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

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Administrivia

No office hour for me on Wednesday this week (today is as usual).
No office hour for Kousuke on Tuesday.

Please take the anonymous "quiz" on Canvas to give feedback to Swabha!

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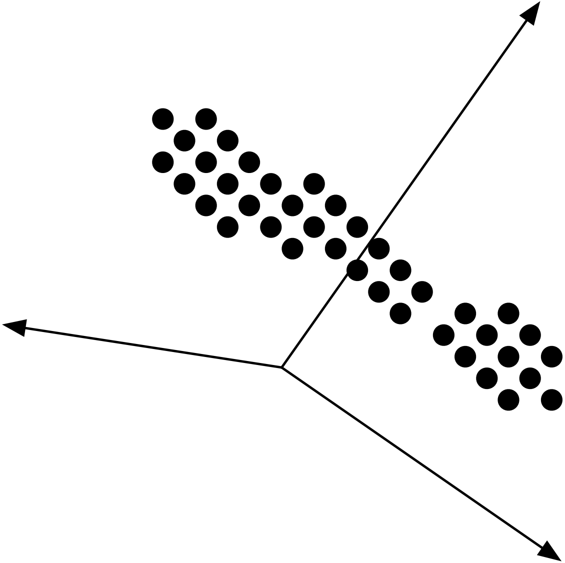
(Why would we want to do this?)

Dimension of Greatest Variance



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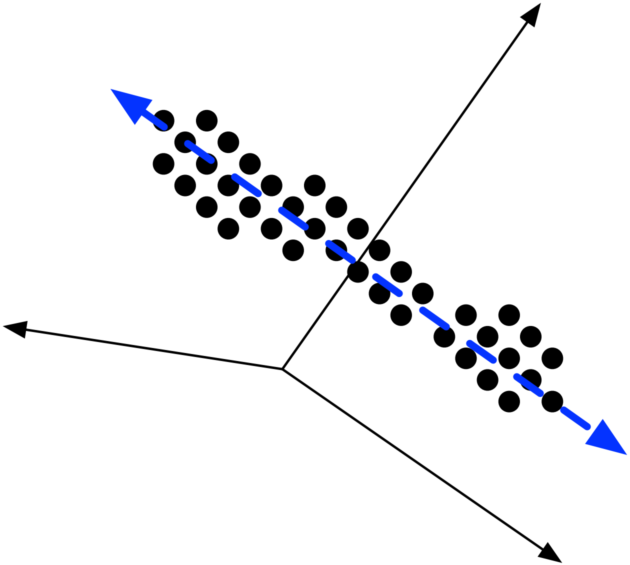

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(Where did N go?)

Finding the Maximum-Variance Direction

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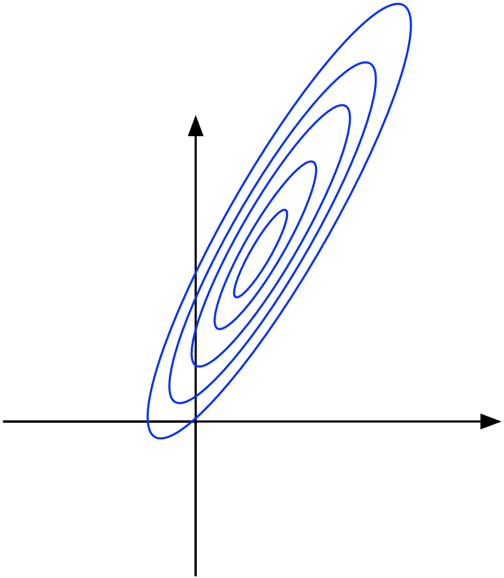
If we let $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix}$, then we want: $\underset{\mathbf{u}}{\operatorname{argmax}} \|\mathbf{X}\mathbf{u}\|_2^2$, s.t. $\|\mathbf{u}\|_2^2 = 1$.

Constrained Optimization



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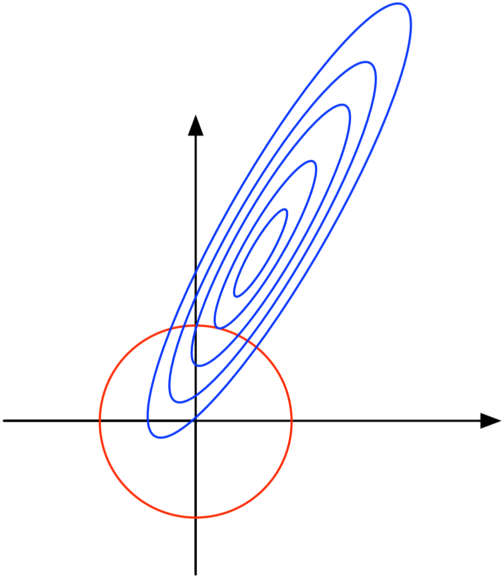

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The red circle is all points with a norm of 1. It represents a constraint like the one we have in the maximum-variance projection problem.

Deriving the Solution

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- We take the first (largest) eigenvalue.

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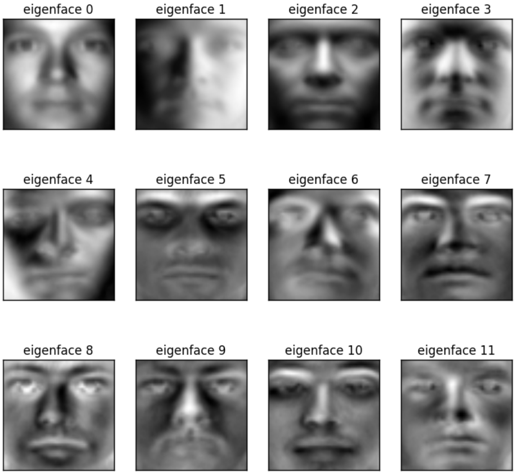
Following the same steps we had for $\mathbf{u}$, we can show that the solution will be the *second* eigenvector.

"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;
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Algorithm 2: PCA

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

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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).

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Both could be used to create new features for supervised learning!

References I

Hal Daume. *A Course in Machine Learning (v0.9)*. Self-published at http://ciml.info/, 2017.