Overview	Manifolds	Clustering	Self-Supervision	Summary

## Lecture 24: Unsupervised Learning

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#### **5** Summary

# What is Unsupervised Learning?

- Supervised learning: given pairs of data, (x<sub>i</sub>, y<sub>i</sub>), learn a mapping f(x) ≈ y.
- **Unsupervised learning:** given unlabeled training examples, *x<sub>i</sub>*, learn something about them.
  - Can  $x_i$  be decomposed into signal + noise?
  - Can we group the x's into "natural classes," i.e., groups of tokens that are similar to one another?
  - Can we design a classifier that puts  $x_i$  into its natural class?

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Some types of unsupervised learning

- Manifold learning: decompose x<sub>i</sub> into signal + noise
- **Clustering:** group the x's into natural classes
- **Self-supervised learning:** learn a classifier that puts x<sub>i</sub> into its natural class

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- Signals lie on a manifold if some perturbations are impossible ("perpendicular" to the manifold)
- If signals are on a manifold, then perturbations perpendicular to the manifold are always noise, and can be ignored.

CC-SA 4.0, https:

//commons.wikimedia.org/wiki/File:Insect\_on\_a\_

torus\_tracing\_out\_a\_non-trivial\_geodesic.gif

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Speech Ma	nifolds			

- The signal manifold: Each sample is
   s[n] = d[n] + ∑ a<sub>m</sub>s[n m]. The excitation, d[n], is sparse:
   only about 10% of its samples should be nonzero.
- **The articulatory manifold:** The formant frequencies and bandwidths change slowly as a function of time, because they are shaped by positions of the tongue, jaw, and lips, and those things have mass.







Fig. 4. Top to bottom: Original spectrogram from the test set; reconstruction from the 312-bit VQ coder; reconstruction from the 312-bit auto-encoder (2304-1000-312); coding errors as a function of time for the VQ coder (blue) and auto-encoder (red); spectrogram of the VQ coder residual; spectrogram of the auto-encoder residual.

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 PCA:
 Manifold = Hyperplane
 Hyperplane
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If the signal is constrained to lie on a hyperplane, then the hyperplane can be found using principal components analysis (PCA).



CC-SA 4.0, Principal\_Component\_Analyses\_for\_the\_

morphological\_and\_molecular\_surveys\_of\_seagrass\_



A one-layer autoencoder (one matrix multiply, then a hidden layer, then the inverse of the same matrix) computes the PCA of its input.





https://commons.wikimedia.org/wiki/File:

Autoencoder\_schema.png



Two-layer autoencoder can compute a nonlinear manifold

- A two-layer autoencoder constrains the data, x, to lie on a **nonlinear** manifold of dimension = dim(z).
- The first layer nonlinearly transforms the input, then the second layer computes PCA of the result.



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https://commons.wikimedia.org/wiki/File:

Autoencoder\_structure.png

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- Speech lies on manifolds of (at least) two timescales
  - **Signal manifold:** samples are predictable from previous samples
  - Articulatory manifold: formant frequencies and bandwidths are predictable from previous formants and bandwidths

- By learning to represent the manifolds, the early layers of an ASR learn to reject irrelevant variation (noise) and keep only relevant variation (signal)
- Autoencoders explicitly learn manifolds

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- The idea of clustering is to group the observed data into natural classes (things that sound similar).
- After grouping them into natural classes, we can then assign a label to each natural class.

Peterson and Barney, 1952. Copyright Acoustical Society of America.



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 K-Means
 Clustering
 (https://en.wikipedia.org/wiki/K-means\_clustering)
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**Step 0:** Choose random initial "means"



**Step 1:** Group each token with its closest mean



**Step 2:** Mean = average of its tokens







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Gaussian mixture modeling is like K-means, except that each cluster has a different covariance matrix. Result can be very similar to a natural vowel space.



Fig. 1, "Building a Statistical Model of the Vowel Space for Phoneticians," (c) Matthew Aylett, 1998

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In 1965, Scudder ("Probability of Error of Some Adaptive Pattern-Recognition Machines") considered the following example:

- $Z_1, \ldots, Z_n, \ldots$  is a series of vectors.
- Each vector either contains signal + noise (Z<sub>n</sub> = X + N<sub>n</sub>), or just noise (Z<sub>n</sub> = N<sub>n</sub>).
- The signal, X, is the same every time it appears, but it is unknown.
- The noise,  $N_n$ , is zero-mean Gaussian noise with covariance matrix  $K_N = \sigma^2 I$ .

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Unsupervised Classifier Example

Here are the questions Scudder asked:

- Suppose a classifier was asked to determine whether or not the pattern is present. What it the optimum decision rule?
- Suppose a classifier was trained without any training labels. Can it learn the optimum decision rule?



First, consider the supervised case. We don't know X, but we are given labels:  $\theta_n = 1$  if  $Z_n = X + N_n$ , otherwise  $\theta_n = 0$ . The optimum decision rule turns out to be:

• Update the matched filter covariance estimate:

$$K_{n+1} = \left(K_n^{-1} + \theta_n K_N^{-1}\right)^{-1}$$

• Update the matched filter estimate:

$$H_{n+1} = H_n + K_N^{-1} K_{n+1} (Z_n - H_n) \theta_n$$

• Calculate the log likelihood ratio (LLR):

$$Q_n = Z_n K_n^{-1} Z_n - (Z_n - H_n)^T (K_N + K_n)^{-1} (Z_n - H_n)$$

• Threshold the LLR:

$$\hat{\theta}_n = \begin{cases} 1 & Q_n > \text{threshold} \\ 0 & Q_n \leq \text{threshold} \end{cases}$$

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In the supervised case, as

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ightarrow\infty$  ,

- The matched filter converges  $H_n \rightarrow X$ .
- The matched filter covariance disappears  $K_n \rightarrow 0$
- The LLR converges to a linear function of Z<sub>n</sub>:

$$Q_n \rightarrow 2H_n^T K_N^{-1} Z_n$$
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• The optimal classifier converges to a linear classifier.



Fig. 2, "Probability of Error of Some Adaptive Pattern-Recognition

Machines", (c) IEEE, 1965

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# The Self-supervised Case

Now, consider the self-supervised case. We don't know X, and we don't know  $\theta_n$ . Instead, all we have is our own classifier output,  $\hat{\theta}_n$ , at each time step. Can we learn the optimum classifier?

• Calculate the log likelihood ratio (LLR):

$$Q_n = Z_n K_n^{-1} Z_n - (Z_n - H_n)^T (K_N + K_n)^{-1} (Z_n - H_n)$$

• Threshold the log likelihood ratio:

$$\hat{ heta}_n = \left\{ egin{array}{cc} 1 & Q_n > {
m threshold} \ 0 & Q_n \leq {
m threshold} \end{array} 
ight.$$

• Update the matched filter covariance estimate:

$$K_{n+1} = \left(K_n^{-1} + \hat{\theta}_n K_N^{-1}\right)^{-1}$$

• Update the matched filter estimate:

$$H_{n+1} = H_n + K_N^{-1} K_{n+1} (Z_n - H_n) \hat{\theta}_n$$

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Figure at right shows the **supervised** case. Can we match it using a **self-supervised** learner?

- The n = 0 classifier is still a circle: any small vector is classified as  $\hat{\theta}_n = 0$ , any large vector is classified as  $\hat{\theta}_n = 1$ .
- This is a good thing! Some of the large vectors are, indeed, signals. But not all!



Fig. 2, "Probability of Error of Some Adaptive Pattern-Recognition

Machines", (c) IEEE, 1965

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The self-supervised learner learns a "matched filter,"  $H_n$ , such that

- The hyperplane is  $H_n^T Z_n =$ threshold.
- *H<sub>n</sub>* is the average of all of the *Z* vectors on the right side of the hyperplane.



Fig. 4, "Probability of Error of Some Adaptive Pattern-Recognition

Machines", (c) IEEE, 1965



- The classifier learns to call all big vectors "signal," and all small vectors "noise."
- It is biased: small signal vectors get misclassified as "noise."
- There is a threshold effect: if the noise covariance matrix,  $K_N$ , is too large, then the learner fails to converge.

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- Manifold learning
  - Learn a low-dimensional representation that captures most of the signal variation
- Clustering
  - Classify each token to its nearest mean
  - Recompute each mean as the average of its tokens
- Self-supervised learning
  - The hyperplane is  $H_n^T Z_n =$ threshold.
  - *H<sub>n</sub>* is the average of all of the *Z* vectors on the right side of the hyperplane.