Carnegie Mellon University
Heinz College

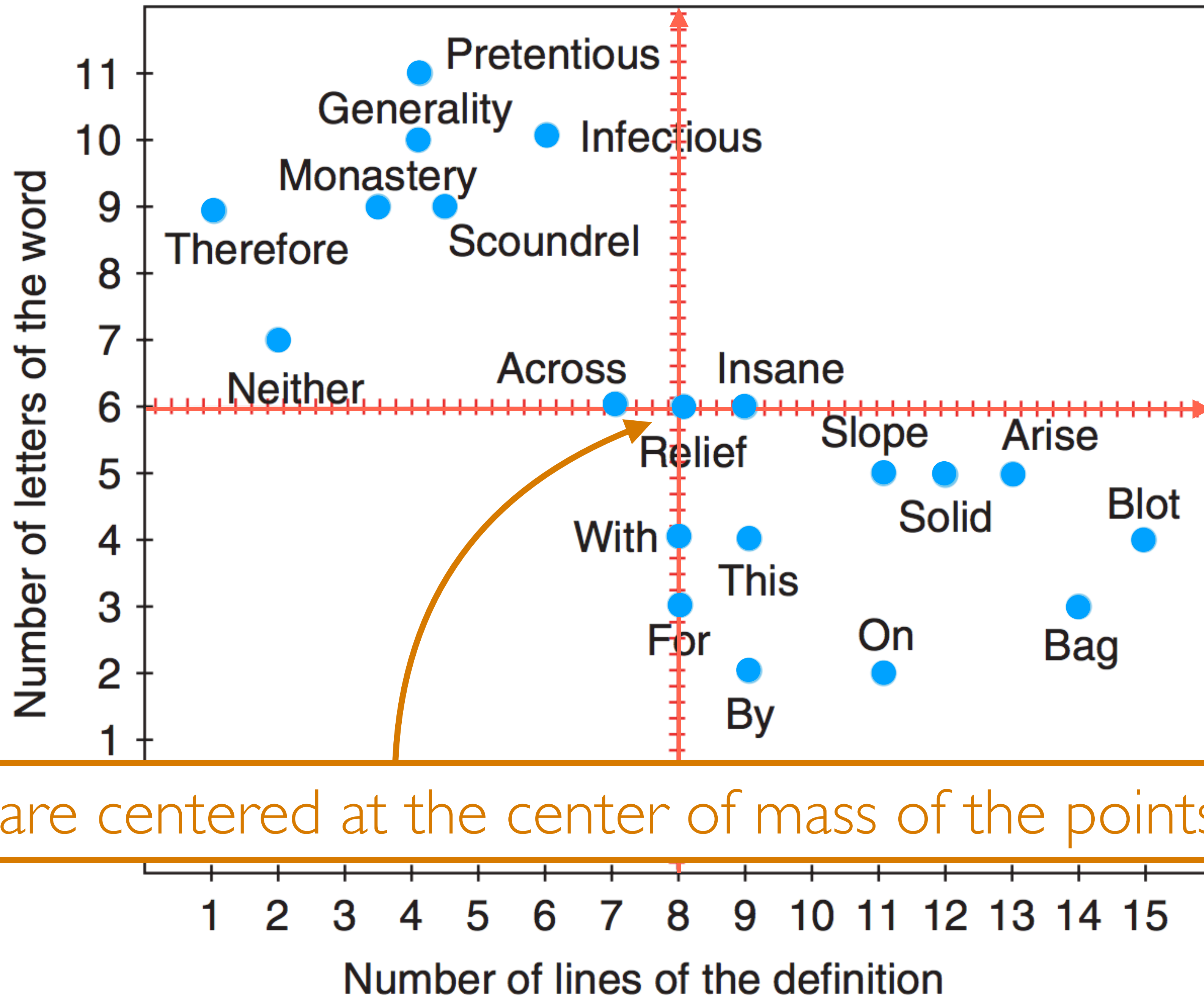
Unstructured Data Analytics for Policy

Lecture 4: PCA, manifold learning

George Chen

Principal Component Analysis (PCA)

How to project 2D data down to 1D?



Note: axes are centered at the center of mass of the points and not at (0, 0)

Hervé Abdi and Lynne J. Williams. Principal component analysis. Wiley Interdisciplinary Reviews: Computational Statistics. 2010.

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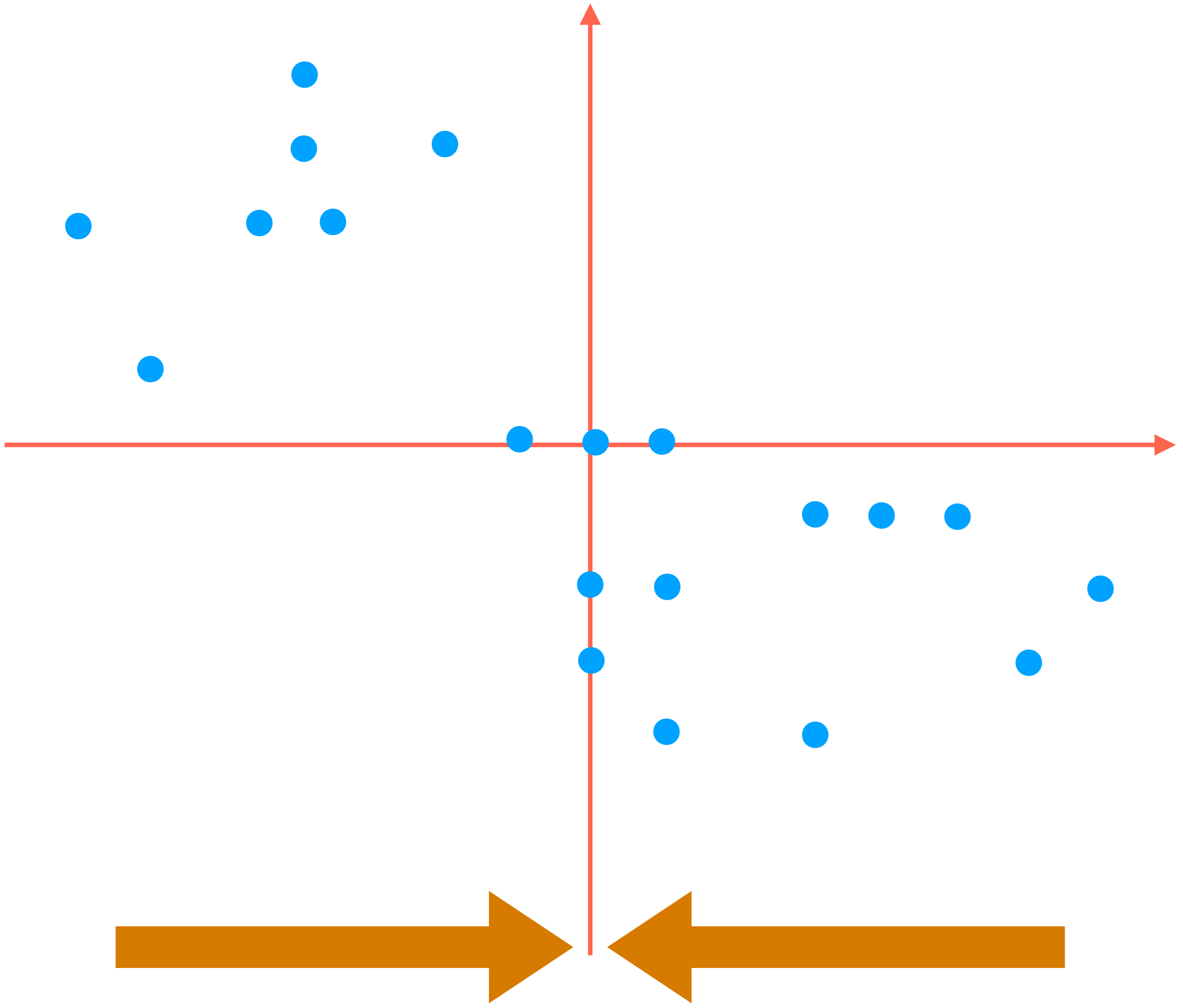

Simplest thing to try: flatten to one of the red axes

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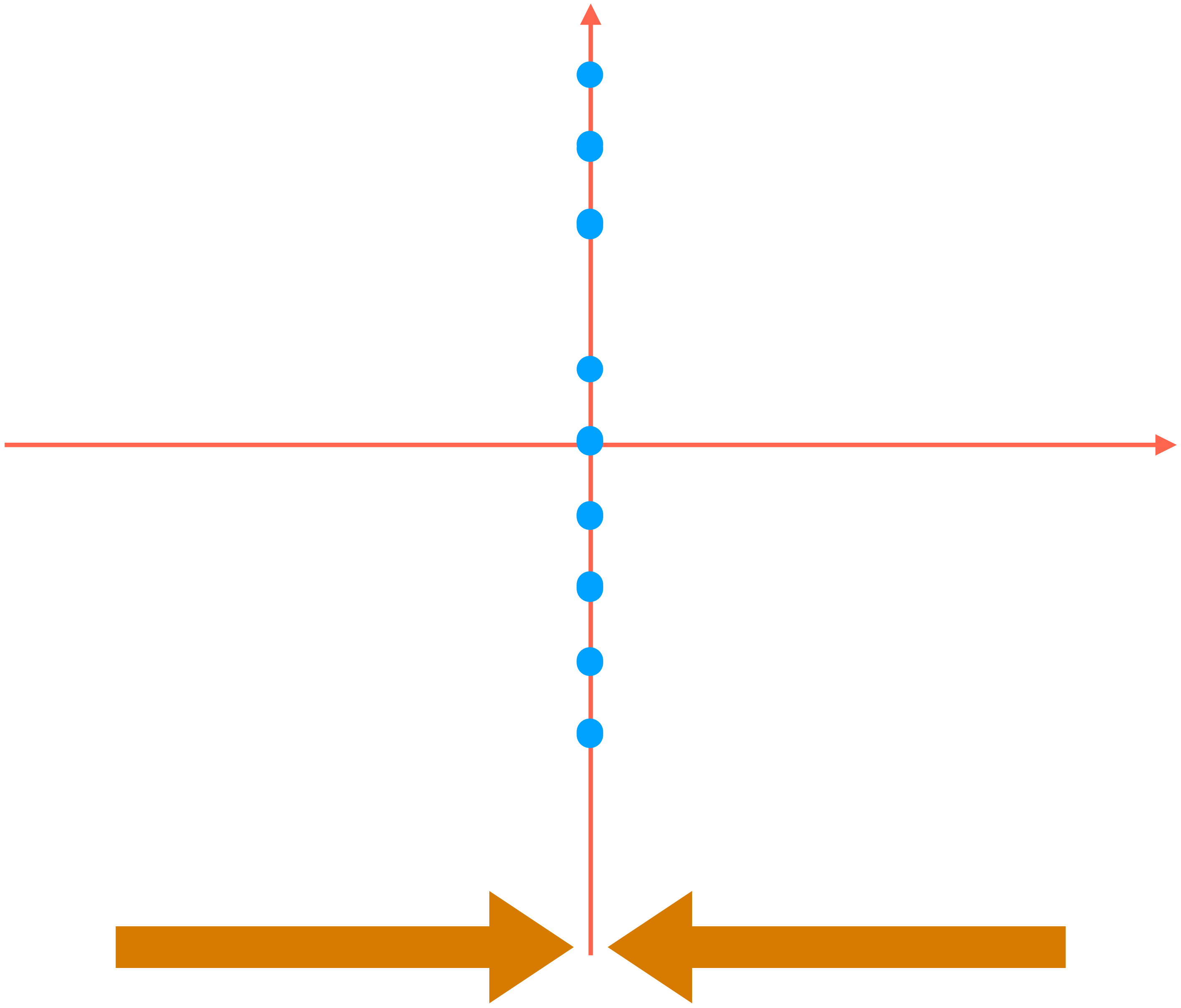

Simplest thing to try: flatten to one of the red axes

(We could of course flatten to the other red axis)

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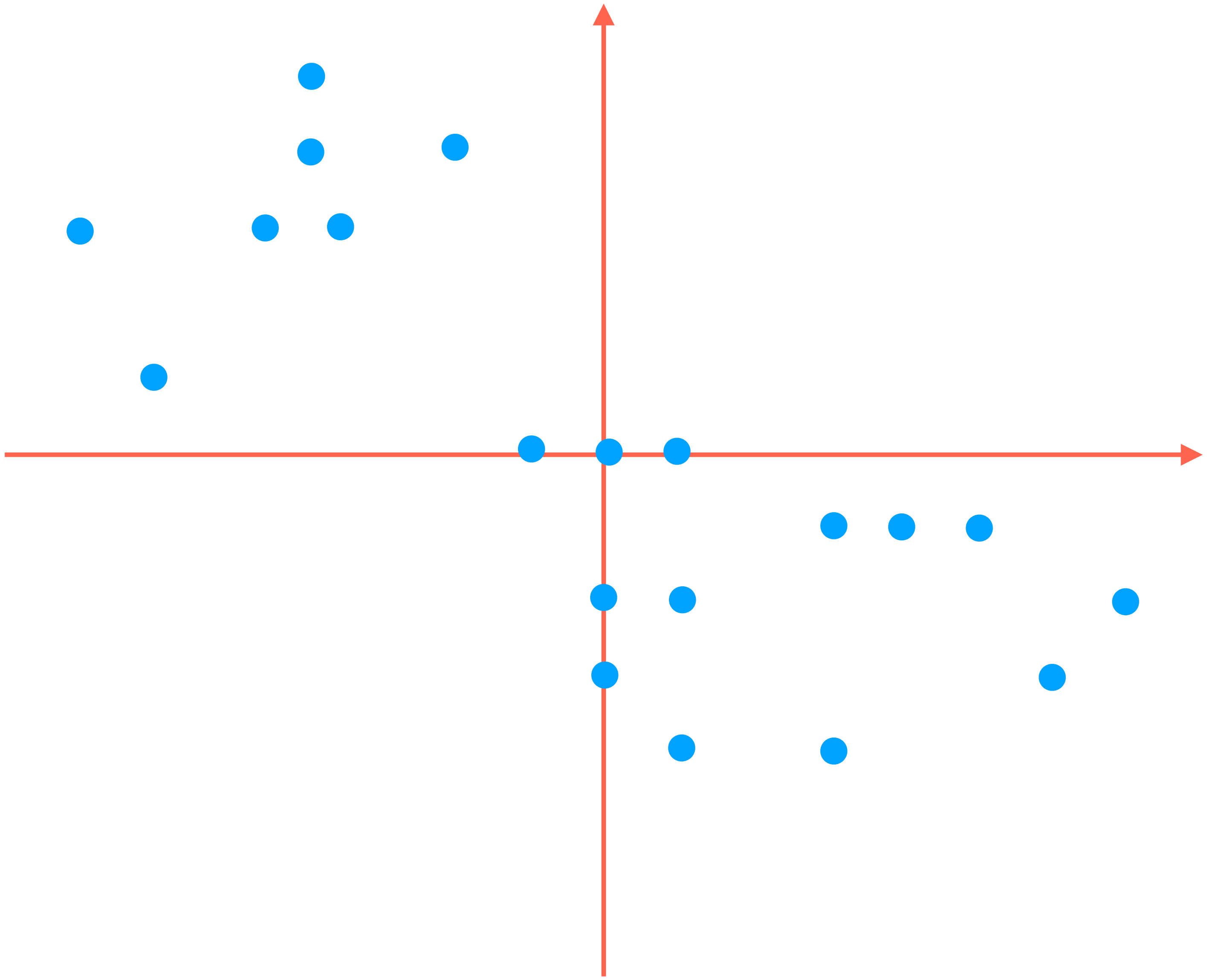

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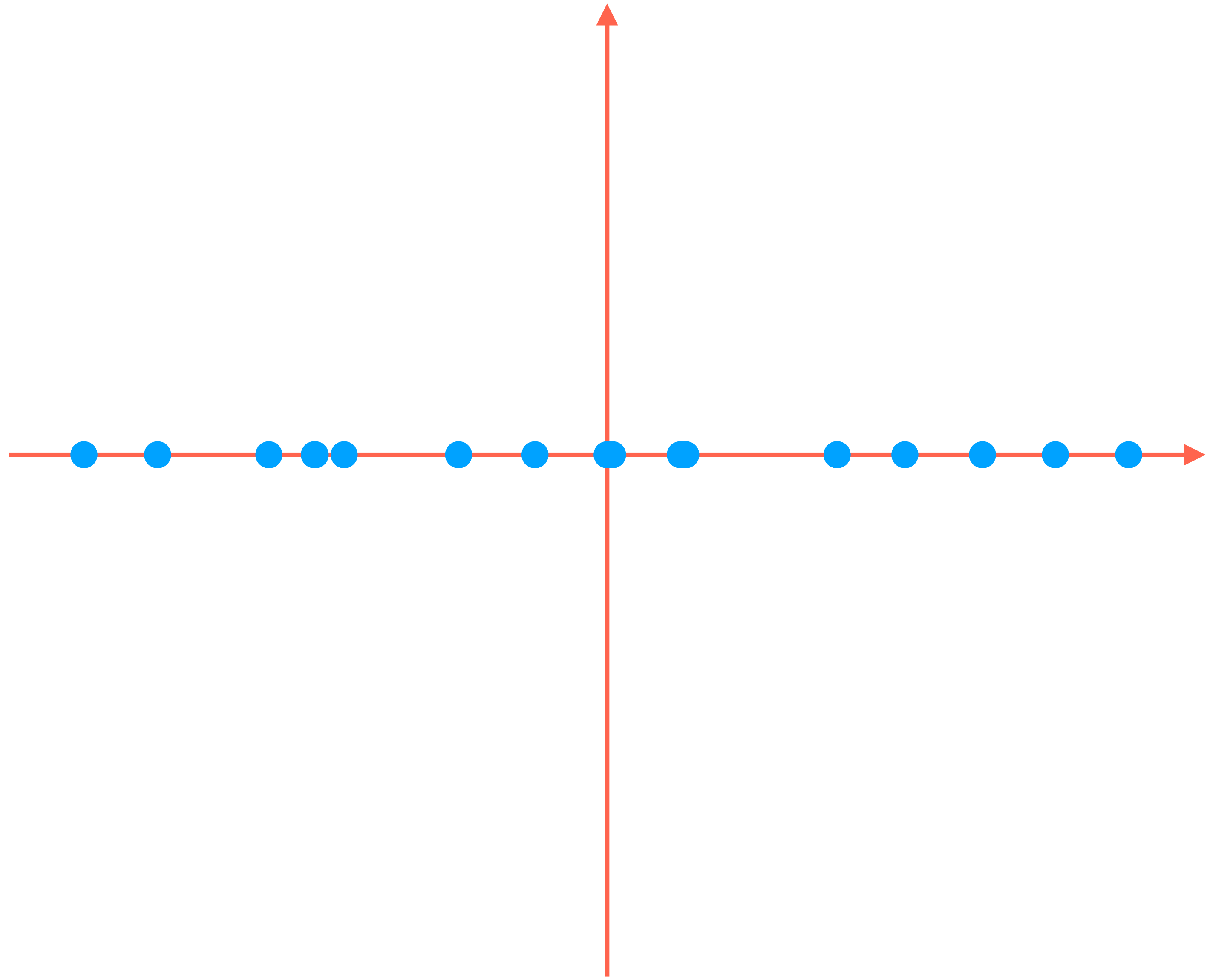

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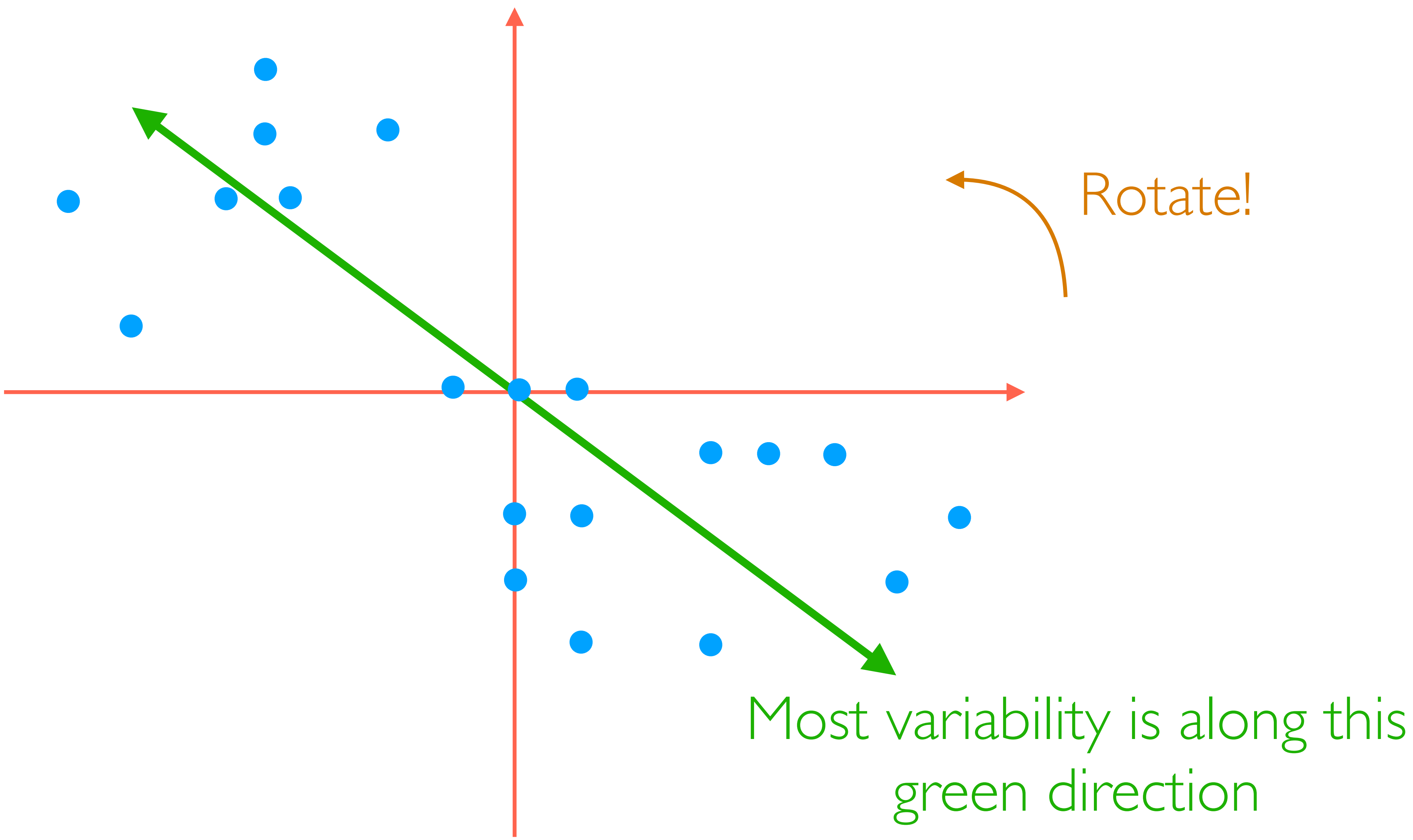

But notice that most of the variability in the data is *not* aligned with the red axes!

Principal Component Analysis (PCA)

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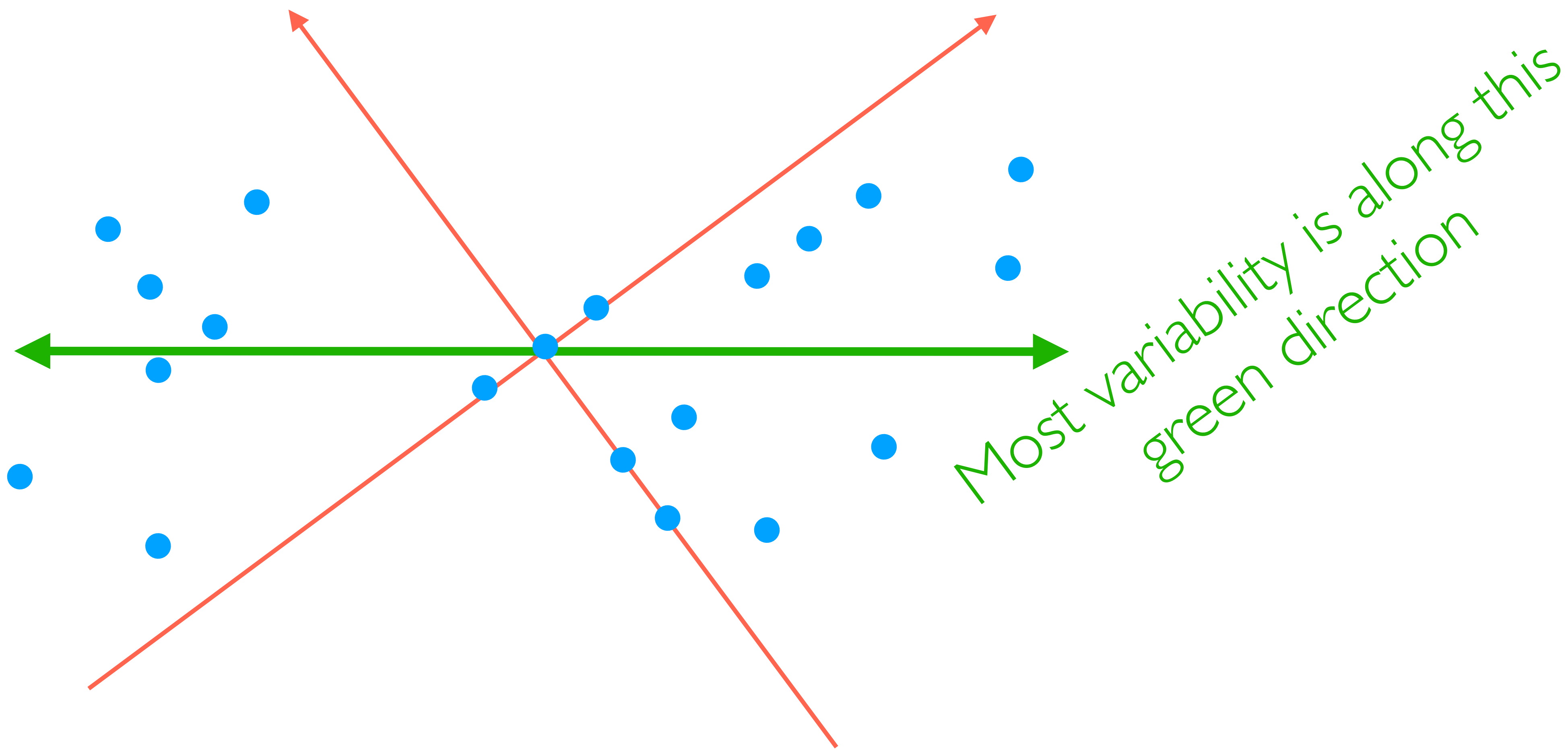

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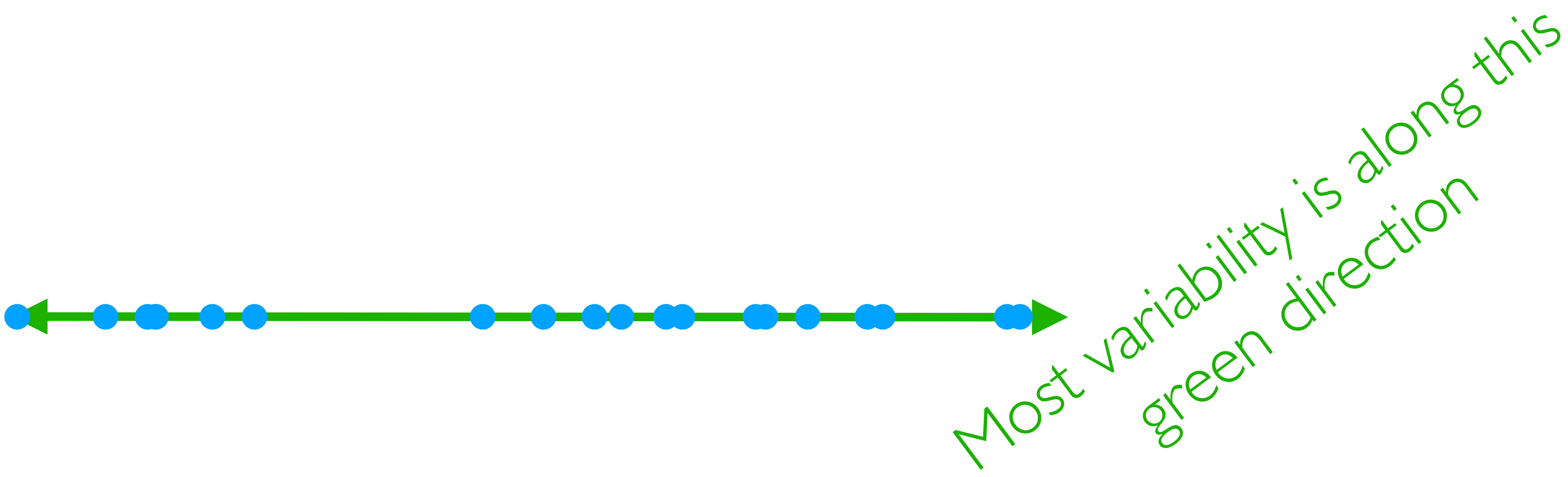
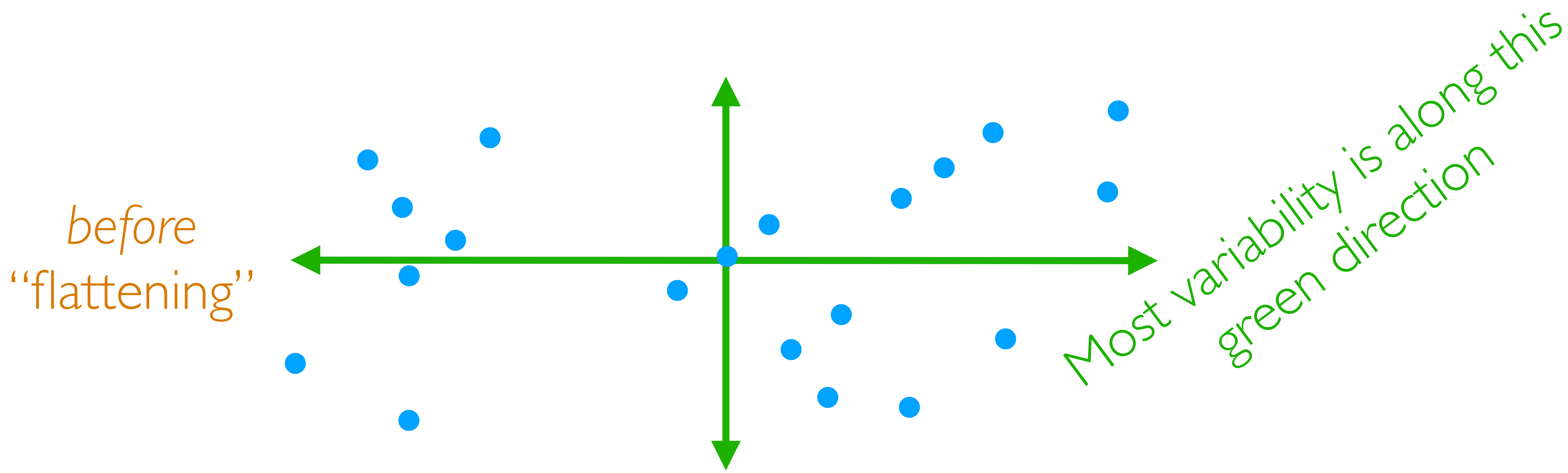


The idea of PCA actually works for 2D ➔ 2D as well
(and just involves rotating, and not "flattening" the data)

Principal Component Analysis (PCA)

~~How to project 2D data down to 1D?~~

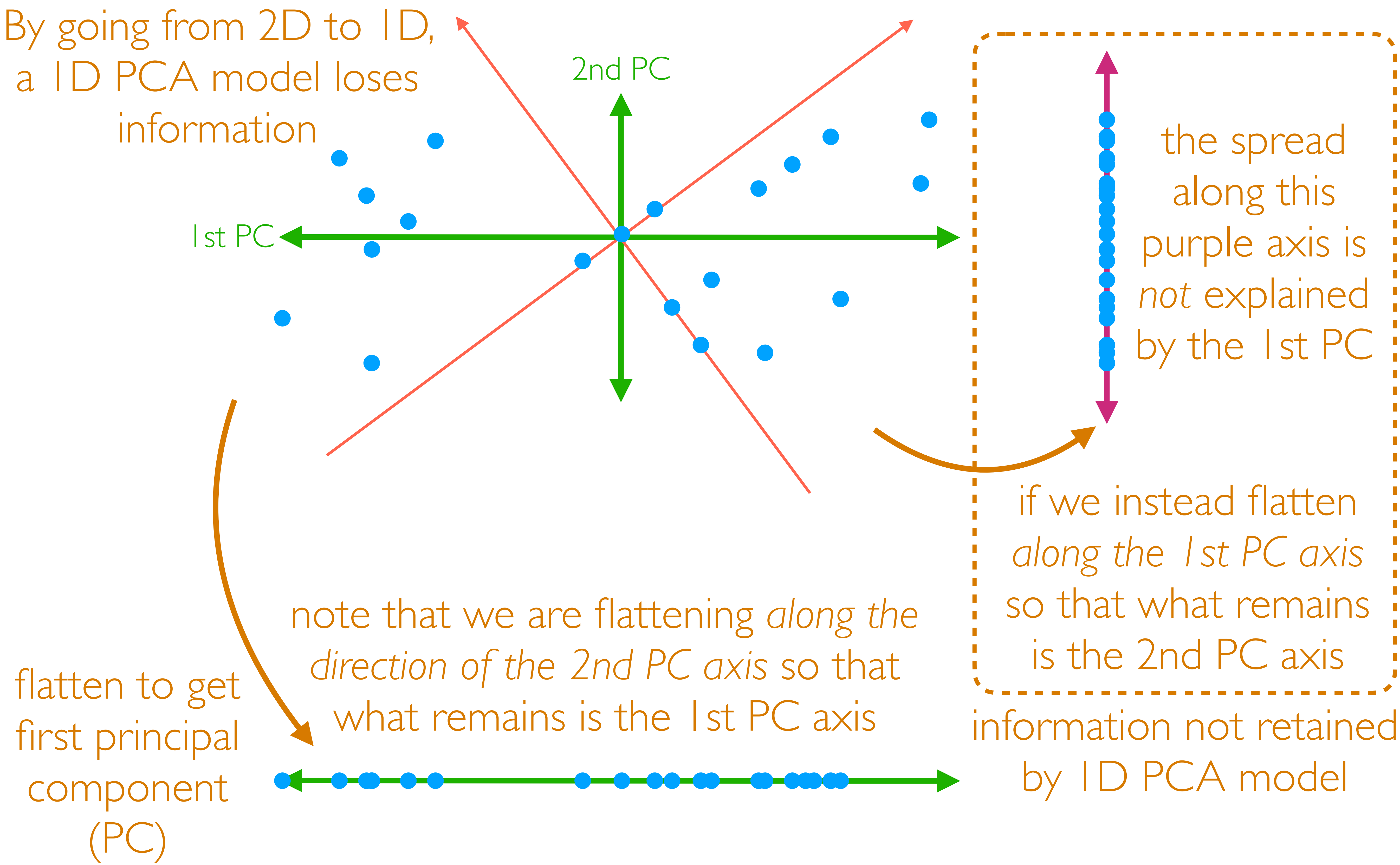
How to rotate 2D data so 1st axis has most variance



The idea of PCA actually works for 2D ➔ 2D as well
(and just involves rotating, and not "flattening" the data)

2nd green axis chosen to be 90° ("orthogonal") from first green axis

PCA: The Unexplained Variability



3D Dataset Example

http://setosa.io/ev/principal-component-analysis/

PCA in Higher Dimensions

- Finds top *k* orthogonal directions that explain the most variance in the data
  - 1st component: explains most variance along 1 dimension
  - 2nd component: explains most of **remaining** variance along next dimension that is orthogonal to 1st dimension
  - …
- "Flatten" data by retaining only the top *k* dimensions (if $k <$ original dimension, then we are doing dimensionality reduction)

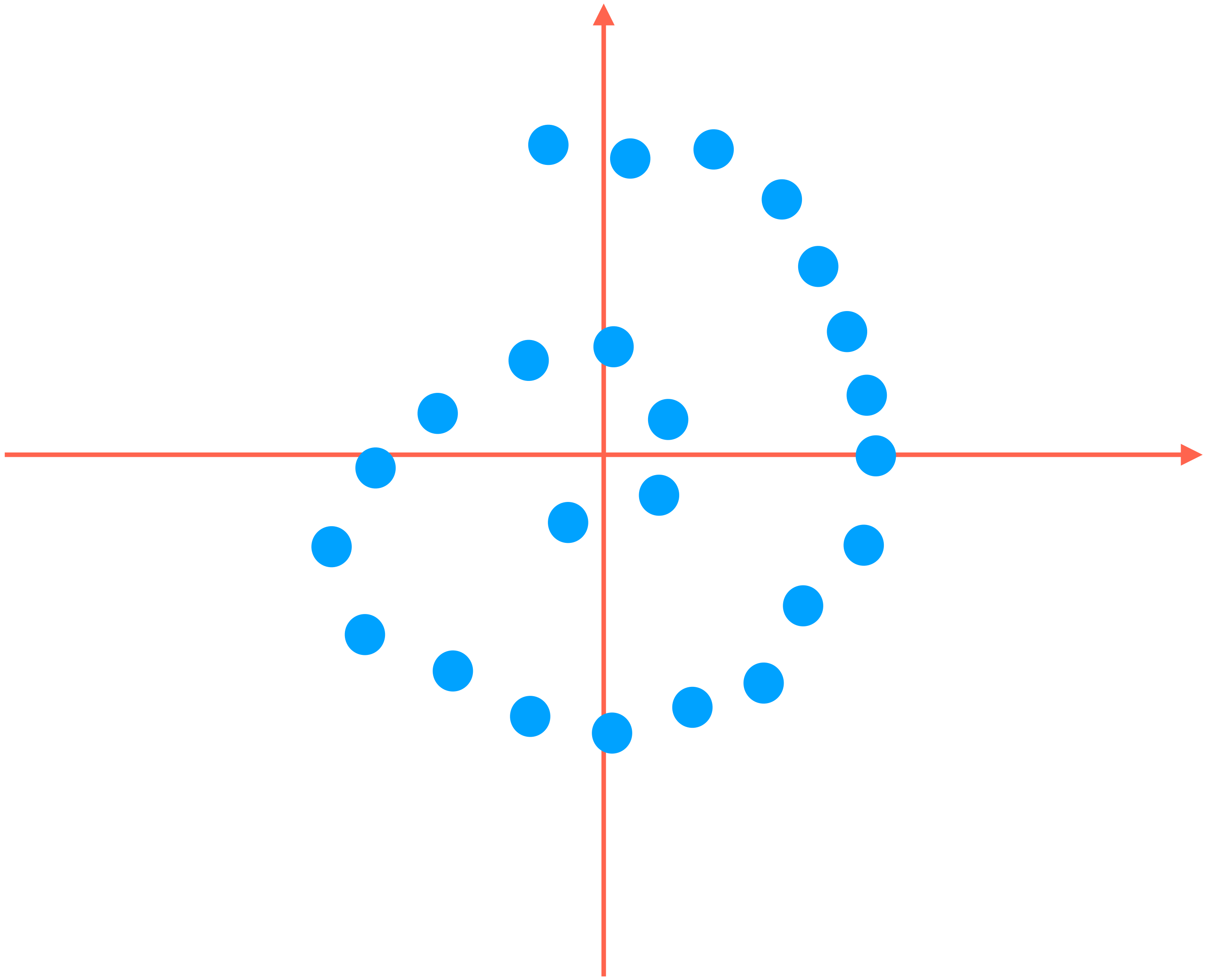
Principal Component Analysis (PCA)

Demo

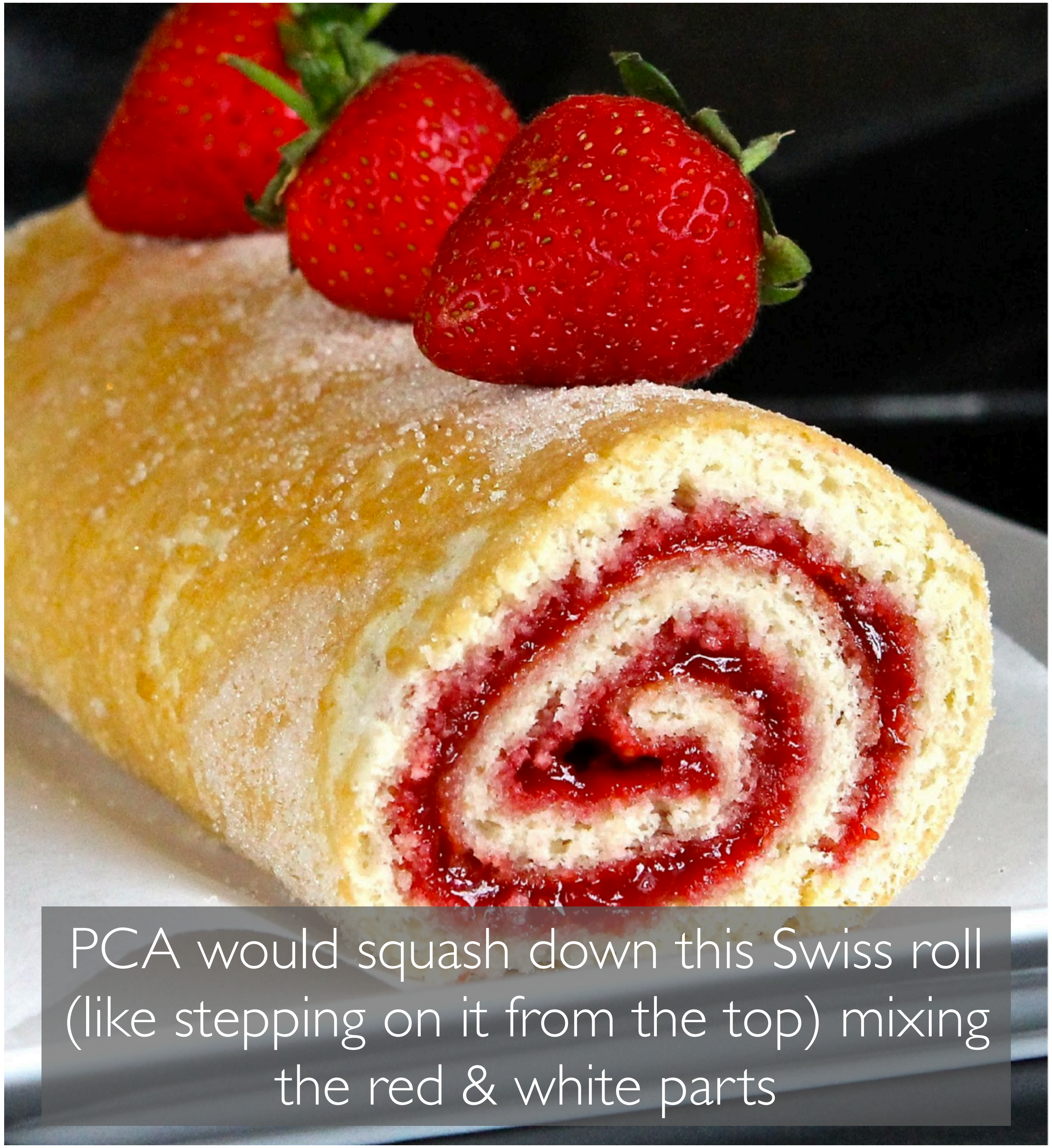
PCA reorients data so axes explain variance in "decreasing order"
→ can "flatten" (*project*) data onto a few axes that captures most variance

Image source: http://4.bp.blogspot.com/-USQEgoh1jCU/VfncdNOETcI/AAAAAAAAGp8/Hea8UtE_1c0/s1600/Blog%2B1%2BIMG_1821.jpg

2D Swiss Roll



PCA would just flatten this thing and
lose the information that the data actually lives on a 1D line that has been curved!



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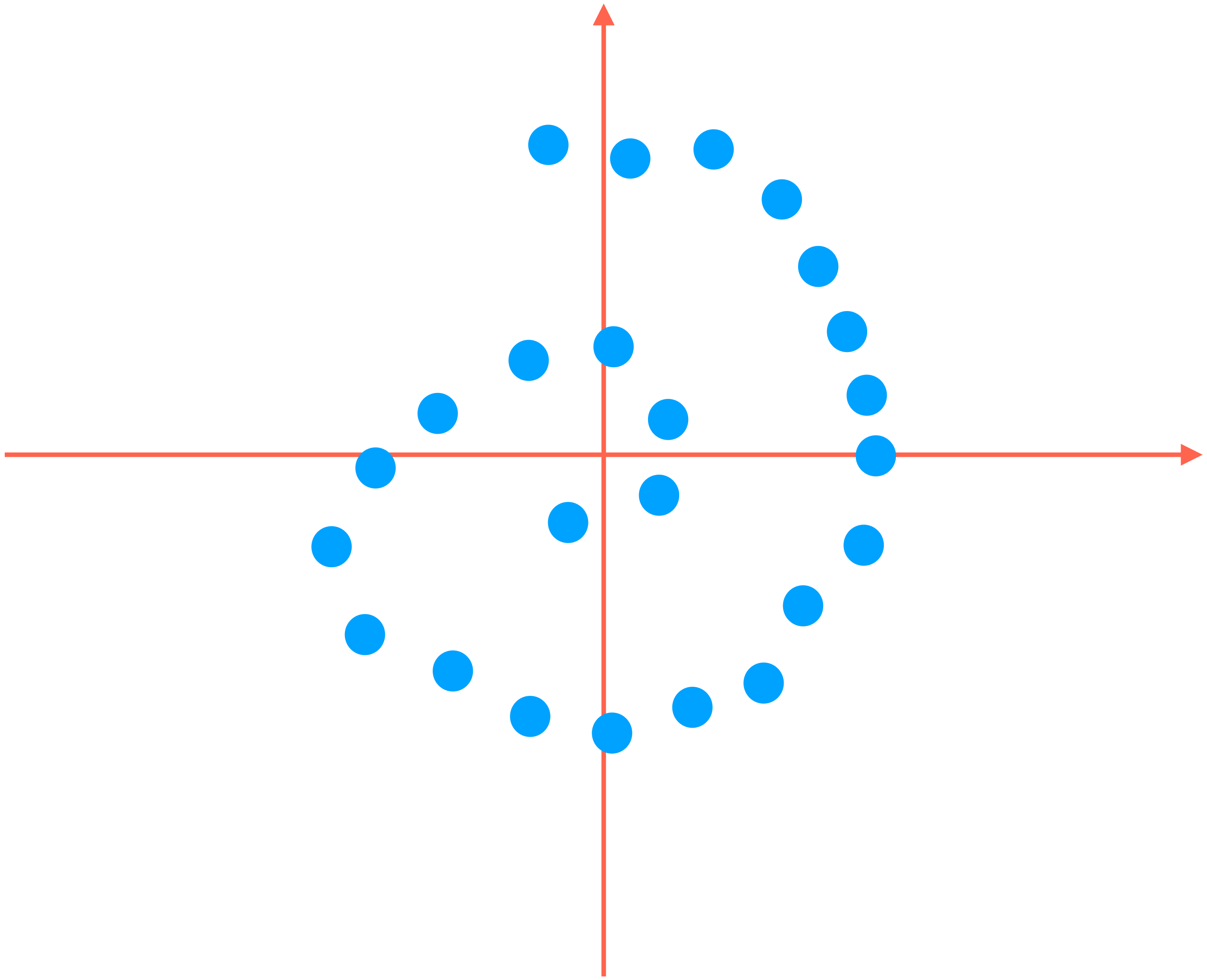

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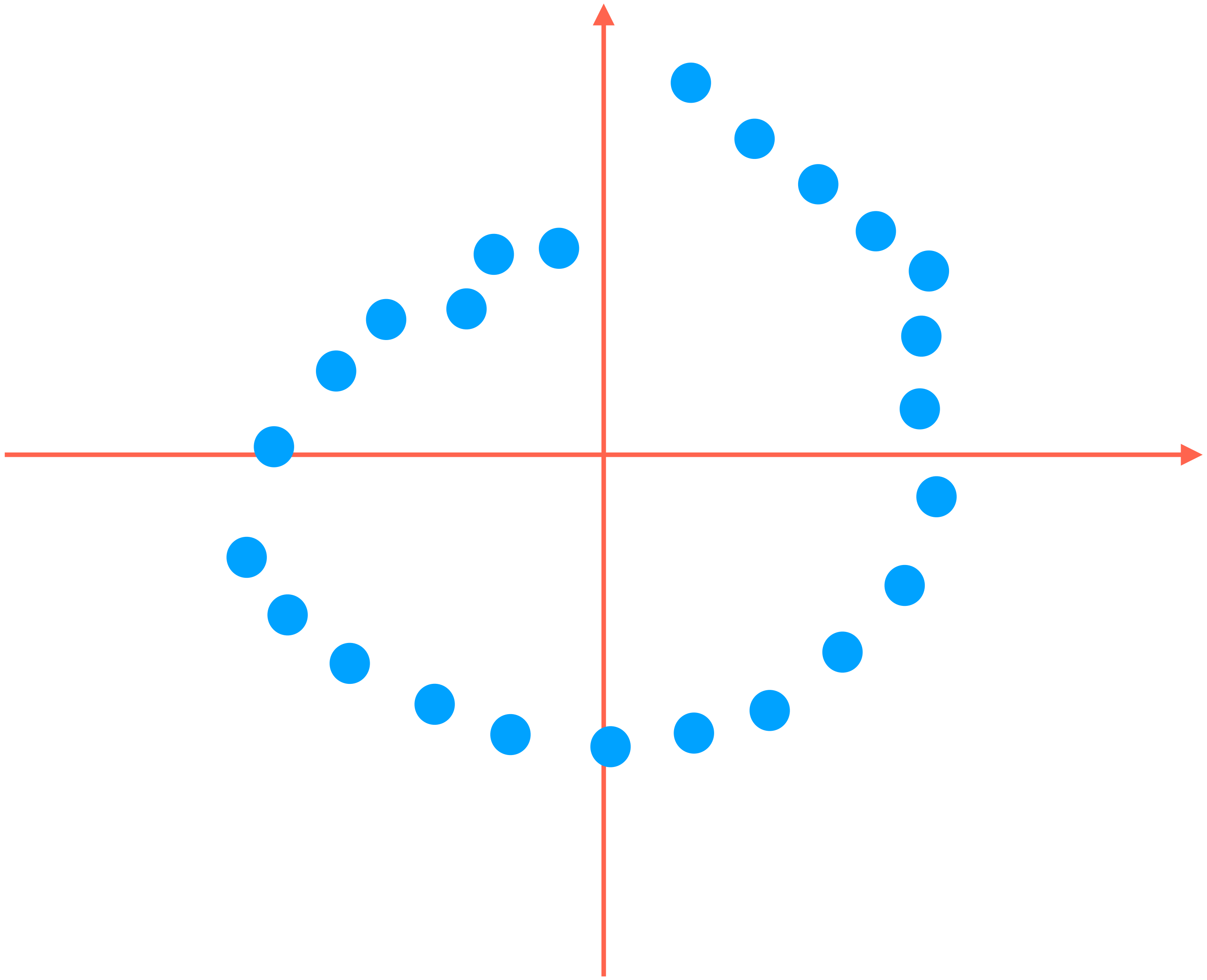

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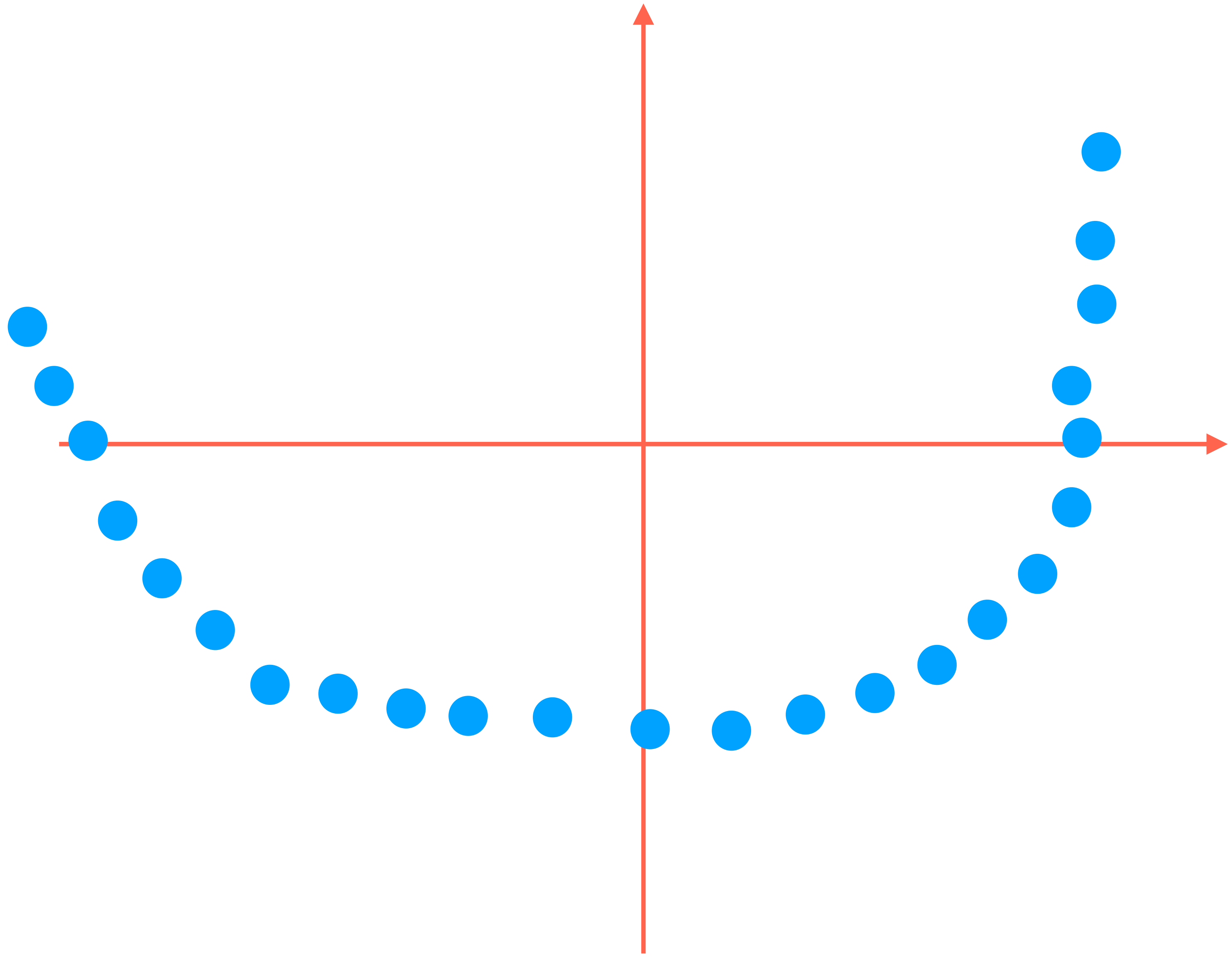

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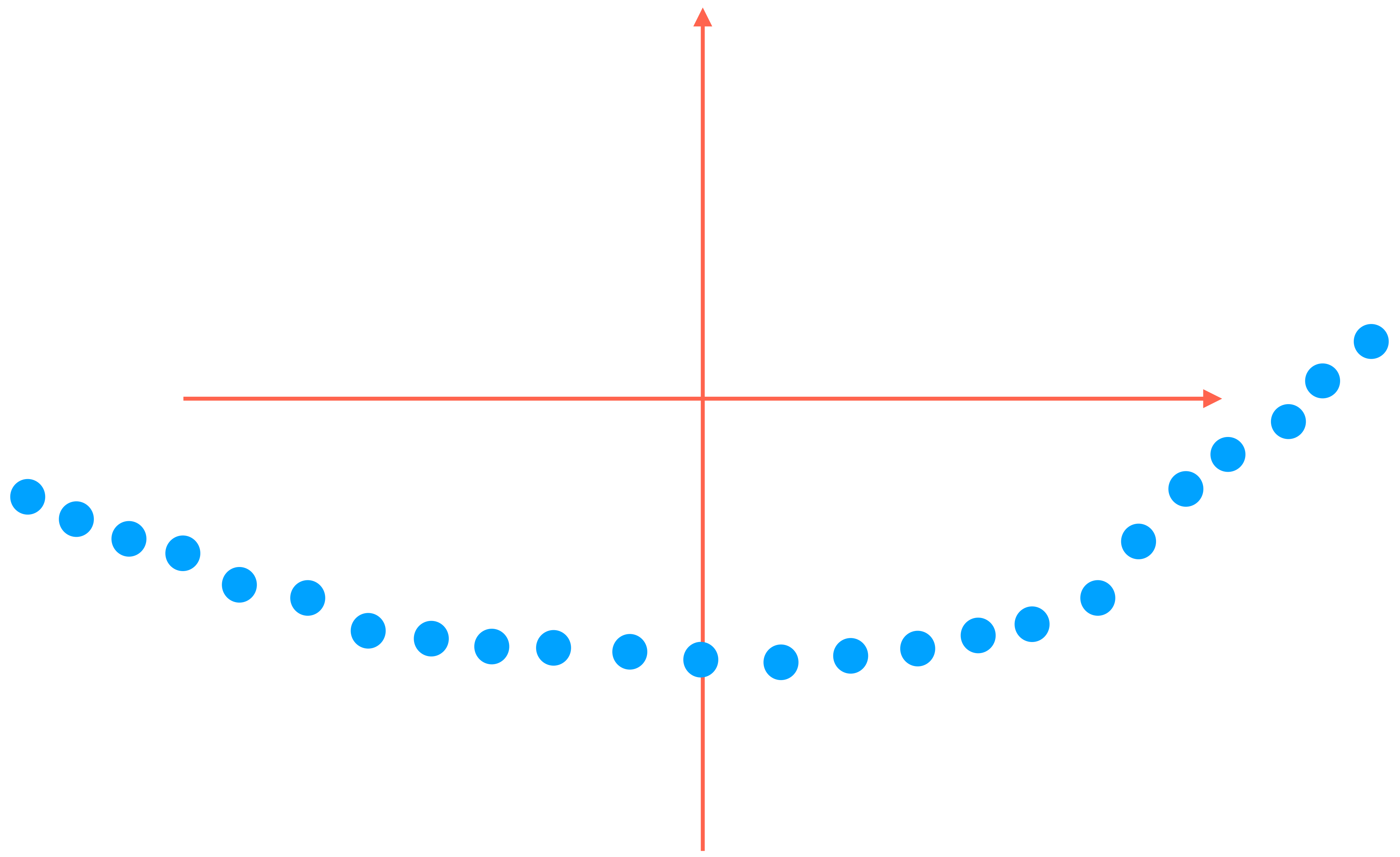

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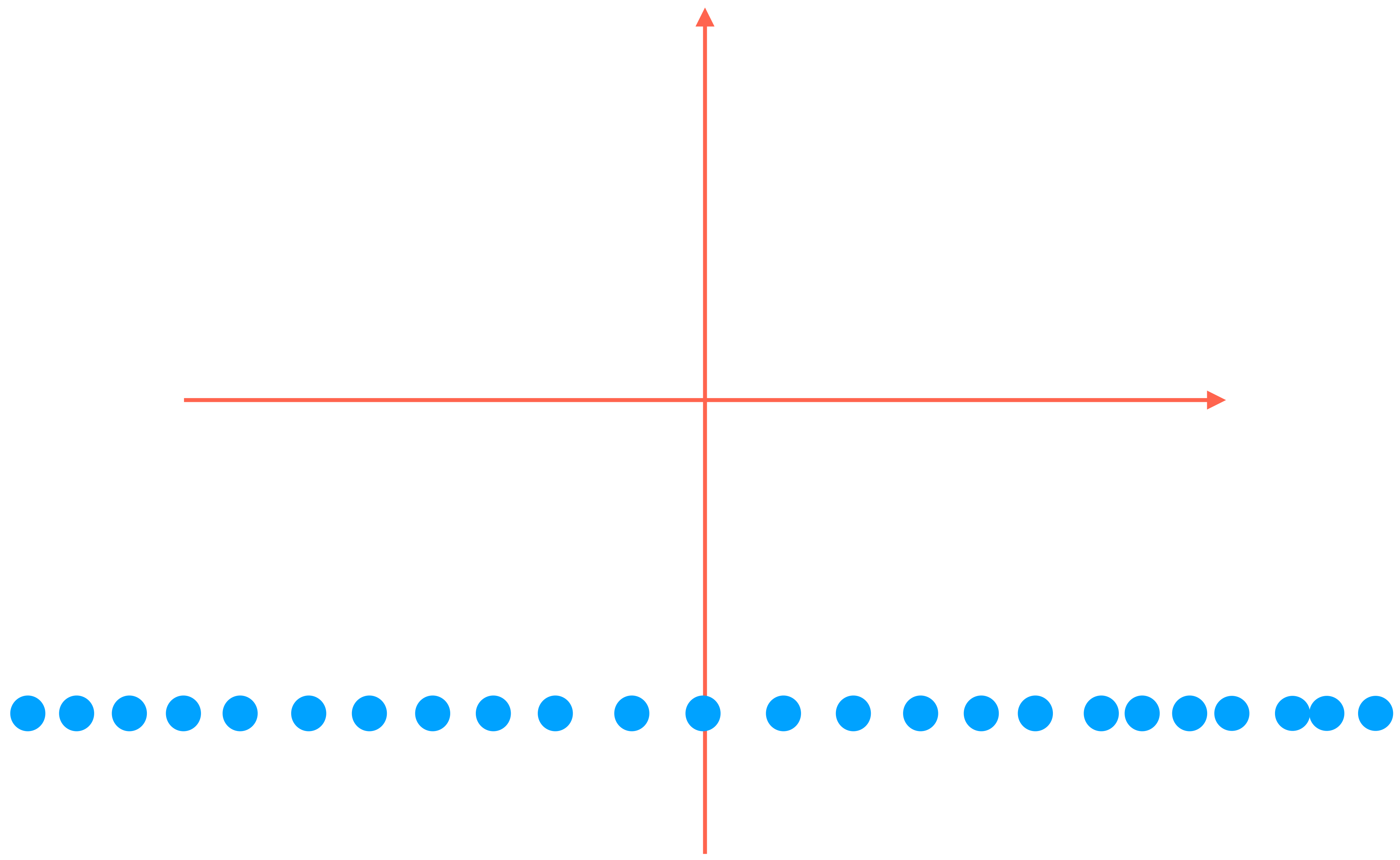

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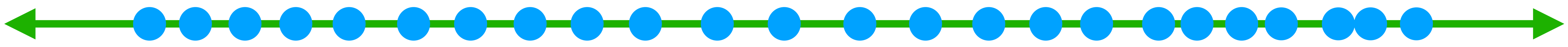
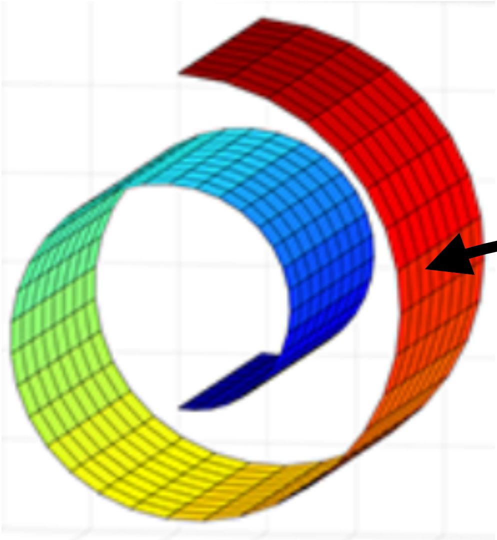


This is the desired result

Manifold Learning



The dataset here is clearly 3D

But when we zoom in a lot on any point, around the point it looks like a flat 2D sheet!

Another example: Earth is approximately a 3D sphere, but zooming a lot on any point, around the point it's approximately a 2D sheet

In general: if we have ***d***-dimensional data where when you zoom in a lot, the data dimensionality is smaller than ***d***, then the lower-dimensional object is called a **manifold**

- We have the data's high-dim. coordinates, but we want to find the low-dim. coordinates (on the manifold) ➜ this is **manifold learning**
- Manifold learning is *nonlinear* whereas PCA is linear (this will make more sense after we see code demos)

Image source: "Head Pose Estimation via Manifold Learning" (Wang et al 2017)