Machine Learning (CSE 446): Unsupervised Learning: Linear Dimensionality Reduction

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Announcements

- Qz section: margins, SVD
- Today:
  Linear diemsionality reduction

Review

Margins, precisely

A linearly separable dataset $D = \langle (\mathbf{x}_n, y_n) \rangle_{n=1}^{N}$. Assume scaling $\|x_n\| \leq 1$.

- Margin of a **particular** $\mathbf{w}$:

$$\text{margin}(\mathbf{w}, D) := \begin{cases} -\infty & \text{if } \mathbf{w} \text{ does not separate D} \\ \min_n y_n \left(\mathbf{w} \cdot \mathbf{x}_n\right) \end{cases}$$

- Geometric Margin (or "maximal" margin): (HW uses this)

$$\gamma = \text{GeometricMargin}(\mathbf{w}, D) := \sup_{\|\mathbf{w}\|=1} \text{margin}(\mathbf{w}, D)$$

- Smallest norm $\|\mathbf{w}_*\|$ at margin 1:

$$\|\mathbf{w}_*\| := \inf_{\mathbf{w} \text{ such that margin}(\mathbf{w}, D)=1} \|\mathbf{w}\|$$

- It holds that $\|\mathbf{w}_*\| = 1/\gamma$.
- The perceptron algorithm makes at most $\|\mathbf{w}_*\|^2$ (or, equivalently, $1/\gamma^2$) mistakes.

Today

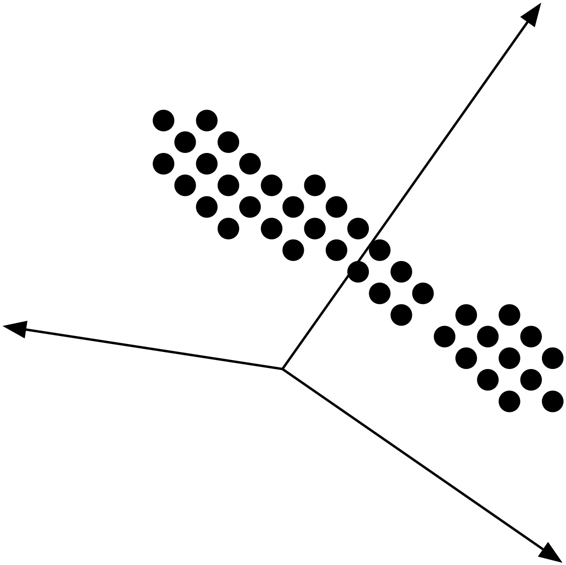
Linear Dimensionality Reduction

As before, you only have a training dataset consisting of $\langle \mathbf{x}_n \rangle_{n=1}^{N}$.

Is there a way to represent each $\mathbf{x}_n \in \mathbb{R}^d$ as a lower-dimensional vector?

(Why would we want to do this?)

Dimension of Greatest Variance



Assume that the data are *centered*,
i.e., that
mean $\left(\langle \mathbf{x}_n \rangle_{n=1}^{N}\right) = \mathbf{0}$.

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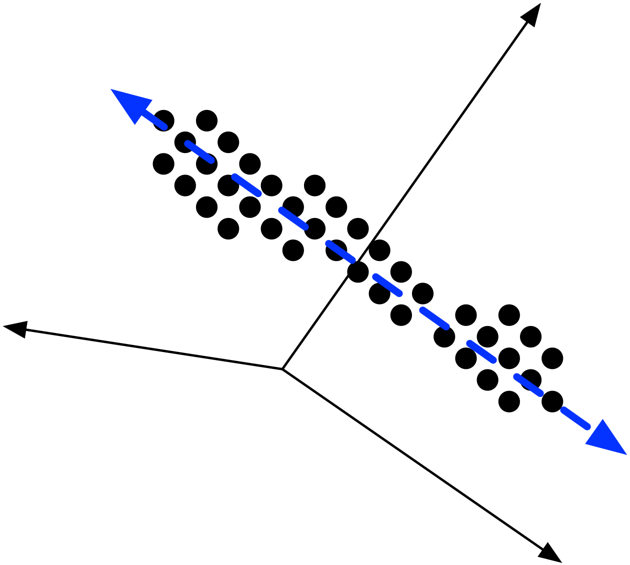

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Projection into One Dimension

Let $\mathbf{u}$ be the dimension of greatest variance, and (without loss of generality) let $\|\mathbf{u}\|_2^2 = 1$.

$p_n = \mathbf{x}_n \cdot \mathbf{u}$ is the projection of the nth example onto $\mathbf{u}$.

Since the mean of the data is $\mathbf{0}$, the mean of $\langle p_1, \ldots, p_N \rangle$ is also 0.

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This implies that the variance of $\langle p_1, \ldots, p_N \rangle$ is $\frac{1}{N} \sum_{n=1}^{N} p_n^2$.

The $\mathbf{u}$ that gives the greatest variance, then, is:

$$\underset{\mathbf{u}}{\operatorname{argmax}} \sum_{n=1}^{N} (\mathbf{x}_n \cdot \mathbf{u})^2$$

(Where did N go?)

Finding the Maximum-Variance Direction

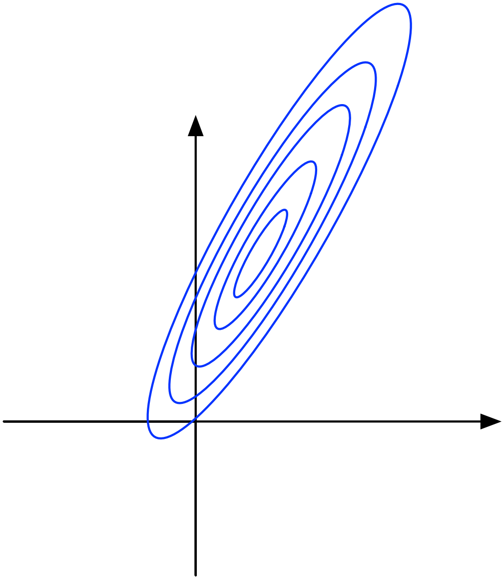
$$\operatorname*{argmax}_{\mathbf{u}} \sum_{n=1}^{N} (\mathbf{x}_n \cdot \mathbf{u})^2$$
$$\text{s.t. } \|\mathbf{u}\|_2^2 = 1$$

(Why do we constrain $\mathbf{u}$ to have length 1?)

If we let $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix}$, then we want: $\operatorname*{argmax}_{\mathbf{u}} \|\mathbf{X}\mathbf{u}\|_2^2$, s.t. $\|\mathbf{u}\|_2^2 = 1$.

2-**This is PCA in one dimension!**

Constrained Optimization



The blue lines represent *contours*: all points on a blue line have the same objective function value.

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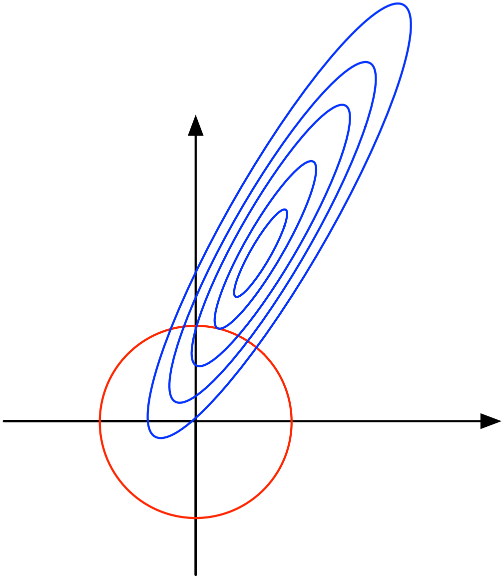

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The red circle is all points with a norm of 1. It represents a constraint like the one we have in the maximum-variance projection problem.

Deriving the Solution

Don't panic.

$$\operatorname*{argmax}_{\mathbf{u}} \|\mathbf{X}\mathbf{u}\|_2^2, \text{ s.t. } \|\mathbf{u}\|_2^2 = 1$$

- The Lagrangian encoding of the problem moves the constraint into the objective:

$$\max_{\mathbf{u}} \min_{\lambda} \|\mathbf{X}\mathbf{u}\|_2^2 - \lambda(\|\mathbf{u}\|_2^2 - 1) \quad \Rightarrow \quad \min_{\lambda} \max_{\mathbf{u}} \|\mathbf{X}\mathbf{u}\|_2^2 - \lambda(\|\mathbf{u}\|_2^2 - 1)$$

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- Gradient (first derivatives with respect to $\mathbf{u}$): $2\mathbf{X}^\top\mathbf{X}\mathbf{u} - 2\lambda\mathbf{u}$
- Setting equal to $\mathbf{0}$ leads to: $\lambda\mathbf{u} = \mathbf{X}^\top\mathbf{X}\mathbf{u}$
- You may recognize this as the definition of an eigenvector ($\mathbf{u}$) and eigenvalue (λ) for the matrix $\mathbf{X}^\top\mathbf{X}$.
- We take the first (largest) eigenvalue.

Projecting into Multiple Dimensions

So far, we've projected each $\mathbf{x}_n$ into one dimension.

To get a second projection $\mathbf{v}$, we solve the same problem again, but this time with another constraint:

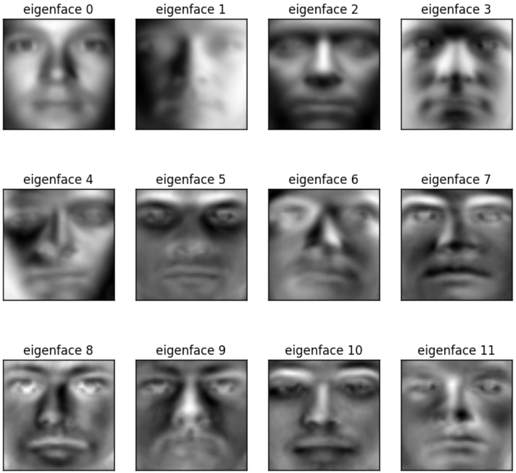
$$\underset{\mathbf{v}}{\text{argmax}} \, \|\mathbf{X}\mathbf{v}\|_2^2, \text{ s.t. } \|\mathbf{v}\|_2^2 = 1 \text{ and } \boxed{\mathbf{u} \cdot \mathbf{v} = 0}$$

(That is, we want a dimension that's orthogonal to the $\mathbf{u}$ that we found earlier.)

Following the same steps we had for $\mathbf{u}$, we can show that the solution will be the *second* eigenvector.

"Eigenfaces"

Fig. from `https://github.com/AlexOuyang/RealTimeFaceRecognition`



Principal Components Analysis

Data: unlabeled data with mean $\mathbf{0}$, $\mathbf{X} = [\mathbf{x}_1 | \mathbf{x}_2 | \cdots | \mathbf{x}_N]^\top$, and dimensionality $K < d$
Result: K-dimensional projection of $\mathbf{X}$
let $\langle \lambda_1, \ldots, \lambda_K \rangle$ be the top K eigenvalues of $\mathbf{X}^\top \mathbf{X}$
  and $\langle \mathbf{u}_1, \ldots, \mathbf{u}_K \rangle$ be the corresponding eigenvectors;
let $\mathbf{U} = [\mathbf{u}_1 | \mathbf{u}_2 | \cdots | \mathbf{u}_K]$;
return $\mathbf{XU}$;

Algorithm 1: PCA

On your own time, you can read up about many algorithms for finding eigenstuff of a matrix.

Alternate View of PCA

Think of $\mathbf{p}_n = \mathbf{x}_n \mathbf{U}$ as a new, K-dimensional representation of $\mathbf{x}_n$.

This means that $\mathbf{p}_n \mathbf{U}^\top \approx \mathbf{x}_n$. The closer these vectors are, the lower our reconstruction error, $\|\mathbf{x}_n - \mathbf{p}_n \mathbf{U}^\top\|_2^2$.

We could have derived PCA by saying that our goal is to minimize the total reconstruction error on the data:

$$\min_{\mathbf{U}} \left\| \mathbf{X} - \mathbf{X}\mathbf{U}\mathbf{U}^\top \right\|_2^2$$
$$\text{s.t. } \mathbf{U}^\top \mathbf{U} = \mathbf{1}$$

Choosing K (Hyperparameter Tuning)

To select K for PCA, you can use the same criteria we discussed for K-Means (BIC and AIC).

PCA and Clustering

There's a unified view of both PCA and clustering.

- K-Means chooses cluster-means so that squared distances to data are small.
- PCA chooses projections so that reconstruction error of data is small.

Both are trying to find a "simple" way to summarize the data; fewer points, or fewer dimensions.

Both could be used to create new features for supervised learning