6.7900: Machine Learning
Lecture 19

Lecture start: Tues/Thurs 2:35pm
Who's speaking today? Prof. Tamara Broderick
Course website: gradml.mit.edu
Questions? Ask here or on piazza.com/mit/fall2024/67900/
Materials: Slides, video, etc linked from gradml.mit.edu after the lecture (but there is no livestream)

Last Time

I. How to proceed when data is missing
II. Dimensionality reduction
III. Principal components analysis (PCA)

Today

I. Another perspective on PCA
II. Successes and challenges of PCA
III. t-SNE

Motivating example for Principal Components Analysis (PCA)

[Example thanks to Schlens 2014]

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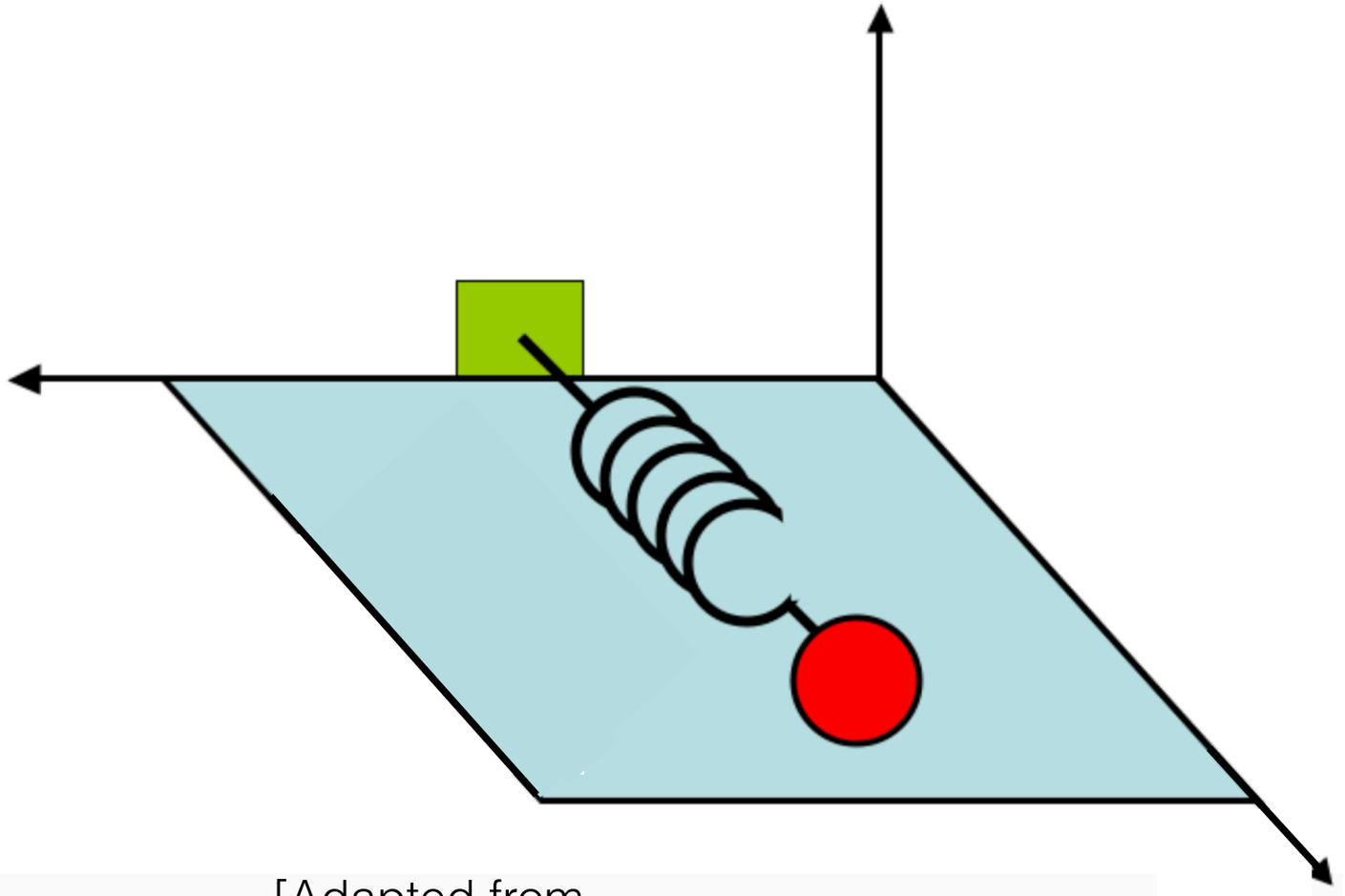

[Adapted from Schlens 2014]

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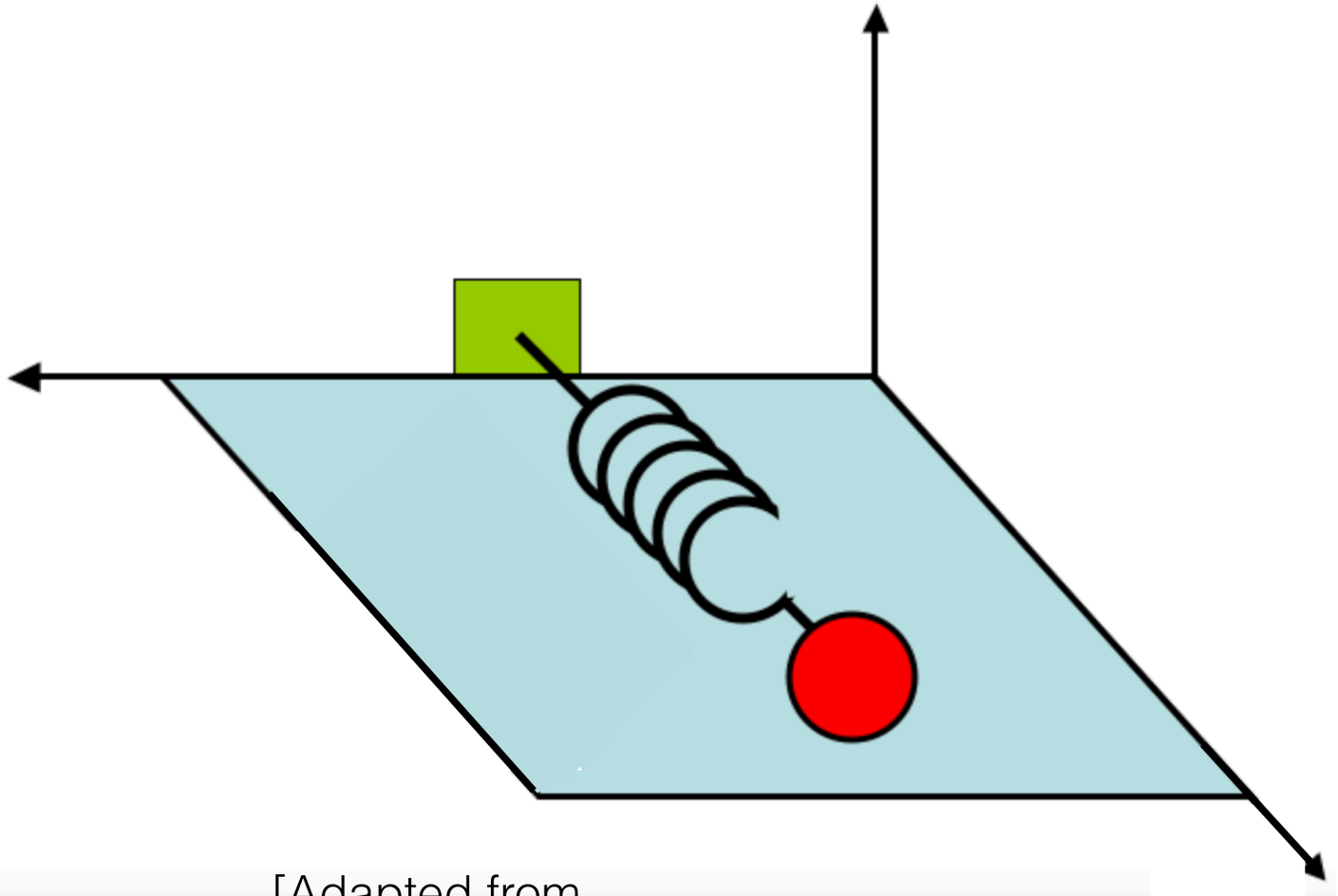

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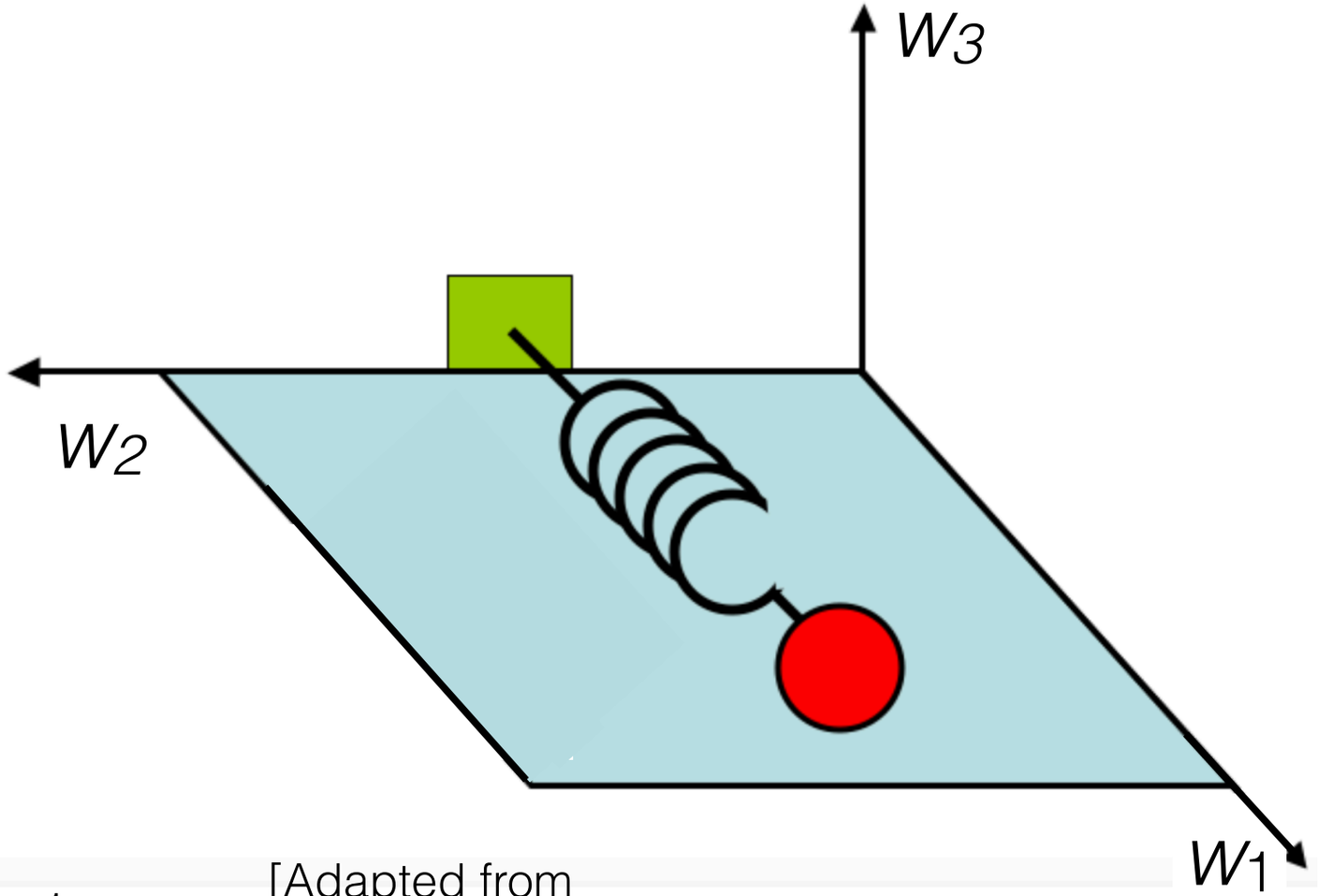

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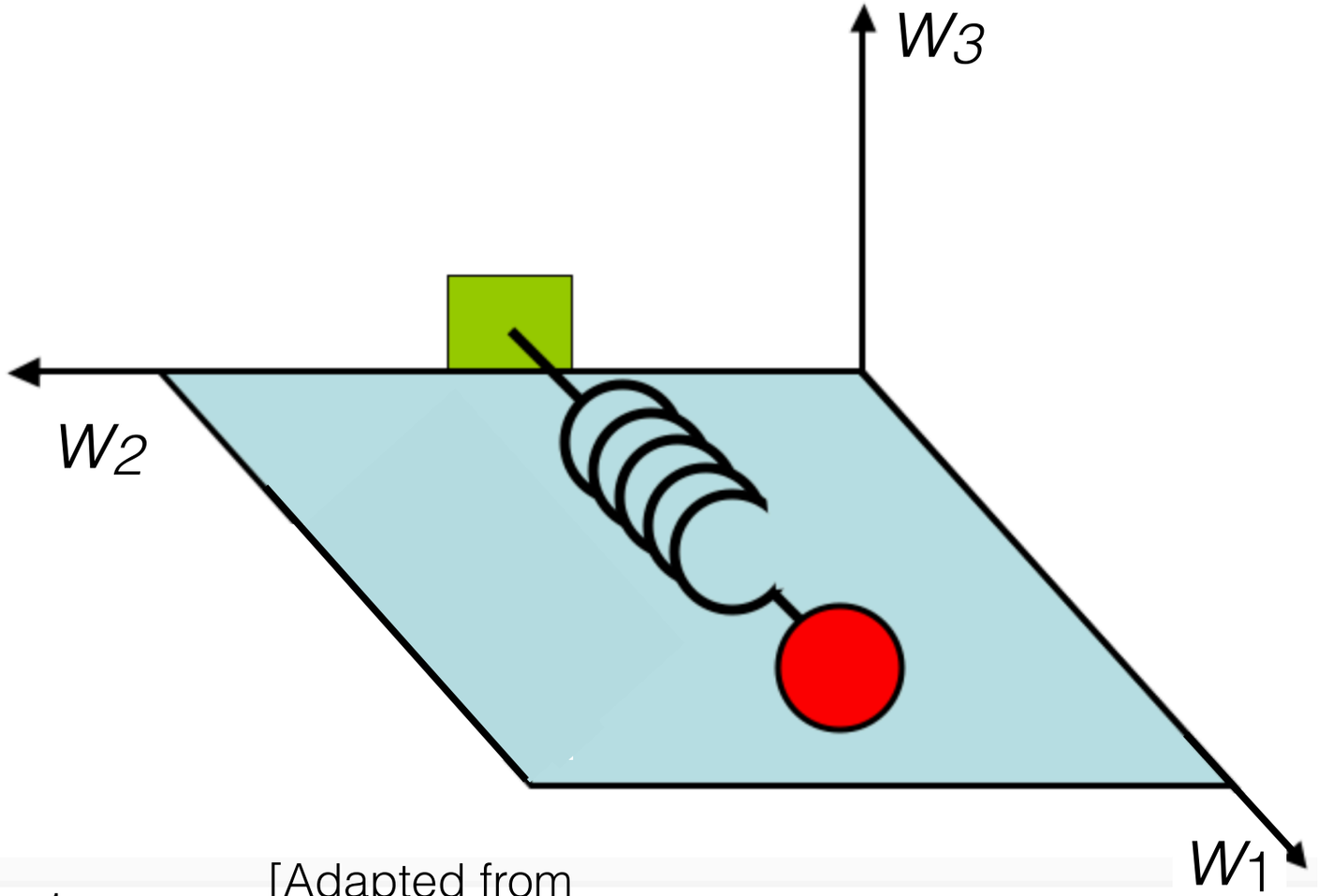

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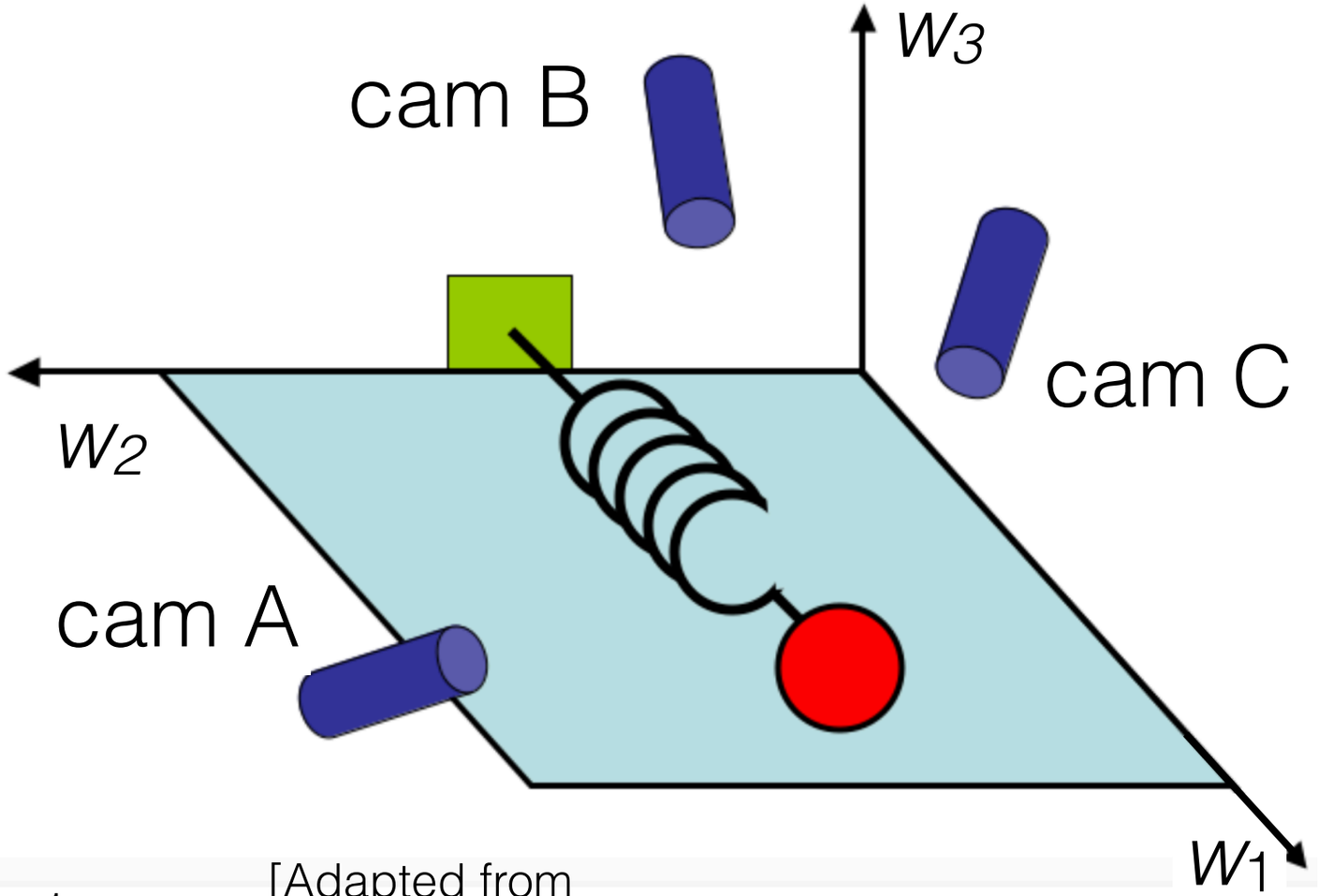

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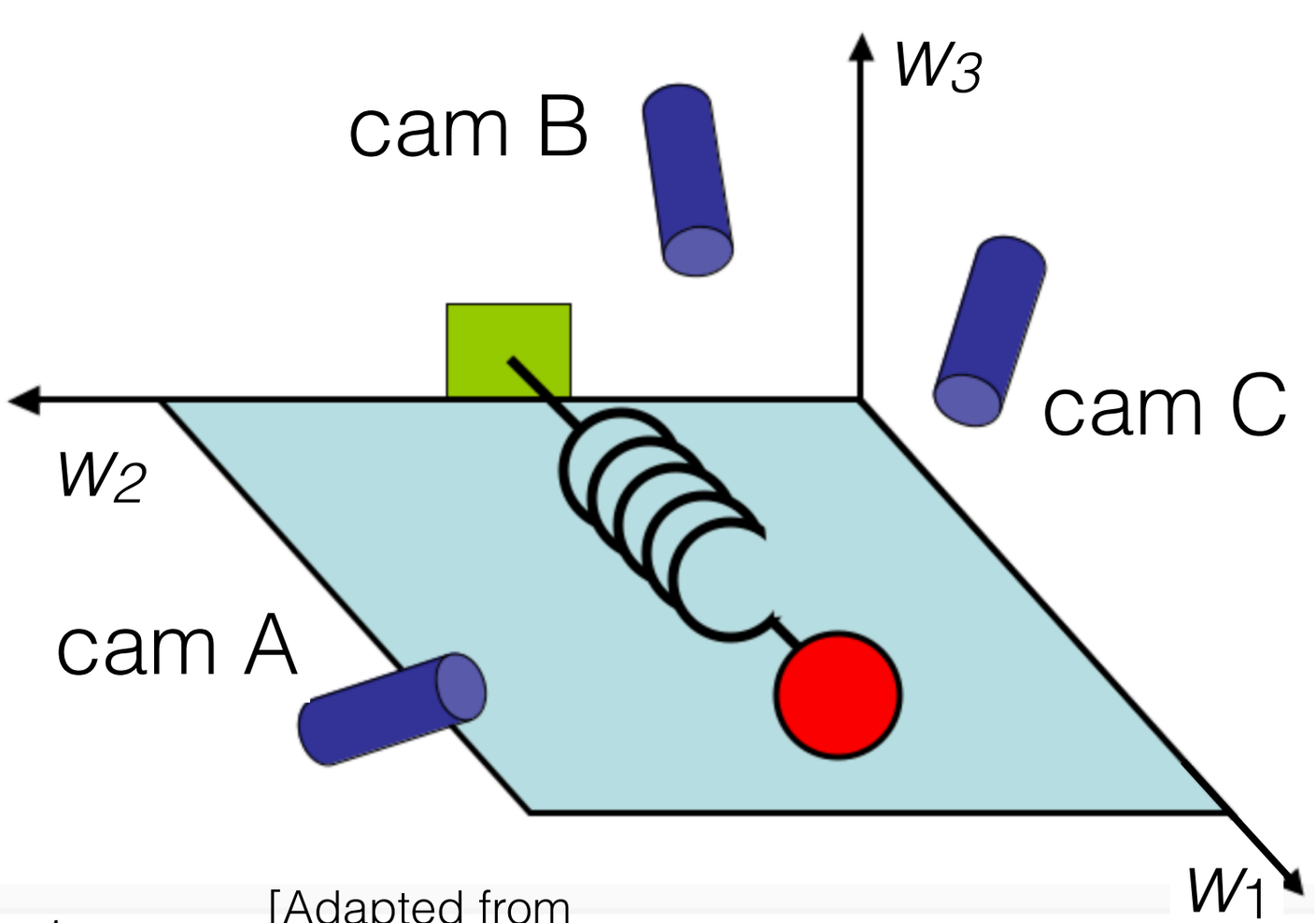

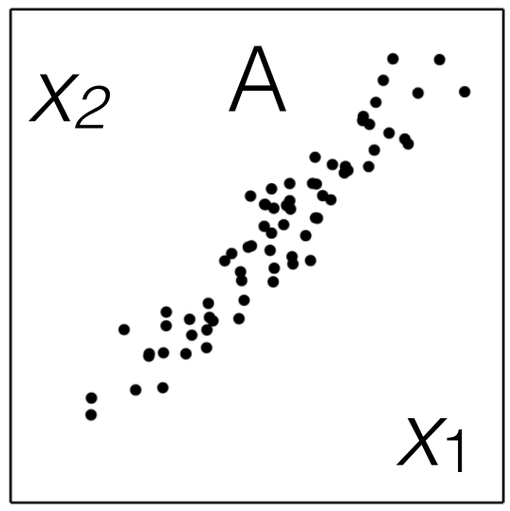

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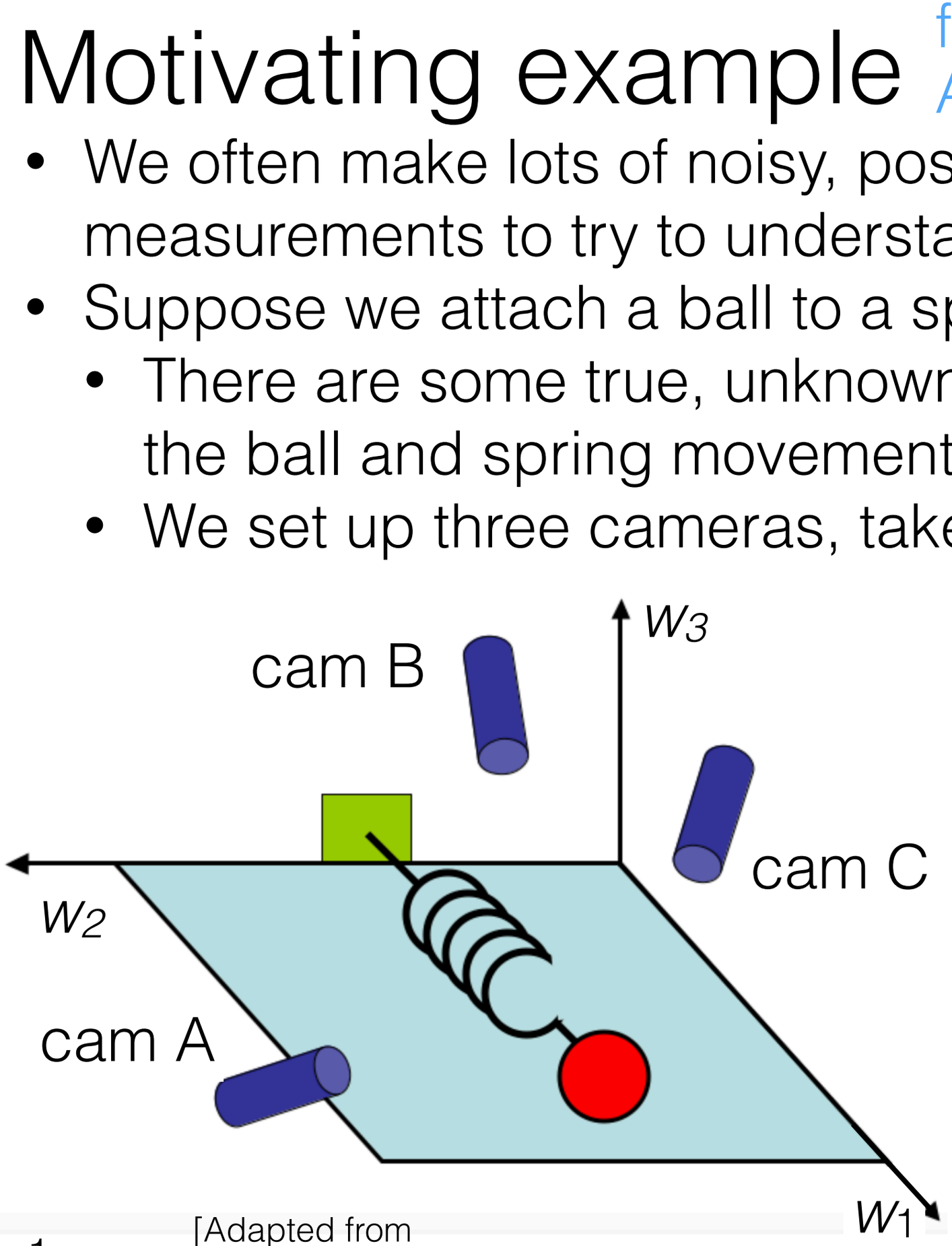

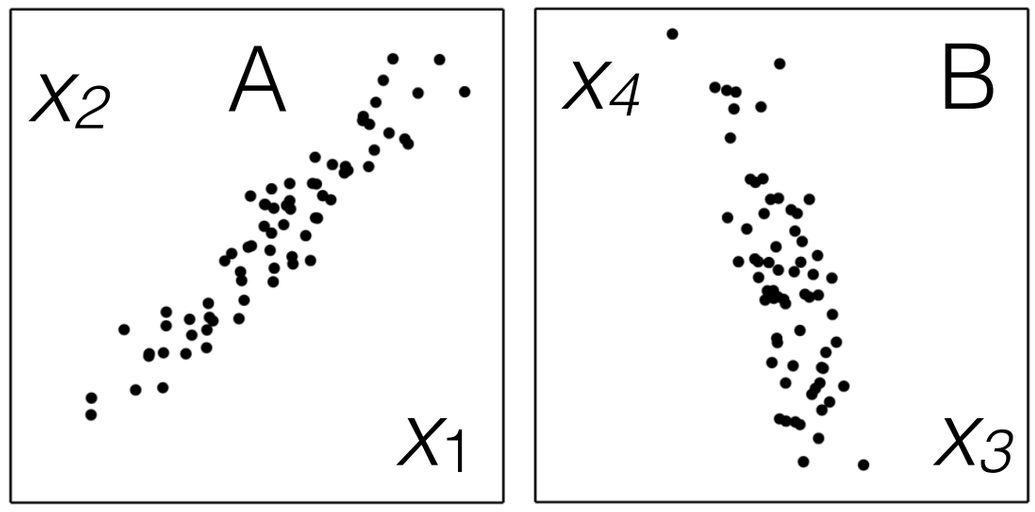

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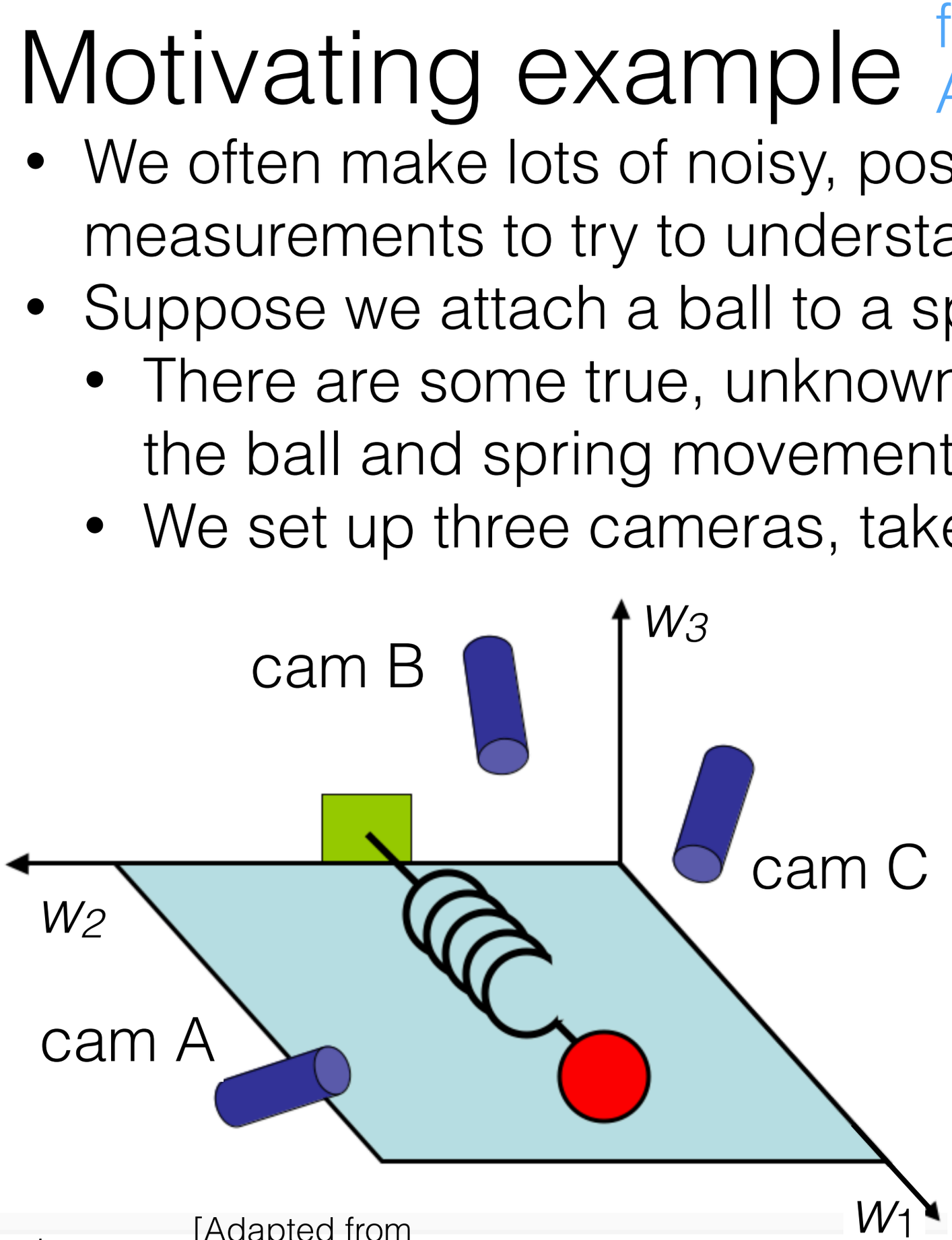

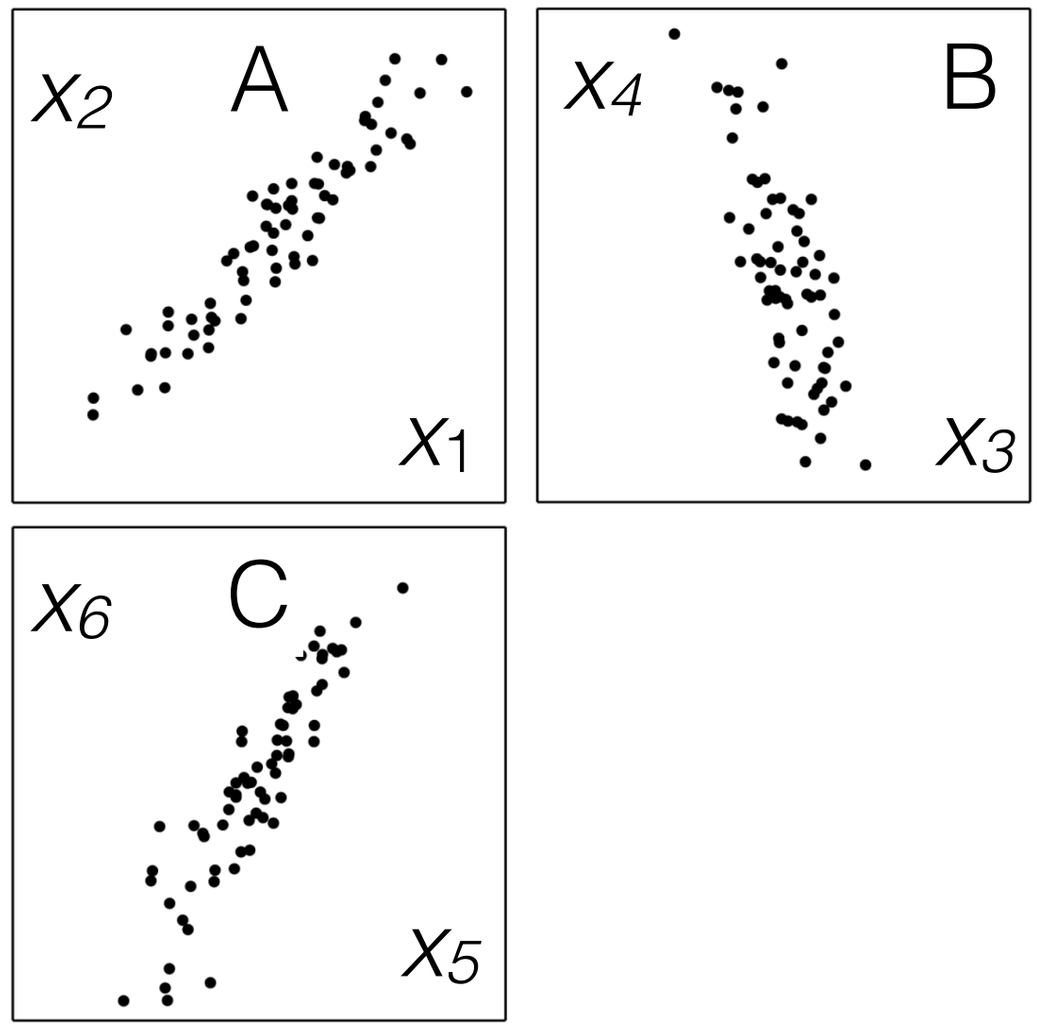

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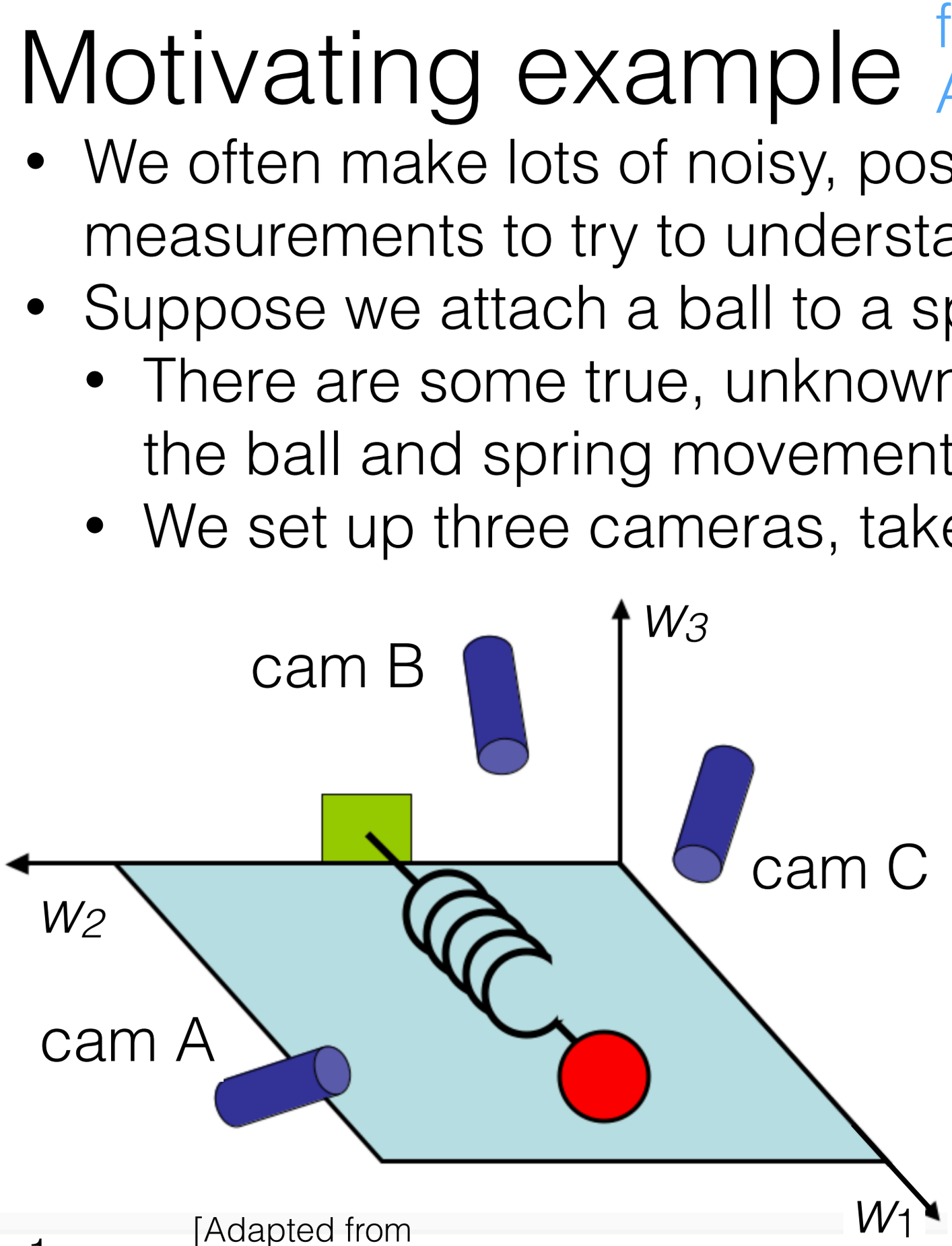
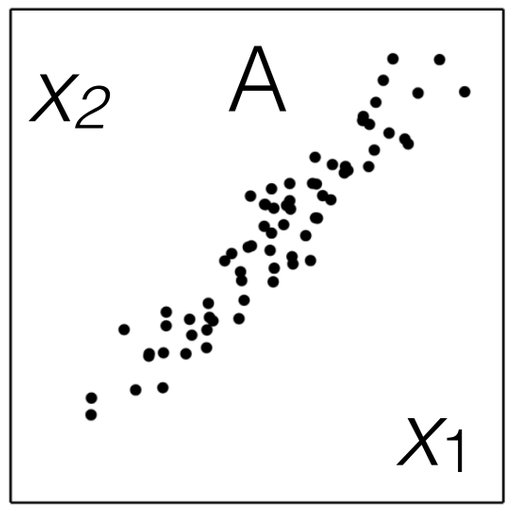
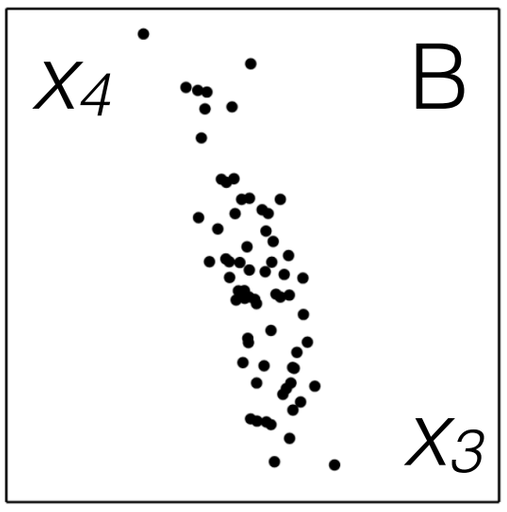
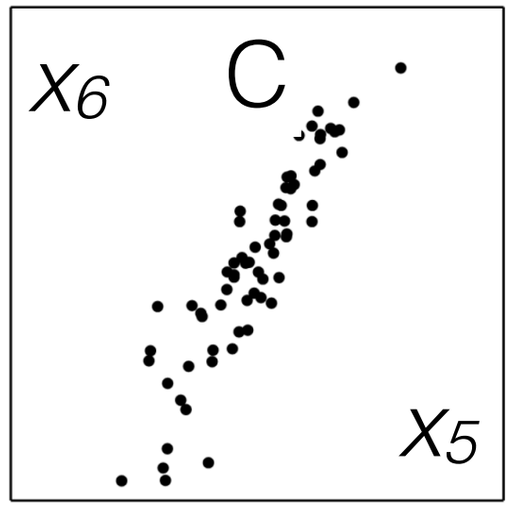




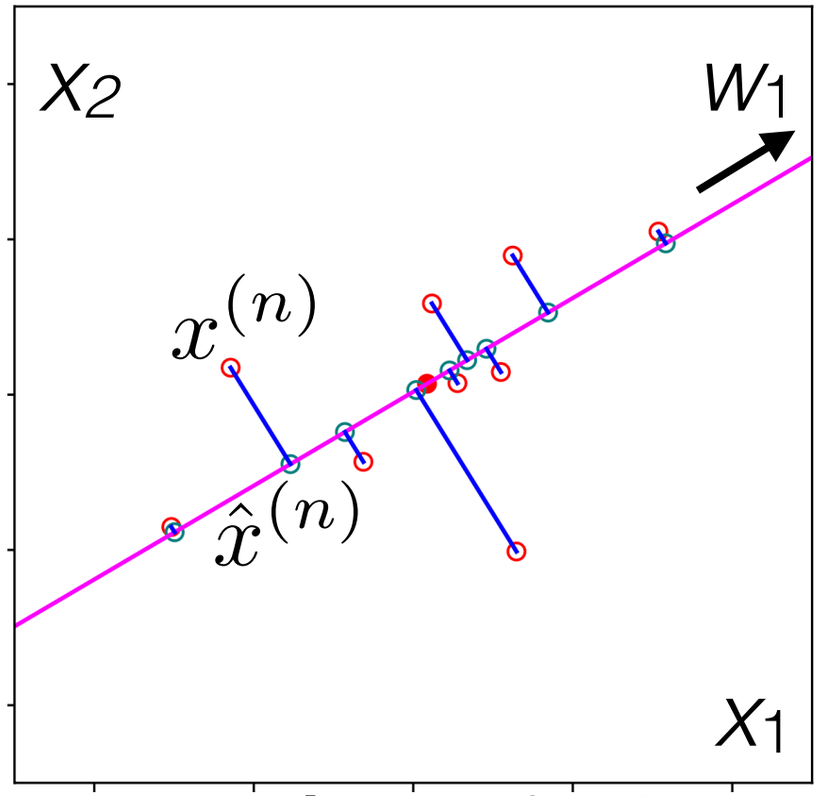




- We have 6 features, but need only 1

[Adapted from Schlens 2014]

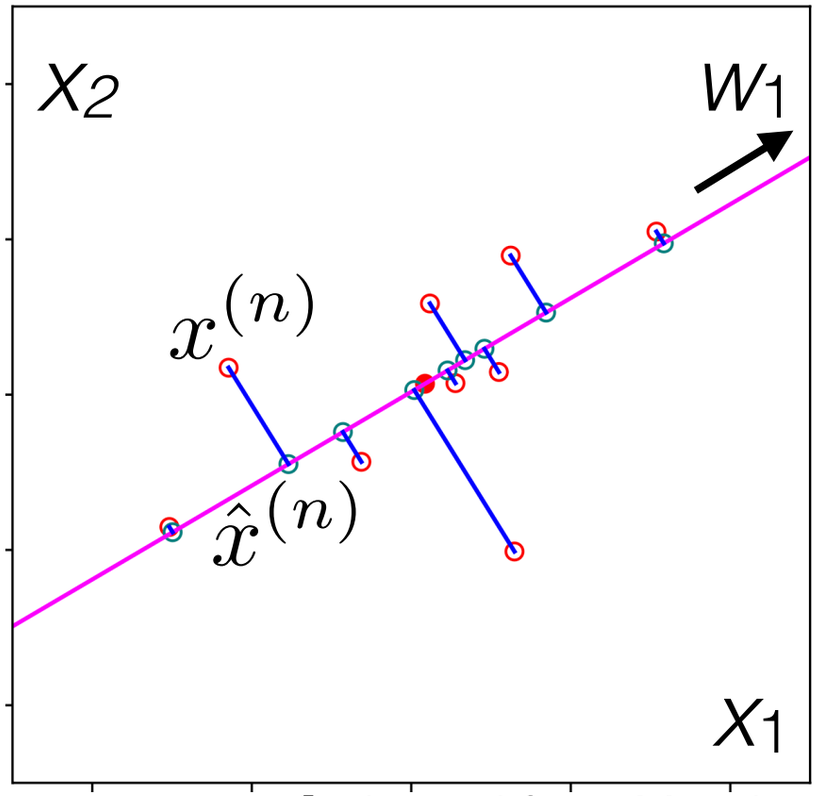
Problem setup for PCA



[adapted from Murphy 2022, Fig 20.1]

Problem setup for PCA

- Pre-process so $\frac{1}{N}\sum_{n=1}^{N} x^{(n)} = 0_D$



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- Pre-process so $\frac{1}{N}\sum_{n=1}^{N} x^{(n)} = 0_D$
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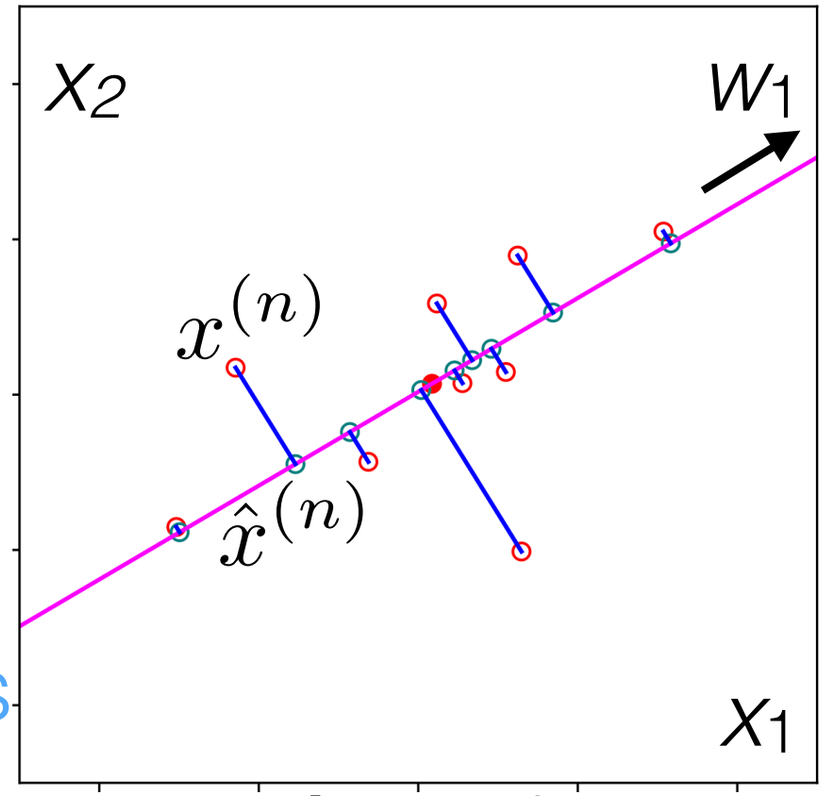
principal components



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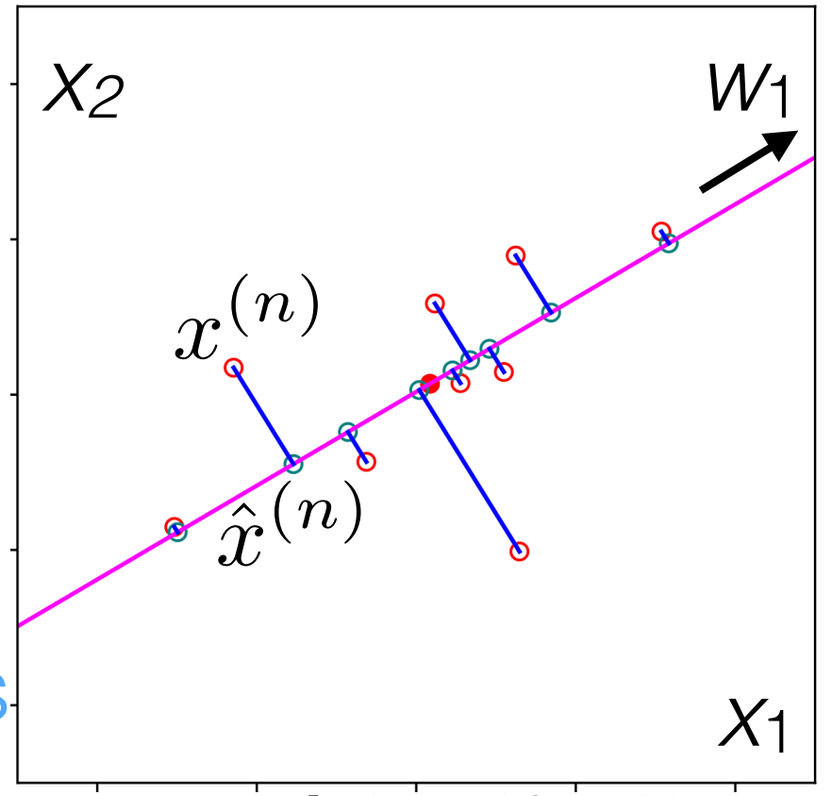

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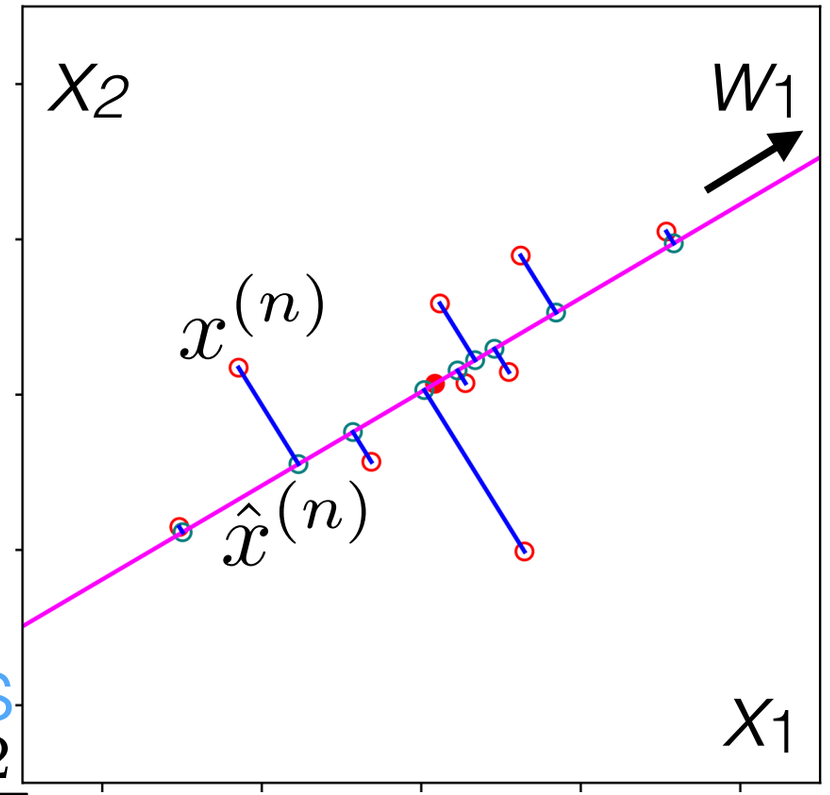

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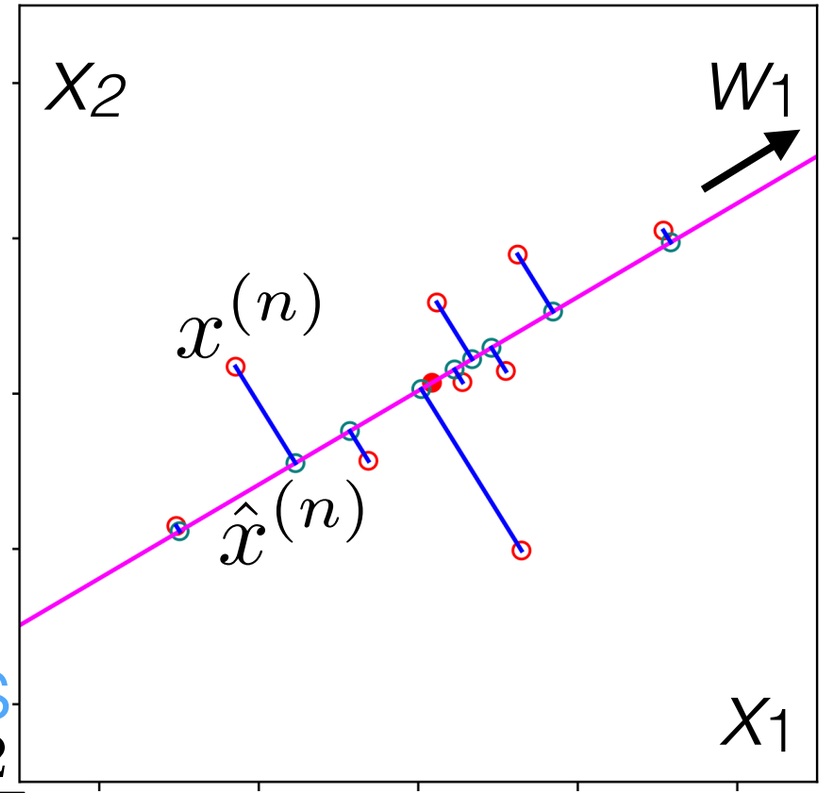

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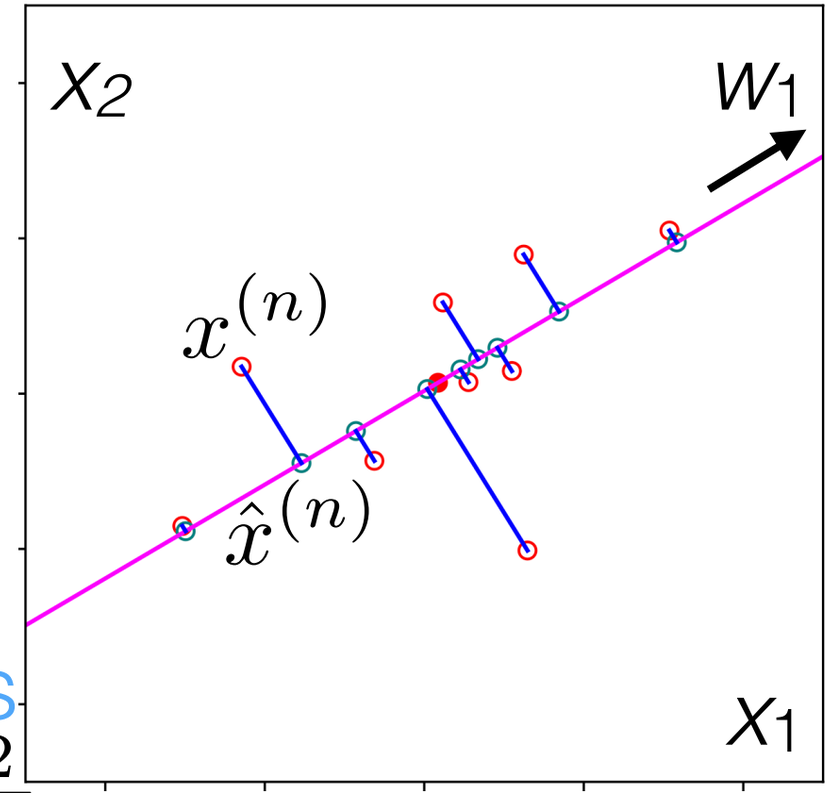

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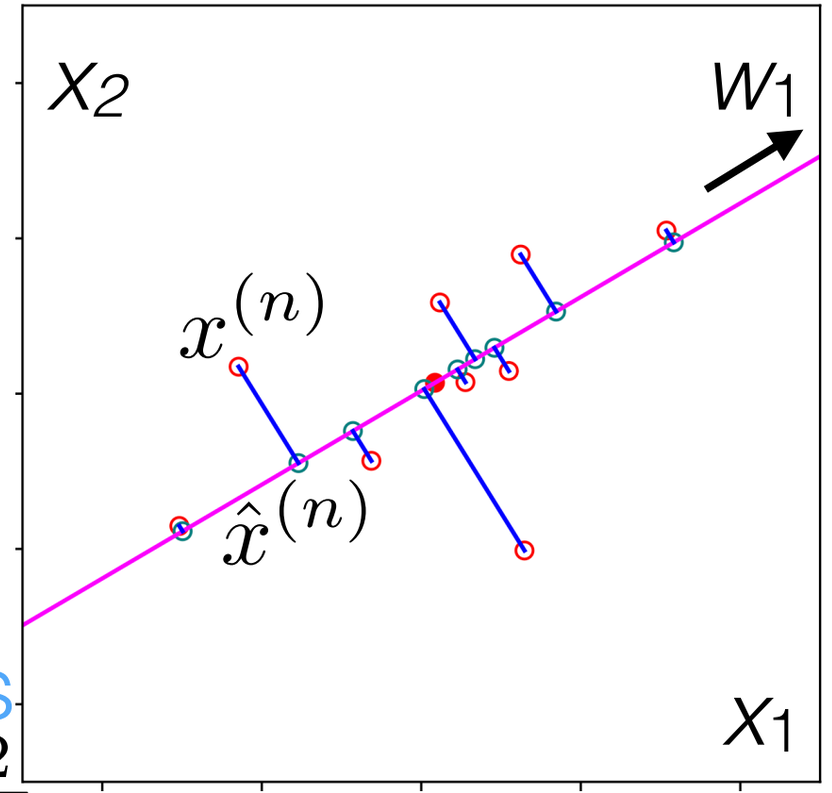

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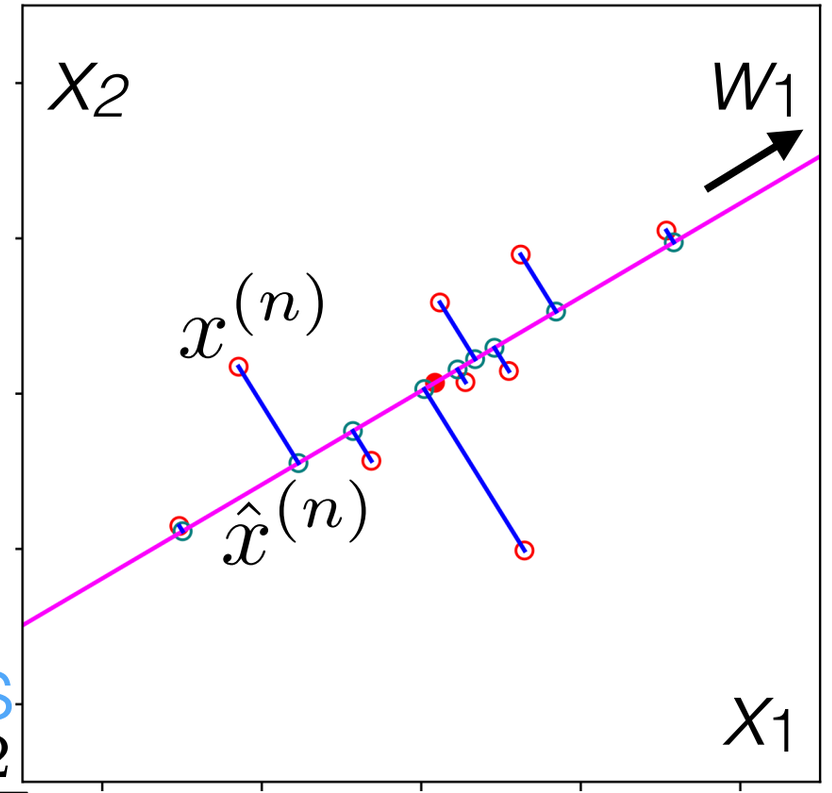

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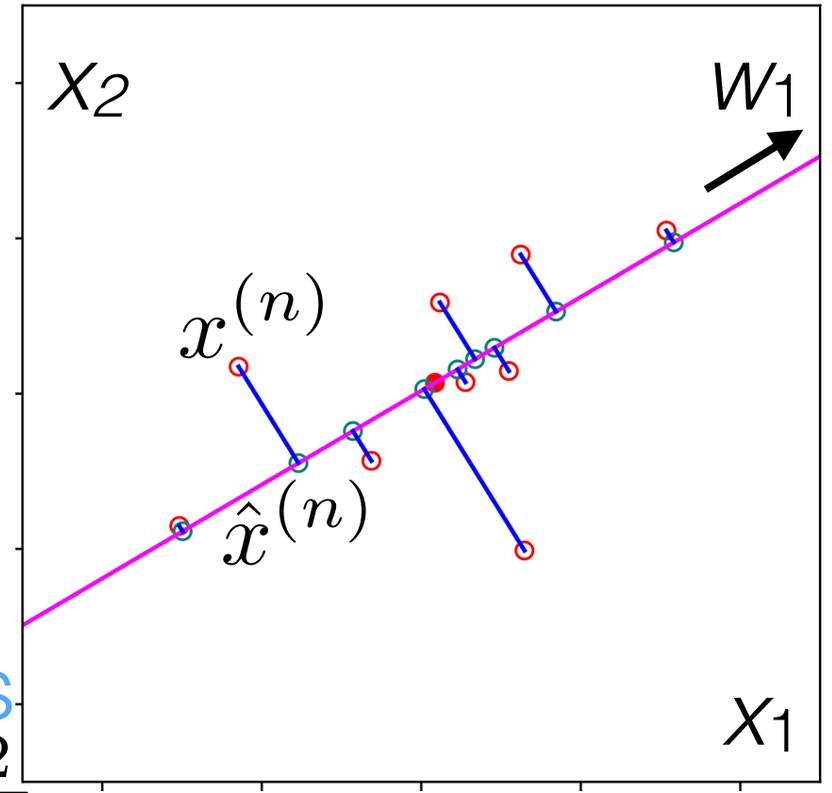

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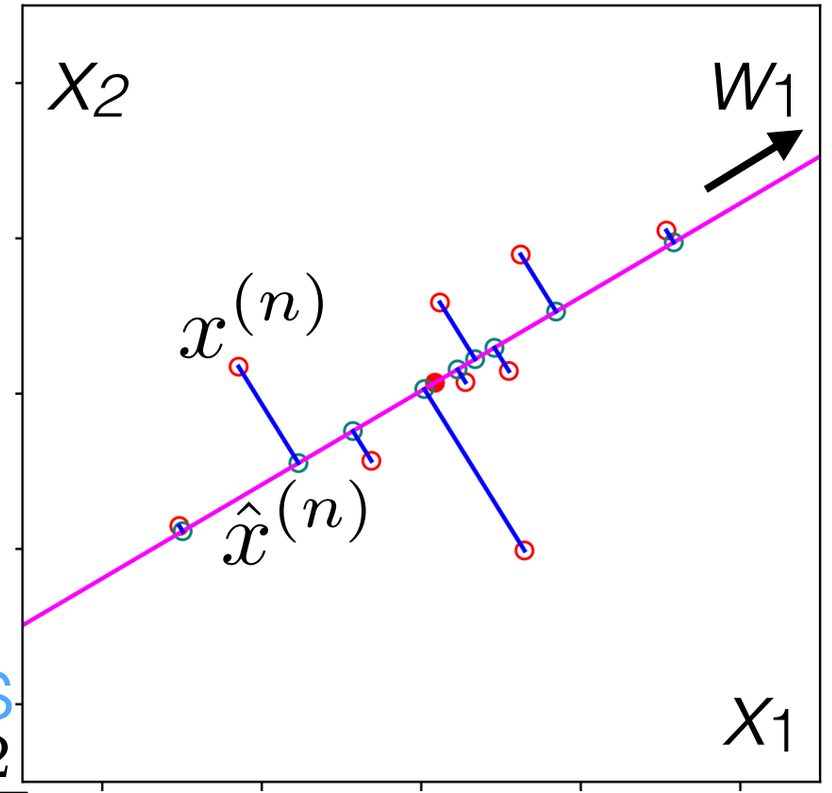

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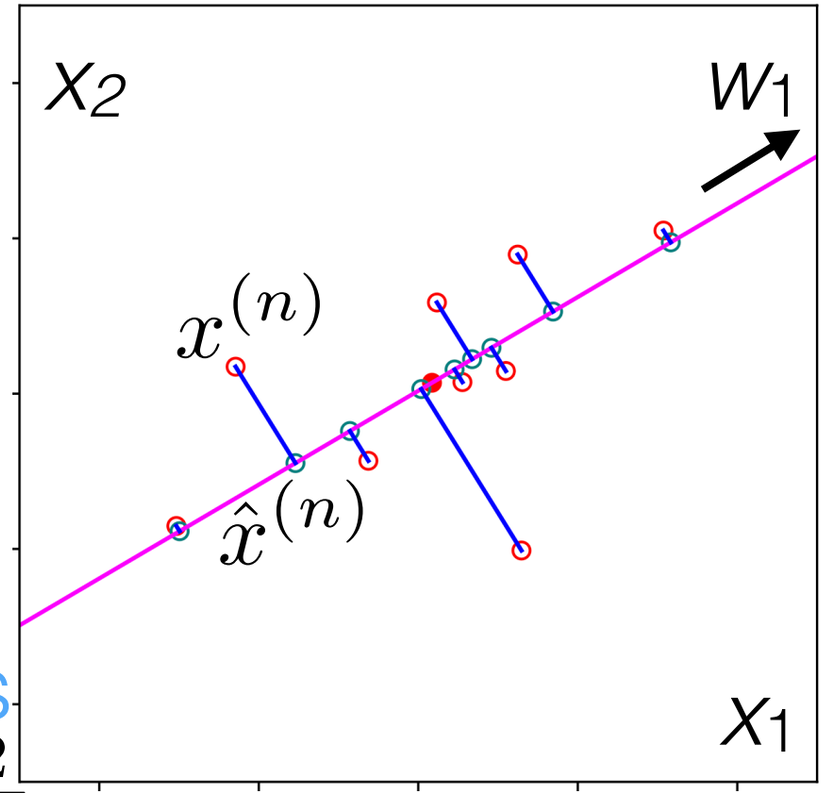

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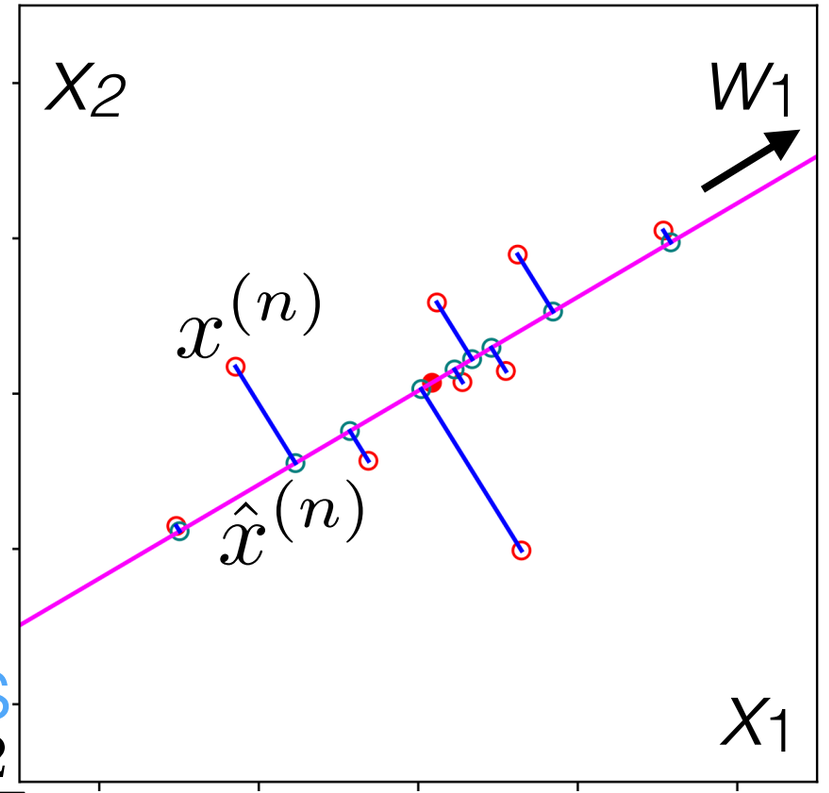

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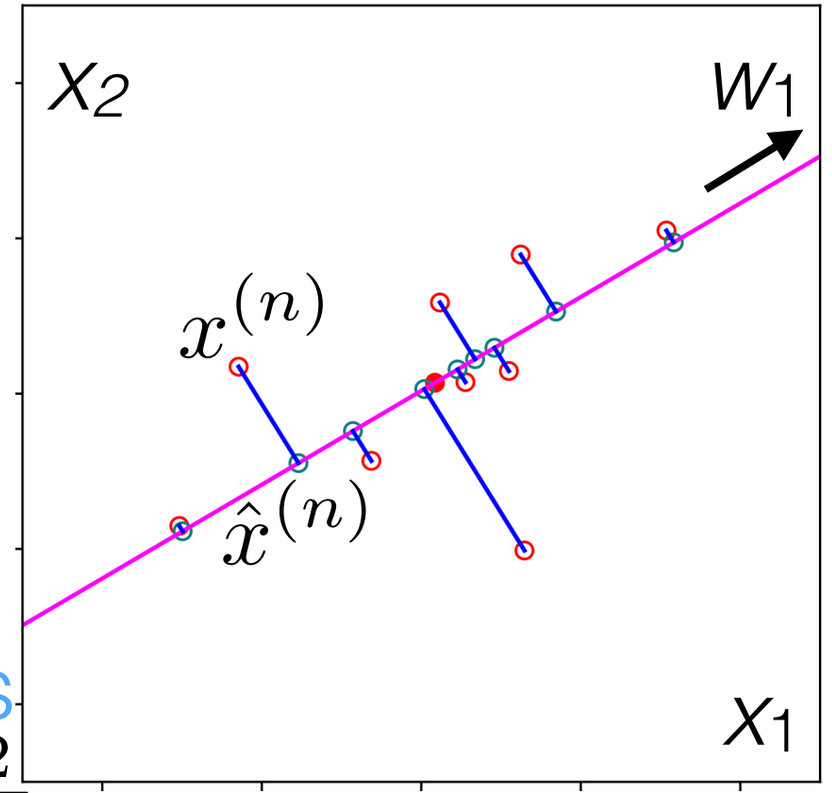

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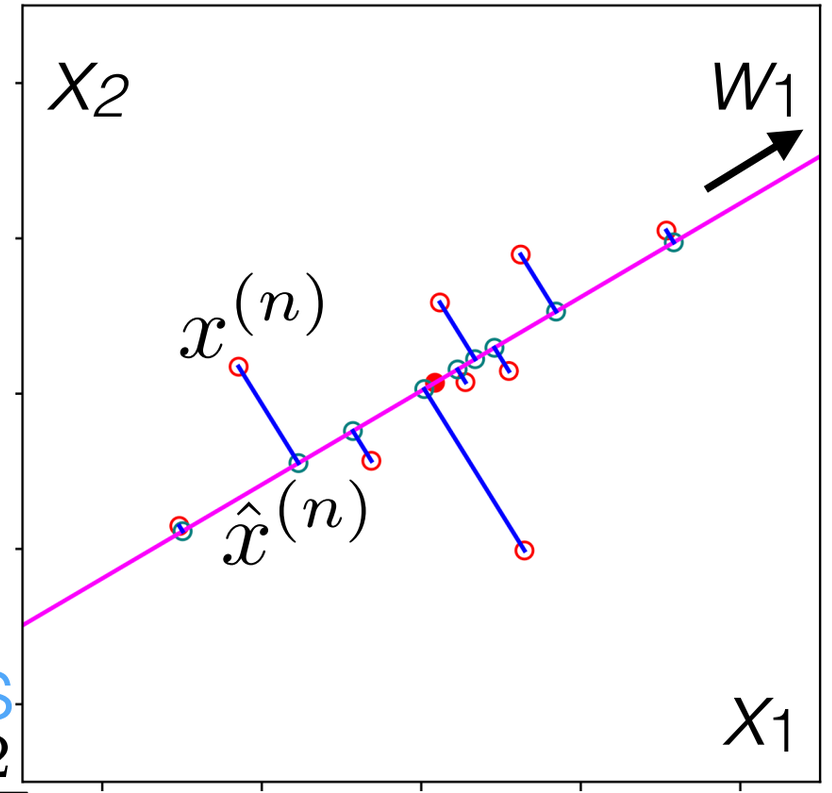

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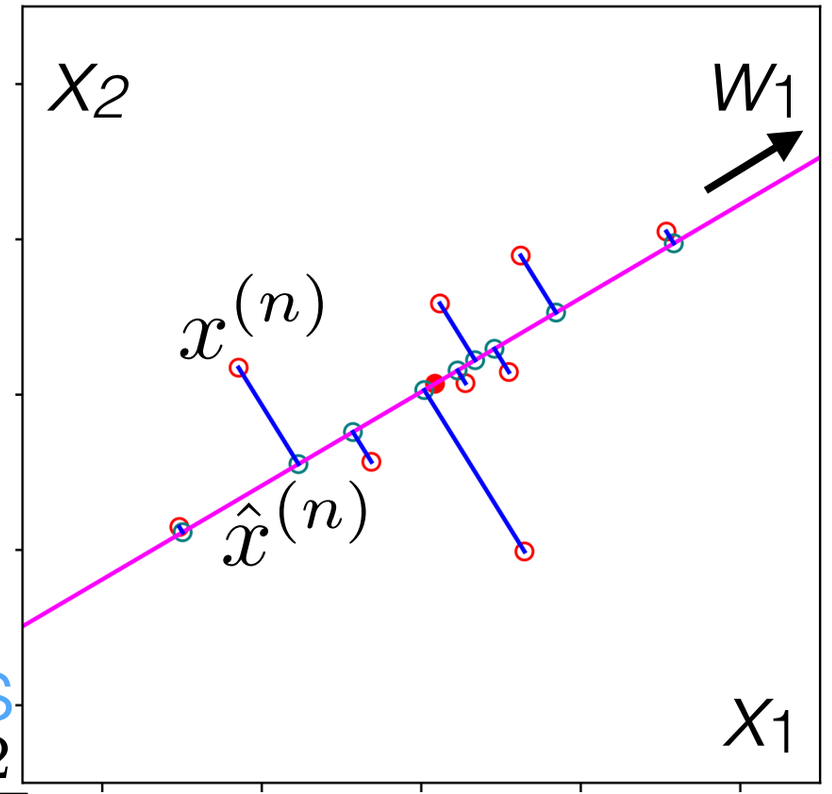

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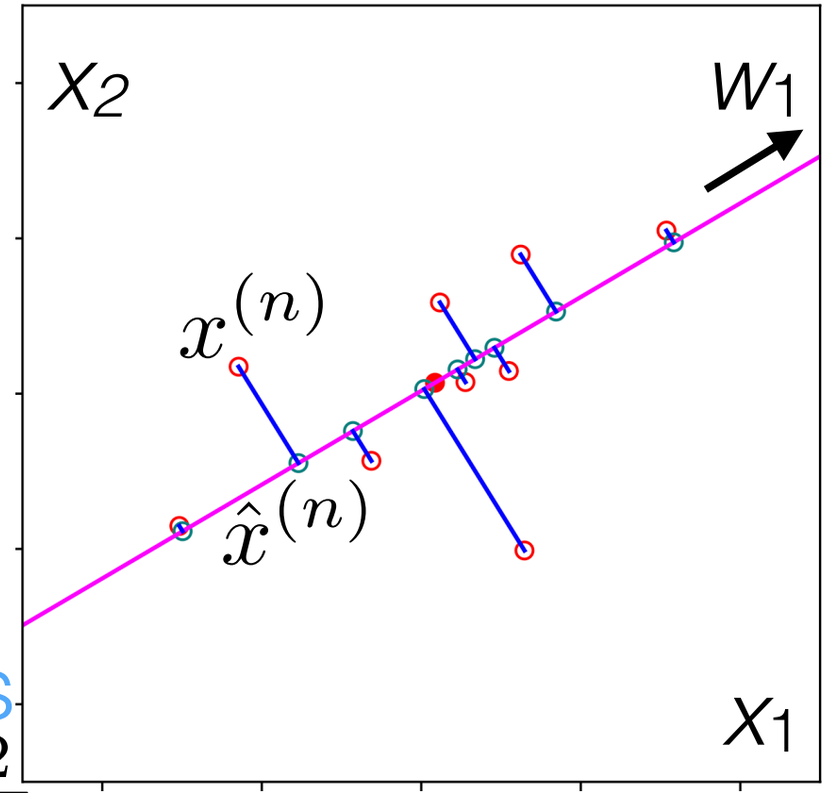

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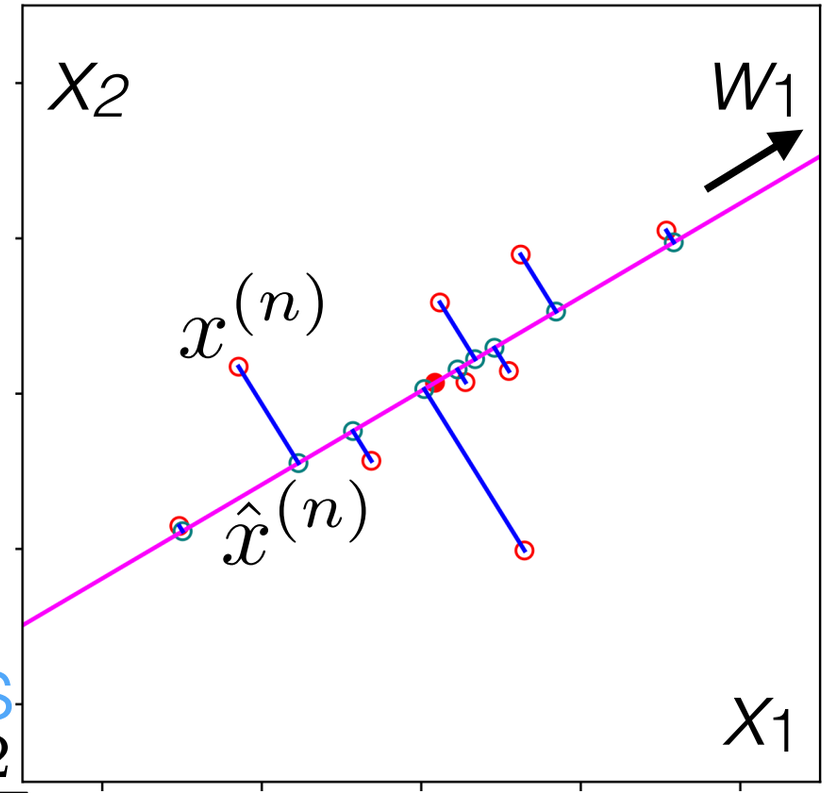

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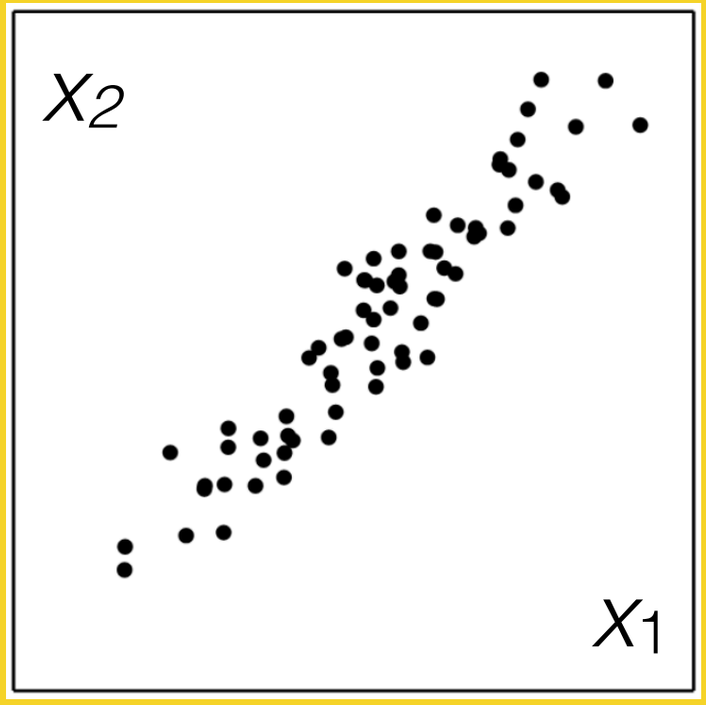

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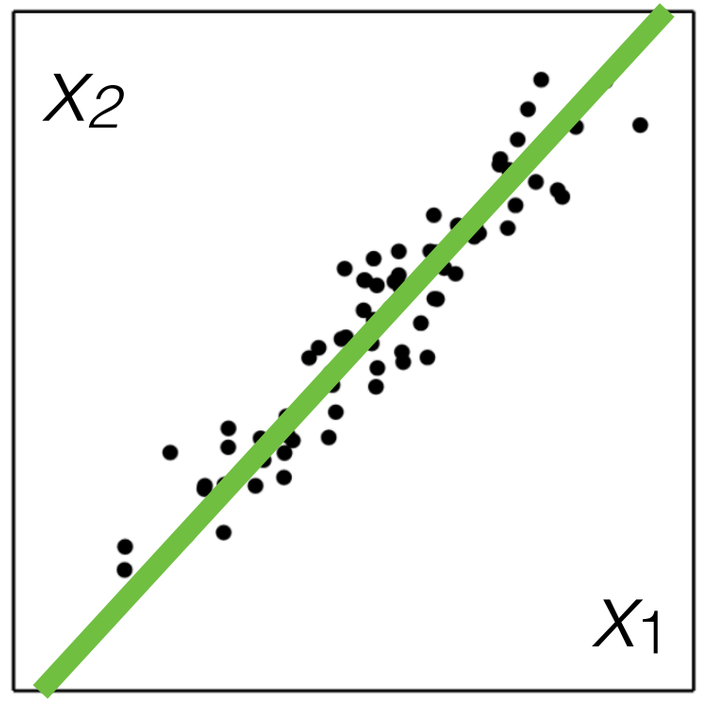

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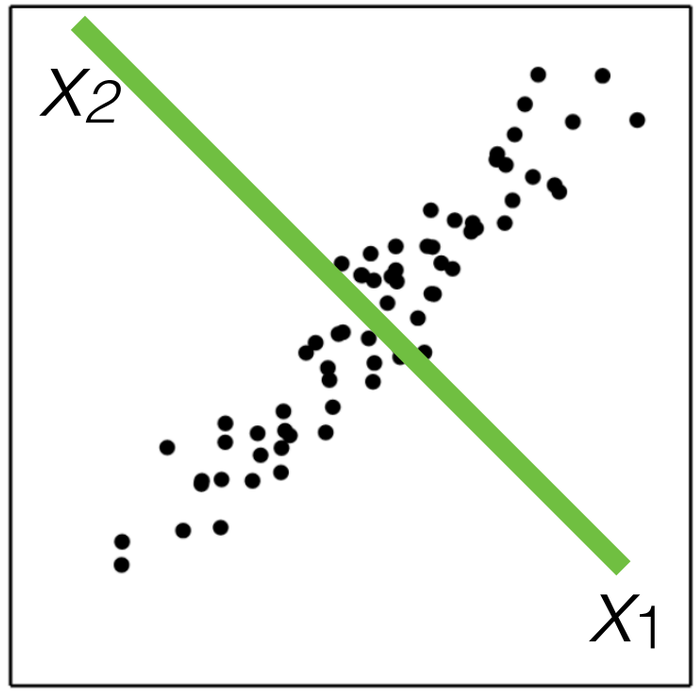

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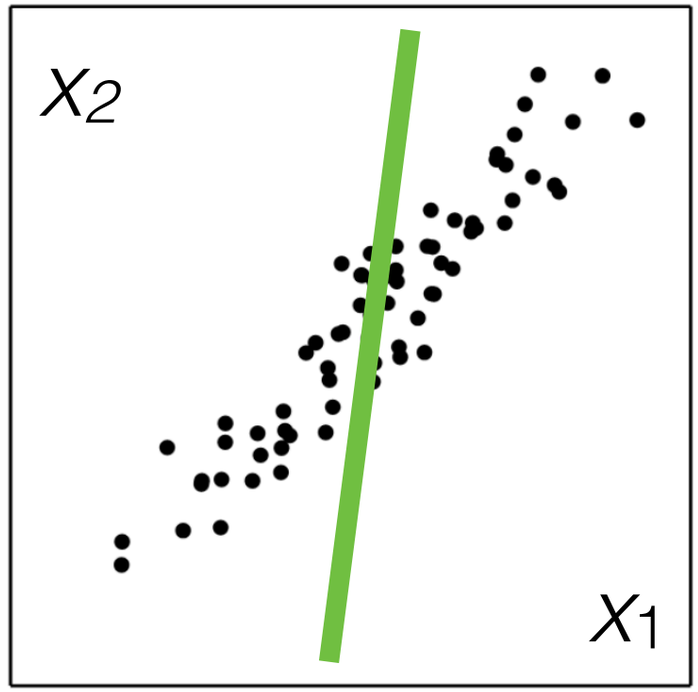

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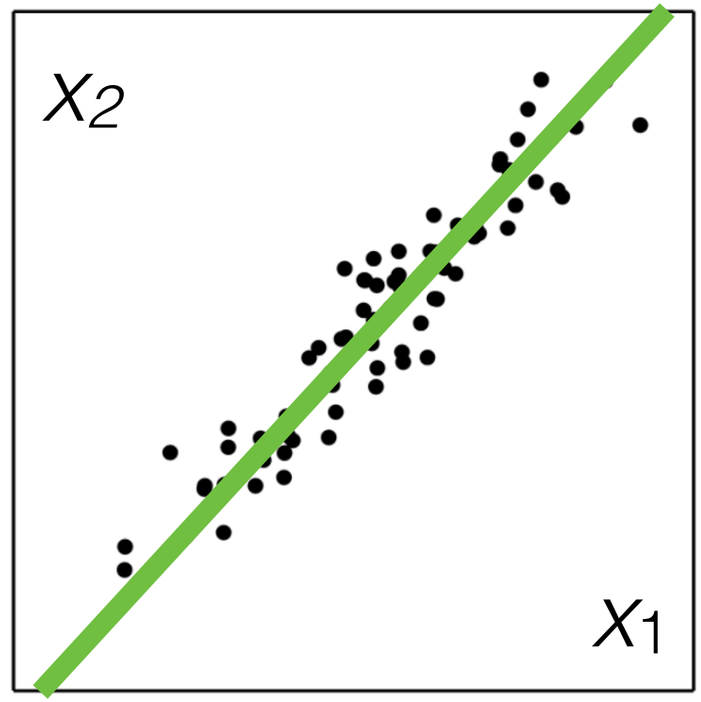

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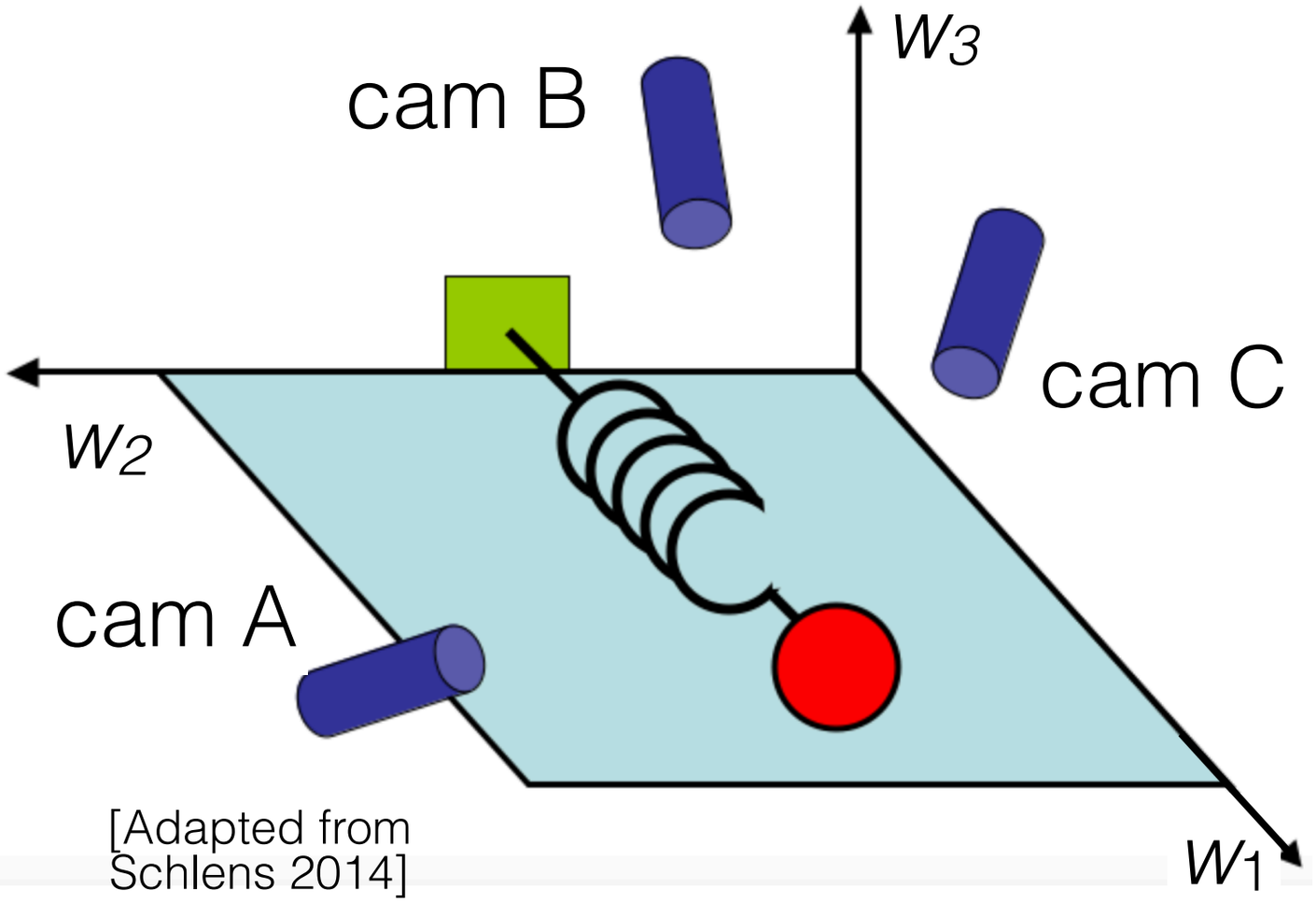

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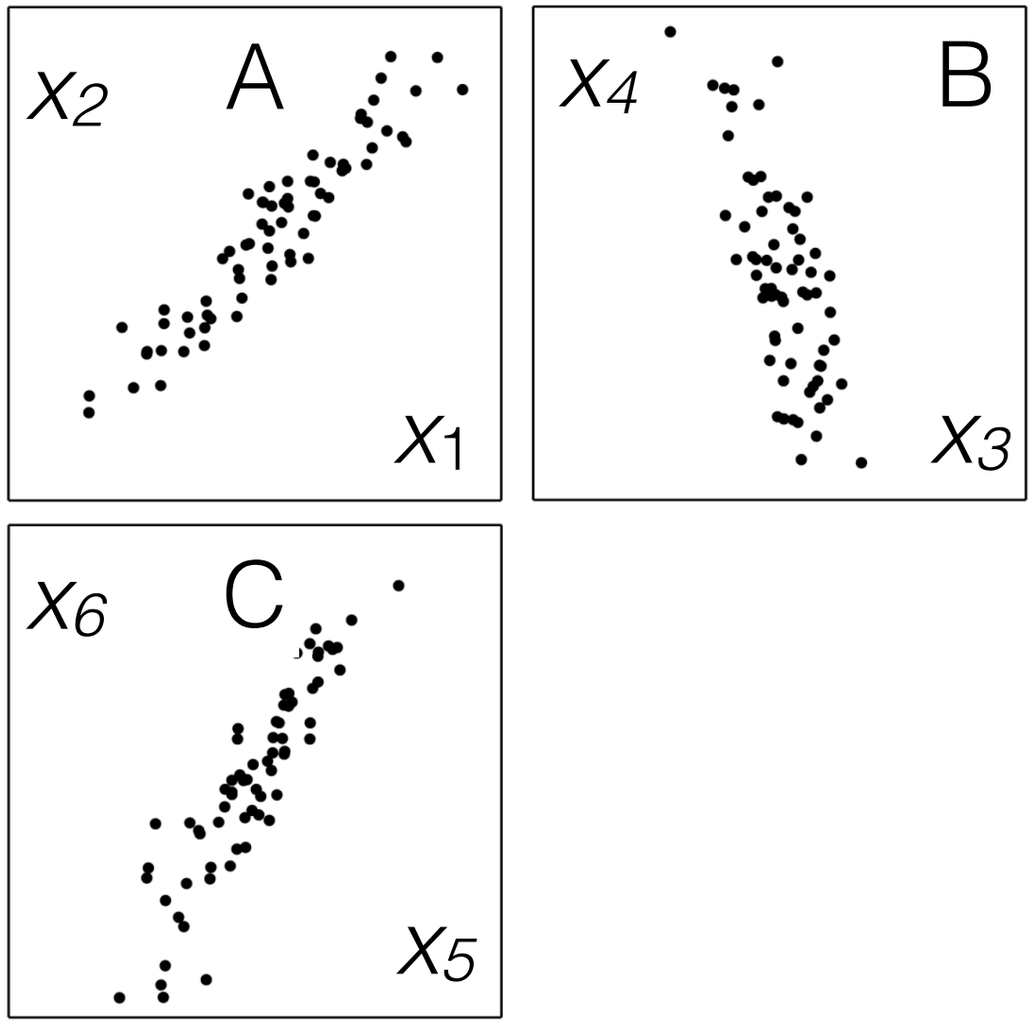

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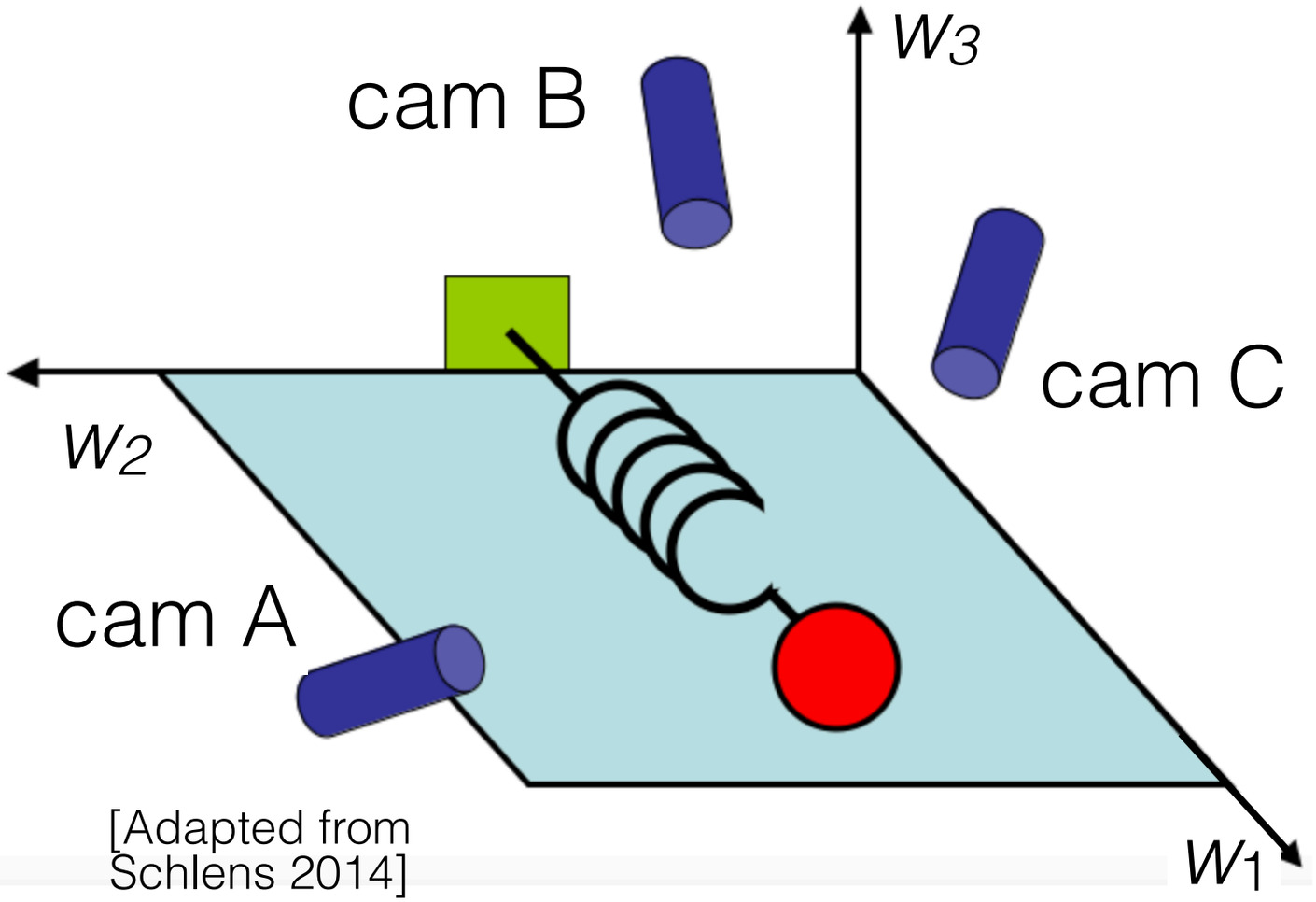

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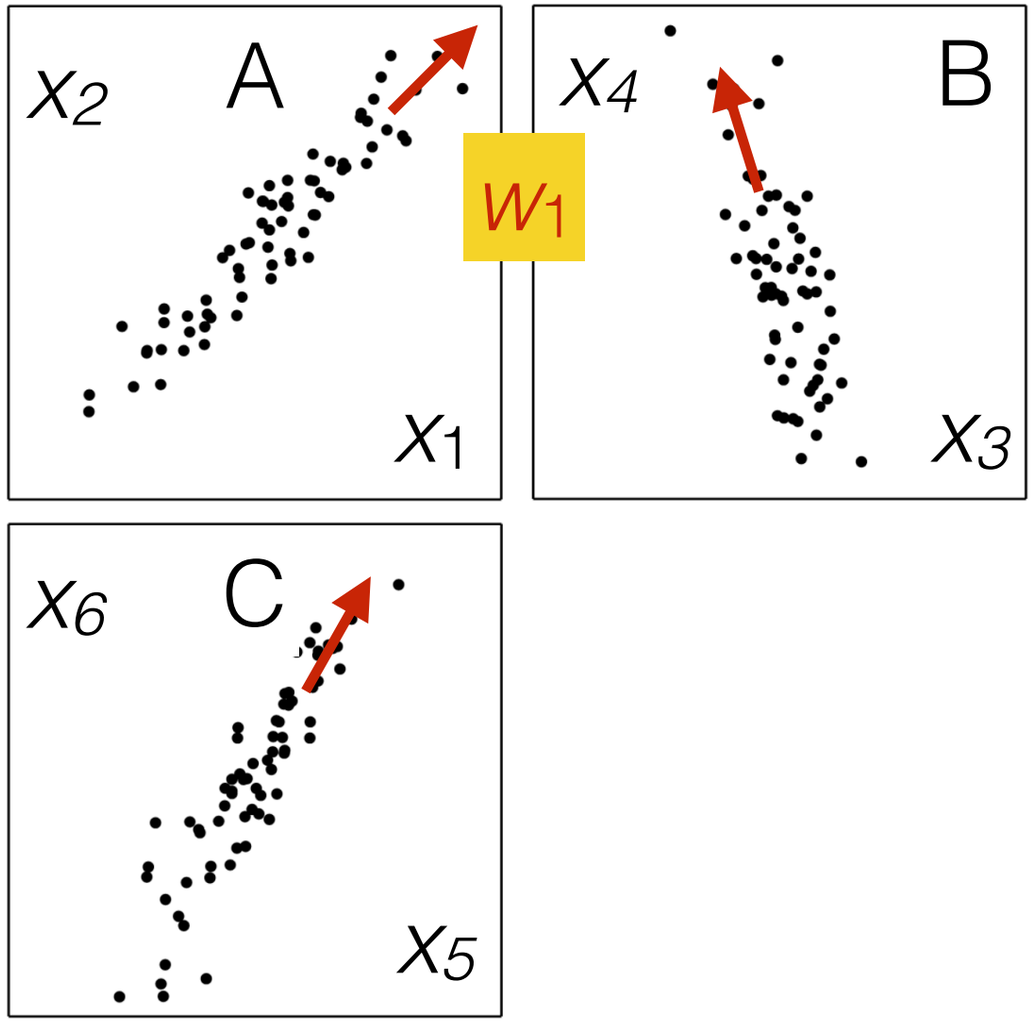

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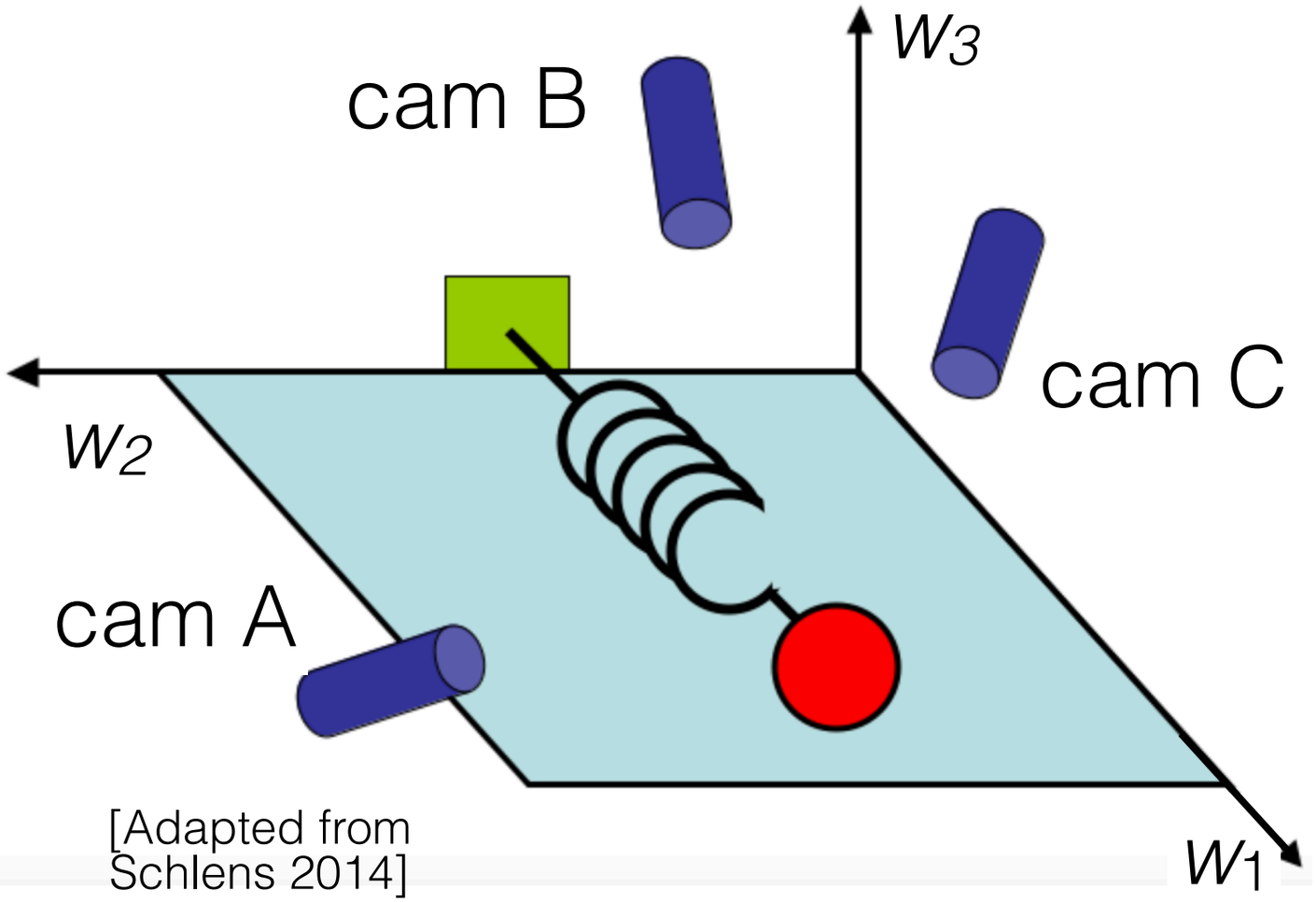

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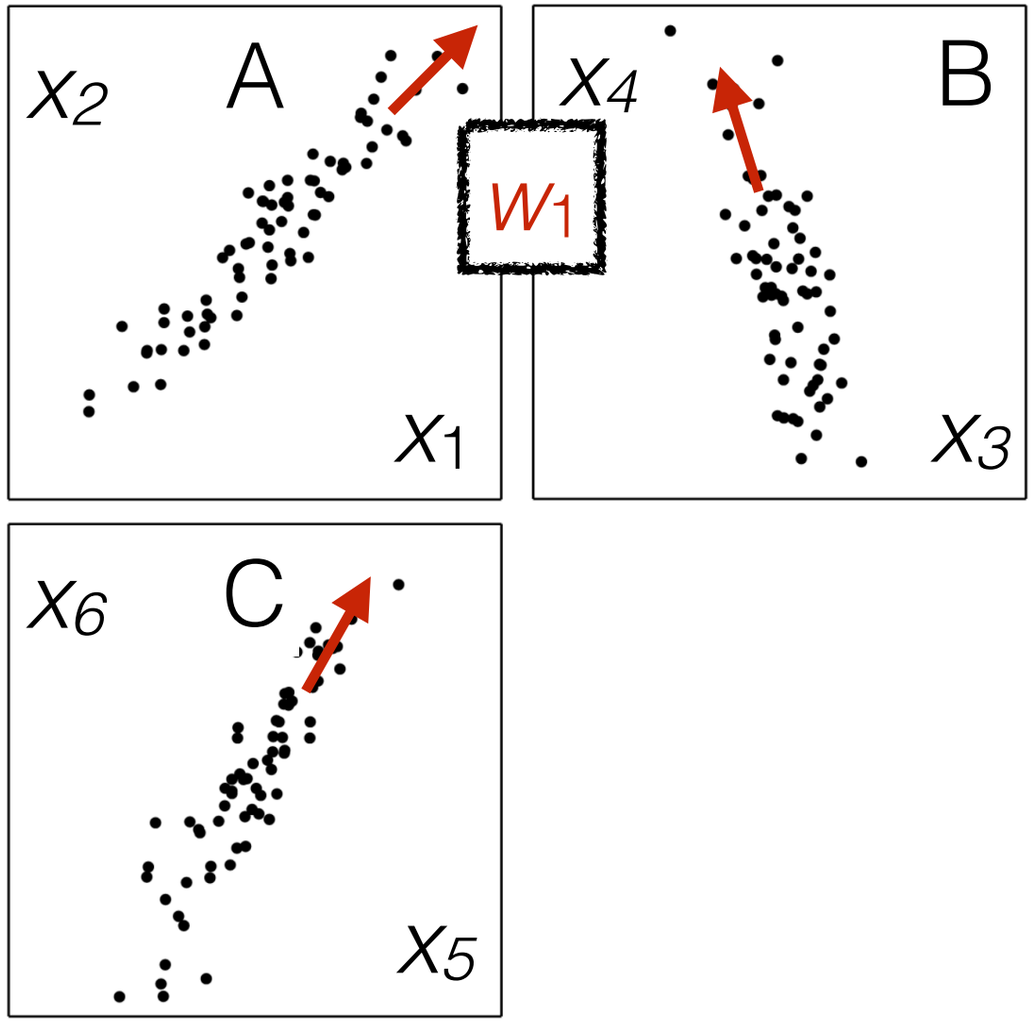

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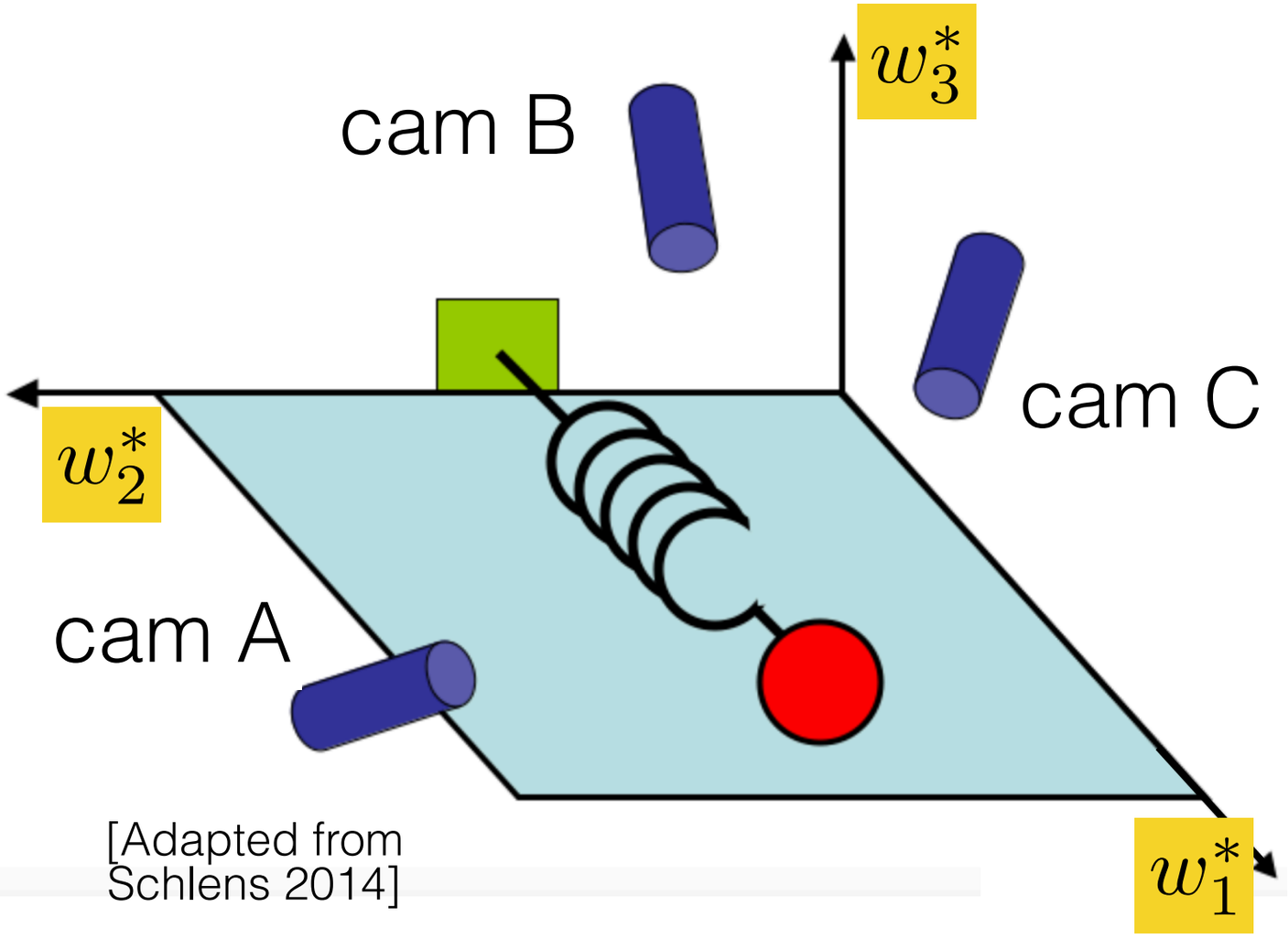

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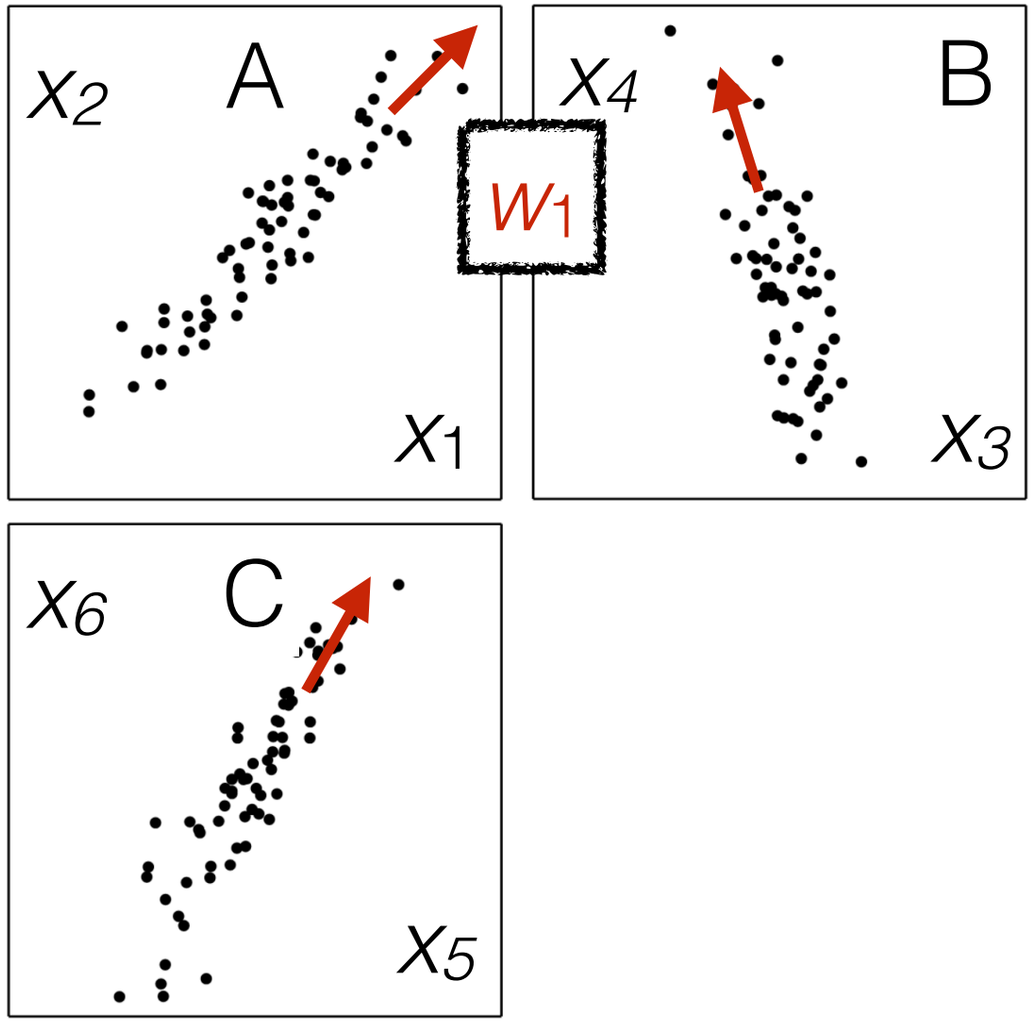

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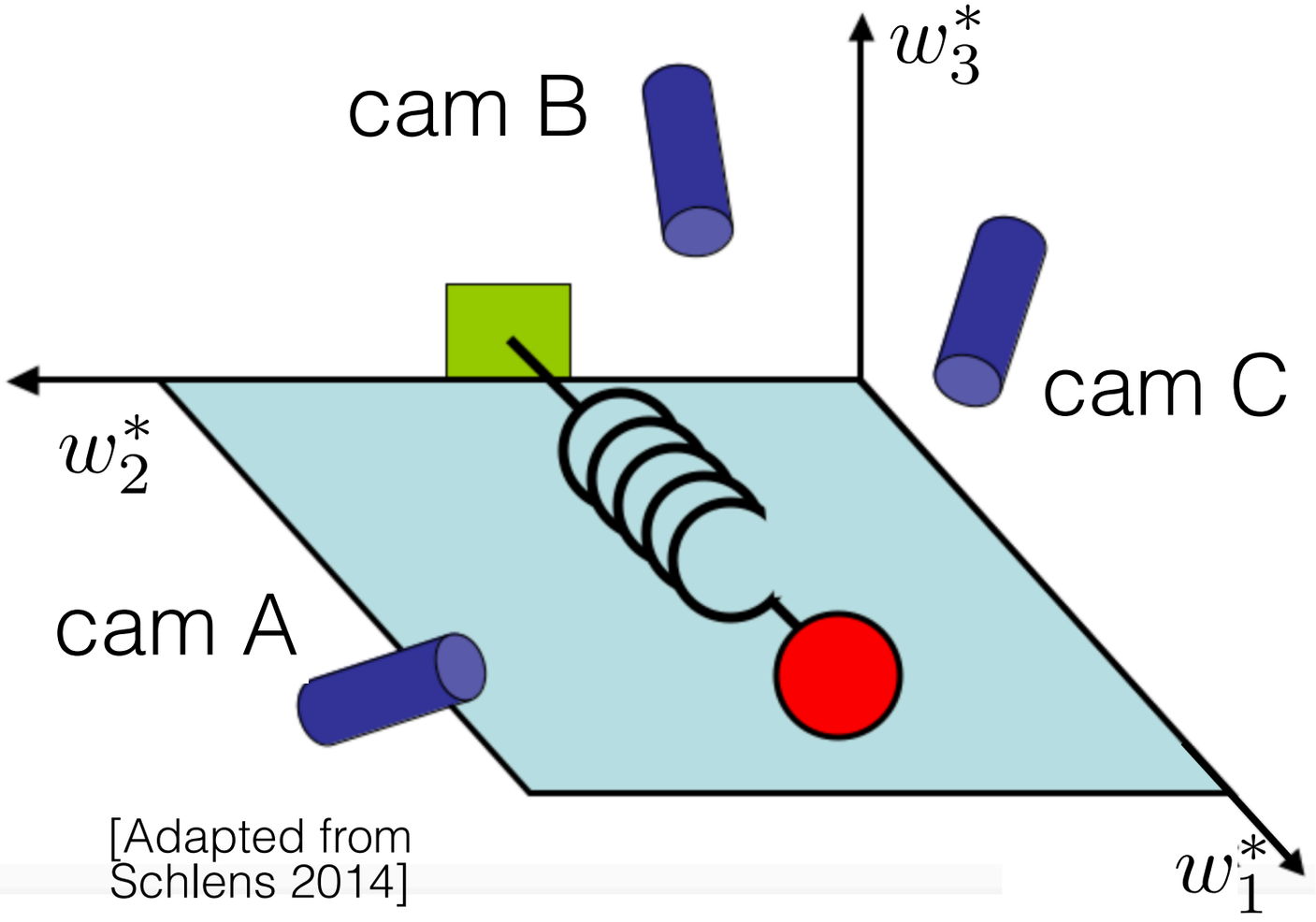

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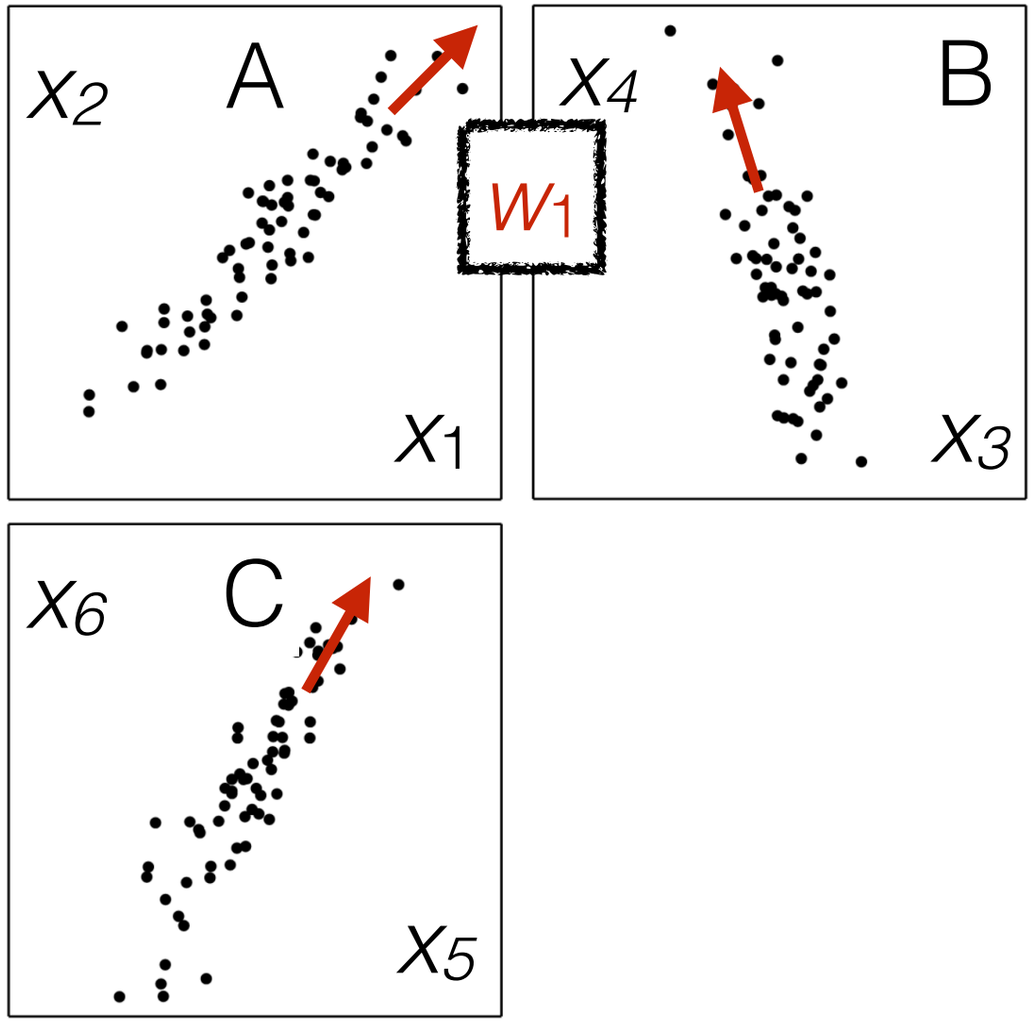

- In our motivating example, we expect PCA to estimate direction of interest well from the observed data

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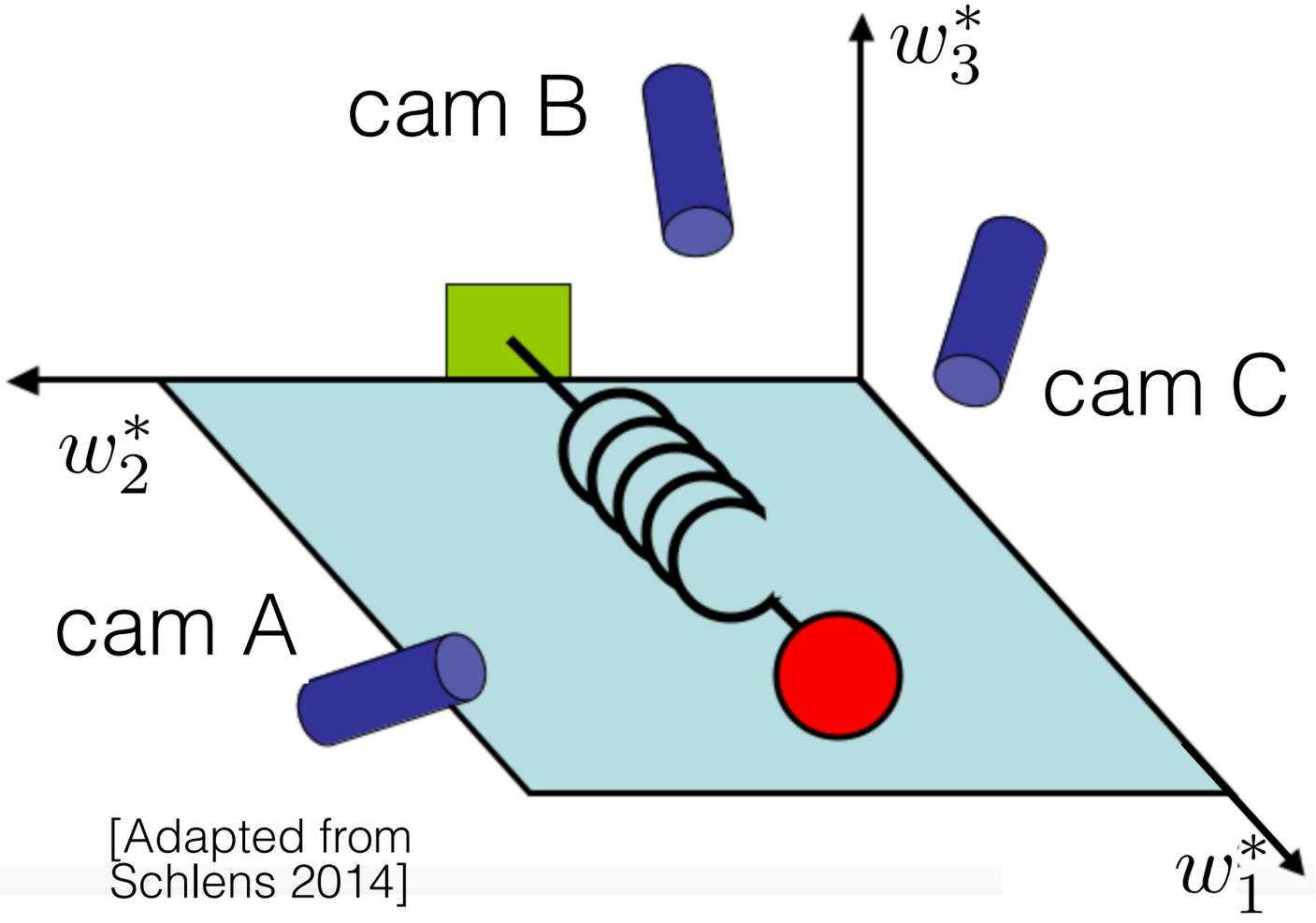

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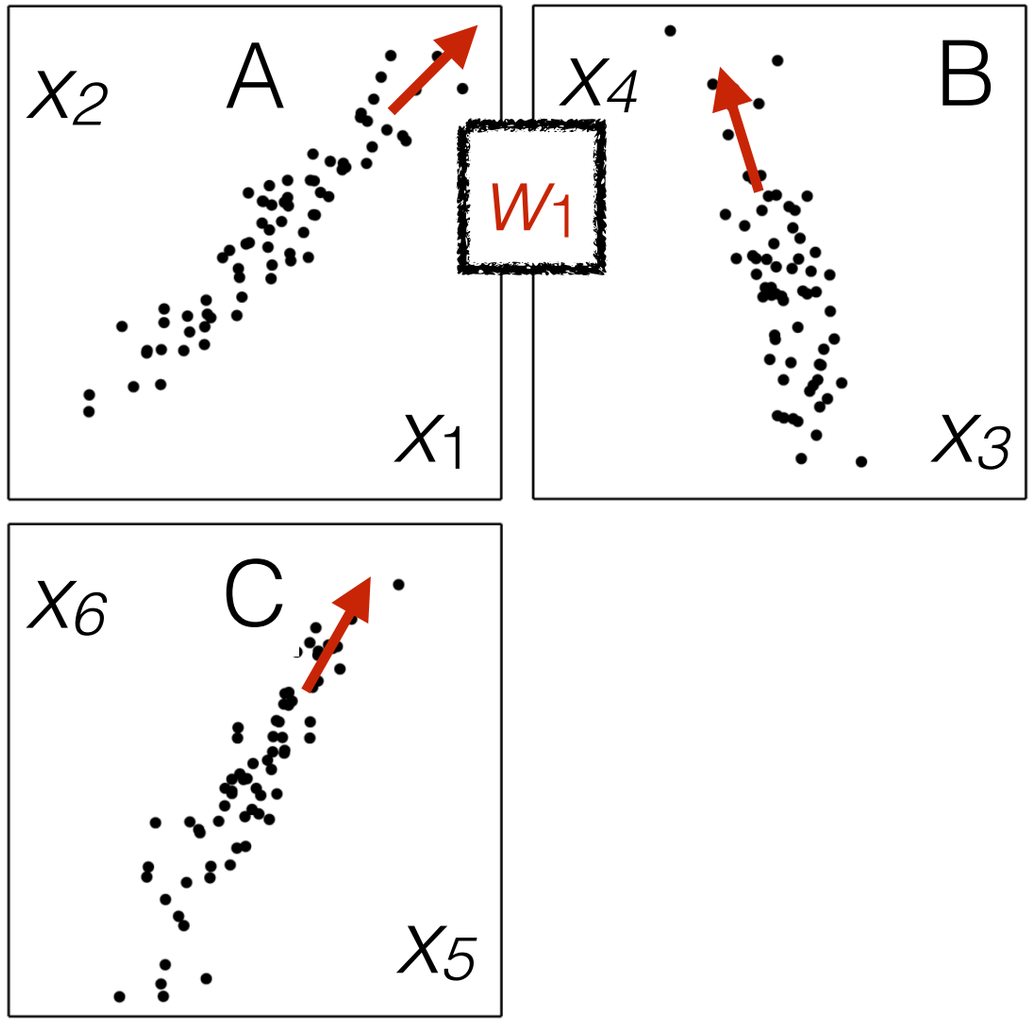
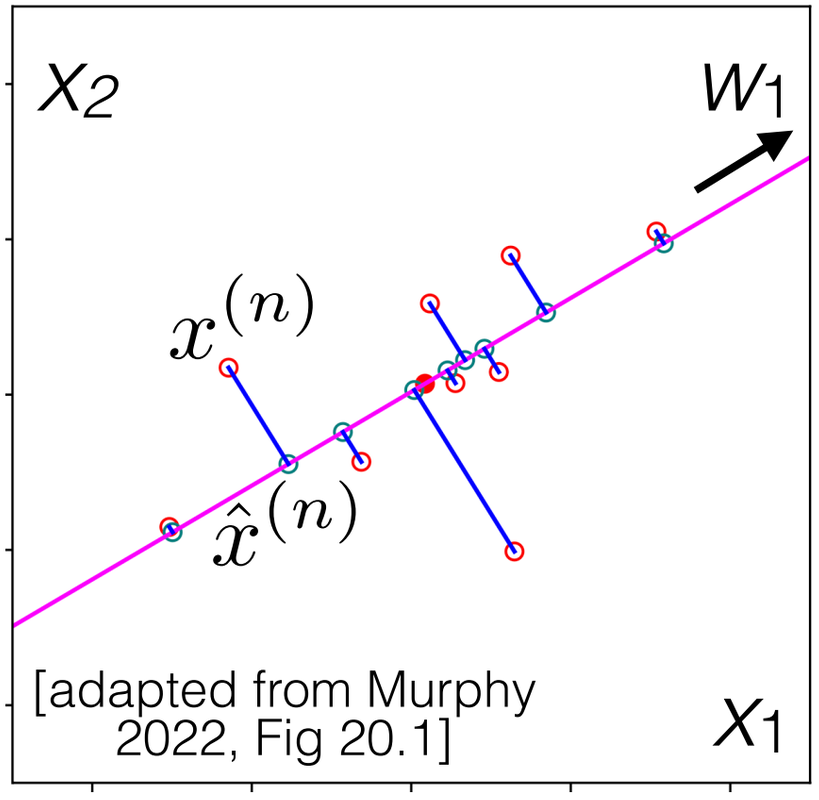


- In our motivating example, we expect PCA to estimate direction of interest well from the observed data
- When plotting, we expect PCA to find coordinates that most distribute the data out across the plot (max variance)

Challenges of PCA



Challenges of PCA

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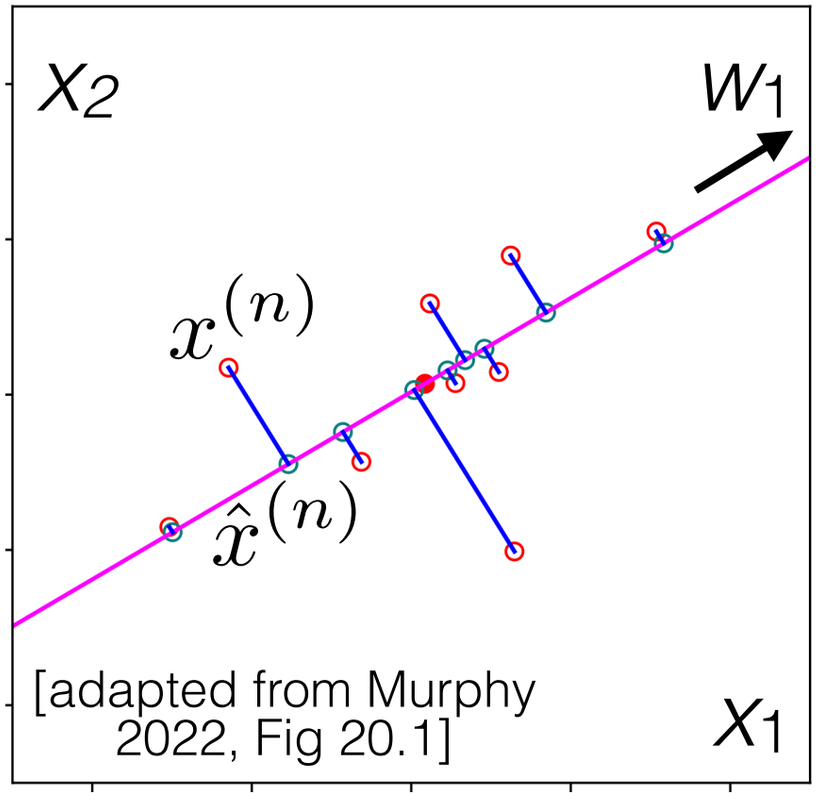

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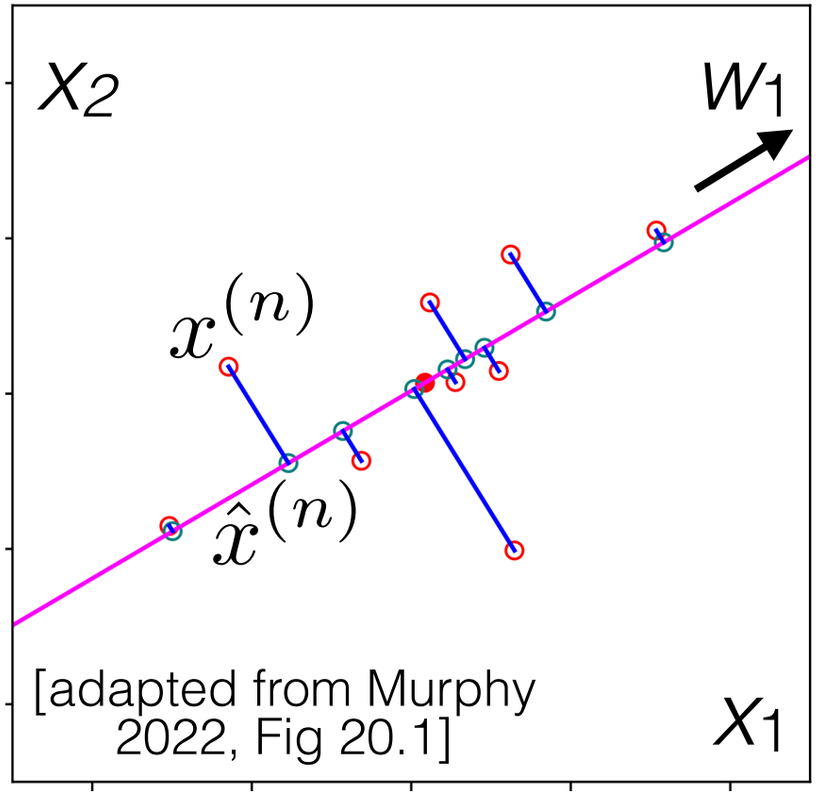

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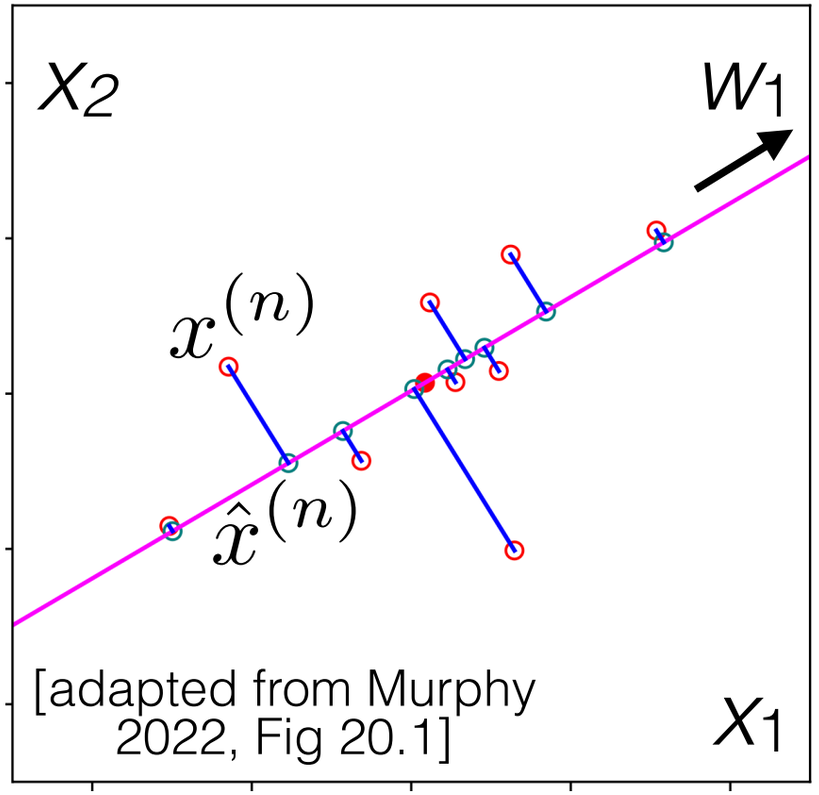

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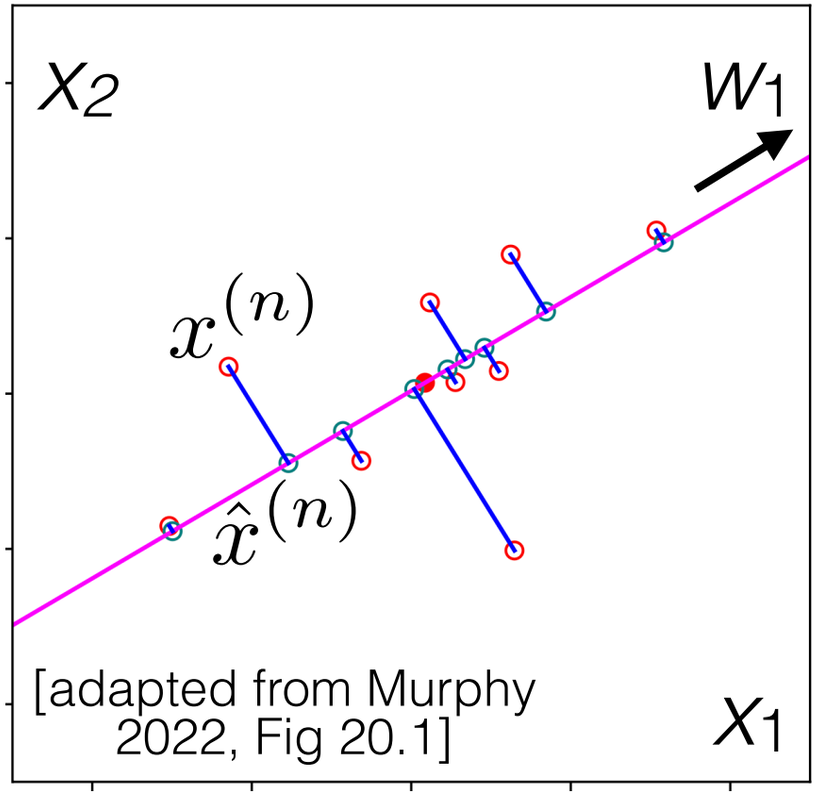

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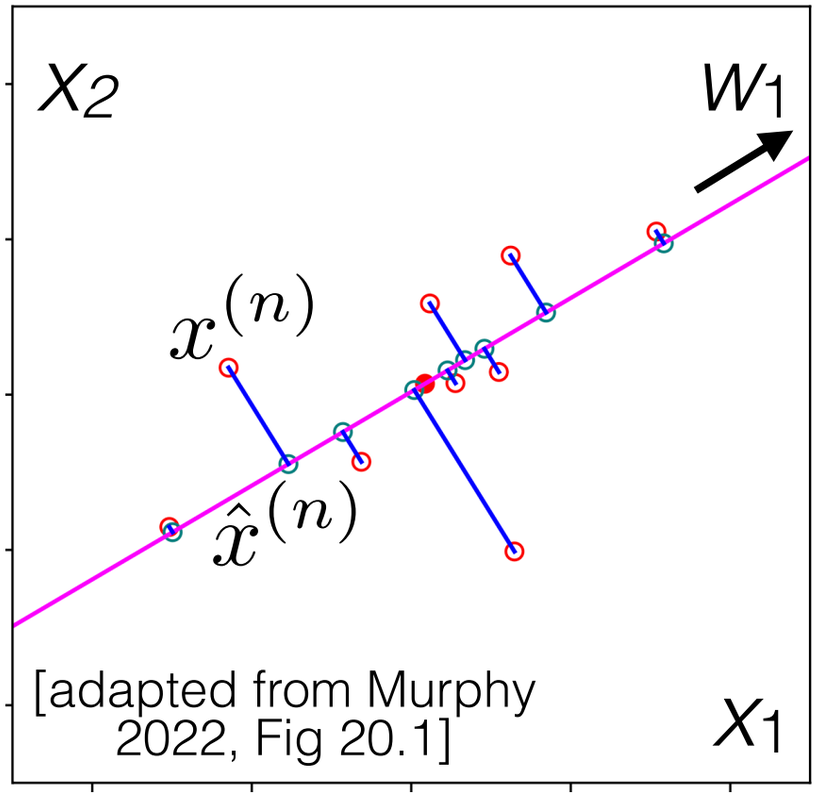

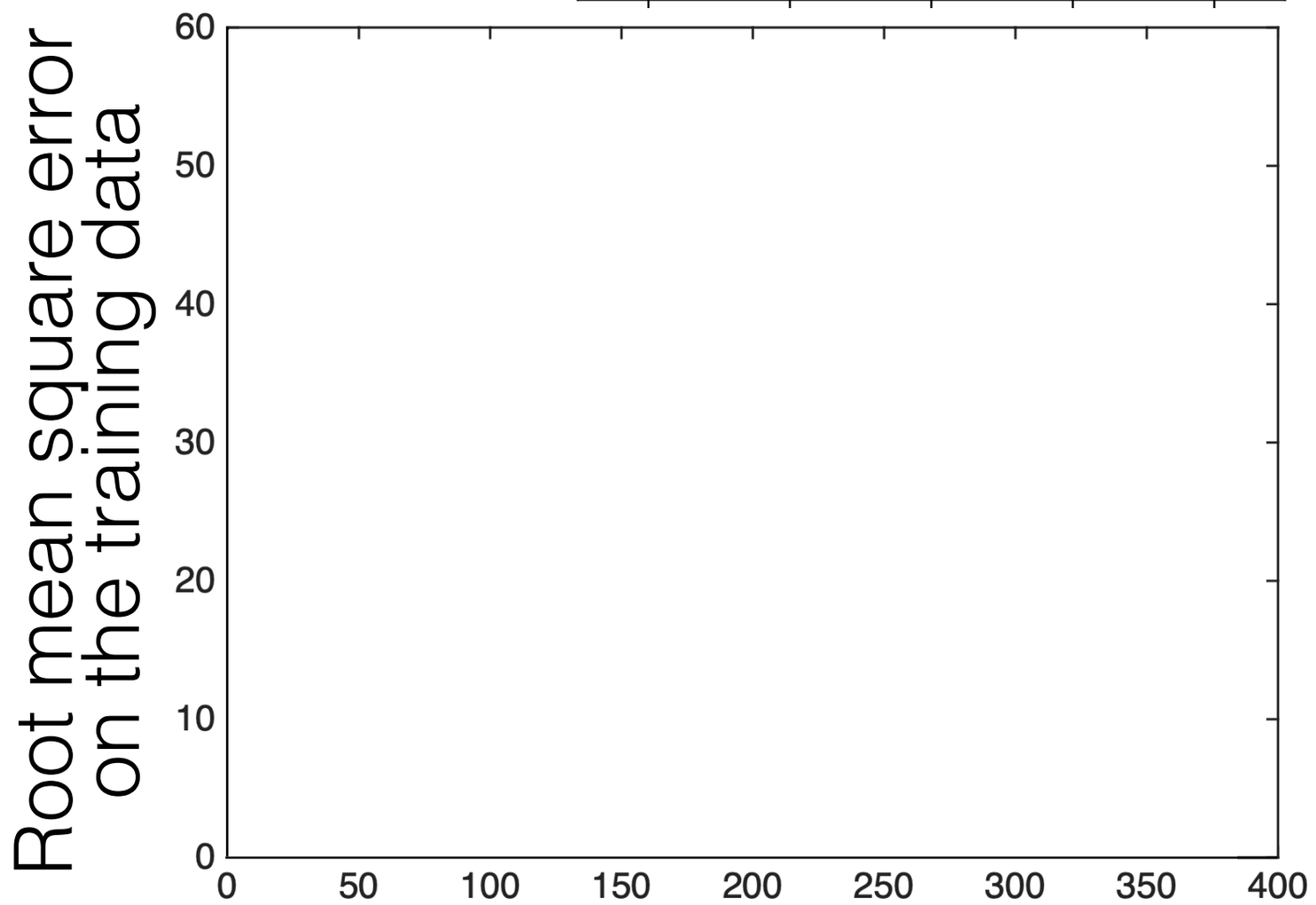

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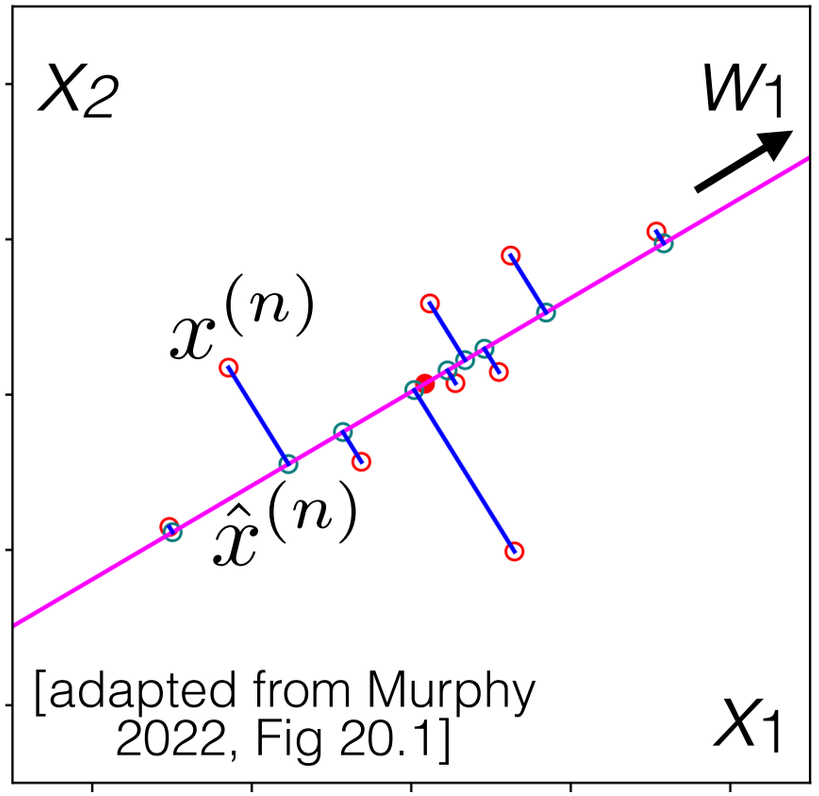

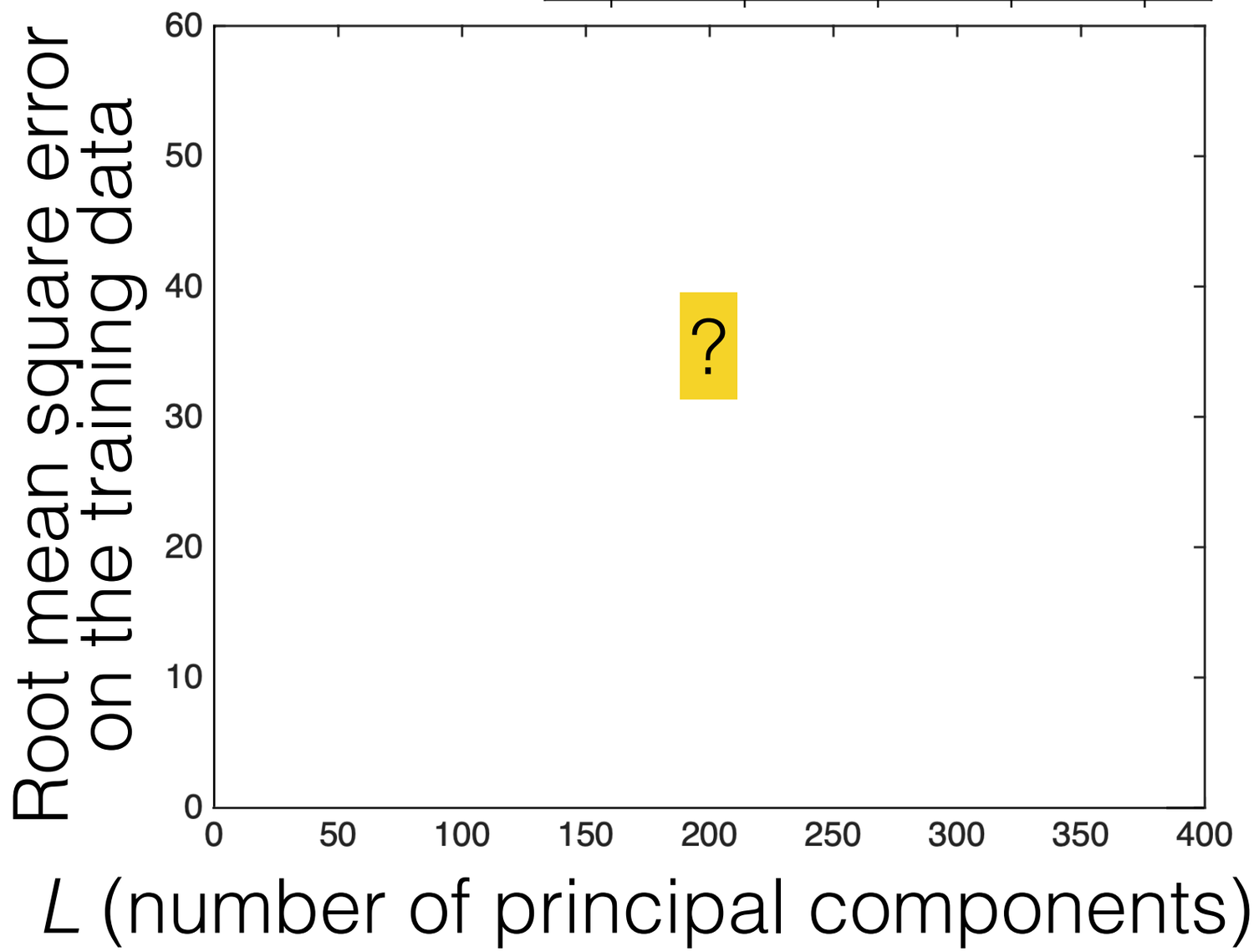

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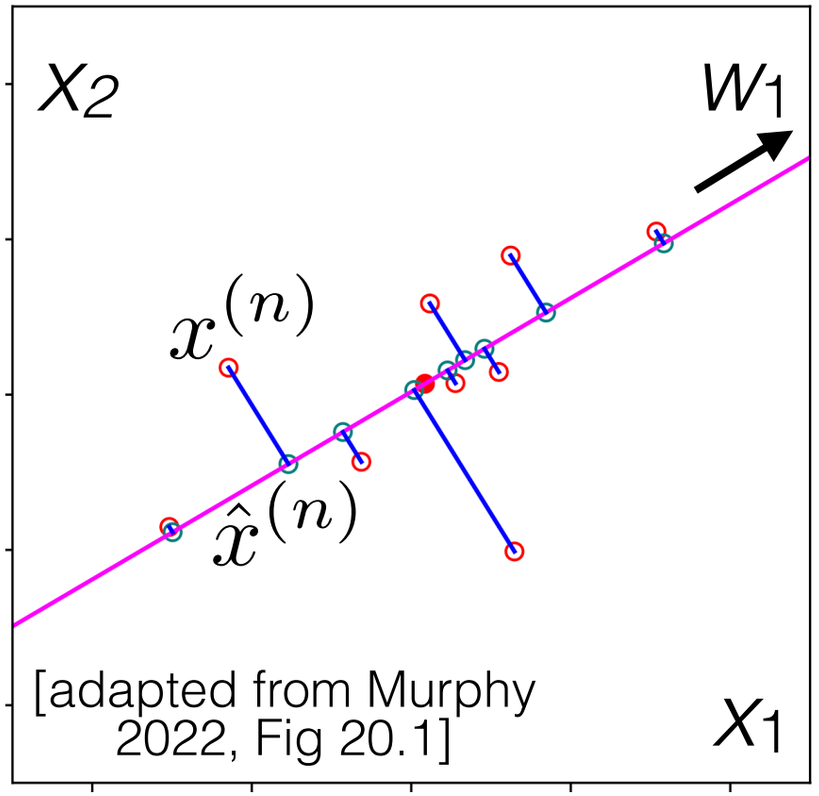

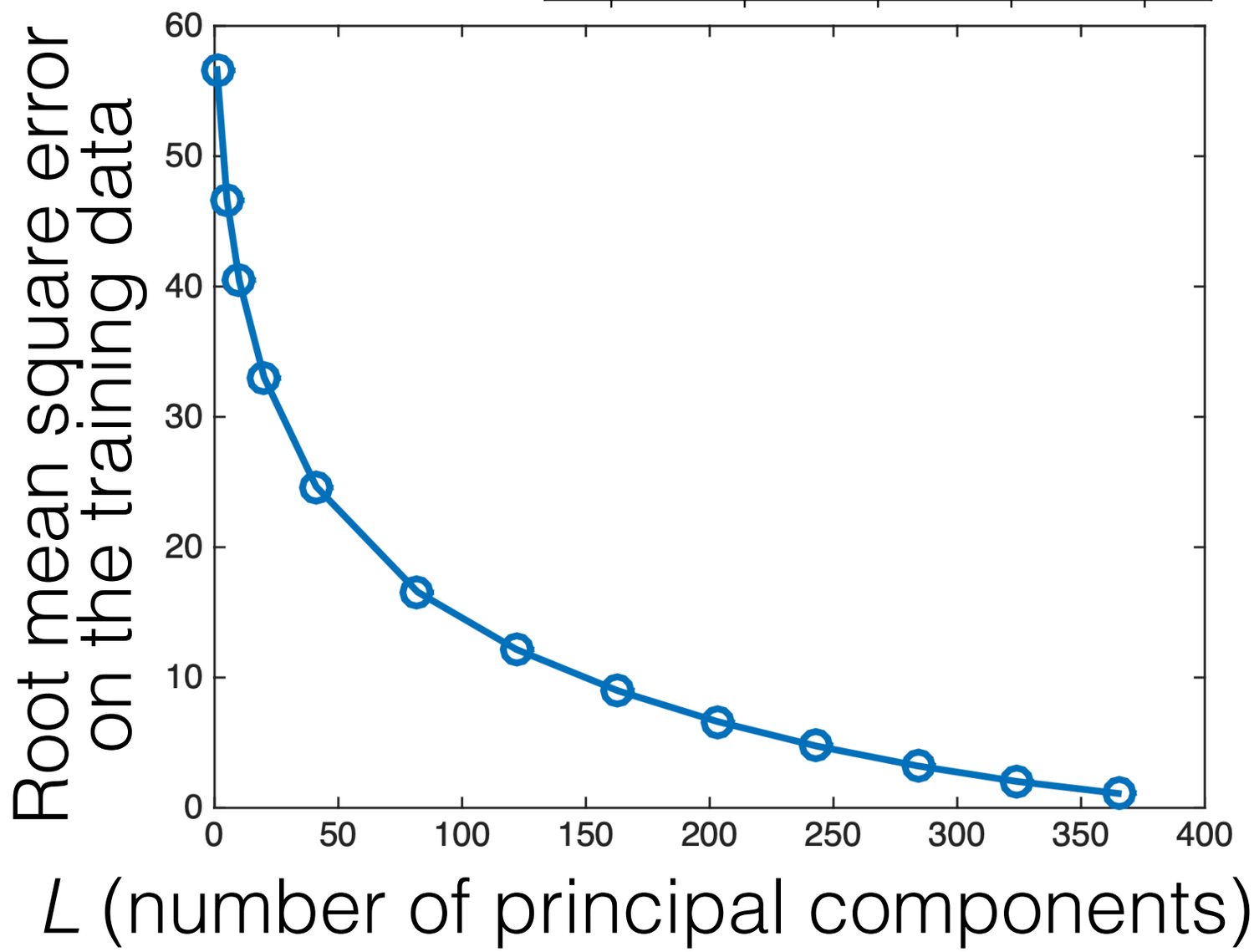

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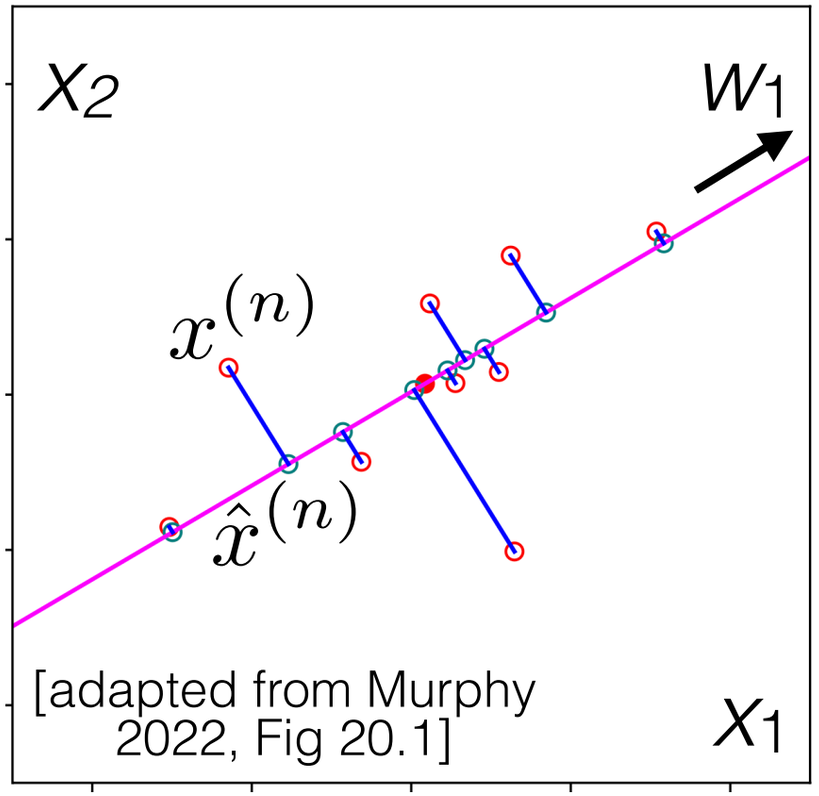

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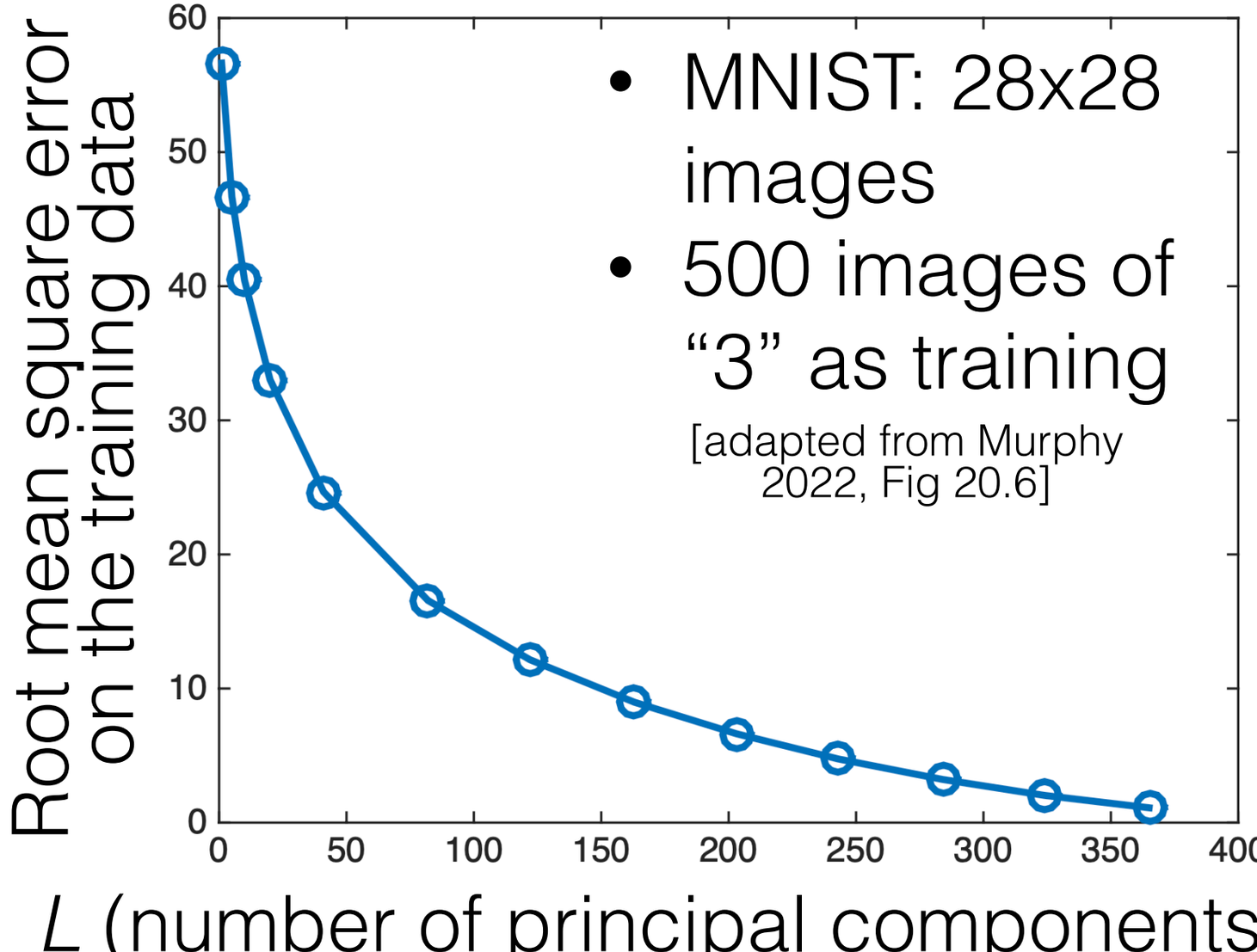

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- 500 images of "3" as training

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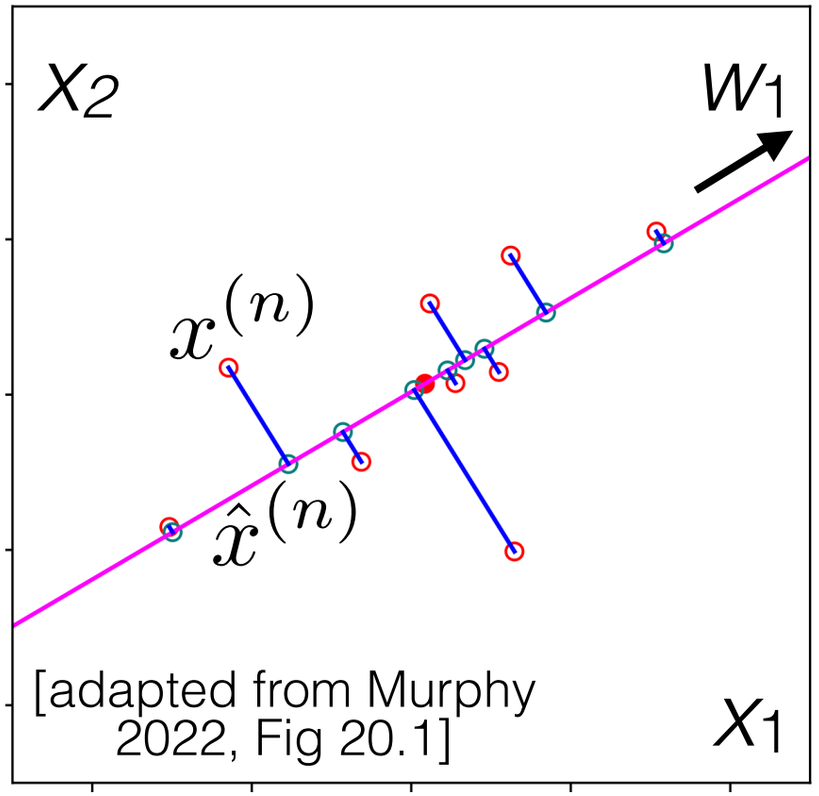

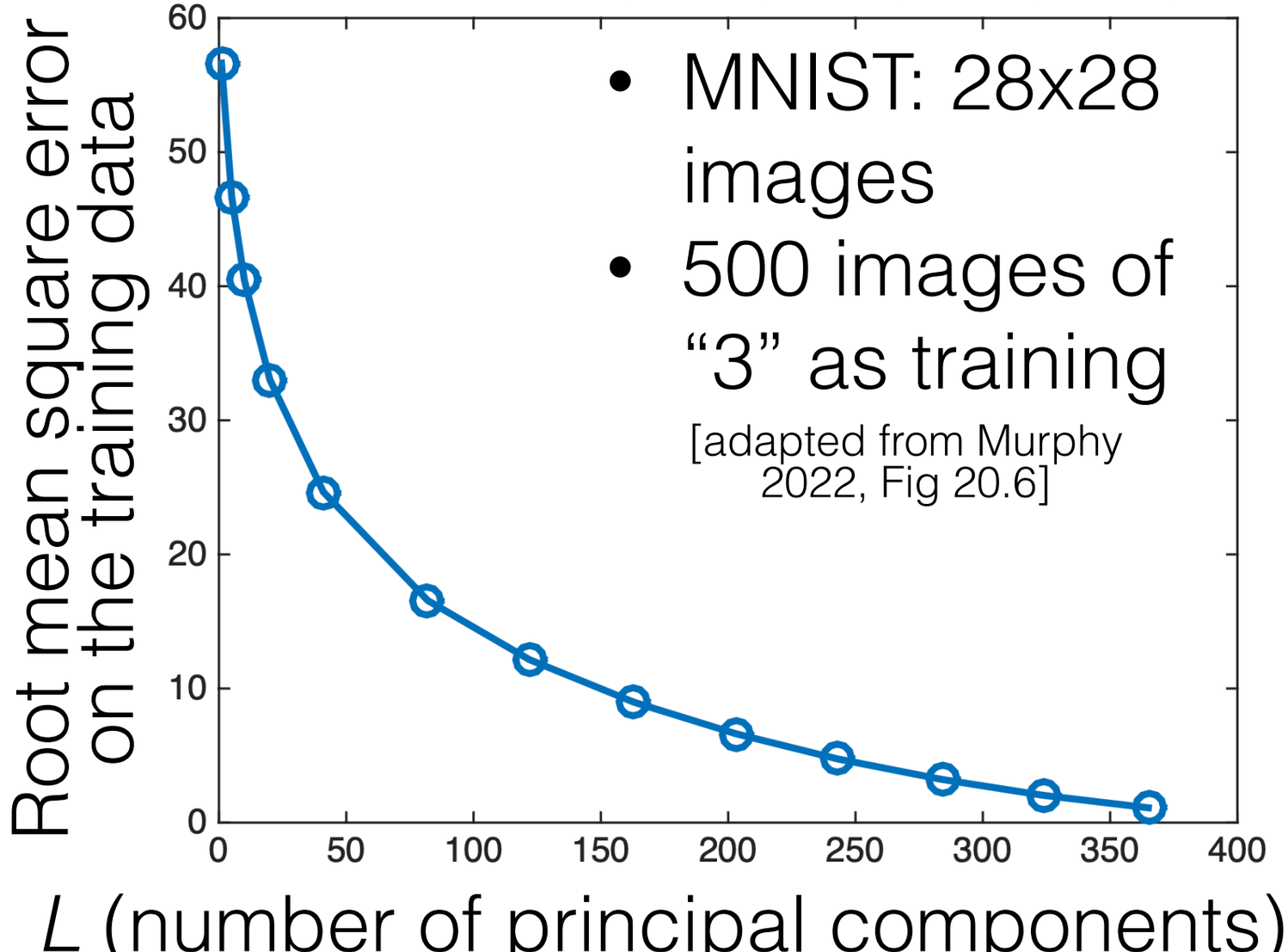

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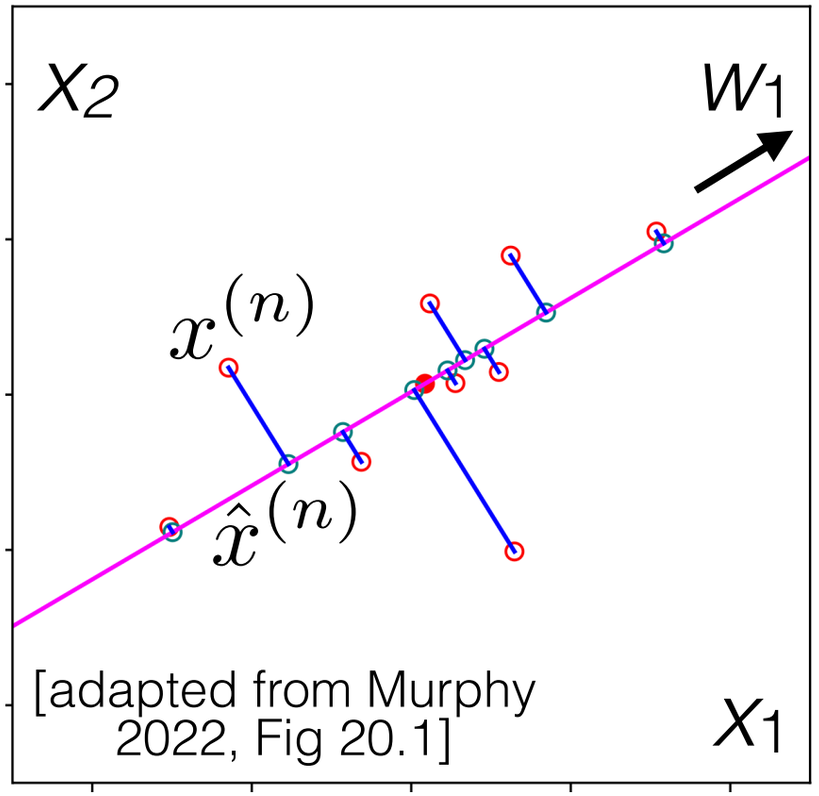

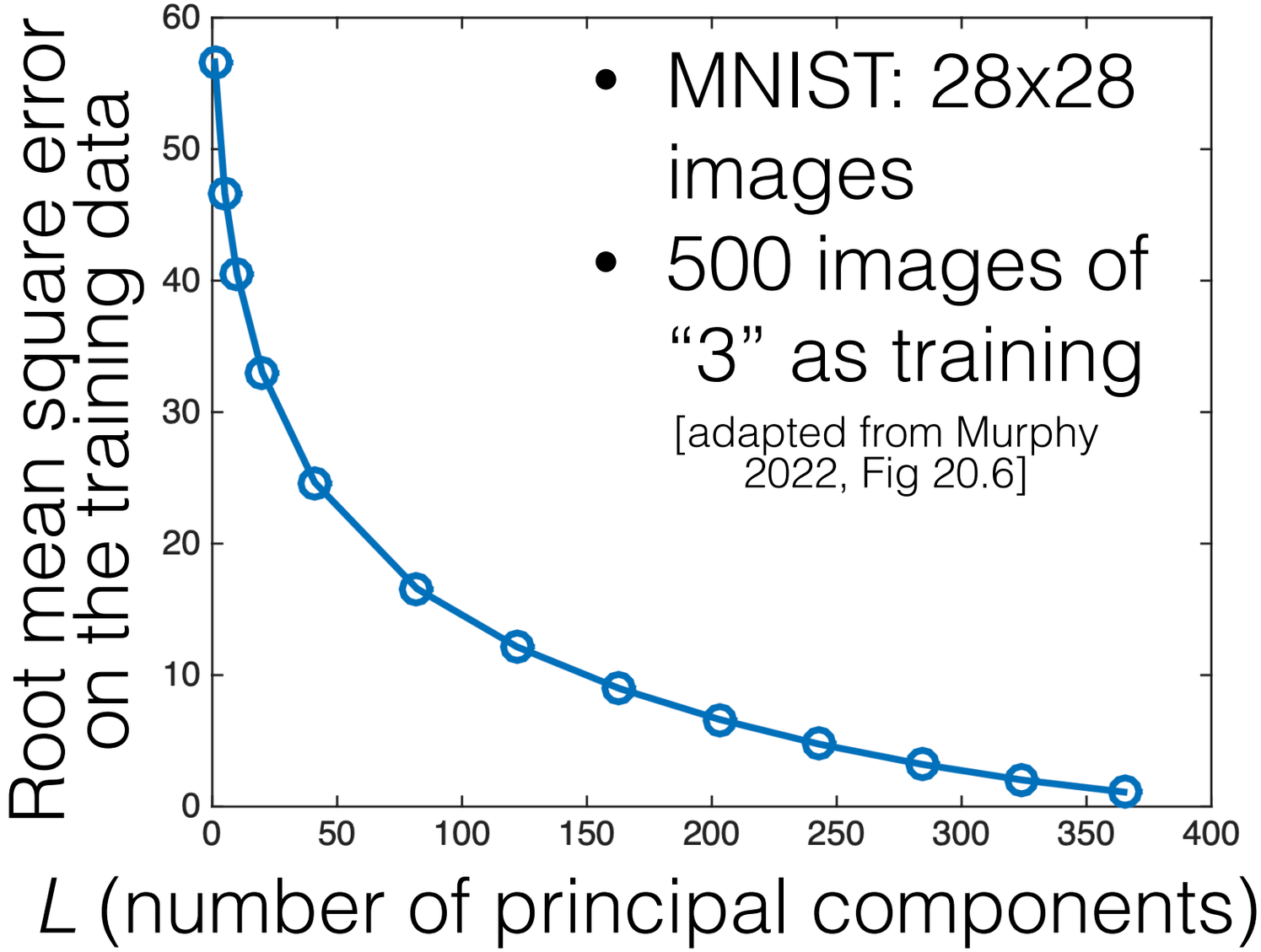

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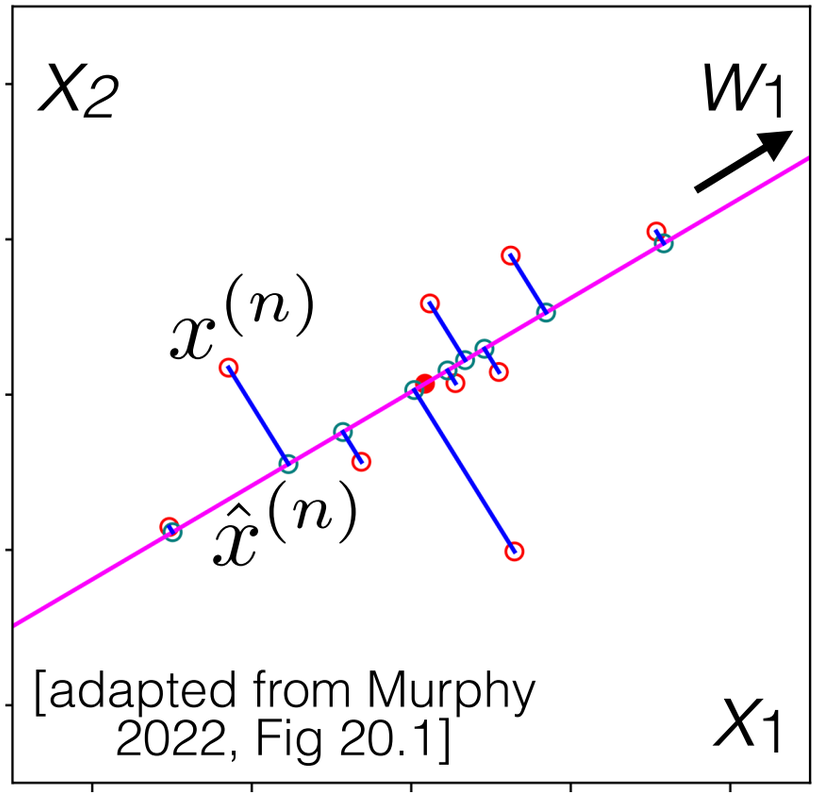

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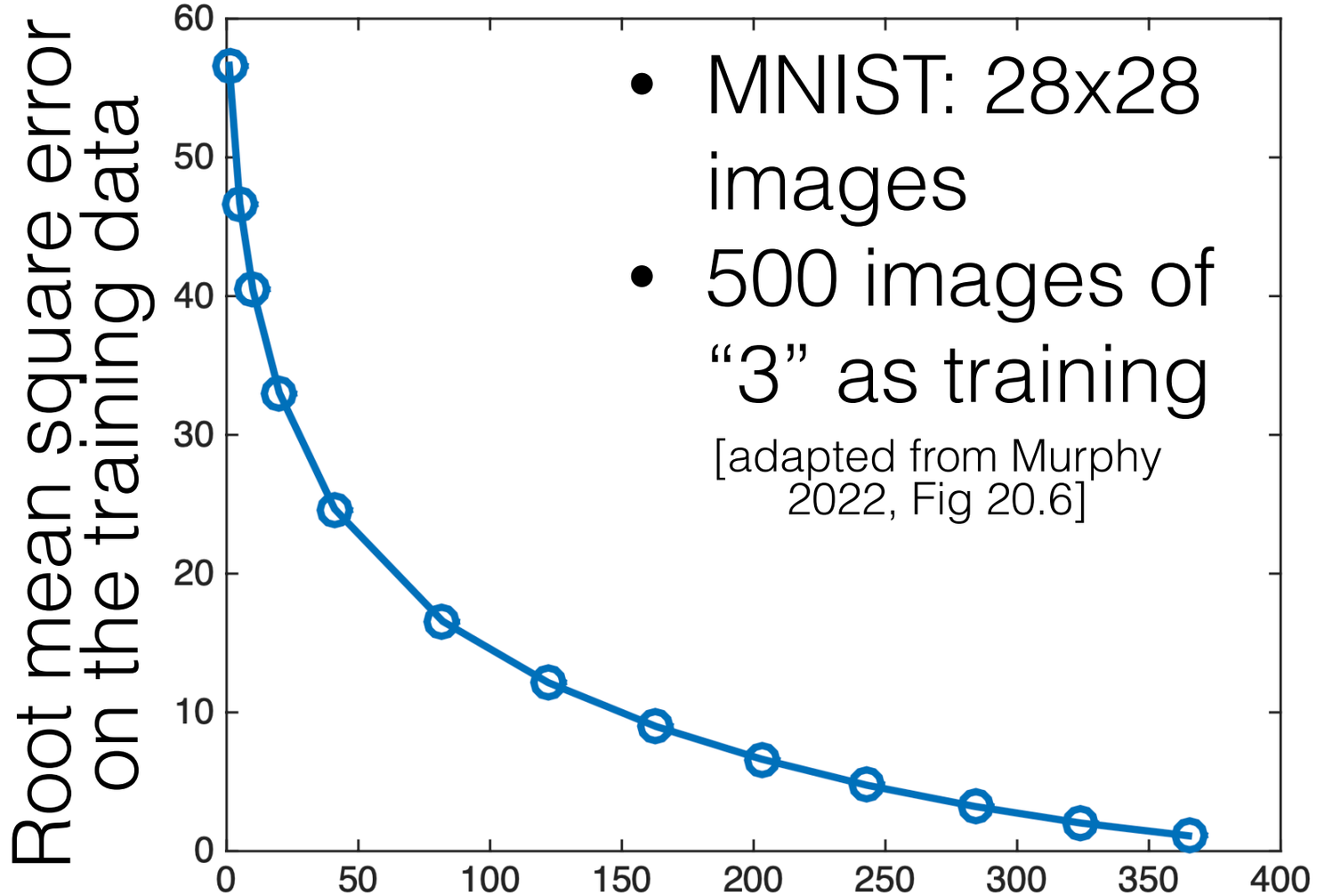

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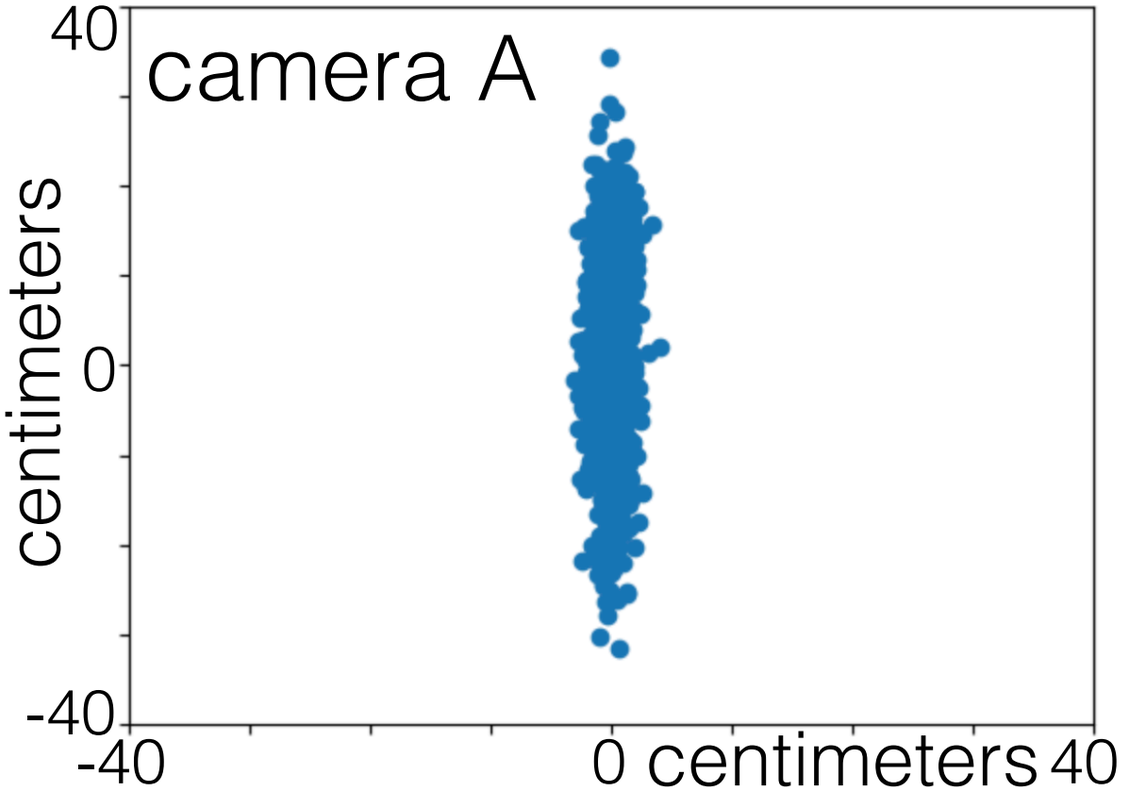

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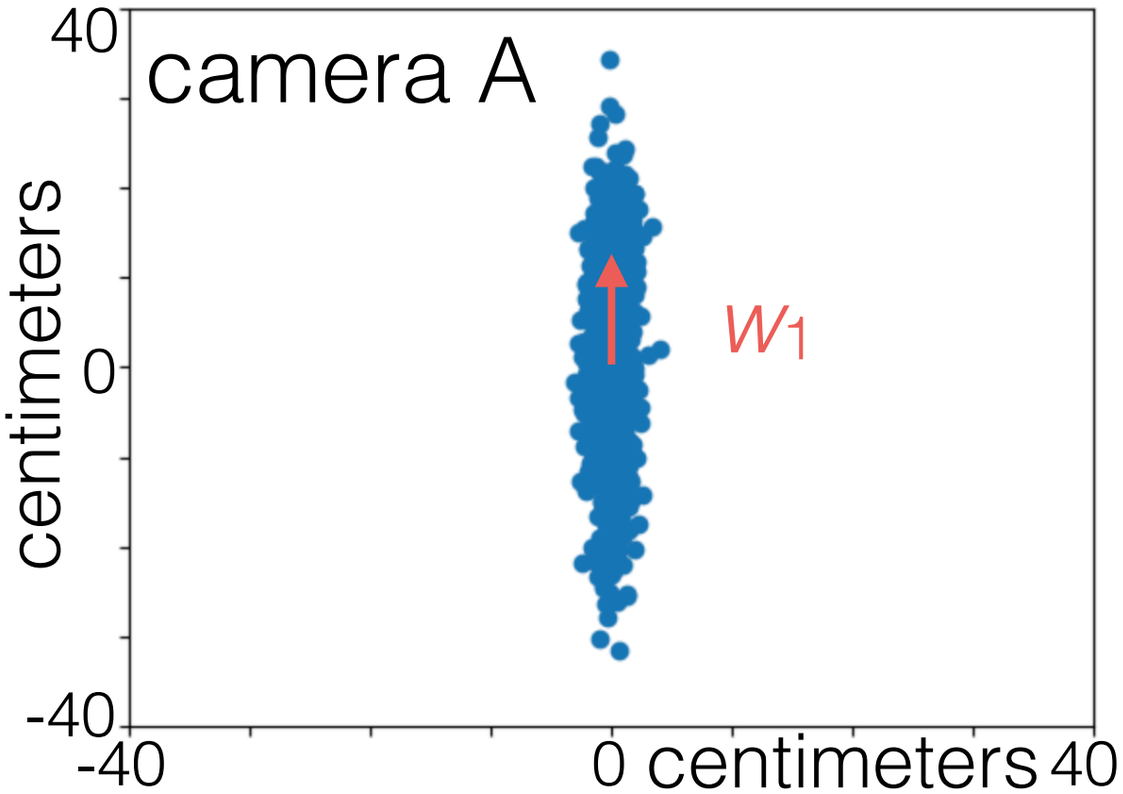

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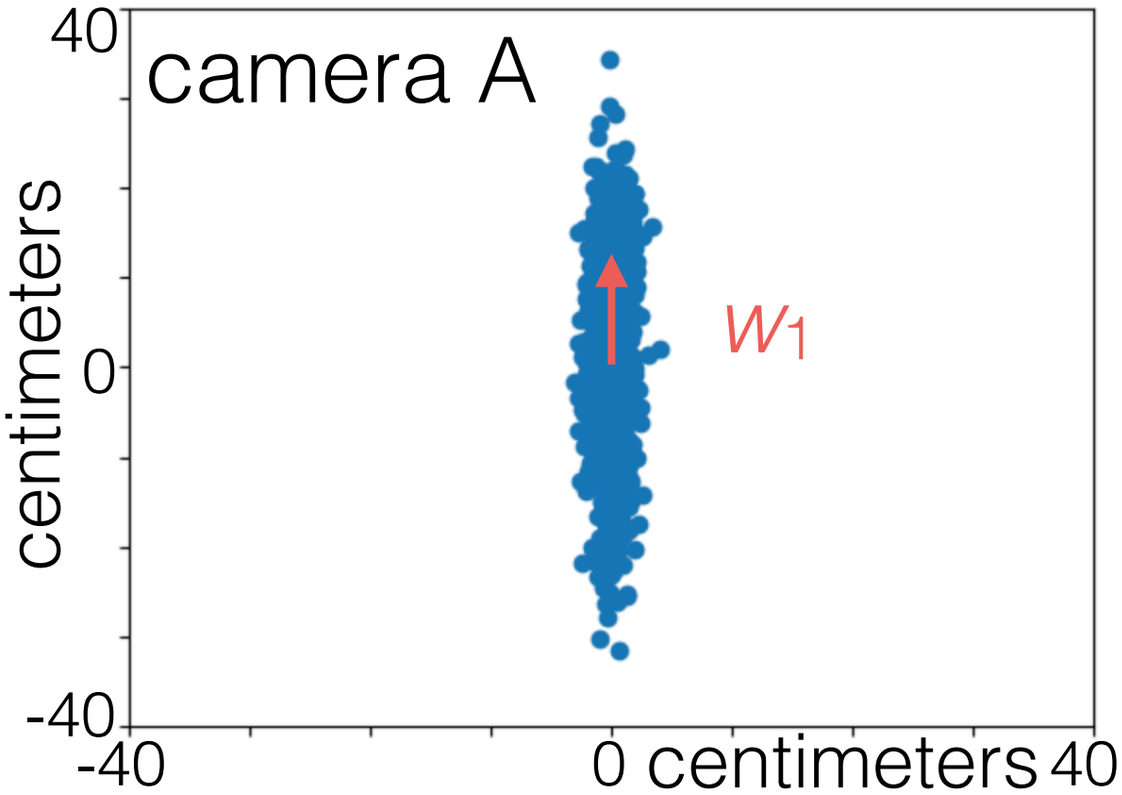

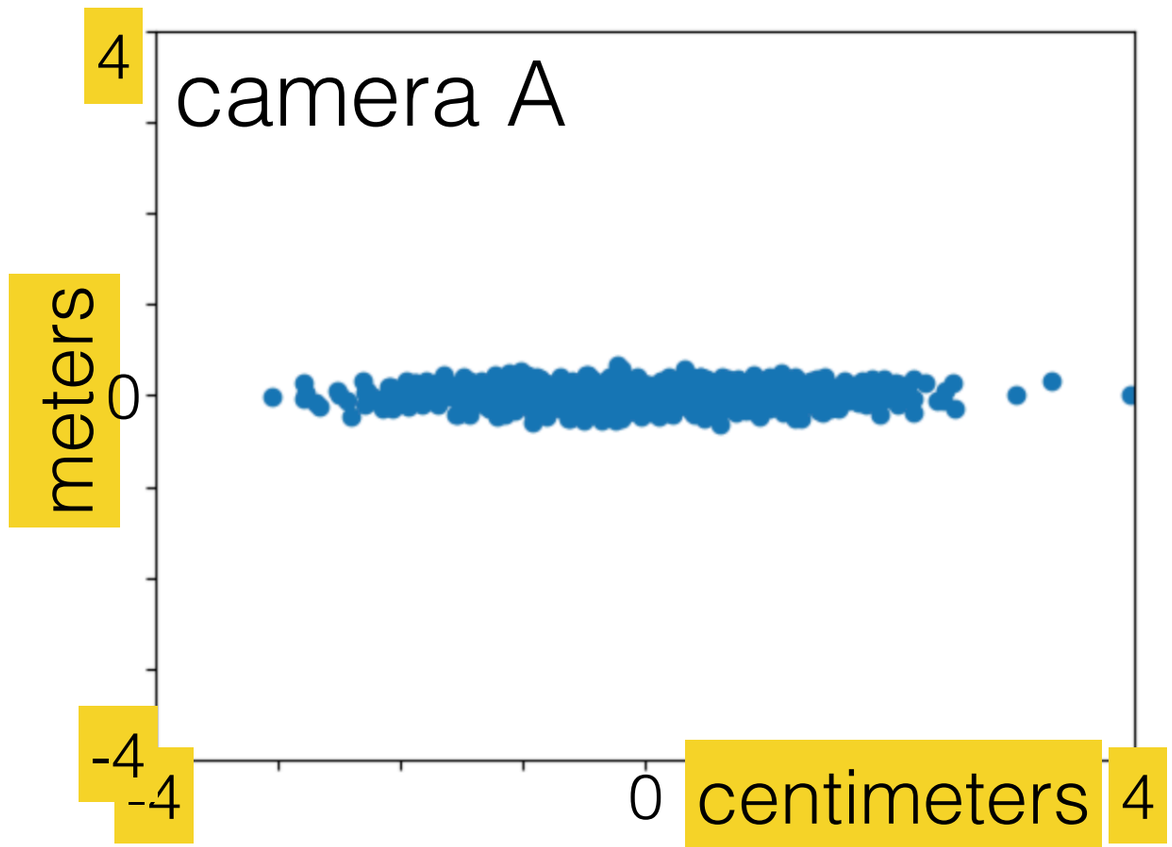

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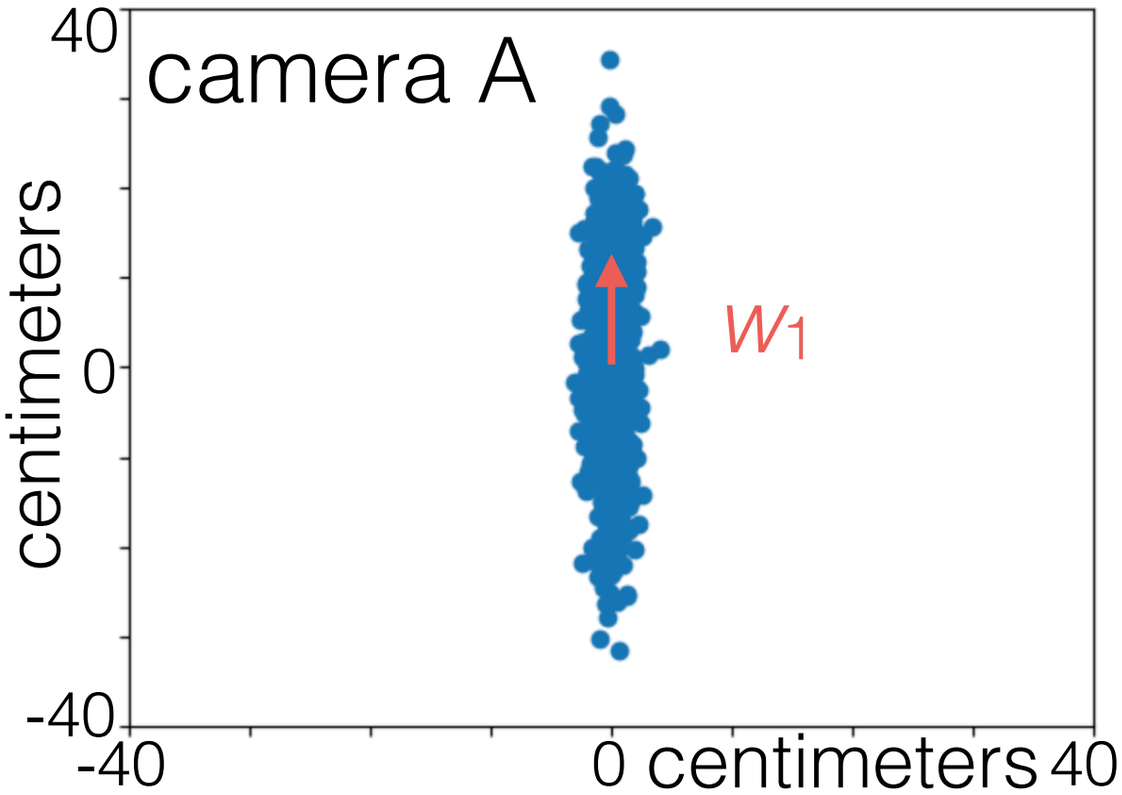

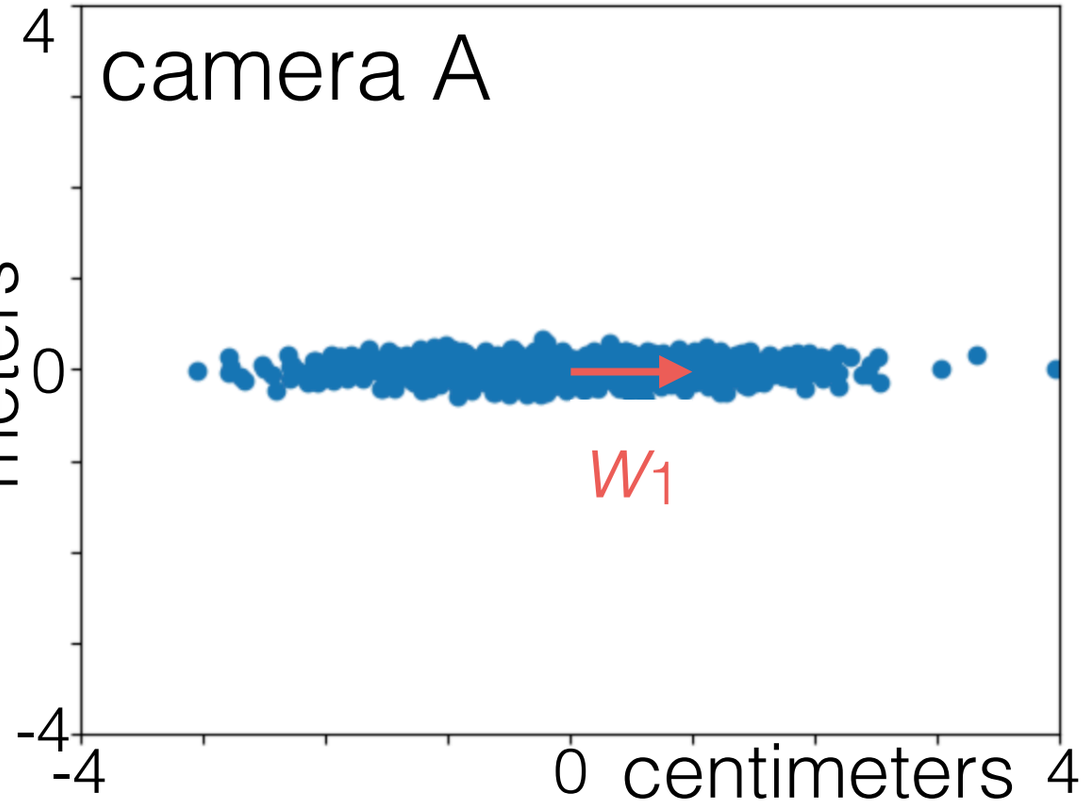

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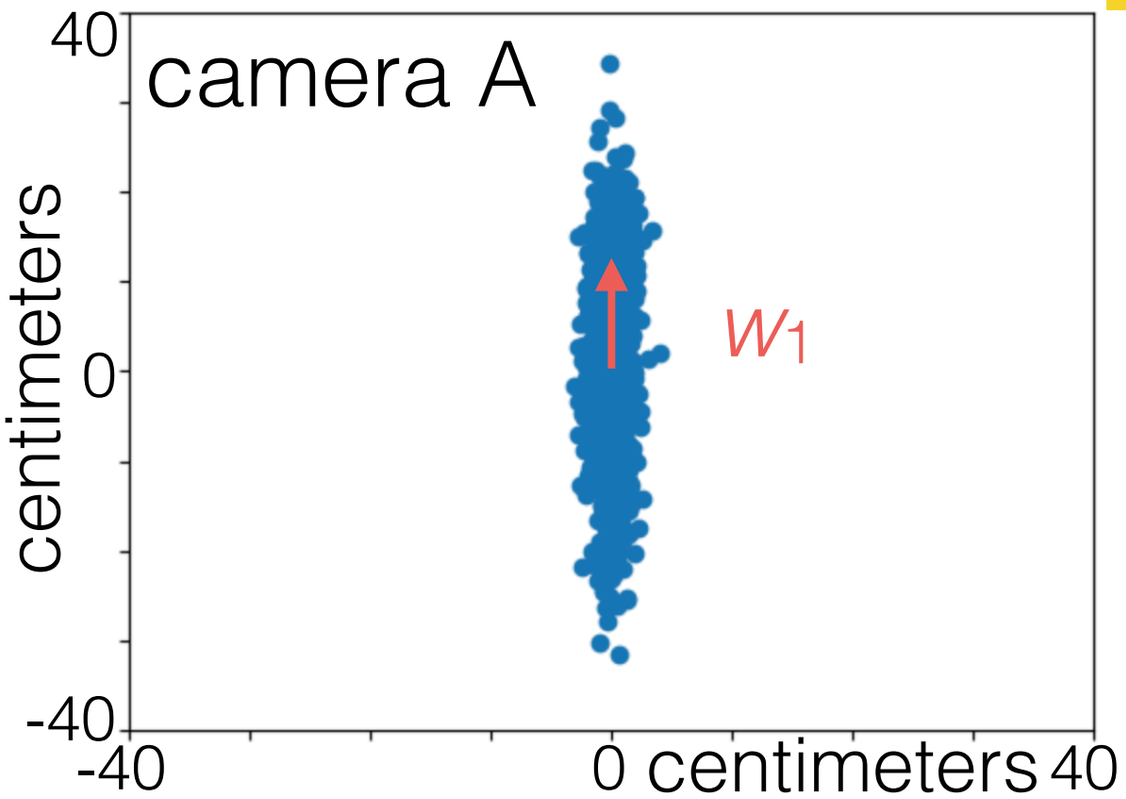

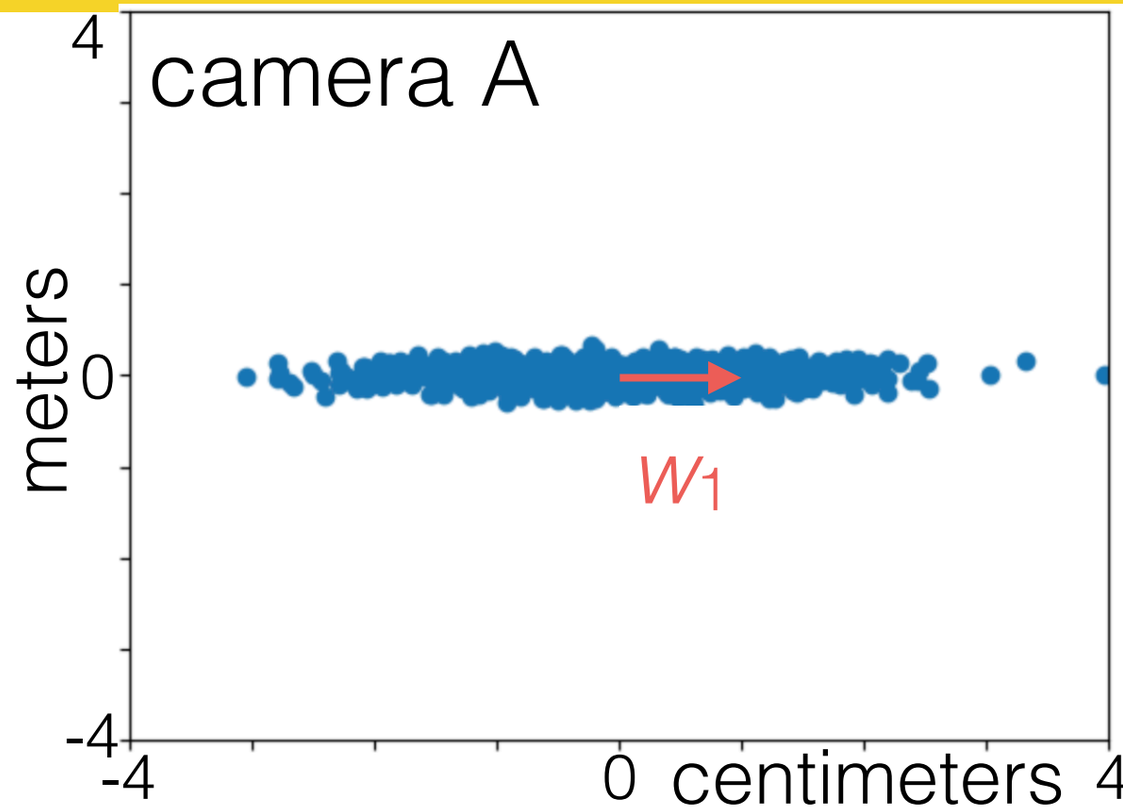

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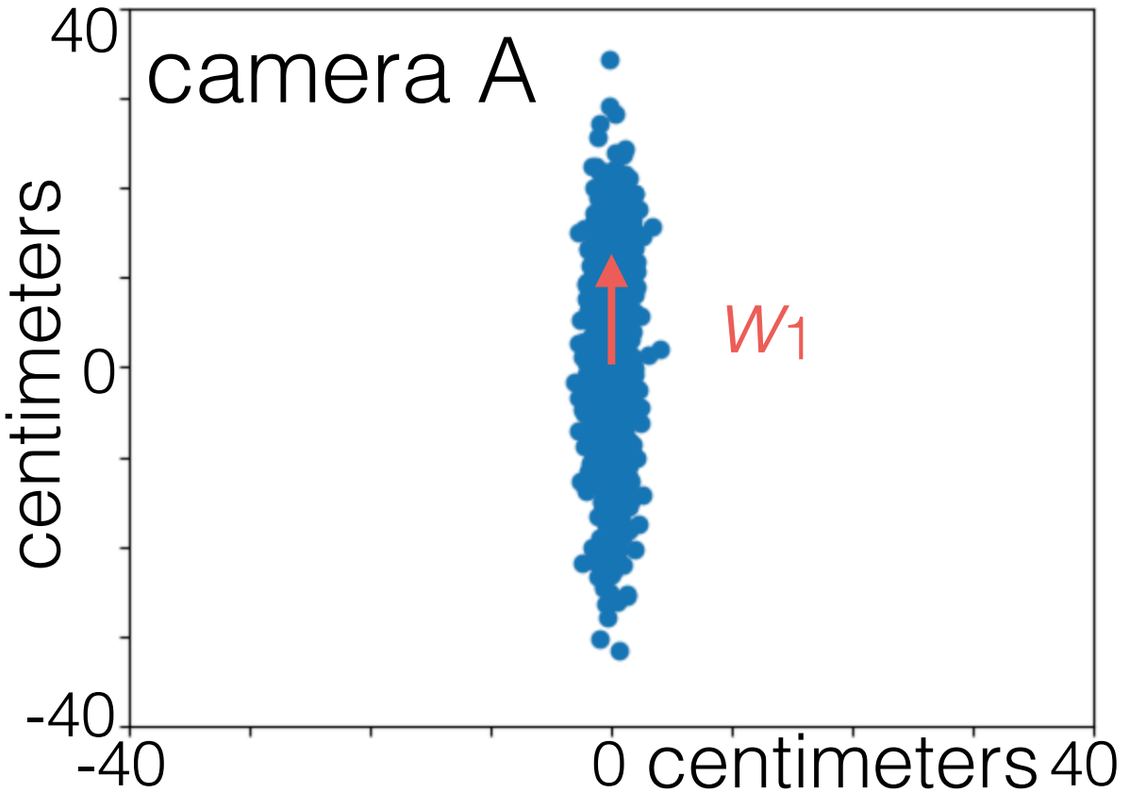

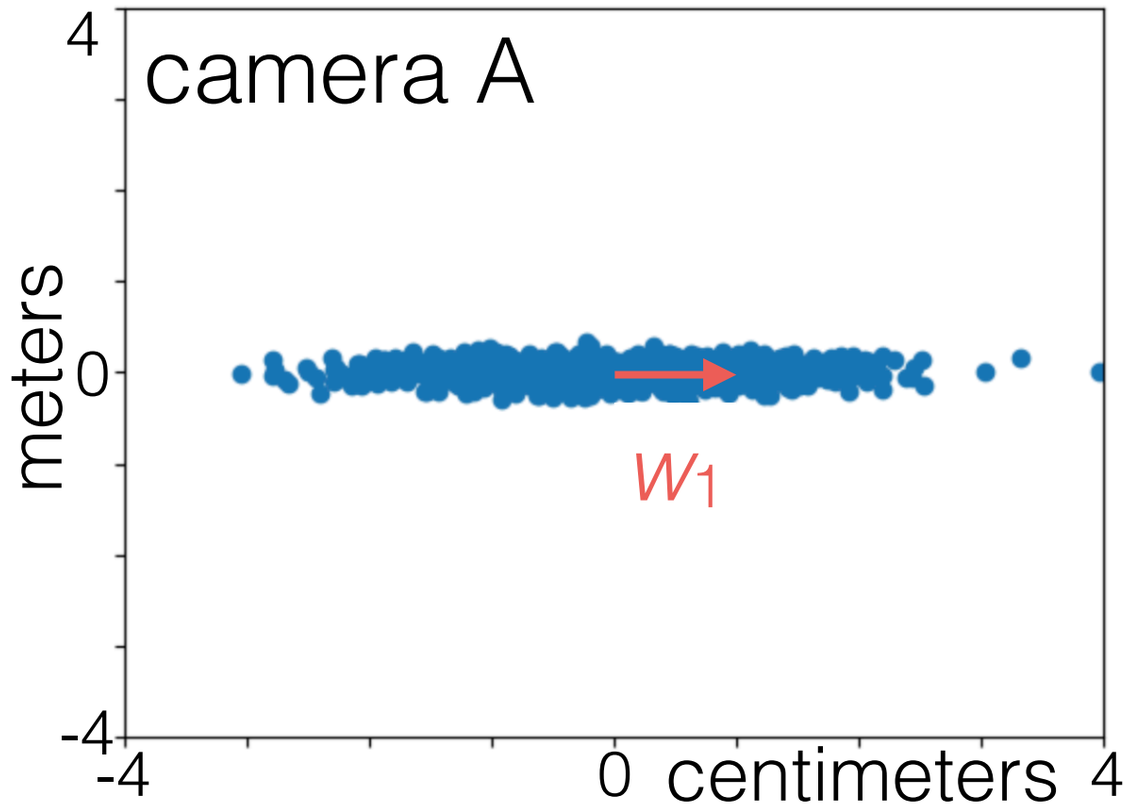

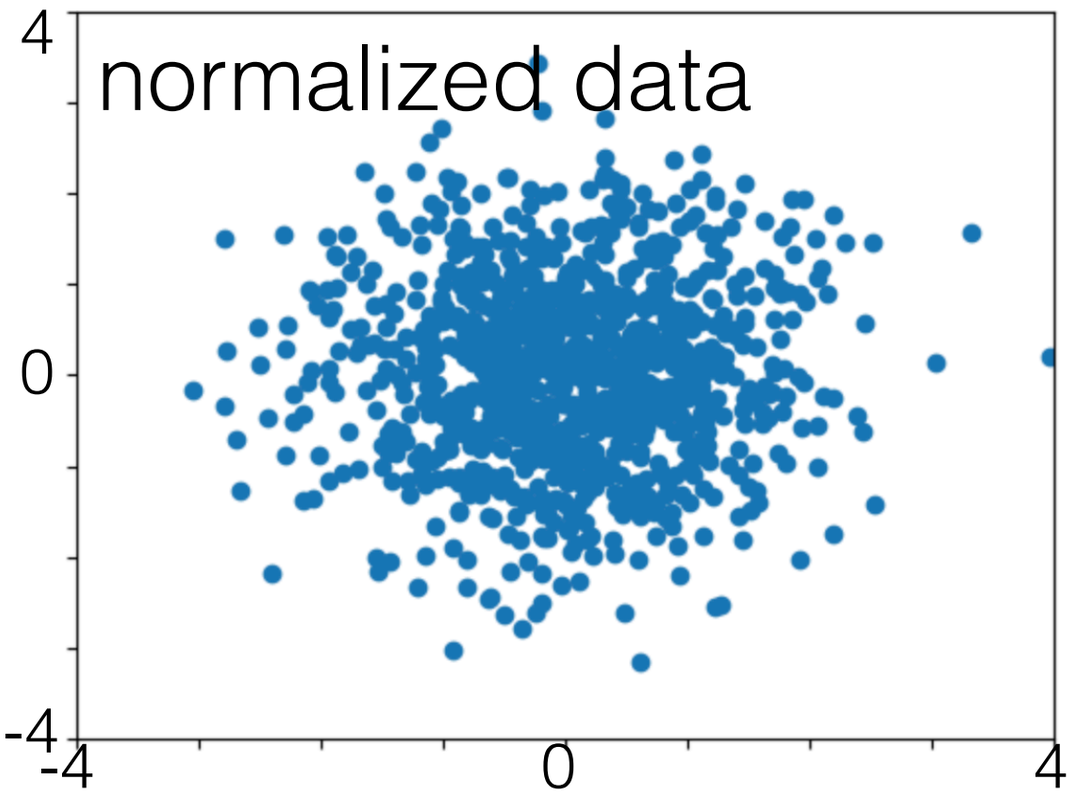

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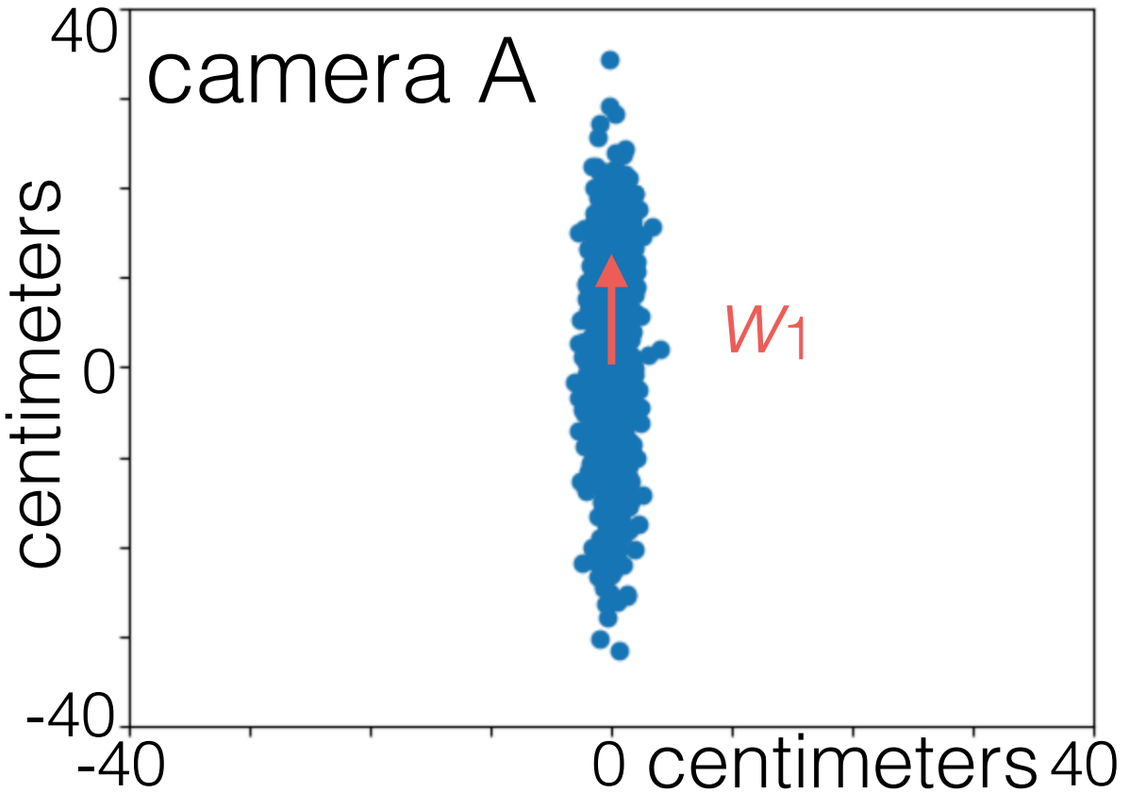

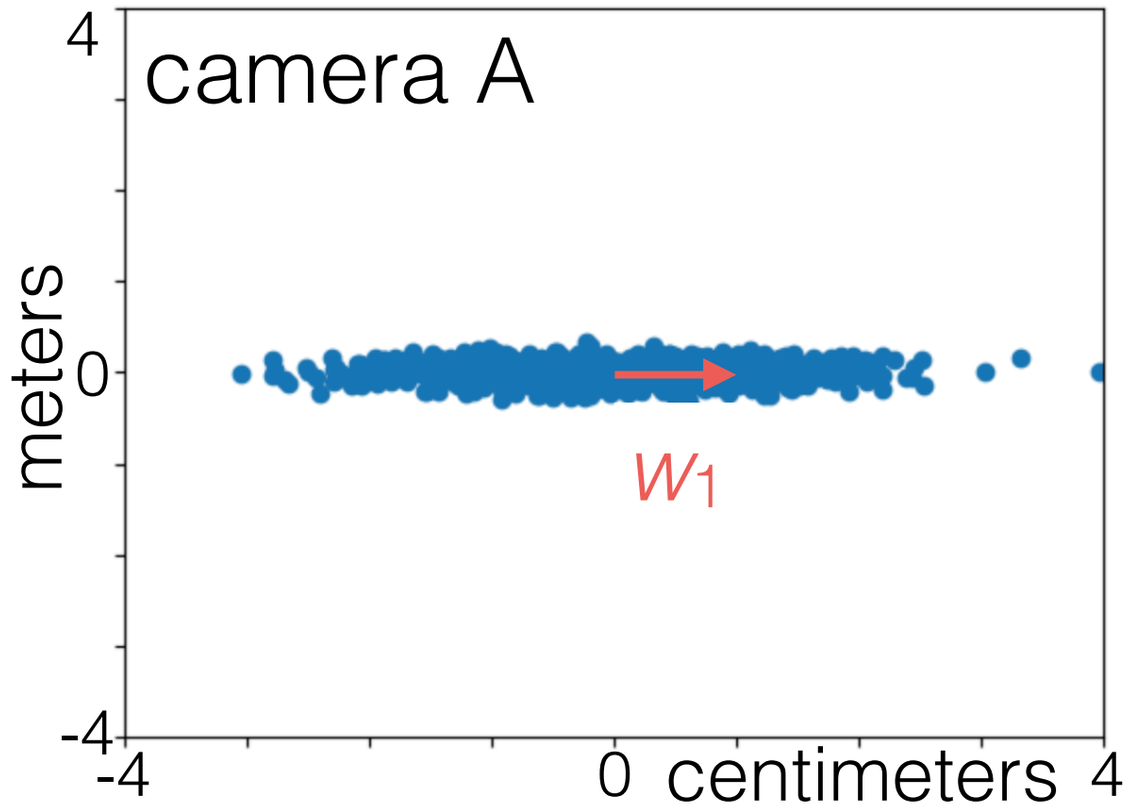

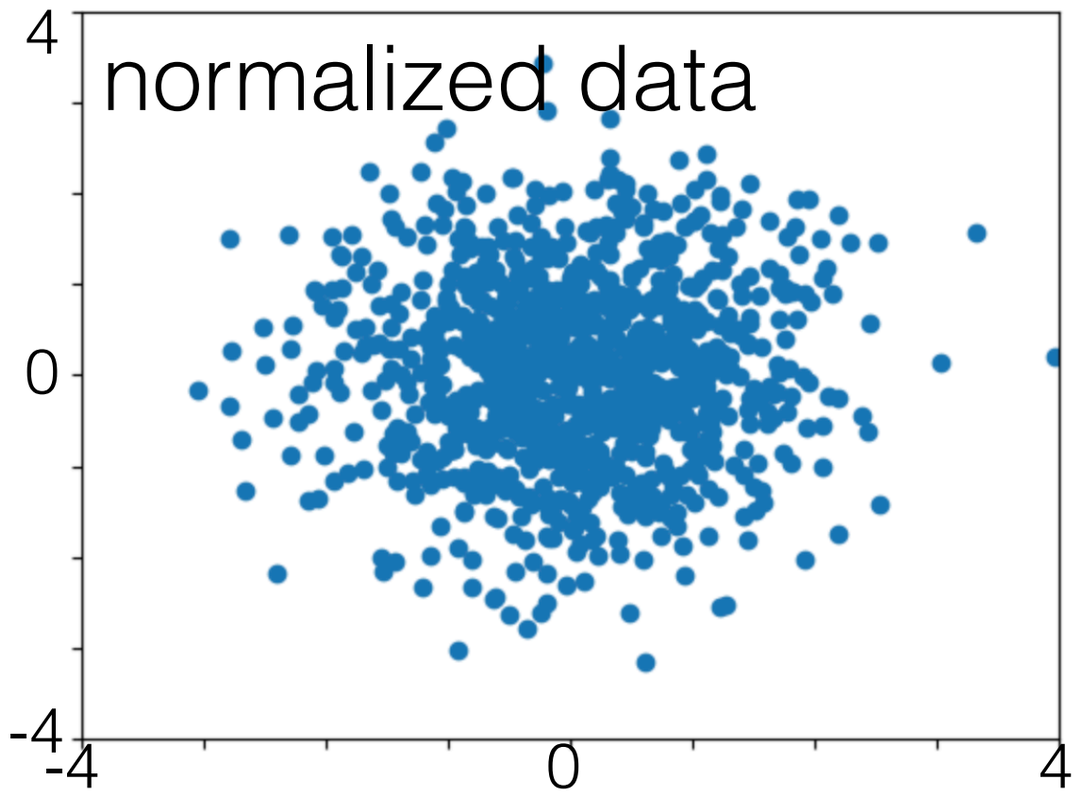

"We have been working with the eigendecomposition of the covariance matrix. However, it is better to use the correlation matrix instead. […O]therwise PCA can be "misled" by directions in which the variance is high merely because of the measurement scale." [Murphy 2022, 20.1.3.1]

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- Proposal: reduce the dimensionality of the feature space with PCA before running supervised learning

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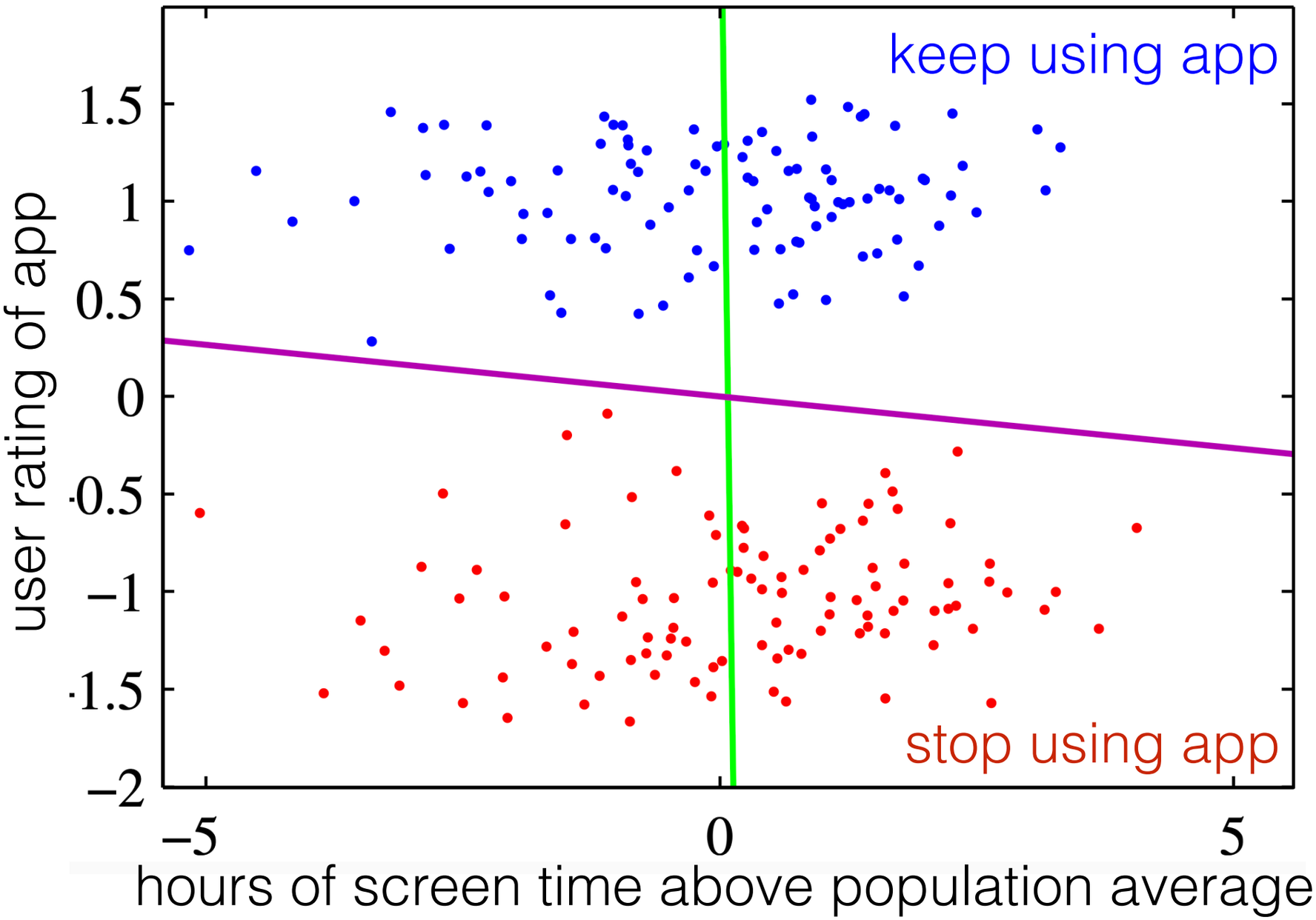

[adapted from Bishop 2006, Fig 12.7]

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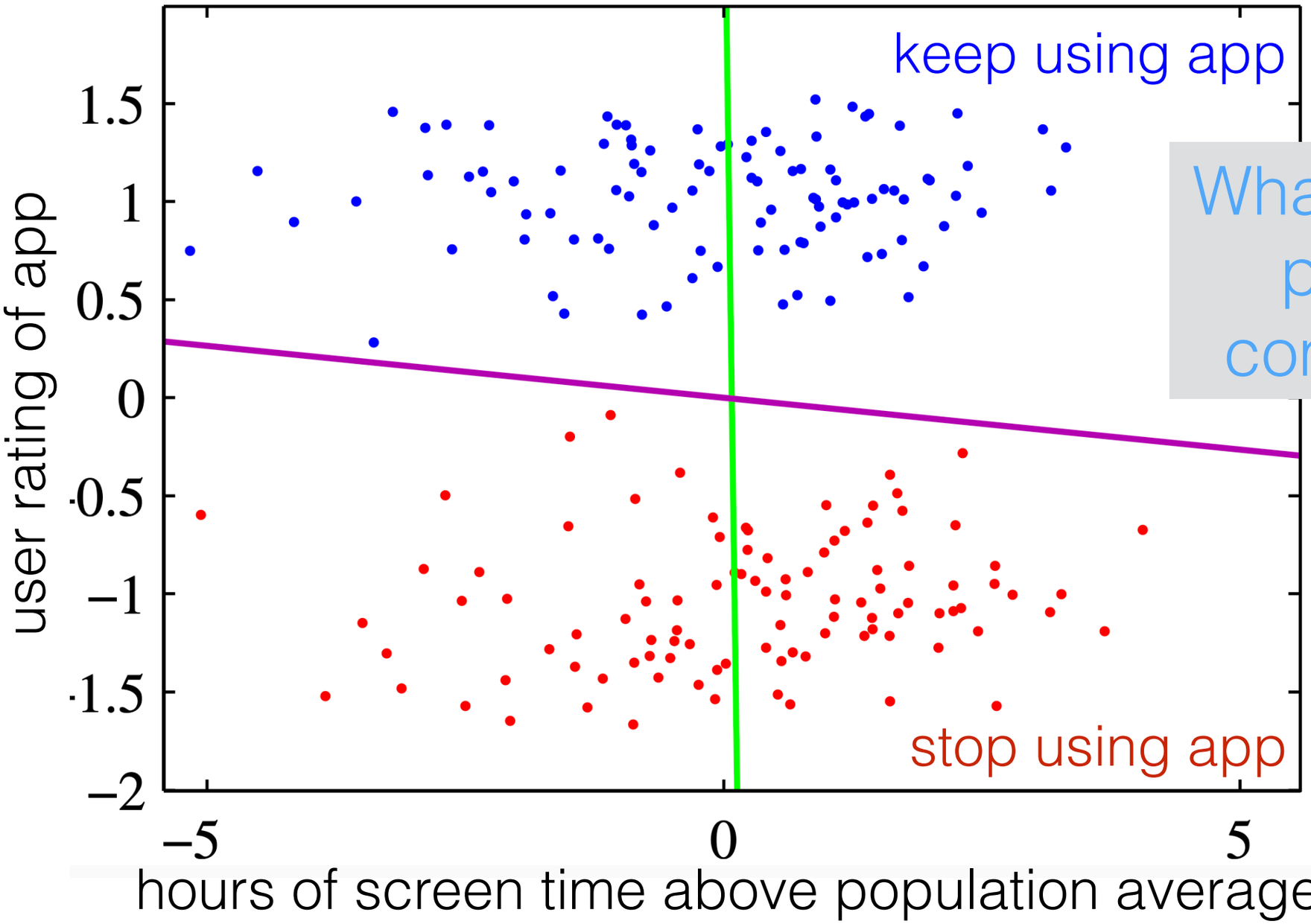

What's the first principal component?

[adapted from Bishop 2006, Fig 12.7]

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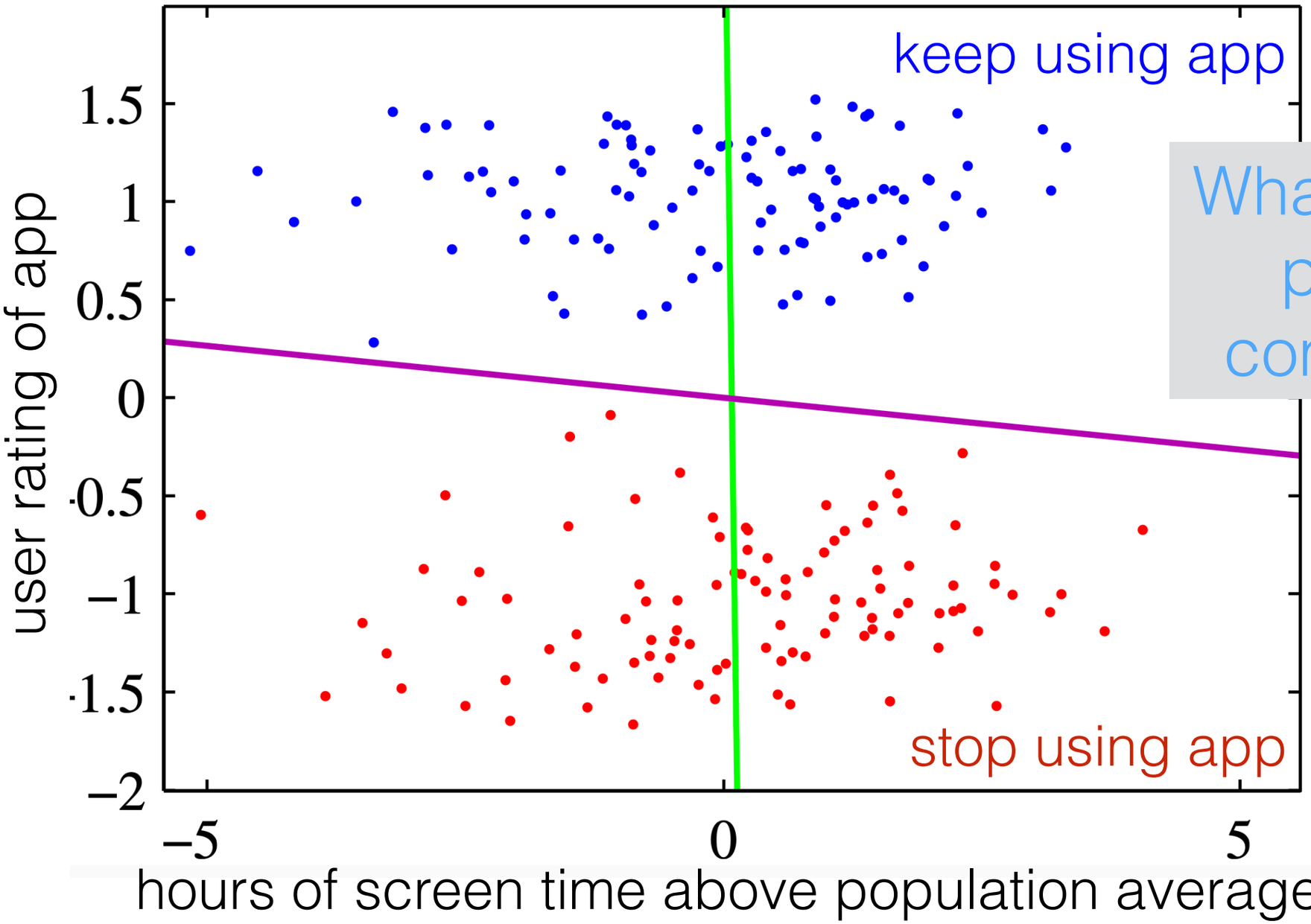

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- This pre-processing assumes directions of highest feature variance are the meaningful ones for prediction

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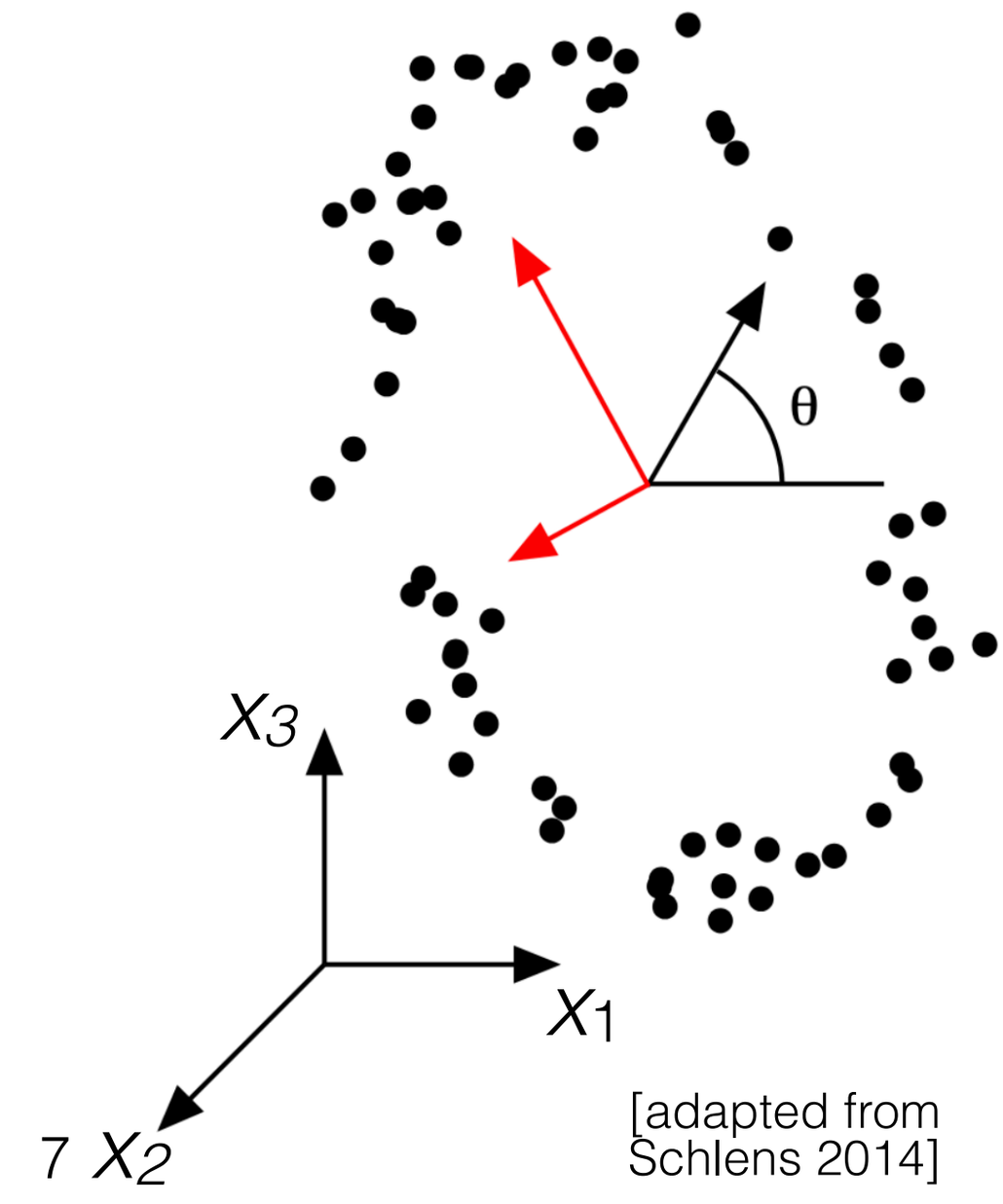

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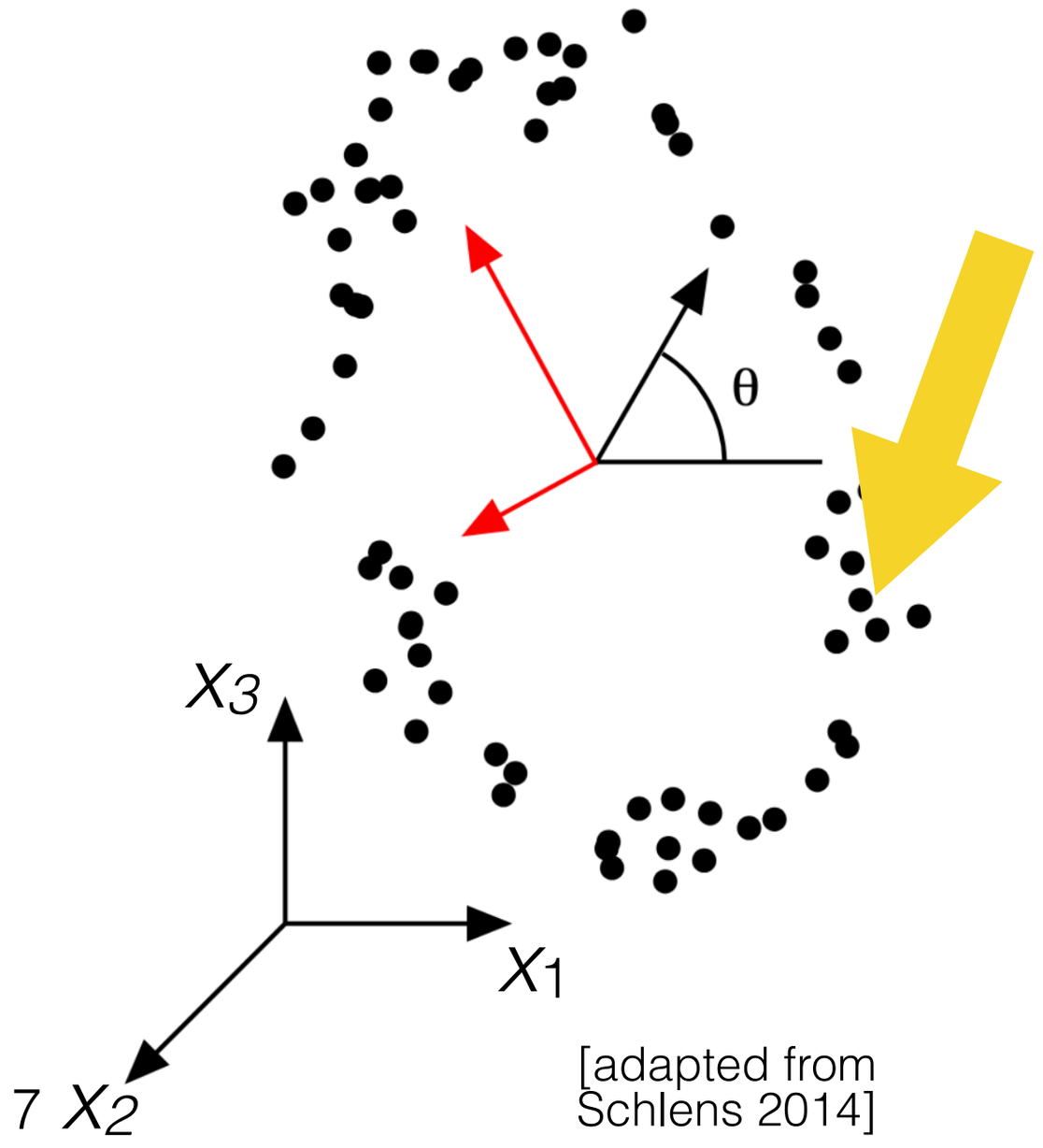

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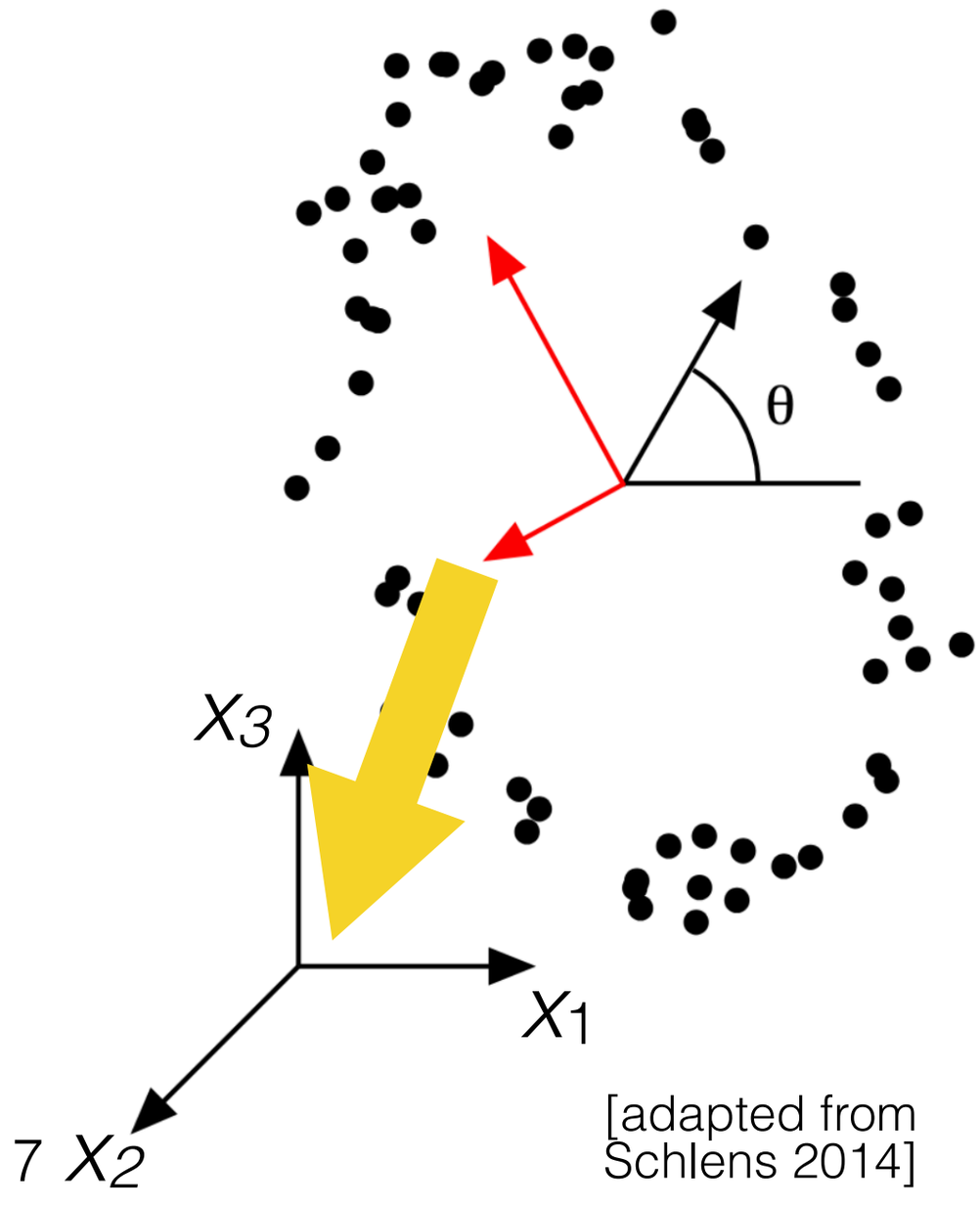

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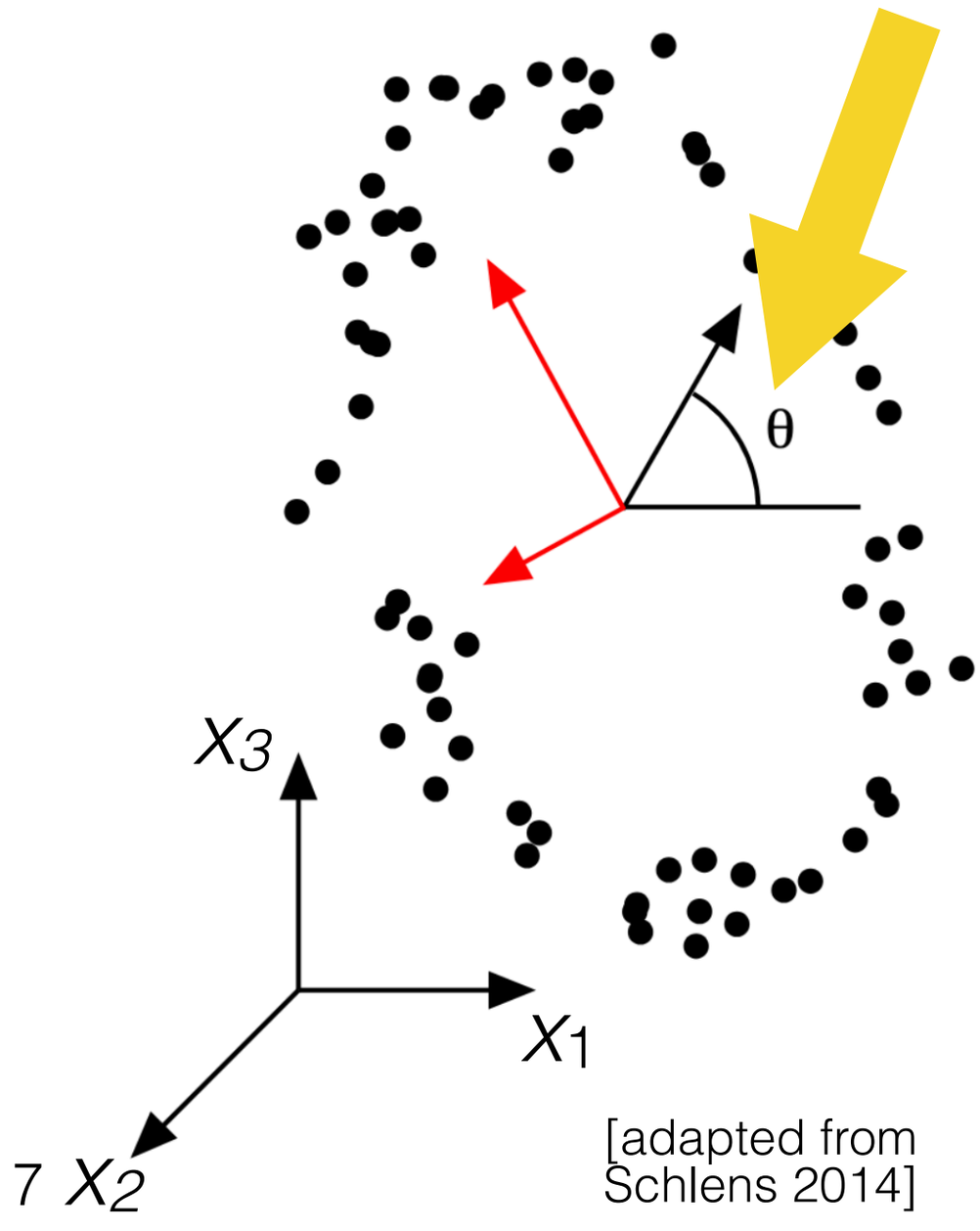

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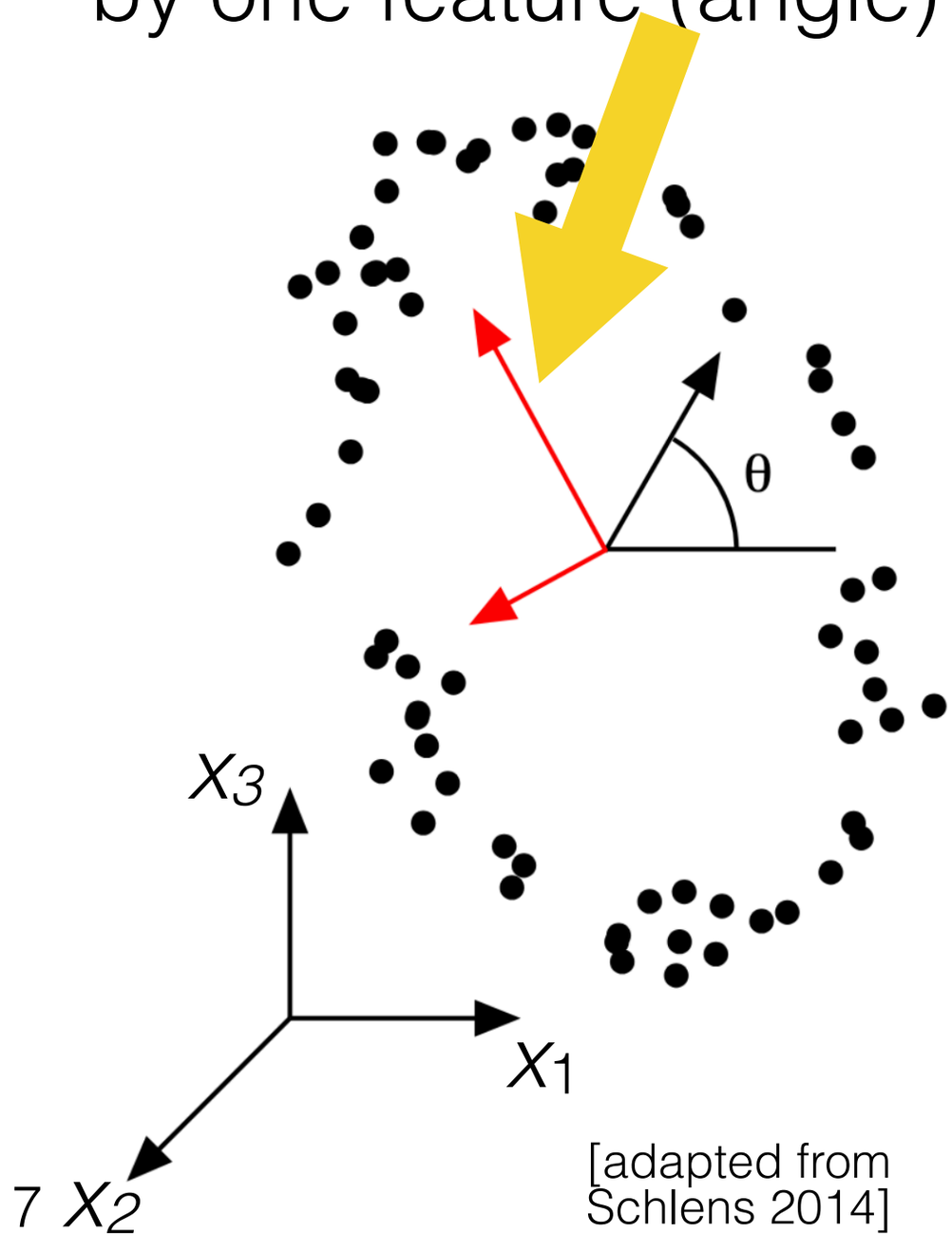

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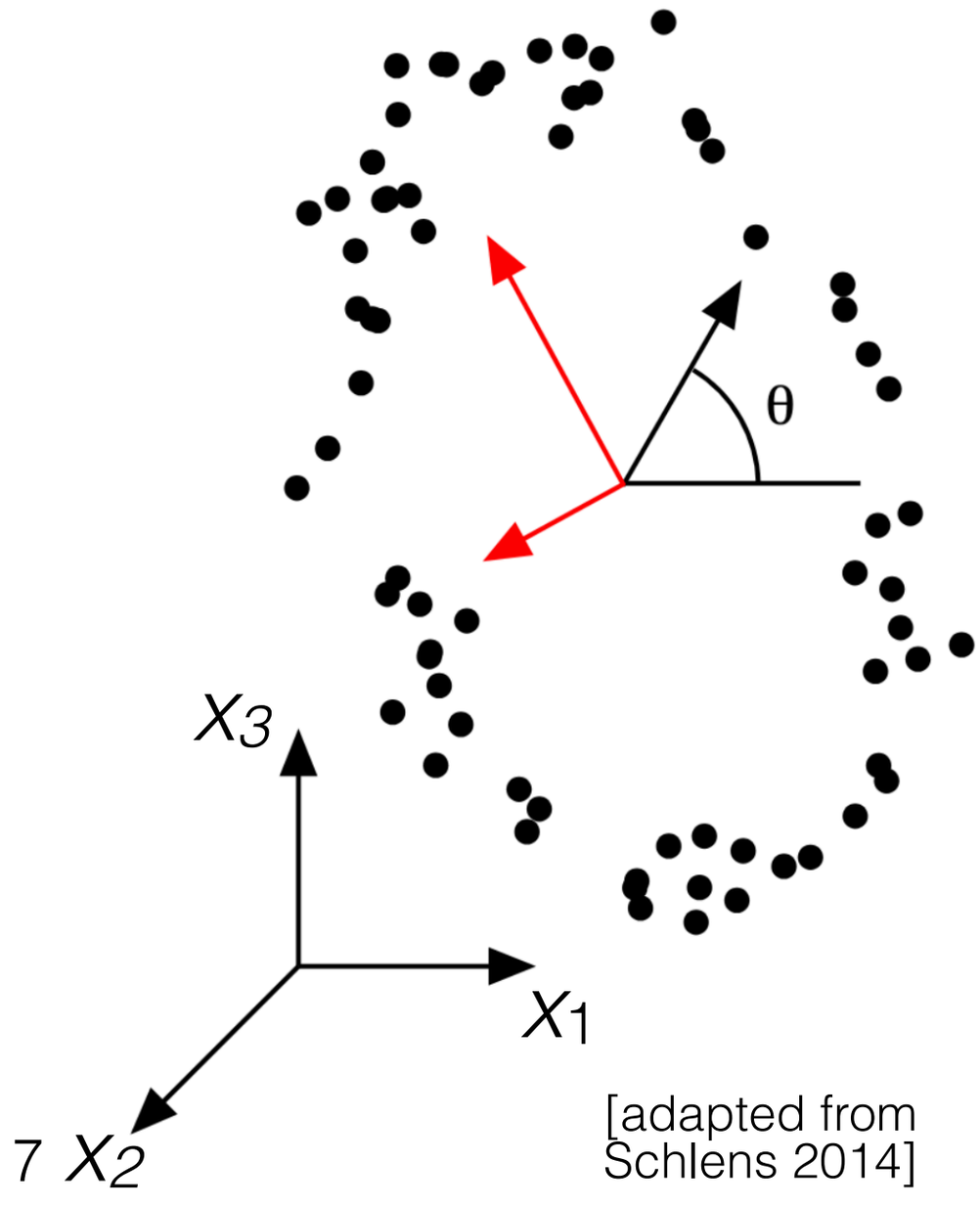

[adapted from Schlens 2014]

- Suppose all the activity in a town is on two main streets

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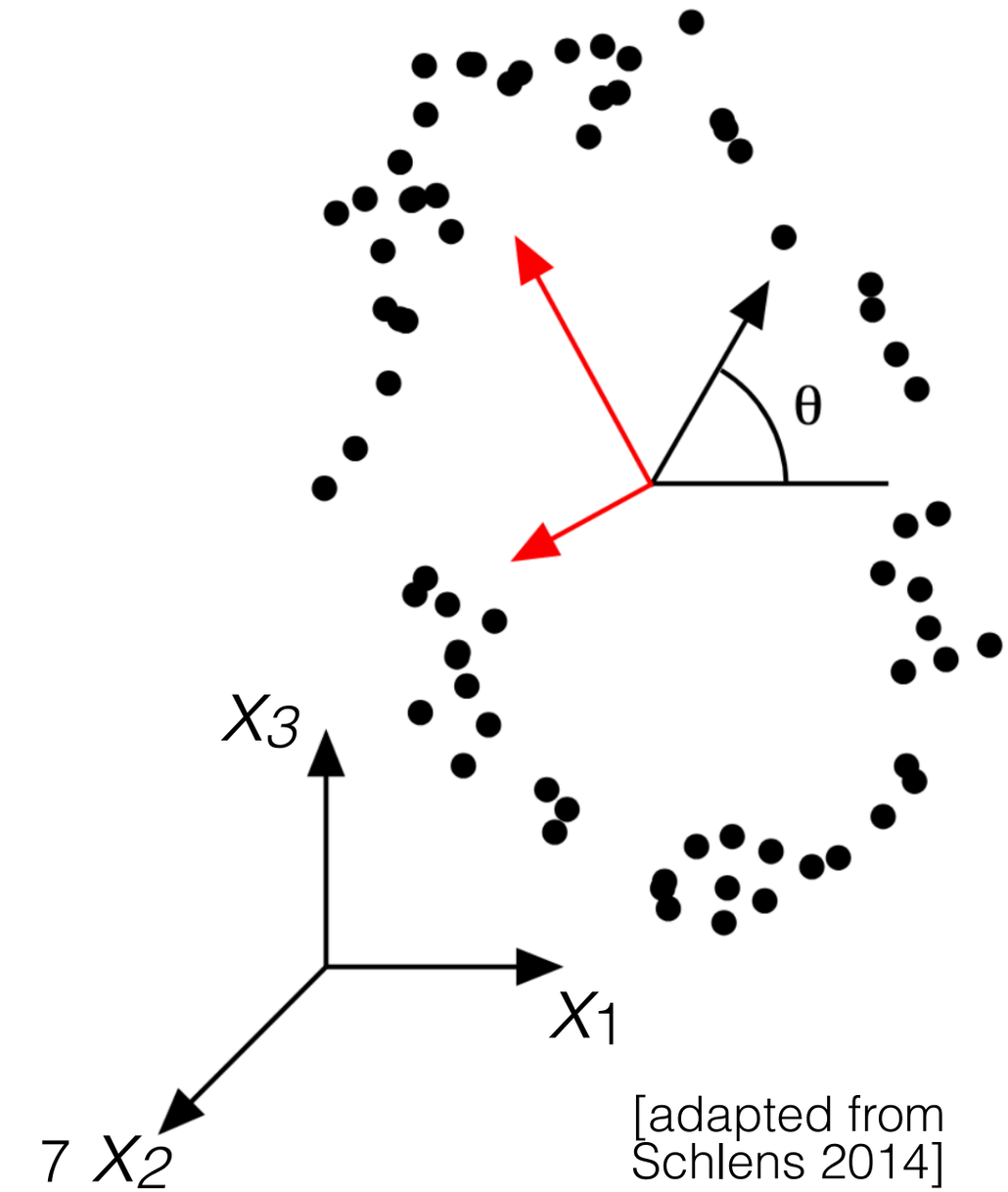

[adapted from Schlens 2014]

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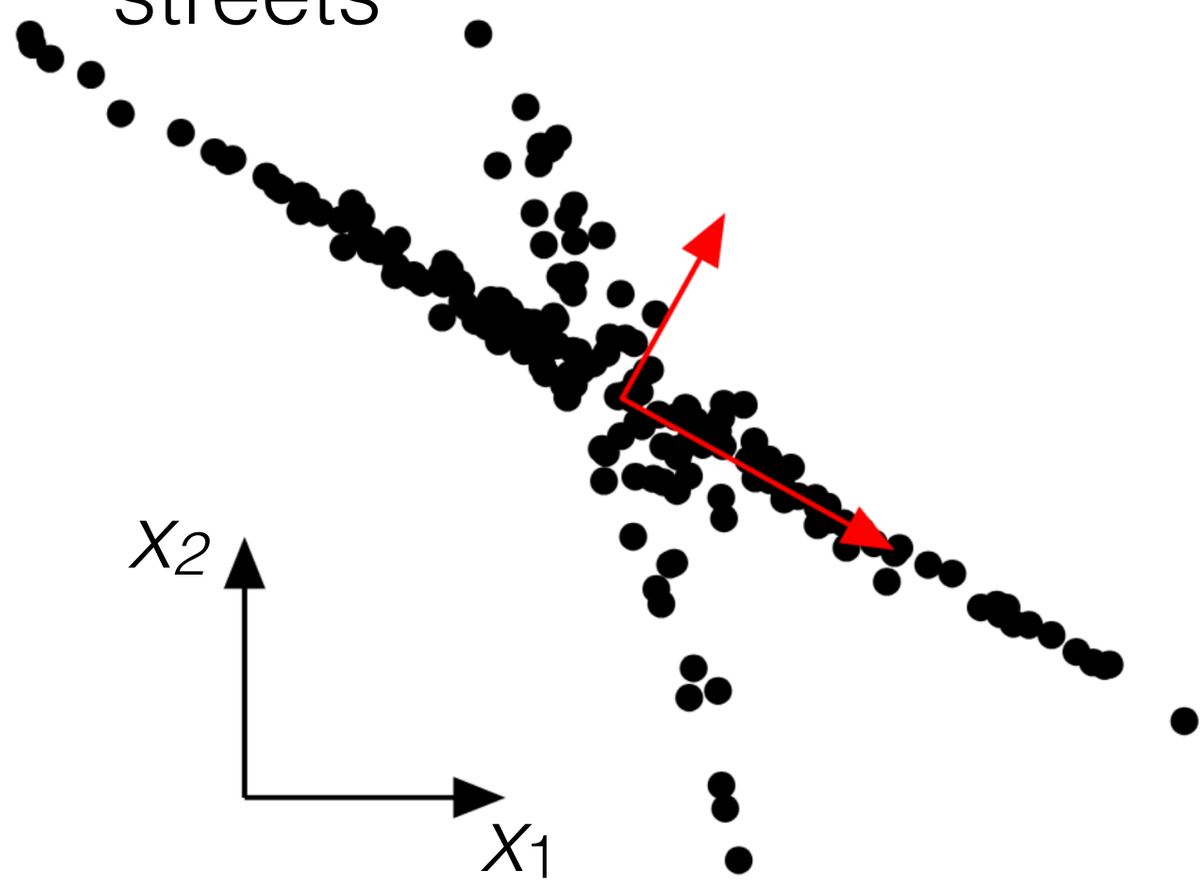

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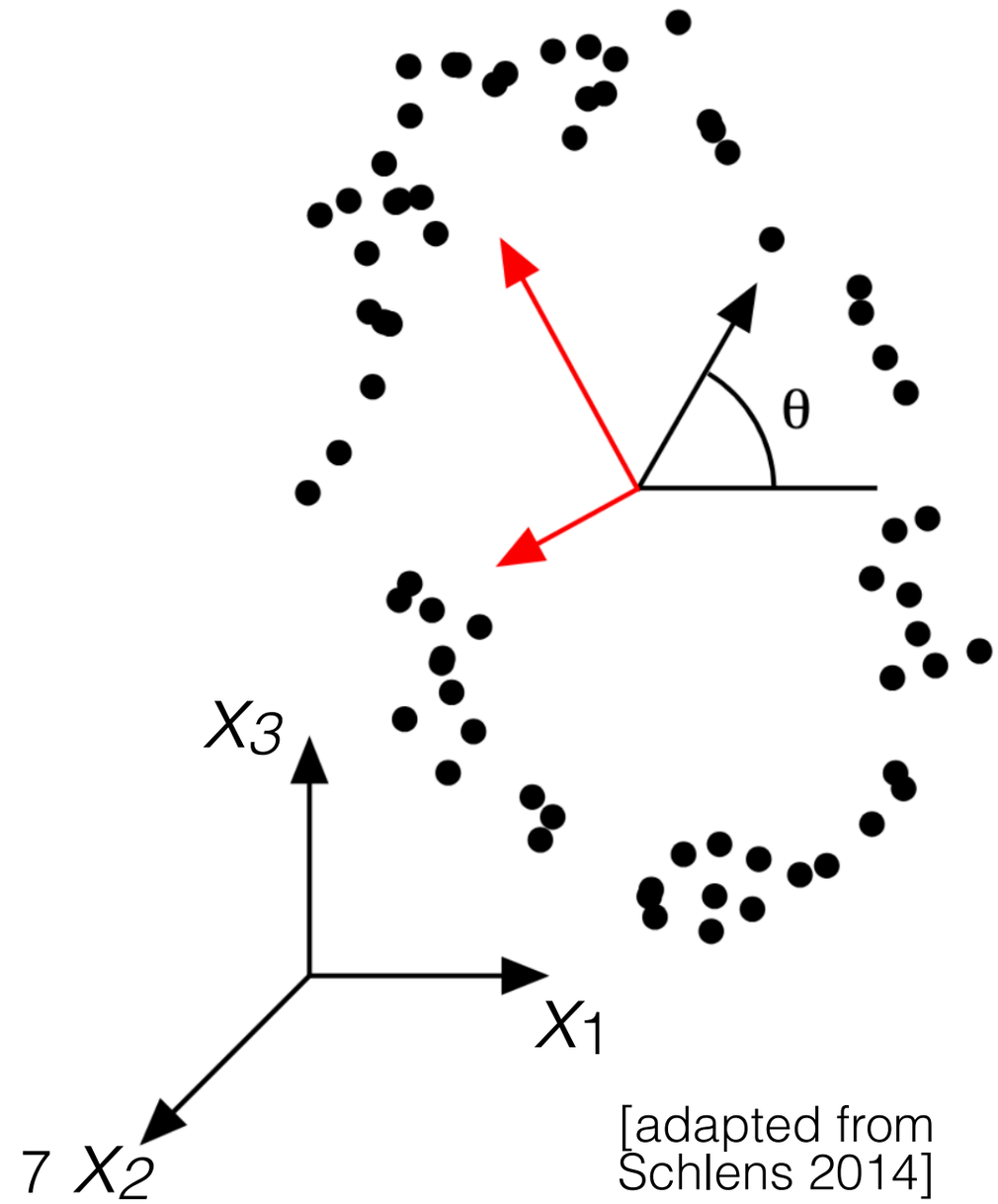

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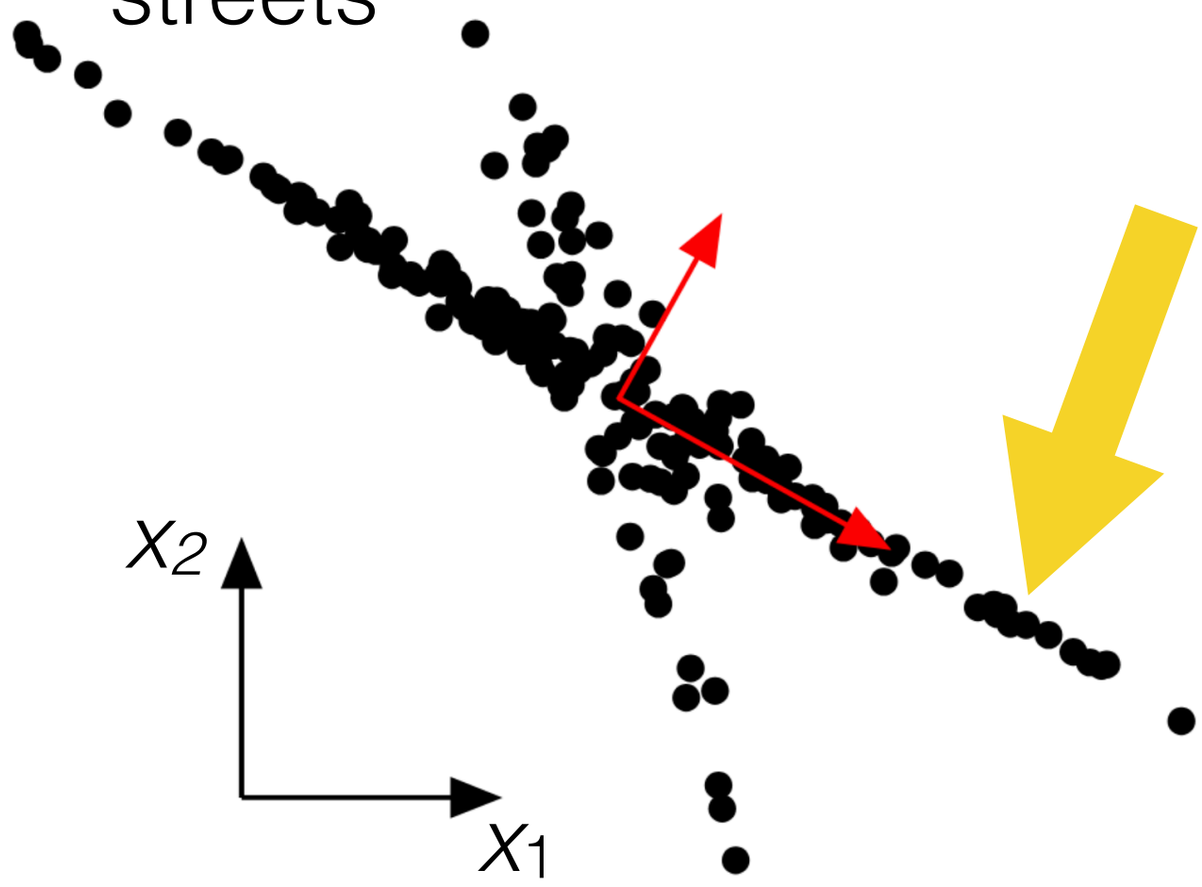

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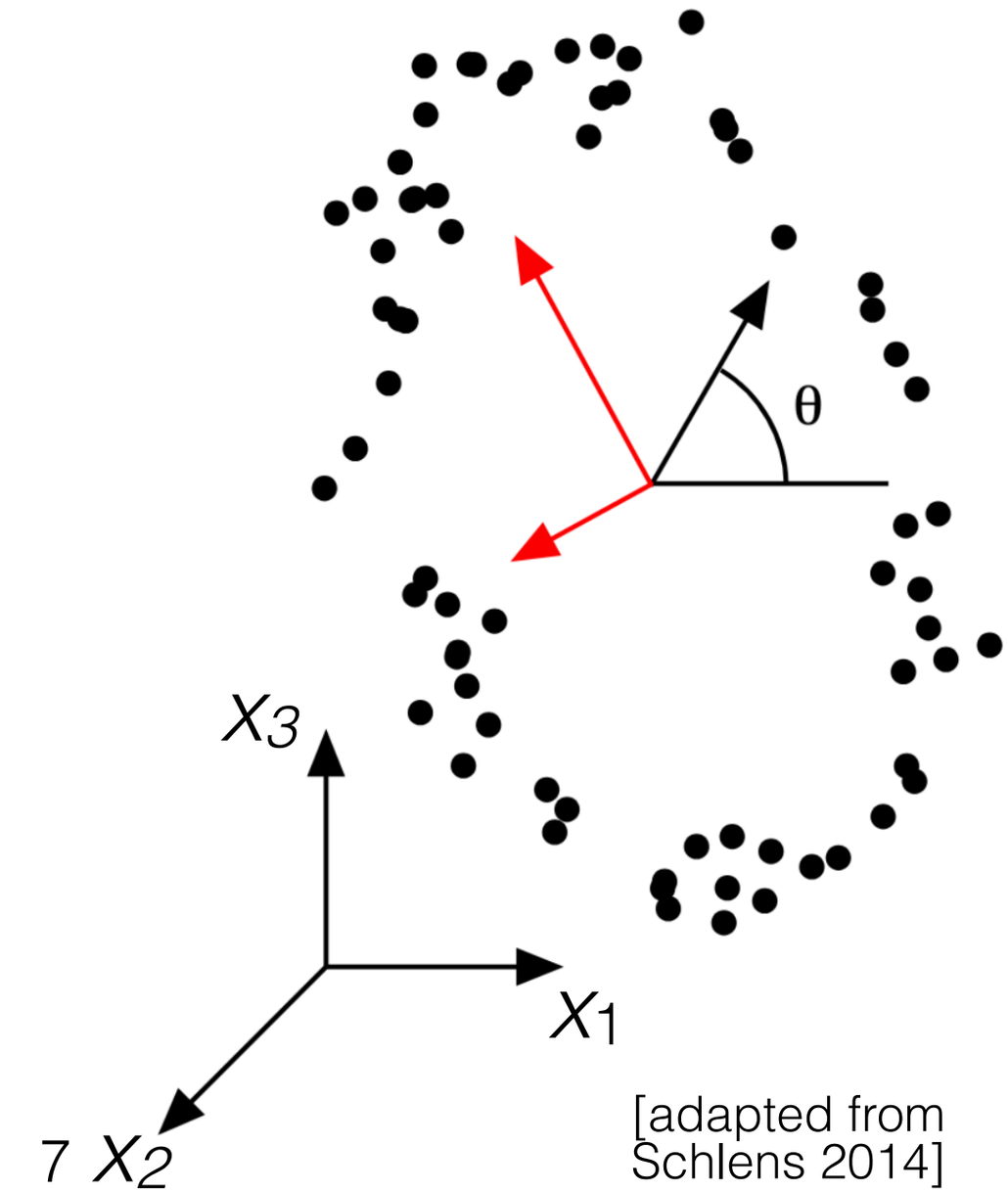

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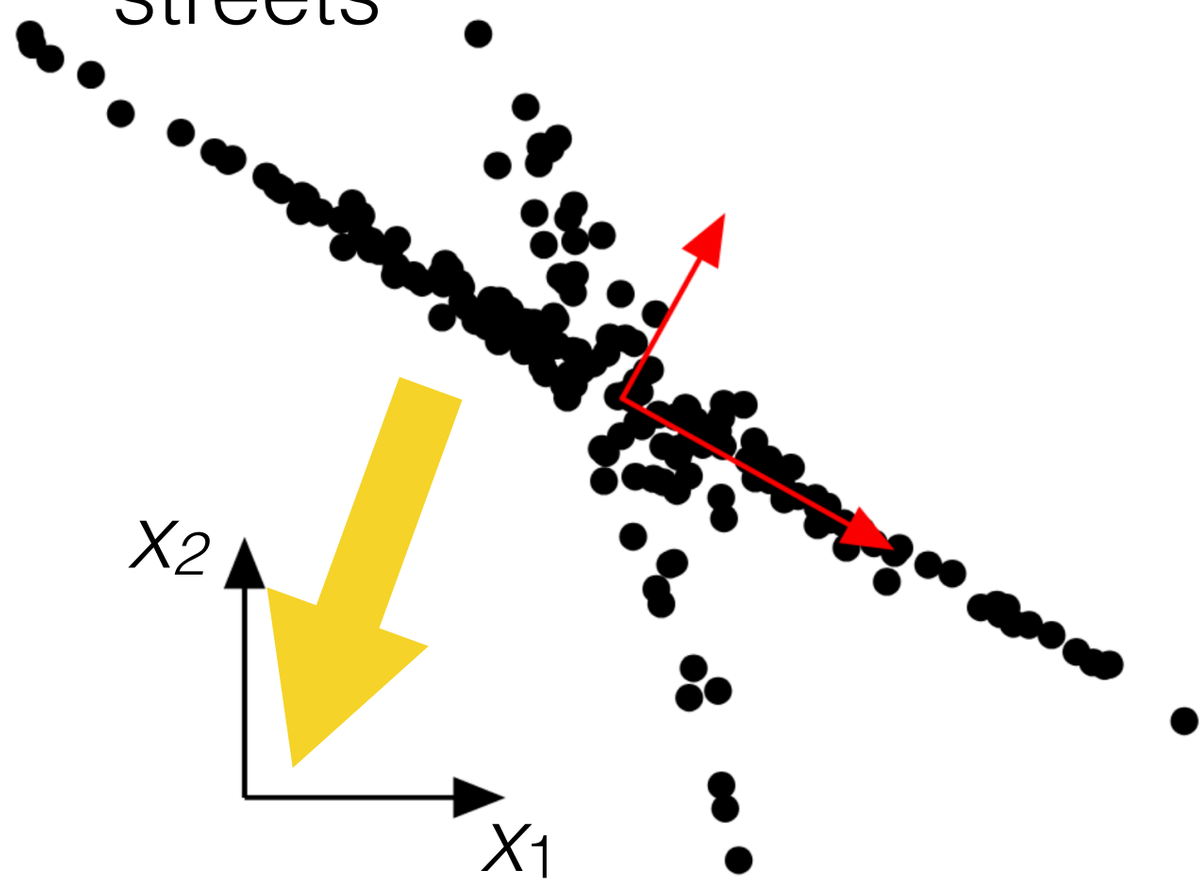

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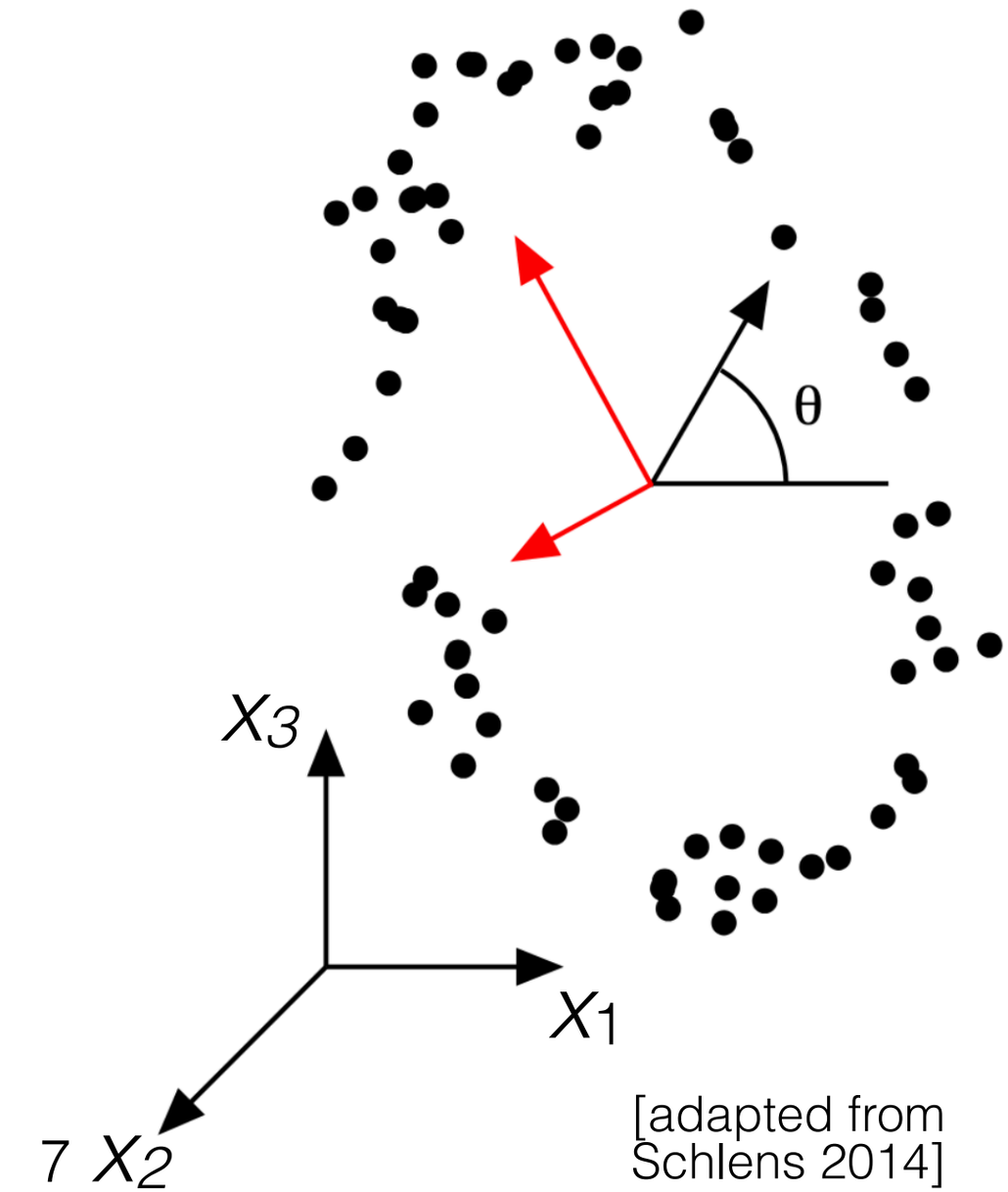

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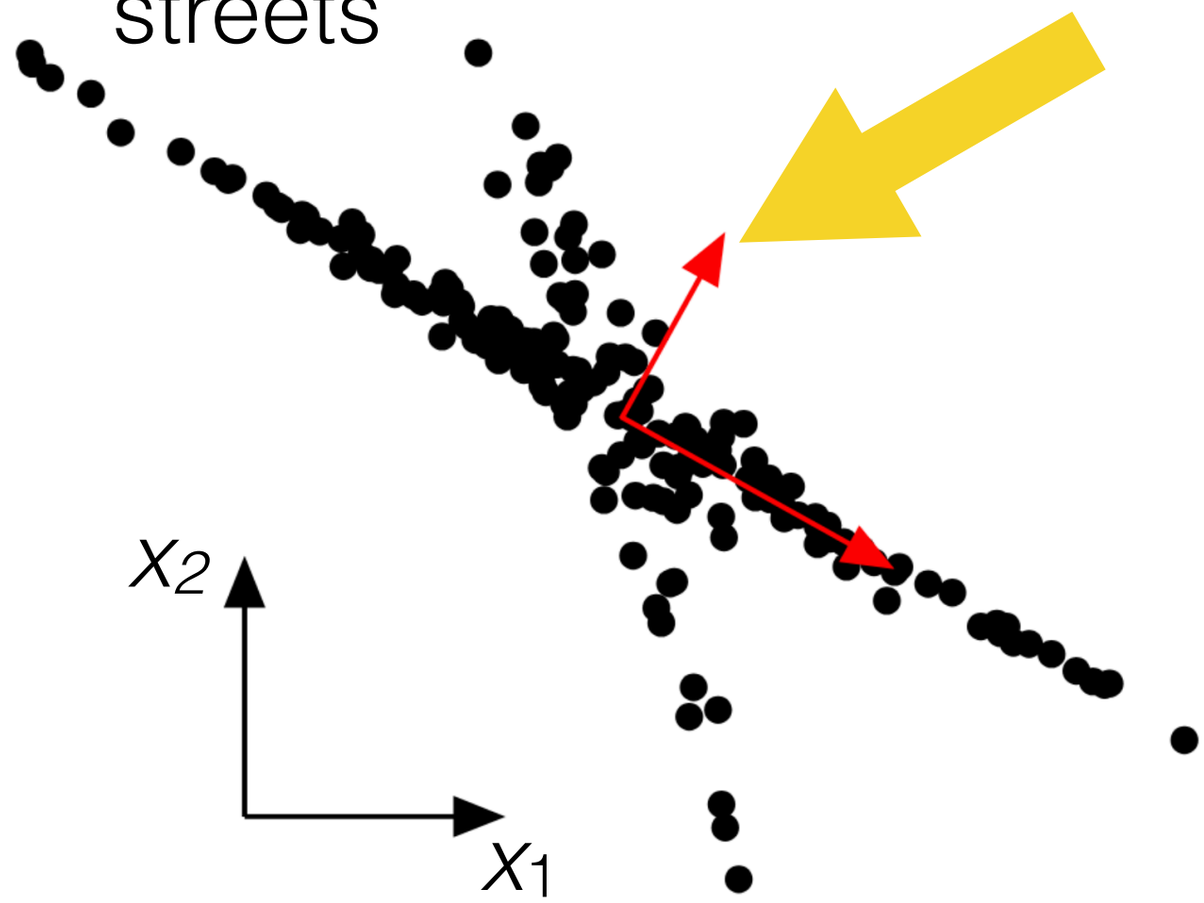

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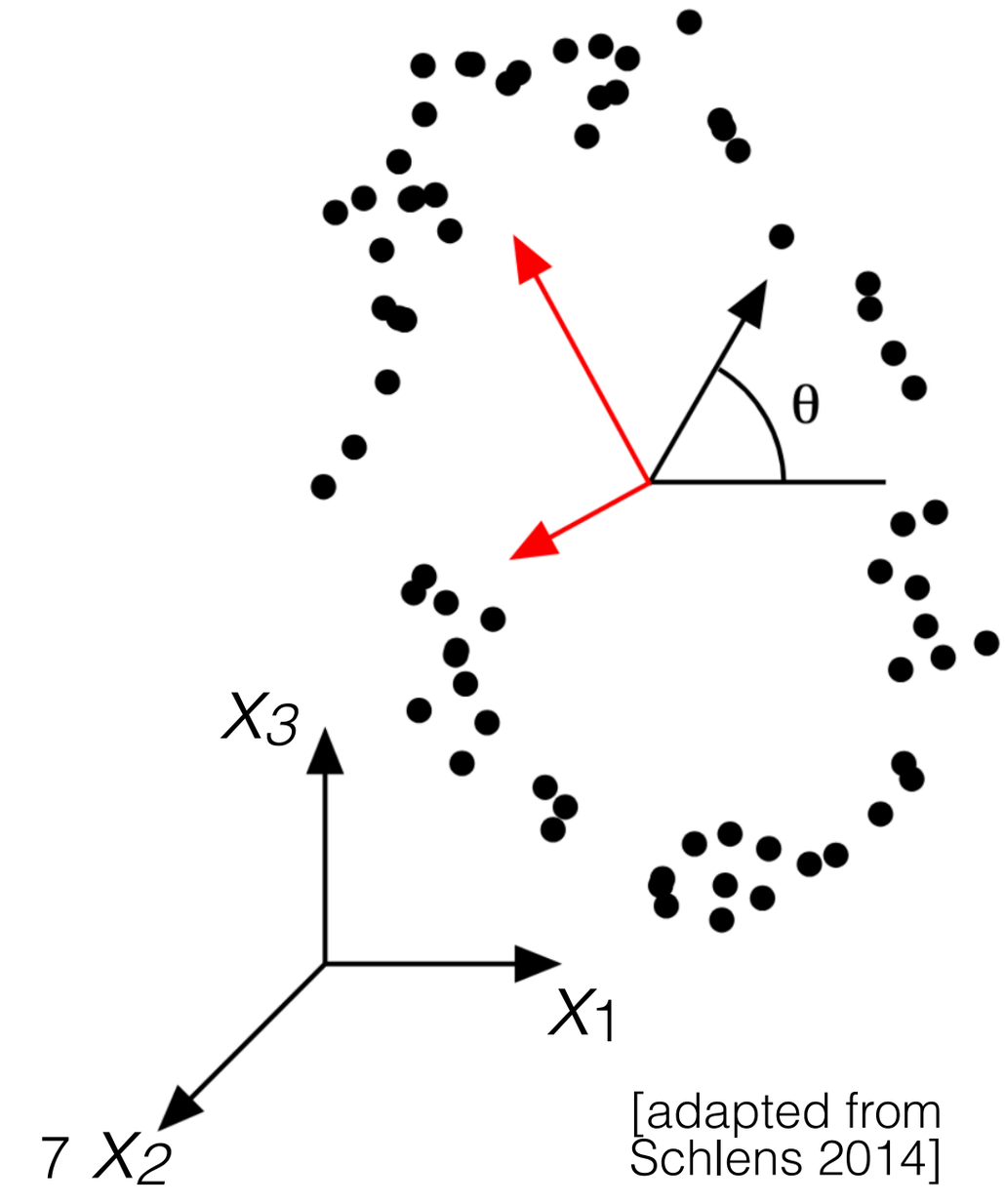

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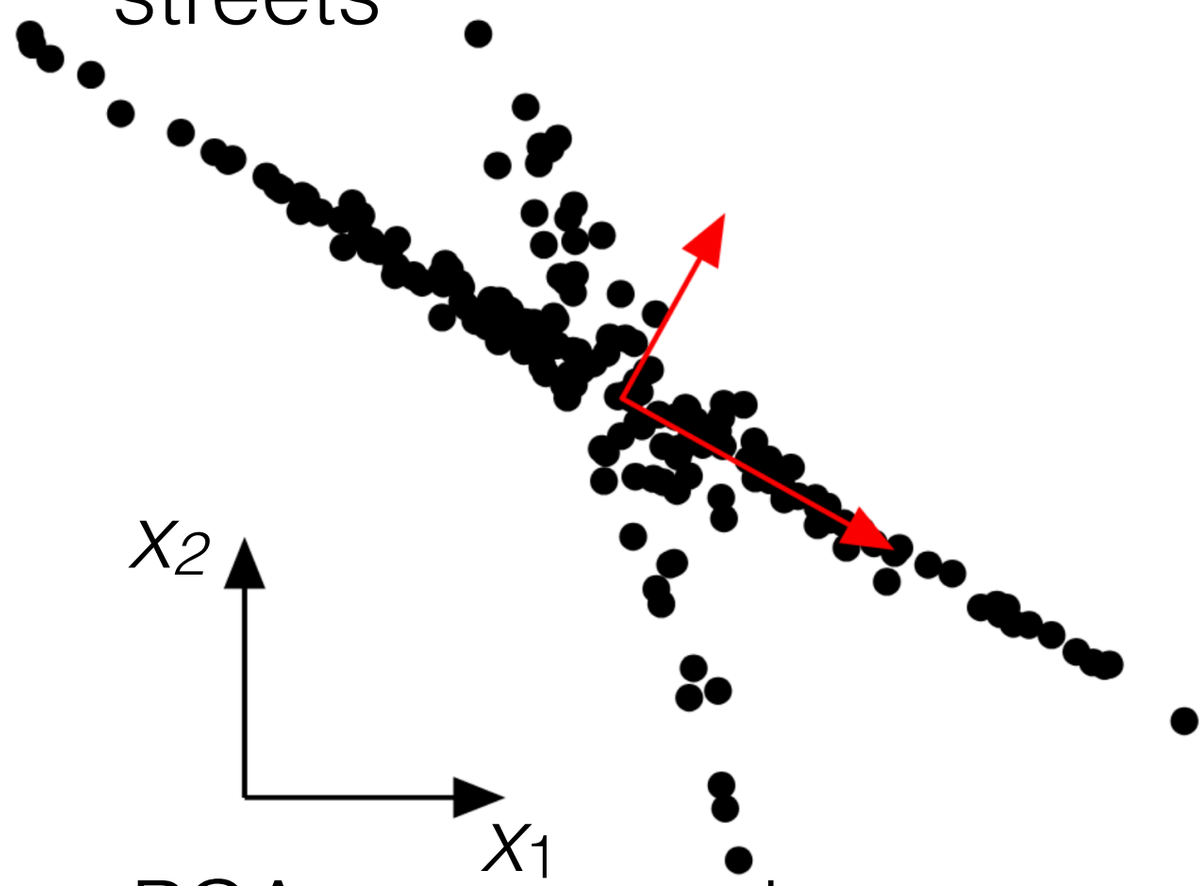

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[Bishop 2006, 12.1]

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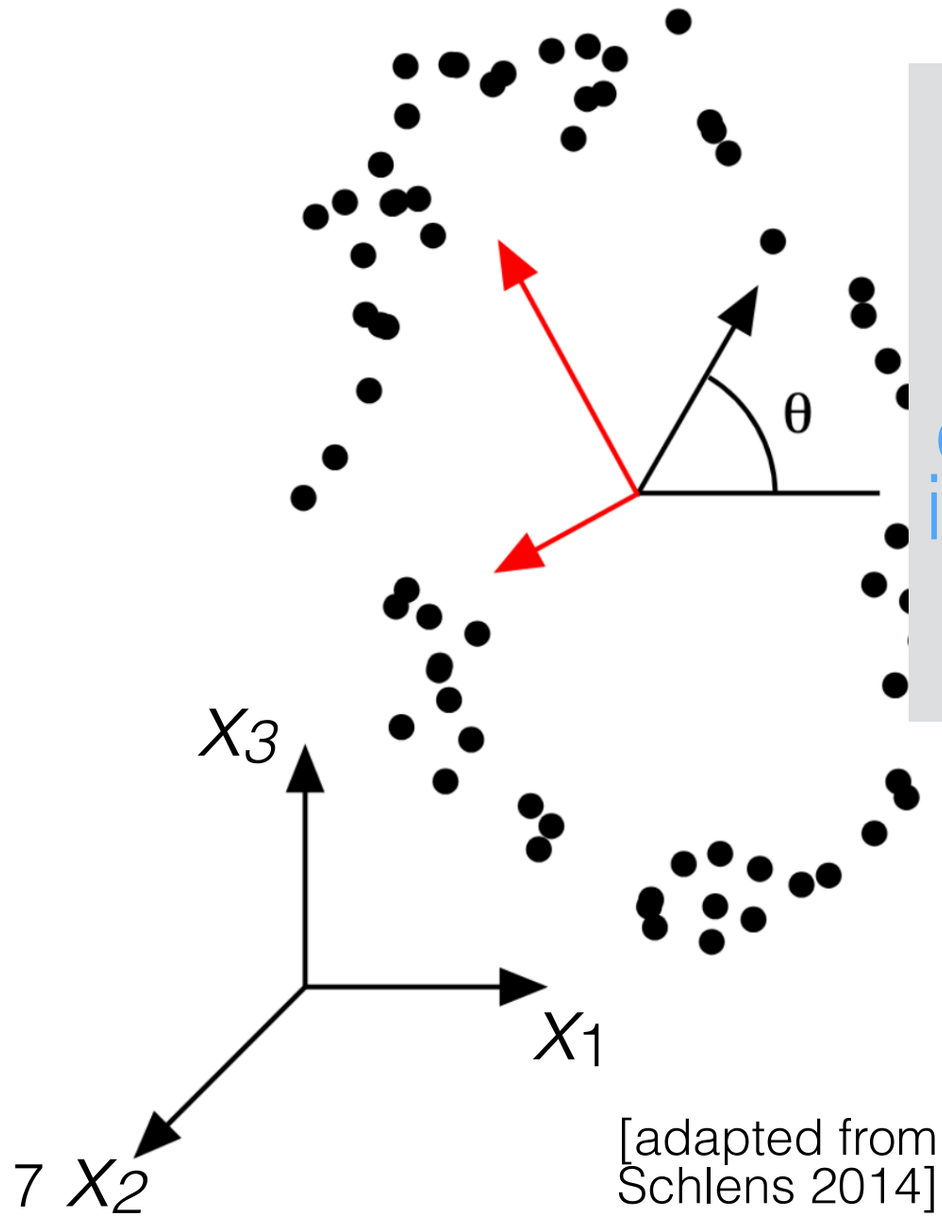

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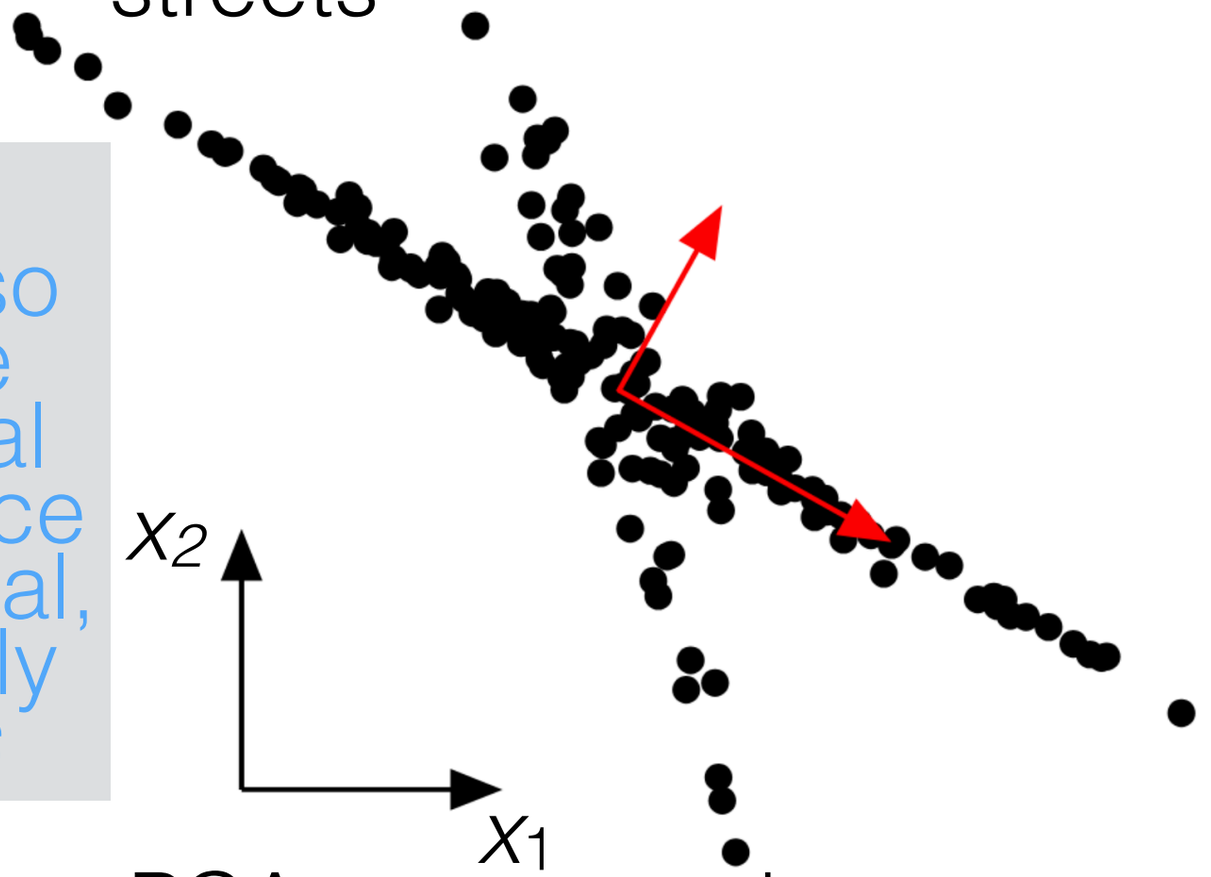

PCA rotates so that the empirical covariance is diagonal, but it only *rotates*

[adapted from Schlens 2014]

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Another option: t-SNE

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UCI digits
cf. analysis of cells

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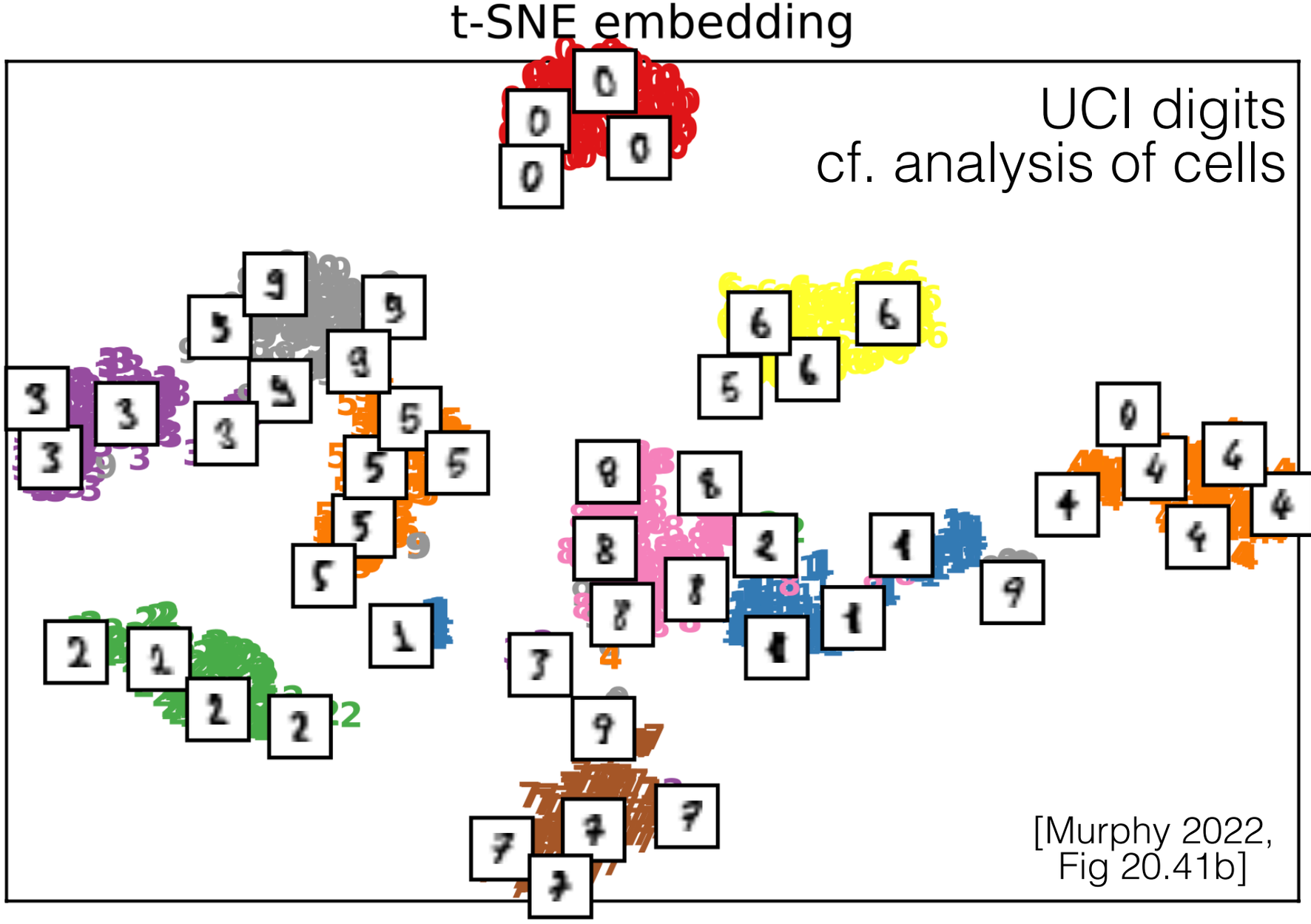

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- t-SNE: Practical behavior is better with a heavier-tailed distribution (student's-t/Cauchy instead of Gaussian)

Challenges of t-SNE

- The choice of perplexity matters

[Largely borrowed from Wattenberg et al 2016 "How to use t-SNE effectively." Check it out!]

Challenges of t-SNE

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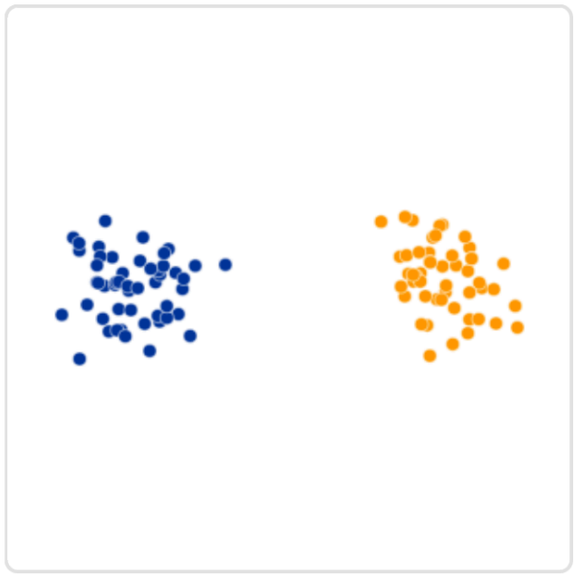

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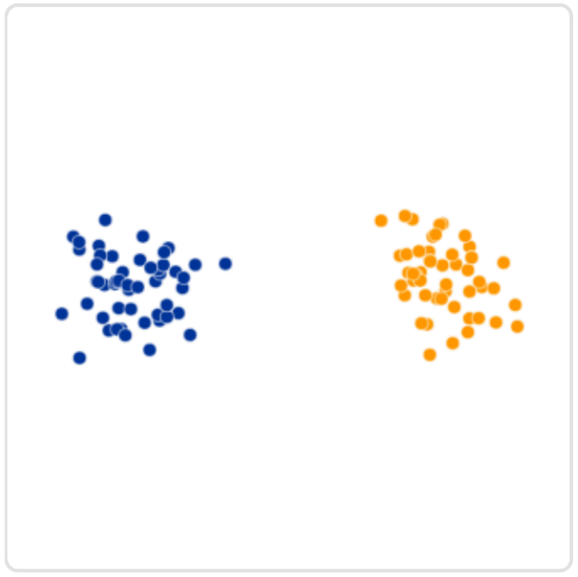

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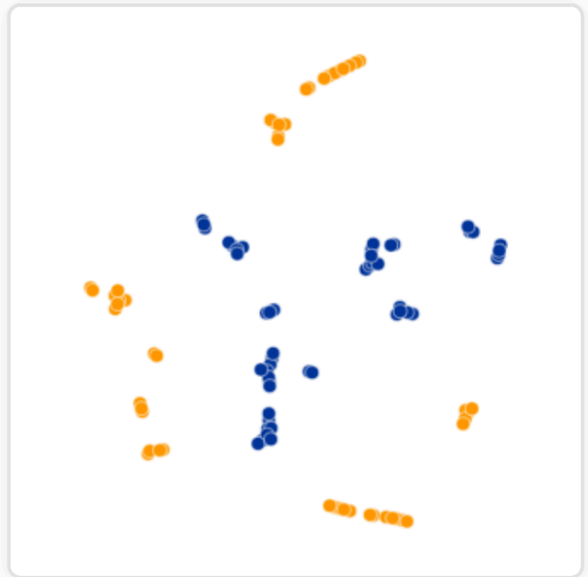
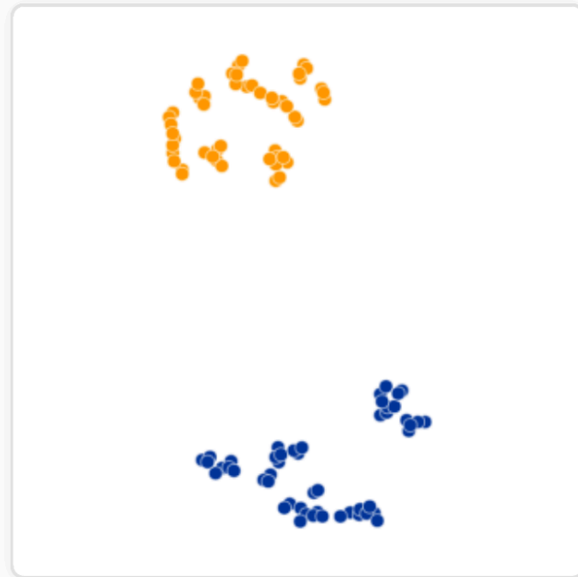
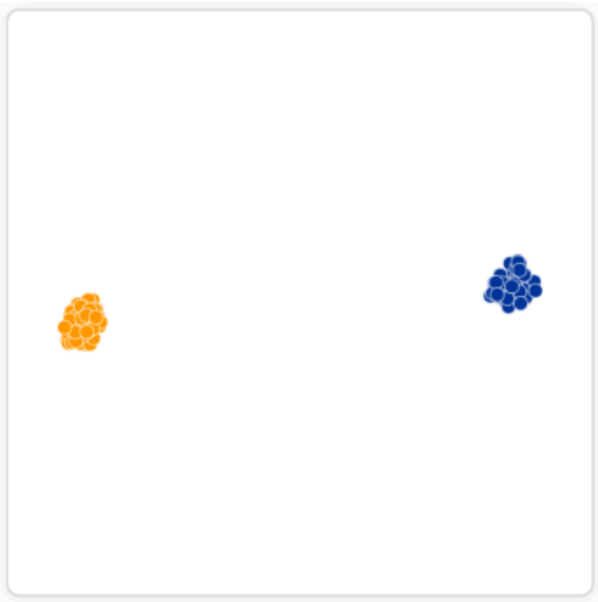


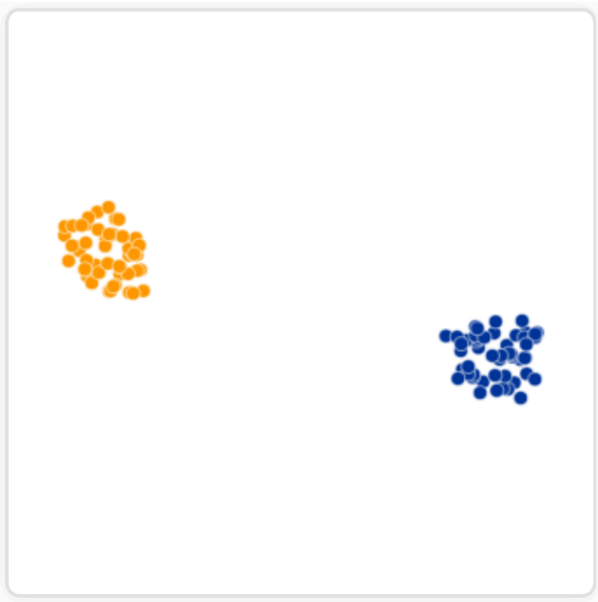
Perplexity: 2
Step: 5,000



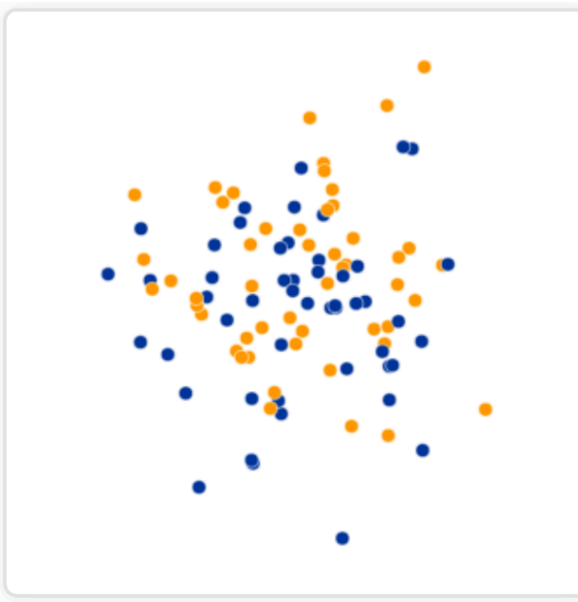
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000



Perplexity: 100
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Challenges of t-SNE

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- The choice of perplexity matters
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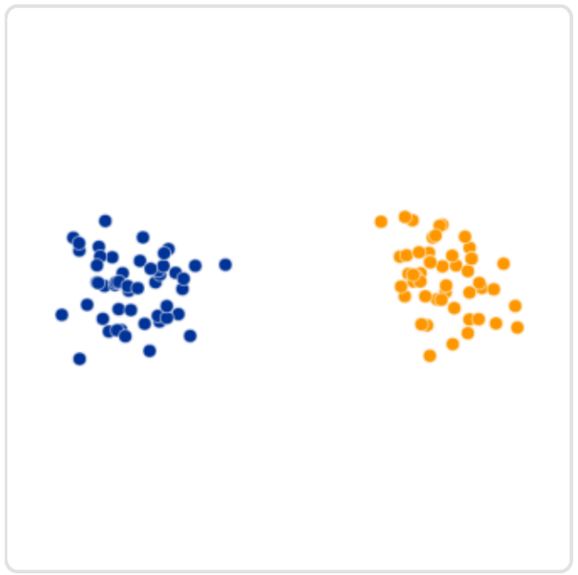
- t-SNE paper suggests perplexity between 5 and 50



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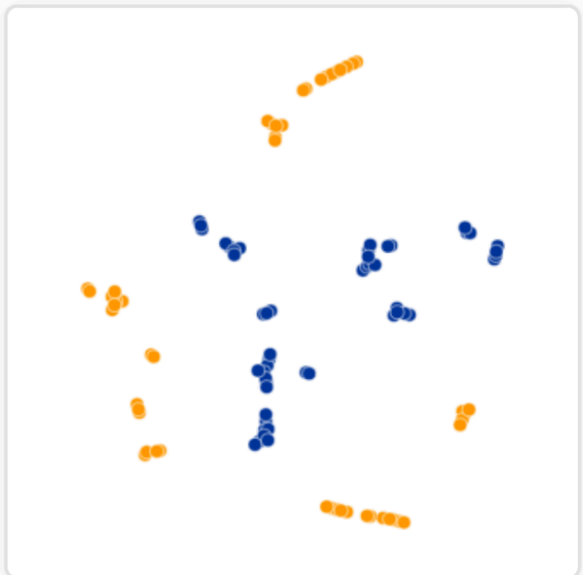
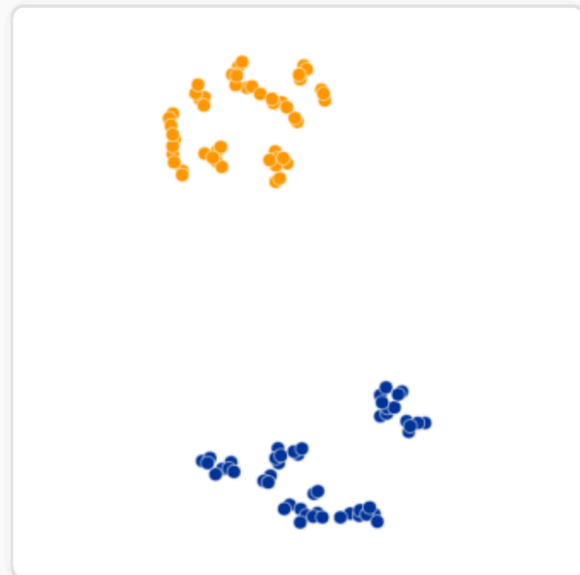
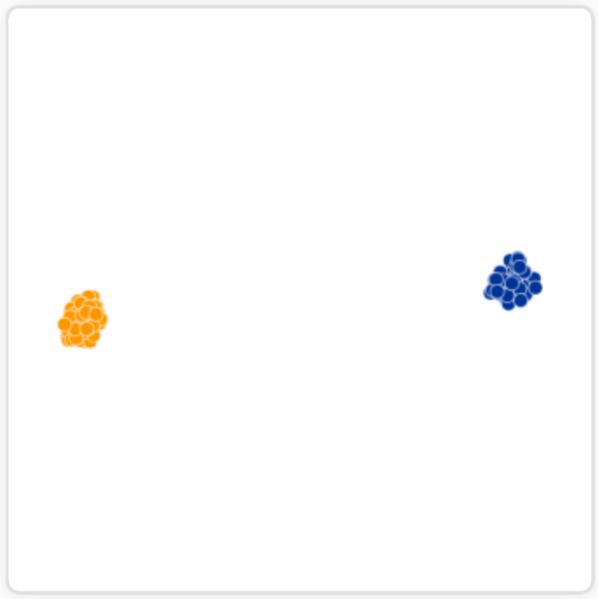


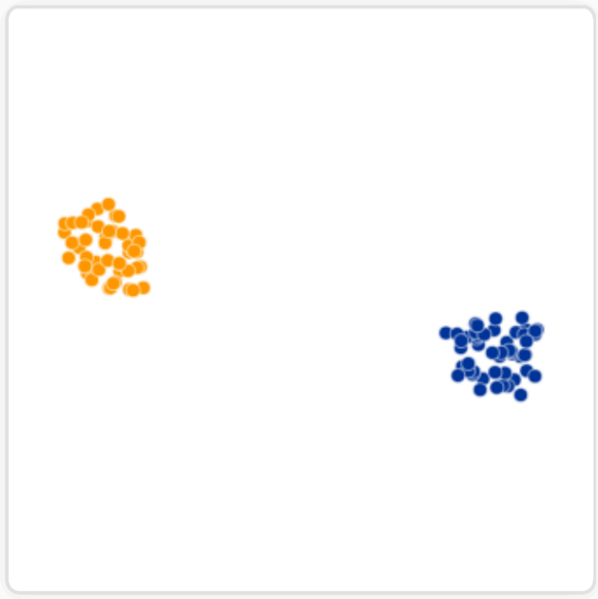
Perplexity: 2
Step: 5,000



Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



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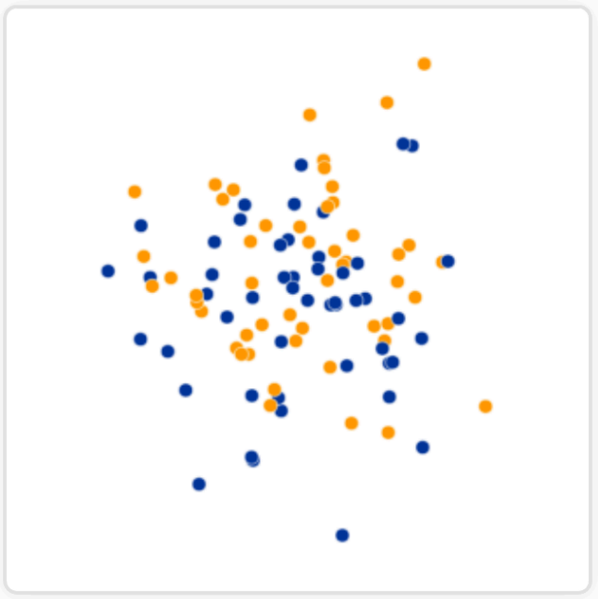

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Challenges of t-SNE

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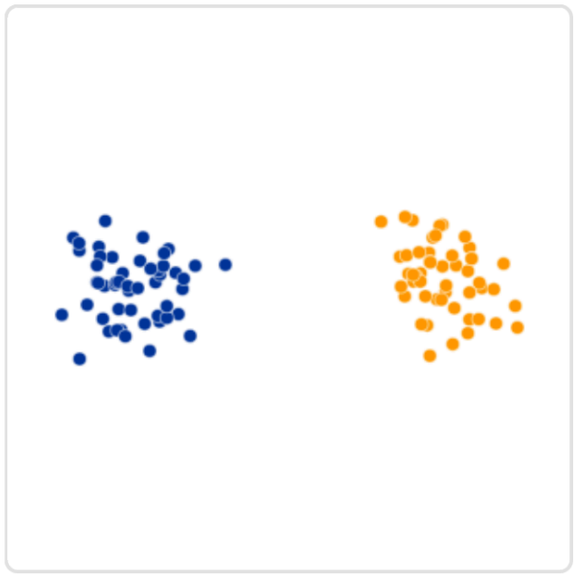
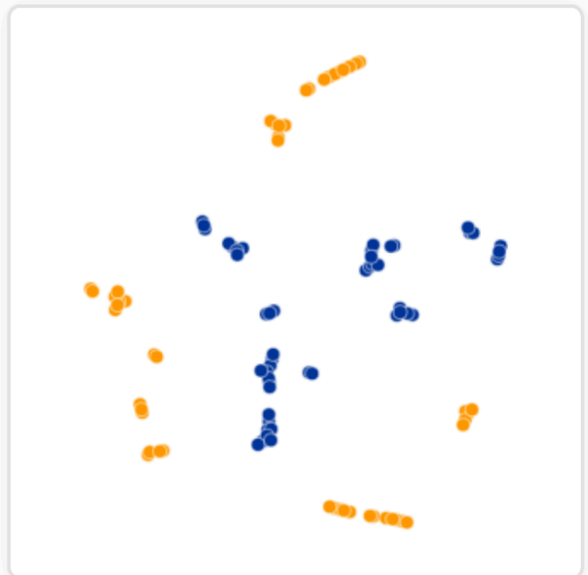
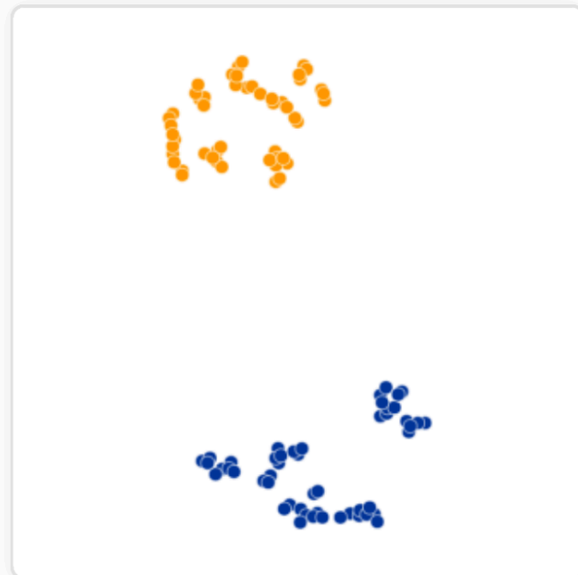
- The choice of perplexity matters
- Data 2D here
- t-SNE paper suggests perplexity between 5 and 50
- Default is often 30



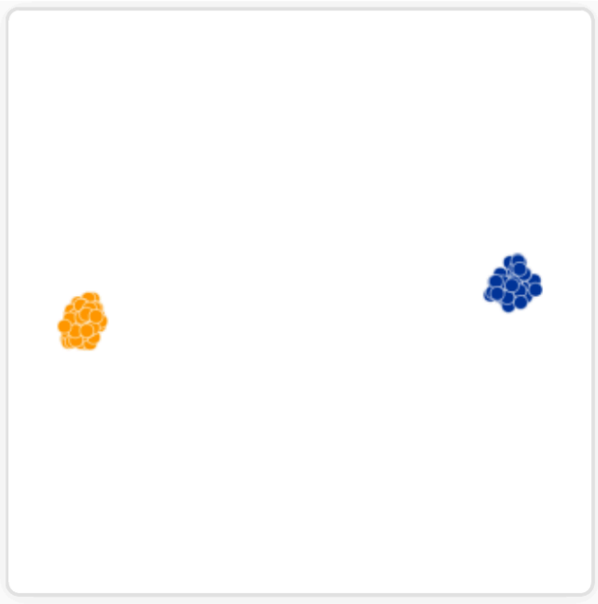
Original



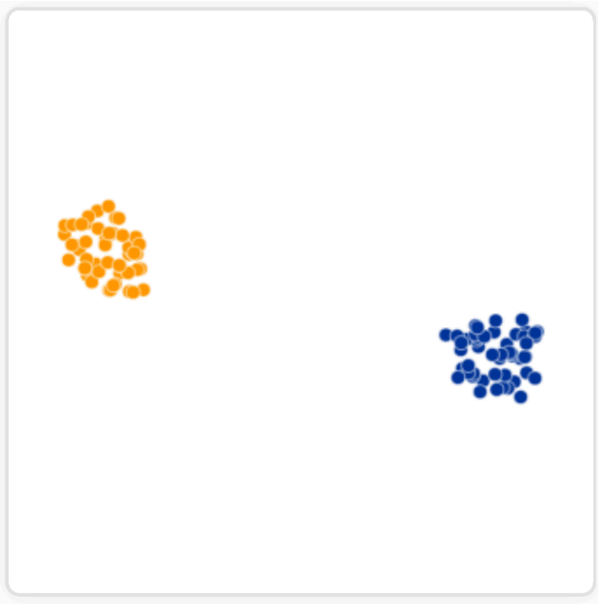
Perplexity: 2
Step: 5,000



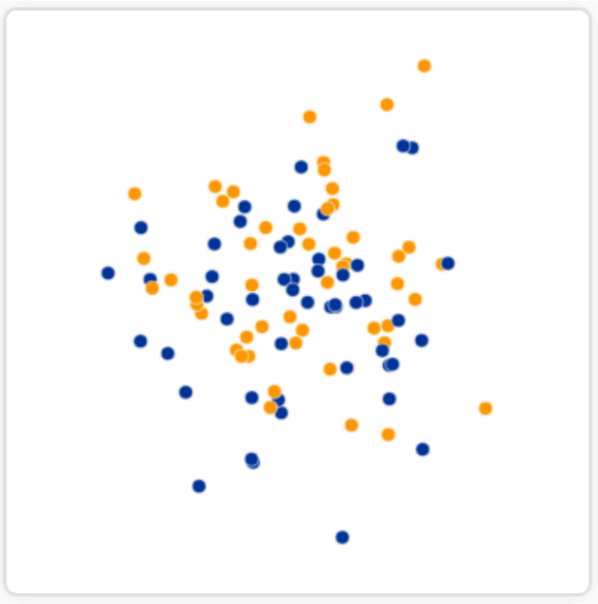
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000

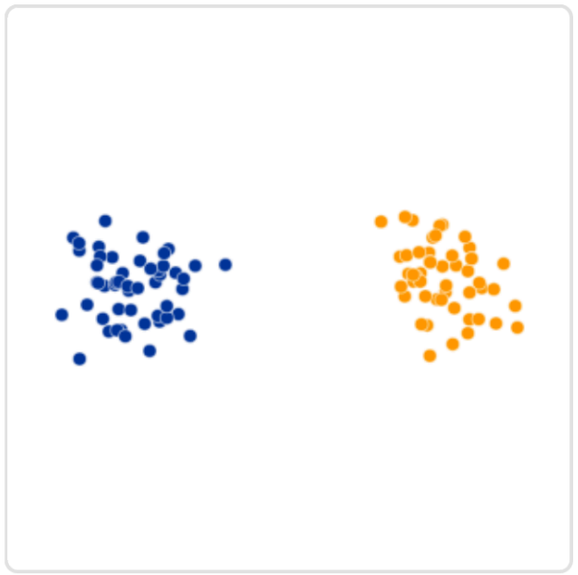


Perplexity: 100
Step: 5,000

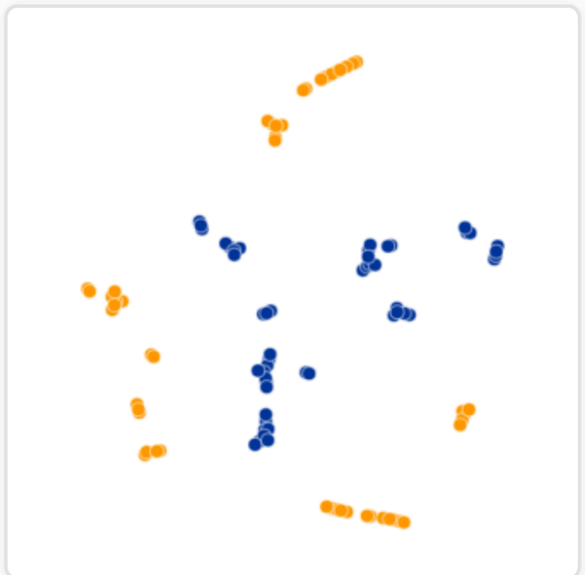
Challenges of t-SNE

[Largely borrowed from Wattenberg et al 2016 "How to use t-SNE effectively." Check it out!]

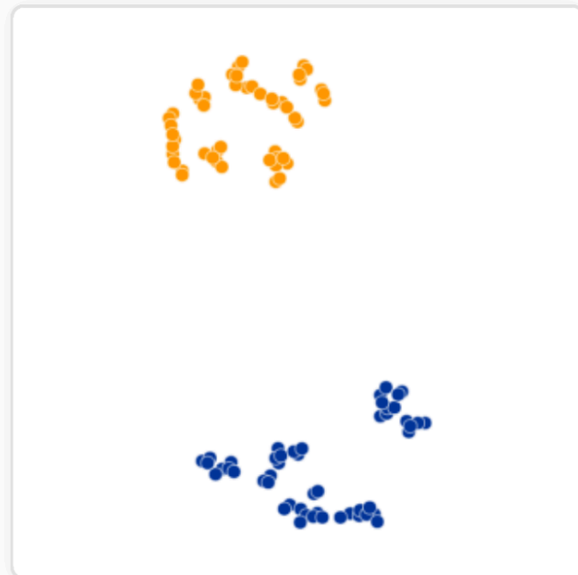
- The choice of perplexity matters
- Data 2D here
- t-SNE paper suggests perplexity between 5 and 50
- Default is often 30
- Have to choose learning rate & # steps (optimization matters)



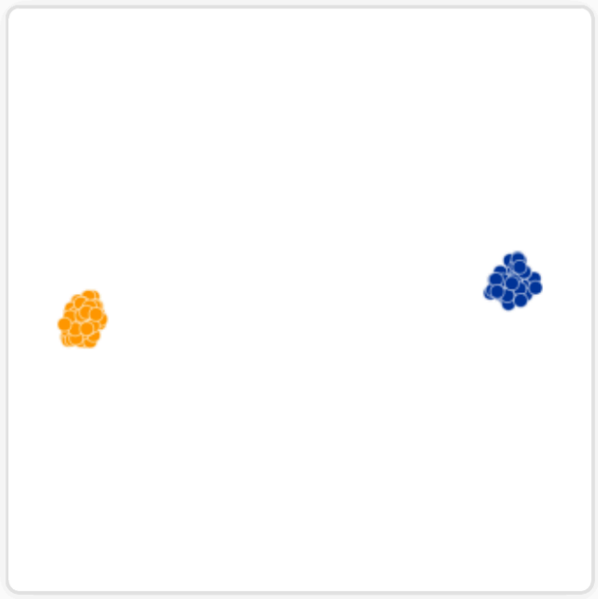
Original



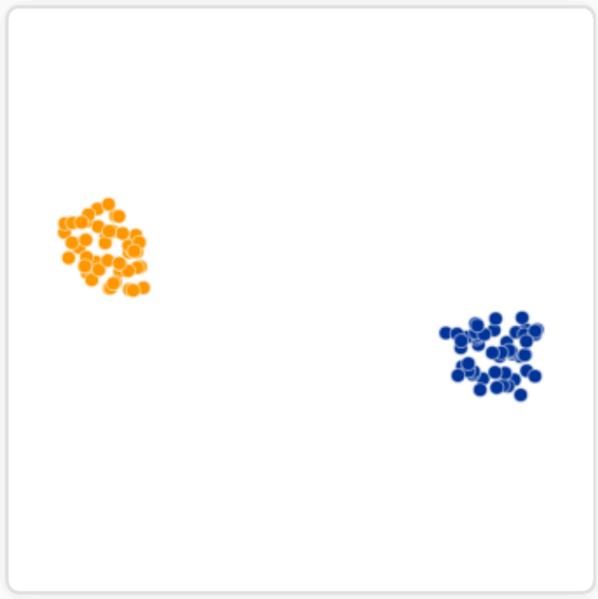
Perplexity: 2
Step: 5,000



Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000

Perplexity: 100
Step: 5,000

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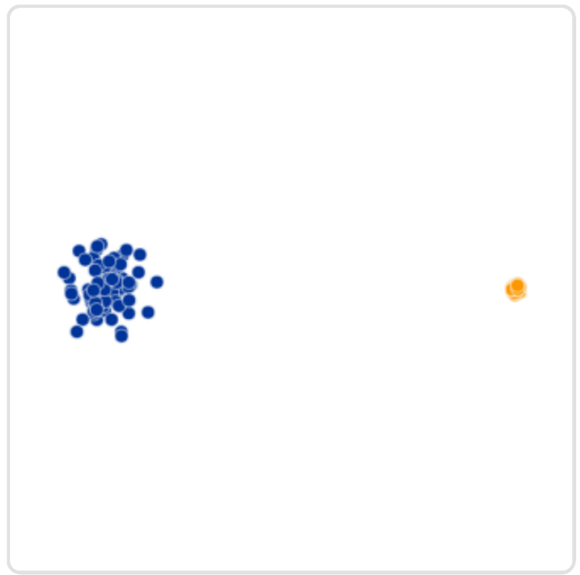

Original

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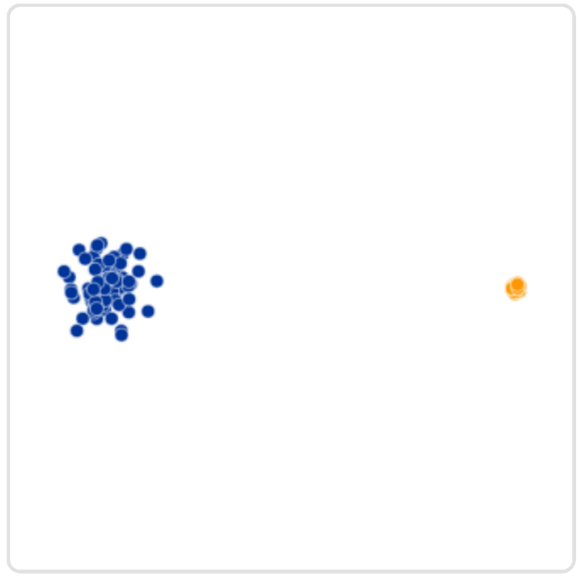
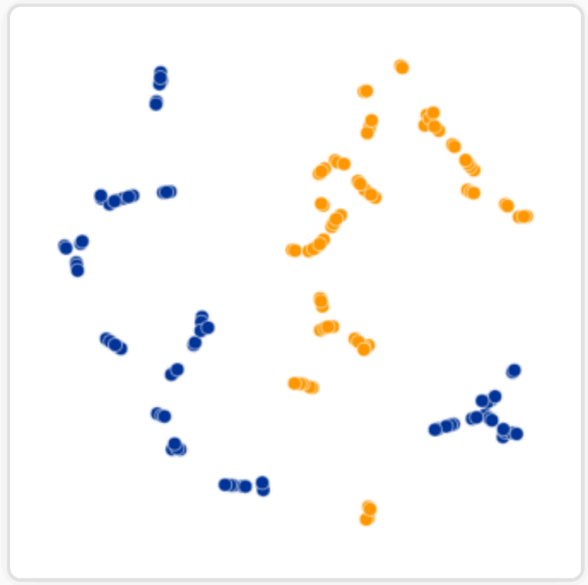
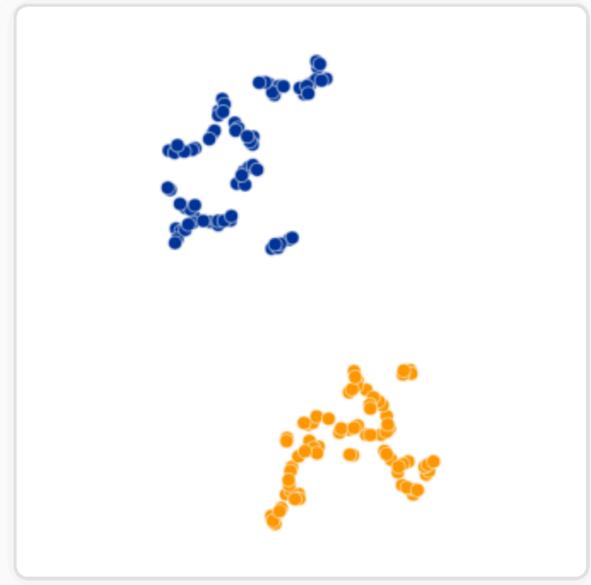


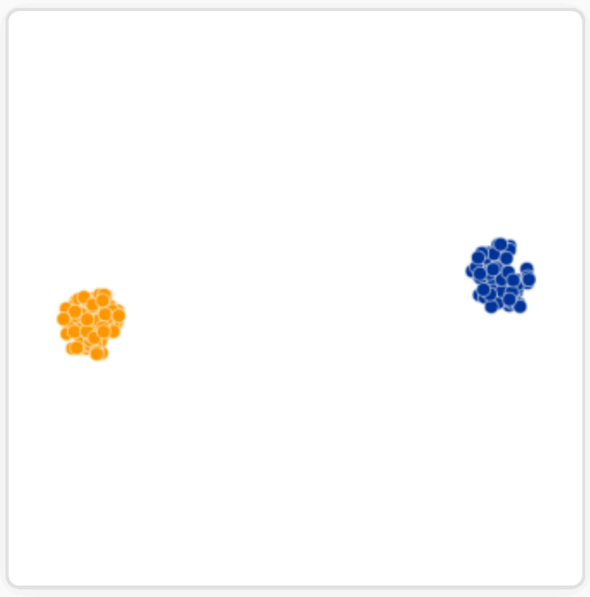
Original



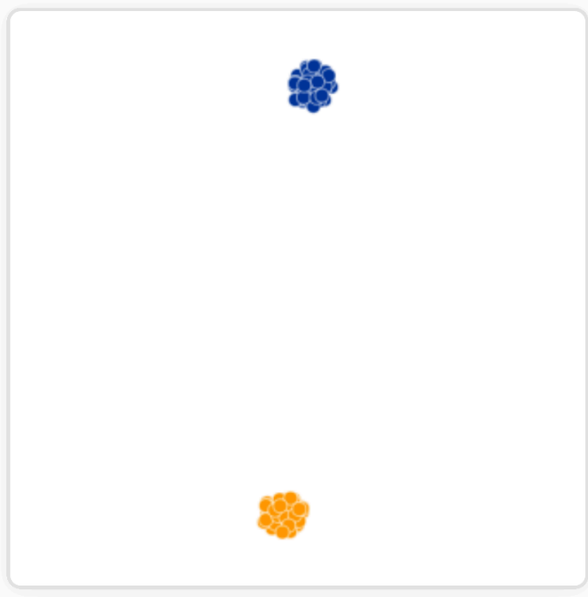
Perplexity: 2
Step: 5,000



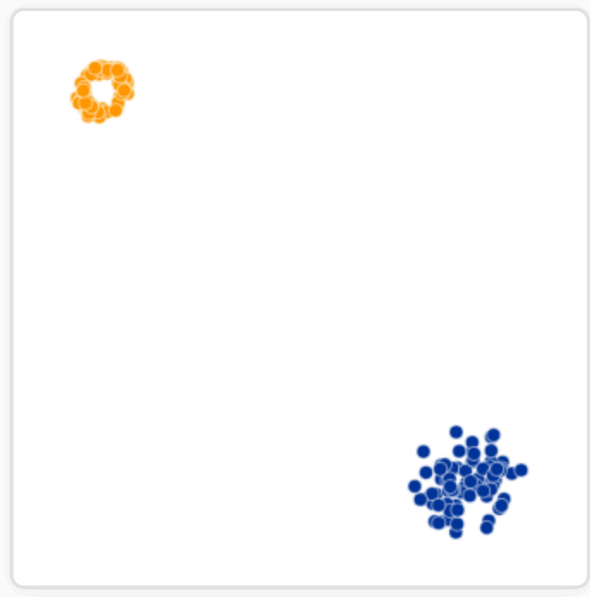
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000



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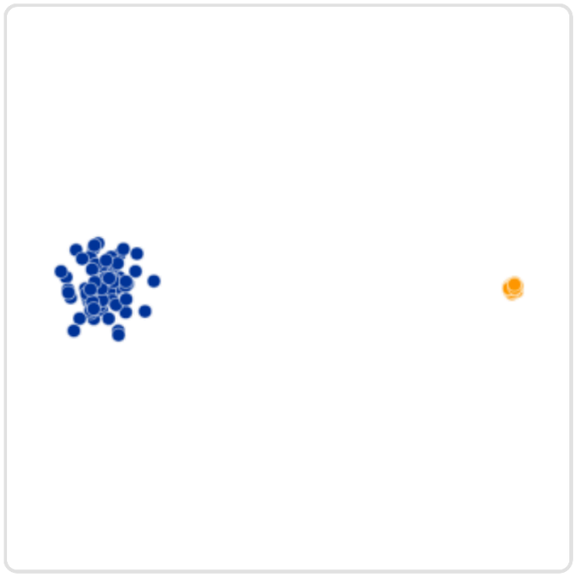
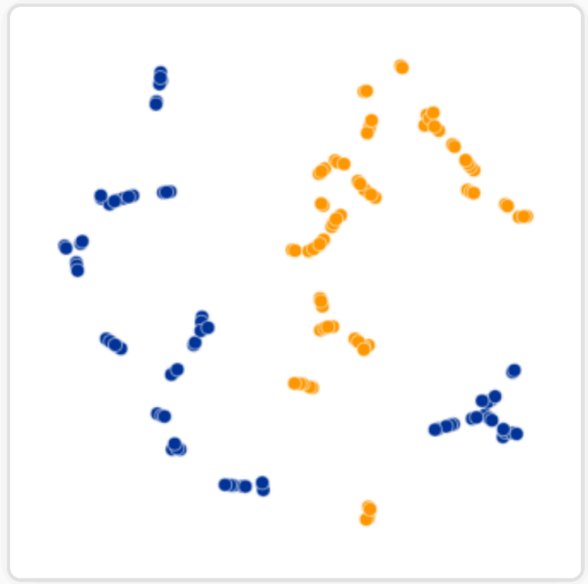
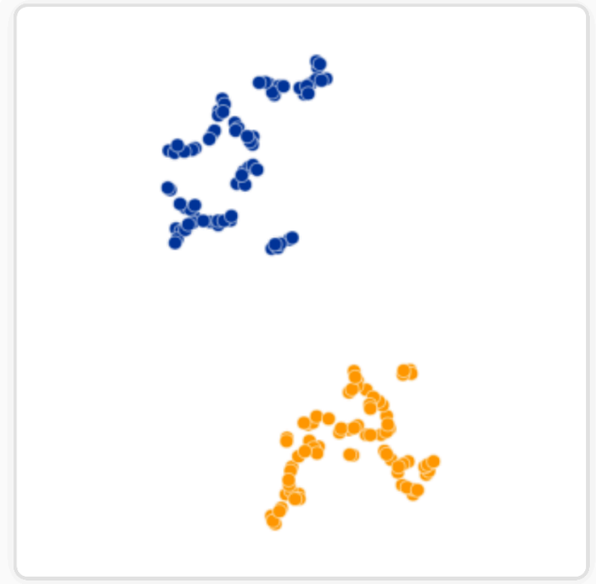


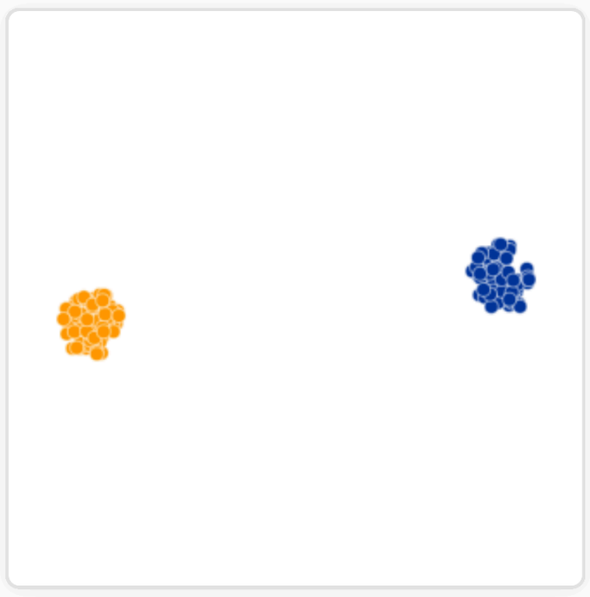
Original



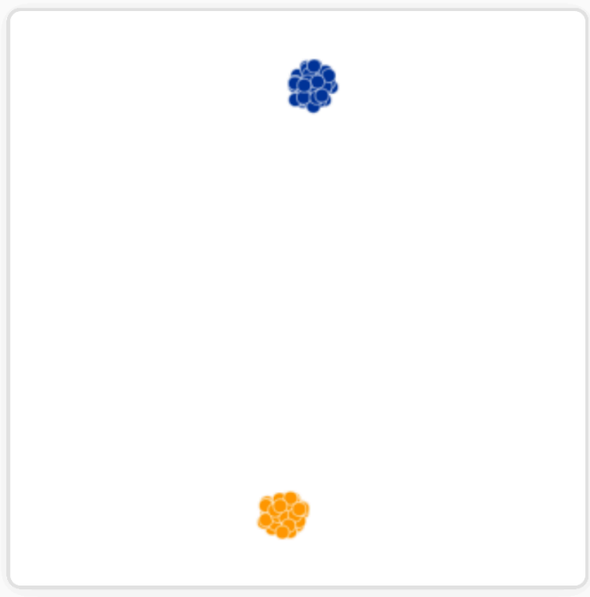
Perplexity: 2
Step: 5,000



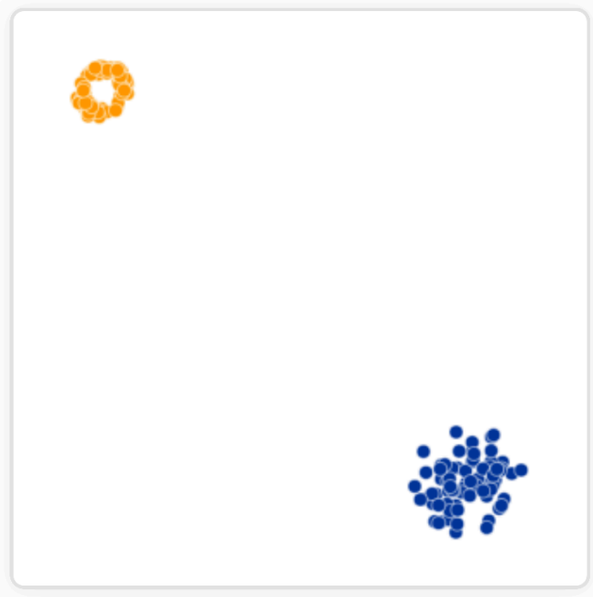
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000

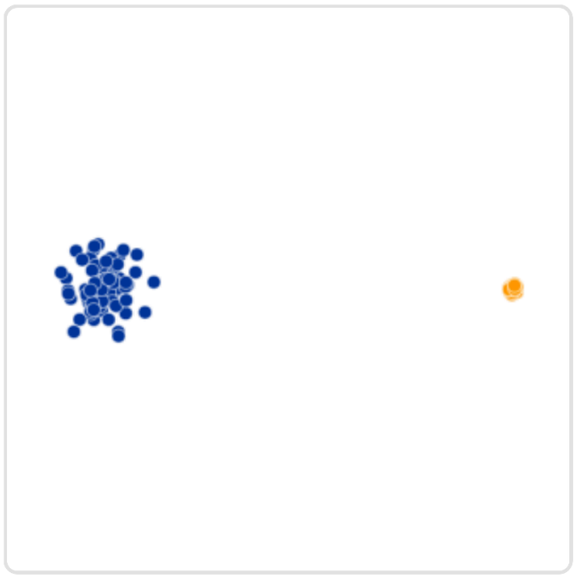


Perplexity: 100
Step: 5,000

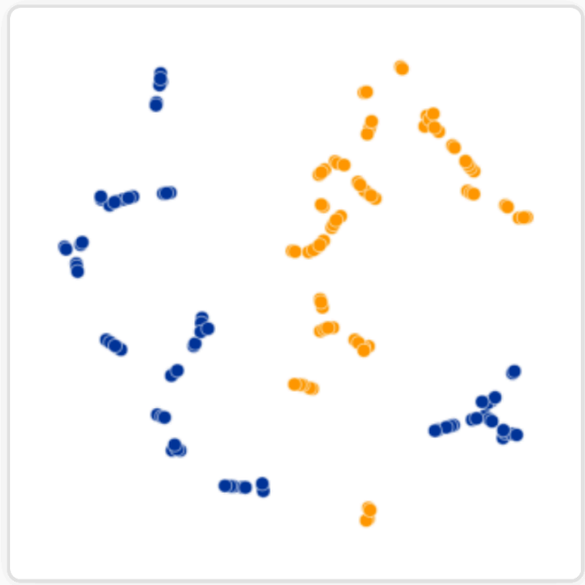
Challenges of t-SNE

[Largely borrowed from Wattenberg et al 2016 “How to use t-SNE effectively.” Check it out!]

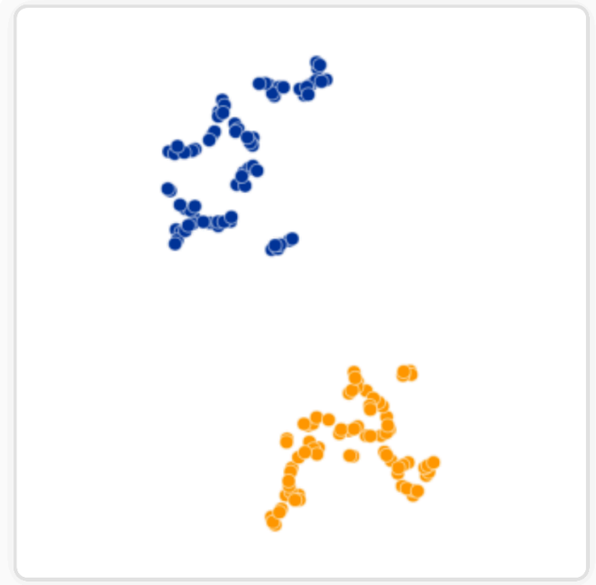
- t-SNE cluster diameters need not reflect original diameters
- Data 2D here
- By design, t-SNE adapts its notion of distance around each point / locally
- Recall that the global perplexity (~controls # of neighbors) $\Rightarrow \{\sigma_n^2\}_{n=1}^N$



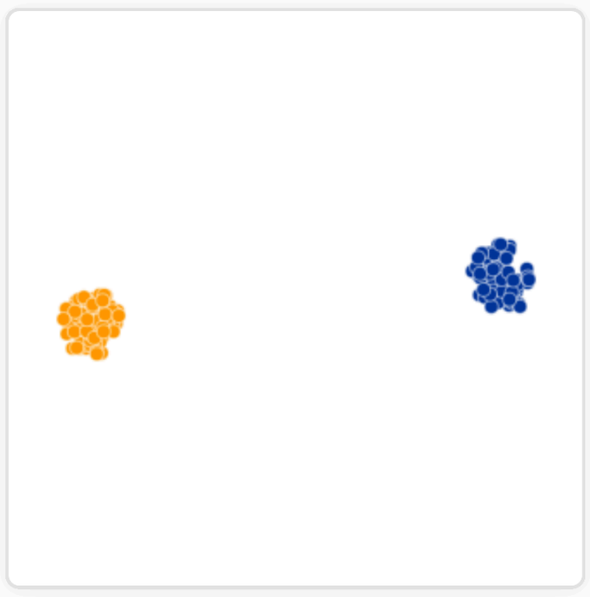
Original



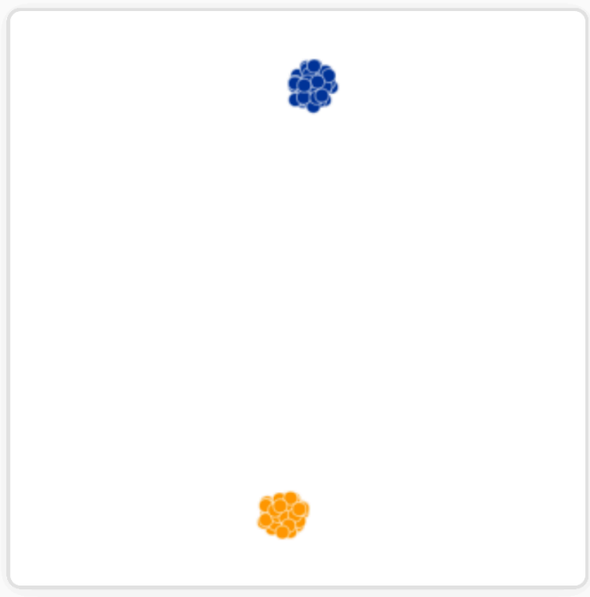
Perplexity: 2
Step: 5,000



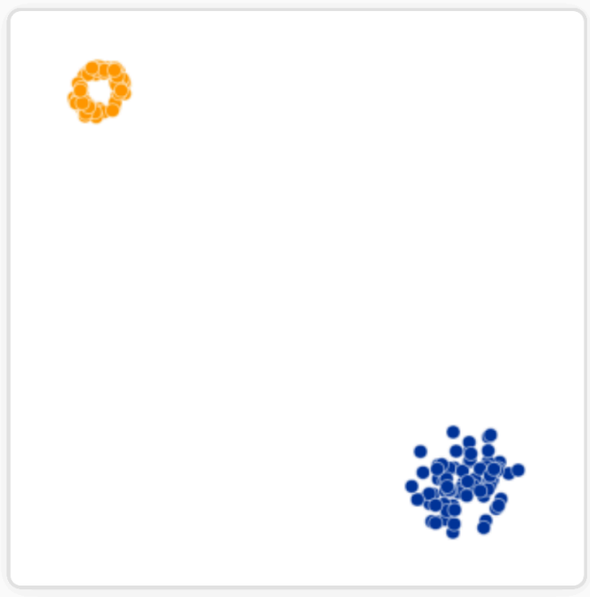
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000



Perplexity: 100
Step: 5,000

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[Largely borrowed from Wattenberg et al 2016 “How to use t-SNE effectively.” Check it out!]

- t-SNE distances between clusters need not reflect originals

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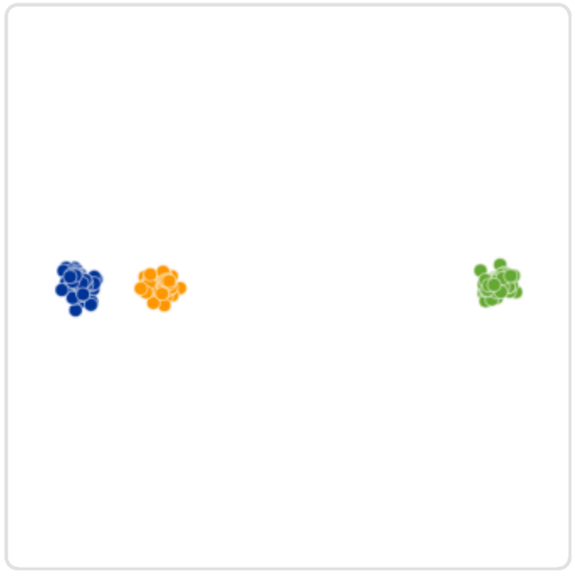

Original

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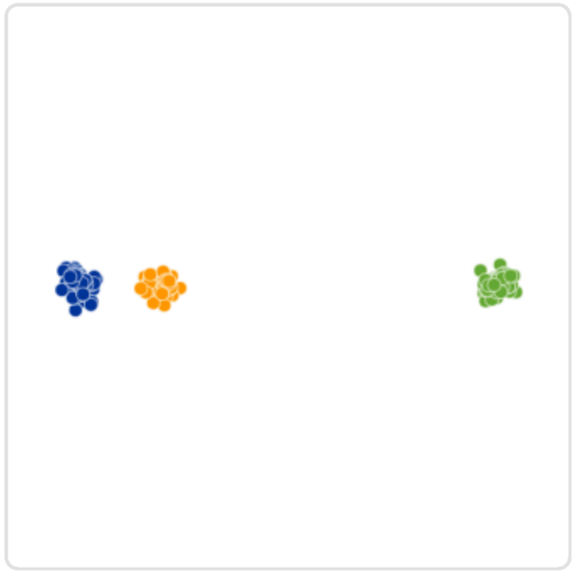
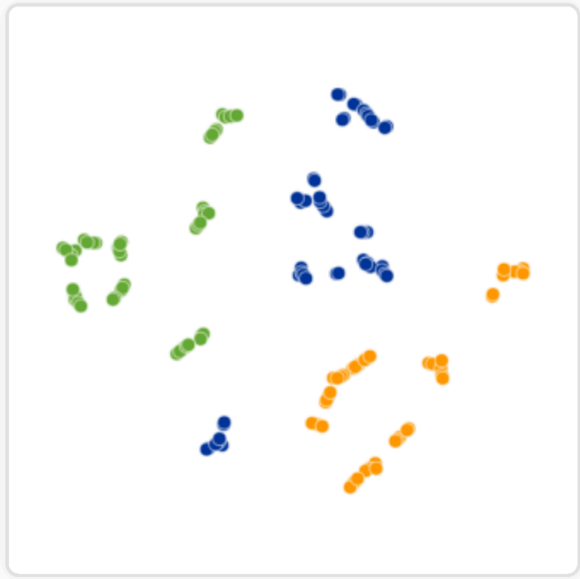
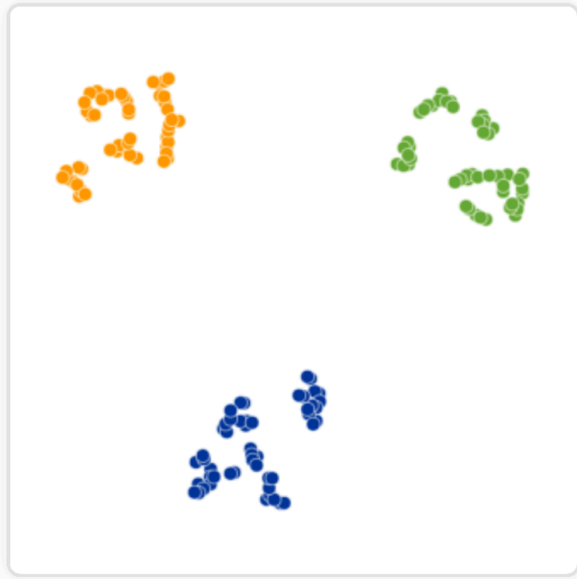


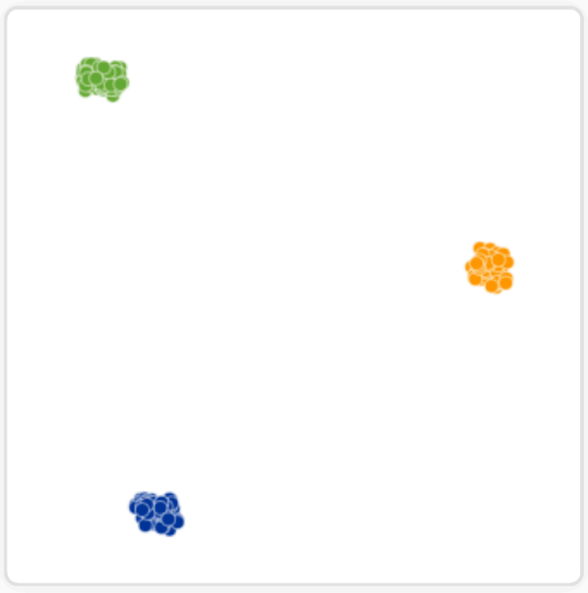
Original



Perplexity: 2
Step: 5,000



Perplexity: 5
Step: 5,000



Perplexity: 30
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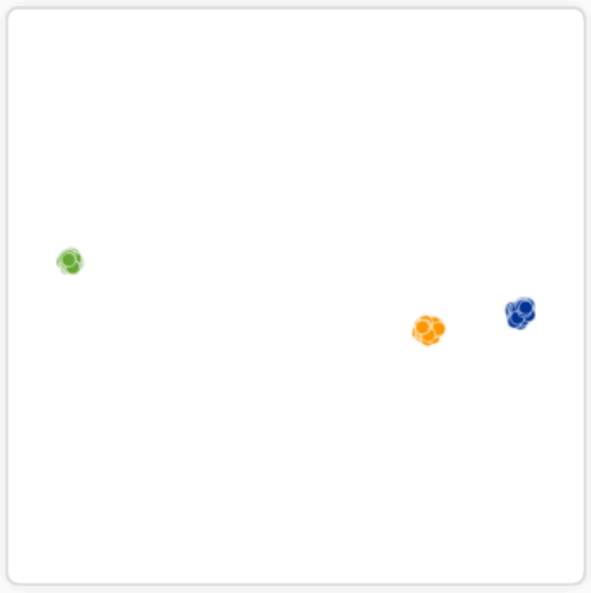
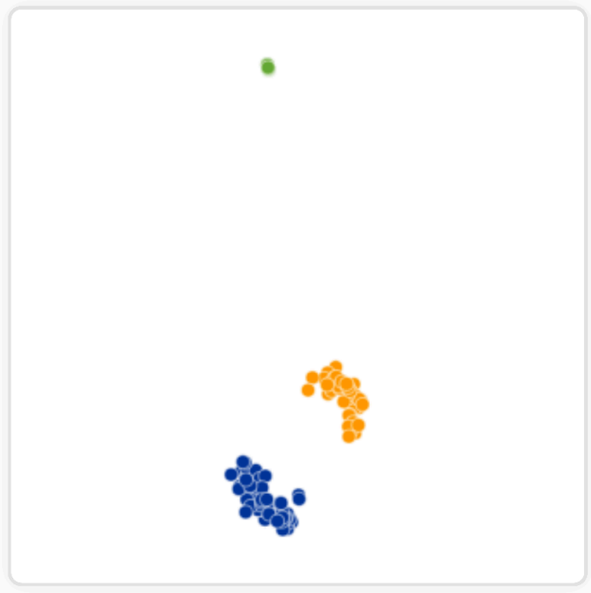


Perplexity: 50
Step: 5,000



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Challenges of t-SNE

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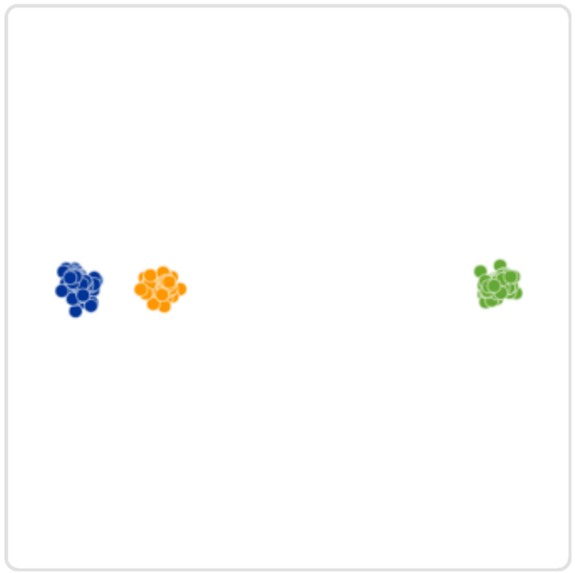
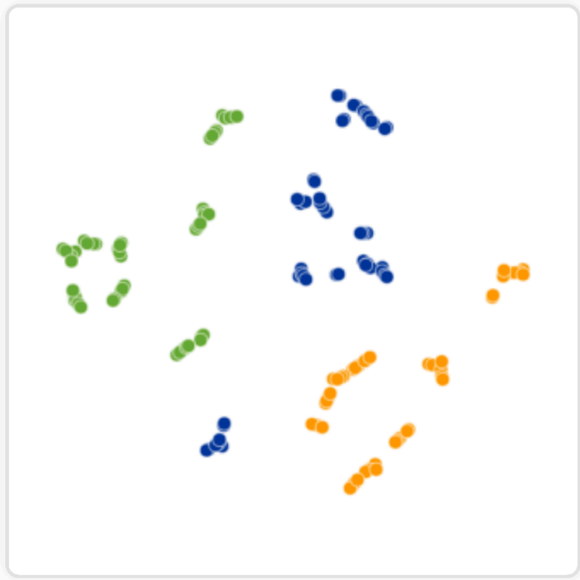
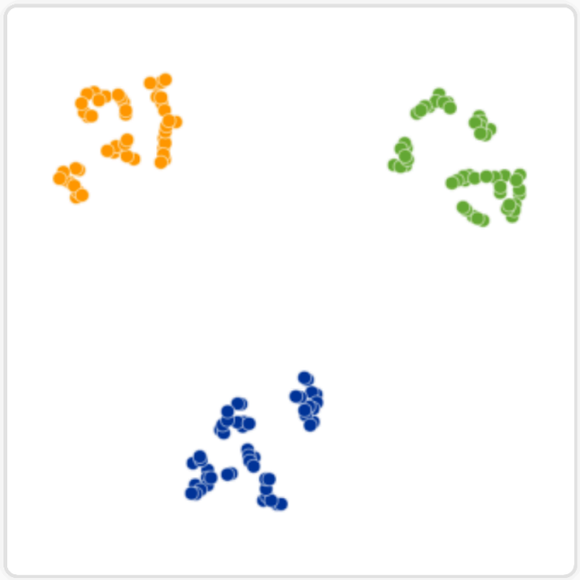
- t-SNE distances between clusters need not reflect originals
- Data 2D here
- Perplexity 50 and above capture the relative distances between clusters; can we count on that in general?



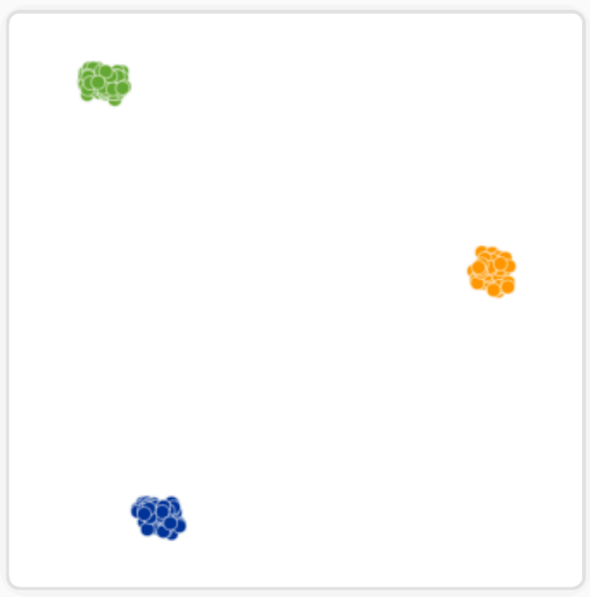
Original



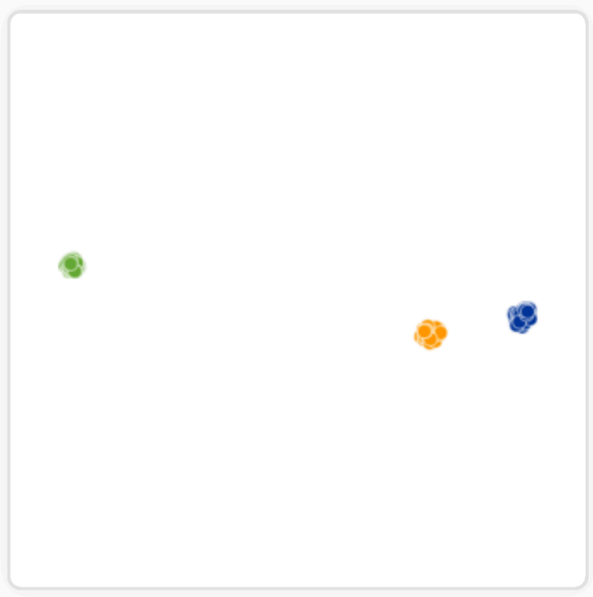
Perplexity: 2
Step: 5,000



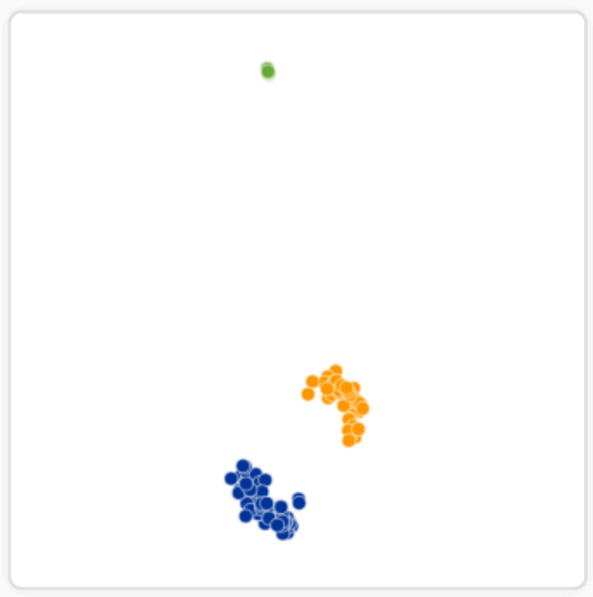
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000



Perplexity: 100
Step: 5,000

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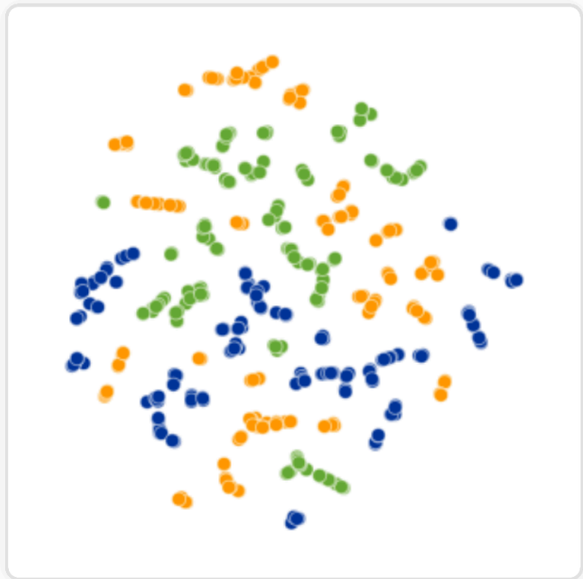
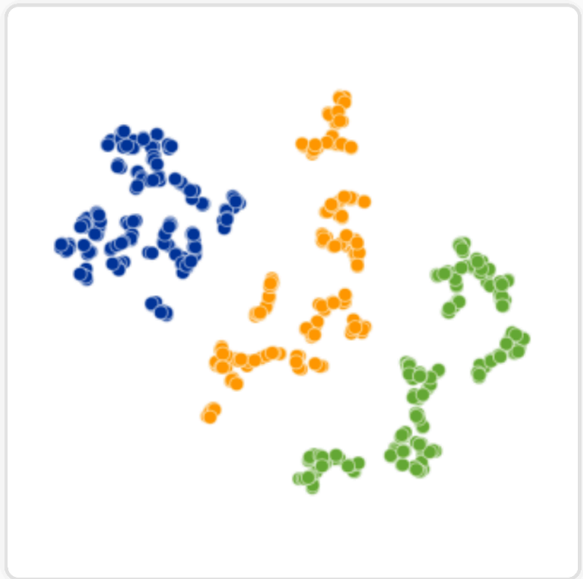
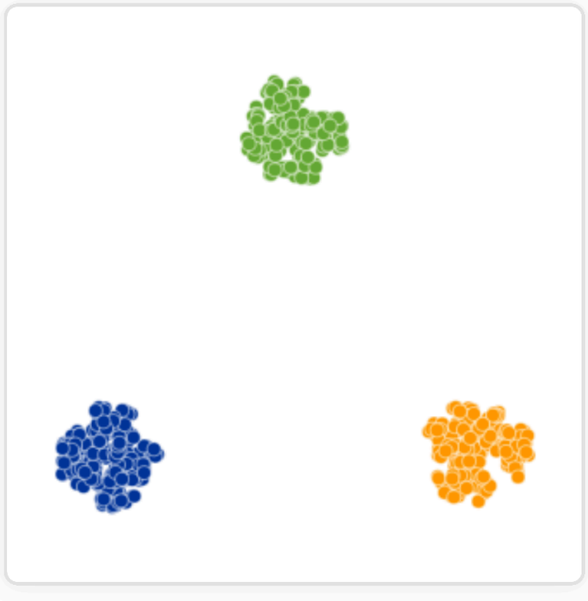


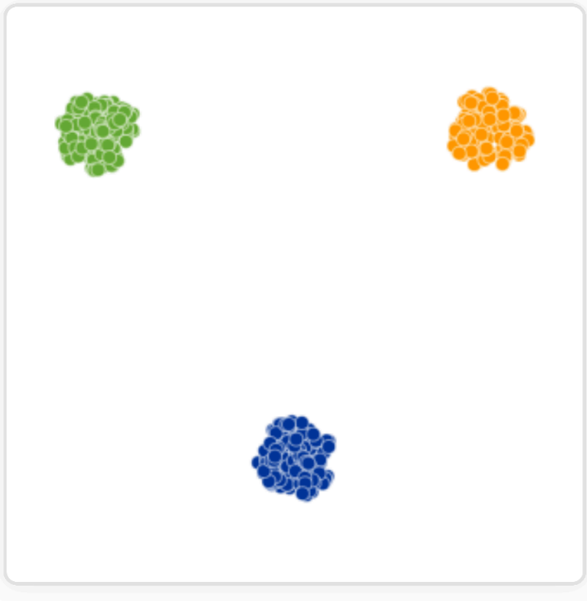
Perplexity: 2
Step: 5,000



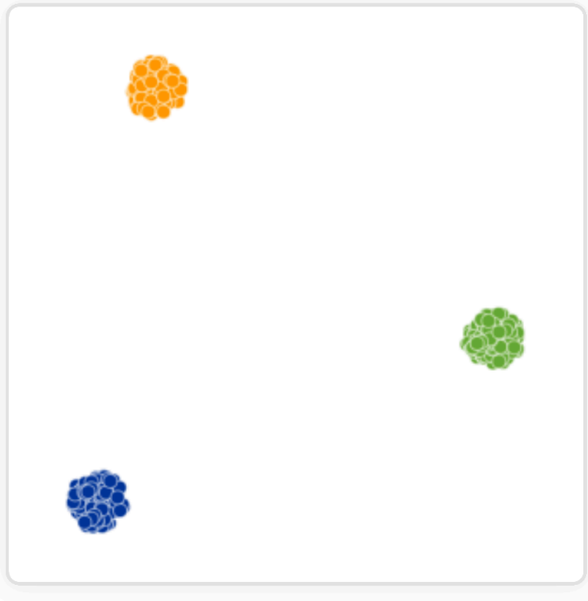
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000



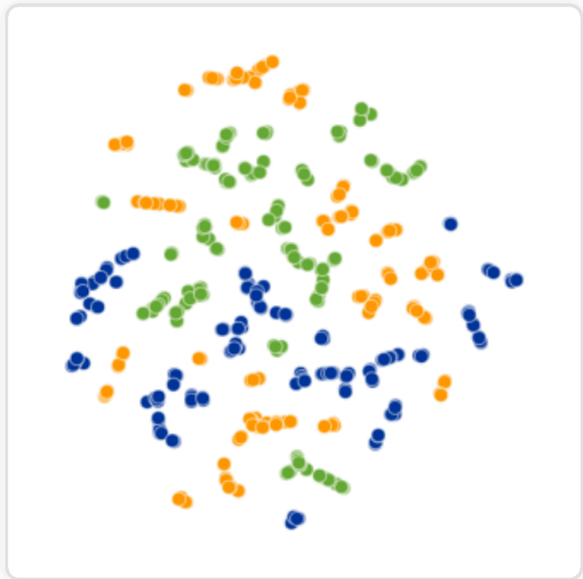
Perplexity: 100
Step: 5,000

Challenges of t-SNE

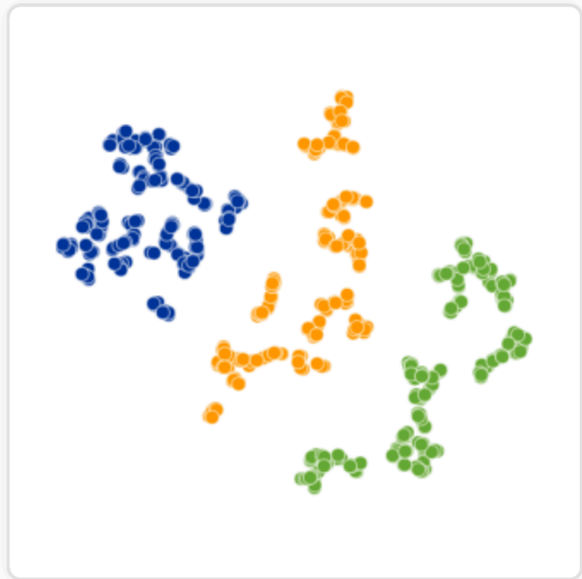
[Largely borrowed from Wattenberg et al 2016 “How to use t-SNE effectively.” Check it out!]

- t-SNE distances between clusters need not reflect originals
- Data 2D here
- Same setup but with 200 data points per cluster (previous slide had 50 per cluster)
- Now none of the plots reflect the distances in the original data

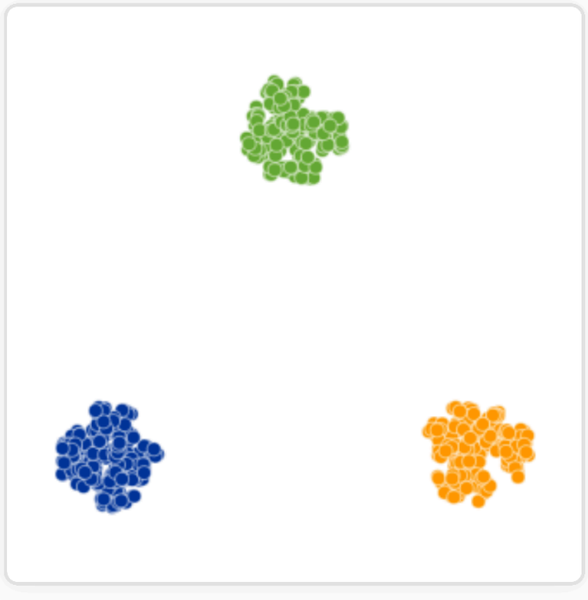
Original



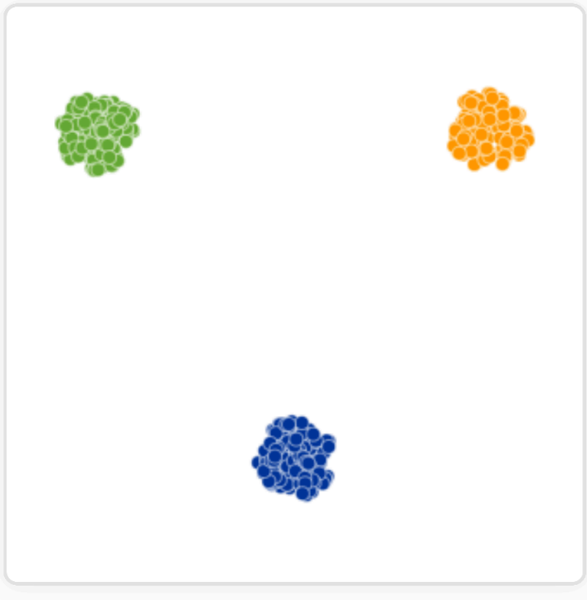
Perplexity: 2
Step: 5,000



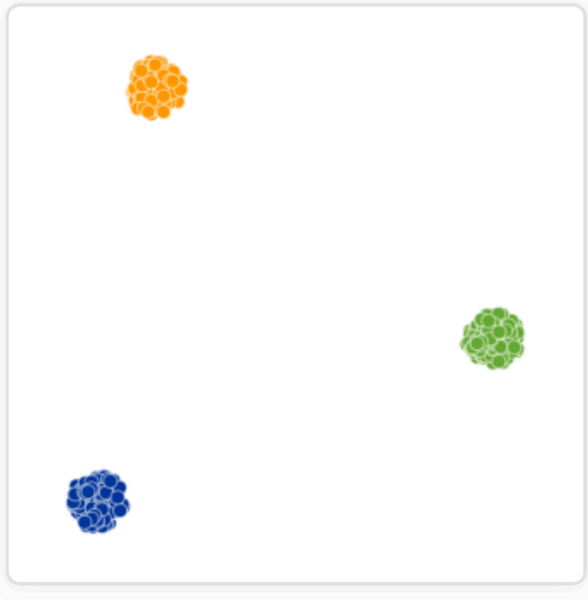
Perplexity: 5
Step: 5,000



Perplexity: 30
Step: 5,000



Perplexity: 50
Step: 5,000



Perplexity: 100
Step: 5,000

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