EECS 545: Machine Learning

Lecture 16. Unsupervised Learning: EM & PCA

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3/12/2025

UNIVERSITY OF MICHIGAN

Logistics

- HW4 due 03/18/25
- Project progress report due 03/14/25
- See project information document for detailed info

Additional tips: Recommended content in the report

- Dataset and/or data collection
- Pre-processing
- Feature representation
- Pipeline of the method
- Initial results
  - Tables
  - Plots
  - Figures (e.g., qualitative examples)
  - Visualization of results/models
- Hyperparameters and how they were tuned
  - make it clear how you performed cross-validation (hold-out CV, or K-fold CV, etc.)
  - For hold-out CV, specify whether you separated training, validation, and test set
  - For K-fold CV, specify K value.
- Error and failure case analysis
- Summary and future work

In your project progress report, please include the following:

- Project Title
  - Please put a specific and informative title (that describes what your project is about)
  - For example, “545 Project Progress Report” is NOT a specific and informative title
- Team members (* Please put these at the beginning of your report)
  - Please specify the full name and email addresses in uniquename@umich.edu
  - You can specify the names and emails as the following format
    - author1, author2, author3, …, authorN
    - {email1, email2, …, emailN}@umich.edu
- Abstract (1 paragraph)
- Section 1. Introduction:
  - Problem description and motivation.
  - Why do you want to solve this problem?
  - What's the impact if you can solve this problem?
- Section 2. Proposed method:
  - How are you going to solve this problem?
  - Why should the proposed method work?
  - Provide explanations/rationale of why you chose this specific method
  - Provide technical details of your approach if you are proposing a novel method.
  - Description of the pipeline. Including a figure (e.g., block diagram) that explains the pipeline will be very helpful
- Section 3. Related work:
  - What are existing methods?
  - What are the state-of-the-art methods for this problem?
  - How is your approach similar to other existing work?
  - How is your approach different from the related work?
- Section 4. (Preliminary) Experimental results:
  - Milestones achieved so far (add all relevant experimental results).
  - How do these results support your claim?
- Section 5. Future milestones: Dates and sub-goals (please set sub-goals on a weekly basis so that they can be done in a week)
- Section 6. Conclusion: Summary of your progress and your final expected goal (what do you expect to achieve or demonstrate for the final project?)
- Author Contributions
  - Please see the guideline “Contribution of each team member” below
- References

Outline

Unsupervised Learning for Clustering:

- Recap: Expectation Maximization
- Gaussian Mixtures with EM (derivation)

Unsupervised Learning for Finding Subspace:

- Principal Component Analysis (PCA)
- Probabilistic PCA
- Kernel PCA

Expectation Maximization

(Recap) Expectation Maximization

- Parameter learning for latent variable models: when the data is not fully observed.
  - **X**: observed variables, **Z**: hidden (latent) variables
- Main idea:

  (E-step) Run inference about **Z** given **X**: $q(\mathbf{Z}) = p(\mathbf{Z} \mid \mathbf{X}, \theta)$

  (M-step) Update parameters by treating *q* as observation (i.e., fractional pseudo-counts)!

  $$\text{argmax}_\theta \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\theta)$$

- Example:
  - K-means (a special case of Gaussian mixtures)
  - Gaussian mixtures

The EM Algorithm in a nutshell

- Variational lower bound on the data likelihood:

$$\log p(\mathbf{X} \mid \theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z} \mid \theta)}{q(\mathbf{Z})} + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{q(\mathbf{Z})}{p(\mathbf{Z} \mid \mathbf{X}, \theta)}$$
$$= \mathcal{L}(q, \theta) + KL(q(\mathbf{Z}) \,\|\, p(\mathbf{Z}|\mathbf{X}, \theta))$$
$$\geq \mathcal{L}(q, \theta)$$

Evidence Lower bound (ELBO) or variational lower bound

with equality holding if and only if $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta)$

- **EM algorithm**:

  * E: expectation
  * M: maximization

  Repeat alternating optimization until convergence:
  - E-step: for fixed θ, find q that maximizes $\mathcal{L}(q, \theta)$
  - M-step: for fixed q, find θ that maximizes $\mathcal{L}(q, \theta)$

Note: For M-step, we need to sum the lower bound for all the training samples. See later slides.

(Recap) The EM Algorithm: E-step

- Variational lower bound on the data likelihood:

$$\log p(\mathbf{X} \mid \theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z} \mid \theta)}{q(\mathbf{Z})} + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{q(\mathbf{Z})}{p(\mathbf{Z} \mid \mathbf{X}, \theta)}$$

$$= \mathcal{L}(q, \theta) + KL(q(\mathbf{Z}) \,\|\, p(\mathbf{Z}|\mathbf{X}, \theta))$$

$$\geq \mathcal{L}(q, \theta)$$

Evidence Lower bound (ELBO) or variational lower bound

with equality holding if and only if $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta)$

- **(E-step)** For a fixed θ, which q maximizes $\mathcal{L}(q, \theta)$?

$\Rightarrow p(\mathbf{Z} \mid \mathbf{X})$, because all other q would make $\mathcal{L}(q, \theta)$ strictly less than $\log p(\mathbf{X} \mid \theta)$

(Recap) The EM Algorithm: M-step

- We also note that for a fixed q, the $\mathcal{L}(q, \theta)$ term can be decomposed into two terms:

$$\begin{aligned}\mathcal{L}(q, \theta) &= \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z} \mid \theta)}{q(\mathbf{Z})} \\ &= \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} \mid \theta) - \sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})\end{aligned}$$

  - (1) A weighted sum of log $p(\mathbf{X}, \mathbf{Z}|\theta)$.
    This is tractable and can be optimized w.r.t θ
  - (2) Entropy of $q(\mathbf{Z})$ which is independent of θ since q is fixed.

- **(M-step)** Thus, when q is fixed, we can find θ that maximizes $\mathcal{L}(q, \theta)$.

The EM Algorithm: summary

- Initialize parameters θ randomly
- Repeat until convergence:

  (optimize $\mathcal{L}(q, \theta)$ w.r.t. q and θ alternatingly.)
  - "E-step": Set $q(\mathbf{Z}) = p(\mathbf{Z} \mid \mathbf{X}, \theta)$ compute posterior → optimal q(Z)!
  - "M-step": Update θ via the following maximization

$$\text{argmax}_\theta \; \mathcal{L}(q, \theta) = \text{argmax}_\theta \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta)$$

use *q*(Z) as (factional) pseudo-counts and maximize the "data completion" log-likelihood

- Note we have assumed that $p(\mathbf{Z} \mid \mathbf{X}, \theta)$ is tractable (i.e., find exact posterior $p(\mathbf{Z} \mid \mathbf{X}, \theta)$) . Q. What if it is not?

The EM Algorithm: Multiple data-points

- Variational lower bound for a single example $\mathbf{x}$:

$$\log p(\mathbf{x}|\theta) = \sum_{\mathbf{z}} q(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}|\theta)}{q(\mathbf{z})} + KL(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \theta))$$
$$\geq \sum_{\mathbf{z}} q(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}|\theta)}{q(\mathbf{z})}$$

- Lower bound on the log-likelihood of the *entire* training data $\mathcal{D} = \{\mathbf{x}^{(1)}, ..., \mathbf{x}^{(N)}\}$:

$$\log p(\mathcal{D}|\theta) = \sum_n \log p(\mathbf{x}^{(n)}|\theta) = \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}^{(n)}|\theta)}{q^{(n)}(\mathbf{z})} + \sum_n KL(q^{(n)}(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}^{(n)}, \theta))$$
$$\geq \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}^{(n)}|\theta)}{q^{(n)}(\mathbf{z})}$$

Note that different $q^{(n)}$ is used for each n

The EM Algorithm: Multiple data-points

$$\log p(\mathcal{D}|\theta) = \sum_n \log p(\mathbf{x}^{(n)}|\theta) = \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}^{(n)}|\theta)}{q^{(n)}(\mathbf{z})} + \sum_n KL(q^{(n)}(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}^{(n)}, \theta))$$

$$\geq \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}^{(n)}|\theta)}{q^{(n)}(\mathbf{z})}$$

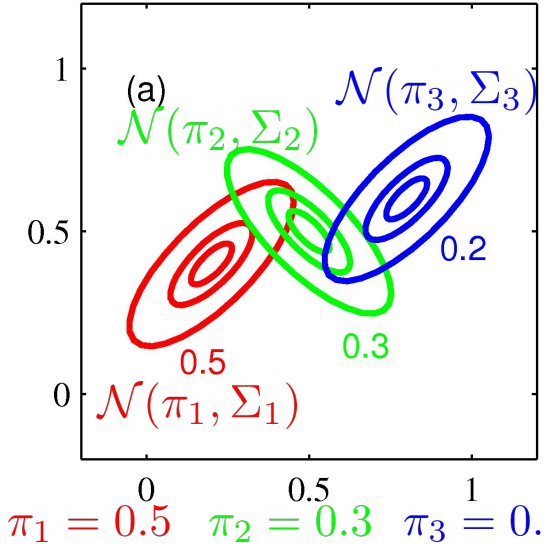
- Initialize random parameters θ
- Repeat until convergence:
  - "**E-step**": Set $q^{(n)}(\mathbf{z}) = p(\mathbf{z} \mid \mathbf{x}^{(n)}, \theta)$, for each training sample n.
  - "**M-step**": Update θ via the following maximization:

$$\arg\max_\theta \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}^{(n)} \mid \theta)$$

Mixtures of Gaussians (recap)

- Let **z** in $\{0,1\}^K$ be a 1-of-*K* random variable;

$$p(z_k = 1) = \pi_k \qquad \sum_{k=1}^{K} \pi_k = 1$$



- Generate **x** from Gaussian given the selected cluster assignment **z**

$$p(\mathbf{x} \mid z_k = 1) = \mathcal{N}(\mathbf{x} \mid \mu_k, \Sigma_k)$$

$$p(\mathbf{x}, \mathbf{z}) = \pi_k \mathcal{N}(\mathbf{x} | \mu_k, \Sigma_k)$$

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x} \mid \mu_k, \Sigma_k)$$

Summary: EM for Gaussian Mixtures

- Initialize parameters randomly $\theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$
- Repeat until convergence (alternating optimization)
  - E Step: Given fixed parameters θ, set $q^{(n)}(\mathbf{z}) = p(\mathbf{z} \mid \mathbf{x}^{(n)}, \theta)$

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)} | \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}^{(n)} | \mu_j, \Sigma_j)} = P(z_k = 1 | \mathbf{x}^{(n)})$$

  - M Step: Given fixed $q(\mathbf{z}^{(n)})$'s for $\mathbf{x}^{(n)}$'s (or $\gamma(z_{nk})$), update θ:

$$\pi_k^{\text{new}} = \frac{N_k}{N} = \frac{\sum_n \gamma(z_{nk})}{N}$$

$$\arg\max_\theta \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}^{(n)} \mid \theta)$$

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) \mathbf{x}^{(n)}$$

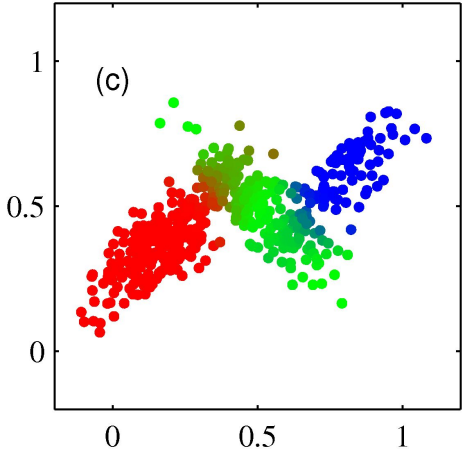
$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) (\mathbf{x}^{(n)} - \mu_k^{\text{new}})(\mathbf{x}^{(n)} - \mu_k^{\text{new}})^\top$$

Mixtures of Gaussians: E-step

- Need to calculate $p(\mathbf{Z} \mid \mathbf{X}, \theta)$, i.e., *soft assignments*
- Responsibility is the degree (posterior prob.) to which each Gaussian explains an observation **X**.

Q. Verify this! (Hint: Use Bayes Rule)

$$q^{(n)}(\mathbf{z}_k) = p(\mathbf{z}_k|\mathbf{x}^{(n)}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} =: \gamma(\mathbf{z}_{nk})$$



Mixtures of Gaussians: M-step

General formula for M-step:

$$\arg\max_\theta \ \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}^{(n)} \mid \theta)$$

Plug in for GMM: $\theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k \mid k \in \{1 \dots K\}\}$

$$\operatorname{argmax}_{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}} \quad \underbrace{\sum_{n=1}^{N} \sum_{k=1}^{K} q^{(n)}(\mathbf{z}_k) \log p(\mathbf{z}_k, \mathbf{x}^{(n)} | \pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{= J(\pi, \boldsymbol{\mu}, \boldsymbol{\Sigma})}$$

$$\text{s.t.} \sum_{k=1}^{K} \pi_k = 1$$

Mixtures of Gaussians: M-step

Let's first simplify the expression $J(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$
\begin{aligned}
J(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) &= \sum_{n=1}^{N} \sum_{k=1}^{K} q^{(n)}(\mathbf{z}_k) \log p(\mathbf{z}_k, \mathbf{x}^{(n)} \mid \pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \left(\log \pi_k + \log \frac{1}{(2\pi)^{m/2} (\det \boldsymbol{\Sigma}_k)^{1/2}} - \frac{1}{2} (\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) \right) \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k - \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \left((2\pi)^{m/2} (\det \boldsymbol{\Sigma}_k)^{1/2} \right) \\
&\qquad - \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) (\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k - \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \det \boldsymbol{\Sigma}_k \\
&\qquad - \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) (\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) + \text{ const}
\end{aligned}
$$

Mixtures of Gaussians: M-step

$$J(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k - \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \det \boldsymbol{\Sigma}_k$$
$$- \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) + \text{ const}$$

- Maximize *J* w.r.t. $\boldsymbol{\mu}_k$ by differentiating w.r.t. $\boldsymbol{\mu}_k$ and setting the gradient to 0:

$$\frac{\partial J}{\partial \boldsymbol{\mu}_k} = \sum_{n=1}^{N} \gamma(\mathbf{z}_{nk}) \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) = 0$$

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk}) \mathbf{x}^{(n)}}{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})}$$

Mixtures of Gaussians: M-step

$$J(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k - \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \det \boldsymbol{\Sigma}_k$$
$$- \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) + \text{ const}$$

- To find $\boldsymbol{\Sigma}_k$, we use change of variables: $\mathbf{M}_k = \boldsymbol{\Sigma}_k^{-1}$

$$J(\boldsymbol{\pi}, \boldsymbol{\mu}, \mathbf{M}) = \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k + \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \det \mathbf{M}_k$$
$$- \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \mathbf{M}_k(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) + \text{ const}$$

Mixtures of Gaussians: M-step

$$J(\boldsymbol{\pi}, \boldsymbol{\mu}, \mathbf{M}) = \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k + \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log\det \mathbf{M}_k$$
$$- \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top \mathbf{M}_k(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) + \text{ const}$$

- Maximize *J* w.r.t. $\mathbf{M}_k$ by differentiating w.r.t. $\mathbf{M}_k$ and setting the gradient to 0:

*Note: $\frac{\partial \log|\det \mathbf{X}|}{\partial \mathbf{X}} = (\mathbf{X}^{-1})^\top$ $\frac{\partial \mathbf{a}^\top \mathbf{X}\mathbf{b}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{b}^\top$

$$\frac{\partial J}{\partial \mathbf{M}_k} = \frac{1}{2}\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})\mathbf{M}_k^{-1} - \frac{1}{2}\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top = 0$$

$$\boldsymbol{\Sigma}_k = \mathbf{M}_k^{-1} = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top}{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})}$$

Mixtures of Gaussians: M-step

$$J(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(\mathbf{z}_{nk})\log\pi_k - \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(\mathbf{z}_{nk})\log\det\boldsymbol{\Sigma}_k$$
$$- \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top\boldsymbol{\Sigma}_k^{-1}(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k) + \text{ const}$$

- Finally we need: $\max_{\boldsymbol{\pi}} \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(\mathbf{z}_{nk})\log\pi_k \quad \text{s.t.} \sum_{k=1}^{K}\pi_k = 1$
- Use Lagrange multipliers

$$L(\boldsymbol{\pi}, \alpha) = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(\mathbf{z}_{nk})\log\pi_k - \alpha\left(\sum_{k=1}^{K}\pi_k - 1\right)$$

Mixtures of Gaussians: M-step

- Finally we need: $\max_{\boldsymbol{\pi}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k \quad \text{s.t.} \sum_{k=1}^{K} \pi_k = 1$
- Use Lagrange multipliers

$$L(\boldsymbol{\pi}, \alpha) = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(\mathbf{z}_{nk}) \log \pi_k - \alpha \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

- Setting $\frac{\partial L}{\partial \pi_k} = \sum_{n=1}^{N} \gamma(\mathbf{z}_{nk}) \frac{1}{\pi_k} - \alpha = 0$ gives $\pi_k = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})}{\alpha}$
- Using the constraint $\sum_{k=1}^{K} \pi_k = 1$, we get:

$$\pi_k = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})}{\sum_{k=1}^{K} \sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})} = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})}{N}$$

Mixtures of Gaussians: M-step
(putting together)

- The mean of a cluster is the weighted mean, weighted by the responsibilities.

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk}) \mathbf{x}^{(n)}}{N_k}$$

[N_k = sum of pseudo-counts γ_{nk} over n.]

  - N_k is the effective number of points in cluster *k*

$$N_k = \sum_{n=1}^{N} \gamma(\mathbf{z}_{nk}) \qquad \pi_k = \frac{N_k}{N}$$

- Likewise for covariance:

$$\boldsymbol{\Sigma}_k = \frac{\sum_{n=1}^{N} \gamma(\mathbf{z}_{nk})(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k)^\top}{N_k}$$

EM for Gaussian Mixtures: Summary

- Initialize means, covariances, and mixing coefficients for the *K* Gaussians.
- E Step: Given the parameters, evaluate the responsibilities or the posterior

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\mu_j, \Sigma_j)} = P(z_k = 1|\mathbf{x}^{(n)})$$

EM for Gaussian Mixtures: Summary

- M Step: Given the responsibilities, re-evaluate the coefficients.

$$\pi_k^{\text{new}} = \frac{N_k}{N} = \frac{\sum_n \gamma(z_{nk})}{N}$$

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}^{(n)}$$

$$\sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}^{(n)} - \mu_k^{\text{new}})(\mathbf{x}^{(n)} - \mu_k^{\text{new}})^\top$$

- Stop when either coefficients or log likelihood converges.

Summary: EM for Gaussian Mixtures

- Initialize parameters randomly $\theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$
- Repeat until convergence (alternating optimization)
  - E Step: Given fixed parameters θ, set $q^{(n)}(\mathbf{z}) = p(\mathbf{z} \mid \mathbf{x}^{(n)}, \theta)$

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)} | \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}^{(n)} | \mu_j, \Sigma_j)} = P(z_k = 1 | \mathbf{x}^{(n)})$$

  - M Step: Given fixed $q(\mathbf{z}^{(n)})$'s for $\mathbf{x}^{(n)}$'s (or $\gamma(z_{nk})$), update θ:

$$\pi_k^{\text{new}} = \frac{N_k}{N} = \frac{\sum_n \gamma(z_{nk})}{N}$$

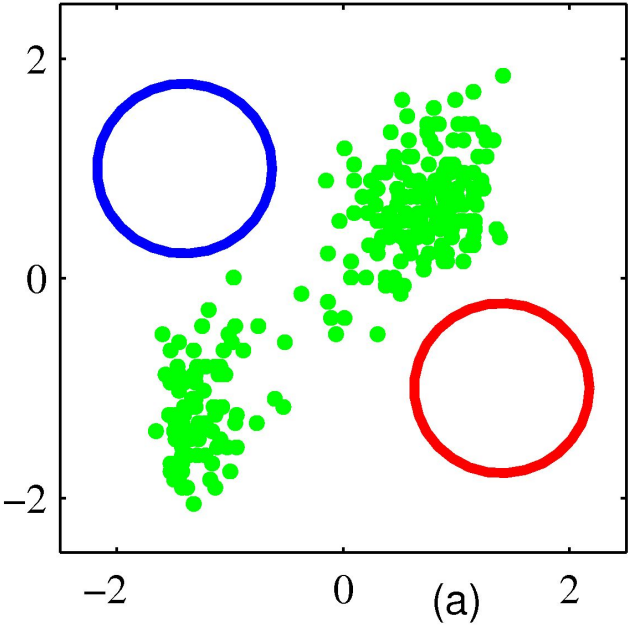
$$\arg\max_\theta \sum_n \sum_{\mathbf{z}} q^{(n)}(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}^{(n)} \mid \theta)$$

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) \mathbf{x}^{(n)}$$

$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) (\mathbf{x}^{(n)} - \mu_k^{\text{new}})(\mathbf{x}^{(n)} - \mu_k^{\text{new}})^\top$$

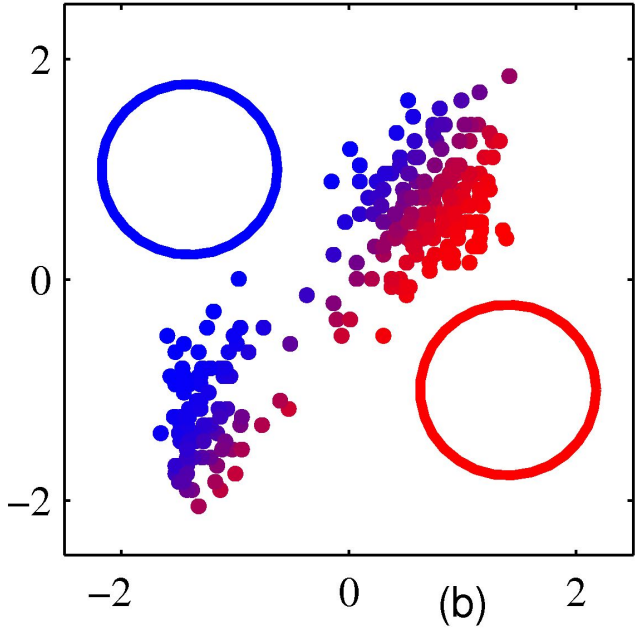
EM Example

- Initialize parameters: means, covariances, and mixing coefficients.



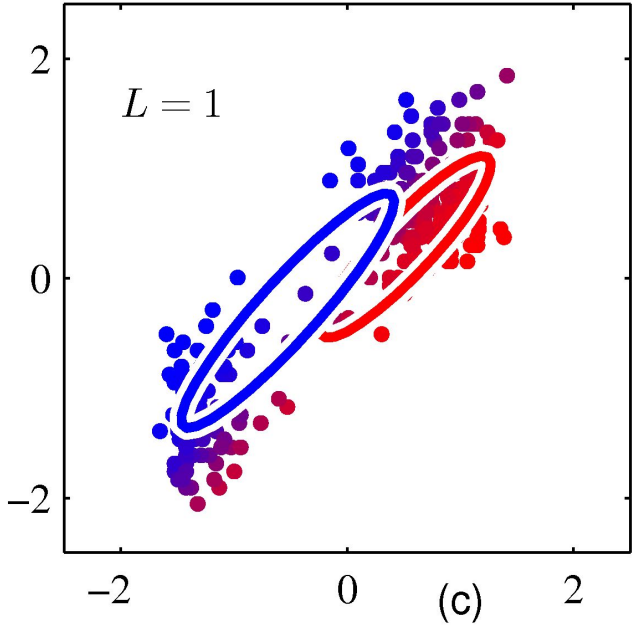
EM Example

- First E Step



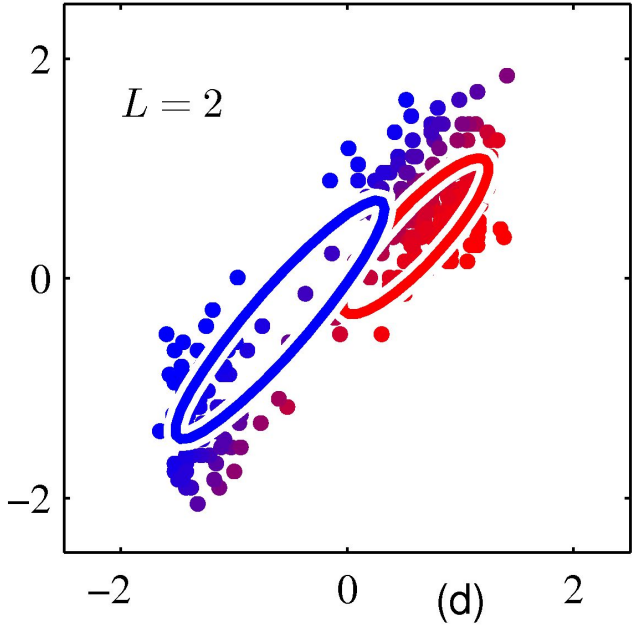
EM Example

- First M Step



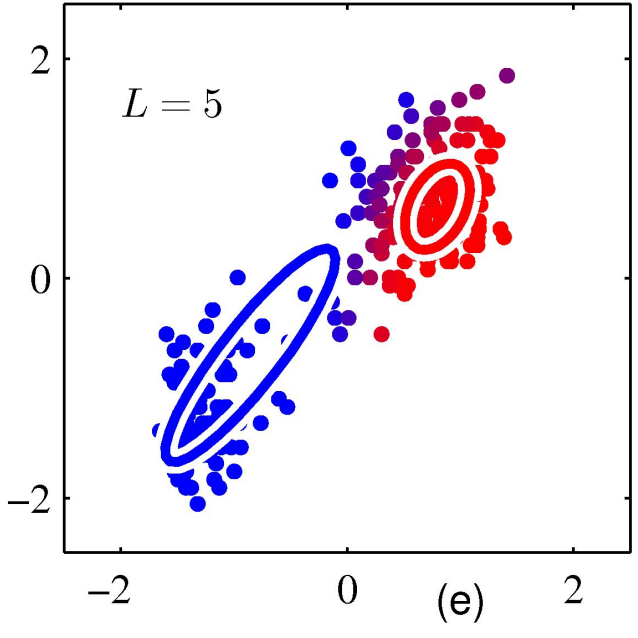
EM Example

- Second E and M Steps



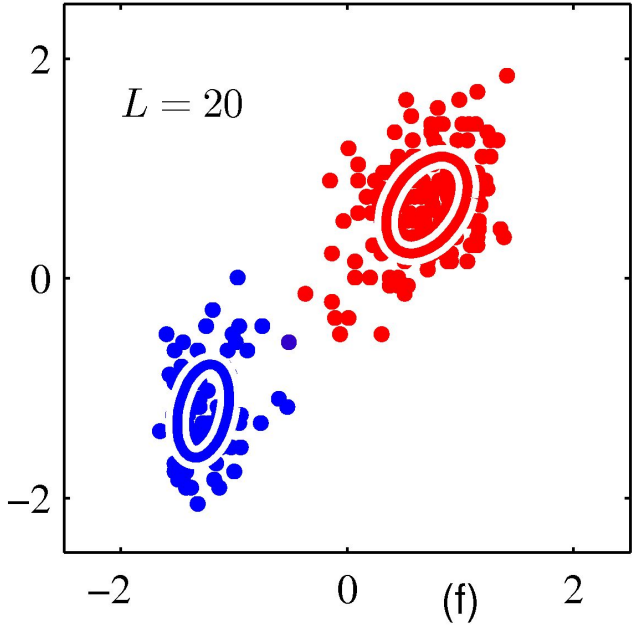
EM Example

- Three more E-M cycles



EM Example

- Fifteen E-M cycles later



Summary: Expectation Maximization

Core Idea:

- Iterative method for parameter estimation with hidden data (latent variables).
- Finds maximum likelihood estimates (local optimum) via EM.

Steps: (alternating optimization until convergence)

- **E-Step:** Estimate the posterior probability (expected value) of latent variables.
- **M-Step:** Maximize the “expected” likelihood to update parameters.

Key Points:

- Converges to a local optimum (initialization matters).
- Commonly used in clustering (e.g., Gaussian Mixture Models) and other models with missing data.

Summary: K-Means vs Gaussian Mixtures

K-means:

- Clusters data by minimizing within-cluster variance.
- Hard assignments; best for spherical, similar-sized clusters.
- Fast, but sensitive to initialization.

Gaussian Mixture Models (GMM):

- Models data as a mix of Gaussian distributions via EM.
- Soft assignments; handles elliptical, overlapping clusters.
- More flexible yet computationally intensive.
- K-means can be shown to be a special case of GMM

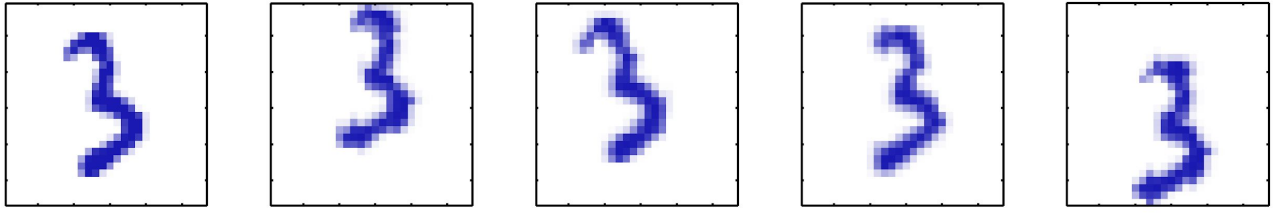
Key Considerations:

- Both need pre-specified # clusters and careful initialization.
- Use K-means for speed; choose GMM for probabilistic clustering or probabilistic modeling of data.

Principal Component Analysis (PCA)

High-Dimensional Data

- ... may have low-dimensional structure.



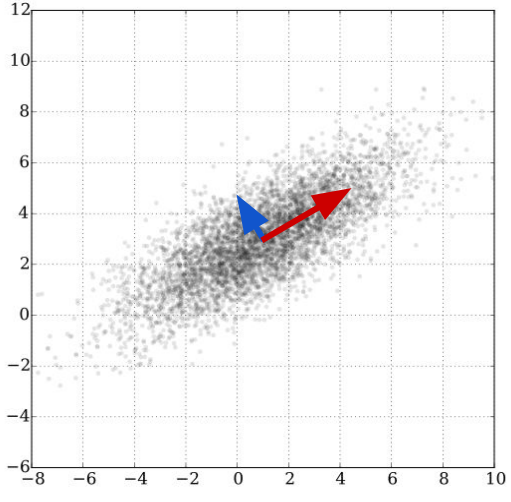
(above: images of digit “3” via translations and rotations)

- The data is 100x100-dimensional.
- But there are only three degrees of freedom, so it lies on a 3-dimensional subspace (x, y, angle).
  - (on a non-linear manifold, in this case)

Principal Component Analysis

- Given a set of $\{\mathbf{x}^{(n)}\}_{n=1,\ldots,N}$ of observations
  - in a space of dimension *D*, i.e., $\mathbf{x}^{(n)} \in \mathbb{R}^D$
  - find a subspace of dimension $M < D$
  - that captures most of its *variability*. (i.e., approximate $x^{(n)}$'s using principal components as basis vectors)

2nd principal component



1st principal component (largest variance)

Image source: Wikipedia

Principal Component Analysis

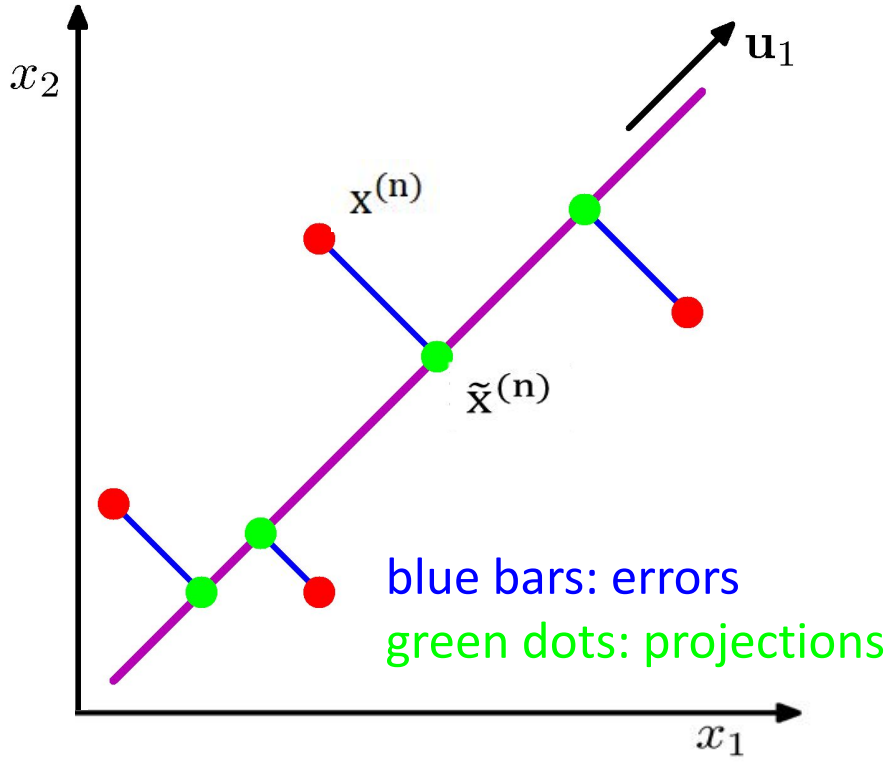
- Given a set of $\{\mathbf{x}^{(n)}\}_{n=1,\ldots,N}$ of observations
  - in a space of dimension *D*,
  - find a subspace of dimension *M* < *D*
  - that captures most of its *variability*. (i.e., approximate $x^{(n)}$'s using principal components as basis vectors)
- PCA can be described as either:
  - maximizing the variance of the projection, or
  - minimizing the squared approximation error.
  - (both are equivalent; see the next slide)

Two Descriptions of PCA

Approximate the data with *projection*

(i.e., for each $x^{(n)}$, find closest point on on the subspace spanned by principal components):

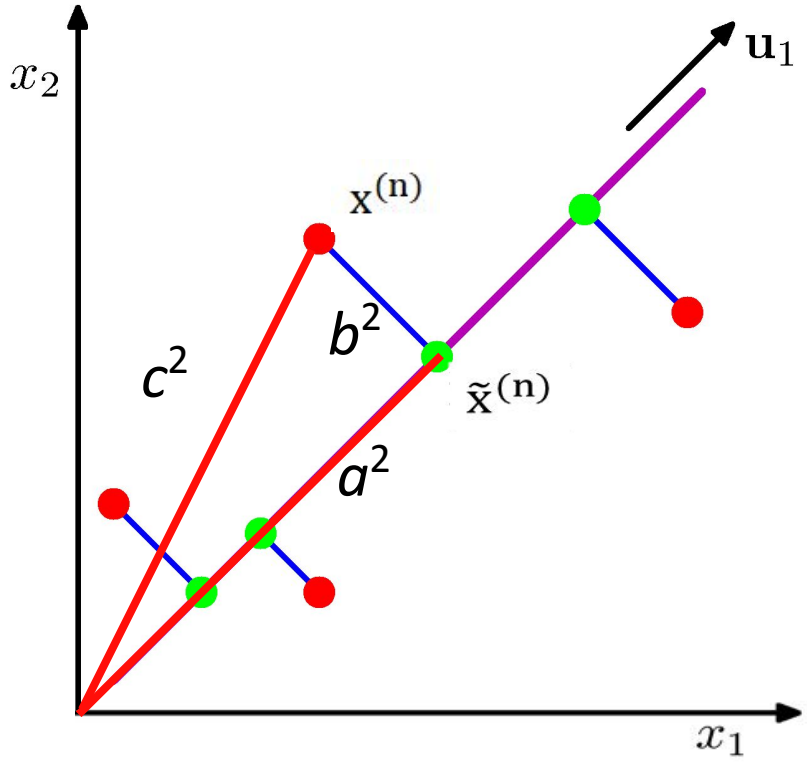
- Maximize variance, or
- Minimize squared error



Main idea: We want to find a basis vector (e.g. $\mathbf{u}_1$) (= principal component) that does the best approximation or best preserves the variance when projected

Equivalent Descriptions

- With mean at the origin $c_i^2 = a_i^2 + b_i^2$
- With constant $\sum_i c_i^2$
  - Minimizing $\sum_i b_i^2$
  - Maximizes $\sum_i a_i^2$
  - … and vice versa



Note: without loss of generality, here we assume that the input data x has zero mean.

First Principal Component

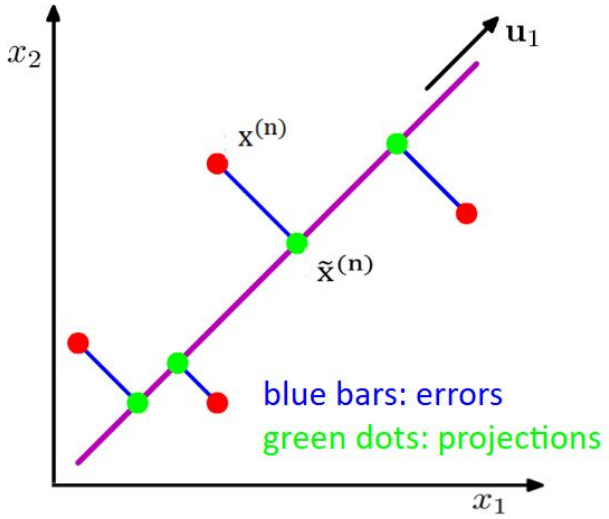
- Given data points $\{\mathbf{x}^{(n)}\}$ in a D-dim space,
  - Mean $\overline{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}^{(n)}$
  - Data covariance $\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}^{(n)} - \overline{\mathbf{x}})(\mathbf{x}^{(n)} - \overline{\mathbf{x}})^{\top}$

D x D matrix

First Principal Component

- Given data points $\{\mathbf{x}^{(n)}\}$ in a D-dim space,
- Let $\mathbf{u}_1$ be the PC maximizing variance of projection:
  - It should have length 1: $\mathbf{u}_1^\top \mathbf{u}_1 = 1$
  - Projection of $\mathbf{x}^{(n)}$ to $\mathbf{u}_1$ subspace:

$$(\mathbf{u}_1^\top \mathbf{x}^{(n)})\mathbf{u}_1$$



- Remark: More generally, projection of $\mathbf{x}^{(n)}$ to subspace spanned by $\mathbf{u}_1,\ldots,\mathbf{u}_M$:

$$\sum_{j=1}^{M} (\mathbf{u}_j^\top \mathbf{x}^{(n)})\mathbf{u}_j$$

First Principal Component

- Maximize the projection variance:

$$\frac{1}{N}\sum_{n=1}^{N}(\mathbf{u}_1^\top \mathbf{x}^{(n)} - \mathbf{u}_1^\top \overline{\mathbf{x}})^2 = \mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1$$

- Use a Lagrange multiplier to enforce $\mathbf{u}_1^\top \mathbf{u}_1 = 1$
- Maximize: $\mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1 + \lambda_1(1 - \mathbf{u}_1^\top \mathbf{u}_1)$

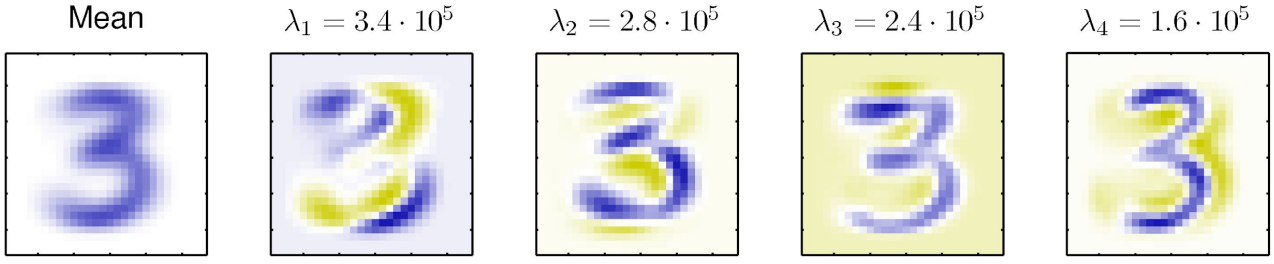
- Derivative is zero when $\mathbf{S}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$
  - That is, $\mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1 = \lambda_1$
- So $\mathbf{u}_1$ is eigenvector with largest eigenvalue.

PCA by Maximizing Variance

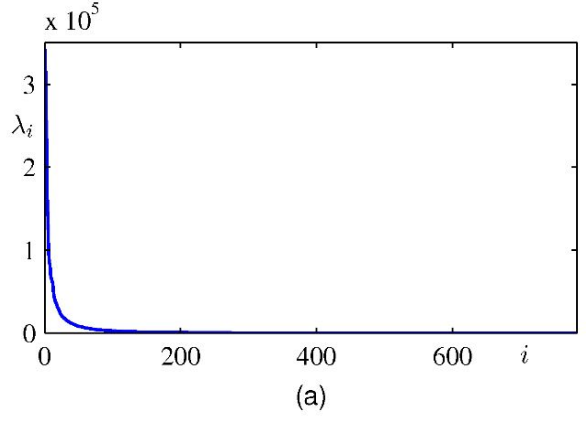
- Repeat to find the *M* eigenvectors of the data covariance matrix **S** corresponding to the *M* largest eigenvalues.
  - The *total variance* is the sum of variances of all individual principal components
  - Principal components are orthogonal to each other
- We can also do the same thing from a "minimizing (projection) squared error" viewpoint.

Digit Image Example

- The mean and first four PCA eigenvectors.

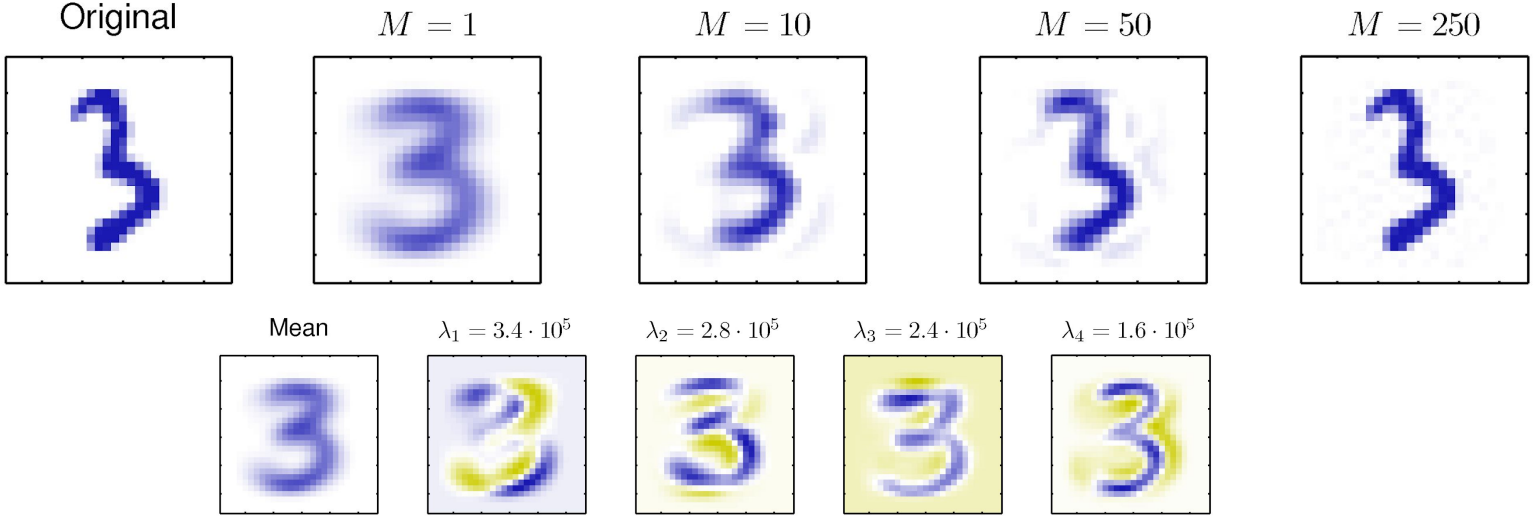


- The eigenvalue spectrum:



Reconstructing the Image

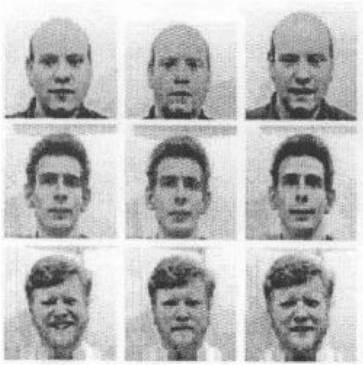
- Compress the image representation by using only first M eigenvectors, and discarding the less important information.



Learning features via PCA

- Example: Eigenfaces

Training face images



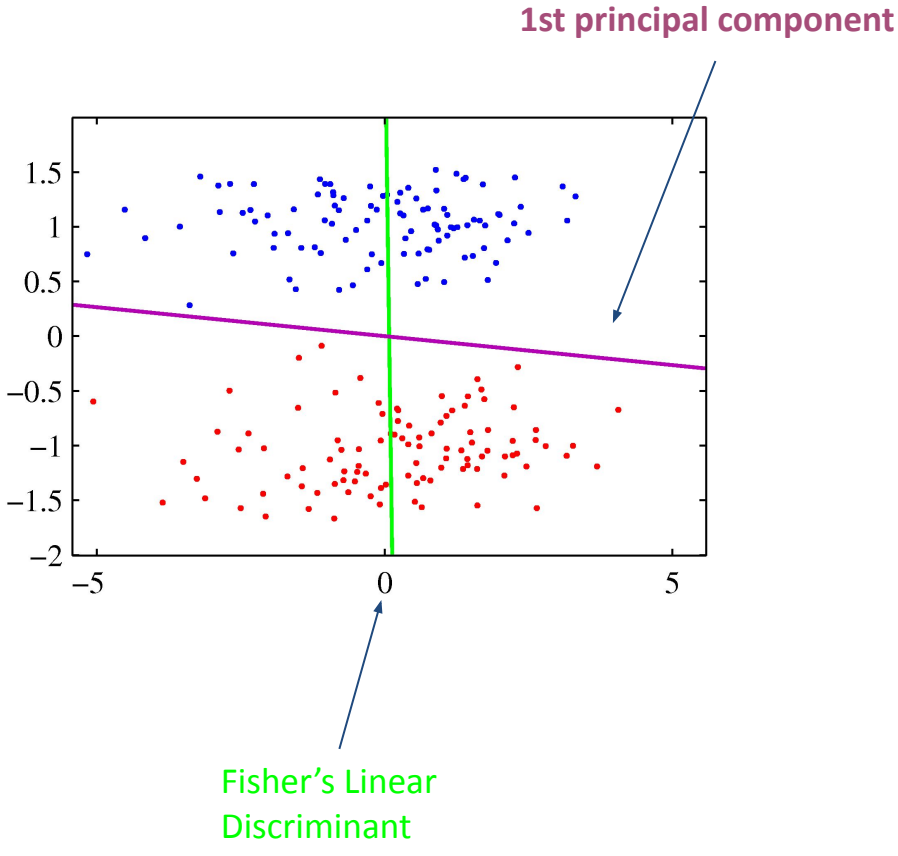
Learned PCA bases

Test example

Images from www.cse.unr.edu/~bebis/CS485/Lectures/Eigenfaces.ppt

Limits to PCA

- Maximizing variance is not always the best way to make the structure visible.
- PCA vs Fisher's linear discriminant



Probabilistic PCA

- We can view PCA as solving a probabilistic latent variable problem.
- Describe a distribution $p(\mathbf{x})$ in *D*-dimensional space, in terms of a latent variable $\mathbf{z}$ in *M*-dimensional space.

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon} \qquad p(\mathbf{z}) = \mathcal{N}(\mathbf{z} \mid \mathbf{0}, \mathbf{I}) \qquad \epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$$

- **W** is a *D* by *M* linear transformation from **z** to **x**

$$p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mathbf{x} \mid \mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$

Probabilistic PCA

- Given the generative model

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

- we can infer

$$\mathbb{E}[\mathbf{x}] = \mathbb{E}[\mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}] = \boldsymbol{\mu}$$

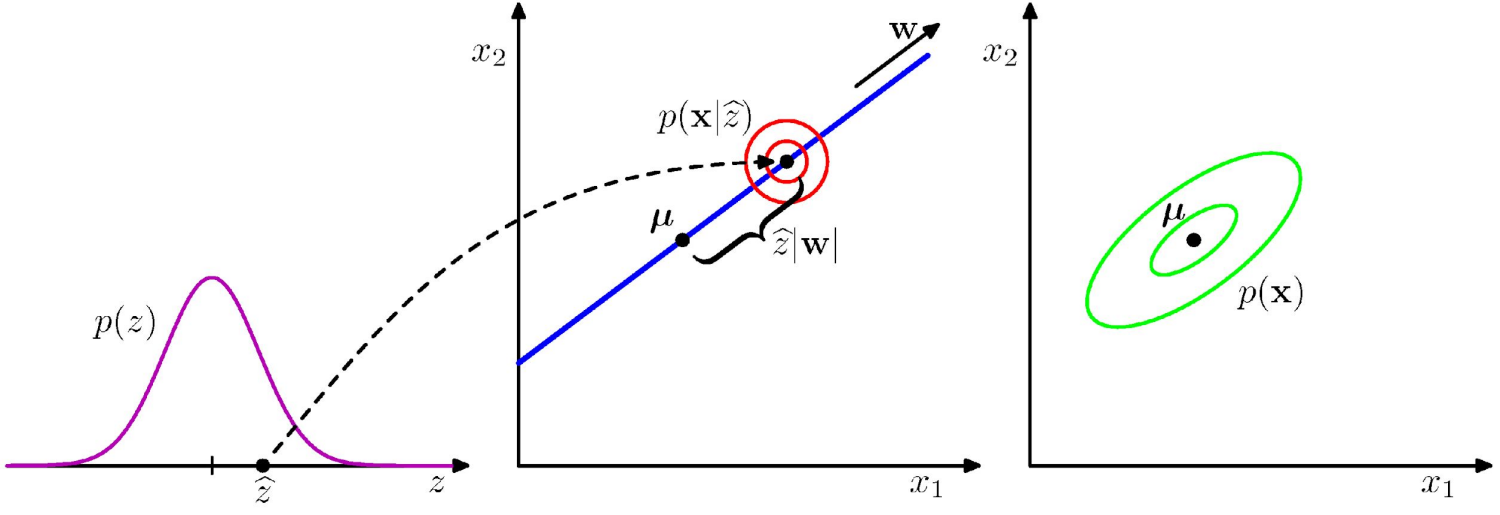
$$\begin{aligned} \mathrm{cov}[\mathbf{x}] &= \mathbb{E}[(\mathbf{W}\mathbf{z} + \boldsymbol{\epsilon})(\mathbf{W}\mathbf{z} + \boldsymbol{\epsilon})^\top] \\ &= \mathbb{E}[\mathbf{W}\mathbf{z}\mathbf{z}^\top\mathbf{W}^\top] + \mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top] = \mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I} \end{aligned}$$

Probabilistic PCA

- The generative model

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

can be illustrated as:



Likelihood of Probabilistic PCA

- (Marginal) likelihood:

$$\log p(\mathbf{x} \mid \mathbf{W}, \boldsymbol{\mu}, \sigma^2)$$
$$= \sum_i p(\mathbf{x}^{(i)} \mid \mathbf{W}, \boldsymbol{\mu}, \sigma^2)$$
$$= -\frac{ND}{2} \log 2\pi - \frac{N}{2} \log |C| - \frac{1}{2} \sum_i (\mathbf{x}^{(i)} - \boldsymbol{\mu})^\top C^{-1} (\mathbf{x}^{(i)} - \boldsymbol{\mu})$$
$$\text{where} \quad C = \mathbf{W}\mathbf{W}^\top + \sigma^2 \mathbf{I}$$

- We can simply maximize this likelihood function with respect to $\mathbf{W}, \boldsymbol{\mu}, \sigma^2$.

Maximum Likelihood Parameters

- Mean: $\boldsymbol{\mu} = \overline{\mathbf{x}}$
- Noise: $\sigma^2_{\mathrm{ML}} = \frac{1}{D-M} \sum_{i=M+1}^{D} \lambda_i$
- **W**: $\mathbf{W}_{\mathrm{ML}} = \mathbf{U}_M (\mathbf{L}_M - \sigma^2 \mathbf{I})^{1/2} \mathbf{R}$

where

- $\mathbf{L}_M$ is diag with the *M* largest eigenvalues
- $\mathbf{U}_M$ is the M corresponding eigenvectors
- **R** is an arbitrary *M* by *M* orthogonal matrix (rotation matrix) (i.e., **z** can be defined by rotating "back")

Maximum likelihood by EM

- Latent variable model

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z} \mid \mathbf{0}, \mathbf{I})$$

$$p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mathbf{x} \mid \mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$

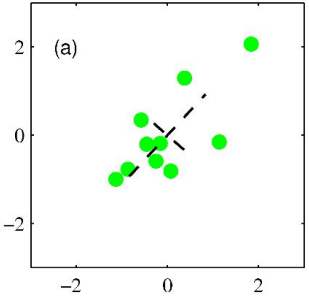
- E-step: Estimate the posterior $q(\mathbf{z}) = p(\mathbf{z} \mid \mathbf{x})$
  - Use linear Gaussian

- M-step: Maximize the data-completion likelihood given $q(\mathbf{z})$

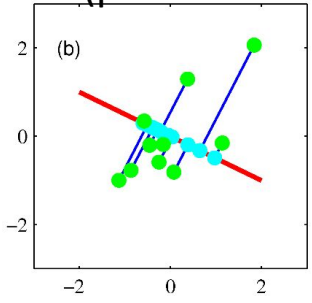
$$\text{maximize}_{\theta=\{\mathbf{W},\boldsymbol{\mu},\sigma\}} \sum_i \sum_{\mathbf{z}^{(i)}} q(\mathbf{z}^{(i)}) \log p_\theta(\mathbf{x}^{(i)}, \mathbf{z}^{(i)})$$

Finding PCA params by EM

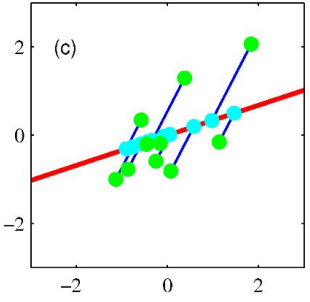
Data points



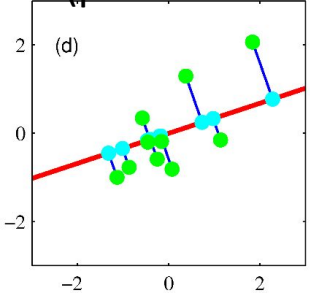
E-step: projection (posterior of **z**)



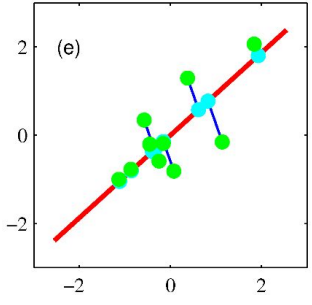
M-step: update **W**



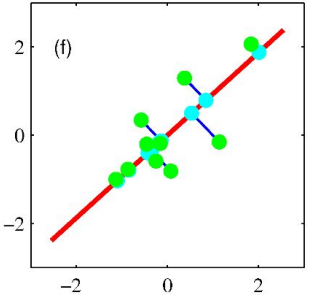
E-step: projection (posterior of **z**)



M-step: update **W**



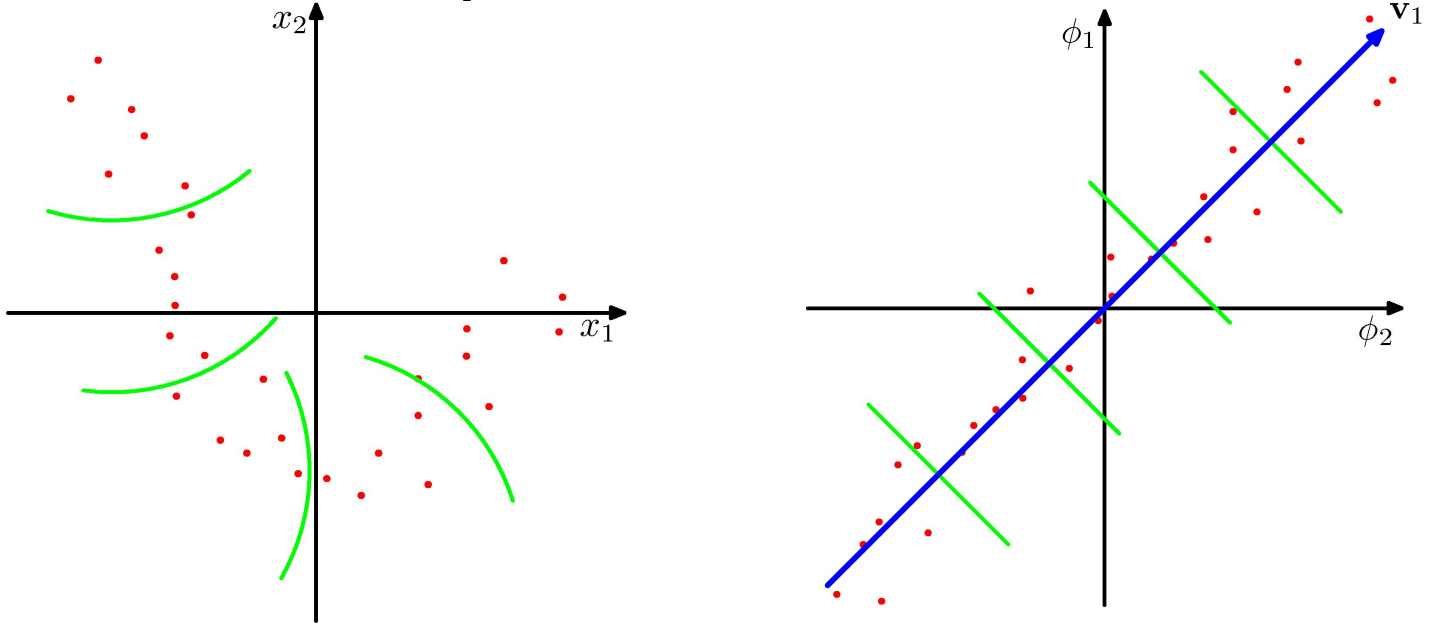
After convergence



- Illustrating EM on simulated data

Kernel PCA

- Suppose the regularity that allows dimensionality reduction is non-linear.



Kernel PCA

- As with regression and classification, we can transform the raw input data $\{\mathbf{x}^{(n)}\}$ to a set of feature values

$$\{\mathbf{x}^{(n)}\} \rightarrow \{\ \phi(\mathbf{x}^{(n)})\ \}$$

- Linear PCA (on the nonlinear feature space) gives us a linear subspace in the feature value space, corresponding to nonlinear structure in the data space.

Kernel PCA

- Define a kernel, to avoid having to evaluate the feature vectors explicitly.

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^\top \phi(\mathbf{x}')$$

- Express PCA in terms of the kernel,
  - Some care is required to centralize the data.

$$K_{nm} = \phi(\mathbf{x}^{(n)})^\top \phi(\mathbf{x}^{(m)}) = k(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$$

Kernel PCA

- Assume that $\{\phi(\mathbf{x}^{(n)})\}$ have zero mean.
- Sample covariance matrix: $S = \frac{1}{N}\sum_{n=1}^{N}\phi(\mathbf{x}^{(n)})\phi(\mathbf{x}^{(n)})^\top = \frac{1}{N}\mathbf{\Phi}^\top\mathbf{\Phi}$
- Let **v** be an eigenvector for *S*

$$S\mathbf{v} = \lambda\mathbf{v} \quad \Longrightarrow \quad \lambda\mathbf{v} = \mathbf{\Phi}^\top\left(\frac{1}{N}\mathbf{\Phi}\mathbf{v}\right)$$

$$\therefore \ \mathbf{v} = \mathbf{\Phi}^\top\boldsymbol{\alpha} \ \text{ for some } \boldsymbol{\alpha} \in \mathbb{R}^N$$

- Thus, $S\mathbf{v} = \lambda\mathbf{v} \quad \Longrightarrow \quad \lambda\mathbf{\Phi}^\top\boldsymbol{\alpha} = \frac{1}{N}\mathbf{\Phi}^\top\mathbf{\Phi}\mathbf{\Phi}^\top\boldsymbol{\alpha} = \frac{1}{N}\mathbf{\Phi}^\top K\boldsymbol{\alpha}$
- Multiply Φ on both sides and cancel out $K = \mathbf{\Phi}\mathbf{\Phi}^\top$

$$\lambda N\boldsymbol{\alpha} = K\boldsymbol{\alpha} \quad \Longrightarrow \quad \boldsymbol{\alpha} \text{ is an eigenvector of } K$$

Kernel PCA

- We thus have $\mathbf{v} = \mathbf{\Phi}^\top \boldsymbol{\alpha}$, where $\boldsymbol{\alpha}$ is eigenvector of the kernel matrix *K*.
- Now, $\|\mathbf{v}\| = 1 \implies \boldsymbol{\alpha}^\top K \boldsymbol{\alpha} = \boldsymbol{\alpha}^\top \lambda_K \boldsymbol{\alpha} = 1 \implies \|\boldsymbol{\alpha}\| = \lambda_K^{-1/2}$
- It is often infeasible to obtain $\mathbf{v}$ (depends on dim of Φ), but we can compute projections:

$$\mathbf{v}^\top \phi(\mathbf{x}) = \boldsymbol{\alpha}^\top \mathbf{\Phi} \phi(\mathbf{x}) = \boldsymbol{\alpha}^\top k(\mathbf{x}) \quad \text{where} \quad k(\mathbf{x}) = \left[k(\mathbf{x}^{(1)}, \mathbf{x}), \ldots, k(\mathbf{x}^{(N)}, \mathbf{x})\right]$$

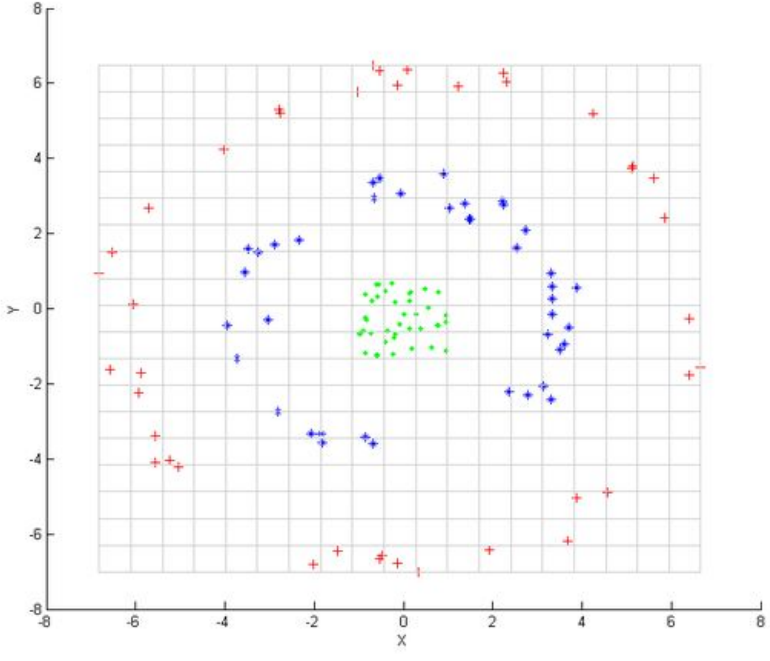
- Finally, some care is required to centralize data (to ensure that features have zero mean):

$$K' = K - \mathbf{1}_N K - K \mathbf{1}_N + \mathbf{1}_N K \mathbf{1}_N$$

$$\text{where} \quad \mathbf{1}_N \in \mathbb{R}^{N \times N} \quad \text{is a matrix of ones.}$$

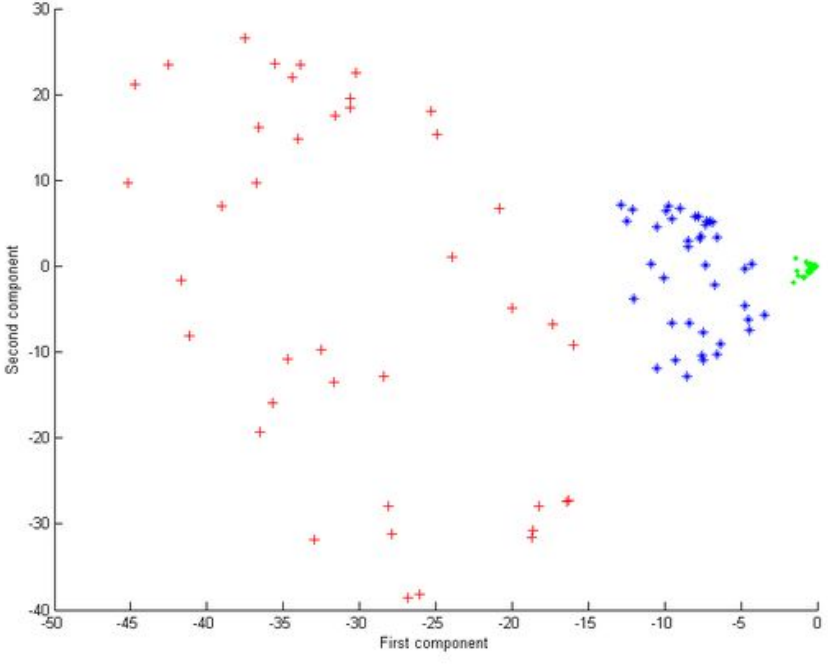
Kernel PCA

Linear PCA operates only in the given (in this case two-dimensional) space, in which these concentric point clouds are not linearly separable.



Data

The first principal component is enough to distinguish the three different groups

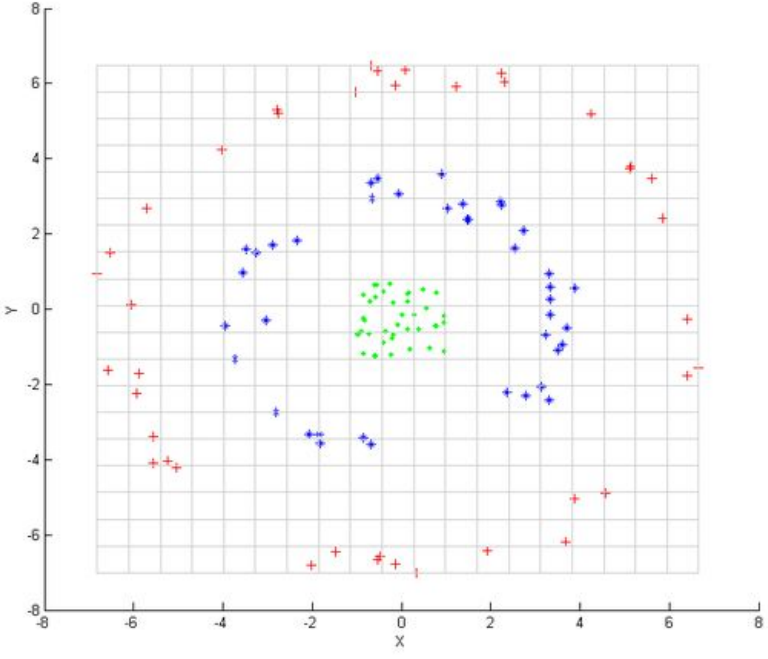


Kernel PCA with

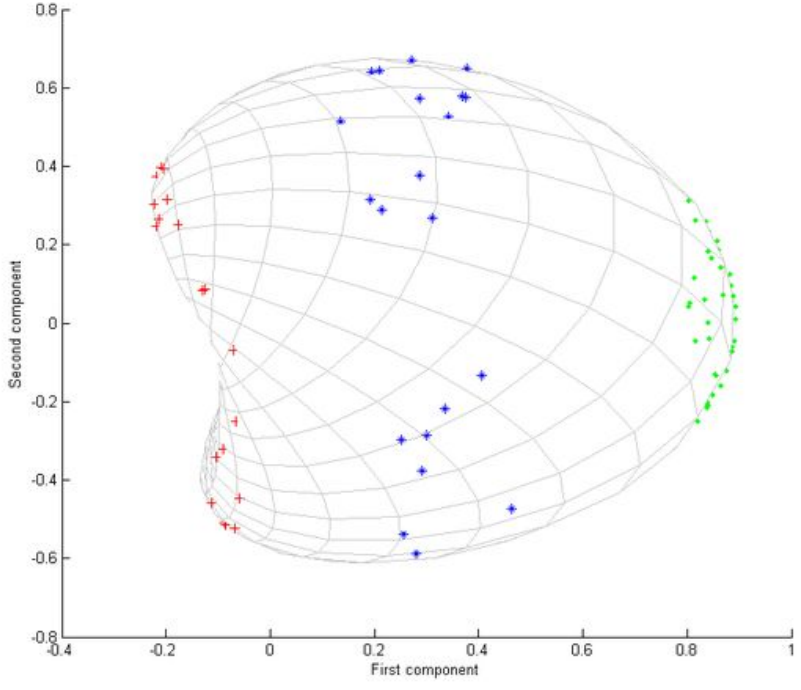
$$k(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^\top \mathbf{y} + 1)^2$$

Source: https://en.wikipedia.org/wiki/Kernel_principal_component_analysis

Kernel PCA



Data



Kernel PCA with Gaussian kernel

Source: https://en.wikipedia.org/wiki/Kernel_principal_component_analysis

Any feedback (about lecture, slide, homework, project, etc.)?

(via **anonymous** google form: https://forms.gle/fpYmiBtG9Me5qbP37)

Change Log of lecture slides:
https://docs.google.com/document/d/e/2PACX-1vSSIHJjkIypK7rKFSR1-5GYXyBCEW8UPtpSfCR9AR6M1l7K9ZQEmxfFwaWaW7kLDxusthsF8WlCyZJ-/pub