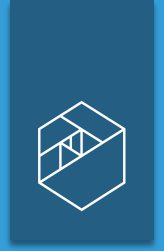
Dimensionality Reduction: SVD, Featuring PCA

Agenda

- Dimensionality reduction
  - Assumptions
- Matrix decomposition
  - In linear algebra
  - Singular value decomposition (SVD) in particular
  - Relation to dimensionality reduction
- Principal Component Analysis (PCA)
  - As a technique for dimensionality reduction / feature extraction
- Preview of applications



Dimensionality Reduction

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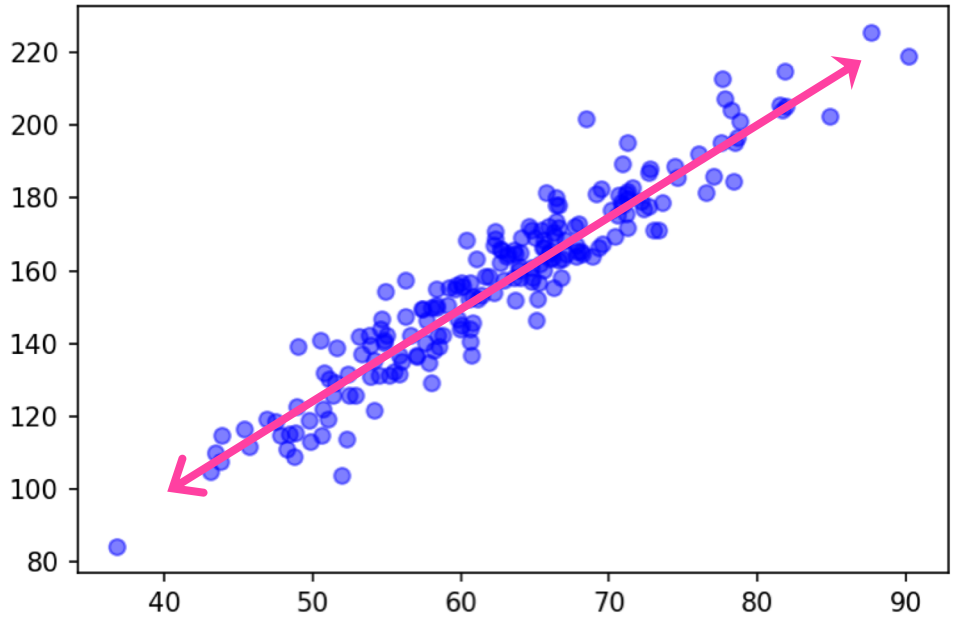

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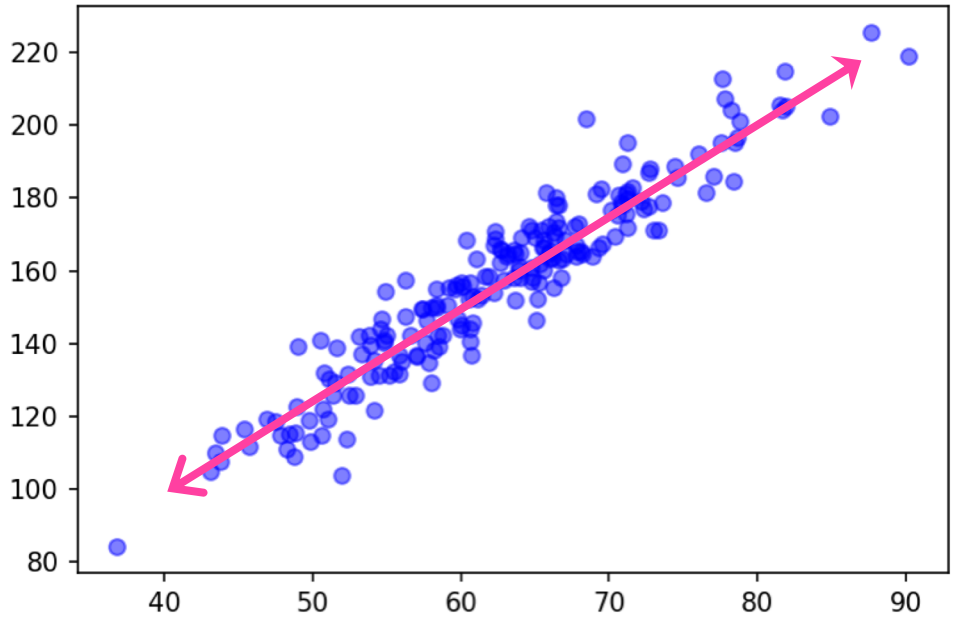

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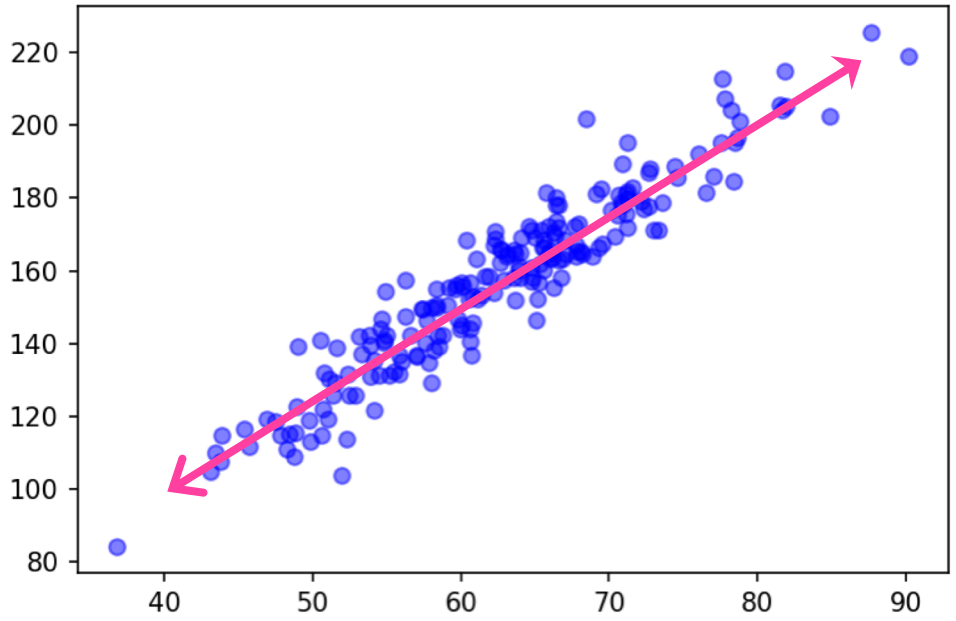

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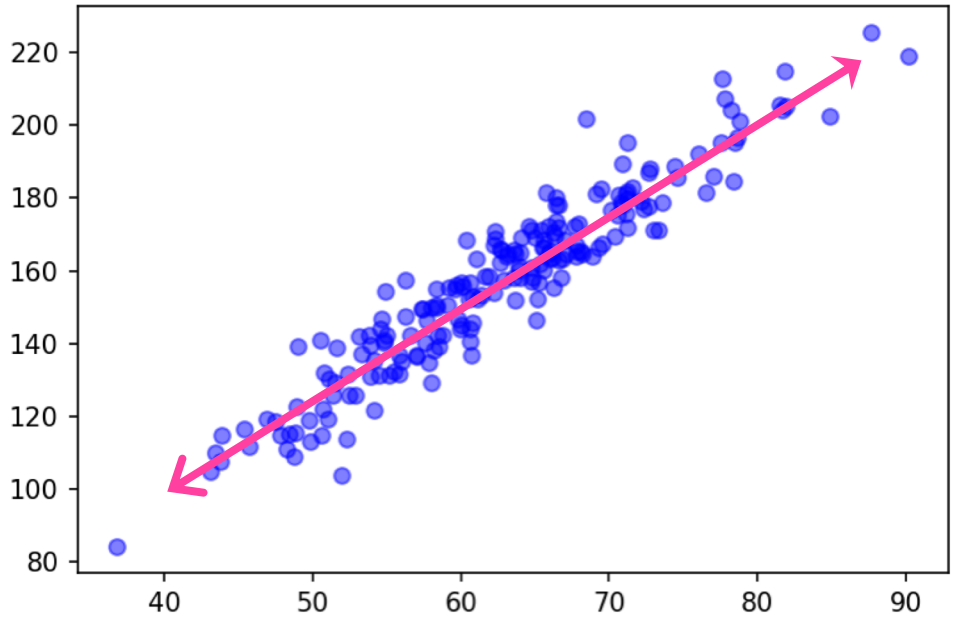
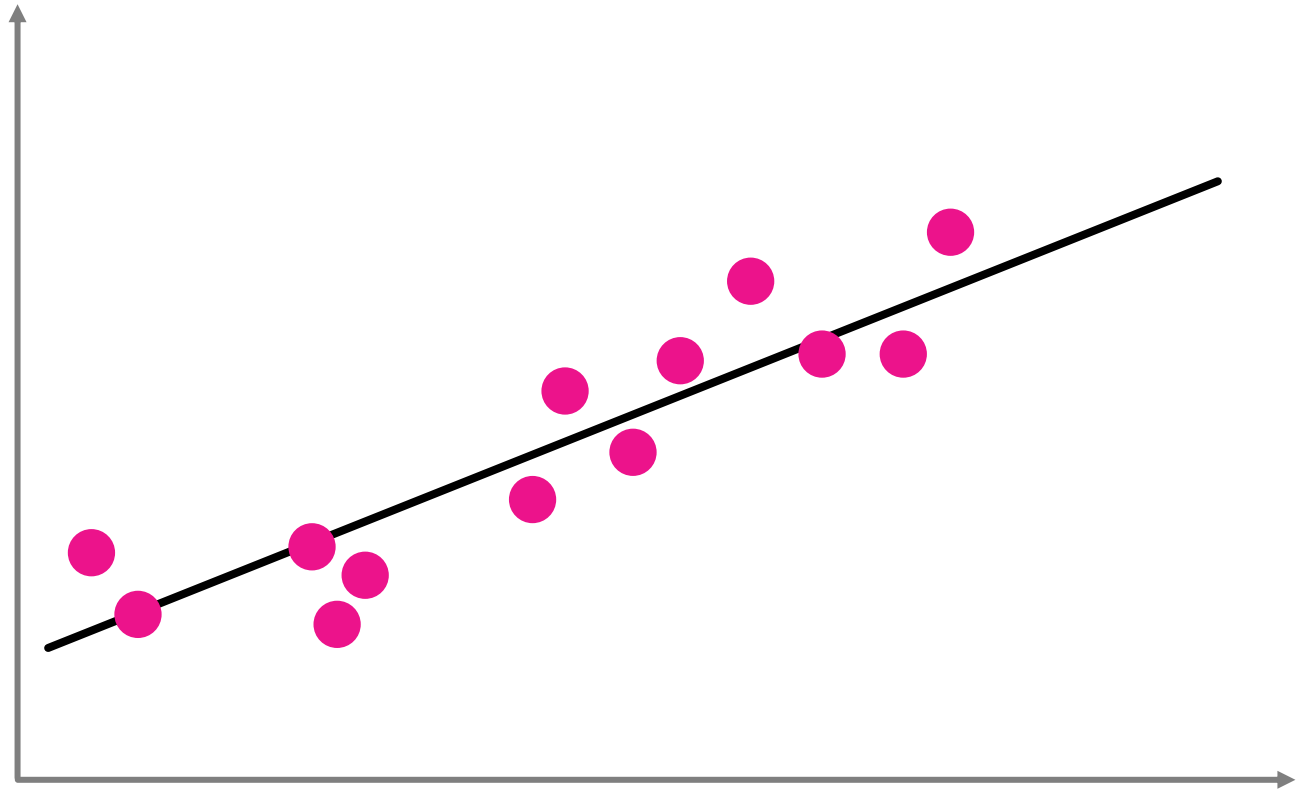


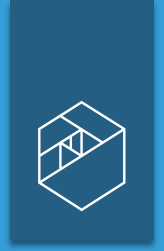
Check for understanding:

Given what we learned in the curse of dimensionality lecture, what do we think some positives of dimensionality reduction might be?

Dimensionality reduction is finding new axis



- The new, reduced axis could be encoding important information!
- We can learn about our data by getting rid of extraneous dimensions that are just noise
  - Some dimensions with little variance might be, e.g., measurement error (imprecise instruments)
  - If a dimension is low variance, not super helpful for modeling



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If you remember nothing else, take away these points:

1) Decomposition is multiplying matrices in a standard form
2) Different subparts of the standard form have special meanings

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- SVD gives us categories in our data that we might not be able to see by looking at all of the data together! This will become more clear with an example

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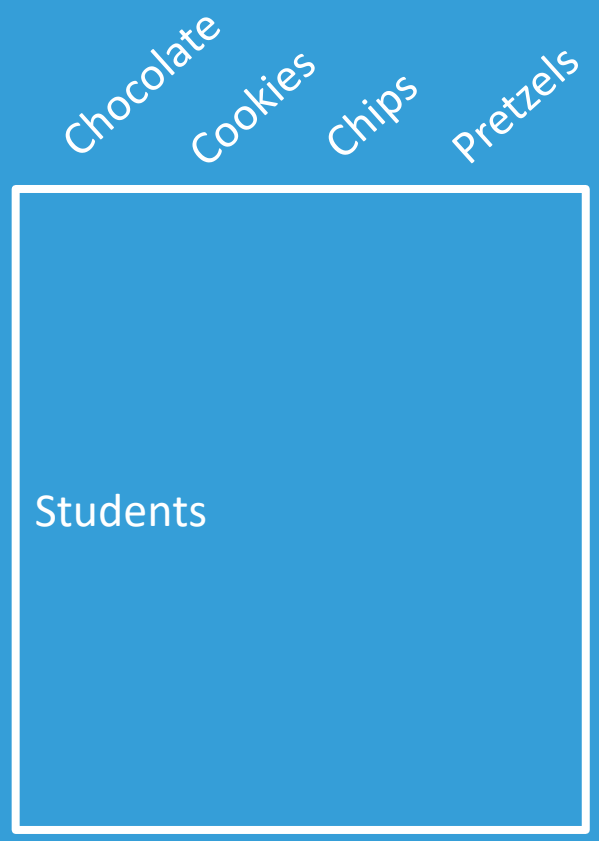

Singular Value Decomposition (SVD)

Data matrix:
Ratings of snack foods

Chocolate	Cookies	Chips	Pretzels
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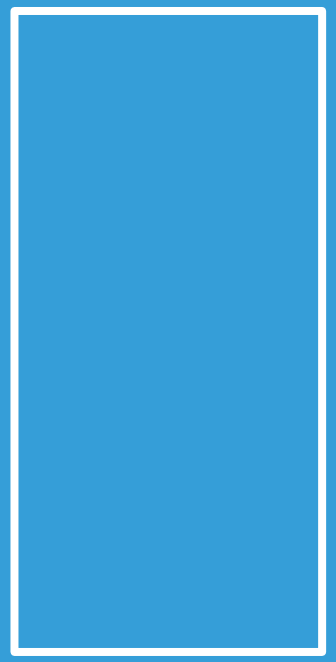

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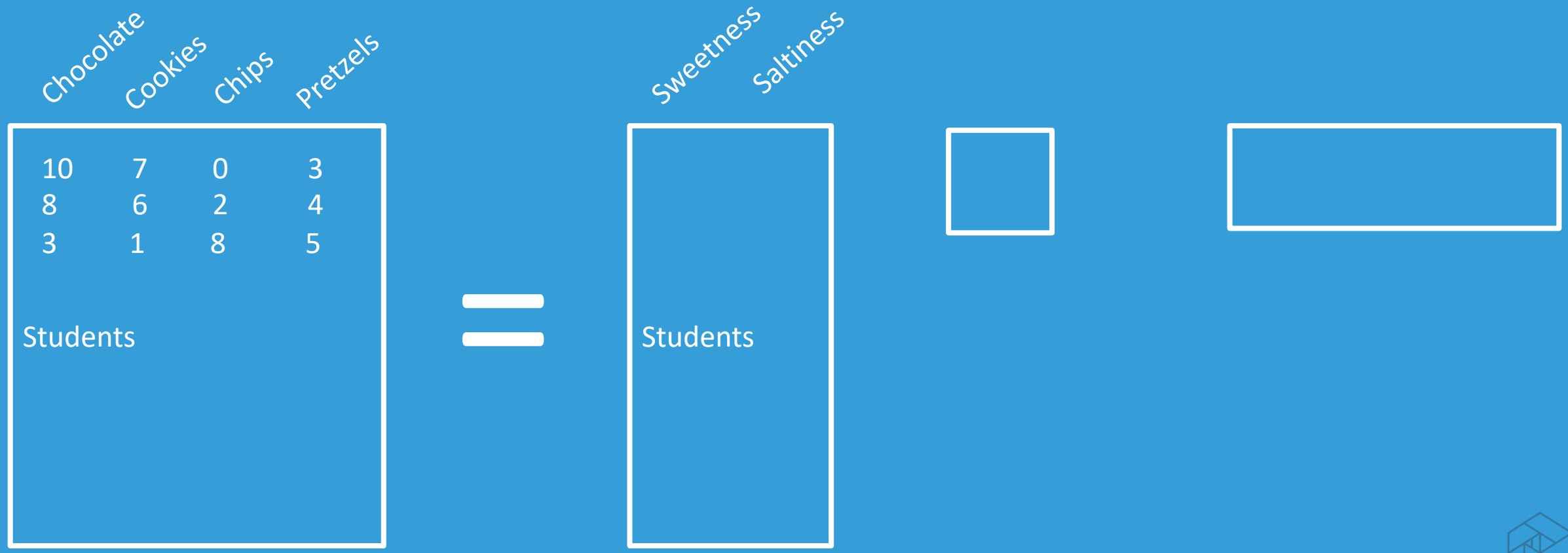

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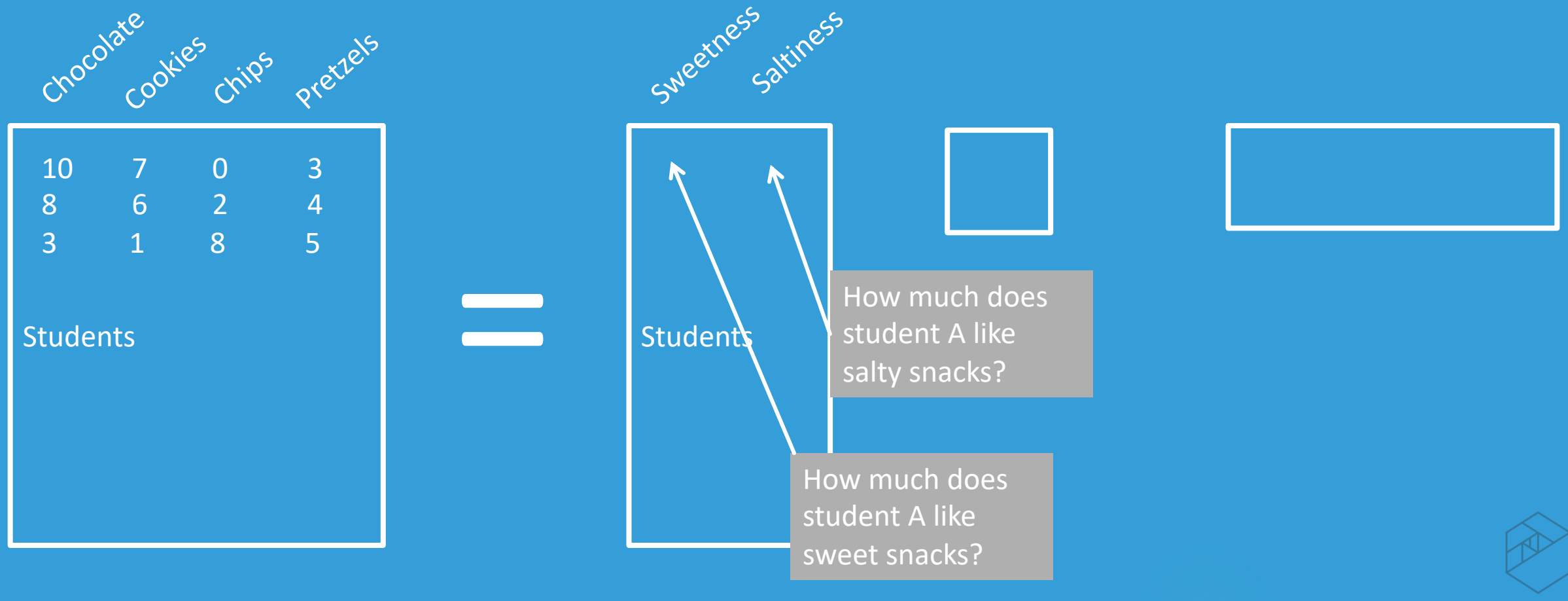

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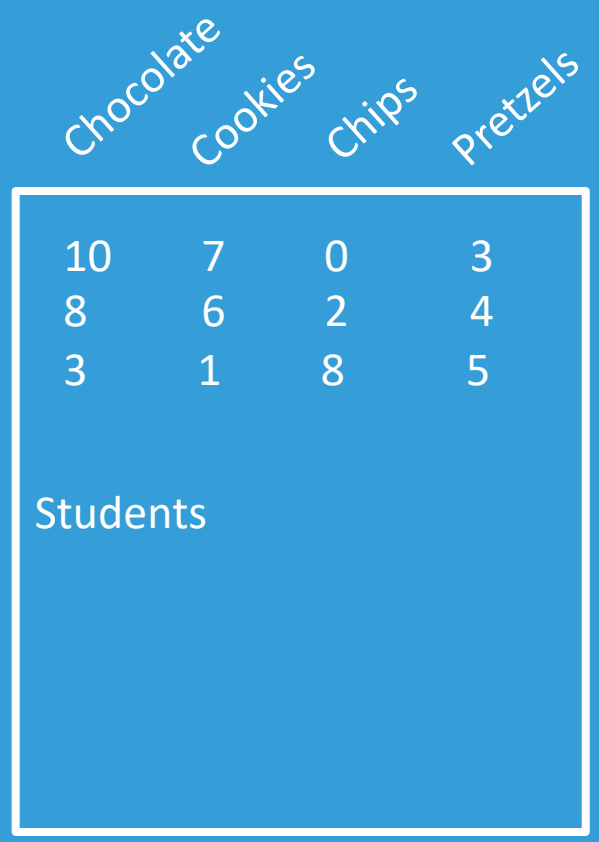

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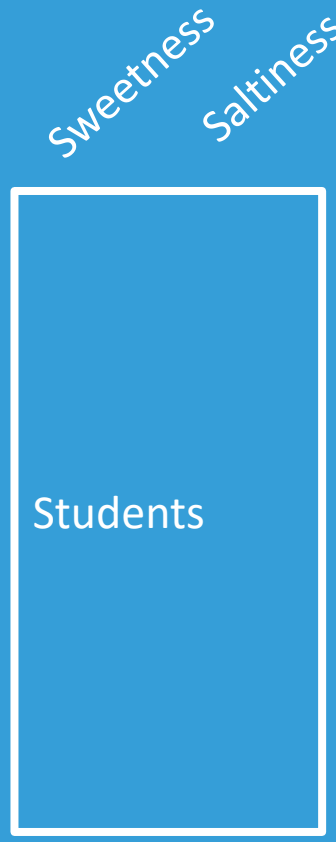

On the diagonal, the strength of sweetness and saltiness (variance)

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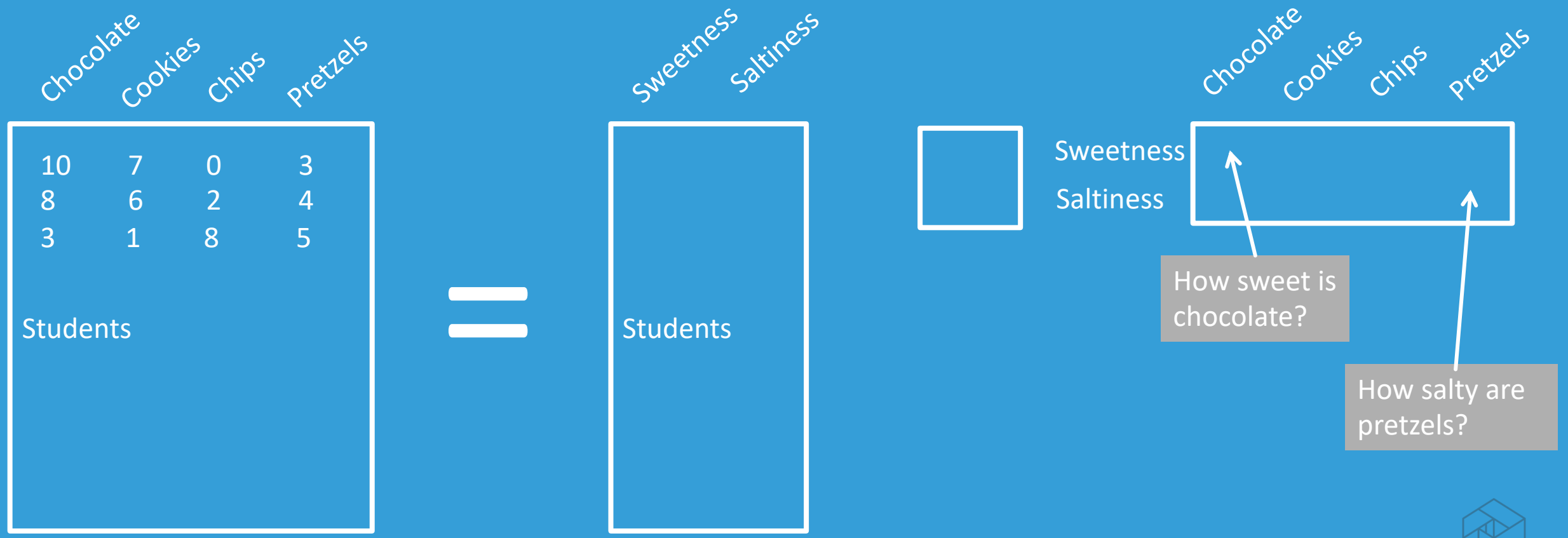

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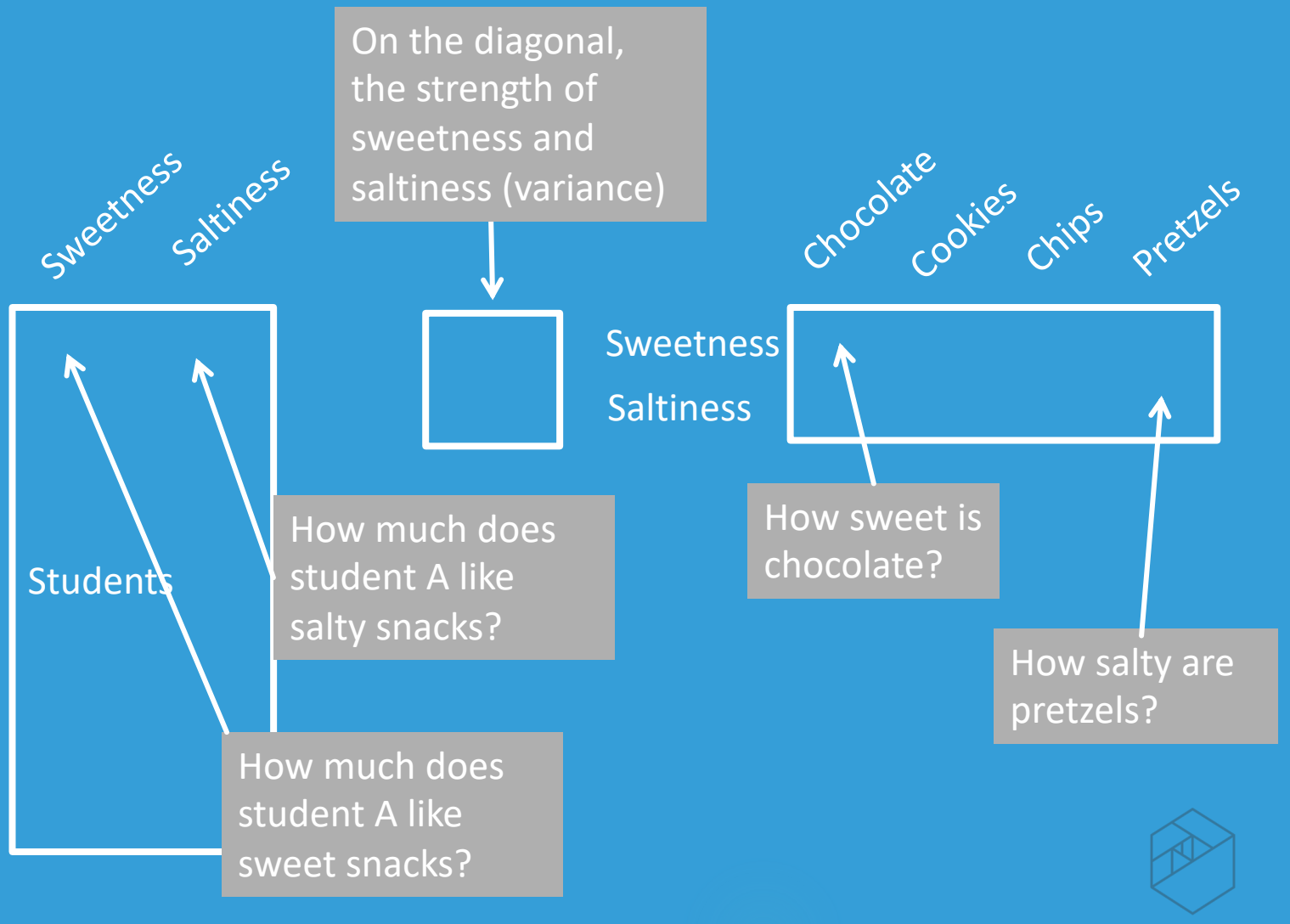

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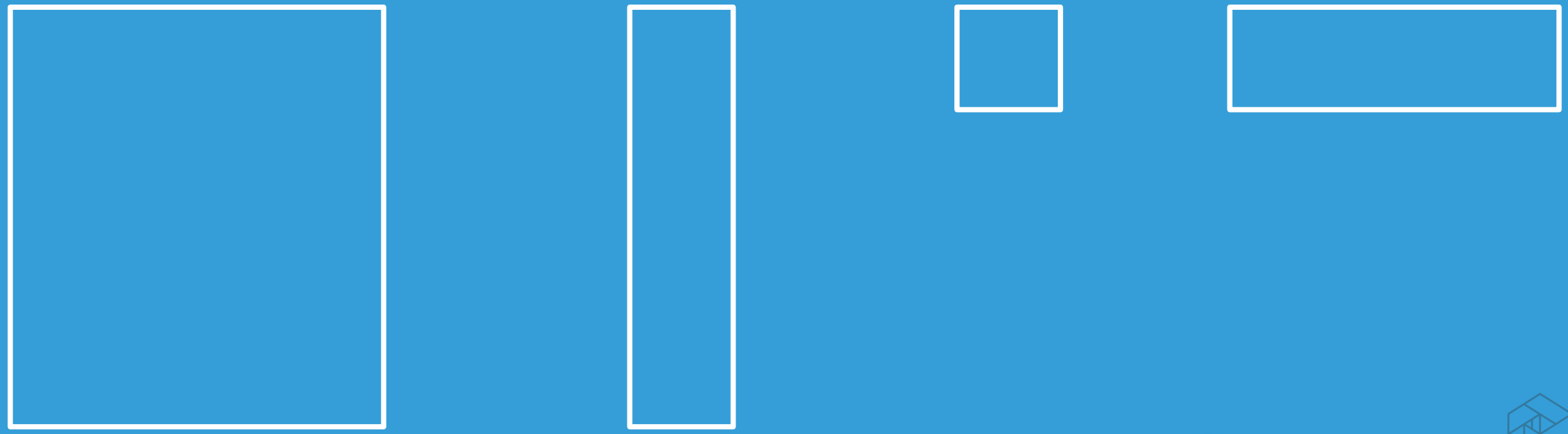
$$A_{m \times n} = U_{m \times r} \Sigma_{r \times r} V'_{n \times r}$$



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- **A:** Our data matrix, where rows are observations and columns are covariates/features
- **U:** Left singular vectors, or decomposing each of our observations into how well they're represented by a category
- **Σ:** Diagonal matrix (all off-diagonal entries are 0) of singular values, or the strengths of our categories
- **V:** Right singular vectors, or decomposing our covariates into categories

- It's always possible to do this decomposition, and **the decomposition is unique for each data matrix A**

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- We can reduce dimensionality by dropping categories with very low strengths (set them to zero)
  - This will drop the rightmost columns of U and the last rows of V'
  - Multiply what's left to get the new data matrix A

Using Σ for dimensionality reduction

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Using Σ for dimensionality reduction

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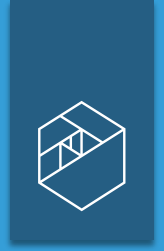
- Depends, but good rule of thumb is ~70-80% of variance explained
- Note that, in practice, we can't usually interpret the singular values like we did here
  - That is, we can't really see that the first component is sweetness and the second is saltiness
  - Similar to how in clustering we usually can't put a category on each cluster (e.g. high spenders)

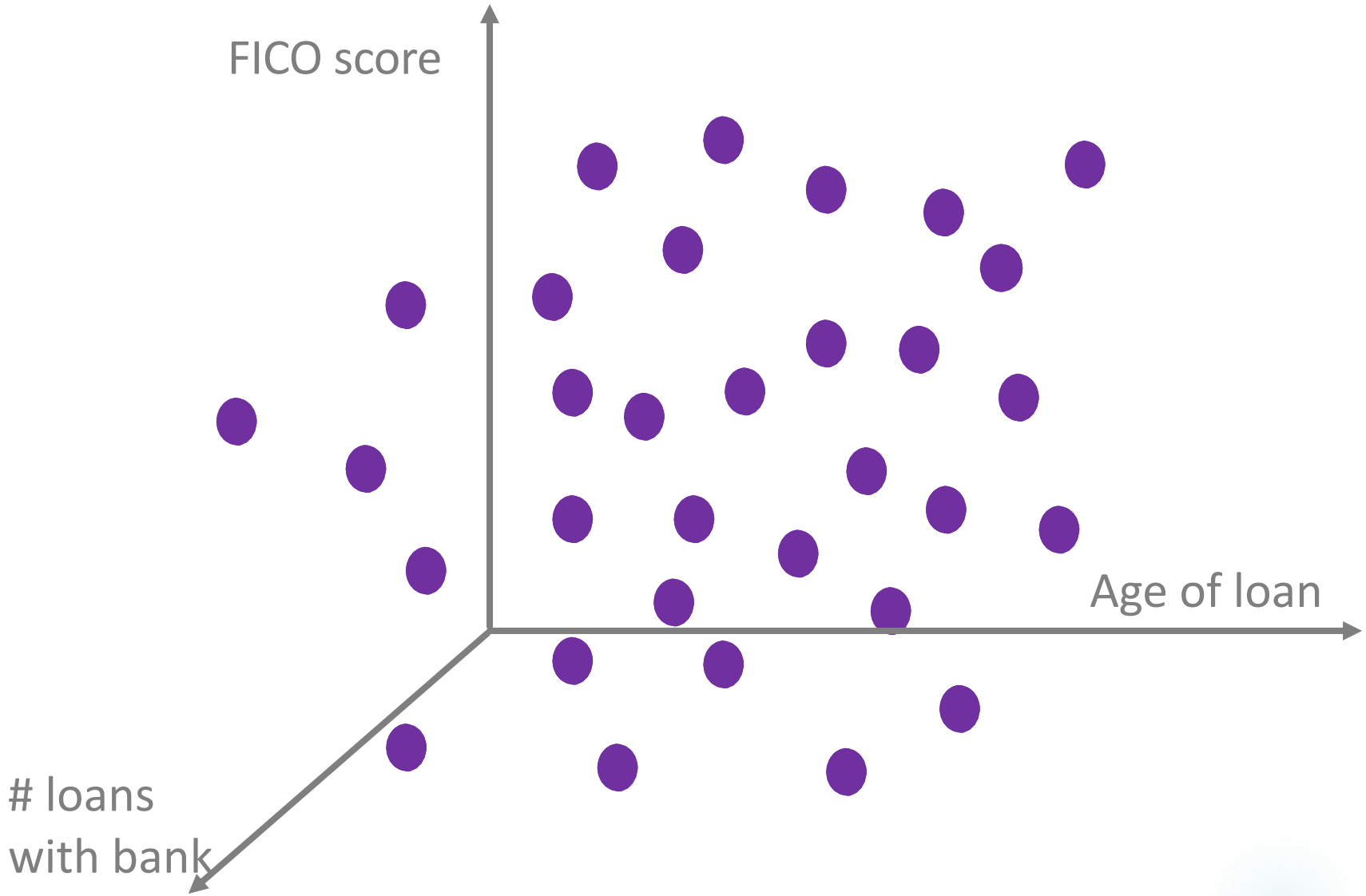


Feature Selection vs. Feature Extraction

Feature **selection** vs feature **extraction**

- Feature selection involves removing features that aren't helpful
  - They may not be predictive of our dependent variable
  - They may not have a lot of variation
- Feature extraction uses information from all features, but creates artificial new features that are composites
  - Uses information from all features
  - May put more weight on certain features

3D → 2D Feature **Selection**



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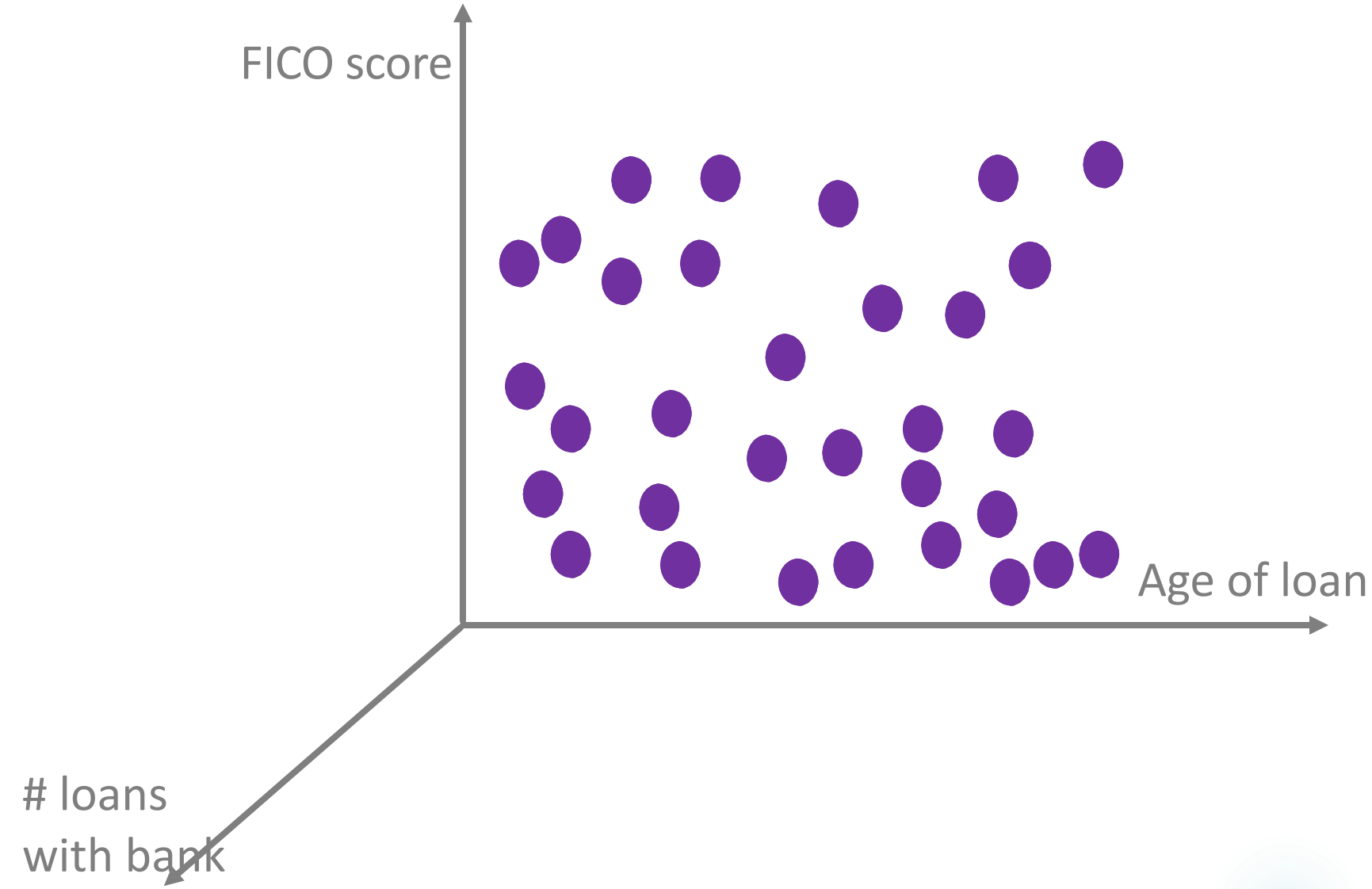

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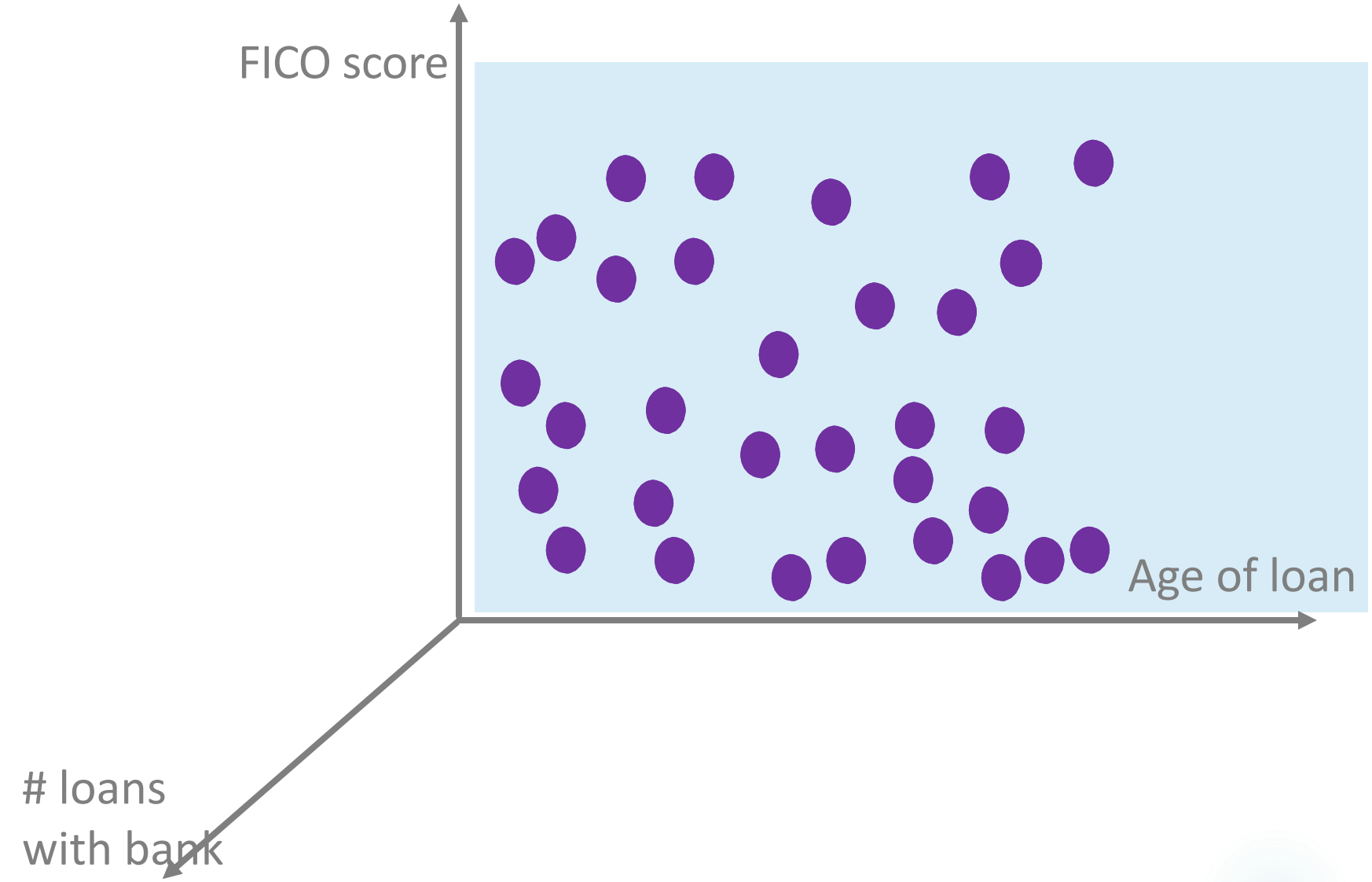
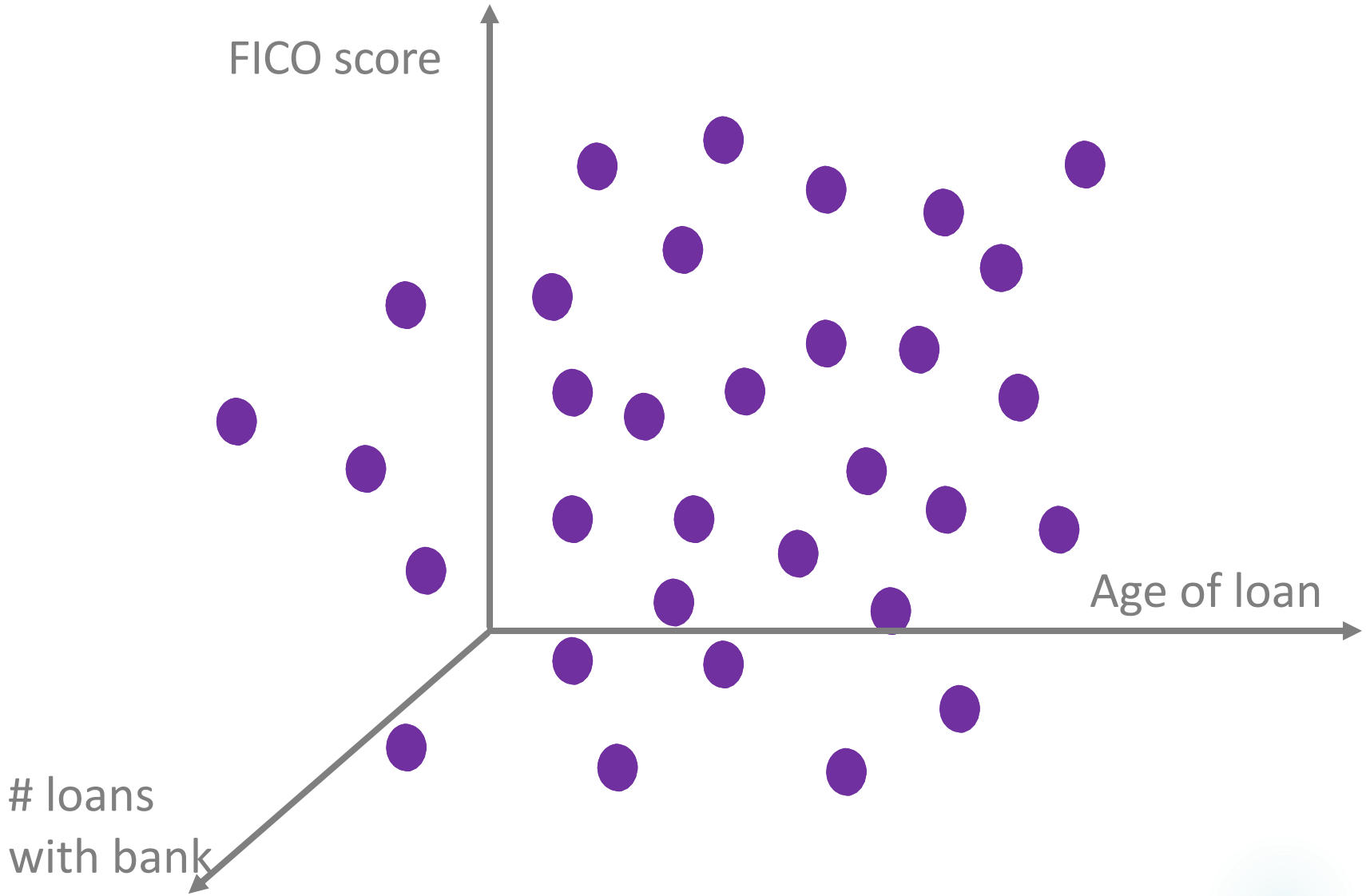


Feature selection

- Feature selection is an art
  - Try fitting with some features, remove some features, re-fit and compare
  - Regularization
  - Feature importance scores (only for some types of models)

3D → 2D Feature **Extraction** (e.g. PCA)



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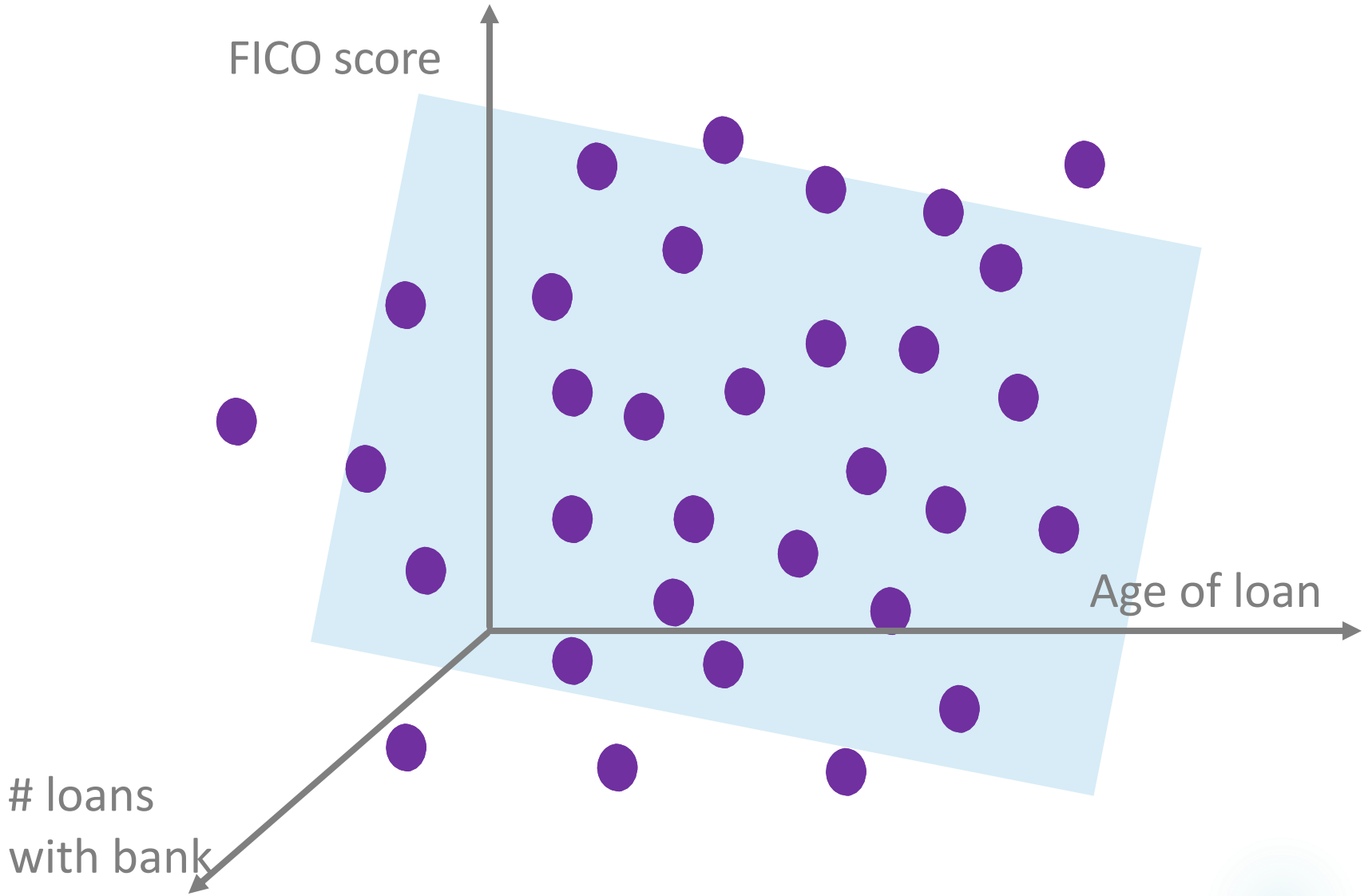

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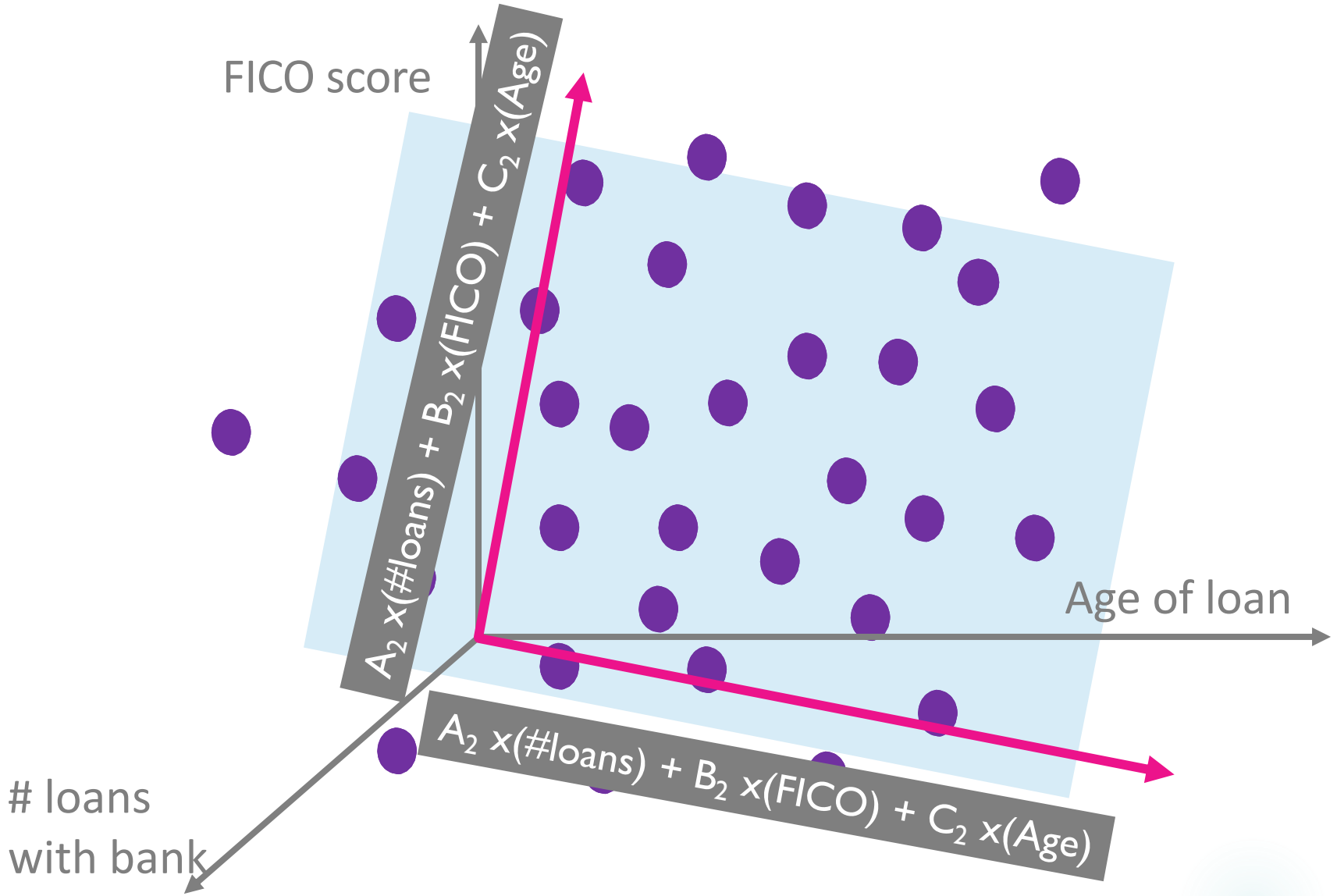

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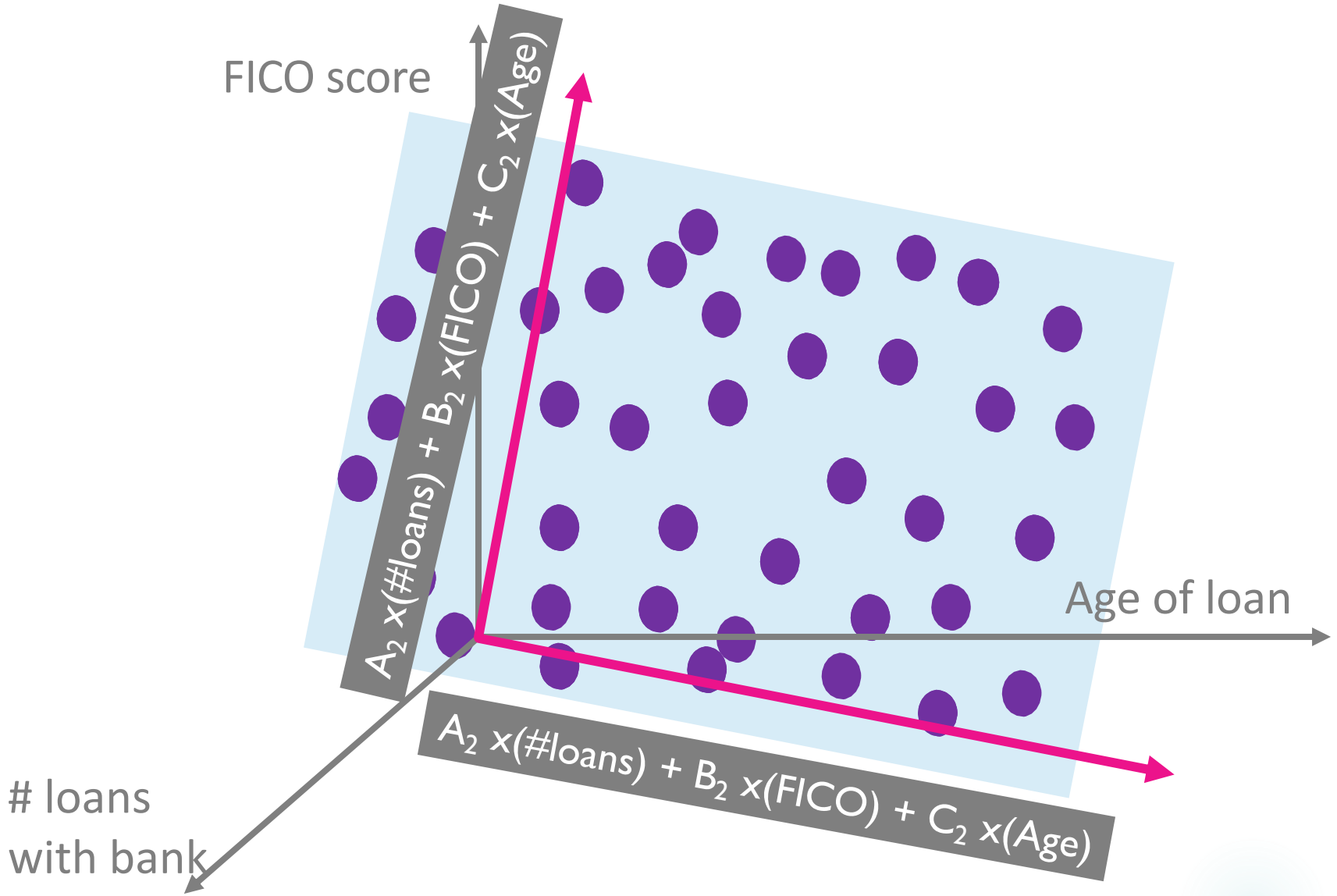

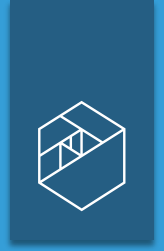

Principal Components Analysis (PCA)

A method of feature extraction

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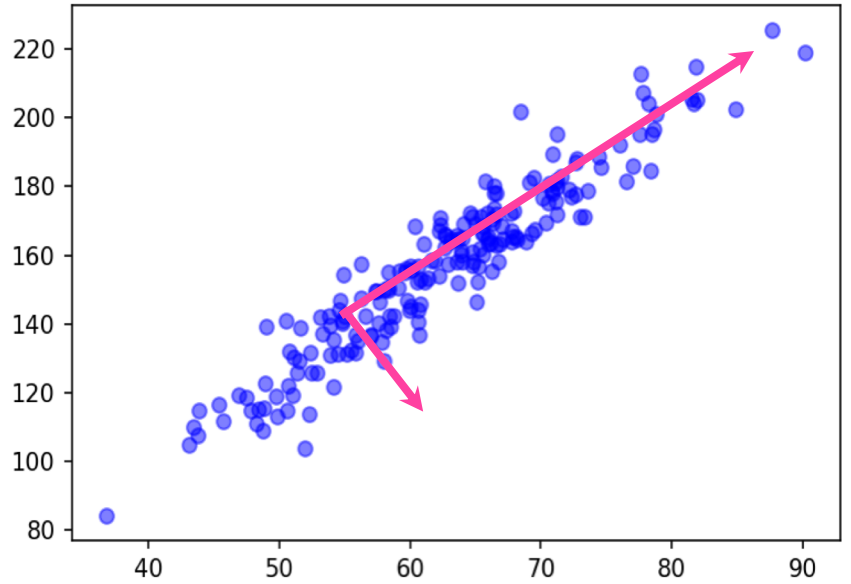

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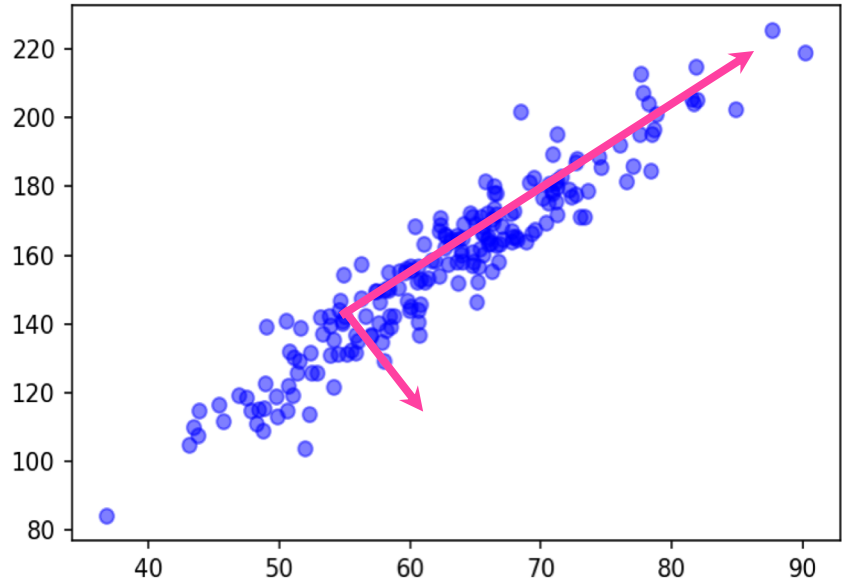

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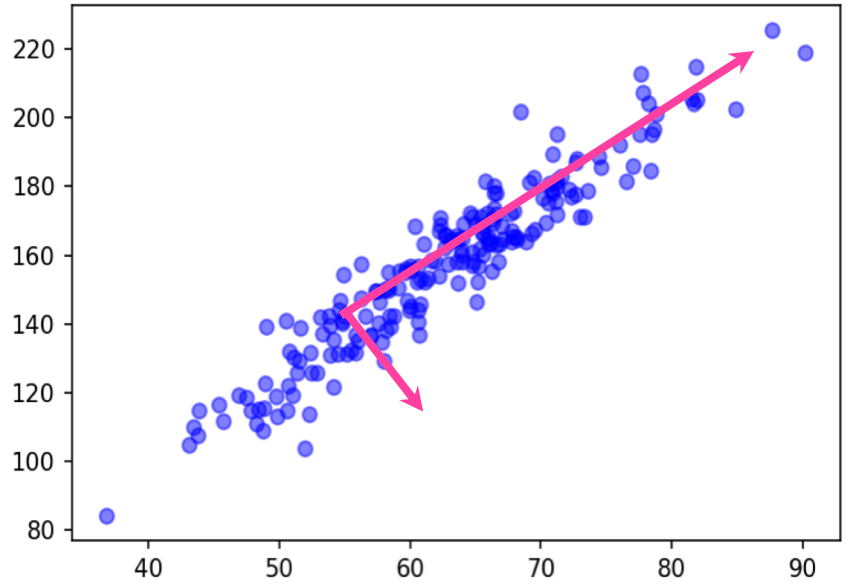

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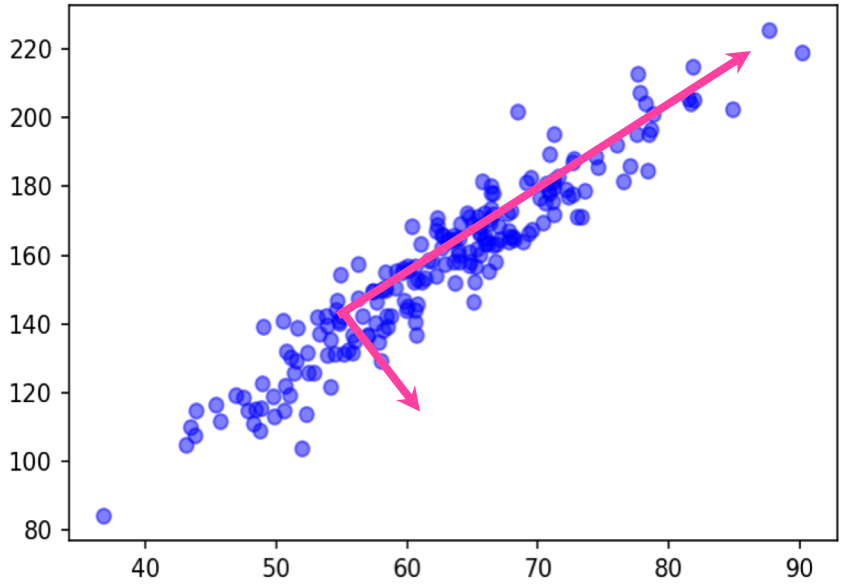

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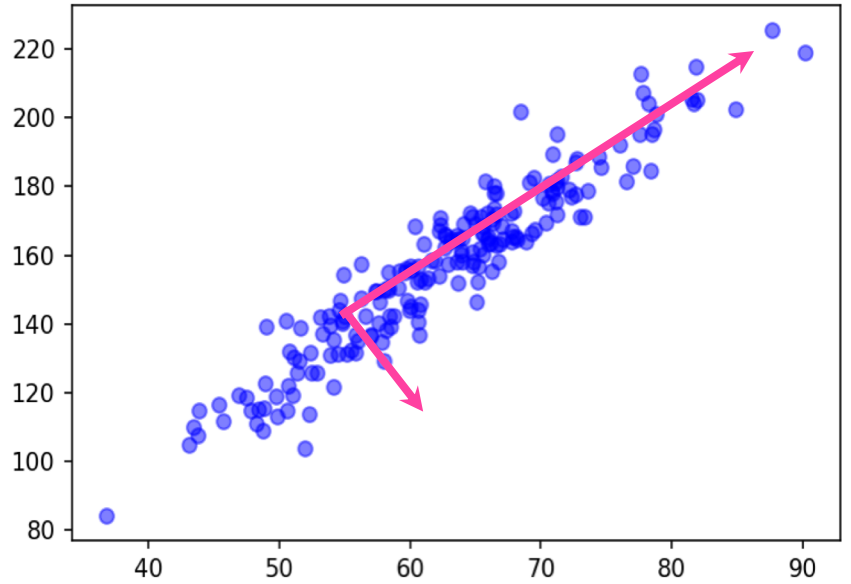
- Behind the scenes, many PCA implementations are doing SVD



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  - Begin by centering all columns/variables (mean 0)
  - Solve the maximization problem of finding a linear combination of Xs with max variance
  - Continue to find linear combinations with the next-highest variance, but where the component is uncorrelated with all components that came before

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- Turns out, being uncorrelated is the same thing as being orthogonal (perpendicular)

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  - Eigenvectors = directions
  - Eigenvalues = variances

PCA is not a panacea for high dimensions

- PCA is looking for linear relationships between variables; if they're related in some different way, PCA won't help us
- **Standardize your data, otherwise PCA will just pick out variables that are on larger scales (higher variance)**
- Since we're not using Y, the variance PCA picks up on may not be as meaningful for our use case
- Components are not easy to interpret, so you lose interpretability

Applications of dimensionality reduction

- NLP
  - Topic modeling: axes are topics and documents cluster around axes
  - Recommender systems
- Visualization
- Reduce computational complexity by reducing amount of data we're storing and processing
- Data compression with little loss (e.g. image compression)