Multivariate Modelling: Latent Variables & Dimensionality Reduction

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Introduction to Neuroimaging

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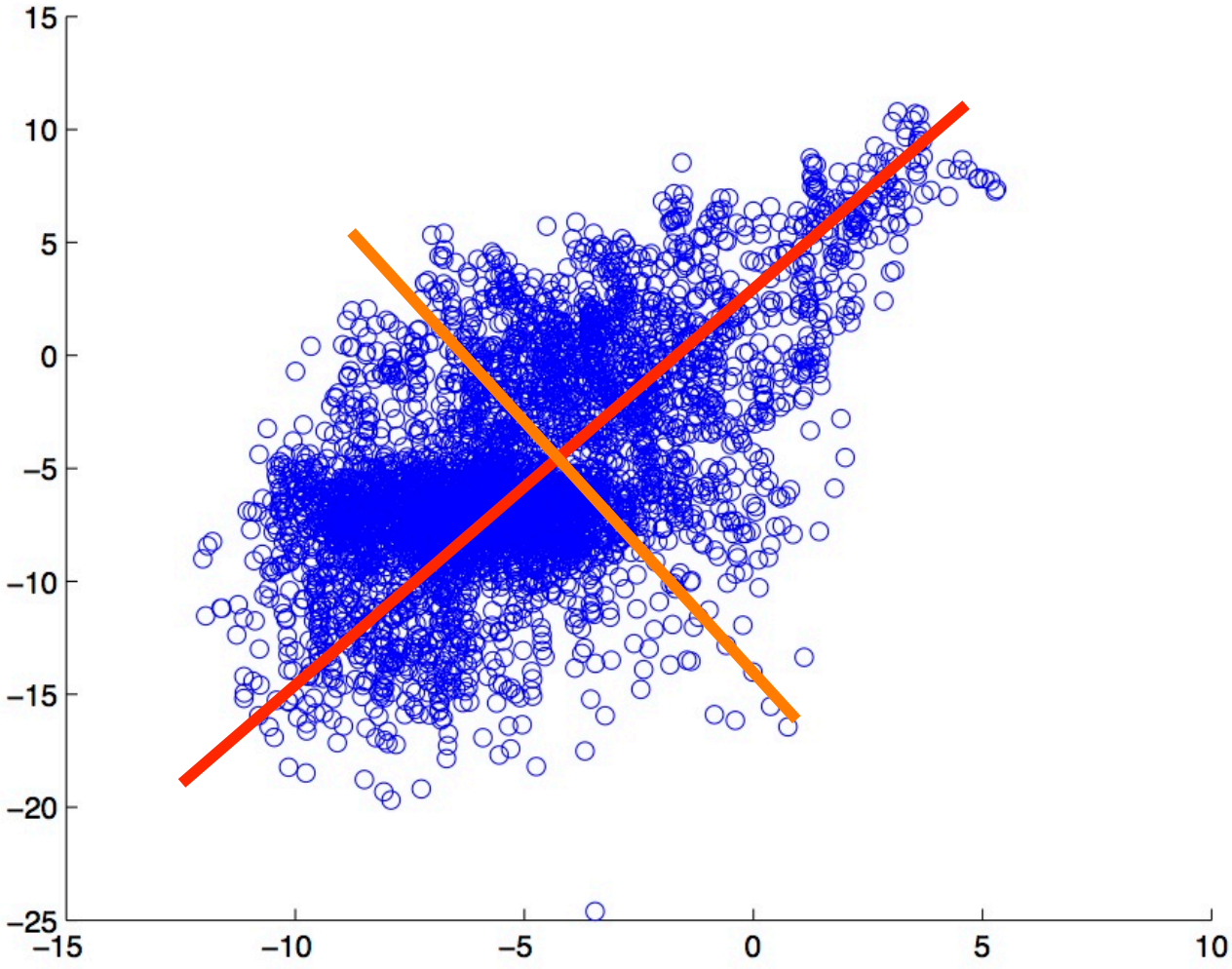
Latent Variable Modelling

- Model high dimensional Y with a lower-dimensional approximation F that has N rows, but typically far fewer columns
- Latent variable modelling is used for:
  - Dimensionality reduction: replace Y with a lower-dimensional F
  - Outlier detection
  - Data visualization: display F in a scatterplot.
  - Factor discovering: discover important hidden **factors** underlying data.

PCA

Projects the data into a sub-space such that the projected data has maximum variance.



Principal Component Analysis (PCA)

- Projects the data into a sub-space such that the projected data has maximum variance.

$$\Upsilon \approx F\Lambda',$$

where $\Upsilon \in \mathbb{R}^{N\times P}$; $\Lambda \in \mathbb{R}^{P\times K}$ principal axis; $F \in \mathbb{R}^{N\times K}$ and $K << P$. PCA derivations:

- choose Λ minimizes construction error: $\text{argmin}\|\Upsilon - F\Lambda'\|_{\text{F}}^2$
- choose Λ maximises the variance: $\text{argmax}\sum_{i=1}^{N}\|\Lambda'\Upsilon_i\|^2 = \text{Tr}(\Lambda'\Upsilon'\Upsilon\Lambda)$
- Λ is the eigenvetor of sample covariance matrix $S = \frac{1}{N}\Upsilon'\Upsilon$

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Factor Analysis (FA)

Describes the correlation among variables using few latent variables. Projects the data into a space that are not correlated

$$\boldsymbol{y}_i = \boldsymbol{f}_i \boldsymbol{\Lambda}' + \boldsymbol{\epsilon}_i, \tag{1}$$

where $k \ll N$ is; $\boldsymbol{f}_t \in \mathbb{R}^K$ is the k vector of latent variables (scores); and $\boldsymbol{\Lambda} \in \mathbb{R}^{P \times k}$ is the loadings matrix. It is assumed that

- Latent variables are independent $\boldsymbol{f}_i \sim N(\boldsymbol{0}, \boldsymbol{I}_{k \times k})$
- Residuals are independent with $\boldsymbol{\epsilon}_t \sim N(\boldsymbol{0}, \boldsymbol{\Psi})$ where $\boldsymbol{\Psi} = \text{diag}(\sigma_1^2, \cdots, \sigma_P^2)$
- The latent variables and residuals are mutually independent $\text{Cov}(\boldsymbol{f}_t, \boldsymbol{\epsilon}_s) = 0$ for all t and s.

Factor Analysis

The FA model:

$$\boldsymbol{y}_i = \boldsymbol{f}_i \boldsymbol{\Lambda}' + \boldsymbol{\epsilon}_i,$$

- $\boldsymbol{y}_i | \boldsymbol{f}_i \sim \mathcal{N}(\boldsymbol{f}_i \Lambda', \boldsymbol{\Psi})$
- $\boldsymbol{y_i} \sim \mathcal{N}(0, \Sigma)$, $\Sigma = \Lambda\Lambda' + \boldsymbol{\Psi}$
- log-likelihood function

$$l(\Lambda, \boldsymbol{\Psi}) \propto -\frac{N}{2} \log |\boldsymbol{\Psi}| - \frac{N}{2} \mathrm{Tr}(S\boldsymbol{\Psi}^{-1})$$

  where $S = \frac{1}{N} \boldsymbol{Y}' \boldsymbol{Y}$ is the sample covariance matrix
- Parameter estimation: Maximise likelihood function
- Varimax rotation for interpretation

Dimensionality Reduction: Unified Approach

$$
\begin{aligned}
\boldsymbol{Y} &= \boldsymbol{F}\Lambda' + \boldsymbol{E}, \\
\boldsymbol{F} &\sim \mathcal{N}(\boldsymbol{0}, I), \quad E \sim \mathcal{N}(\boldsymbol{0}, \Psi), \\
\boldsymbol{Y} &\sim \mathcal{N}(\boldsymbol{0}, \Lambda\Lambda' + \Psi), \\
\boldsymbol{F}|\boldsymbol{Y}, \Lambda, \Psi &\sim \mathcal{N}(m, V) \\
V &= \left(I - \Lambda'\Psi^{-1}\Lambda\right)^{-1}, \quad m = V\Lambda'\Psi^{-1}\boldsymbol{Y}
\end{aligned}
$$

- PCA [1]
  - $\Psi = \sigma^2 I$
  - $\sigma^2 \to 0$ recovers classic PCA
- FA
  - $\Psi = \mathrm{diag}(\sigma_1^2, \cdots, \sigma_P^2)$

Identifiability

The model (Eq., 1) is invariant under any orthogonal transformation:

$$\boldsymbol{y} = (\boldsymbol{F}P)(\boldsymbol{\Lambda}P)' + \boldsymbol{\epsilon} = \boldsymbol{F}^*\boldsymbol{\Lambda}^* + \boldsymbol{\epsilon}$$

where $PP' = I$. That is mean that the rotated parameters $(\boldsymbol{F}^*, \boldsymbol{\Lambda}^*)$ and $(\boldsymbol{F}, \boldsymbol{\Lambda})$ are not distinguishable, hence further restrictions, so called identifiability condition, should be imposed to achieve unique solution.

Identifiability

- Constraint parameter space
  - Block of lower triangular matrix
  - Sparse mode
- Post process MCMC outputs or MAP estimates

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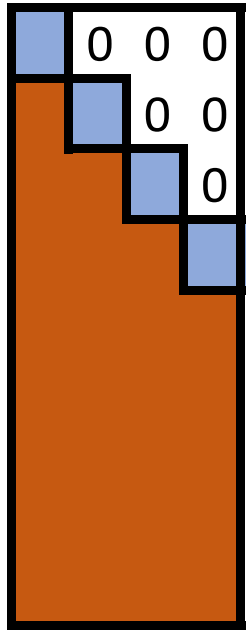
Bayesian FA: Identifiability

Identifiability condition breaks the symmetry of likelihood function and guarantees unique mode of the posterior[2]:

- Λ is full column rank and has a square block of lower triangular with positive diagonal elements (LT).
- $\exists B$ of size Λ and full column rank such that $B'\Lambda$ has a block of lower triangular matrix.
- $\Lambda'\Lambda$ or $\Lambda'\Sigma^{-1}\Lambda$ is diagonal and diagonal elements are unique and arranged in descending order.



Inference

- Bayes rule:

$$\pi(\theta|Y) \propto \pi(\theta)\pi(Y|\theta),$$

  where $\theta = (\Lambda, \boldsymbol{F}, \Psi)$
- MCMC algorithm
- MAP estimates: Expectation Maximisation (EM)

$$\begin{aligned} Q(\theta) &= E_{\boldsymbol{F}|.} \log(\pi(\theta|Y)) \\ \hat{\theta} &= \operatorname{argmax}(Q(\theta)) \end{aligned}$$

Identifiability: LT

- Caveats:
  - Posterior may suffer from local maxima that affects the MCMC sampling schemes.
  - Reduces the accuracy of parameter estimations [3].
  - Ordering problem: LT constraint is invariant to order of variables
  - Number of latent variables is influenced by order of variables [4].

Identifiability

- Identifiability condition that $\mathbf{\Lambda}\mathbf{\Lambda}'$ is diagonal with unique diagonal elements in descending order.
- Kaufmann and Schumacher[5] used the following specification for the FA model in Eq.,(1)

$$\begin{aligned} \boldsymbol{y}_t &= (\boldsymbol{f}_t^* P)(\mathbf{\Lambda}^* P)' + \boldsymbol{\epsilon}, \\ &= \boldsymbol{f}_t \mathbf{\Lambda}' + \boldsymbol{\epsilon}, \end{aligned}$$

  where $\mathbf{\Lambda}^*$ is sparse; $\boldsymbol{f}_t^*$ is the latent variable vector corresponds to the sparse loading and P is an orthogonal matrix such that $\mathbf{\Lambda}'\mathbf{\Lambda}$ is diagonal with unique elements in descending order.
- P is derived from eigenvalue decomposition of $\mathbf{\Lambda}^*\mathbf{\Lambda}^*$.
- In their approach, a draw from $\mathbf{\Lambda}^*$ is used to get an identified solution, then latent variables correspond to the sparse loading is derived using the identified latent variable as $\boldsymbol{f}_t^* = \boldsymbol{f}_t P'$.

Identifiability: Sparse Modes

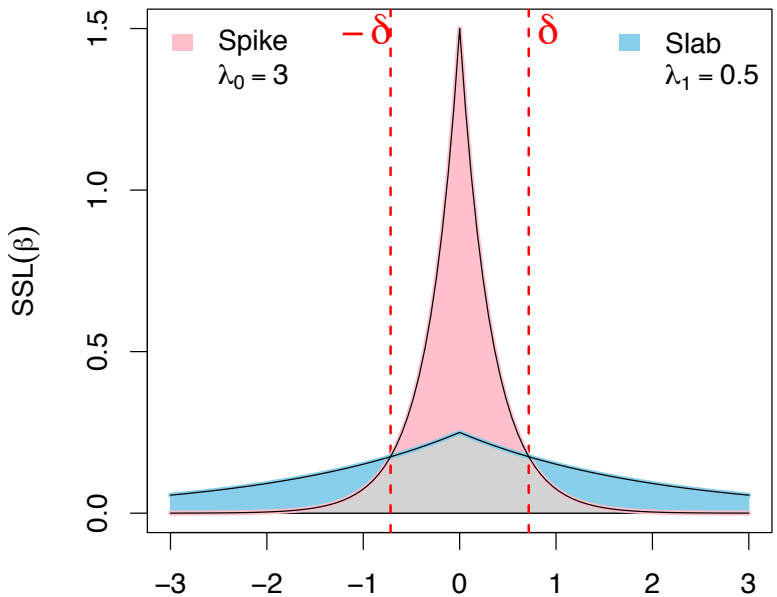
- Sparsity inducing priors can be used to achieve unique solution
- Helps interoperability of latent variables while only few variables enter to each latent variables.
- Improves predictive performances [6].
- Shrinkage prior:
  - Automatic relevance determination (ARD)
  - Horseshoe
- No exact zeros
- spike and slap prior

Spike and Slab prior

Spike and Slab (SSL) prior with Laplace components

$$\pi(\lambda|\gamma) = \gamma \text{Laplace}(\lambda|\sigma_1^2) + (1-\gamma)\text{Laplace}(\lambda|\sigma_0^2)$$

- σ_1^2 **small**: to avoid over-shrinkage of large effects
- σ_0^2 **large**: to shrink ignorable coefficients to zero
- θ controls sparsity, $P(\gamma = 1|\theta) = \theta$
- Point-mass spike-and-slab is a limiting case as $\sigma_0^2 \to 0$



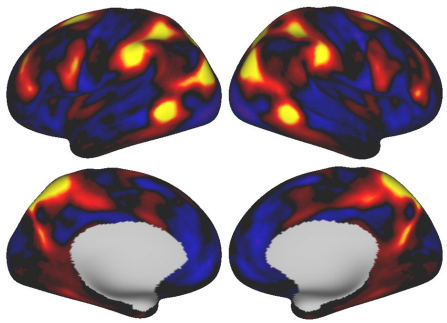
Latent variable: Spike and Slab prior

Hierarchical spike and slab prior[7]:

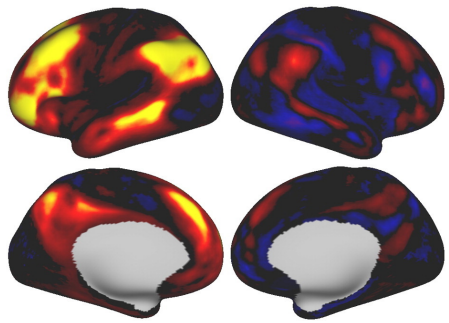
$$
\begin{aligned}
\pi(\lambda_{jk}|\gamma_{jk}) &\sim \gamma \text{Laplace}(\lambda_{jk}|\sigma_1^2) + (1-\gamma)\text{Laplace}(\lambda_{jk}|\sigma_0^2) \\
\gamma_{jk} &\sim \text{Bernoulli}(\theta_k) \\
\theta_k &= \prod_{l=1}^{k} \nu_l \\
\nu_l &\sim^{iid} \text{B}(\alpha, 1)
\end{aligned}
$$

An Example: rsfMRI Modelling[8]

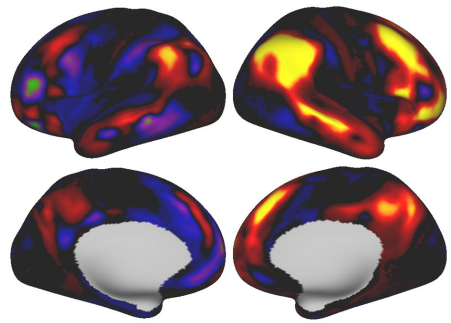
$$\boldsymbol{Y} = \boldsymbol{F}\Lambda' + E$$



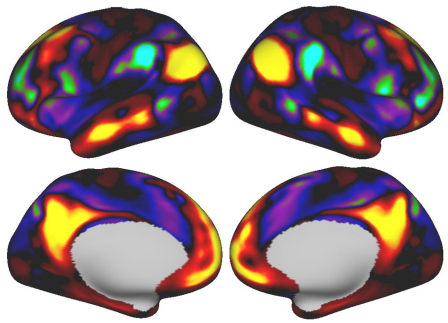
(a) PFM 13 (0.86). Dorsal attention (DA).



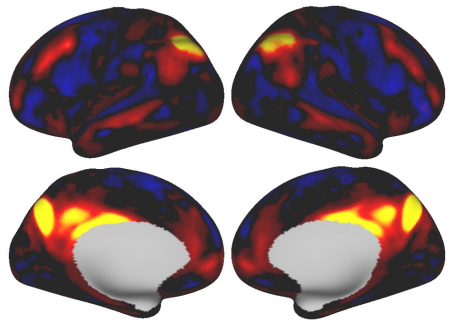
(b) PFM 18 (0.95). Left fronto-parietal control (lFPC).



(c) PFM 17 (0.77). Right fronto-parietal control (rFPC).



(d) PFM 15 (0.90). Default mode (DM).



(e) PFM 16 (0.98). Posteriomedial cortex, inferior parietal lobule (PMPL).

Posterior mean

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Canonical Correlation Analysis

Linear combination such that maximises the correlation

$$\underset{(P_1 \times N)}{Y_1} = \underset{(P_1 \times K)}{\Lambda_1} \times \underset{(K \times N)}{F} + \epsilon_1$$

$$\underset{(P_2 \times N)}{Y_2} = \underset{(P_2 \times K)}{\Lambda_2} \times \underset{(K \times N)}{F} + \epsilon_2$$

CCA Application: UKBB

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Canonical Correlation Analysis (CCA)

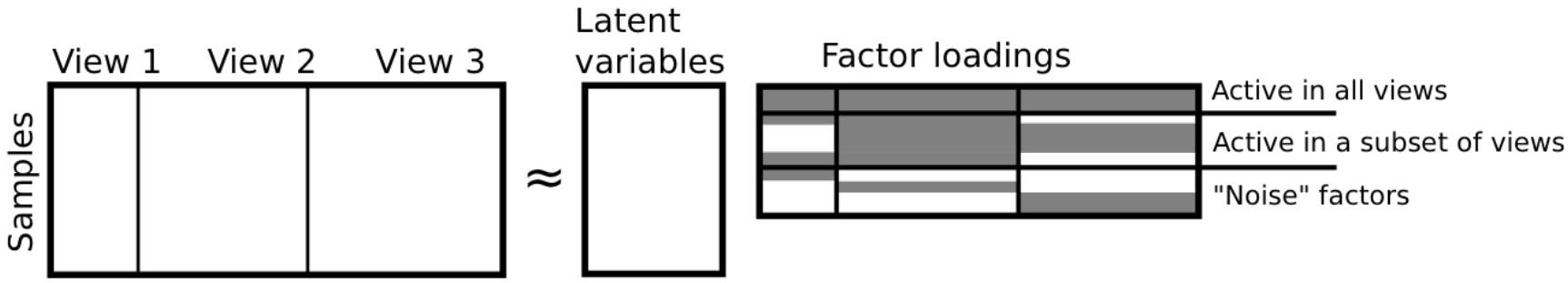
Bayesian CCA [9]

$$\begin{aligned} \boldsymbol{y}_i^{(1)} &= \boldsymbol{A}^{(1)}\boldsymbol{f}_i^{(0)} + \boldsymbol{B}^{(1)}\boldsymbol{f}_i^{(1)} + \boldsymbol{\epsilon}_i^{(1)}, \\ \boldsymbol{y}_i^{(2)} &= \boldsymbol{A}^{(2)}\boldsymbol{f}_i^{(0)} + \boldsymbol{B}^{(1)}\boldsymbol{f}_i^{(2)} + \boldsymbol{\epsilon}_i^{(2)}, \end{aligned}$$

where $\boldsymbol{f}_i^{(0)} \in \mathbb{R}^{k_0 \times 1}$ is the shared latent variable; $\boldsymbol{f}_i^{(1)} \in \mathbb{R}^{k_1 \times 1}$ and $\boldsymbol{f}_i^{(2)} \in \mathbb{R}^{k_2 \times 1}$ are the view specific latent variables.

- $\boldsymbol{\epsilon}_i^{w} \sim \mathcal{N}(\boldsymbol{0}, \Psi^{(w)})$, $w = 1, 2$
- $\boldsymbol{f}_i^{(w)} \sim \mathcal{N}(\boldsymbol{0}, I)$
- Marginal distributions: $\mathrm{cov}(\boldsymbol{y}_i)^{(w)} = \Sigma^{(w)} = \boldsymbol{B}^{(w)}\boldsymbol{B}'^{(w)} + \Psi^{(w)}$

Multi-view Learning



Generative model: Extend CCA to more than 2 views [10]

$$
\begin{aligned}
\boldsymbol{y}_i^{(w)} &= \boldsymbol{A}^{(w)}\boldsymbol{f}_i^{(0)} + \boldsymbol{B}^{(w)}\boldsymbol{f}_i^{(w)} + \boldsymbol{\epsilon}_i^{(w)}, \quad \text{for} \quad w = 1, \cdots, m \\
\boldsymbol{y}_i &= \Lambda \boldsymbol{f}_i + \boldsymbol{\epsilon}_i, \\
\Lambda &= \begin{bmatrix} \boldsymbol{A}^{(1)} & \boldsymbol{B}^{(1)} & \cdots & \boldsymbol{0} \\ \boldsymbol{A}^{(2)} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ \boldsymbol{A}^{(m)} & 0 & 0 & \boldsymbol{B}^{(m)} \end{bmatrix}
\end{aligned}
$$

Multi-view Learning[10]

- Column-wise shrinkage: ARD prior on the loading columns

$$\begin{aligned} \lambda_{jh}^{w} &\sim \mathcal{N}\left(0, \left(\alpha_{h}^{(w)}\right)\right) \\ \alpha_{h}^{(w)} &\sim Ga(a_0, b_0) \end{aligned}$$

- Caveats:
  - Structured covariance matrix: Large m intractable
  - Can not capture covariance among arbitrary subset of data
  - ARD prior: Only induces column-wise sparsity

Multi-view Learning

$$\boldsymbol{y}_i = \Lambda \boldsymbol{f}_i + \boldsymbol{\epsilon}_i,$$

Structured sparsity prior on loadings [11]: sparse and dense factors

$$
\begin{aligned}
\text{Global} \quad \{ \quad & \gamma^{(w)} \sim Ga(f, \nu) \\
& \eta^{(w)} \sim Ga(e, \gamma^{(w)}) \\
\text{Factor} - \text{specific} \quad \{ \quad & \tau_h^{(w)} \sim Ga(d, \eta^{(w)}) \\
& \phi_h^{(w)} \sim Ga(c, \tau_h^{(w)}) \\
\text{Local} \quad \{ \quad & \delta_{jh}^{w} \sim Ga(b, \phi_h^{(w)}) \\
& \theta_{jh}^{(w)} \sim \pi^{(w)} Ga(a, \delta_{jh}^{w}) + (1 - \pi^{(w)}) \delta_{\phi_h^{(w)}}(.) \\
\lambda_{jh}^{w} \quad \sim \quad & \mathcal{N}(0, \theta_{jh}^{(w)})
\end{aligned}
$$

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