

# Classtering: Joint Classification and Clustering with Mixture of Factor Analysers

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# Motivation

## Semi-supervised learning (SSL)

Classification

Clustering

- Problem of label propagation
- Cluster assumption

Discriminative

Generative

$$f : y \rightarrow c$$

$$p(c|y) = \frac{p(y|c)p(c)}{Z}$$

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- No wrong label propagation
- Relaxing the cluster assumption

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- Model inter- and intra-class variabilities
- Achieve possibly “good performance”

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Discover the structure of data while preserving the discrimination among classes

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## Why jointly addressing classification and clustering?

**Medicine:** discrimination between healthy and pathological cases is often hard (lack of complete understanding of the pathology, data collection)



Healthy vs. pathological case + Different forms of disease

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Clustering and Classification with limited amount of supervised information

# Model

## **Assumptions:**

1. Class-conditional densities are well approximated by a Gaussian mixture
2. i.i.d. samples
3. Data lie on a manifold



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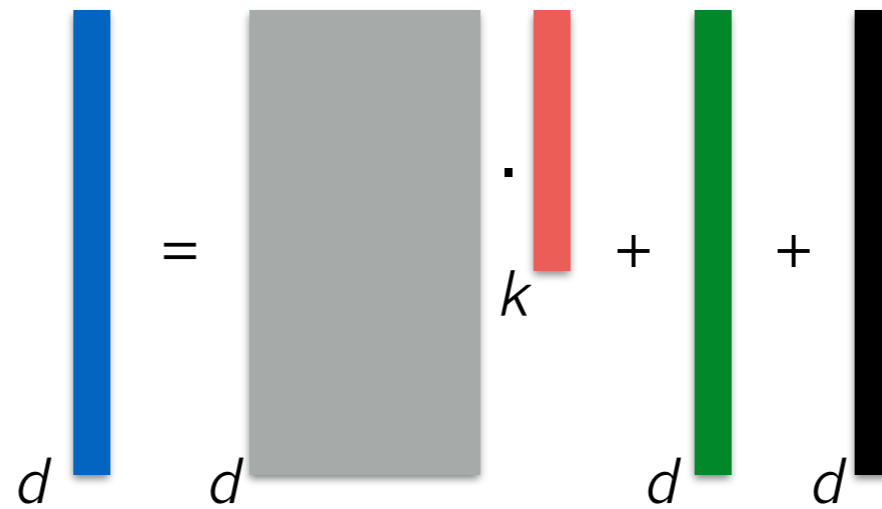
Model based on Mixture of Factor Analysers  
(MFA)

Note: the MFA model is used in unsupervised learning (e.g. model-based clustering, local dimensionality reduction)

# Model

Given an **unlabeled** training dataset  $D = \{\mathbf{y}_n\}_{n=1}^N$

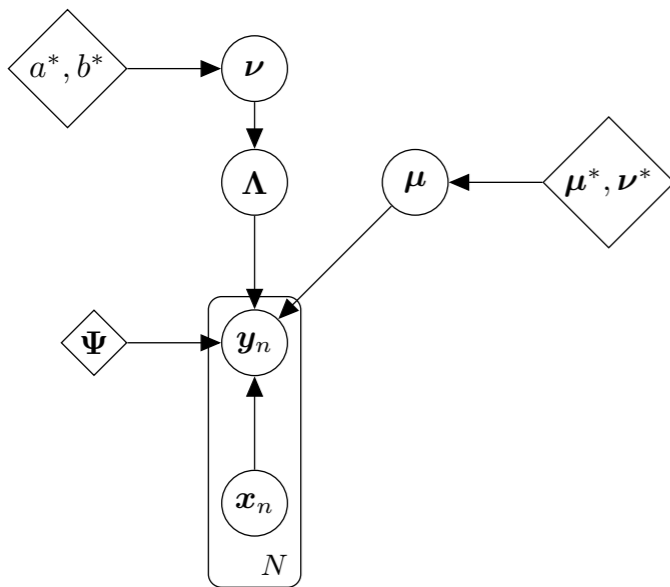
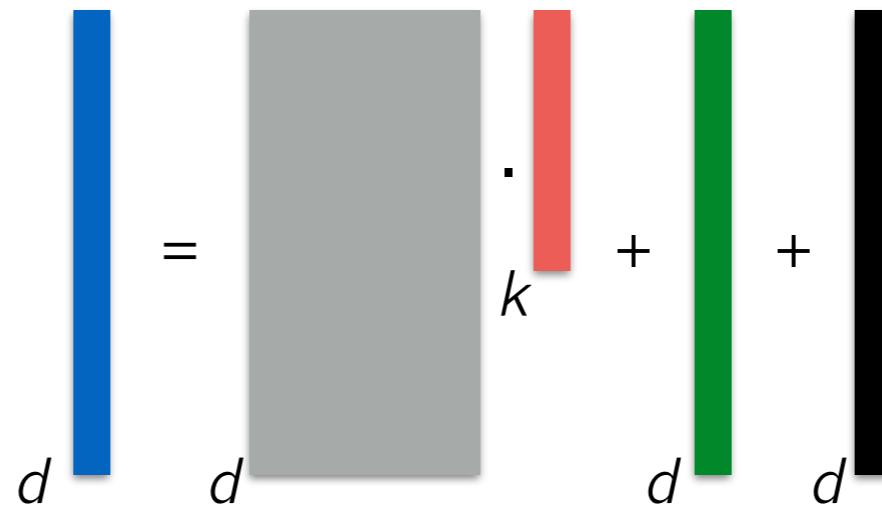
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$$\Lambda \sim \prod_{j=1}^k \mathcal{N}\left(\mathbf{0}, \frac{\mathbf{I}}{\nu(j)}\right)$$

$$\mathbf{x}_n \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\boldsymbol{\mu} \sim \mathcal{N}(\boldsymbol{\mu}^*, \text{diag}(\boldsymbol{\nu}^*)^{-1})$$

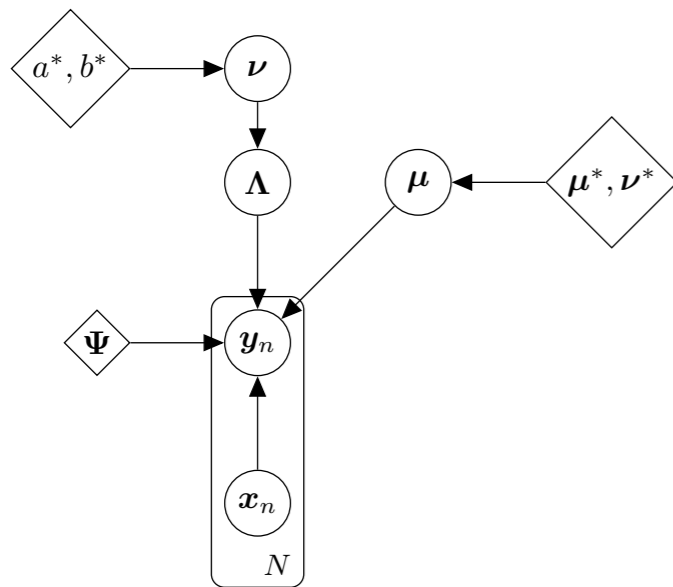
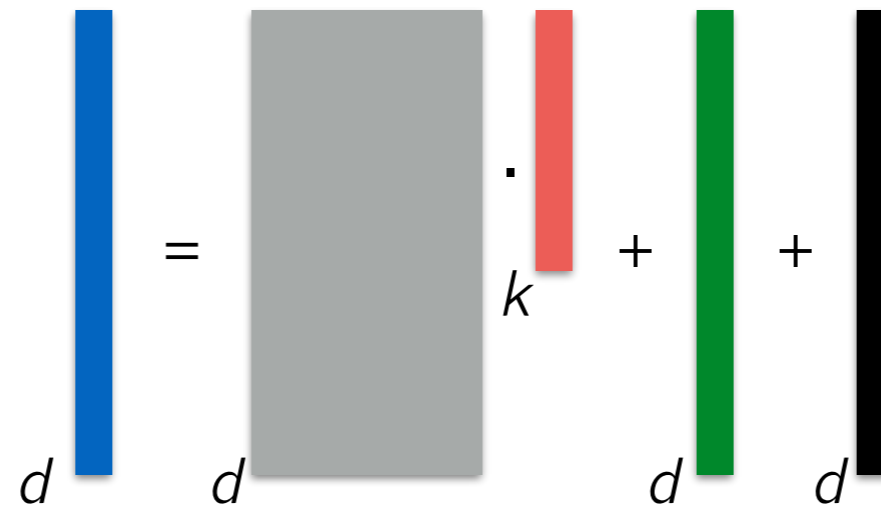
$$\boldsymbol{\xi} \sim \mathcal{N}(\mathbf{0}, \Psi)$$

$$\boldsymbol{\nu} \sim \prod_{j=1}^k \text{Gamma}(\nu(j) | a^*, b^*)$$

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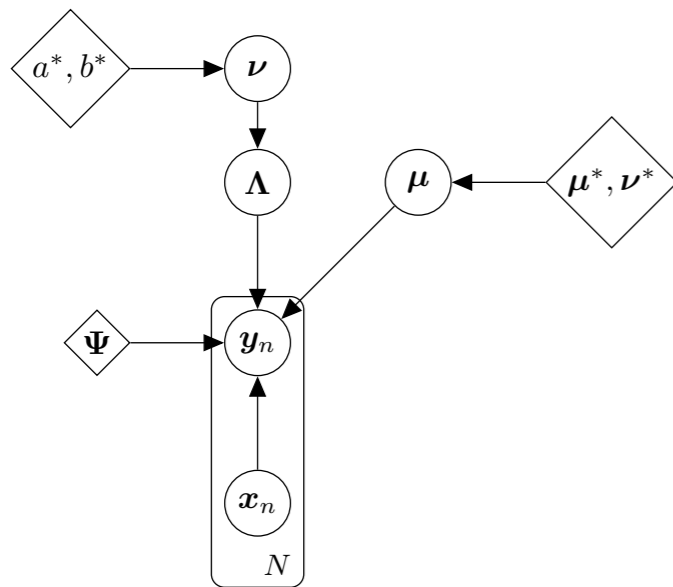
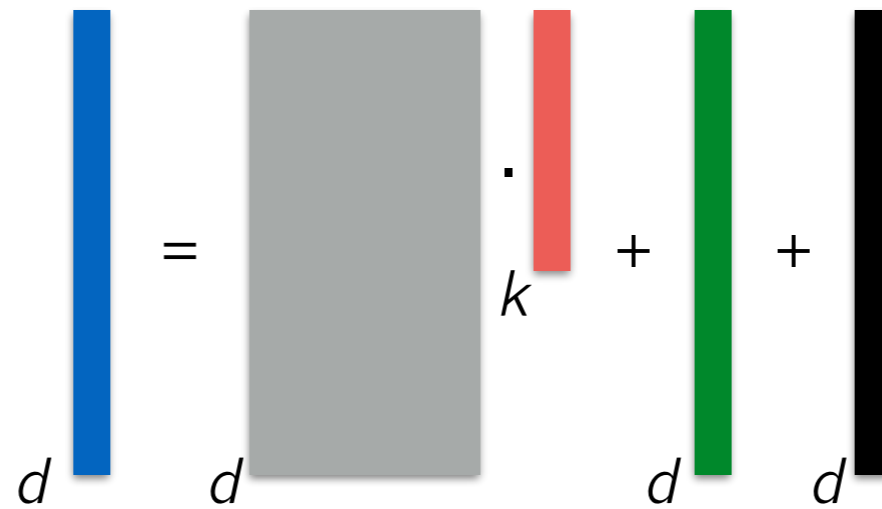
$$p(\mathbf{y}_n | \Lambda, \boldsymbol{\mu}, \Psi) \sim \mathcal{N}(\boldsymbol{\mu}, \Lambda \Lambda' + \Psi)$$

Analyser is described only by  $\Lambda, \boldsymbol{\mu}$

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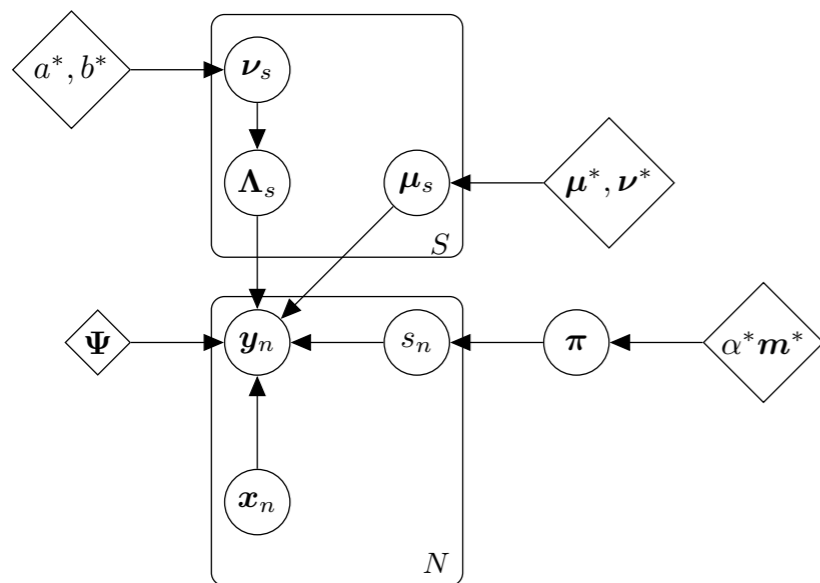
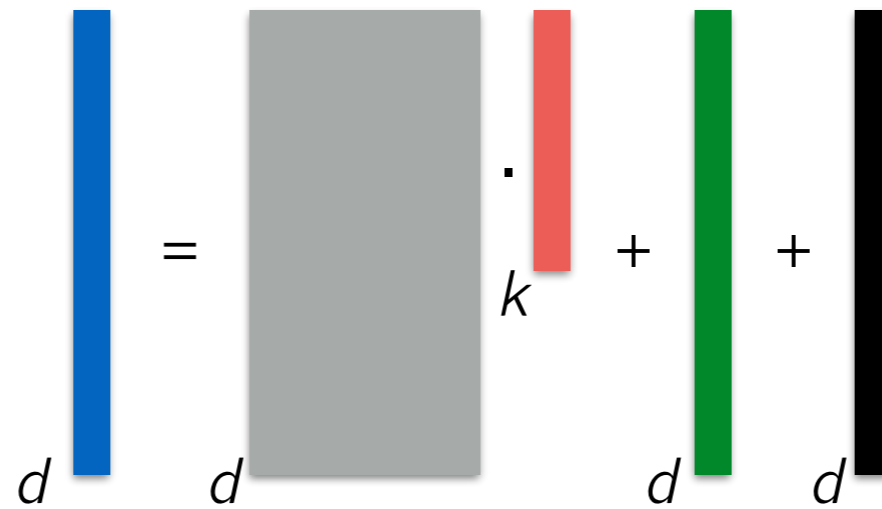
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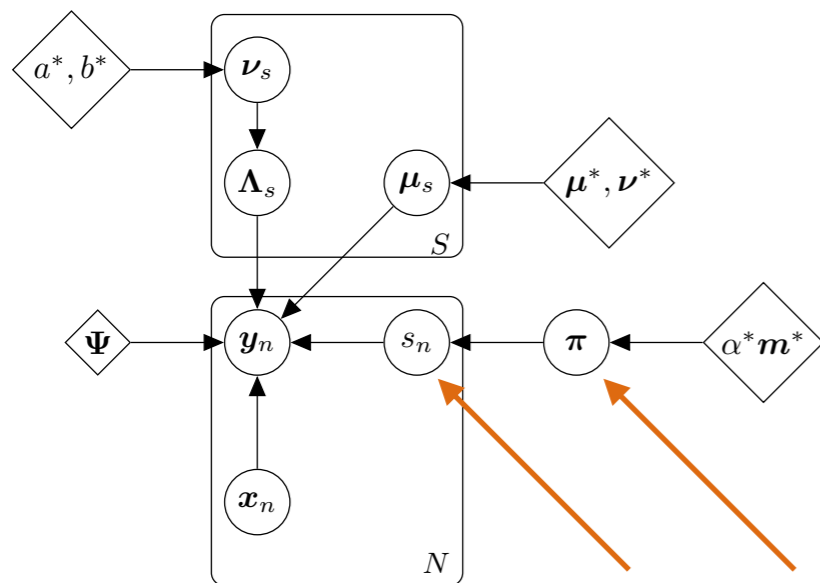
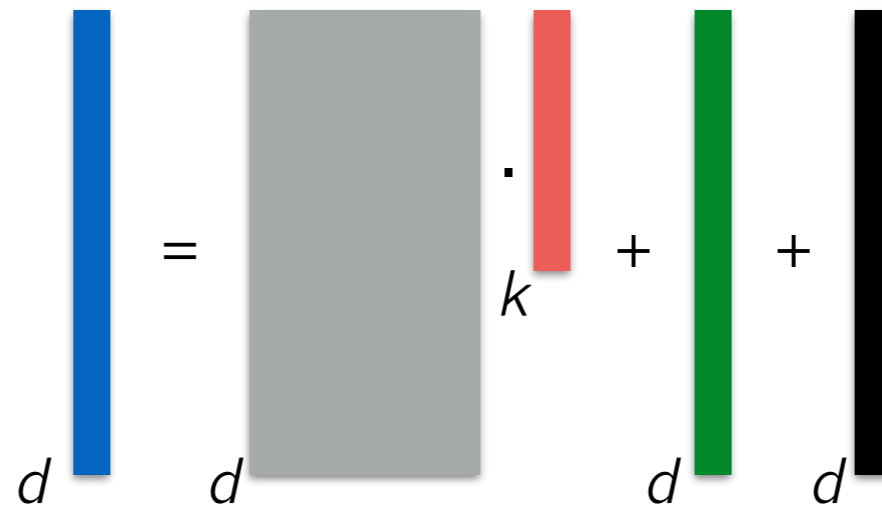
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$$s_n \sim \prod_{s=1}^S \pi_s^{1_{s_n}(s)}$$

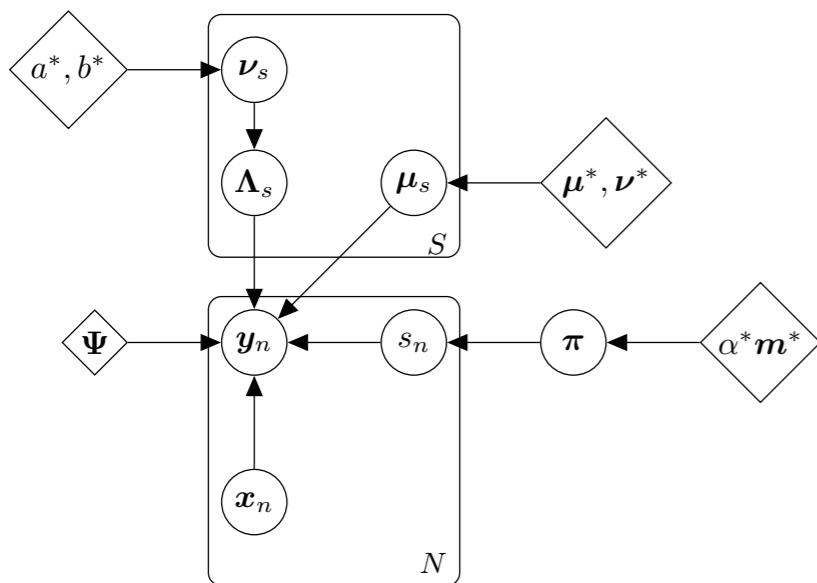
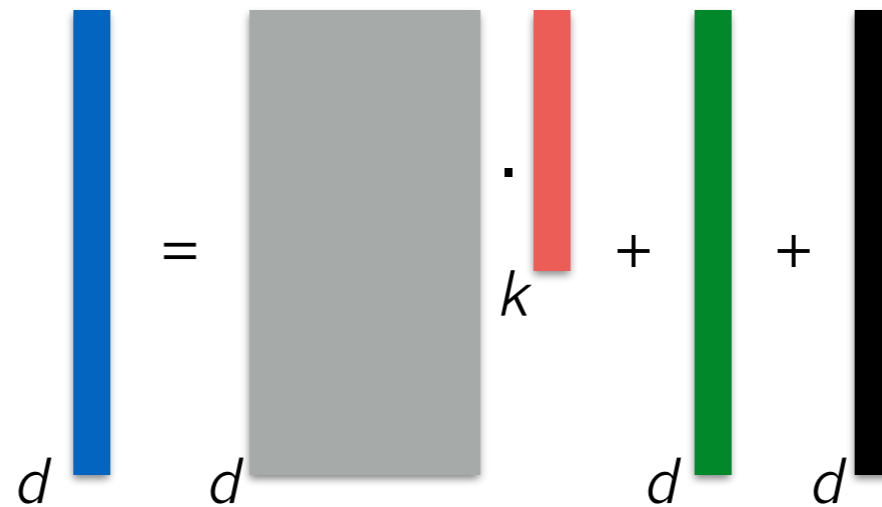
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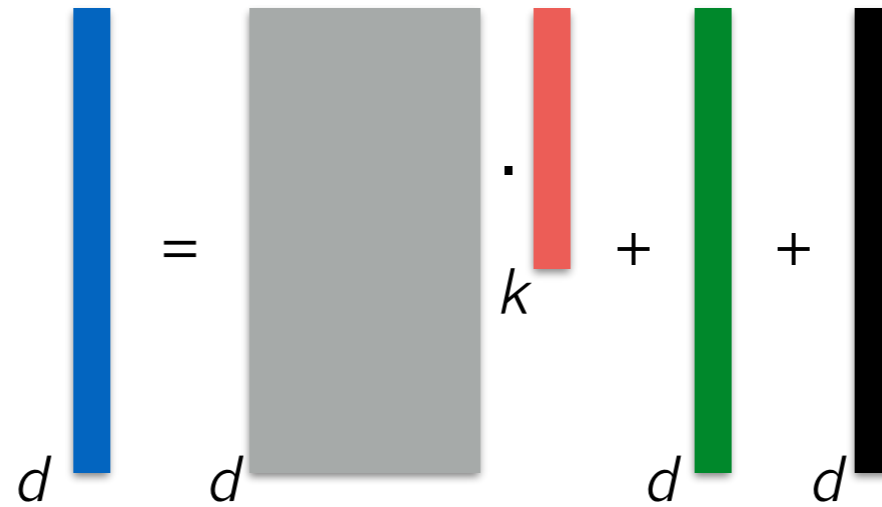
$$p(\mathbf{y}_n | \boldsymbol{\Lambda}, \boldsymbol{\mu}, \boldsymbol{\Psi}) \sim \sum_{s_n=1}^S \pi_{s_n} \mathcal{N}(\boldsymbol{\mu}_{s_n}, \boldsymbol{\Lambda}_{s_n} \boldsymbol{\Lambda}_{s_n}^T + \boldsymbol{\Psi})$$



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Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$

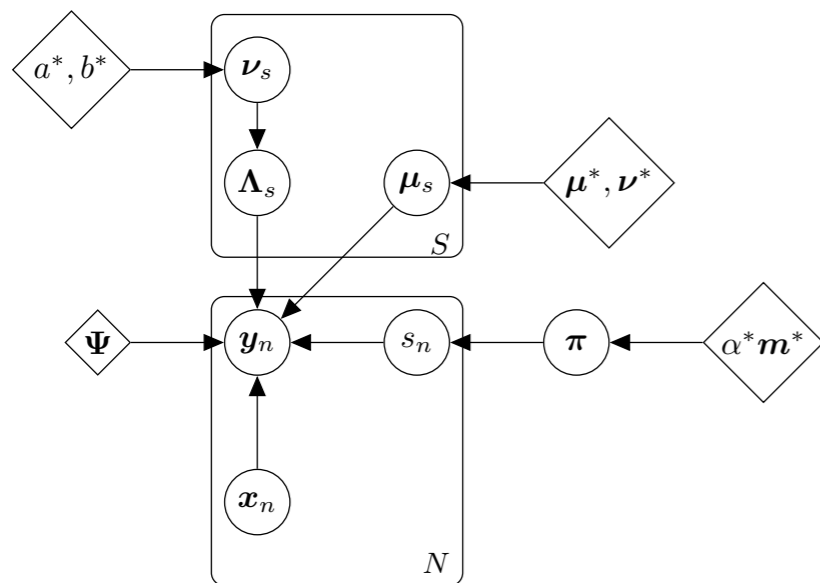
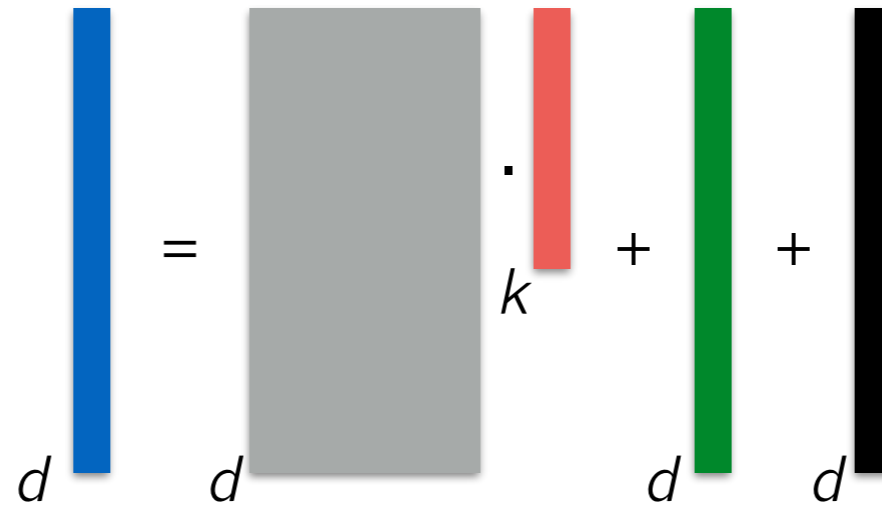
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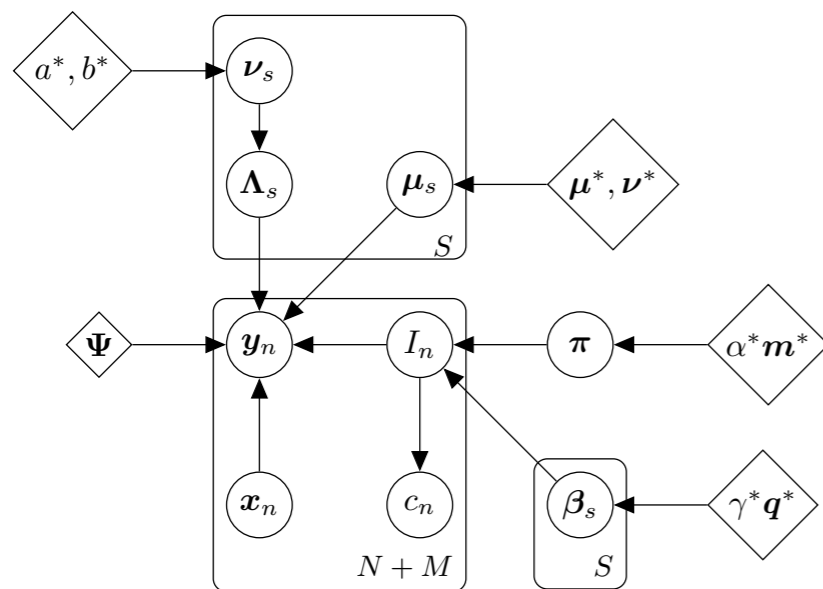


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$$d \quad = \quad d \cdot k \quad + \quad d \quad + \quad d$$

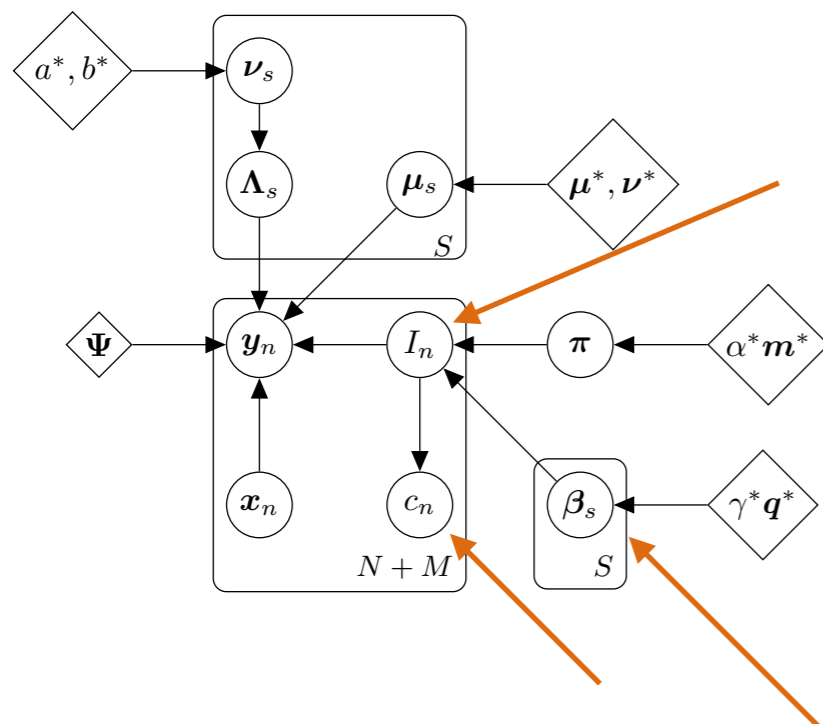


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$$c_n \sim \delta(c_n - \ell_n)$$

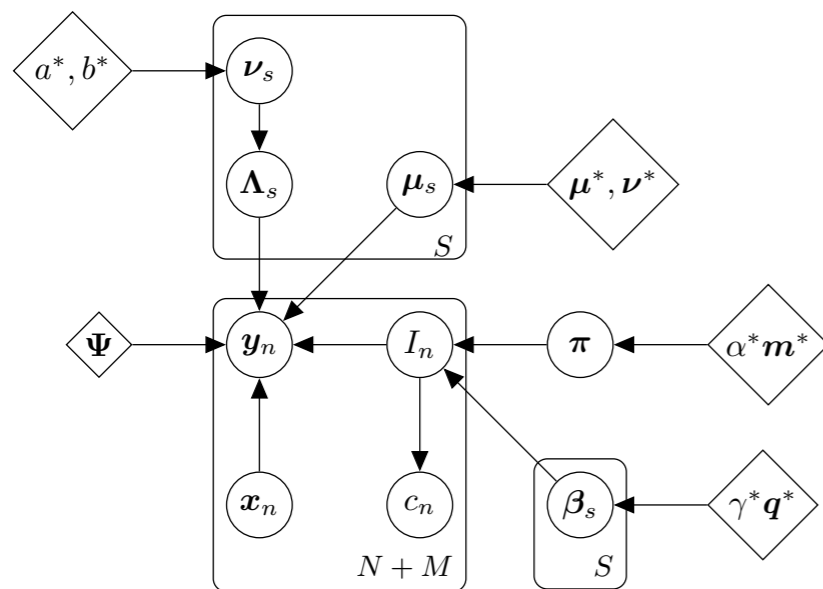
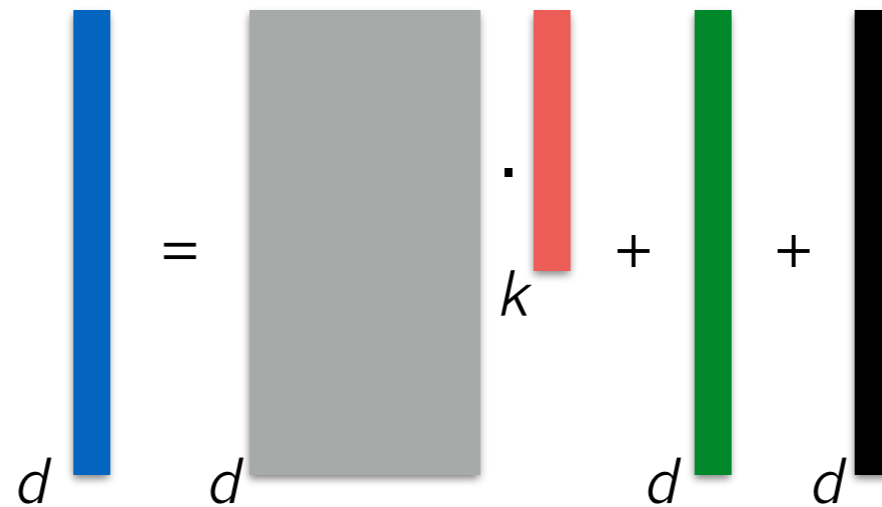
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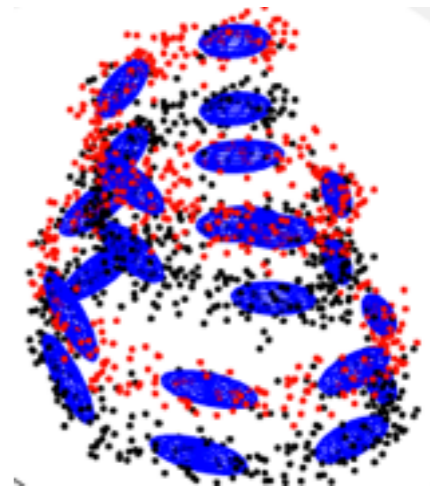
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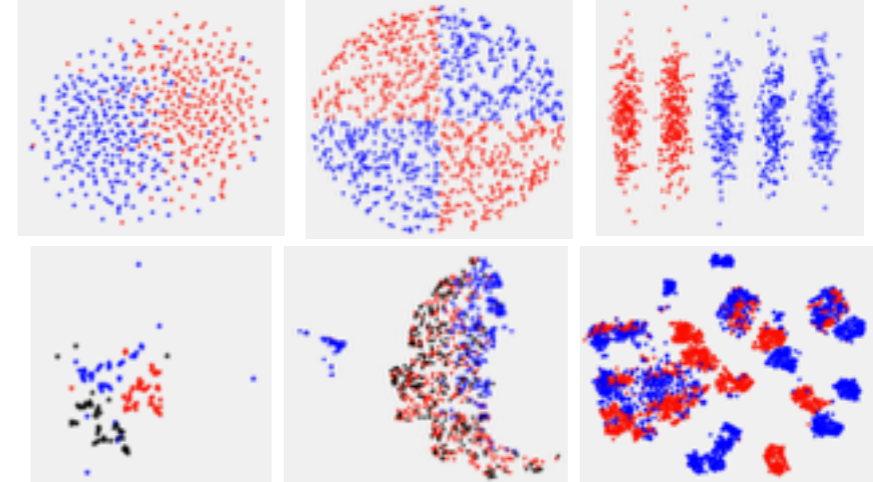


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Information about clusters vs. classes

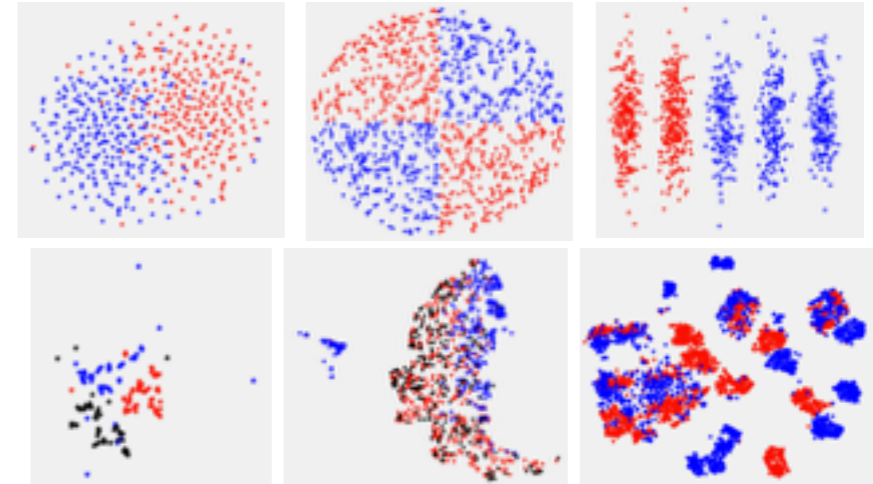
# Experiments

<b>Data sets</b>	<b>Classes</b>	<b>Features</b>	<b>Instances</b>
G50C	2	50	550
CAKE	2	2	1000
TOES	2	2	1000
IRIS	3	4	150
USPS	3	256	1918
ISOLET	2	617	3119

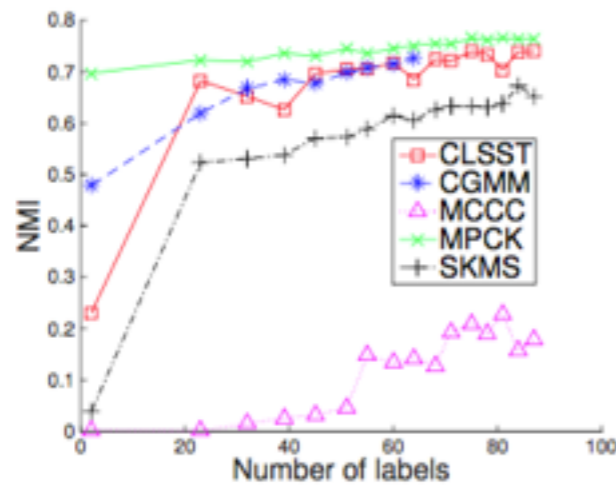


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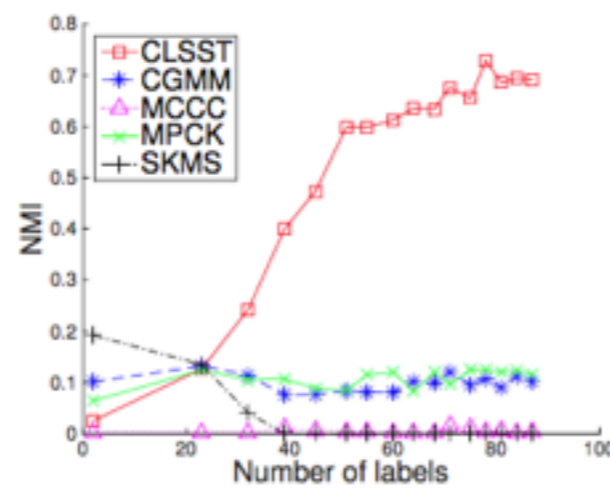
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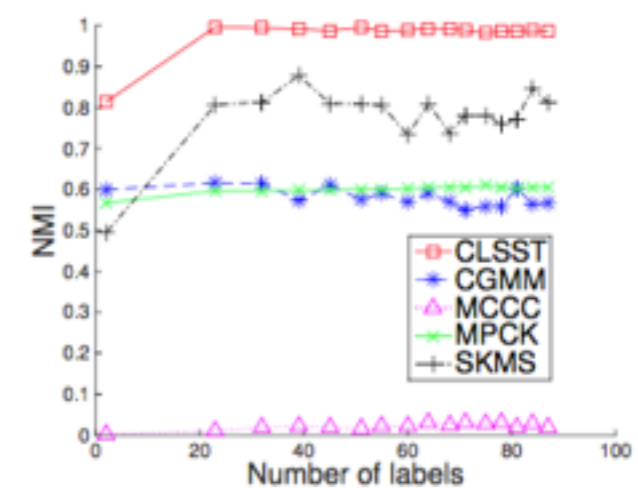
## Clustering



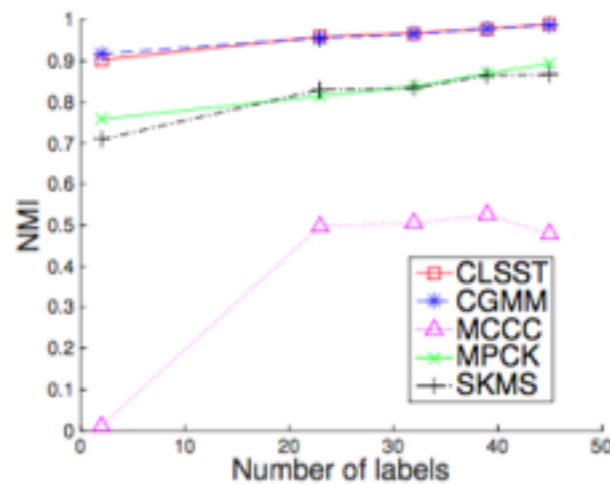
(a) G50C



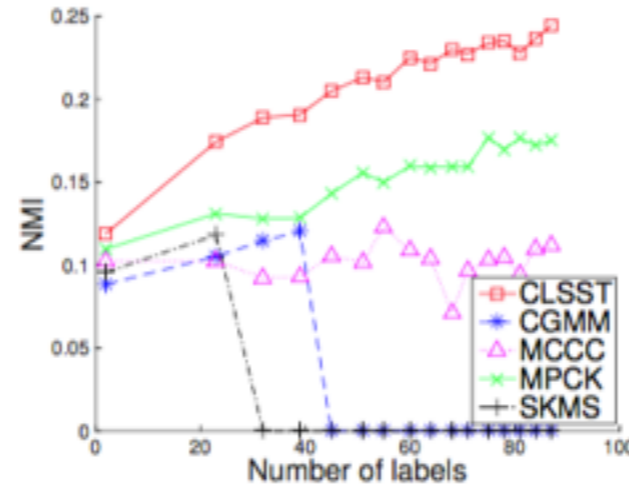
(b) CAKE



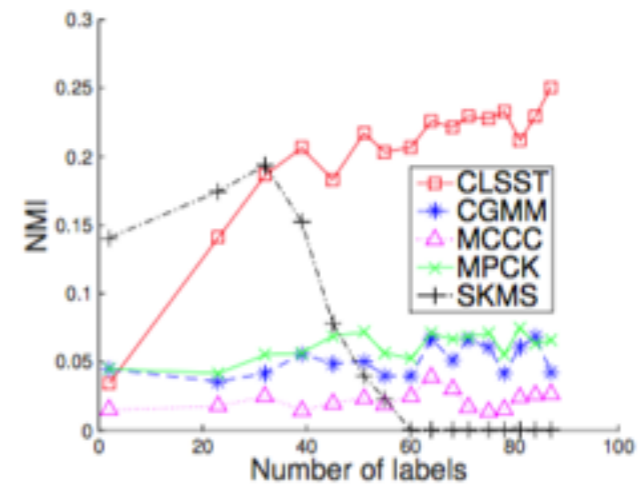
(c) TOES



(d) IRIS



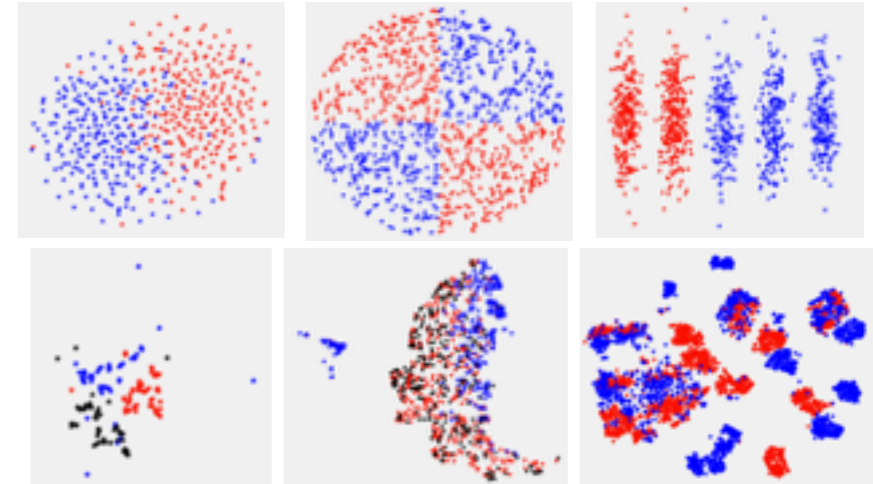
(e) USPS



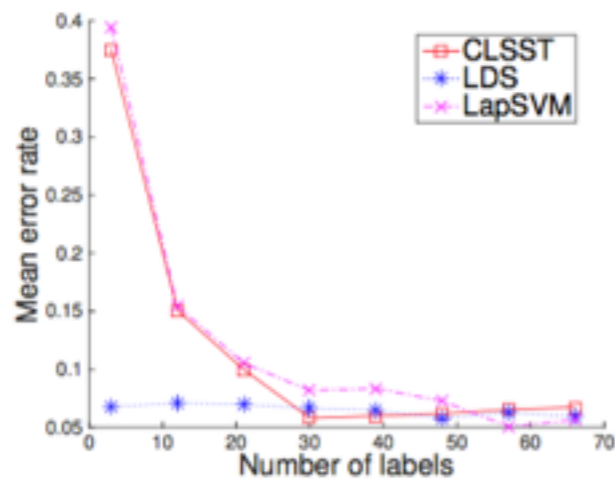
(f) ISOLET

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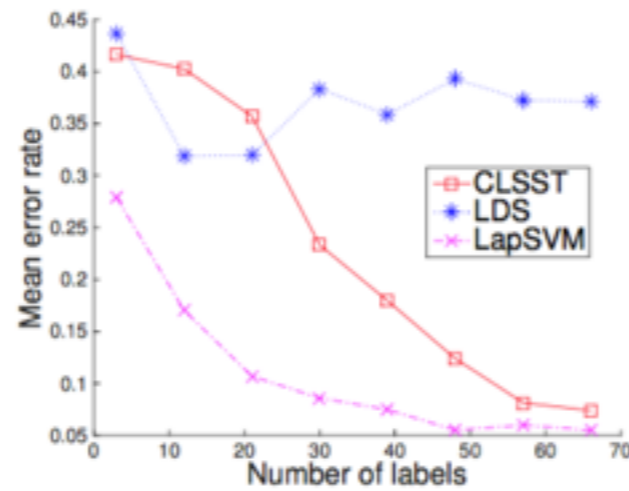
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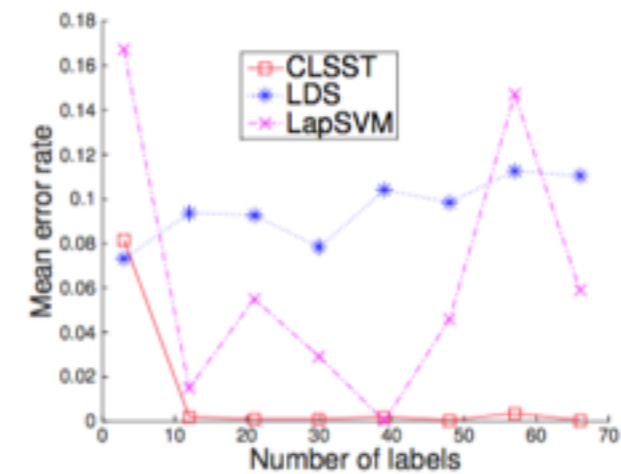
## Classification



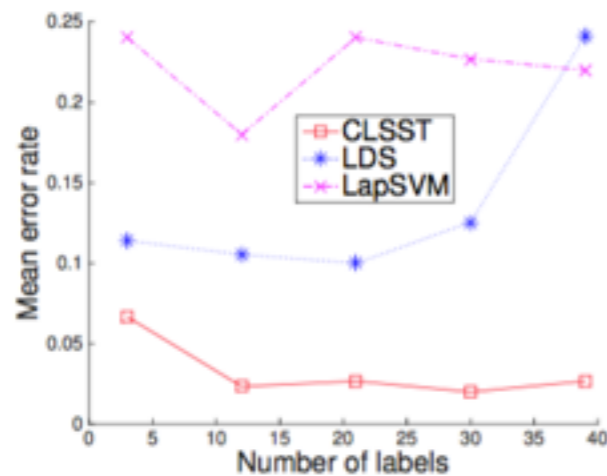
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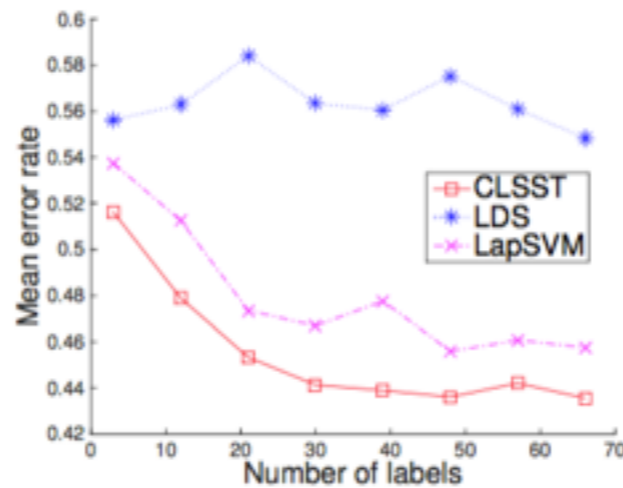
(b) CAKE



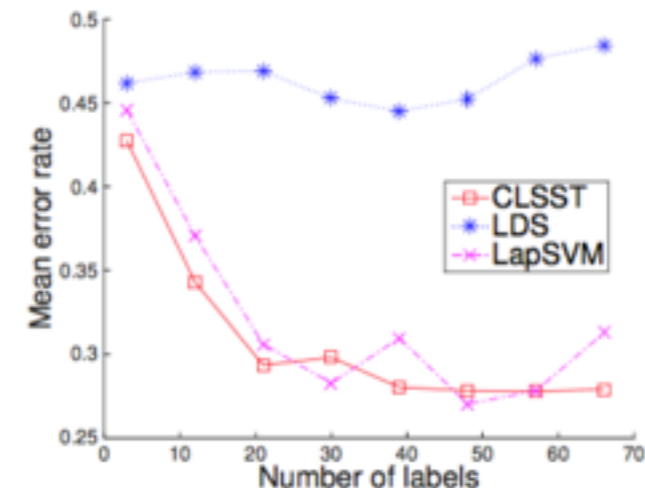
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# Experiments

<b>Dataset</b>	<b>Classes</b>	<b>Features</b>	<b>Instances</b>
Breast cancer (discovery)	5	754	997
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<b>Cluster</b>	<b>[13]</b>	<b>CLSST (fixed <math>S</math>)</b>	<b>CLSST (variable <math>S</math>)</b>
1	0.8235	0.9266	0.9117
2	0.8099	0.8639	0.8377
3	0.7281	0.7899	0.7931
4	0.7091	0.6867	0.7730
5	0.6866	0.6842	0.7624
6	0.6455	0.6794	0.5833
7	0.6015	0.6780	0.5745
8	0.5818	0.6000	-
9	0.5072	0.5965	-
10	0.4481	0.5574	-
<b>Avg.</b>	0.654	<b>0.706</b>	<b>0.748</b>
<b>Min.</b>	0.448	<b>0.557</b>	<b>0.575</b>
<b>Max.</b>	0.824	<b>0.927</b>	<b>0.912</b>

IGP is increased at least of 5%! But further analysis is required to prove the biological relevance.

## Conclusions & Future work

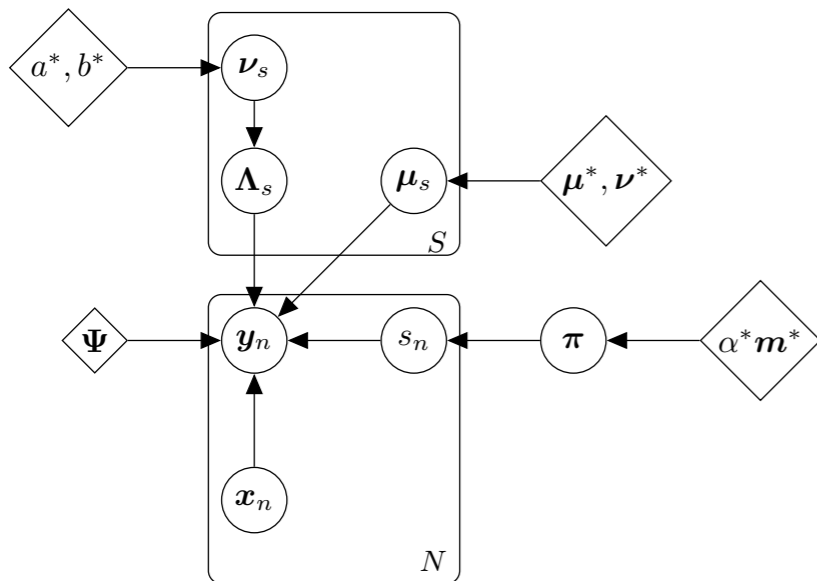
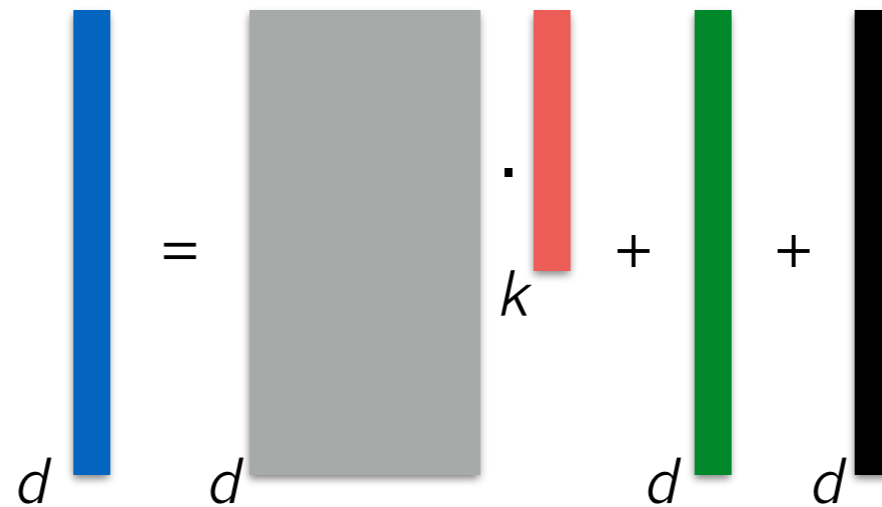
- Proposed model based on MFA for SSL (clustering/classification)
- Clustering: handling multi-groups per class + problem of cluster assumption
- Classification: discovered clusters help classification (comparison with discriminative approaches)
- Real-world problem: promising results (future research)

**Thank You**

# Model

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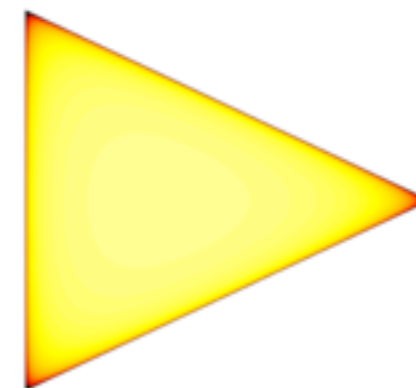


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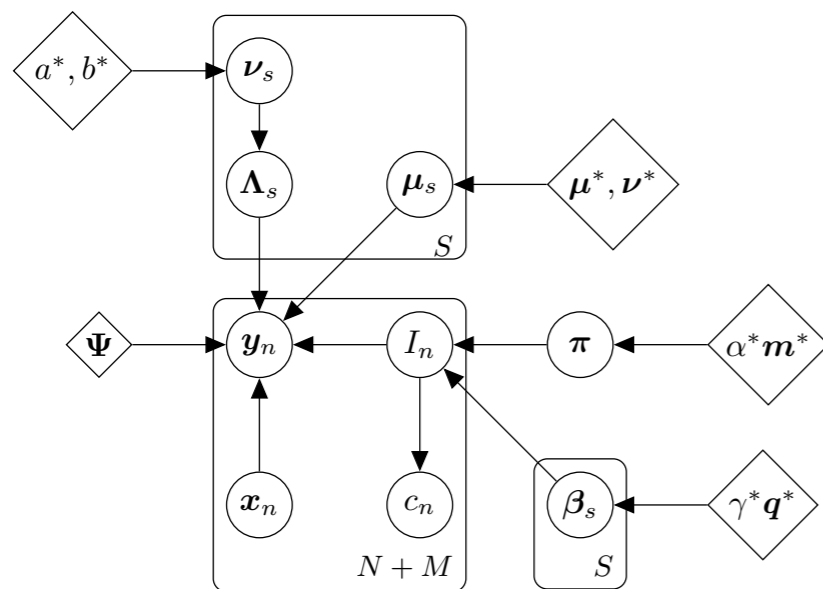
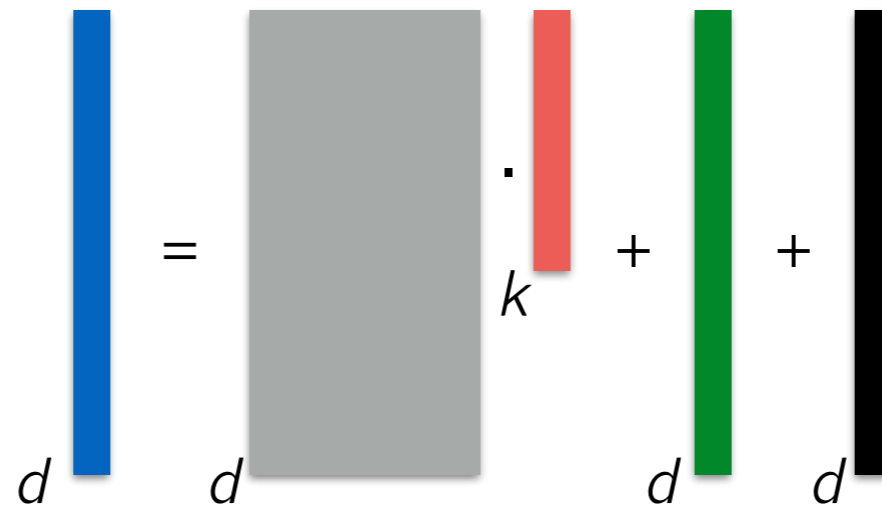
Example with  $S = 3, \alpha^* = 2.1$



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Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$

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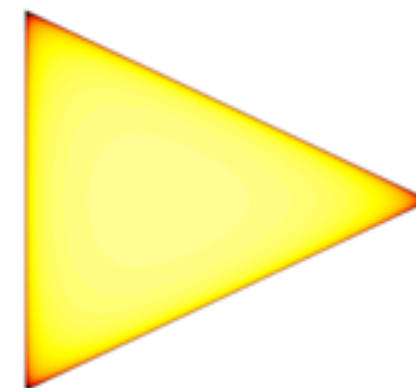
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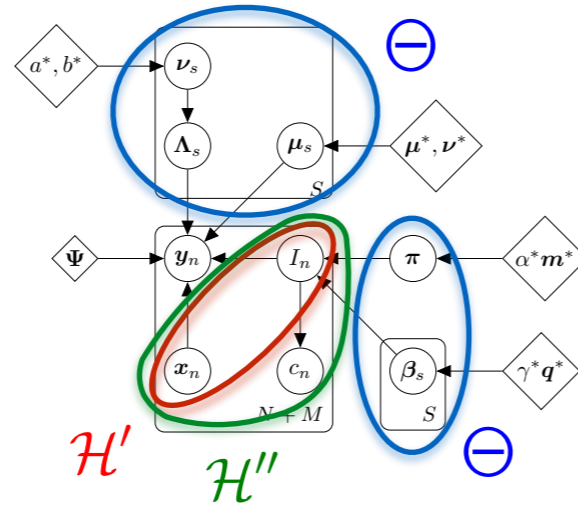
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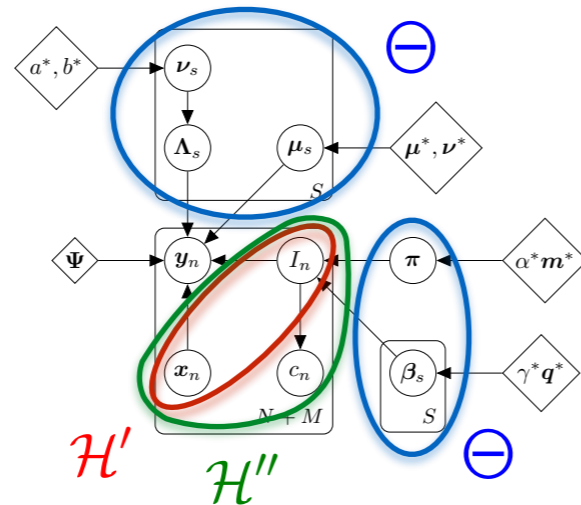
$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

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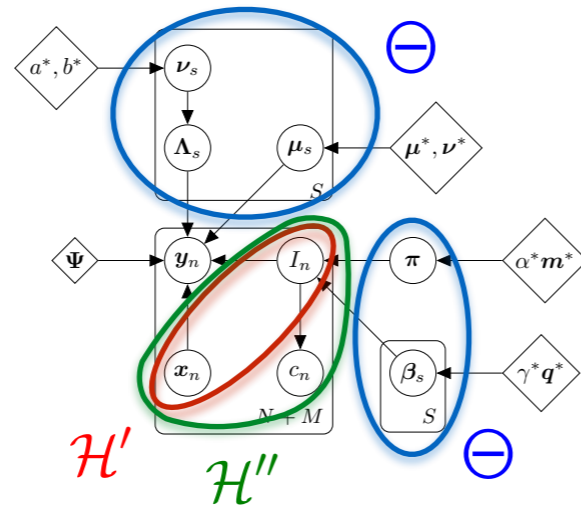
$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, \ell_n), c_n\}_{n=N+1}^M$$

$$\begin{aligned} \log p(D', D'') &= \log \int_{\Theta, \mathcal{H}', \mathcal{H}''} p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'') \\ &= \log \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} \\ &\geq \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} = \mathcal{F}(q(\cdot)) \end{aligned}$$



# Inference

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, l_n), c_n\}_{n=N+1}^M$$

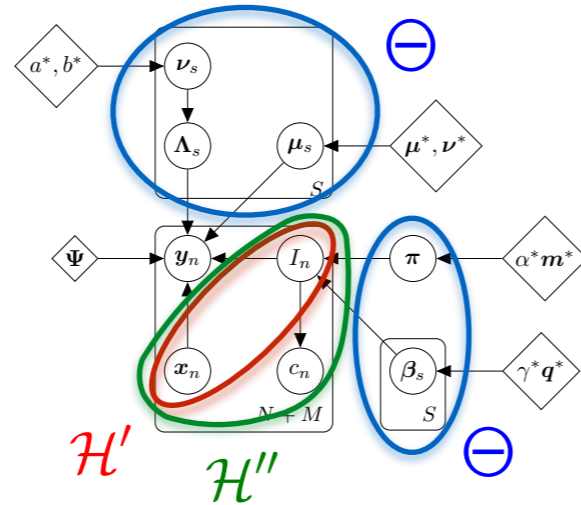
$$\begin{aligned} \log p(D', D'') &= \log \int_{\Theta, \mathcal{H}', \mathcal{H}''} p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'') \\ &= \log \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} \\ &\geq \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} = \mathcal{F}(q(\cdot)) \end{aligned}$$

- Lower bound on the log-likelihood function
- Equality holds when  $q(\Theta, \mathcal{H}', \mathcal{H}'') = p(\Theta, \mathcal{H}', \mathcal{H}'' | D', D'')$
- Given conditional independence properties of graph  $q(\Theta, \mathcal{H}', \mathcal{H}'') = q(\Theta)q(\mathcal{H}' | \Theta)q(\mathcal{H}'' | \Theta)$
- Strict inequality holds in general for:

$$q(\Theta) = q(\pi) \prod_{s=1}^S q(\beta_s) q(\nu_s) q(\Lambda_s, \mu_s) \quad q(\mathcal{H}' | \Theta) = \prod_{n=1}^N q(s_n) q(\mathbf{x}_n | s_n) \quad q(\mathcal{H}'' | \Theta) = \prod_{n=1}^N q(l_n) q(\mathbf{x}_n | l_n)$$

# Inference

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

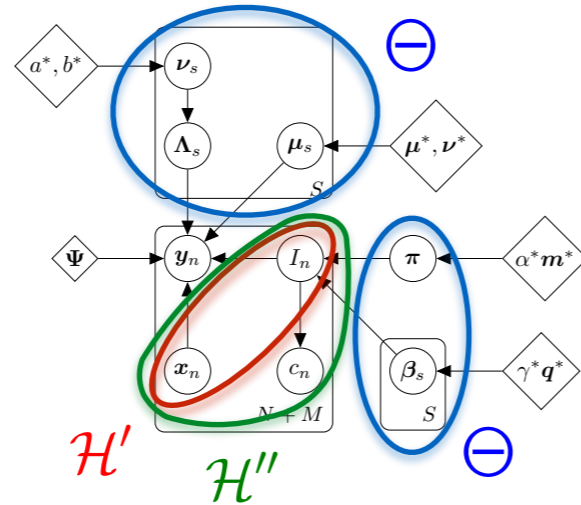
$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, \ell_n), c_n\}_{n=N+1}^M$$

$$\begin{aligned} \log p(D', D'') &= \log \int_{\Theta, \mathcal{H}', \mathcal{H}''} p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'') \\ &= \log \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} \\ &\geq \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} = \mathcal{F}(q(\cdot)) \end{aligned}$$

$$q(\Theta, \mathcal{H}', \mathcal{H}'') = q(\Theta)q(\mathcal{H}'|\Theta)q(\mathcal{H}''|\Theta)$$

# Inference

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

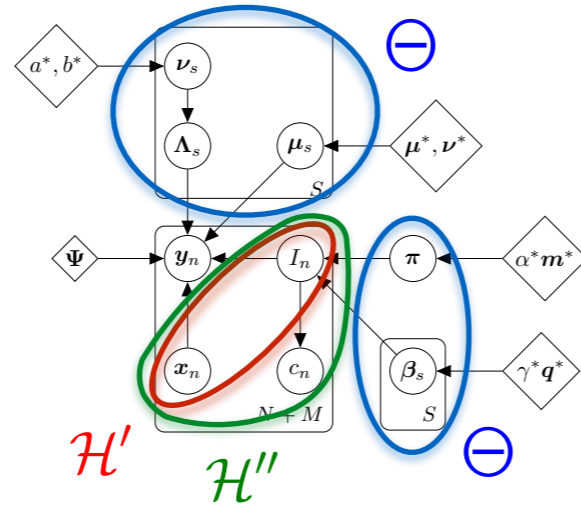
$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, \ell_n), c_n\}_{n=N+1}^M$$

$$\begin{aligned} \mathcal{F}(q(\cdot)) &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} \\ &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta) \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta)} \\ &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta) \log \frac{p(D' | \Theta, \mathcal{H}') p(D'' | \Theta, \mathcal{H}'') p(\mathcal{H}' | \Theta) p(\mathcal{H}'' | \Theta) p(\Theta)}{q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta)} \\ &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta) \left[ \log \frac{p(\Theta)}{q(\Theta)} + \log \frac{p(D' | \Theta, \mathcal{H}') p(\mathcal{H}' | \Theta)}{q(\mathcal{H}' | \Theta)} + \log \frac{p(D'' | \Theta, \mathcal{H}'') p(\mathcal{H}'' | \Theta)}{q(\mathcal{H}'' | \Theta)} \right] \\ &= \int_{\Theta} q(\Theta) \left[ \log \frac{p(\Theta)}{q(\Theta)} + \int_{\mathcal{H}'} q(\mathcal{H}' | \Theta) \log \frac{p(D' | \Theta, \mathcal{H}') p(\mathcal{H}' | \Theta)}{q(\mathcal{H}' | \Theta)} + \int_{\mathcal{H}''} q(\mathcal{H}'' | \Theta) \log \frac{p(D'' | \Theta, \mathcal{H}'') p(\mathcal{H}'' | \Theta)}{q(\mathcal{H}'' | \Theta)} \right] \end{aligned}$$

$$q(\Theta, \mathcal{H}', \mathcal{H}'') = q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta)$$

# Inference

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

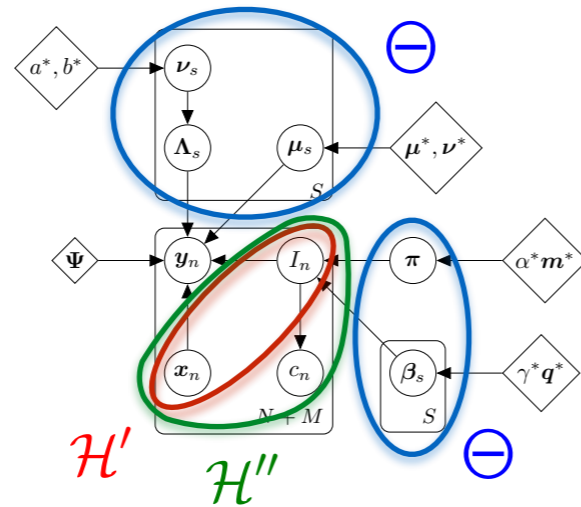
$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, \ell_n), c_n\}_{n=N+1}^M$$

$$\begin{aligned} \mathcal{F}(q(\cdot)) &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta, \mathcal{H}', \mathcal{H}'') \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta, \mathcal{H}', \mathcal{H}'')} \\ &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta) \log \frac{p(D', D'', \Theta, \mathcal{H}', \mathcal{H}'')}{q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta)} \\ &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta) \log \frac{p(D' | \Theta, \mathcal{H}') p(D'' | \Theta, \mathcal{H}'') p(\mathcal{H}' | \Theta) p(\mathcal{H}'' | \Theta) p(\Theta)}{q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta)} \\ &= \int_{\Theta, \mathcal{H}', \mathcal{H}''} q(\Theta) q(\mathcal{H}' | \Theta) q(\mathcal{H}'' | \Theta) \left[ \log \frac{p(\Theta)}{q(\Theta)} + \log \frac{p(D' | \Theta, \mathcal{H}') p(\mathcal{H}' | \Theta)}{q(\mathcal{H}' | \Theta)} + \log \frac{p(D'' | \Theta, \mathcal{H}'') p(\mathcal{H}'' | \Theta)}{q(\mathcal{H}'' | \Theta)} \right] \\ &= \int_{\Theta} q(\Theta) \left[ \log \frac{p(\Theta)}{q(\Theta)} + \int_{\mathcal{H}'} q(\mathcal{H}' | \Theta) \log \frac{p(D' | \Theta, \mathcal{H}') p(\mathcal{H}' | \Theta)}{q(\mathcal{H}' | \Theta)} + \int_{\mathcal{H}''} q(\mathcal{H}'' | \Theta) \log \frac{p(D'' | \Theta, \mathcal{H}'') p(\mathcal{H}'' | \Theta)}{q(\mathcal{H}'' | \Theta)} \right] \end{aligned}$$

Compute functional derivatives with respect to  $q(\Theta)$ ,  $q(\mathcal{H}' | \Theta)$ ,  $q(\mathcal{H}'' | \Theta)$  and equate them to 0.

# Prediction

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

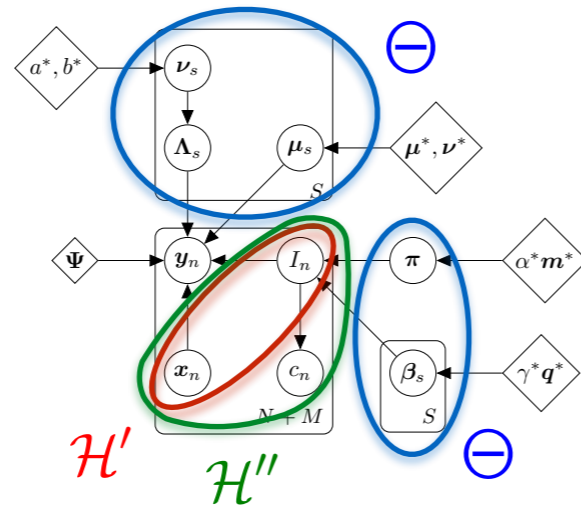
$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, \ell_n), c_n\}_{n=N+1}^M$$

$$q(\Theta), q(\mathcal{H}'|\Theta), q(\mathcal{H}''|\Theta)$$

# Prediction

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, l_n), c_n\}_{n=N+1}^M$$

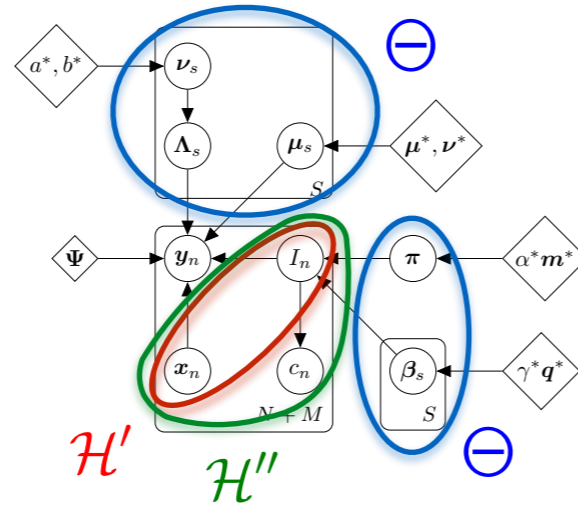
$$q(\Theta), q(\mathcal{H}'|\Theta), q(\mathcal{H}''|\Theta)$$



$$\begin{aligned} \log p(\mathbf{y}_t | D', D'') &= \log \int_{\Theta, \{\mathbf{x}_t, l_t\}} p(\mathbf{y}_t, \mathbf{x}_t, l_t, \Theta | D', D'') \\ &= \log \int_{\Theta} p(\Theta | D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} p(\mathbf{y}_t, \mathbf{x}_t, l_t, \Theta | D', D'') \right] \\ &= \log \int_{\Theta} p(\Theta | D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \frac{p(\mathbf{y}_t, \mathbf{x}_t, l_t, \Theta | D', D'')}{q(\mathbf{x}_t, l_t)} \right] \\ &= \log \int_{\Theta} p(\Theta | D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \frac{p(\mathbf{y}_t | \mathbf{x}_t, l_t, \Theta) p(\mathbf{x}_t, l_t | \Theta)}{q(\mathbf{x}_t, l_t)} \right] \\ &\geq \int_{\Theta} p(\Theta | D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \log \frac{p(\mathbf{y}_t | \mathbf{x}_t, l_t, \Theta) p(\mathbf{x}_t, l_t | \Theta)}{q(\mathbf{x}_t, l_t)} \right] \\ &\approx \int_{\Theta} q(\Theta) \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \log \frac{p(\mathbf{y}_t | \mathbf{x}_t, l_t, \Theta) p(\mathbf{x}_t, l_t | \Theta)}{q(\mathbf{x}_t, l_t)} \right] \end{aligned}$$

# Prediction

Given two sets: **labeled**  $D' = \{(\mathbf{y}_n, c_n)\}_{n=1}^N$  and **unlabeled**  $D'' = \{\mathbf{y}_n\}_{n=N+1}^M$



$$\Theta = \{\pi\} \cup \{\beta_s, \Lambda_s, \mu_s, \nu_s\}_{s=1}^S$$

$$\mathcal{H}' = \{\mathbf{x}_n, s_n\}_{n=1}^N$$

$$\mathcal{H}'' = \{\mathbf{x}_n, (s_n, \ell_n), c_n\}_{n=N+1}^M$$

$$q(\Theta), q(\mathcal{H}'|\Theta), q(\mathcal{H}''|\Theta)$$



$$\begin{aligned} \log p(\mathbf{y}_t|D', D'') &= \log \int_{\Theta, \{\mathbf{x}_t, l_t\}} p(\mathbf{y}_t, \mathbf{x}_t, l_t, \Theta|D', D'') \\ &= \log \int_{\Theta} p(\Theta|D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} p(\mathbf{y}_t, \mathbf{x}_t, l_t, \Theta|D', D'') \right] \\ &= \log \int_{\Theta} p(\Theta|D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \frac{p(\mathbf{y}_t, \mathbf{x}_t, l_t, \Theta|D', D'')}{q(\mathbf{x}_t, l_t)} \right] \\ &= \log \int_{\Theta} p(\Theta|D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \frac{p(\mathbf{y}_t|\mathbf{x}_t, l_t, \Theta)p(\mathbf{x}_t, l_t|\Theta)}{q(\mathbf{x}_t, l_t)} \right] \\ &\geq \int_{\Theta} p(\Theta|D', D'') \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \log \frac{p(\mathbf{y}_t|\mathbf{x}_t, l_t, \Theta)p(\mathbf{x}_t, l_t|\Theta)}{q(\mathbf{x}_t, l_t)} \right] \\ &\approx \int_{\Theta} q(\Theta) \left[ \int_{\{\mathbf{x}_t, l_t\}} q(\mathbf{x}_t, l_t) \log \frac{p(\mathbf{y}_t|\mathbf{x}_t, l_t, \Theta)p(\mathbf{x}_t, l_t|\Theta)}{q(\mathbf{x}_t, l_t)} \right] \end{aligned}$$

Compute  $q(\mathbf{x}_t, l_t)$  for a test sample