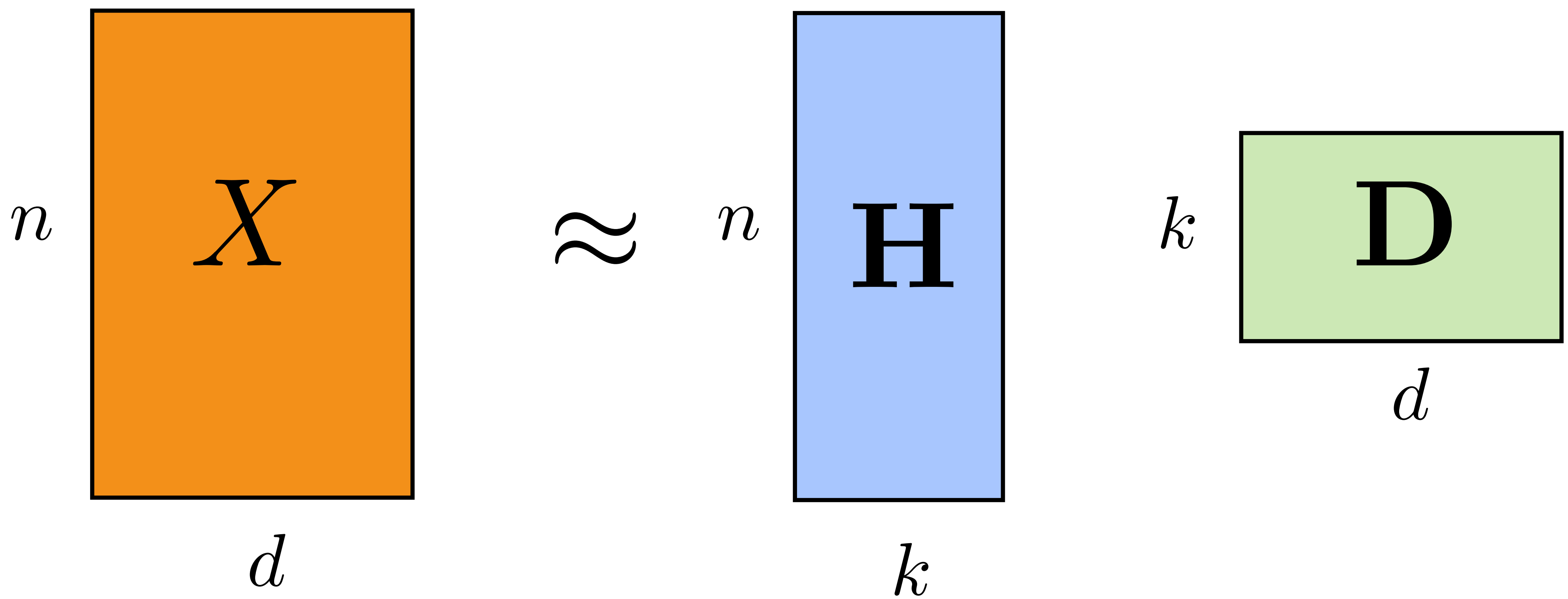
Matrix factorization and embeddings



Reminders/Comments

- Initial draft of Mini-project due today

Today

- Back to representation learning
- How do we transform an input x into a new vector phi(x) that is
  - composed of real values
  - enables nonlinear functions in terms of x, using only a generalized linear model with phi(x)
  - and has other potentially desirable properties, like compactness or…

Neural networks summary

- Discussed basics, including
- Basic architectures (fully connected layers with activations like sigmoid, tanh, and relu)
- How to choose the output loss
    - i.e., still using the GLM formulation
- Learning strategy: gradient descent (called back-propagation)
- Basic regularization strategies

How else can we learn the representation?

- Discussed how learning can be done in simple ways even for “fixed representations”
  - e.g., learn the centres for radial basis function networks
  - e.g., learn the bandwidths for Gaussian kernel
- In general, this problem has been tackled for a long time in the field of unsupervised learning
  - where the goal is to analyze the underlying structure in the data

Using factorizations

- Many unsupervised learning and semi-supervised learning problems can be formulated as factorizations
  - PCA, kernel PCA, sparse coding, clustering, etc.
- Also provides an way to embed more complex items into a shared space using co-occurrence
  - e.g., matrix completion for Netflix challenge
  - e.g., word2vec

Intuition (factor analysis)

- Imagine you have test scores from 10 subjects (topics), for 1000 students
- As a psychologist, you hypothesize there are two kinds of intelligence: verbal and mathematical
- You cannot observe these factors (hidden variables)
- Instead, you would like to see if these two factor explain the data, where x is the vector of test scores of a student
- Want to find: $x = d1\ h1 + d2\ h2$, where d1 and d2 are vectors h1 = verbal intelligence and h2 = mathematical intelligence
- Having features h1 and h2 would give a compact, intuitive rep

Example continued

- Imagine you have test scores from 10 subjects (topics), for 1000 students
- Learned basis vectors d1 and d2 that reflect scores for a student with high verbal or math intelligence, respectively

$$\text{Obtain } \mathbf{x}_5 = \mathbf{d}_1 h_{5,1} + \mathbf{d}_2 h_{5,2}$$

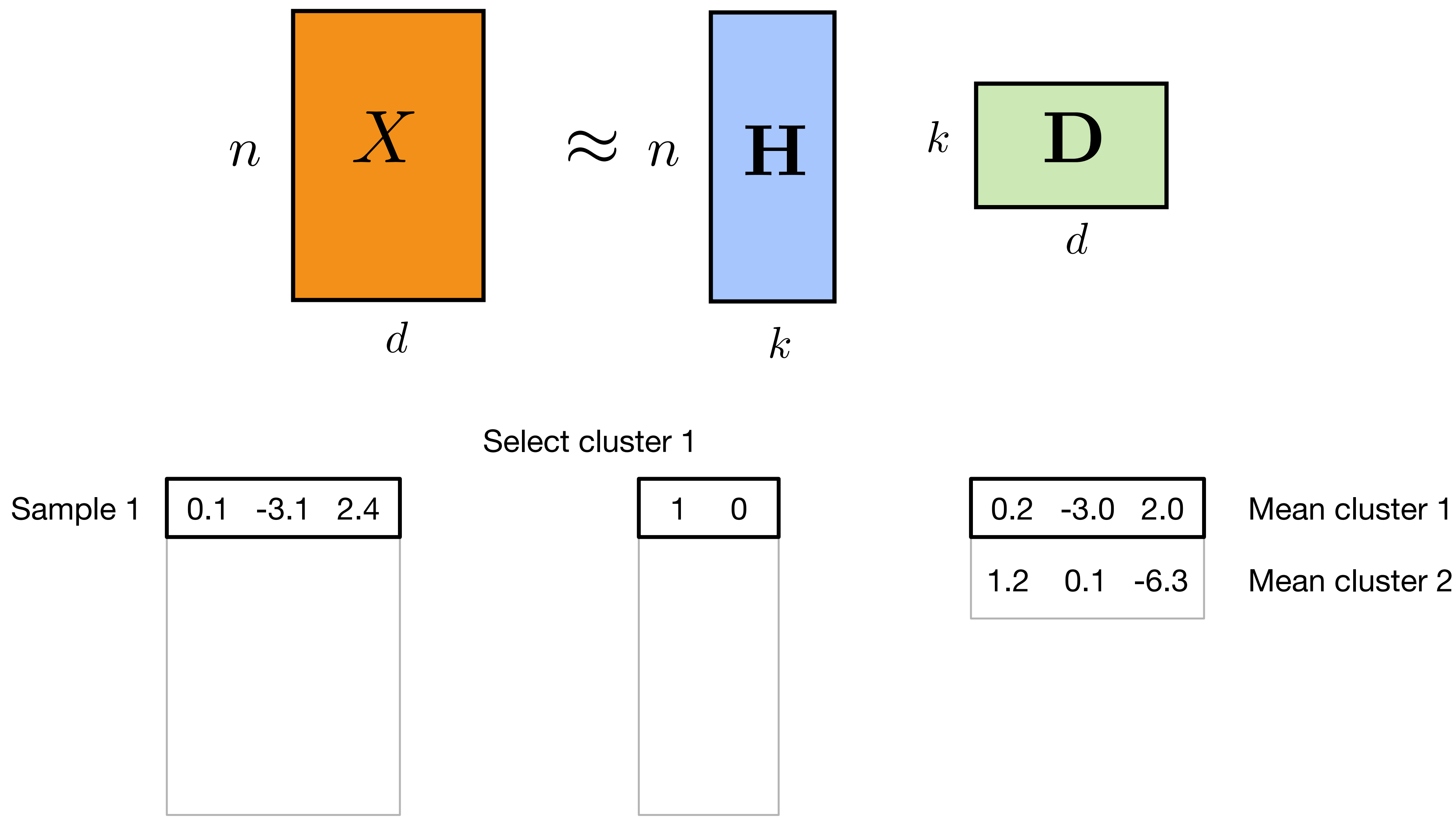
$$\text{where } h_{5,1} = \text{verbal intelligence and } h_{5,2} = \text{math intelligence}$$

- Features [h_{5,1}, h_{5,2}] provide useful attributes about student 5

Whiteboard

- Linear neural network
- Auto-encoders and Matrix factorization
- Learning (latent) attributes of inputs

Example: K-means



$$\|\mathbf{x} - \sum_{i=1}^{2} 1\,(\mathbf{x} \text{ in cluster } i)\,\mathbf{d}_i\|_2^2 = \|\mathbf{x} - \mathbf{h}\mathbf{D}\|_2^2$$

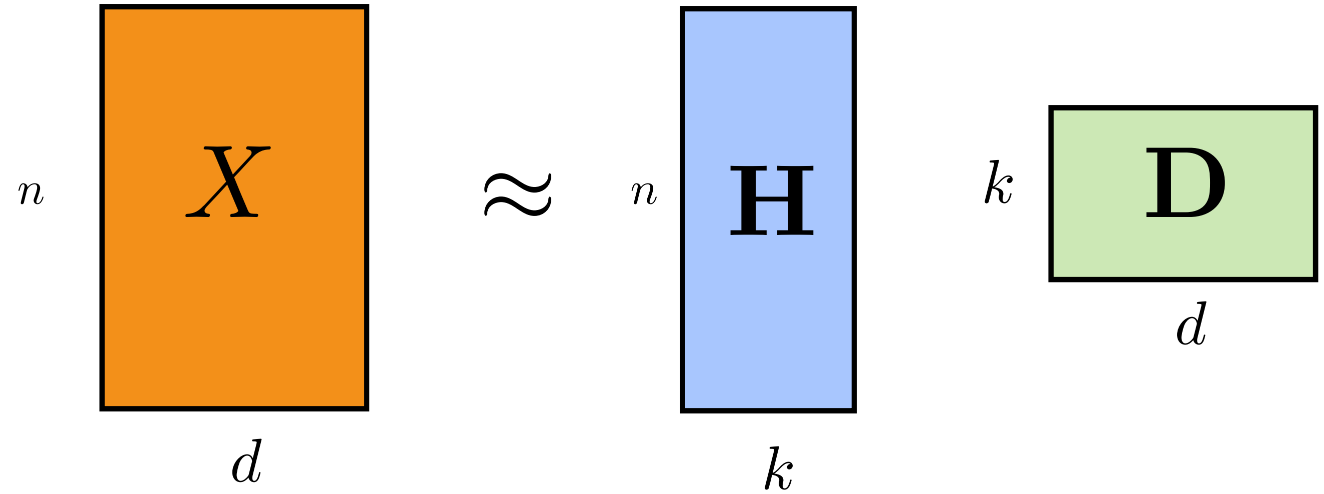
where $\mathbf{h} = [1 \quad 0]$ or $\mathbf{h} = [0 \quad 1]$ and $\mathbf{D} = [\mathbf{d}_1 \ ; \ \mathbf{d}_2]$.

Dimensionality reduction

- If set inner dimension k < d, obtain dimensionality reduction
- Recall that the product of two matrices H and D has rank at most the minimum rank of H and D

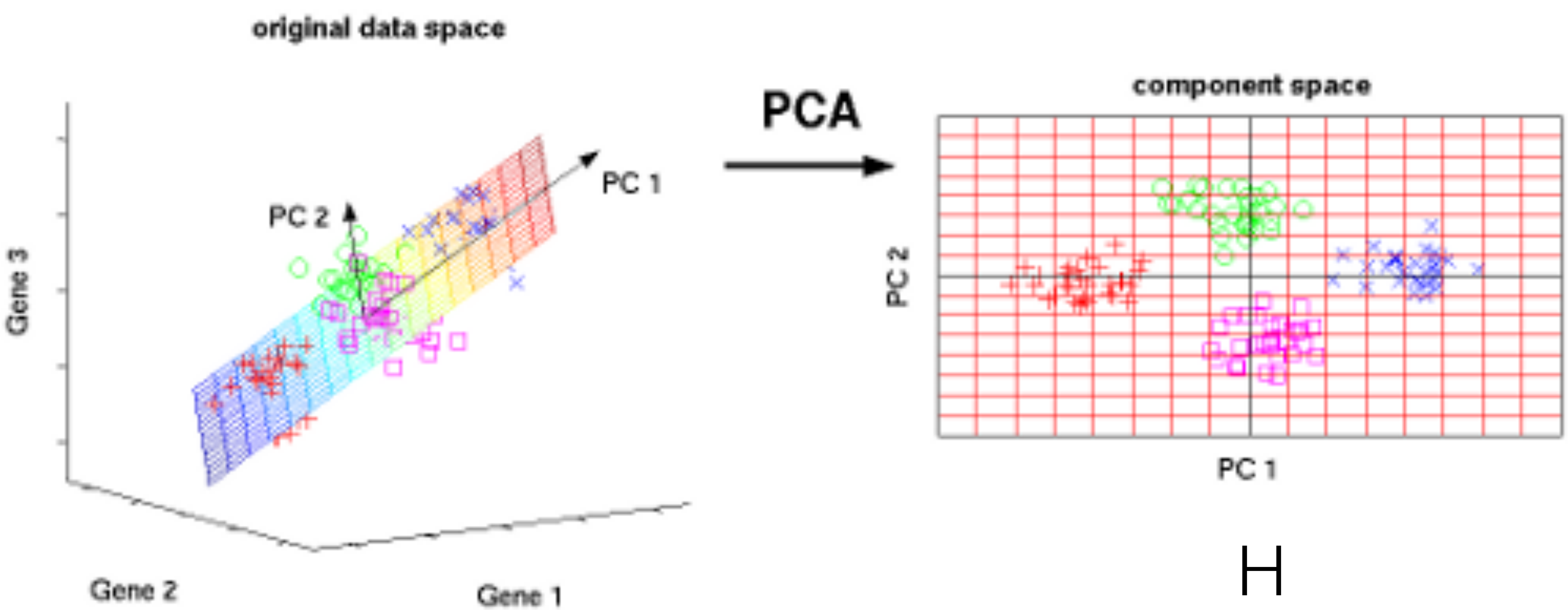
$$\text{rank}(\mathbf{HD}) \leq \min(\text{rank}(\mathbf{H}), \text{rank}(\mathbf{D}))$$

- Even if d = 1000, if we set k = 2, then we get a reconstruction of X that is only two-dimensional
  - we could even visualize the data! How?



Principal components analysis

- New representation is k left singular vectors that correspond to k largest singular values
  - i.e., for each sample x, the corresponding k-dimensional h is the rep
- Not the same as selecting k features, but rather projecting features into lower-dimensional space



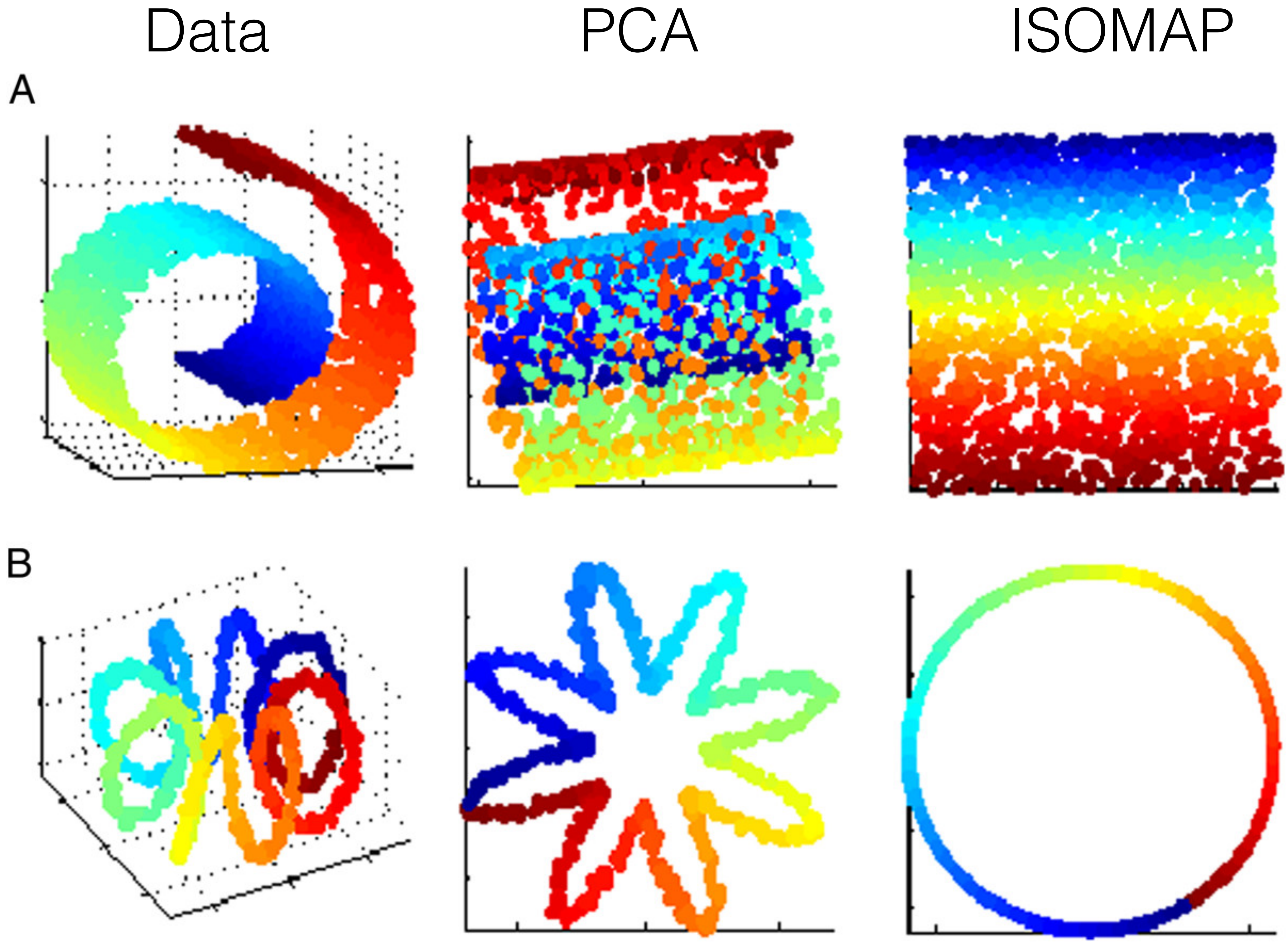
Do these make useful features?

- Before we were doing (huge) nonlinear expansions
- PCA takes input features and reduces the dimension
- This constrains the model, cannot be more powerful
- Why could this be helpful?
  - Constraining the model is a form of regularization: could promote generalization
  - Sometimes have way too many features (e.g., someone overdid their nonlinear expansion, redundant features), want to extract key dimensions and remove redundancy and noise
  - Can be helpful for simply analyzing the data, to choose better models

What if the data does not lie on a plane?

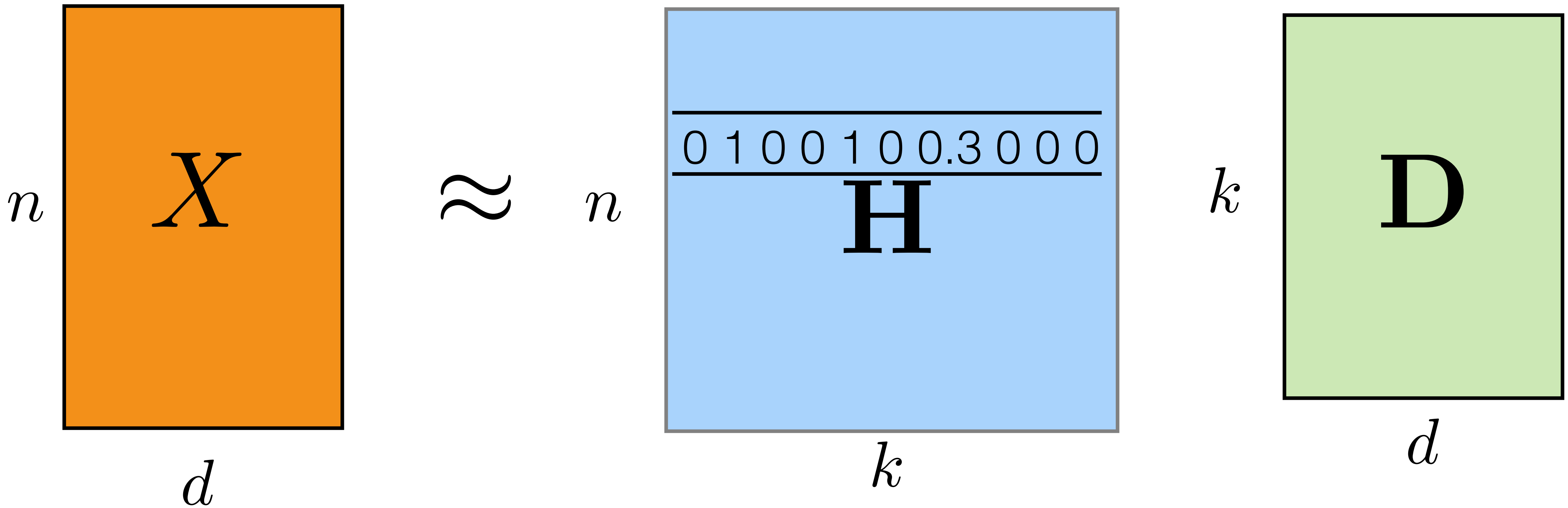
- Can do non-linear dimensionality reduction
- Interestingly enough, many non-linear dimensionality reduction techniques correspond to PCA, but first by taking a nonlinear transformation of the data with a (specialized) kernel
    - Isomap, Laplacian eigenmaps, LLE, etc.
- Can therefore extract a lower-dimensional representation on a curved manifold, can better approximate input data in a low-dimensional space
    - which would be hard to capture on a linear surface

Isomap vs PCA



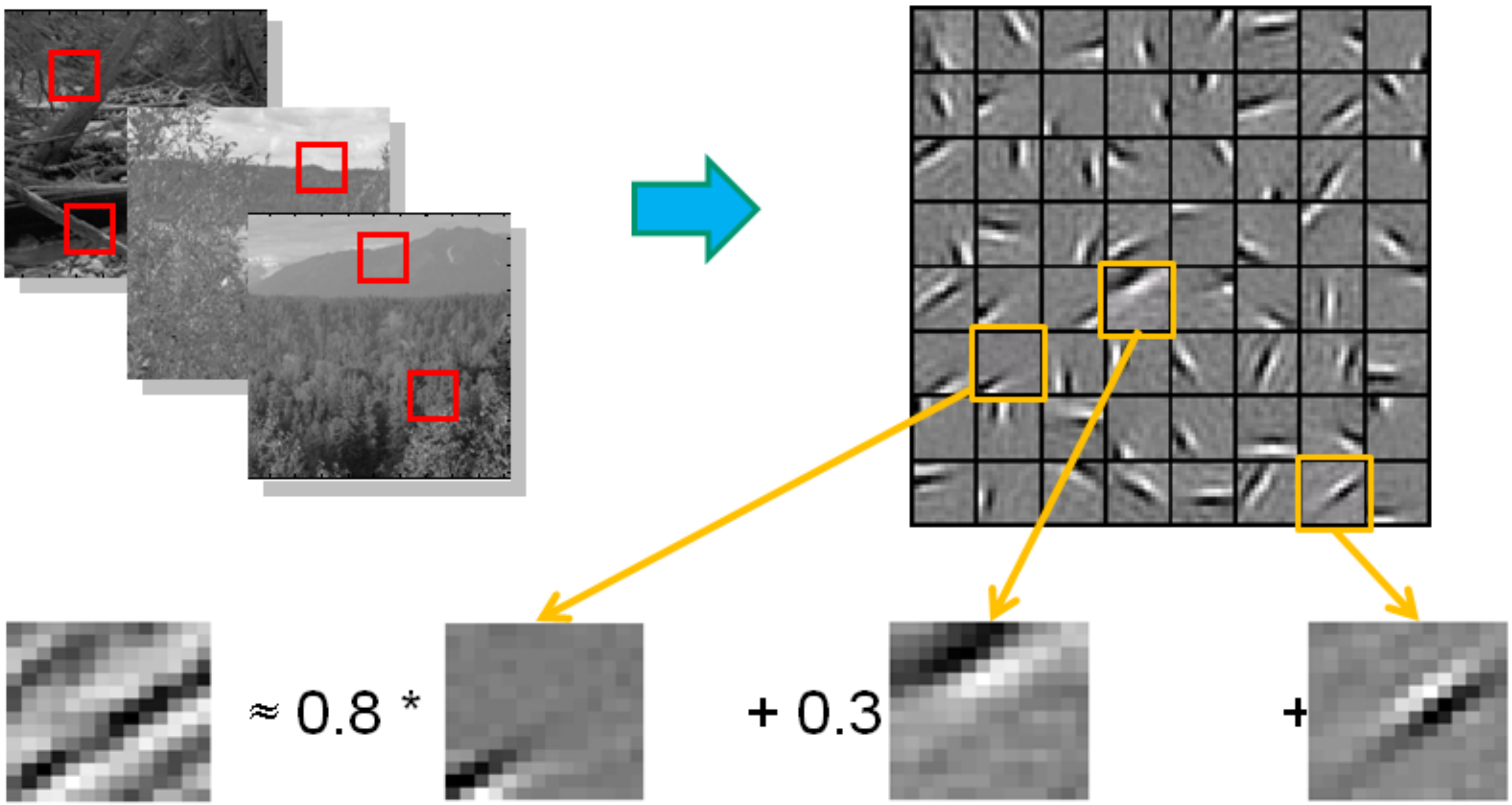
*Note: you don't need to know Isomap, just using it as an example

Sparse coding



- For sparse representation, usually k > d
- Many entries in new representation are zero

Sparse coding illustration



$[a_1, \ldots, a_{64}] = [0, 0, \ldots, 0, \mathbf{0.8}, 0, \ldots, 0, \mathbf{0.3}, 0, \ldots, 0, \mathbf{0.5}, 0]$
(feature representation)

Slide credit: Andrew Ng

Compact & easily interpretable

Embeddings with co-occurence

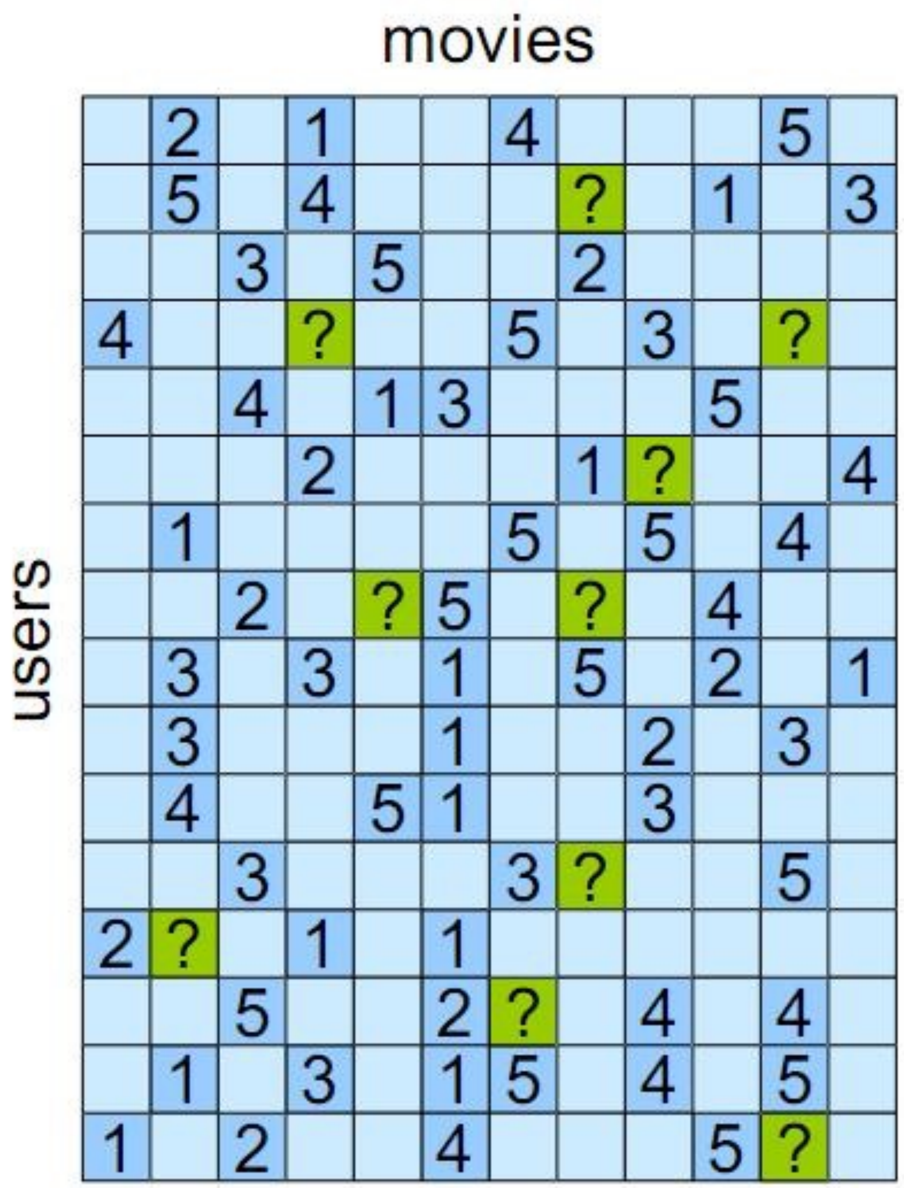
- Embed complex items into a shared (Euclidean) space based on their relationships to other complex items
- Examples:
  - word2vec
  - users and movies
  - gene sequences

Embedding Movies and Users

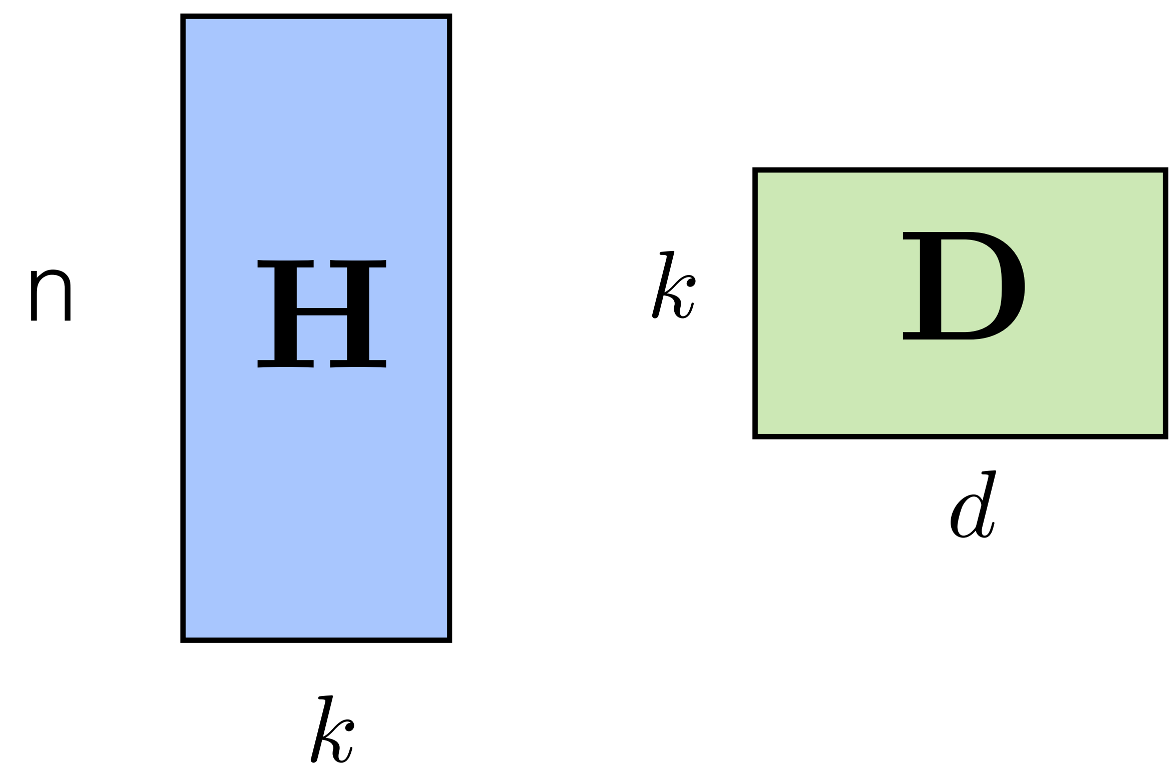
$$\text{Example } \mathbf{H}_{i:} = [\text{like comedies}, \ldots] = [1, \ldots]$$

$$\mathbf{D}_{:j} = [\text{is a comedy}, \ldots] = [1, \ldots]$$

$$\mathbf{H}_{i:}\mathbf{D}_{:j} = 1 + \ldots$$



$\approx$



$\mathbf{H}_{i:}$ is the representation of user i

$\mathbf{D}_{:j}$ is the representation of movie j

Consider word features

- Imagine want to predict whether a sentence is positive or negative (say with logistic regression)

- How do we encode words?

- One basic option: a one-hot encoding. If there are 10000 words, the ith word has a 1 in the ith location of a 10000 length vector, and zero everywhere else.

- This is a common way to deal with categorical variables, but with 10000 words this can get big!

- Can we get a more compact representation of a word?

Co-occurrence matrix example

- X is count of words (rows) and context (columns), where for word i the count is the number of times a context word j is seen within 2 words (say) of word i

- Each word is a one-hot encoding; if there are 10000 words, each row corresponds to 1 word, and X is 10000x10000

  - I like deep learning.
  - I like NLP.
  - I enjoy flying.

counts	I	like	enjoy	deep	learning	NLP	flying	.
I	0	2	1	0	0	0	0	0
like	2	0	0	1	0	1	0	0
enjoy	1	0	0	0	0	0	1	0
deep	0	1	0	0	1	0	0	0
learning	0	0	0	1	0	0	0	1
NLP	0	1	0	0	0	0	0	1
flying	0	0	1	0	0	0	0	1
.	0	0	0	0	1	1	1	0

How obtain embeddings?

- Words i and s that have similar context counts should be embedded similarly
- Factorize co-occurrence matrix
  - or some measure of how items are related, e.g. rank or probability
- $X = H D$ —> What is $H_{i:}$, and what is $D_{:j}$? Which should we use as the embedding for words?

How obtain embeddings?

- $X = H D$ —> What is $H_{i:}$, and what is $D_{:j}$? Which should we use as the embedding for words?
- $H_{i:}$ is the embedding for word i
- Is it possible to get the embedding for a new word, that you did not train on?

Pros/cons of rep learning approaches

- Neural networks
  - ✓ demonstrably useful in practice
  - ✓ theoretical representability results
  - \- can be difficult to optimize, due to non-convexity
  - \- properties of solutions not well understood
  - \- not natural for missing data

- Matrix factorization models
  - ✓ widely used for unsupervised learning
  - ✓ simple to optimize, with well understood solutions in many situations
  - ✓ amenable to missing data
  - \- much fewer demonstrations of utility

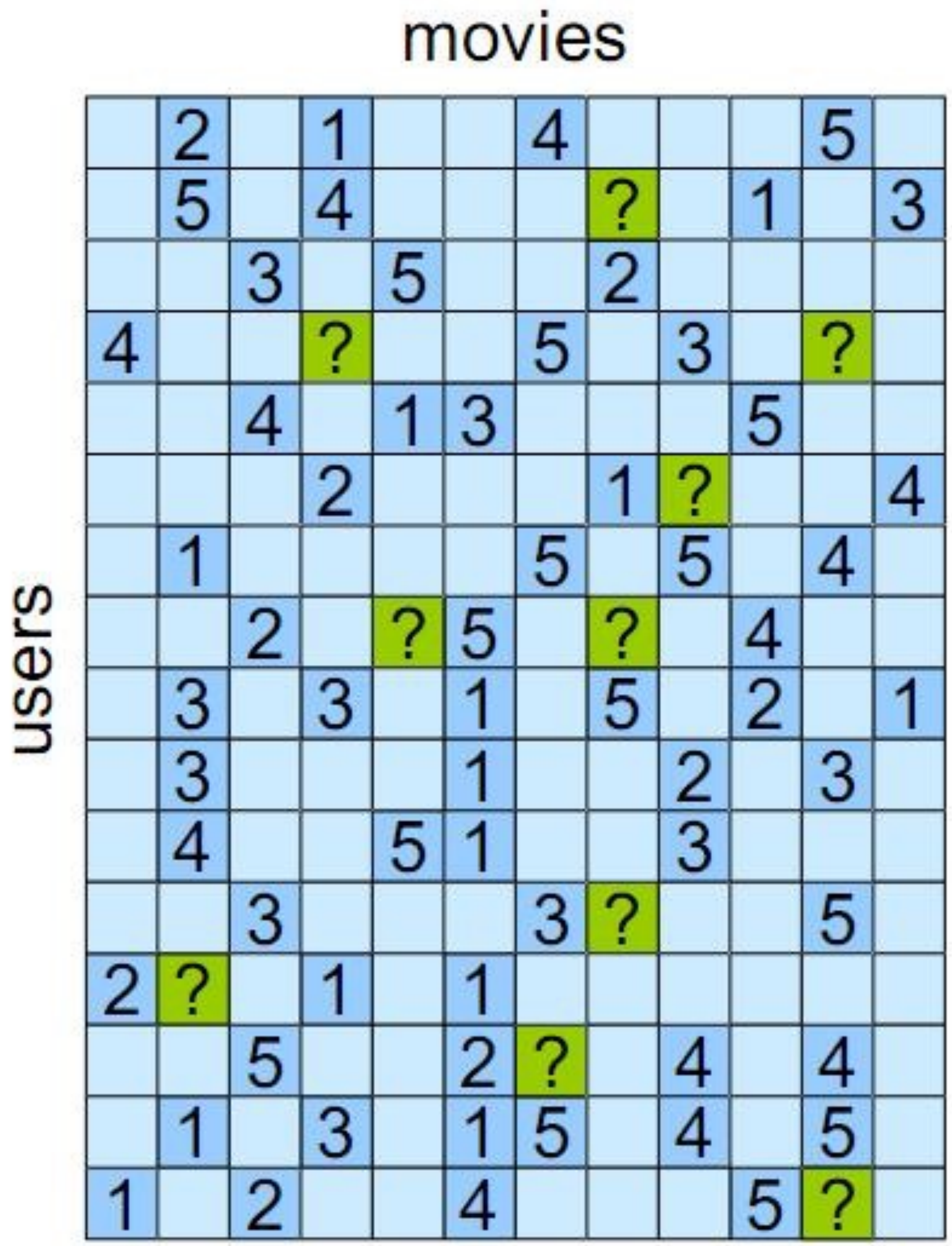
Can they both be used to get embeddings?

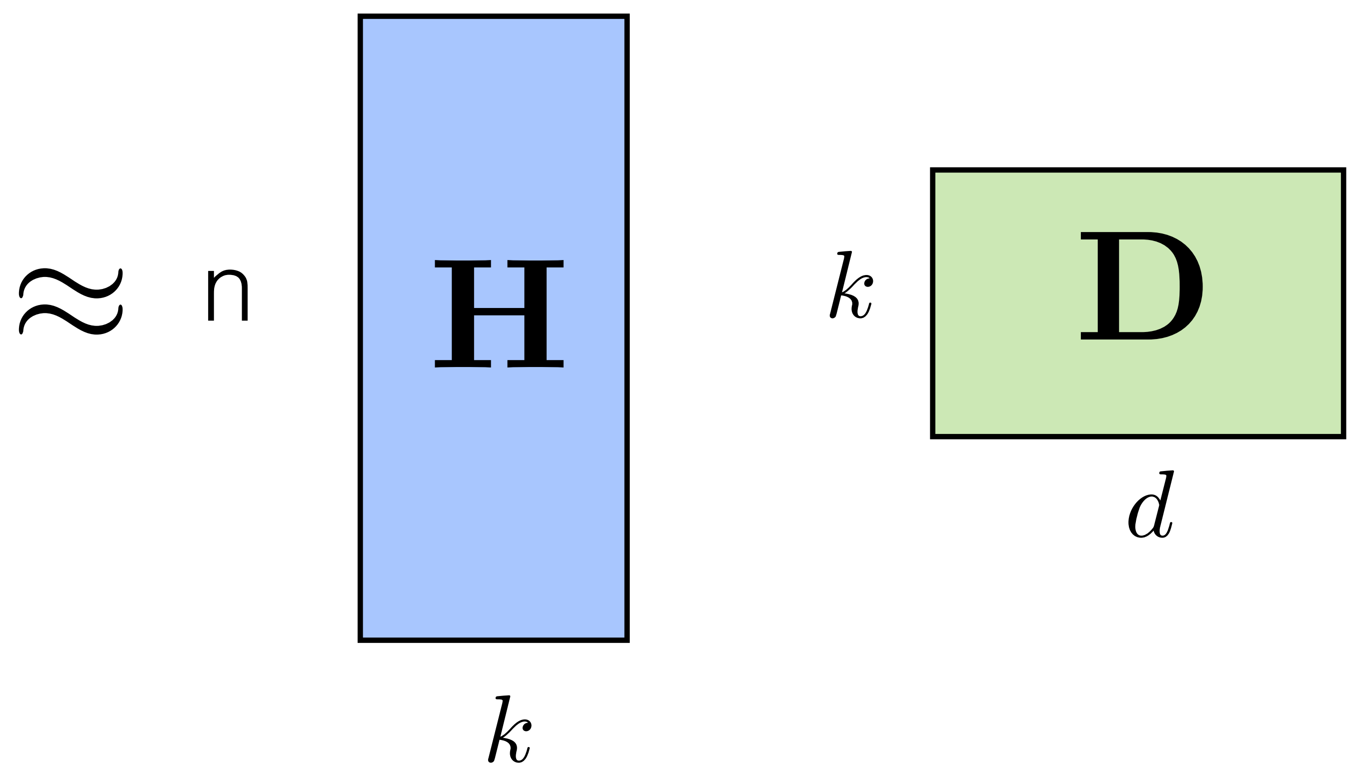
Missing data

- Can easily perform factorization even with missing data
- Important in an area called matrix completion or collaborative filtering
- This contrasts NNs, where it is less clear how to handle missing data (why?)

Matrix completion

Subspace (low-rank) form





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Matrix completion

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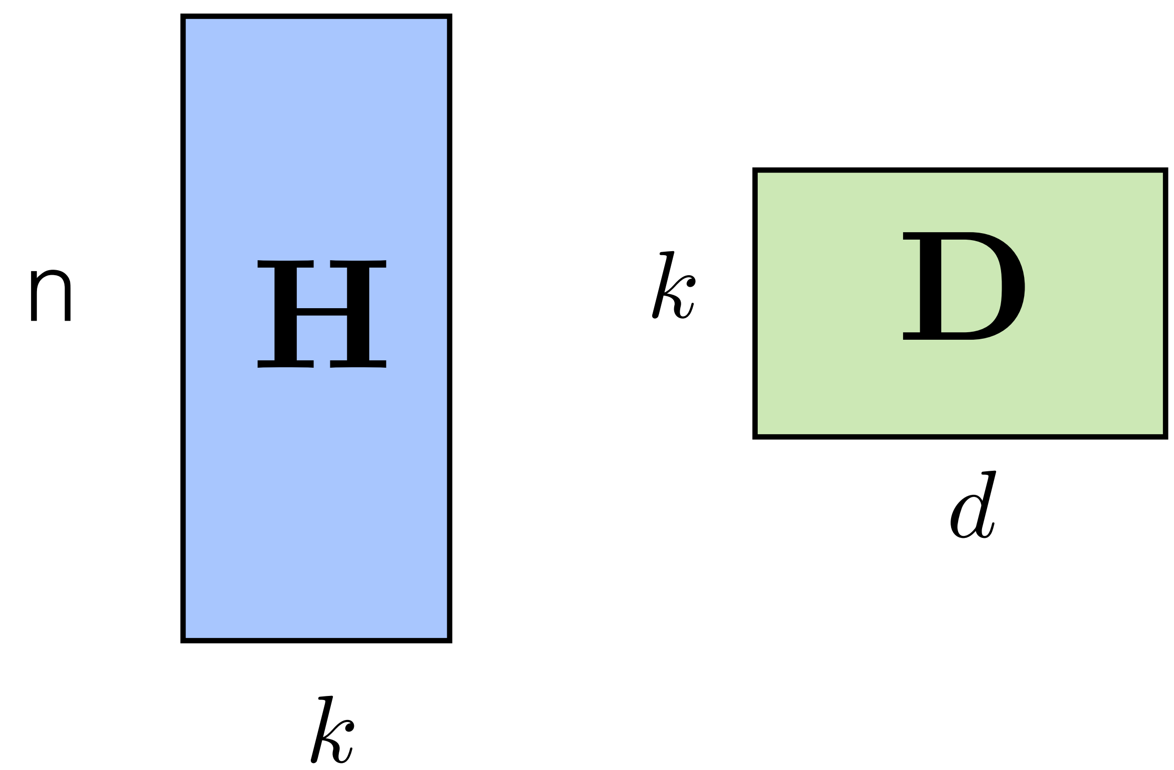

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How fill in missing data?

- The goal in factorization is to find $X = H D$
- This corresponds to finding $X_{ij} = H_{i,:} D_{:j}$ for all i, j
- The $H_{i,:}$ is shared for i, across all j
- The $D_{:,j}$ is shared for j, across all i
- We can learn something about $H_{i,:}$, as long as X_{ij} available for some j
- We can learn something about $D_{:j}$, as long as X_{ij} available for some i

Algorithm

$$\min_{H,D} \sum_{\text{available } (i,j)} (X_{ij} - \mathbf{H}_{i:}\mathbf{D}_{:j})^2$$

$$\nabla_D \sum_{\text{available } (i,j)} (X_{ij} - \mathbf{H}_{i:}\mathbf{D}_{:j})^2 = \sum_{\text{available } (i,j)} \nabla_D (X_{ij} - \mathbf{H}_{i:}\mathbf{D}_{:j})^2$$

$$\nabla_{D_{:j}} (X_{ij} - \mathbf{H}_{i:}\mathbf{D}_{:j})^2 = -2(X_{ij} - \mathbf{H}_{i:}\mathbf{D}_{:j})\mathbf{H}_{i:}$$

Gradient descent on H and D until convergence

Matrix completion solution

- Once learn H and D, can complete the matrix
- Take entry (i,j) that was missing, compute Xij = H_{i:} D_{:j}
- H_{i:} is the representation of user i
  - also called an embedding, where similar users in terms of movie preferences should have similar H_{i:}
- D_{:j} is the representation of movie j

Conclusion: factorization enables missing data to be inferred, and provides a new metric between items

$$\|\mathbf{H}_{i:} - \mathbf{H}_{s:}\|_2$$

Whiteboard

- What do we mean by embedding
- Can we use NNs for embeddings?
- Generalizing how to get embeddings (supervised, sparse embeddings, etc.)