## Announcements

Matlab Grader homework, Binary graded.
168 (HW1), 166,165 (HW2) has done the homework. (If you have not done HW talk to me/TA!)
Homework 3 due 5 May TODAY
Homework 4 (SVM +Dictionary Learning) due ~24 May, released soon

Jupiter "GPU" homework. Due 10 May

Today:

- Stanford CNN 12, K-means, EM (Bishop 9) $\leftarrow$ Mithe Bim Lo
- Play with Tensorflow playground before class http://playground.tensorflow.org Solve the spiral problem

Monday

- Stanford CNN 13, Dictionary Learning,
- 3-4 person groups preferred

Proiects

- Deliverables: Poster, Report \& main code (plus proposal, midterm slide)
- Topics your own or chose form suggested topics. Some physics inspired.
- April 26 groups due to TA. 5 students not signed up 44 Groups formed. Guidelines is on Piazza
- May 5 proposal due. use dropbox Format "Proposal"+groupNumber https://www.dropbox.com/request/XGqCV0qXm9LBYz7J1msS
- Wednesday May 22 Midterm slide presentation.
- Project discussion, 22 May: We split into 6 sub-classes. The purpose is to make sure your project is on track, good progress and good goals.
Each group gives a $\sim 10 \mathrm{~min}$ presentation by all members
- (each person talks for $\sim 2$ min, $\sim 1$ slide)
- Motivation \& background, which data?
- small Example,
- final outcome, (focused on method and data)
- difficulties,
- There are 7 Groups in each sub-class, thus we have 15 min in total/group. And will use the remaining time for discussion.
- June 5, 5-8pm poster. Atkinson Hall with Pizza. Upload June ~3
- Report and code due Saturday 15 June.


## What's going on inside ConvNets?



Input Image: $3 \times 224 \times 224$


What are the intermediate features looking for?

Class Scores: 1000 numbers

The general expression of a convolution is

## Image Processing

$g(x, y)=\omega * f(x, y)=\sum_{s=-a}^{a} \sum_{t=-b}^{b} \omega(s, t) f(x-s, y-t)$,
where $g(x, y)$ is the filtered image, $f(x, y)$ is the original image, $\omega$ is the filter kernel. Every element of the filter kernel is considered by $-a \leq s \leq a$ and $-b \leq t \leq b$.

Depending on the element values, a kernel can cause a wide range of effects.



## Reverse engineering

## First Layer: Visualize Filters



AlexNet:
$64 \times 3 \times 11 \times 11$


ResNet-18:
$64 \times 3 \times 7 \times 7$


ResNet-101:
$64 \times 3 \times 7 \times 7$


DenseNet-121:
$64 \times 3 \times 7 \times 7$


## Similar to human neuron: First observe oriented edges

$w^{T} \underline{x}$ subject to $\|w\|=1$


## Last Layer: Nearest Neighbors

Test image L2 Nearest neighbors in feature space


## Feature Inversion

Given a CNN feature vector for an image, find a new image that:

- Matches the given feature vector
- "looks natural" (image prior regularization)

$$
\begin{aligned}
& \mathbf{x}^{*}=\underset{\mathbf{x} \in \mathbb{R}^{H \times W \times C} \underset{\sim}{\operatorname{argmin}} \ell\left(\Phi(\mathbf{x}), \widehat{\Phi_{0}}\right)+\lambda \mathcal{\mathcal { R }}(\mathbf{x})}{\longrightarrow} \text { Given feature vector } \\
& \ell\left(\Phi(\mathbf{x}), \Phi_{0}\right)=\left\|\Phi(\mathbf{x})-\Phi_{0}\right\|^{2} \\
& \mathcal{R}_{V^{\beta}}(\mathbf{x})=\sum_{i, j}\left(\left(x_{i, j+1}-x_{i j}\right)^{2}+\left(x_{i+1, j}-x_{i j}\right)^{2}\right)^{\frac{\beta}{2}} \searrow \text { Total Variation regularizer }
\end{aligned}
$$

## Feature Inversion

Reconstructing from different layers of VGG-16


## Neural Texture Synthesis: Gram Matrix



This image is in the public domain.


Each layer of CNN gives $\mathrm{C} \times \mathrm{H} \times \mathrm{W}$ tensor of features; $\mathrm{H} \times \mathrm{W}$ grid of C -dimensional vectors

Outer product of two C-dimensional vectors gives C x C matrix measuring co-occurrence

Average over all HW pairs of vectors, giving Gram matrix of shape $\mathrm{C} \times \mathrm{C}$


HWCden
Efficient to compute; reshape features from
$\mathrm{C} \times \mathrm{H} \times \mathrm{W}$ to $=\mathrm{C} \times \mathrm{HW}=\mathrm{F} \sim[\dot{C}] \mathrm{C}$ then compute $G=F^{\top}$

## Neural Texture Synthesis <br> $$
E_{l}=\frac{1}{4 N_{l}^{2} M_{l}^{2}} \sum_{i, j}\left(G_{i j}^{l}-\hat{G}_{i j}^{l}\right)^{2} \quad \mathcal{L}(\vec{x}, \hat{\vec{x}})=\sum_{l=0}^{L} w_{l} E_{l}
$$

- 1 1. Pretrain a CNN on ImageNet (VGG-19)

2. Run input texture forward through CNN, record activations on every layer; layer i gives feature map of shape $\mathrm{C}_{\mathrm{i}} \times \mathrm{H}_{\mathrm{i}} \times \mathrm{W}_{\mathrm{i}}$
3. At each layer compute the Gram matrix giving outer product of features:
$G_{i j}^{l}=\sum_{k} F_{i k}^{l} F_{j k}^{l}\left(\right.$ shape $\left.\mathrm{C}_{\mathrm{i}} \times \mathrm{C}_{\mathrm{i}}\right)$
4. Initialize generated image from random noise
5. Pass generated image through CNN, compute Gram matrix on each layer
6. Compute loss: weighted sum of L 2 distance between Gram matrices
7. Backprop to get gradient on image
8. Make gradient step on image
9. GOTO 5


## Neural Texture Synthesis

Reconstructing texture from higher layers recovers larger features from the input texture

Texture synthesis (Gram reconstruction)


## Neural Style Transfer



Style transfer=Feature reconstruction loss+ Gram matrix


# K-means and Expectation Maximization 

Mike Bianco and Peter Gerstoft
ECE228
5/6/2019

## K-means and expectation maximization (EM) can be considered unsupervised learning

- In supervised learning, we have desired machine learning (ML) model output or 'action' $\mathbf{y}$ based on inputs $\mathbf{x}$ (features), and model parameters $\boldsymbol{\theta}$
- Probabilities of the form: $p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta})$
- Linear regression and classification, support vector machines, etc.
- In unsupervised learning, we are interested in discovering useful patterns in the features. This can be for discovering latent data 'causes' or significant 'groups'
- Probabilities of the form: $p(\mathbf{x} \mid \boldsymbol{\theta})$
- Principal components analysis (PCA), K-means, dictionary learning, etc.


## Unsupervised learning

Unsupervised machine learning is inferring a function to describe hidden structure from "unlabeled" data (a classification or categorization is not included in the observations). Since the examples given to the learner are unlabeled, there is no evaluation of the accuracy of the structure that is output by the relevant algorithm-which is one way of distinguishing unsupervised learning from supervised learning.

We are not interested in prediction

Supervised learning: all classification and regression.

$$
\boldsymbol{Y}=\boldsymbol{w}^{T} \boldsymbol{X}
$$

Prediction is important.

Supervised learning: least square classifier (binary)


$$
\begin{aligned}
& \|y-x w\|_{2} \\
& \mathbf{y}=\mathbf{X w}
\end{aligned}
$$

Training set $\left\{\left(x^{1}, y^{1}\right),\left(x^{2}, y^{2}\right),\left(x^{3}, y^{3}\right)\right\}$
We are given the two classes
(green $=0$, red $=1$ )

## Unsupervised learning: how are features best divided?


$K$-means

Just have features $\left\{\left(x_{1}^{1}, x_{2}^{1}\right),\left(x_{1}^{2}, x_{2}^{2}\right),\left(x_{1}^{3}, x_{2}^{3}\right)\right\}$

## K-means

- Input: Points $\mathbf{x}_{1}, \ldots, \mathbf{x}_{\mathrm{N}} \in \mathrm{R}^{\mathrm{p}}$ integer K
- Output: "Centers", or representatives, $\mu_{1}, \ldots, \mu_{K} \in R^{p}$
- Output also $\mathbf{z}_{1}, \ldots, \mathbf{z}_{\mathrm{N}} \in \mathrm{R}^{\mathrm{K}}$

Goal: Minimize average squared distance between points and their nearest representatives:

- $\operatorname{cost}\left(\mu_{1}, \ldots, \mu_{K}\right)=\sum_{n=1}^{N} \min _{j}\left\|x_{n}-\mu_{j}\right\|$


> The centers carve $\mathbb{R}^{p}$ up into $k$ convex regions: $\mu_{j}$ 's region consists of points for which it is the closest center.

## K-means

$$
\begin{equation*}
J=\sum_{n=1}^{N} \sum_{k=1}^{K} r_{n k}\left\|\mathbf{x}_{n}-\boldsymbol{\mu}_{k}\right\|^{2} \tag{9.1}
\end{equation*}
$$

(1) assign pts. centroids.

## Solving for $r_{n k}$

$$
r_{n k}=\left\{\begin{array}{l}
1 \text { if } k=\arg \min _{j}\left\|\mathbf{x}_{n}-\boldsymbol{\mu}_{j}\right\|^{2} \\
\text { otherwise } .
\end{array}\right.
$$

(2) update
centroids based in per. (9.2)

Differentiating for $\mu_{k}$

$$
\begin{equation*}
2 \sum_{n=1}^{N} r_{n k}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{k}\right)=0 \tag{9.3}
\end{equation*}
$$

which we can easily solve for $\boldsymbol{\mu}_{k}$ to give

$$
\boldsymbol{\mu}_{k}=\frac{\sum_{n} r_{n k} \mathbf{x}_{n}}{\sum_{n} r_{n k}}
$$




## Old Faithful, Kmeans from Murphy



## Application of K-means to data compression:

 Vector QuantizationEach pixel $\mathbf{x}_{i}$ is represented By codebook of K entries $\mu_{k}$
$\operatorname{Encode}\left(\mathbf{x}_{\mathrm{i}}\right)=\underset{k}{\operatorname{argmin}}\left\|x_{i}-\mu_{k}\right\|$
Consider $\mathrm{N}=64 \mathrm{k}$ observations, of $\mathrm{D}=1(\mathrm{~b} / \mathrm{w})$ dimension, $\mathrm{C}=8 \mathrm{bit}$
$N C=513 k$
$\mathrm{Nlog}_{2} \mathrm{~K}+\mathrm{KC}$ bits is needed $K=4$ gives 128 k a factor 4 .
"codebook"


## Mixtures of Gaussians (1)

## Old Faithful geyser:

The time between eruptions has a bimodal distribution, with the mean interval being either 65 or 91 minutes, and is dependent on the length of the prior eruption. Within a margin of error of $\pm 10$ minutes, Old Faithful will erupt either 65 minutes after an eruption lasting less than $21 / 2$ minutes, or 91 minutes after an eruption lasting more than $2 \frac{1}{2}$ minutes.



## Mixtures of Gaussians (2)

Combine simple models into a complex model:

$$
p(\mathbf{x})=\sum_{k=1}^{K} \underbrace{\pi_{k} \mathcal{N}\left(\underset{b}{\mathbf{x}} \mid \boldsymbol{\mu}_{k}, \mathbf{\Sigma}_{k}\right)}_{\text {Component }}
$$

$$
\forall k: \pi_{k} \geqslant 0 \quad \sum_{k=1}^{K} \pi_{k}=1
$$



Mixtures of Gaussians (3)




Mixture of Gaussians

- Mixtures of Gaussians

$$
p(\mathbf{x})=\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)
$$

- Expressed with latent variable z

$$
p(\mathbf{x})=\sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x} \mid \mathbf{z})=\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)
$$

$$
\begin{aligned}
& p\left(\boldsymbol{x} \mid z_{k}=1\right)=N\left(\boldsymbol{x} ; \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right) \\
& p\left(z_{k}=1\right)=\pi_{k} / / \\
& p(\boldsymbol{x} \mid \mathbf{z})=\prod_{k=1}^{k} N\left(\times / \mu_{k}, \sum_{k}\right) \\
& p(\mathbf{z})=\pi_{k} \pi_{k}^{z_{k}} \quad z_{k}=\{0,1\} \\
& p(\boldsymbol{x}, \mathbf{z})=\prod_{k} \frac{(x / z) p(z)}{}=\pi_{k} / \sum_{k=1}^{K} \pi_{k}=1 \\
& \forall k: \pi_{k} \geqslant 0 \quad
\end{aligned}
$$



Want to estimate the latent variables for data X

- Probability of data given latent representation

$$
p(\mathbf{X} \mid \underset{\theta}{\pi, \mu, \Sigma})=\Pi_{N} \sum_{k}^{\prime} \pi_{k} N\left(x \mid \mu_{k}, \Sigma_{k}^{\prime}\right)
$$

- Log likelihood

$$
\begin{gathered}
\ln p(\mathbf{X} \mid \pi, \mu, \Sigma)=\sum_{N} \overbrace{\substack{\sum_{k} \\
\ln N}}\left(X \mid \mu k, \sum_{k}^{\prime}\right) \\
\sum_{k} p(x, z \mid \theta)
\end{gathered}
$$

Can't we just solve for the latent variables by maximimizing log likelihood?

- Log likelihood $\ln p(\mathbf{X} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})=\sum_{n=1}^{N} \ln \left\{\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)\right\}$.
- Take derivative w.r.t. $\left.\mu_{k}: \rightarrow N\left(x_{n} \mid \mu_{k}, \bar{\Sigma}_{k}\right)=\frac{1}{2 \pi^{n / 2}, \sum_{k}}\right)^{1 / L}$

$$
\begin{aligned}
& \frac{\partial}{\partial \mu_{k}} N()=\underbrace{\left.\left(x_{n}-\mu_{k}\right)\right\}}_{\sum_{k}^{-1}\left(x_{2}-\mu_{k}\right) N() \cdot \exp \left\{-\frac{1}{2}\left(x_{n}-\mu_{k}\right)^{\top} \sum_{k}^{-1}\right.}
\end{aligned}
$$

Can't we just solve for the latent variables by maximimizing log likelihood?

- Log likelihood $\ln p(\mathbf{X} \mid \pi, \mu, \Sigma)=\sum_{n=1}^{N} \ln \left\{\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)\right\}$.
- Take derivative w.r.t. $\boldsymbol{\mu}_{k}$ :

$$
\begin{aligned}
& 0=-\sum_{n=1}^{N} \underbrace{\frac{\pi_{k} \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)}{\sum_{j} \pi_{j} \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{j}, \boldsymbol{\Sigma}_{j}\right)}}_{\gamma\left(z_{n k}\right)} \boldsymbol{\Sigma}_{k}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{k}\right) \\
& \text { "responsibility", from Bayes's rule: } \\
& \gamma\left(z_{k}\right) \equiv p\left(z_{k}=1 \mid \mathbf{x}\right)
\end{aligned} \quad=\frac{p\left(z_{k}=1\right) p\left(\mathbf{x} \mid z_{k}=1\right)}{\sum_{j=1}^{K} p\left(z_{j}=1\right) p\left(\mathbf{x} \mid z_{j}=1\right)}, ~=\frac{\pi_{k} \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)}{\sum_{j=1}^{K} \pi_{j} \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{j}, \boldsymbol{\Sigma}_{j}\right)} .
$$

## Solving for $\mu_{k}, \Sigma_{k}$

Take derivative w.r.t. $\mu_{k}$ :

## Solving for $\pi_{k}$

Use Lagrange multipliers with constraint $\quad \sum_{k=1}^{K} \pi_{k}=1$

## EM Gauss Mix

1. Initialize the means $\boldsymbol{\mu}_{n}$ covariances $\boldsymbol{\Sigma}_{k}$ and mixing coefficients $\pi_{k}$, and evaluate the initial value of the $\log$ likelihood.
2. E step. Evaluate the responsibilities using the current parameter values

3. M step. Re-estimate the parameters using the current responsibilities


Important not to have singularities
"maxinum litalinoced"


General EM
Given a joint distribution $p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$ over observed variables $\mathbf{X}$ and latent variables $\mathbf{Z}$, governed by parameters $\boldsymbol{\theta}$, the goal is to maximize the likelihood function $p(\mathbf{X} \mid \boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$.

1. Choose an initial setting for the parameters $\boldsymbol{\theta}^{\text {old }}$.
2. E step Evaluate $p\left(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{\text {old }}\right)$.
3. $\mathbf{M}$ step Evaluate $\boldsymbol{\theta}^{\text {new }}$ given by

$$
\begin{equation*}
\boldsymbol{\theta}^{\text {new }}=\underset{\boldsymbol{\theta}}{\arg \max } \mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text {old }}\right) \tag{9.32}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text {old }}\right)=\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{\text {old }}\right) \ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta}) . \tag{9.33}
\end{equation*}
$$

4. Check for convergence of either the log likelihood or the parameter values. If the convergence criterion is not satisfied, then let

$$
\begin{equation*}
\boldsymbol{\theta}^{\text {old }} \leftarrow \boldsymbol{\theta}^{\text {new }} \tag{9.34}
\end{equation*}
$$

and return to step 2.
"local methad"




## Kmeans and EM (9.3.2)

$$
\boldsymbol{\Sigma}_{k}=\epsilon \boldsymbol{I}
$$

$$
\begin{array}{ll}
p\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}, \Sigma_{k}\right)=\frac{1}{(2 \pi \epsilon)^{1 / 2}} \exp \left\{-\frac{1}{2 \epsilon}\left\|\mathbf{x}-\boldsymbol{\mu}_{k}\right\|^{2}\right\} . \quad \text { (9.41) } \\
\text { reby the responsibilities } & \exp \left(\frac{1}{2 \epsilon} d_{m i n}\right)
\end{array}
$$

Whereby the responsibilities

Becomes delta functions. And the EM means approach the Kmeans

$$
\begin{equation*}
\boldsymbol{\mu}_{k}=\frac{1}{N_{k}} \sum_{n=1}^{N} \gamma\left(z_{n k}\right) \mathbf{x}_{n} \tag{9.17}
\end{equation*}
$$

