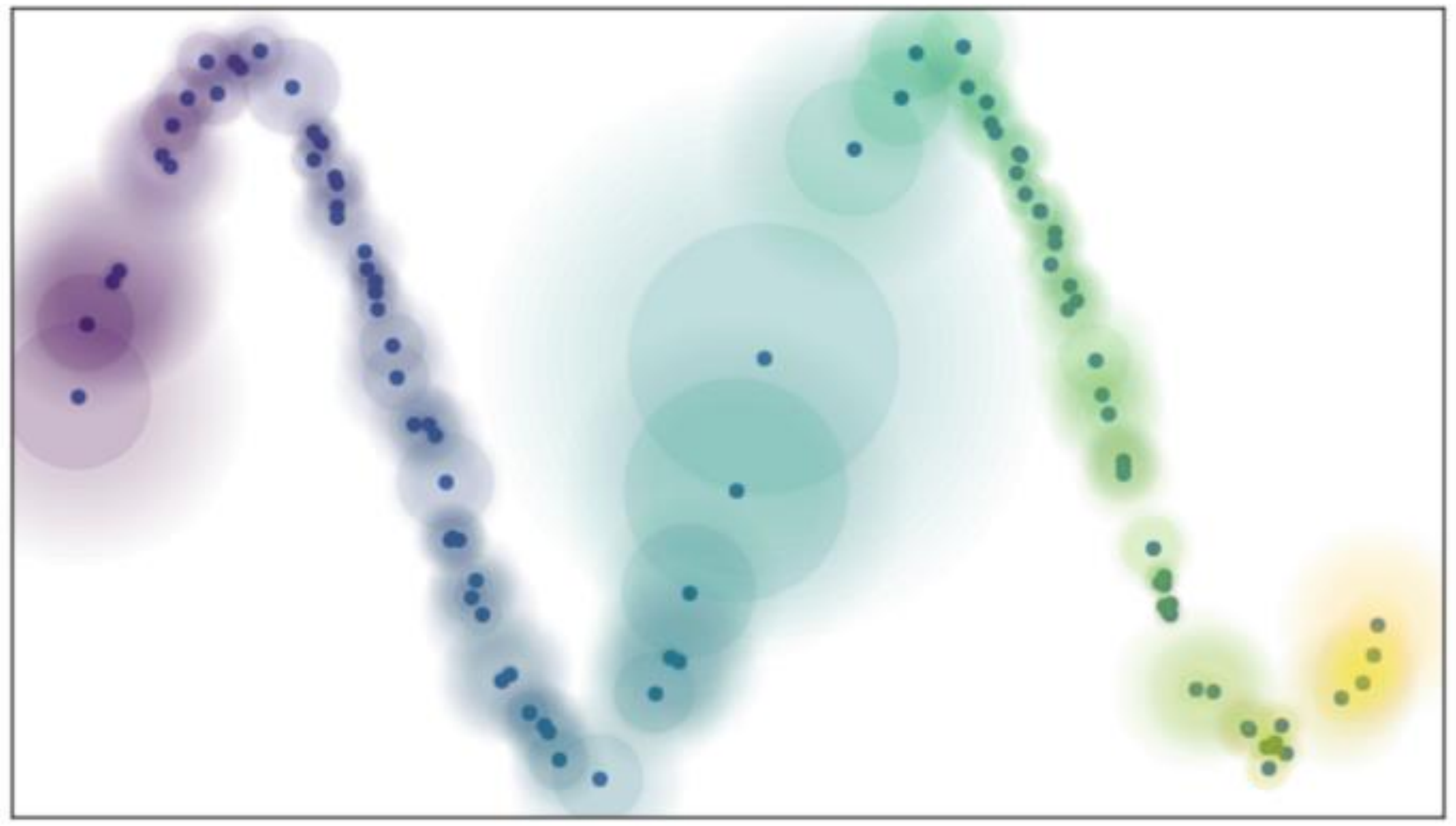
→ If we add more data to a PCA-transformed set of data, we …

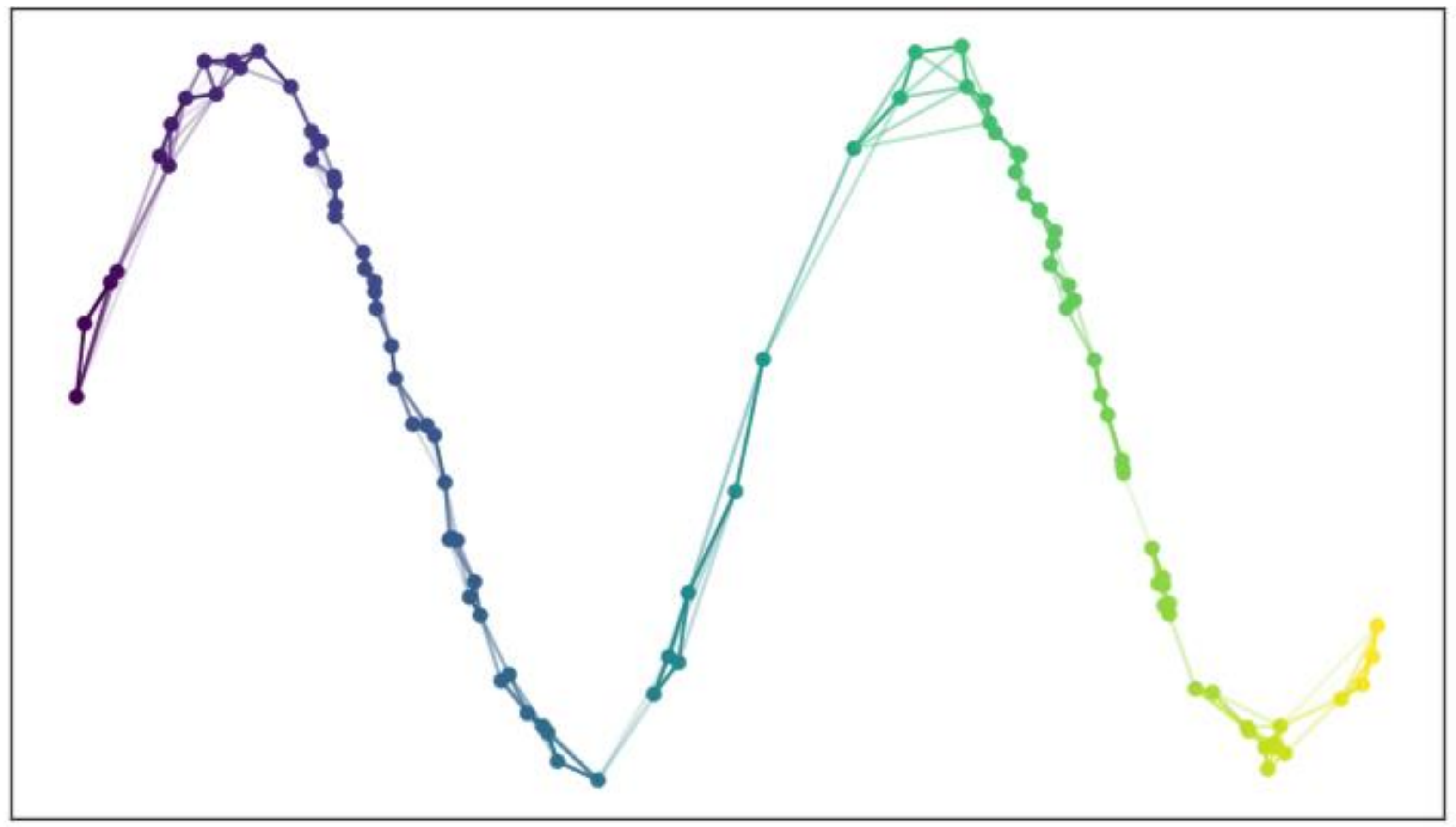
Need to re-run the PCA	Can use the same PCA components	Cannot use PCA at all

→ We can measure meaningful differences between data point in terms of component$_1$ and component$_2$

True	False

UMAP





UMAP:

→ Link neighboring points by introducing point-wise distance metrics

→ "Relax" neighborhood graph to be able to display it in fewer dimensions while preserving its topology

We can measure meaningful differences between data points in terms of UMAP_0 and UMAP_1

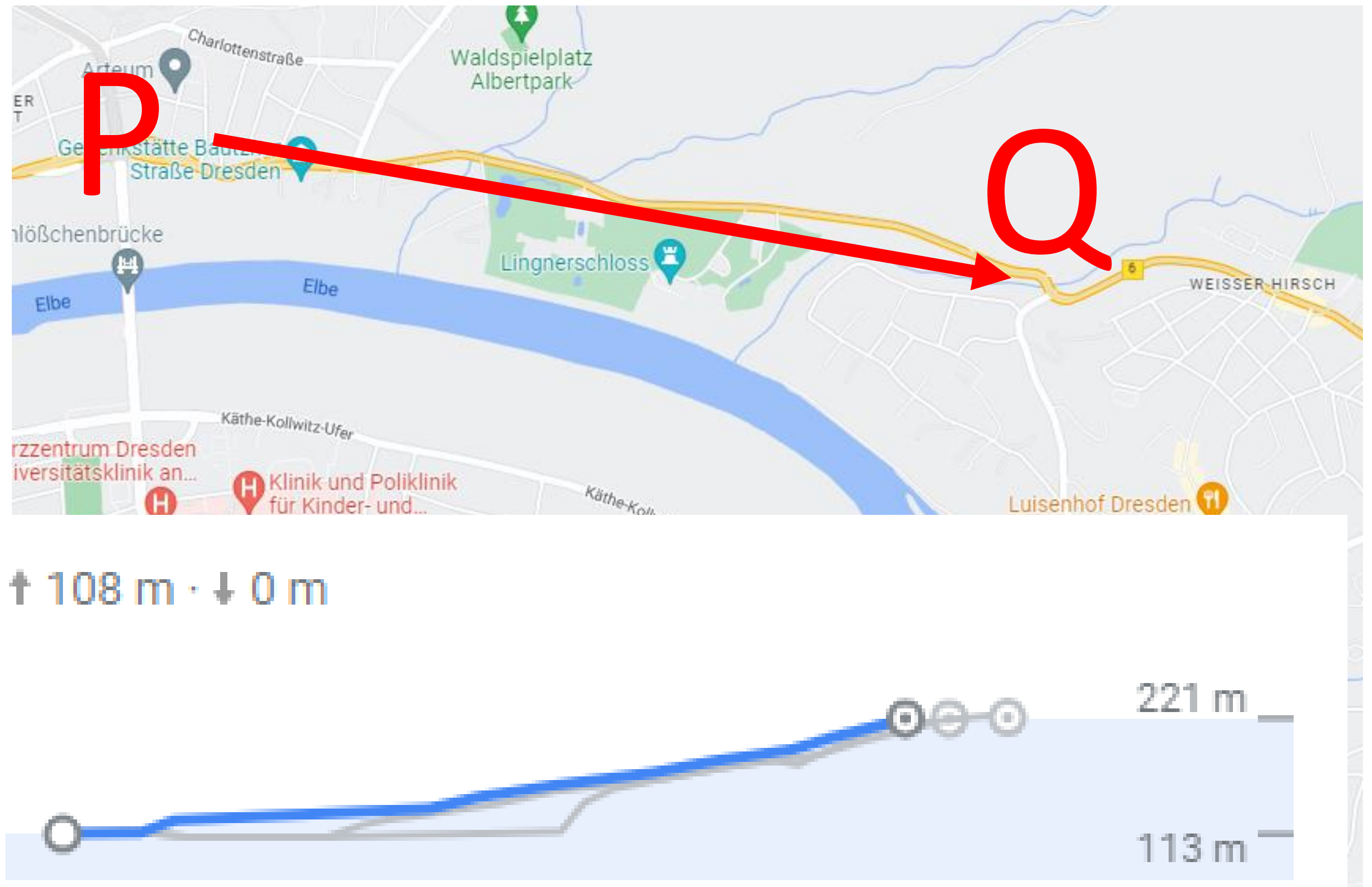
True | False

If we add new points to an existing UMAP projection, we can use the same projection

True | False

Running a UMAP twice will give the same result

True | False



Source: https://hdbscan.readthedocs.io/en/latest/how_hdbscan_works.html

@haesleinhuepf, @jm_mightypirate

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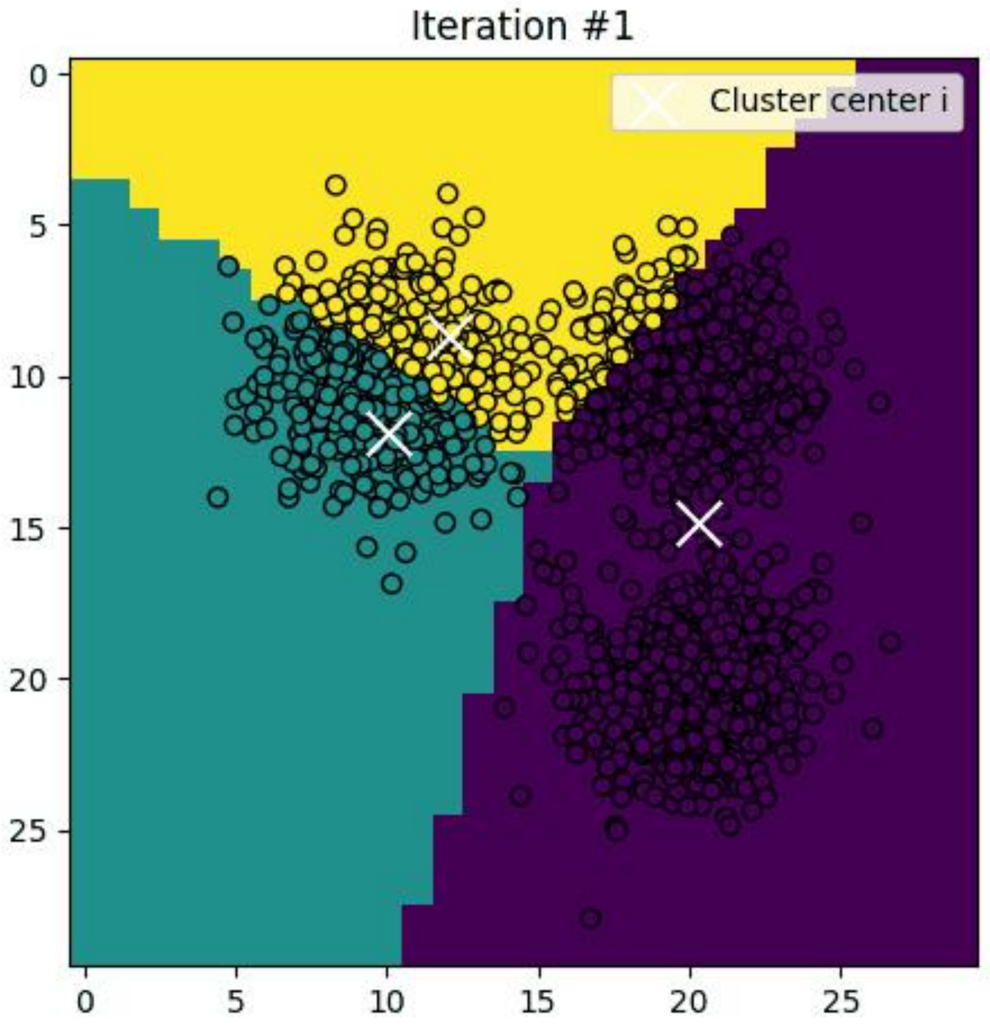
Clustering



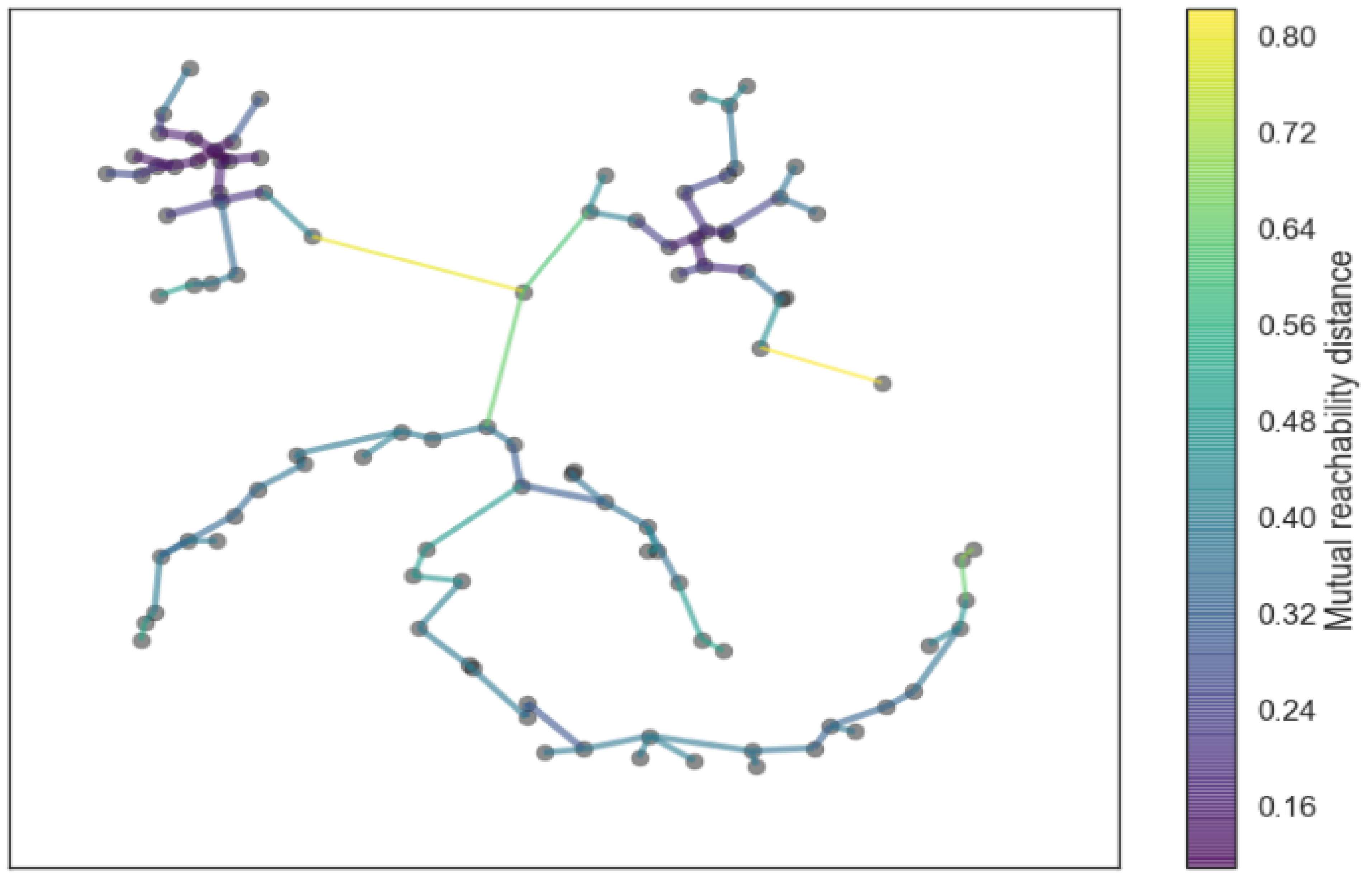
K-Means clustering:

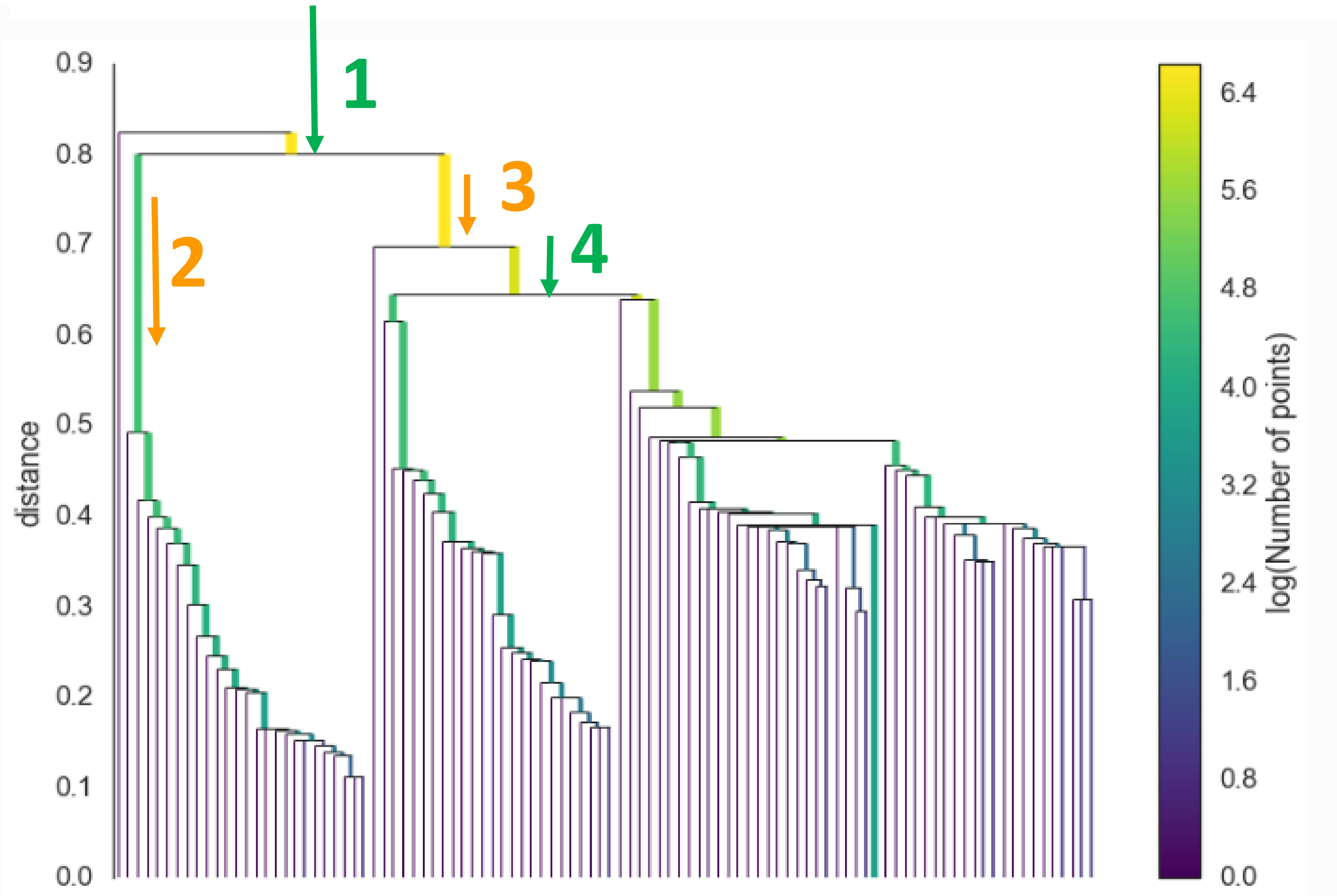
If we add more data to the pool, we can infer the cluster of a new point from the previously determined clusters

True

False

HDBSCAN: If we add more data to the pool, we can infer the cluster of a new point from the previously determined clusters





True

False

An important parameter is…

The point density

Data units

Minimal cluster size

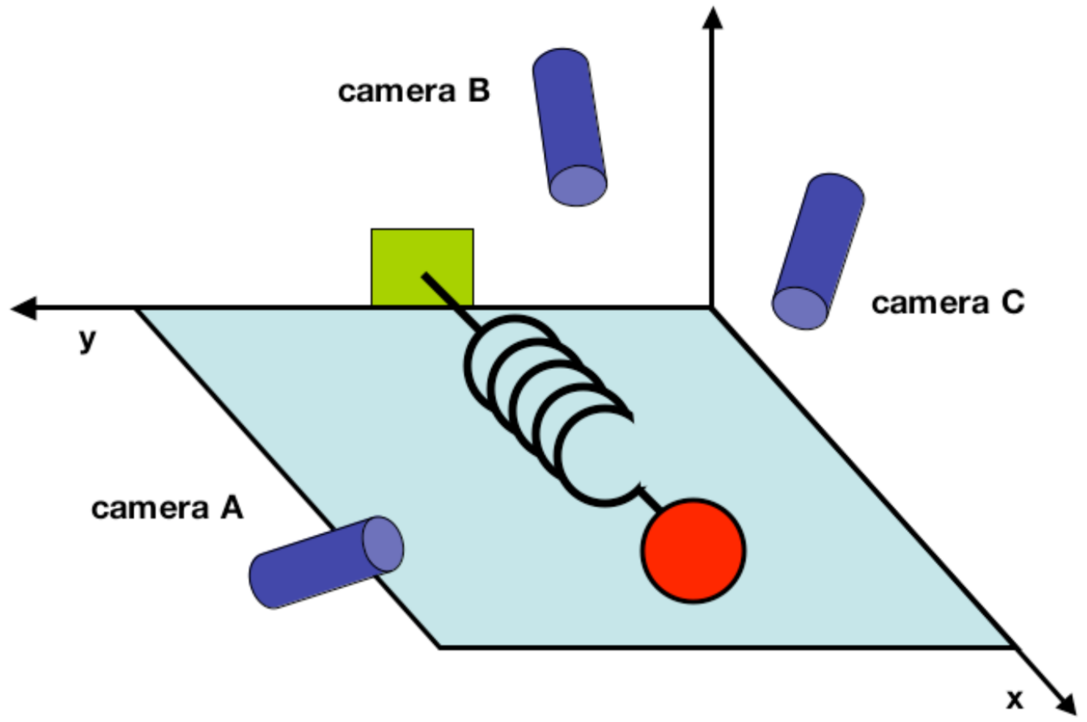
Source: https://hdbscan.readthedocs.io/en/latest/how_hdbscan_works.html

PCA

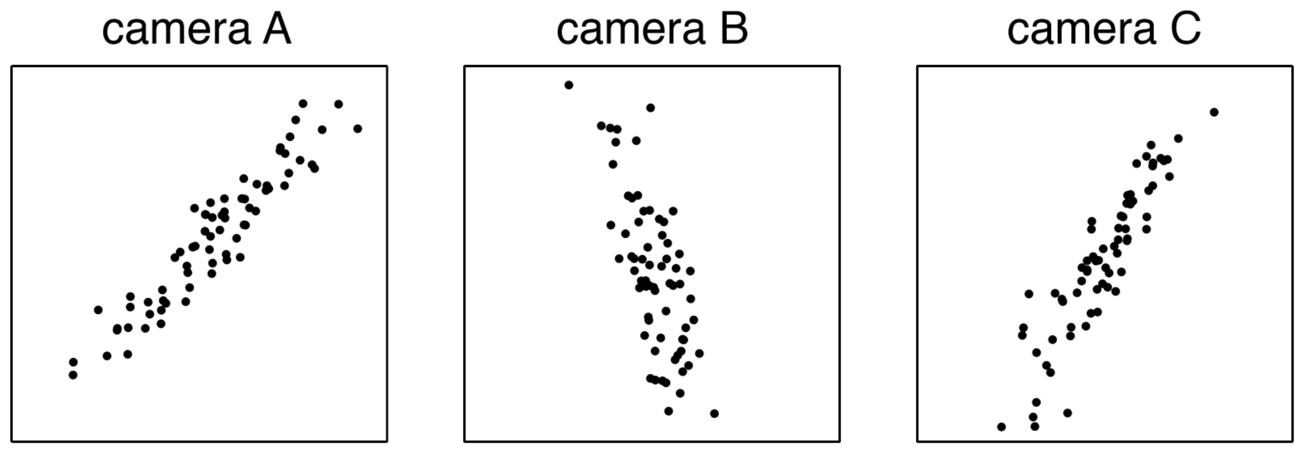
A Tutorial on Principal Component Analysis

Jonathon Shlens

https://arxiv.org/abs/1404.1100



$$\mathbf{X} = \begin{bmatrix} \mathbf{x_1} \\ \vdots \\ \mathbf{x_m} \end{bmatrix}$$



covariance matrix $\mathbf{C_X}$.

$$\mathbf{C_X} \equiv \frac{1}{n}\mathbf{X}\mathbf{X}^T.$$

Is there another basis, which is a linear combination of the original basis, that best re-expresses our data set?

$$\mathbf{PX} = \mathbf{Y}$$

SVD is a more general method for change of basis.

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

$\mathbf{C_X}$ captures the covariance between all possible pairs of measurements. The covariance values reflect the noise and redundancy in our measurements.

- In the diagonal terms, by assumption, large values correspond to interesting structure.
- In the off-diagonal terms large magnitudes correspond to high redundancy.

$$\begin{aligned}
\mathbf{C_Y} &= \frac{1}{n}\mathbf{Y}\mathbf{Y}^T \\
&= \frac{1}{n}(\mathbf{PX})(\mathbf{PX})^T \\
&= \frac{1}{n}\mathbf{P}\mathbf{X}\mathbf{X}^T\mathbf{P}^T \\
&= \mathbf{P}(\frac{1}{n}\mathbf{X}\mathbf{X}^T)\mathbf{P}^T \\
\mathbf{C_Y} &= \mathbf{P}\mathbf{C_X}\mathbf{P}^T
\end{aligned}$$

A symmetric matrix is diagonalized by a matrix of its orthonormal eigenvectors.

$$\mathbf{A} = \mathbf{E}\mathbf{D}\mathbf{E}^T$$

$$\begin{aligned}
\mathbf{C_Y} &= \mathbf{P}\mathbf{C_X}\mathbf{P}^T \\
&= \mathbf{P}(\mathbf{E}^T\mathbf{D}\mathbf{E})\mathbf{P}^T
\end{aligned}$$

If we select P as the eigenvectors of C$_x$: $\mathbf{P} \equiv \mathbf{E}^T$

$$\begin{aligned}
&= \mathbf{P}(\mathbf{P}^T\mathbf{D}\mathbf{P})\mathbf{P}^T \\
&= (\mathbf{P}\mathbf{P}^T)\mathbf{D}(\mathbf{P}\mathbf{P}^T) \\
&= (\mathbf{P}\mathbf{P}^{-1})\mathbf{D}(\mathbf{P}\mathbf{P}^{-1}) \\
\mathbf{C_Y} &= \mathbf{D}
\end{aligned}$$

Quiz

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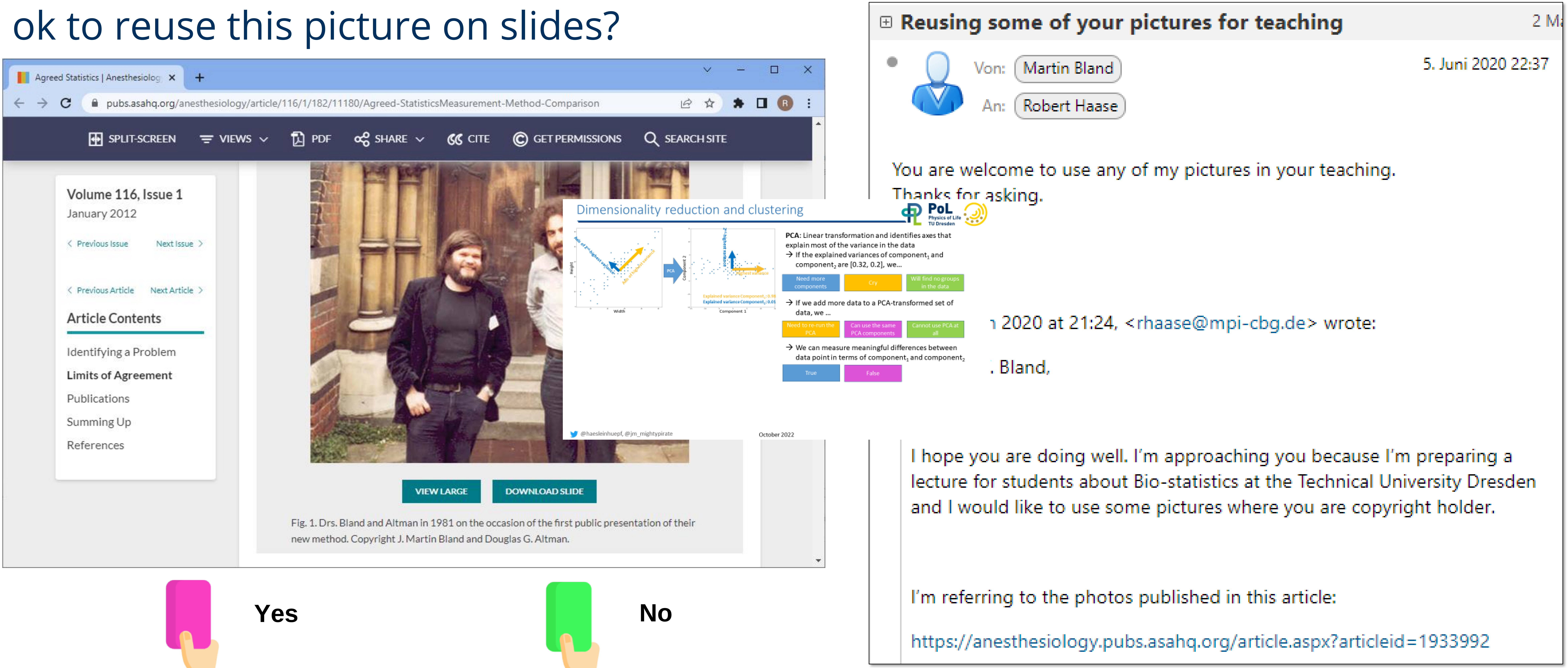

Agreed Statistics | Anesthesiolog ×

pubs.asahq.org/anesthesiology/article/116/1/182/11180/Agreed-StatisticsMeasurement-Method-Comparison

Volume 116, Issue 1
January 2012

Article Contents

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Fig. 1. Drs. Bland and Altman in 1981 on the occasion of the first public presentation of their new method. Copyright J. Martin Bland and Douglas G. Altman.

Dimensionality reduction and clustering

PCA: Linear transformation and identifies axes that explain most of the variance in the data

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True | False

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October 2022

Reusing some of your pictures for teaching

2 M

Von: Martin Bland

An: Robert Haase

5. Juni 2020 22:37

You are welcome to use any of my pictures in your teaching.

Thanks for asking.

ı 2020 at 21:24, <rhaase@mpi-cbg.de> wrote:

. Bland,

I hope you are doing well. I'm approaching you because I'm preparing a lecture for students about Bio-statistics at the Technical University Dresden and I would like to use some pictures where you are copyright holder.

I'm referring to the photos published in this article:

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Yes

No

Source:
https://anesthesiology.pubs.asahq.org/article.aspx?articleid=1933992

Quiz

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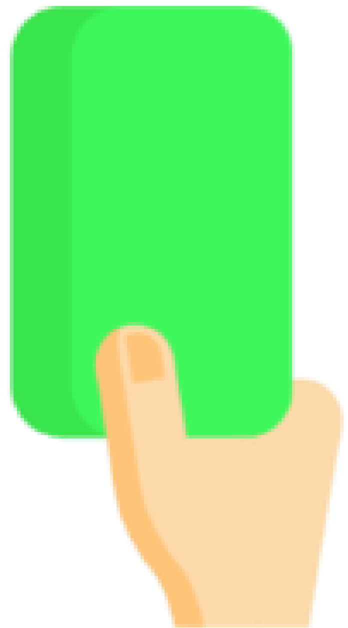

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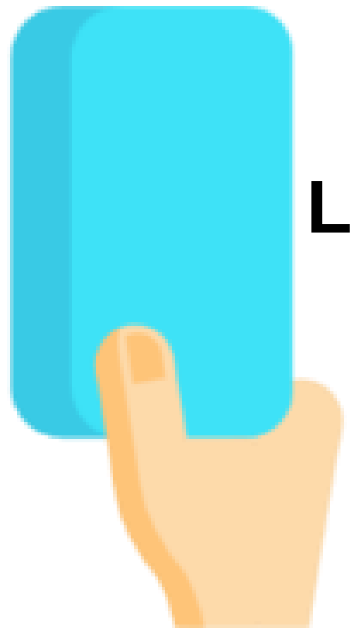

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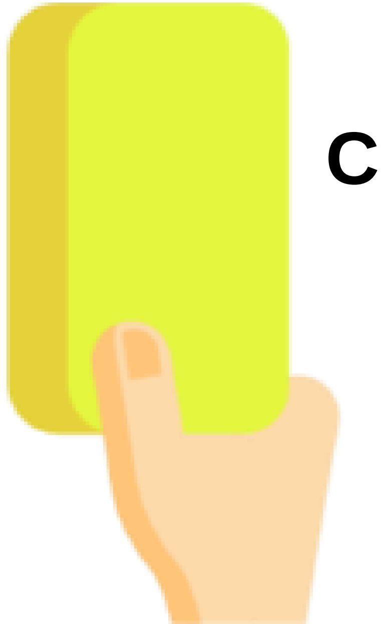

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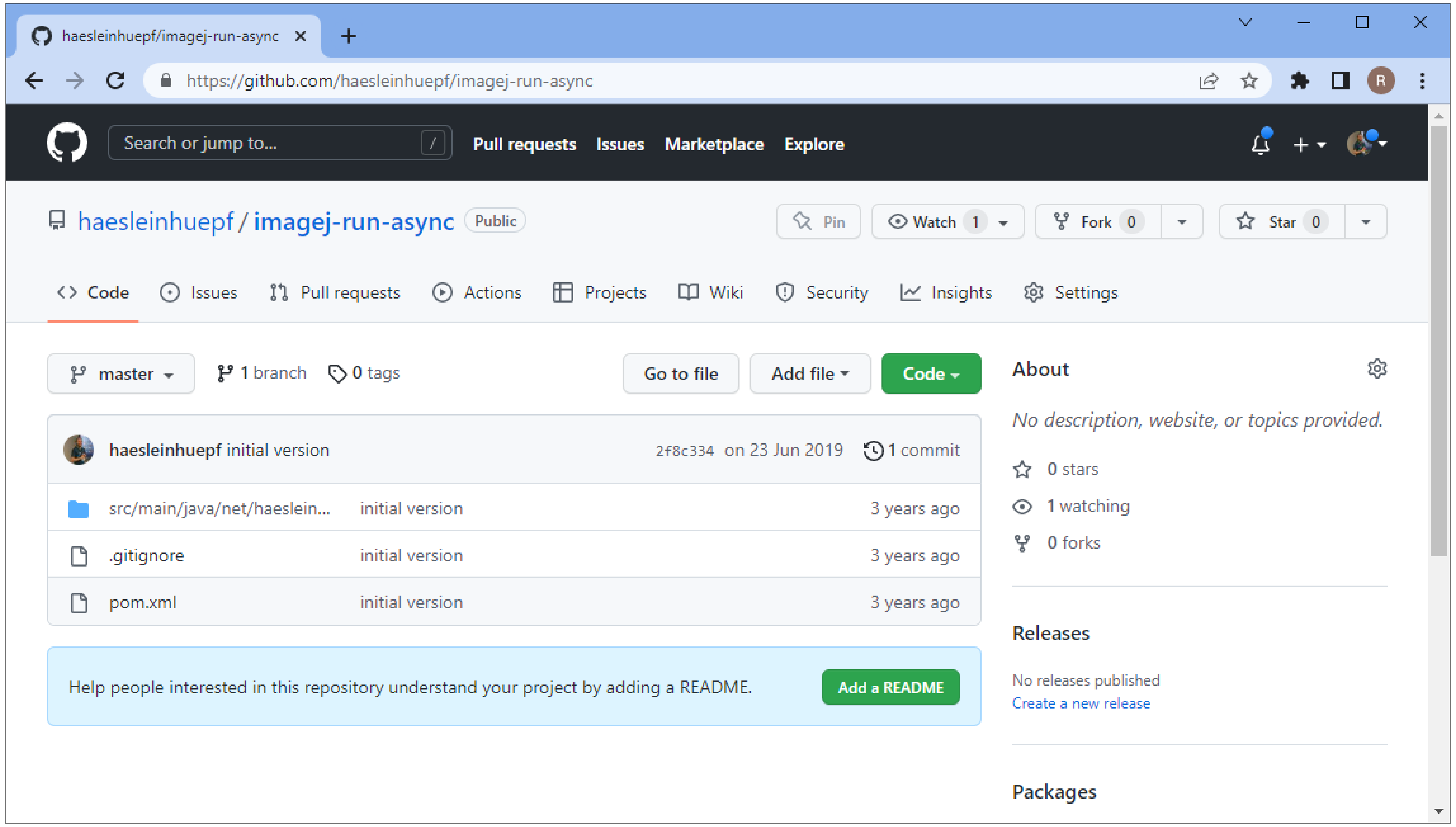

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1 branch 0 tags

haesleinhuepf initial version 2f8c334 on 23 Jun 2019 1 commit

src/main/java/net/haeslein…	initial version	3 years ago
.gitignore	initial version	3 years ago
pom.xml	initial version	3 years ago

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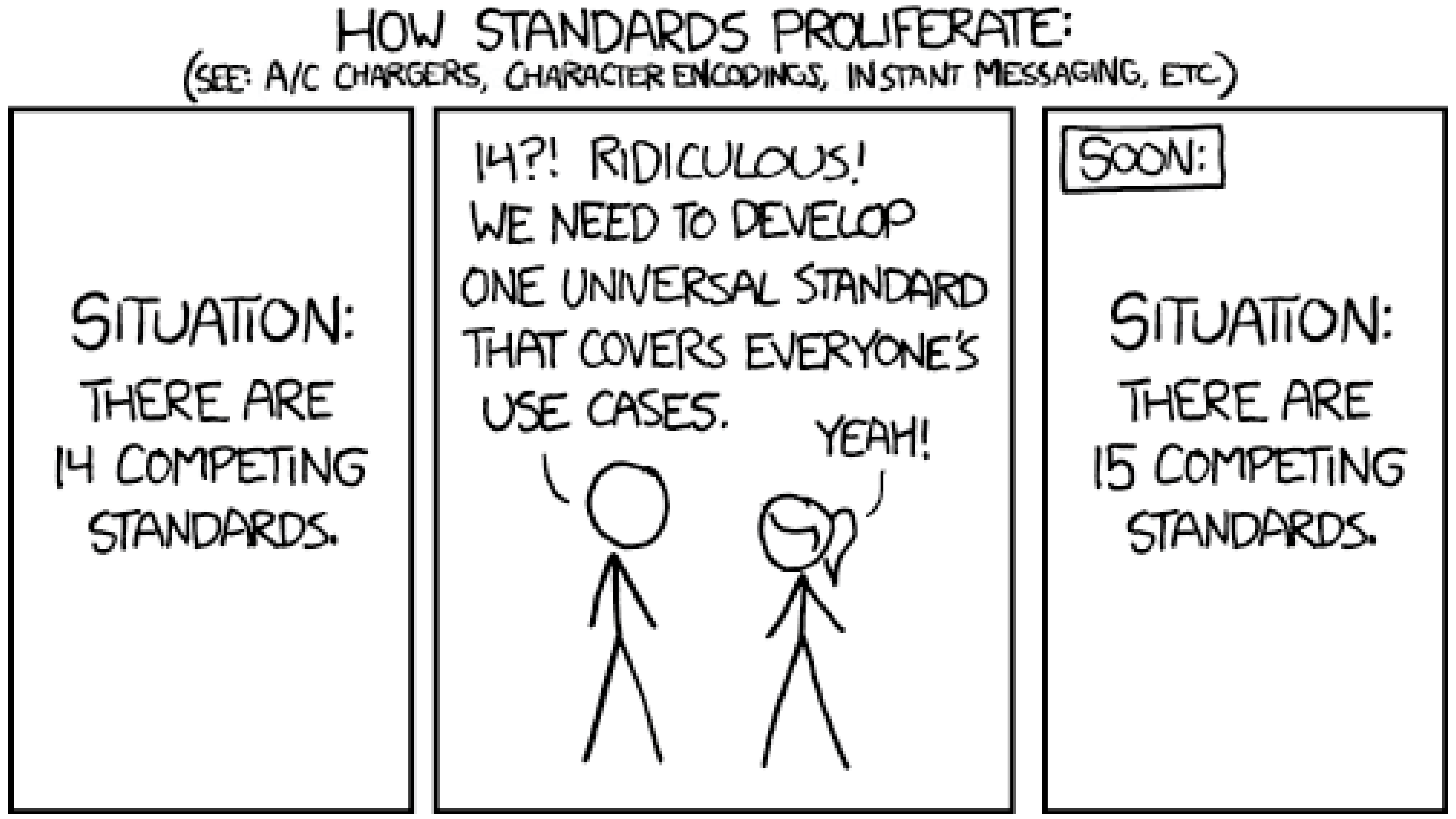
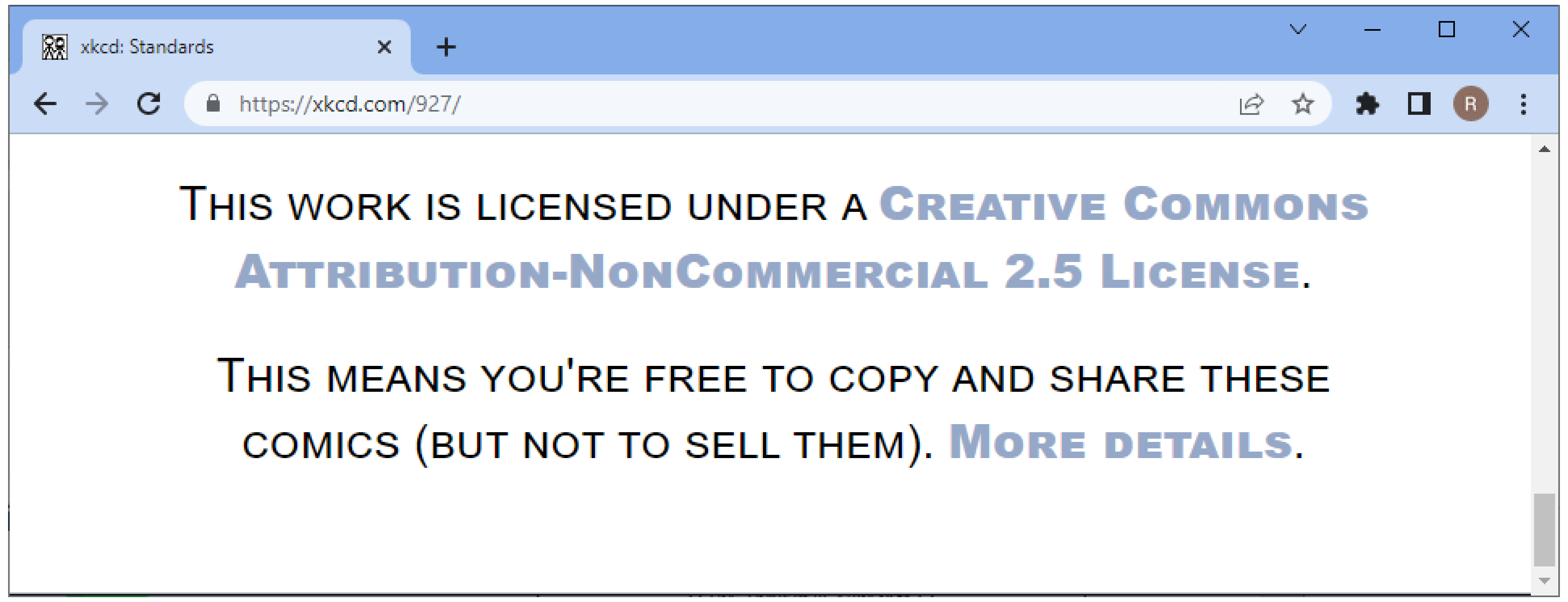

HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC)
SITUATION: THERE ARE 14 COMPETING STANDARDS.
14?! RIDICULOUS! WE NEED TO DEVELOP ONE UNIVERSAL STANDARD THAT COVERS EVERYONE'S USE CASES.
YEAH!
SOON:
SITUATION: THERE ARE 15 COMPETING STANDARDS.



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