GMMs by Maximam Likelihood Estimator

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We are trying to find a set of parameters $\boldsymbol{\theta} = \{\boldsymbol{\pi}, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2, ..., \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_K\}$, to maximize the likelihood function:

$$\mathcal{L}(\boldsymbol{\theta}; \boldsymbol{D}) = \prod_{n} P(\boldsymbol{x}_{n} | \boldsymbol{\theta})$$
$$= \prod_{n} \sum_{i} \pi_{i} \mathcal{N}(\boldsymbol{x}_{n} | \boldsymbol{\mu}_{i}, \boldsymbol{\Sigma}_{i})$$

So our optimization task is:

$$\operatorname{arg\,min}_{\boldsymbol{\theta}} - \ell(\boldsymbol{\theta}; \boldsymbol{D})$$

$$s.t. ||\boldsymbol{\pi}|| = 1, |\boldsymbol{\Sigma}_i| \ge 0, i = 1, 2, ..., K$$

To meet the constraints, set auxiliary variables: $\text{vector}\boldsymbol{\alpha}$ and square matrix $\boldsymbol{A}_i,\ i=1,2,...K$. Let $\pi_i = \frac{\exp(\alpha_i)}{\sum_j \exp(\alpha_j)}$, $\boldsymbol{\Sigma}_i = \boldsymbol{A}_i \boldsymbol{A}_i^T$.

Then we can use standard gradient optimization algorithm to find $\hat{\alpha}$, $\hat{\mu}_1$, \hat{A}_1 , $\hat{\mu}_2$, \hat{A}_2 , ..., $\hat{\mu}_K$, \hat{A}_K , then calculate $\hat{\theta} = \{\hat{\pi}, \hat{\mu}_1, \hat{\Sigma}_1, \hat{\mu}_2, \hat{\Sigma}_2, ..., \hat{\mu}_K, \hat{\Sigma}_K\}$.

Predict z for new x:

After finding the ML estimator, we can predict class labels for new input x.

$$P(z|\mathbf{x})$$

$$\propto P(\mathbf{x}|z)P(z)$$

$$=\hat{\pi}_z \mathcal{N}(\mathbf{x}|\hat{\boldsymbol{\mu}}_z, \hat{\boldsymbol{\Sigma}}_z)$$