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Eidgenössische Technische Hochschule Zürich
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inf | Informatik
Computer Science

Introduction to Machine Learning

Dealing with missing data (Unsupervised learning via prob. modeling)

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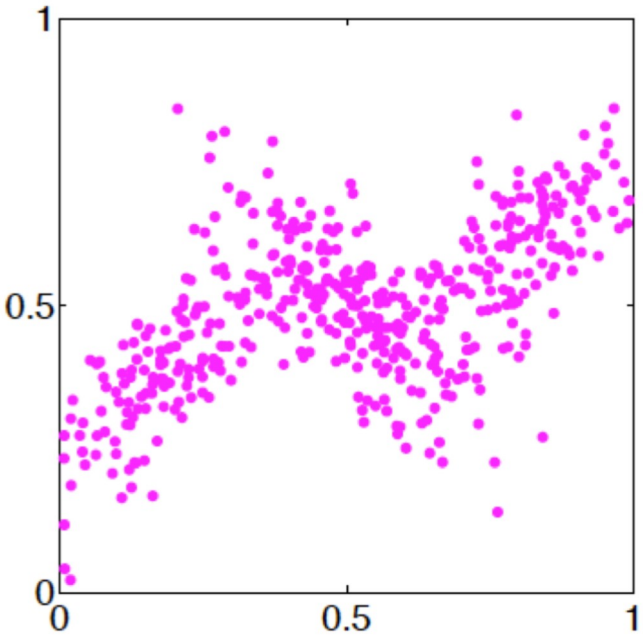
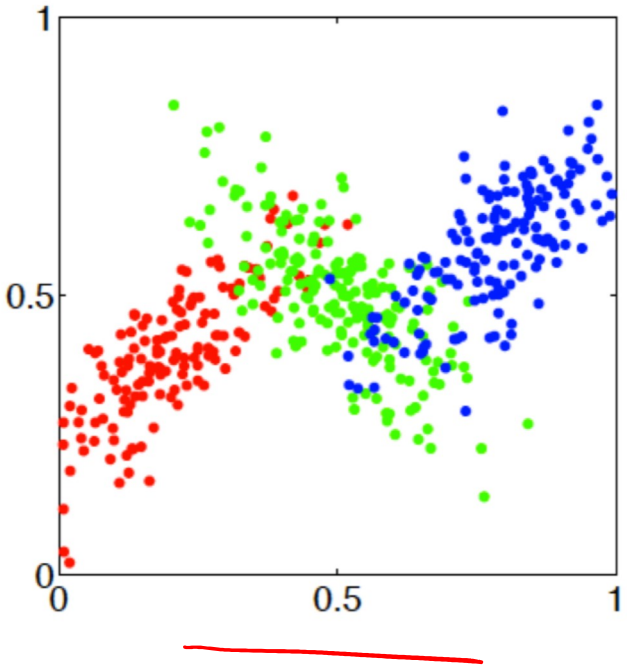
What if we assume P(X | Y) is Gaussian?



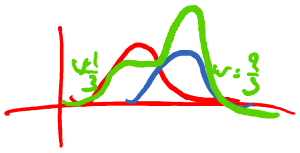


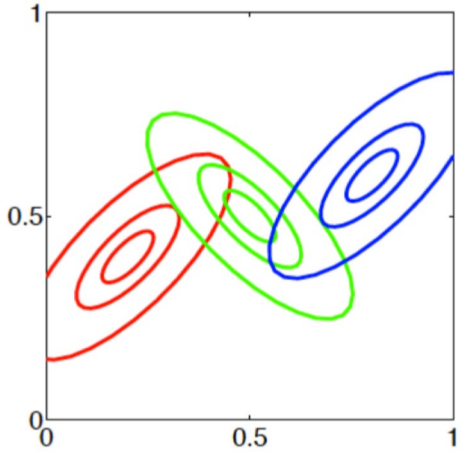
Gaussian mixtures

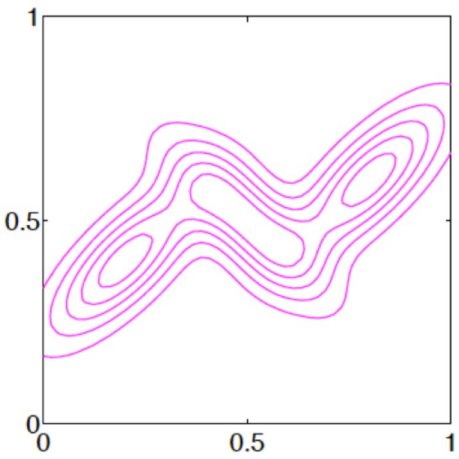
- Convex-combination of Gaussian distributions

$$P(\mathbf{x} \mid \theta) = P(\mathbf{x} \mid \mu, \Sigma, \mathbf{w}) = \sum_{i=1}^{C} w_i \mathcal{N}(\mathbf{x}; \mu_i, \Sigma_i)$$

where $w_i \geq 0$ and $\sum_i w_i = 1$







GMMs vs. Gaussian Bayes Classifiers

- The joint distribution $P(z, \mathbf{x}) = w_z \mathcal{N}(\mathbf{x} \mid \mu_z, \Sigma_z)$ of *(cluster_index,features)* is identical to the generative model used by the Gaussian Bayes Classifier

- **Main difference**: In contrast to GBCs, in GMMs the (label) variable z is *unobserved*!

➔ Fitting a GMM = Training a GBC without labels

➔ Clustering = latent variable modeling

➔ If we could just get the labels, could compute MLE in closed form!

Maximum likelihood estimation

- Can show: At MLE

$$(\mu^*, \Sigma^*, w^*) = \arg\min - \sum_i \log \sum_{j=1}^{k} w_j \mathcal{N}(\mathbf{x_i} \mid \mu_j, \Sigma_j)$$

it must hold that

$$\mu_j^* = \frac{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)\mathbf{x}_i}{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)}$$

$$\Sigma_j^* = \frac{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)(\mathbf{x}_i - \mu_j^*)(\mathbf{x}_i - \mu_j^*)^T}{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)}$$

$$w_j^* = \frac{1}{n} \sum_{i=1}^{n} \gamma_j(\mathbf{x}_i)$$

These equations are *coupled* → difficult to solve jointly

Expectation-Maximization (Soft-EM)

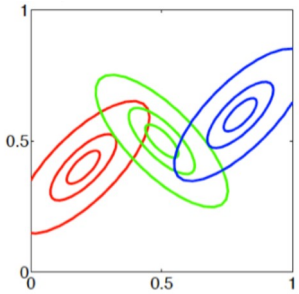
- While not converged
  - E-step: calculate cluster membership weights ("Expected sufficient statistics") for each point (aka "responsibilities"):
    Calculate $\gamma_j^{(t)}(\mathbf{x}_i)$ for each *i* and *j* given estimates of $\mu^{(t-1)}, \Sigma^{(t-1)}, \mathbf{w}^{(t-1)}$ from previous iteration
  - M-step: Fit clusters to weighted data points (closed form Maximum likelihood solution!)

$$w_j^{(t)} \leftarrow \frac{1}{n}\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i) \quad \mu_j^{(t)} \leftarrow \frac{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)\mathbf{x}_i}{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)}$$

$$\Sigma_j^{(t)} \leftarrow \frac{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)(\mathbf{x}_i-\mu_j^{(t)})(\mathbf{x}_i-\mu_j^{(t)})^T}{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)}$$

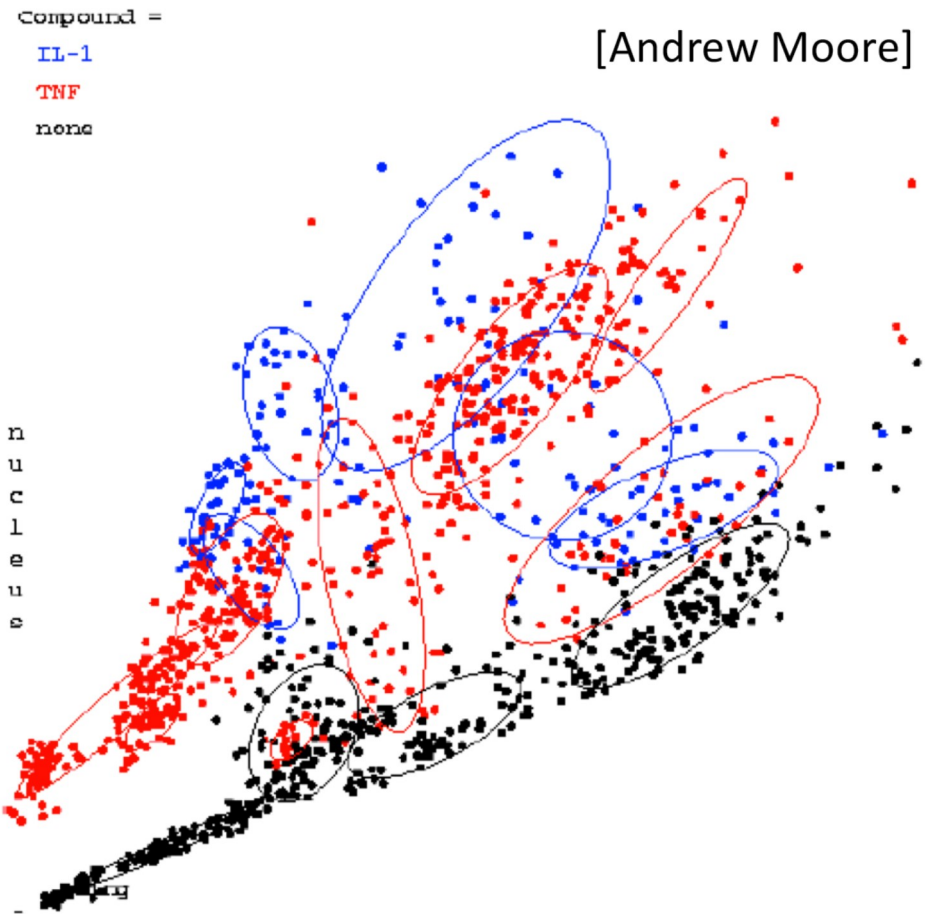
Why are mixture models useful?

- Can encode assumptions about "shape" of clusters
  - E.g., fit ellipses instead of points



- Can be part of more complex statistical models
  - E.g., classifiers (or more general probabilistic models)
- Probabilistic models can output likelihood $P(\boldsymbol{x})$ of a point $\boldsymbol{x}$
  - Useful for anomaly/outlier detection
- Can be naturally used for semi-supervised learning!

Clustering for (nonlinear) classification



Gaussian-*Mixture* Bayes classifiers

- Given *labeled* data set $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$
  - Label $y_i \in \{1, \ldots m\}$
  - Estimate class prior *P(y)*
  - Estimate conditional distribution *for each class*

$$P(\mathbf{x} \mid y) = \sum_{j=1}^{n_y} w_j^{(y)} \mathcal{N}(\mathbf{x}; \mu_j^{(y)}, \Sigma_j^{(y)})$$

  as Gaussian mixture model

- How do we use this model for classification?

$$P(y|x) = \frac{1}{Z} P(y) P(x|y)$$
$$= \frac{1}{Z} P(y) \sum_{j=1}^{n_y} w_j^{(y)} \mathcal{N}(x; \mu_j^{(y)}, \Sigma_j^{(y)})$$

Gaussian-*Mixture* Bayes classifiers

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$$P(\mathbf{x} \mid y) = \sum_j w_j^{(y)} \mathcal{N}(\mathbf{x}; \mu_j^{(y)}, \Sigma_j^{(y)})$$

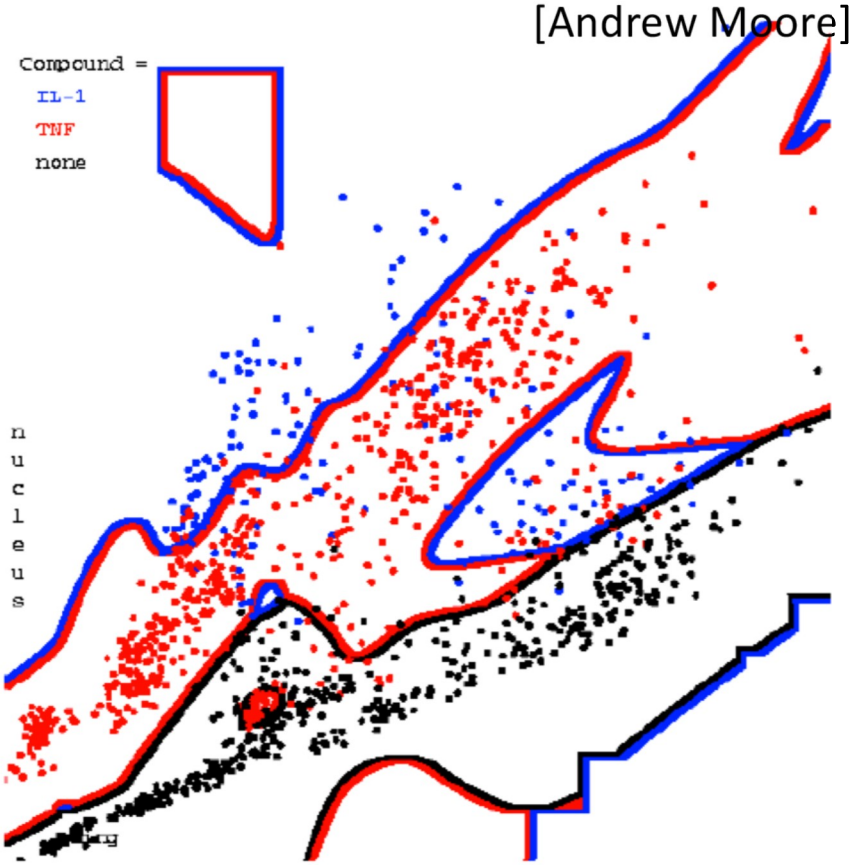
  as Gaussian mixture model

- How do we use this model for classification?

$$P(y \mid \mathbf{x}) = \frac{1}{Z} p(y) \sum_{j=1}^{k_y} w_j^{(y)} \mathcal{N}(\mathbf{x}; \mu_j^{(y)}, \Sigma_j^{(y)})$$

Resulting classifier

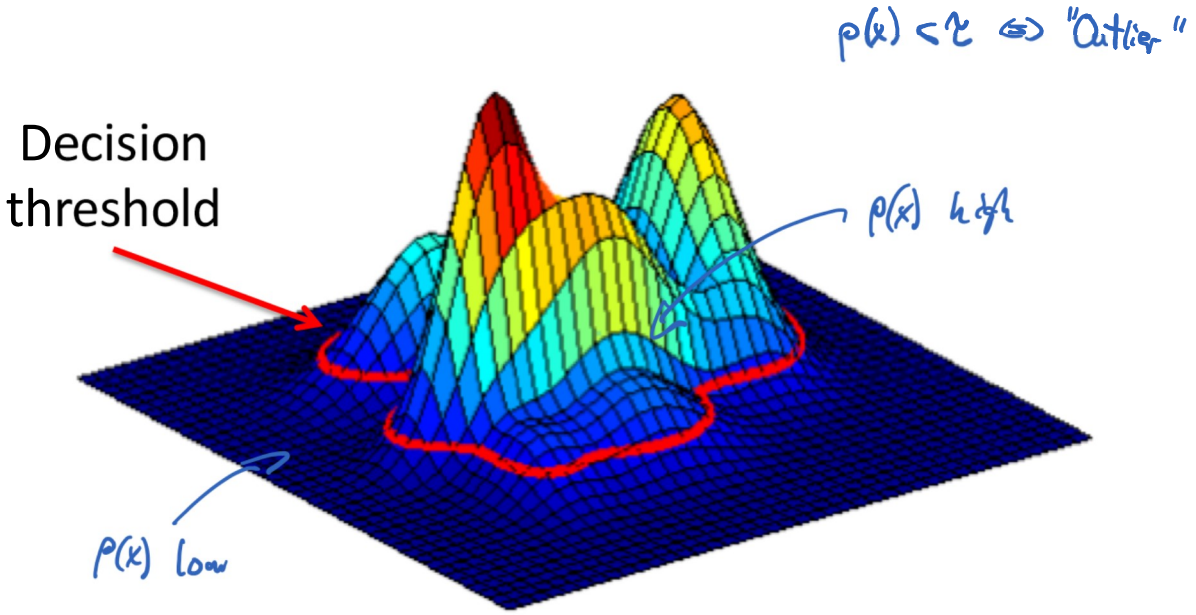
[Andrew Moore]



GMMs for density estimation

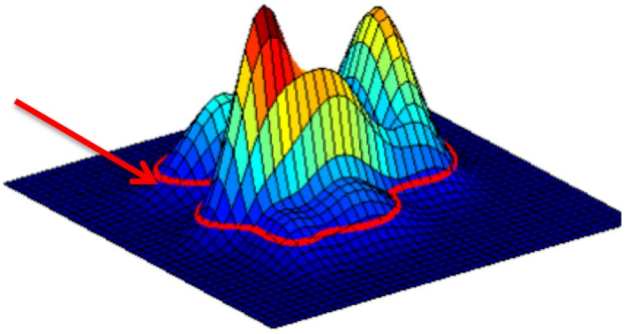
- We may be interested in fitting a Gaussian Mixture Model not for clustering but for density estimation
- E.g.,
  - Model $P(\boldsymbol{x})$ as Gaussian mixture
  - Model $P(y|\boldsymbol{x})$ using logistic regression, neural network, etc.
- Combines the advantage of accurate predictions / robustness from discriminative model, with the ability to detect outliers!

Anomaly detection with mixture models



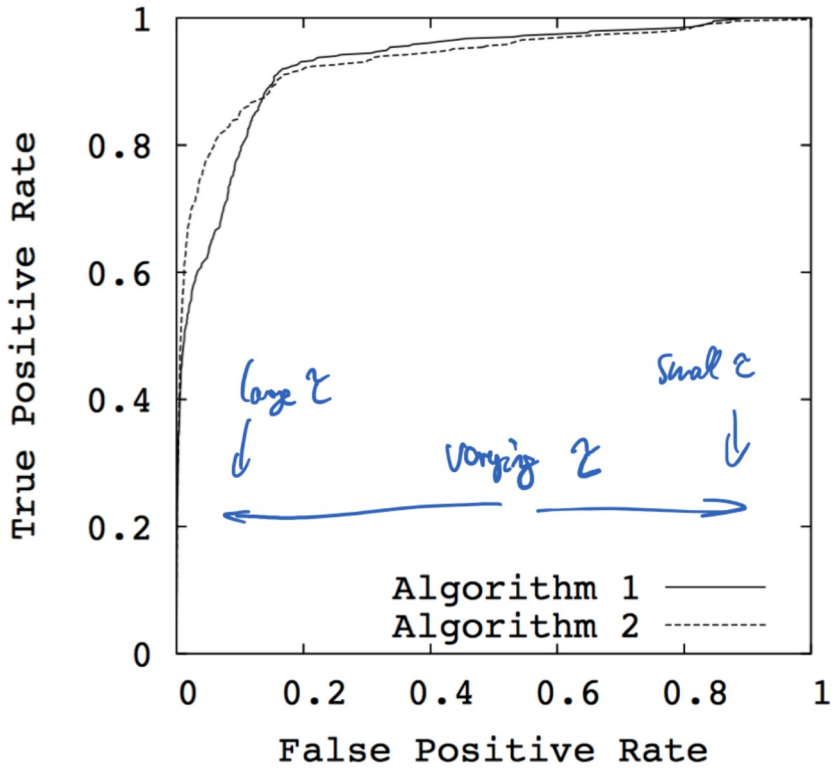
- Can determine outliers by comparing the estimated density of a data point against a threshold

How to pick the threshold?

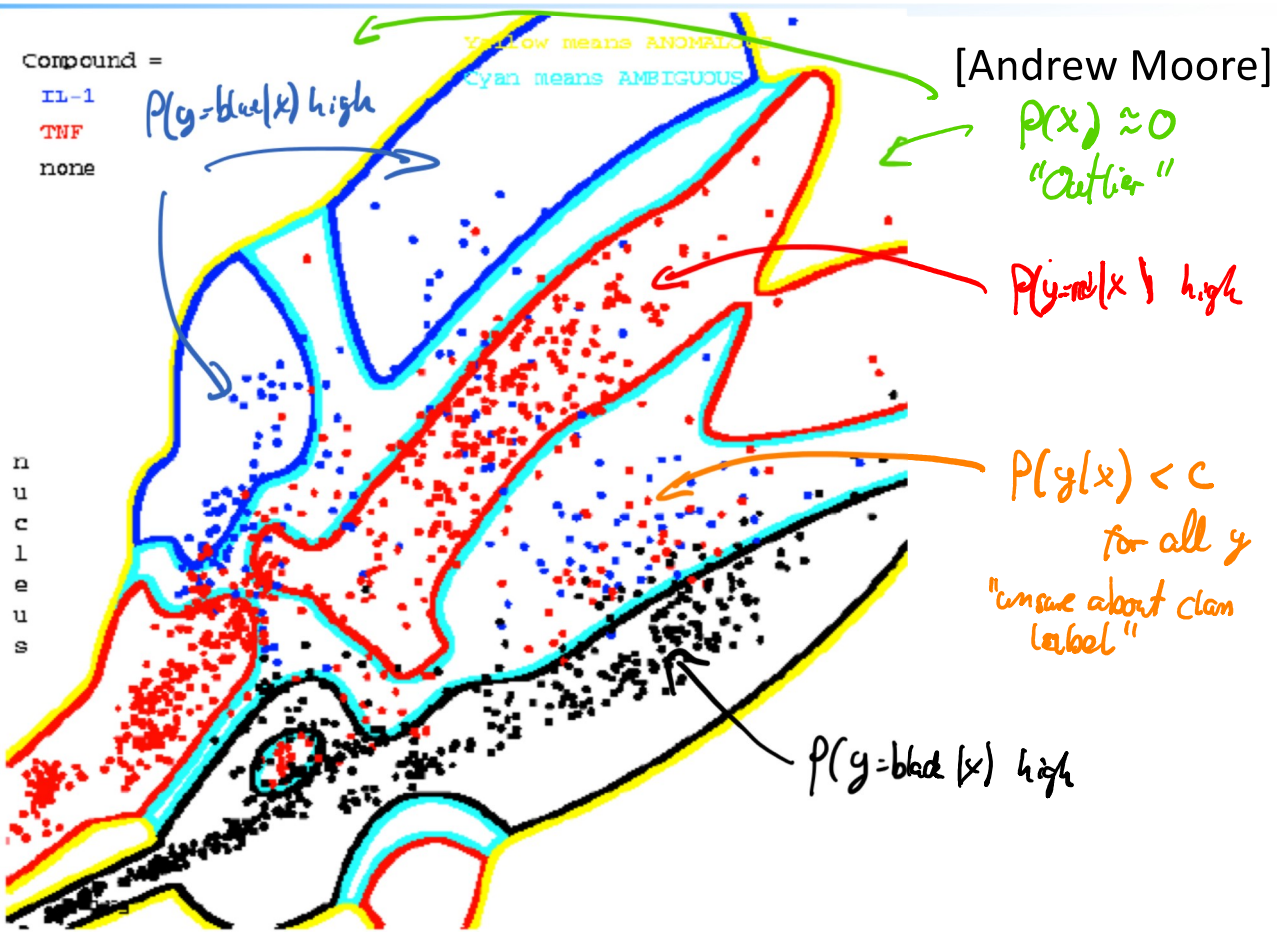


- If we have no examples of anomalies, this is challenging
- If we do have some examples:
  - Varying the threshold trades false-positives and false-negatives
  - Can use precision-recall curves / ROC curves as evaluation criterion; e.g., maximize F1 score
  - This allows to optimize the threshold, e.g., via cross-validation!

Recall: ROC curves



Classification + Anomaly detection



[Andrew Moore]

GMMs for density estimation

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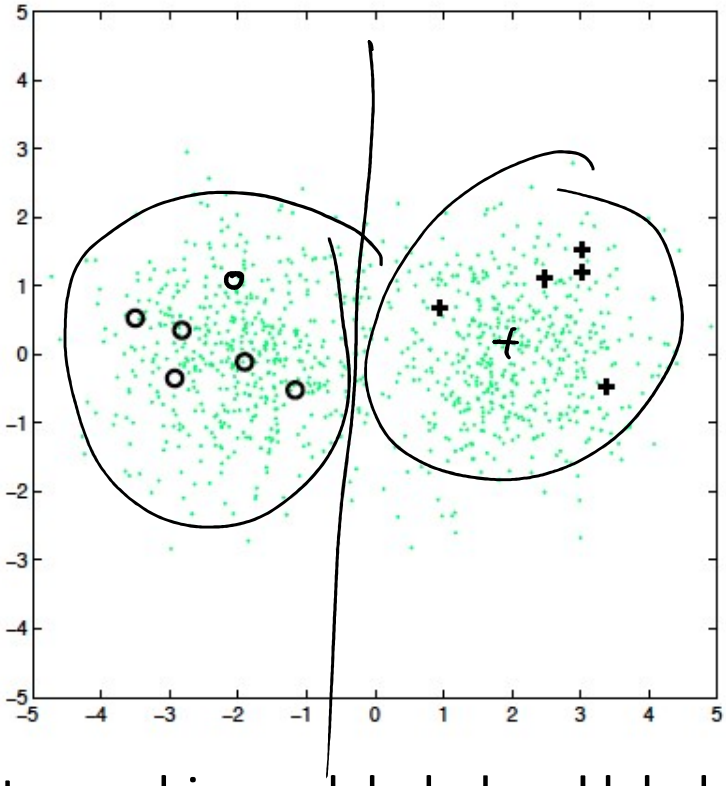
- Combines the advantage of accurate predictions / robustness from discriminative model, with the ability to detect outliers / anomalies!

$$P(x, y) = P(y)\,P(x|y) = p(x)\,p(y|x)$$

Semi-supervised learning with GMMs

[Zhu]



- Want to combine unlabeled and labeled data!

Semi-supervised learning = partially missing labels

X_1	X_2	…	X_d	Y
1.1	.3	…	.5	N/A
.5	.4	…	.7	**+1**
…	…	…	…	…
-.4	-.5	…	.3	N/A

Semi-supervised learning with GMMs

- We have discussed
  - Supervised Learning: Data consists of (feature,label)-pairs
  - Unsupervised Learning: Data consists of feature vectors **only**
- Often, one can obtain large amounts of unlabeled data, but labeled data is expensive
- Semi-supervised learning = learning from (large amounts of) unlabeled data **and** (small amounts of) labeled data

- Easy to do with Gaussian mixture models!

Semi-supervised learning with GMMs

- Recall, for GMMs, at the MLE it holds that

$$\mu_j^* = \frac{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)\mathbf{x}_i}{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)}$$

$$\Sigma_j^* = \frac{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)(\mathbf{x}_i - \mu_j^*)(\mathbf{x}_i - \mu_j^*)^T}{\sum_{i=1}^n \gamma_j(\mathbf{x}_i)}$$

$$w_j^* = \frac{1}{n}\sum_{i=1}^n \gamma_j(\mathbf{x}_i)$$

- where $\gamma_j(\mathbf{x}) = P(z = j \mid \mathbf{x}, \Sigma^*, \mu^*, \mathbf{w}^*)$
- In SSL, for instances ***x*** with observed labels *y*, must hold:

$$\gamma_j(\mathbf{x}_i) = [j = y_i]$$

EM for semi-supervised learning with GMMs

- While not converged
  - E-step: For unlabeled points:

$$\gamma_j^{(t)}(\mathbf{x}_i) = P(Z = j \mid \mathbf{x}_i, \mu^{(t-1)}, \Sigma^{(t-1)}, \mathbf{w}^{(t-1)})$$

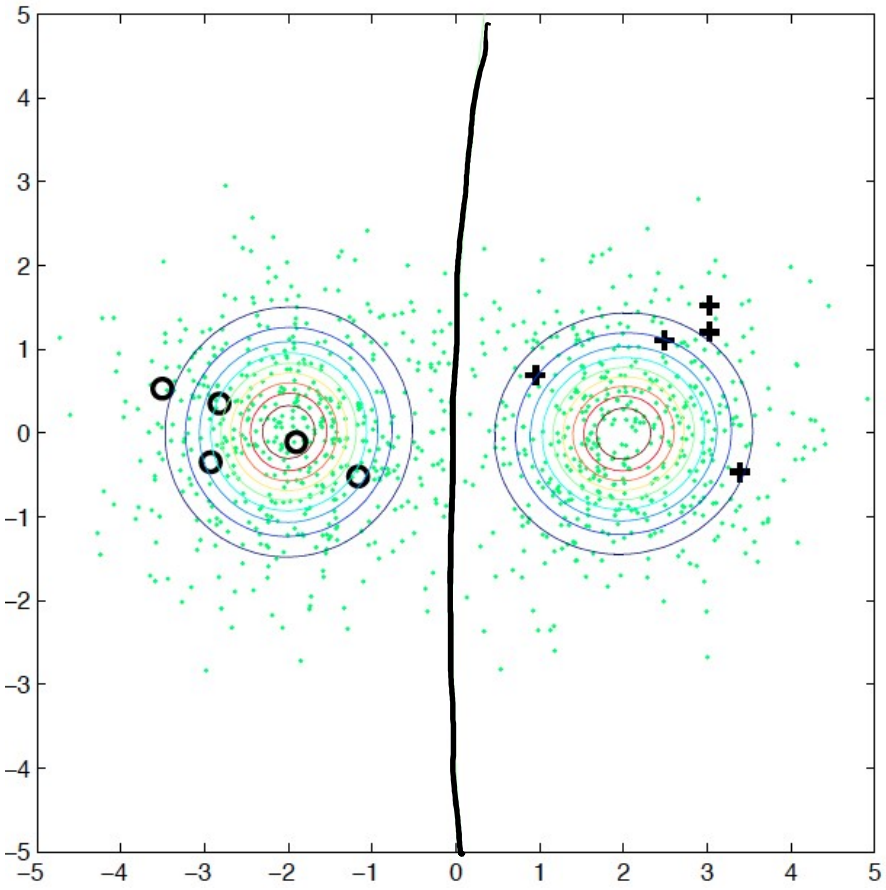
For points with label y_i : $\gamma_j^{(t)}(\mathbf{x}_i) = [j = y_i]$

  - M-step: Fit clusters to weighted data points (closed form Maximum likelihood solution!)

$$w_j^{(t)} \leftarrow \frac{1}{n}\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i) \quad \mu_j^{(t)} \leftarrow \frac{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)\mathbf{x}_i}{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)}$$

$$\Sigma_j^{(t)} \leftarrow \frac{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)(\mathbf{x}_i - \mu_j^{(t)})(\mathbf{x}_i - \mu_j^{(t)})^T}{\sum_{i=1}^{n}\gamma_j^{(t)}(\mathbf{x}_i)}$$

Semi-supervised learning solution



Theory behind the EM Algorithm

- Can show that the EM algorithm is equivalent to the following procedure:

- E-Step: Calculate the expected complete data log-likelihood (= function of θ)

$$Q(\theta; \theta^{(t-1)}) = \mathbb{E}_{\mathbf{z}_{1:n}} \left[\log P(\mathbf{x}_{1:n}, \mathbf{z}_{1:n} \mid \theta) \mid \mathbf{x}_{1:n}, \theta^{(t-1)} \right]$$

$$= \sum_{z_{1:n}} P(z_{1:n} \mid x_{1:n}, \theta^{(t-1)}) \quad \log P(x_{1:n}, z_{1:n} \mid \theta)$$

Complete data log-likelihood

- M-Step: Maximize $\theta^{(t)} = \arg\max_{\theta} Q(\theta; \theta^{(t-1)})$

Details

Notation: $\tilde{\theta} := \theta^{(t-1)}$, $x := x_{1:n}$, $z := z_{1:n}$

- EM-Objective function

$$Q(\theta; \underbrace{\theta^{(t-1)}}_{\tilde{\theta}}) = \mathbb{E}_{\mathbf{z}_{1:n}}\left[\log P(\mathbf{x}_{1:n}, \mathbf{z}_{1:n} \mid \theta) \mid \mathbf{x}_{1:n}, \theta^{(t-1)}\right]$$

can be simplified:

$$Q(\theta;\tilde{\theta}) \overset{iid}{=} \mathbb{E}_z\left[\sum_{i=1}^{n} \log P(x_i, z_i \mid \theta) \mid x, \tilde{\theta}\right]$$

$$= \sum_{i=1}^{n} \mathbb{E}_{z_{1:n}}\left[\log P(x_i, z_i \mid \theta) \mid x_{1:n}, \tilde{\theta}\right]$$

$$= \sum_{i=1}^{n} \mathbb{E}_{z_i}\left[\log P(x_i, z_i \mid \theta) \mid x_i, \tilde{\theta}\right]$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{k} \underbrace{P(z_i = j \mid x_i, \tilde{\theta})}_{\gamma_j(x_i)} \log \underbrace{P(x_i, z_i = j \mid \theta)}_{w_j \mathcal{N}(x_i; \mu_j, \Sigma_j)}$$

Details for E-Step

- Thus, the EM objective function is equivalent to

$$Q(\theta; \theta^{(t-1)}) = \sum_{i=1}^{n} \sum_{z_i=1}^{k} \gamma_{z_i}(\mathbf{x}_i) \log P(\mathbf{x}_i, z_i \mid \theta)$$

  where $\gamma_z(\mathbf{x}) = P(z \mid \mathbf{x}, \theta^{(t-1)})$

- Thus, E-step is equivalent to computing $\gamma_z(\mathbf{x}_i)$ (called Expected Sufficient Statistics)

Details for M-Step

$$Q(\theta; \theta^{(t-1)}) = \sum_{i=1}^{n} \sum_{z_i=1}^{k} \gamma_{z_i}(\mathbf{x}_i) \log P(\mathbf{x}_i, z_i \mid \theta)$$

- In M-Step, need to compute

$$\theta^{(t)} = \arg\max_{\theta} Q(\theta; \theta^{(t-1)})$$

- Note similarity to MLE in Gaussian Bayes Classifiers:

$$\theta^{*} = \arg\max_{\theta} \sum_{i=1}^{n} \log P(\mathbf{x}_i, z_i \mid \theta)$$

- Thus, each iteration in the M-step is equivalent to training a GBC with weighted data!
- Closed form solution (given in EM pseudo-code)

Convergence of EM Algorithm

- Can prove that the EM Algorithm monotonically increases the likelihood

$$\log P(\mathbf{x}_{1:n} \mid \theta^{(t)}) \geq \log P(\mathbf{x}_{1:n} \mid \theta^{(t-1)})$$

- For Gaussian mixtures, EM is guaranteed to converge to a local maximum*
- Quality of solution highly depends on initialization! (as in k-Means)
- **Common strategy**: Rerun algorithm multiple times, and use the solution with largest likelihood

Convergence proof

- **Goal**: Maximize $\theta^* = \arg\max_\theta P(\mathbf{x}_{1:n} \mid \theta)$
- Can rewrite: $P(\mathbf{x}_{1:n} \mid \theta) = \dfrac{P(\mathbf{x}_{1:n}, \mathbf{z}_{1:n} \mid \theta)}{P(\mathbf{z}_{1:n} \mid \mathbf{x}_{1:n}, \theta)}$
- Take logs, and expectation w.r.t. $P(\mathbf{z}_{1:n} \mid \mathbf{x}_{1:n}, \tilde{\theta})$ ($\tilde{\theta} = \theta^{(t-1)}$)

$$\mathbb{E}_z[\log P(x|\theta) \mid x, \tilde{\theta}] = \mathbb{E}_z\left[\log \frac{P(x,z|\theta)}{P(z|x,\theta)} \,\middle|\, x, \tilde{\theta}\right]$$

$\log P(x|\theta)$

$$= \mathbb{E}_z[\log P(x,z|\theta) \mid x, \tilde{\theta}] - \mathbb{E}_z[\log P(z|x,\theta) \mid x, \tilde{\theta}]$$

$Q(\theta, \tilde{\theta})$; ?

Convergence proof

- So far, we have

$$\log P(\mathbf{x} \mid \theta) = Q(\theta, \theta^{(t-1)}) - \mathbb{E}_{\mathbf{z}}[\log P(\mathbf{z} \mid \mathbf{x}, \theta) \mid \mathbf{x}, \theta^{(t-1)}]$$

$\ell(\theta)$

- Want to show $\log P(\mathbf{x} \mid \theta^{(t)}) \geq \log P(\mathbf{x} \mid \theta^{(t-1)})$

Suffices to show that

(1) $Q(\theta^{(t)}, \theta^{(t-1)}) \geq Q(\theta^{(t-1)}, \theta^{(t-1)})$ ✓ Since in M-step $\theta^{(t)} = \arg\max_{\theta} Q(\theta, \theta^{(t-1)})$

(2) $\ell(\theta^{(t)}) \leq \ell(\theta^{(t-1)})$

Convergence proof

- So far, we have

$$\log P(\mathbf{x} \mid \theta) = Q(\theta, \theta^{(t-1)}) - \mathbb{E}_{\mathbf{z}}[\log P(\mathbf{z} \mid \mathbf{x}, \theta) \mid \mathbf{x}, \theta^{(t-1)}]$$

- Want to show $\log P(\mathbf{x} \mid \theta^{(t)}) \geq \log P(\mathbf{x} \mid \theta^{(t-1)})$

- Compare term by term:
  - EM-Algorithm guarantees (strict inequality unless converged):

$$Q(\theta^{(t)}, \theta^{(t-1)}) \geq Q(\theta^{(t-1)}, \theta^{(t-1)})$$

  - Remains to show:

$$\mathbb{E}_{\mathbf{z}}[\log P(\mathbf{z} \mid \mathbf{x}, \theta^{(t-1)}) \mid \mathbf{x}, \theta^{(t-1)}] \geq \mathbb{E}_{\mathbf{z}}[\log P(\mathbf{z} \mid \mathbf{x}, \theta^{(t)}) \mid \mathbf{x}, \theta^{(t-1)}]$$