DSC250: Advanced Data Mining

Topic Models

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Lecture 7, October 19, 2023

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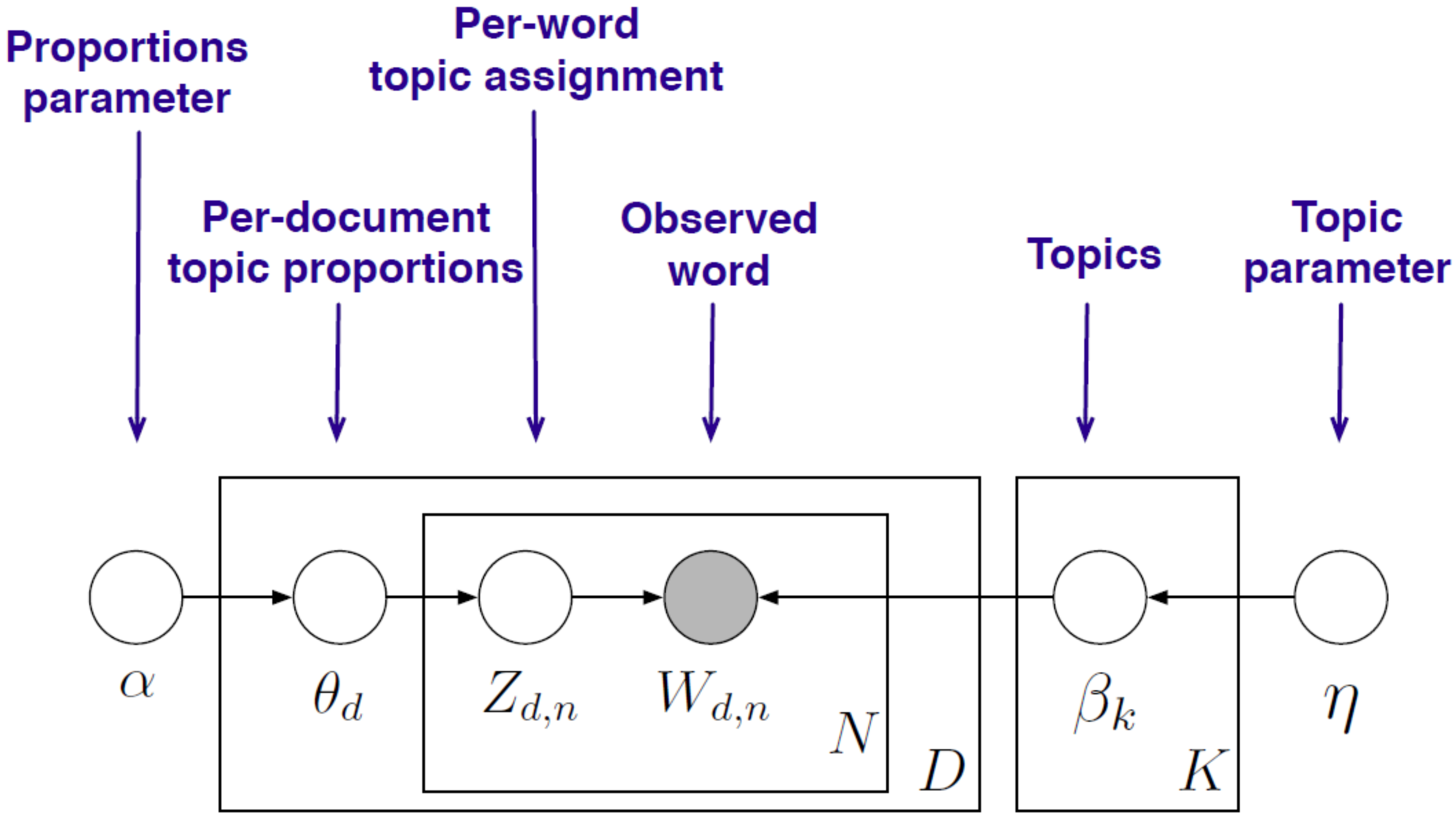
Outline

- Topic Model v3: Latent Dirichlet Allocation (LDA)
- Learning of Topic Model: Expectation Maximization (EM)

Slides adapted from:
- Y. Sun, CS 247: Advanced Data Mining
- M. Gormley, 10-701 Introduction to Machine Learning

Topic Model v3: Latent Dirichlet Allocation (LDA)



$\boldsymbol{\theta_d \sim Dirichlet(\alpha)}$: **address topic distribution for unseen documents**

$\boldsymbol{\beta_k \sim Dirichlet(\eta)}$: **smoothing over words**

Generative Model for LDA

For each topic $k \in \{1, \ldots, K\}$:

$\quad \beta_k \sim \mathrm{Dir}(\eta)$ [*draw distribution over words*]

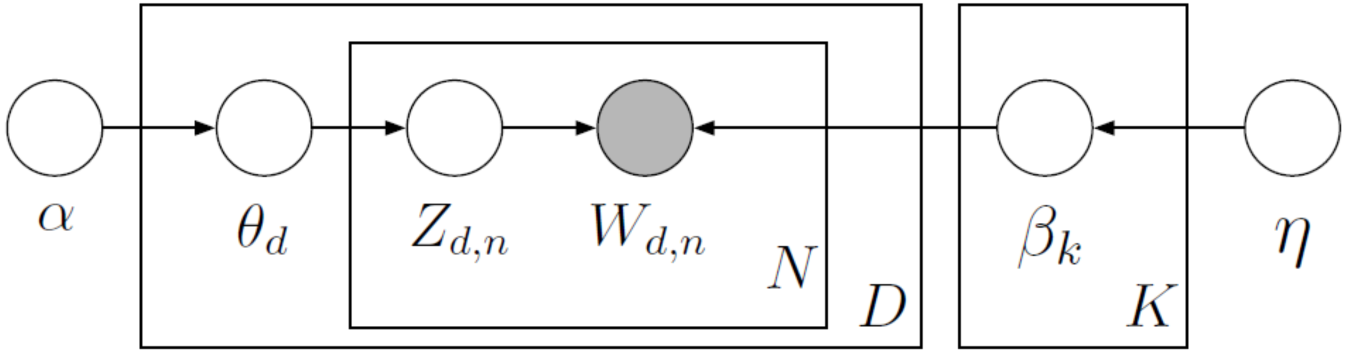
For each document $d \in \{1, \ldots, D\}$

$\quad \boldsymbol{\theta}_d \sim \mathrm{Dir}(\boldsymbol{\alpha})$ [*draw distribution over topics*]

$\quad$ For each word $n \in \{1, \ldots, N_d\}$

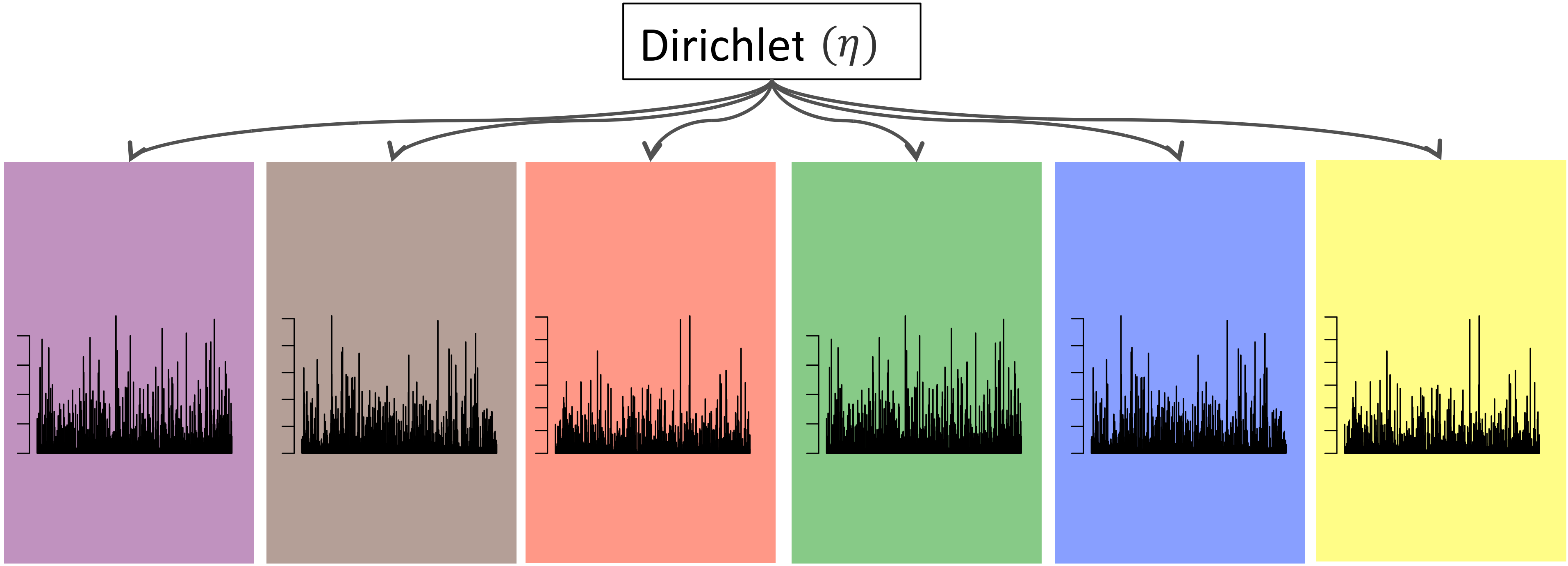
$\quad\quad z_{d,n} \sim \mathrm{Mult}(1, \boldsymbol{\theta}_d)$ [*draw topic assignment*]

$\quad\quad w_{d,n} \sim \theta_{z_{d,n}}$ [*draw word*]



(Blei, Ng, & Jordan, 2003)

LDA for Topic Modeling



- The **generative story** begins with only a **Dirichlet prior** over the topics.
- Each **topic** is defined as a **Multinomial distribution** over the vocabulary, parameterized by $\boldsymbol{\beta}_k$

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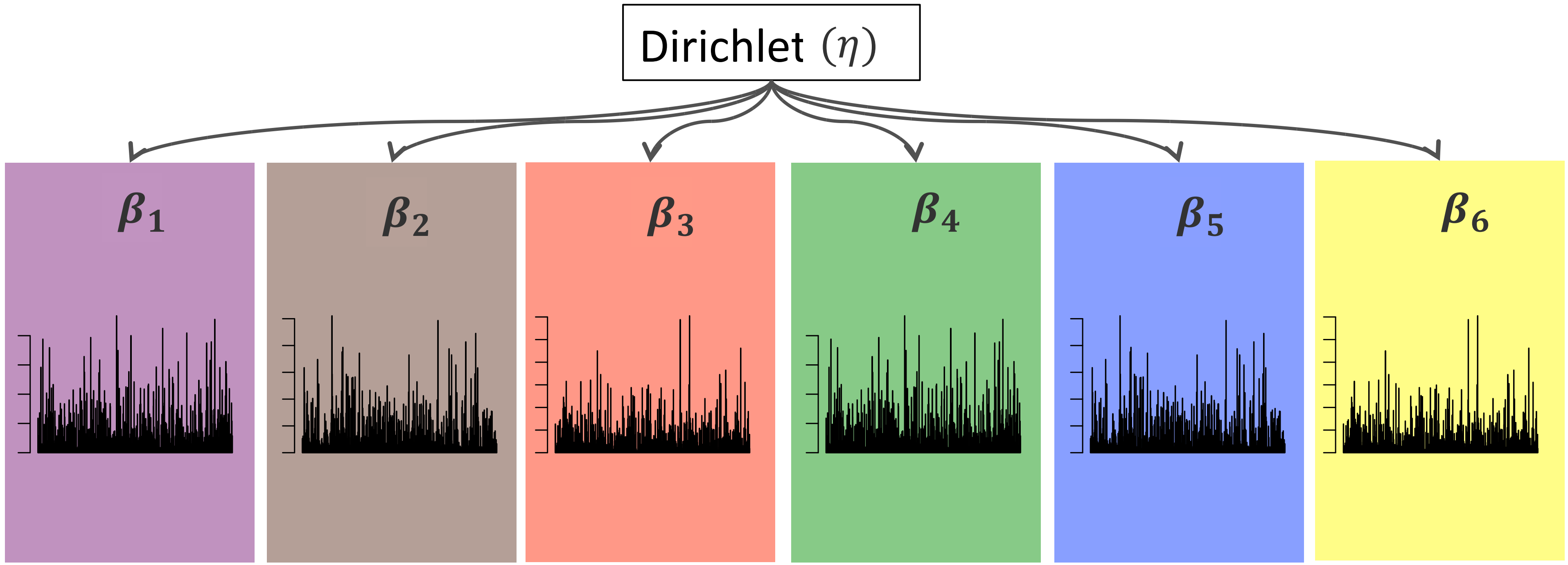

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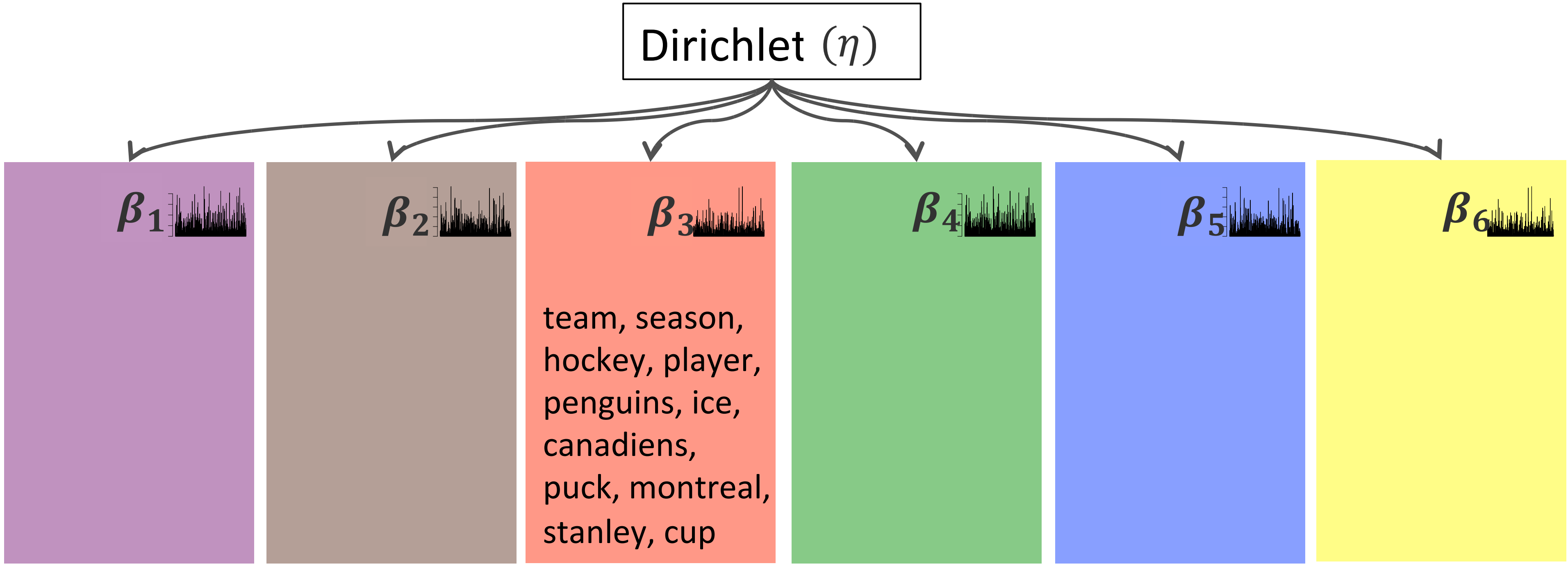

- A topic is visualized as its **high probability words.**

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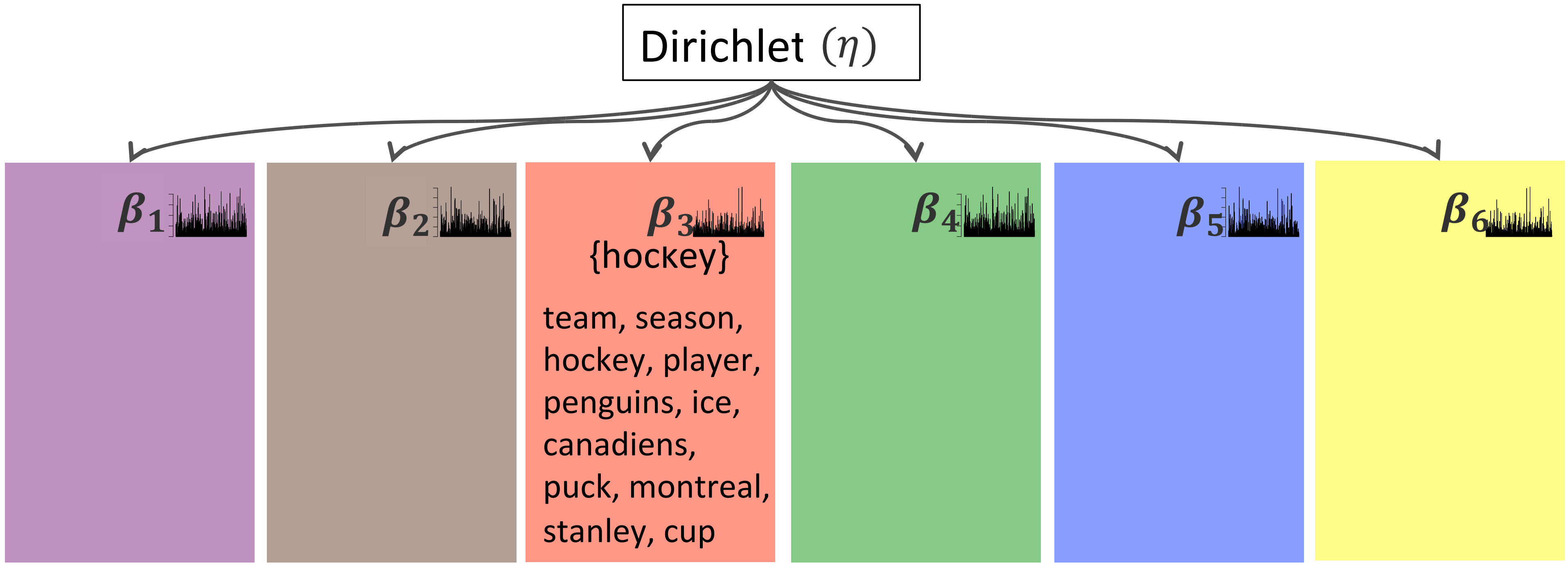

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- A pedagogical **label** is used to identify the topic.

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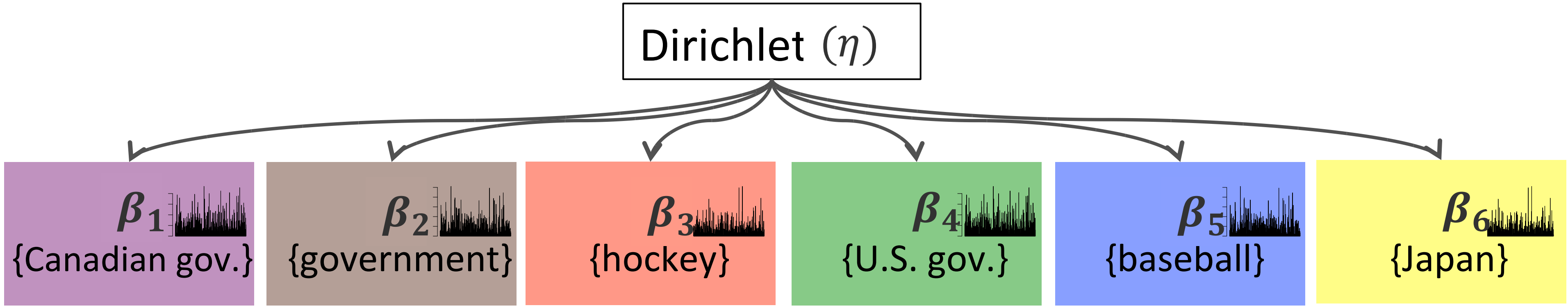

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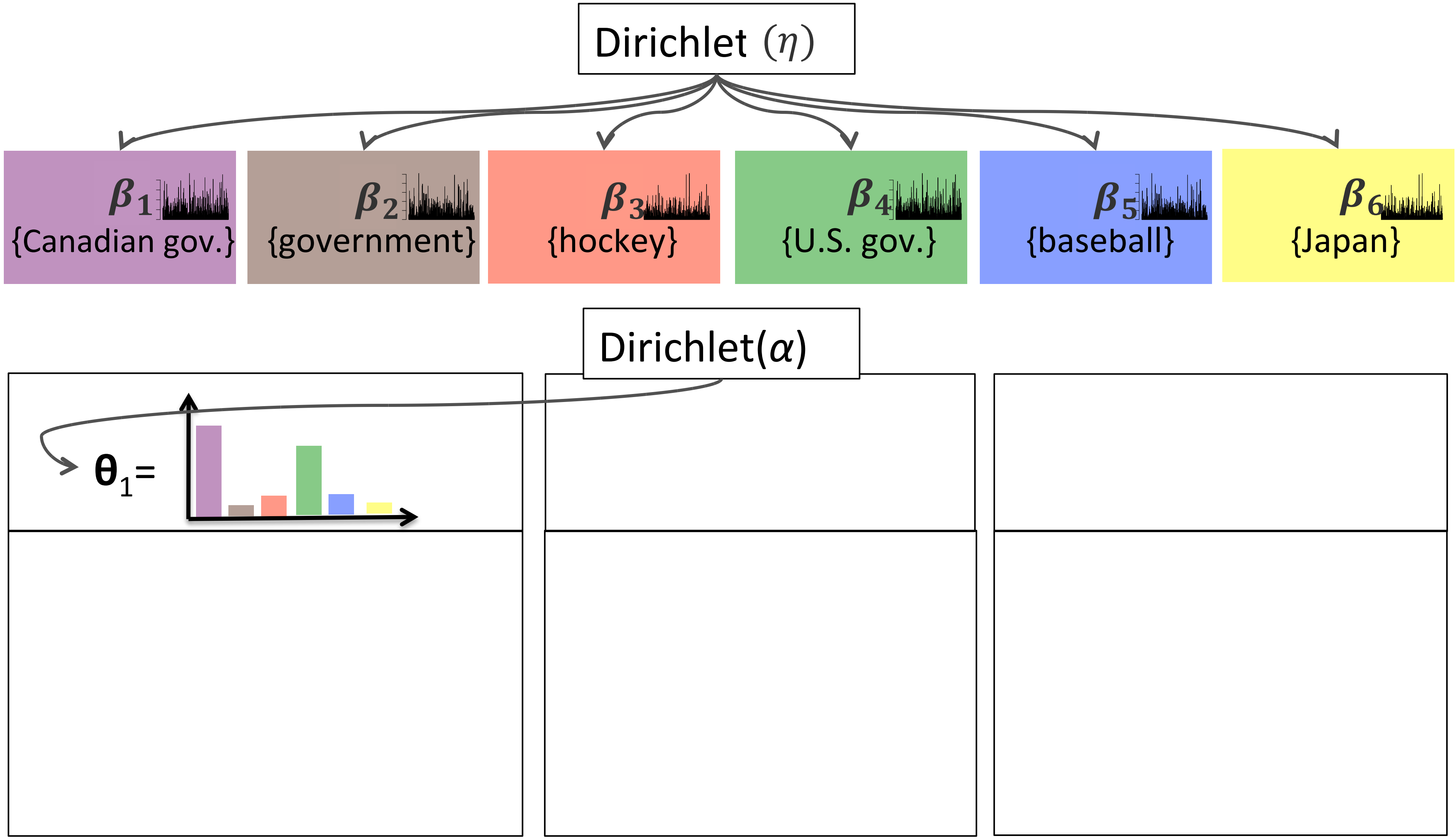

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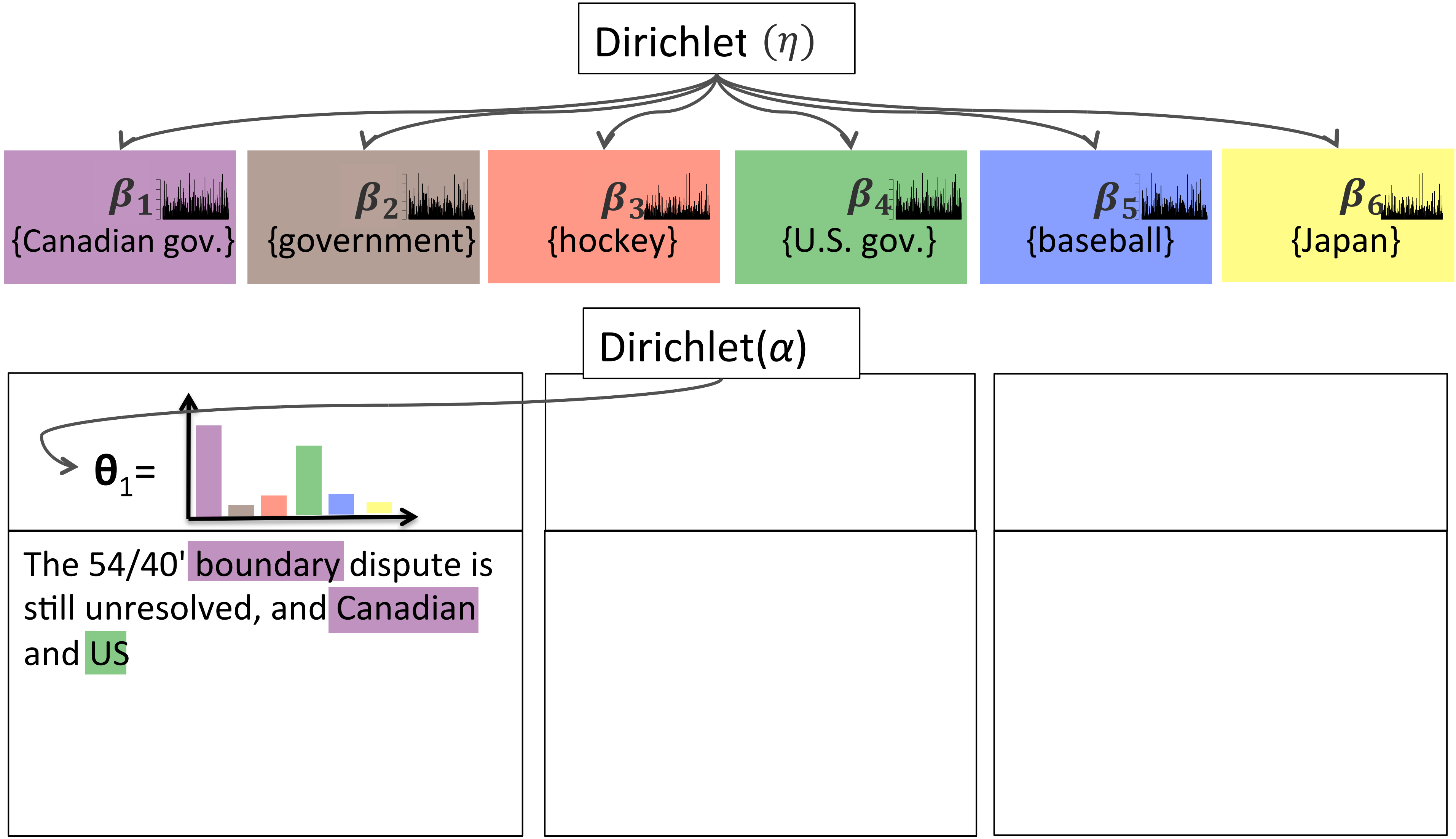

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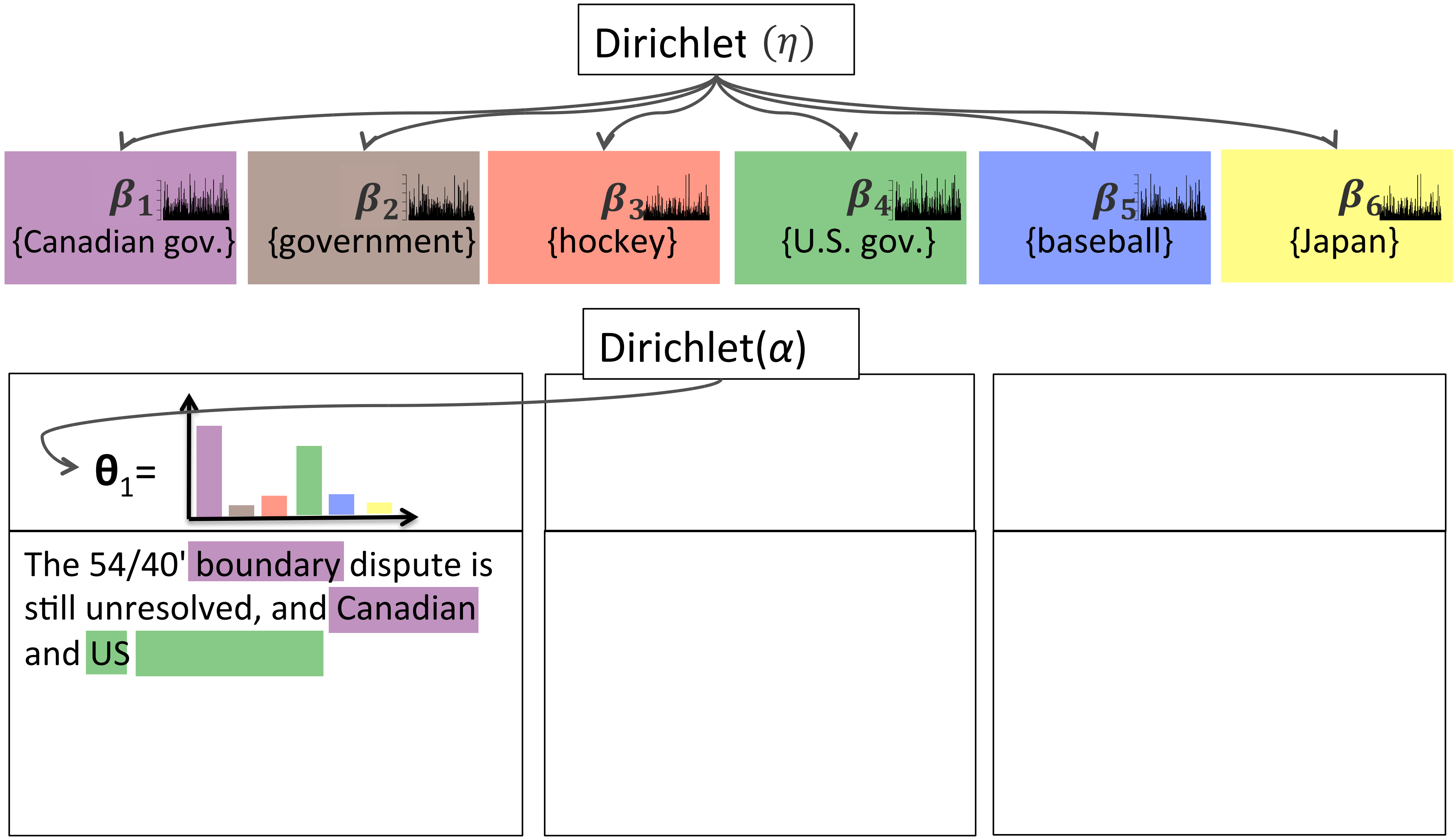

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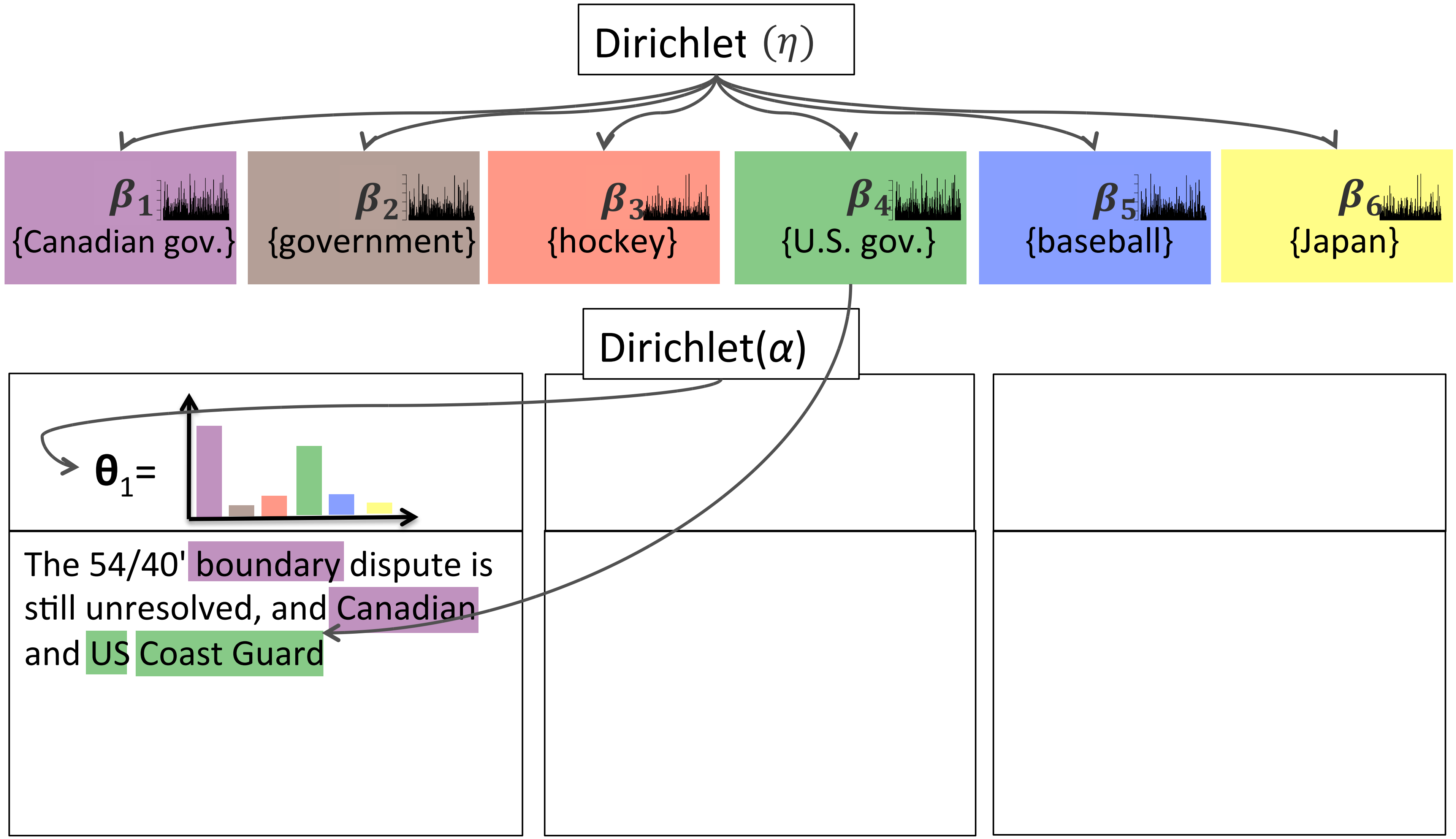

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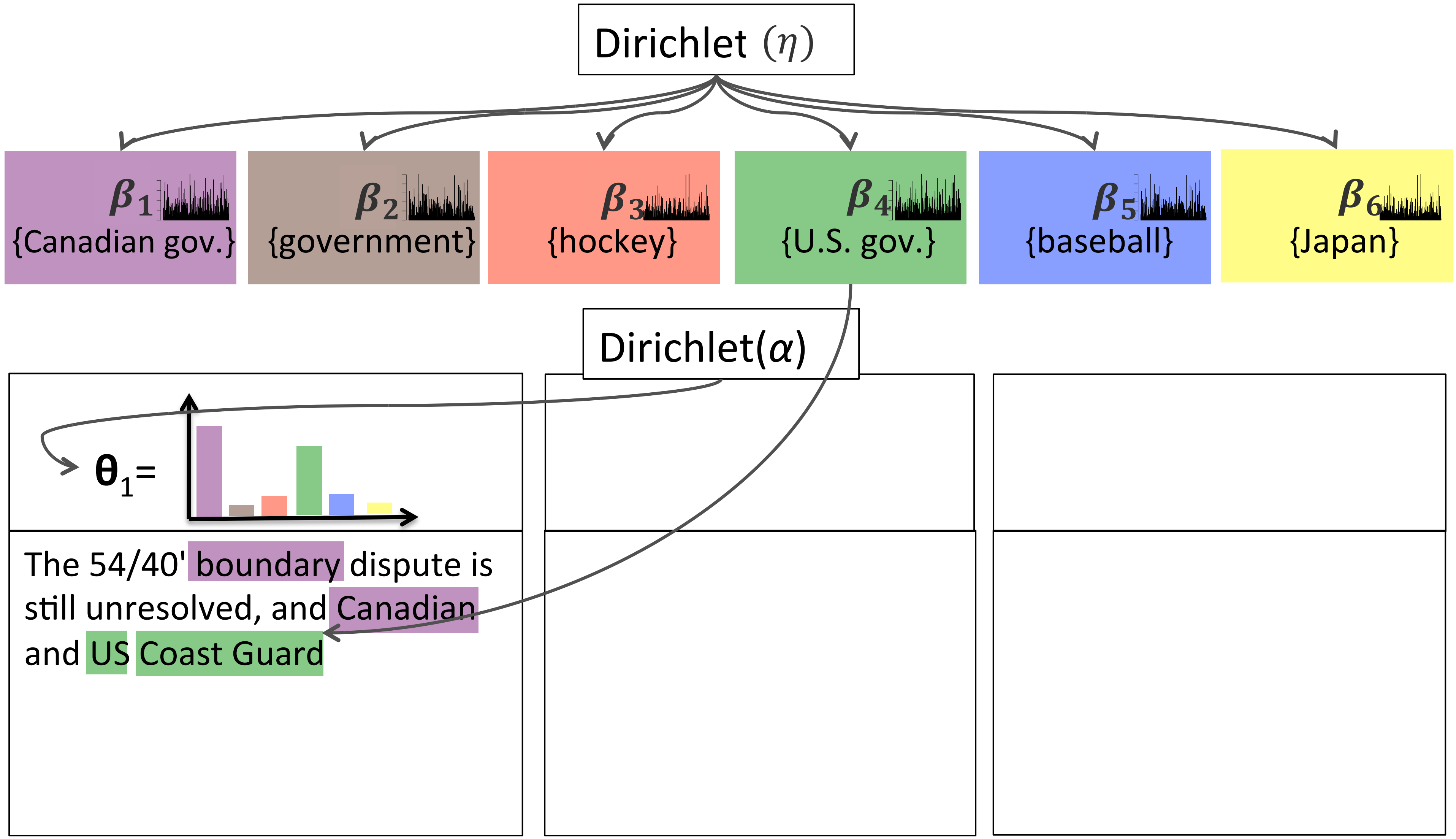

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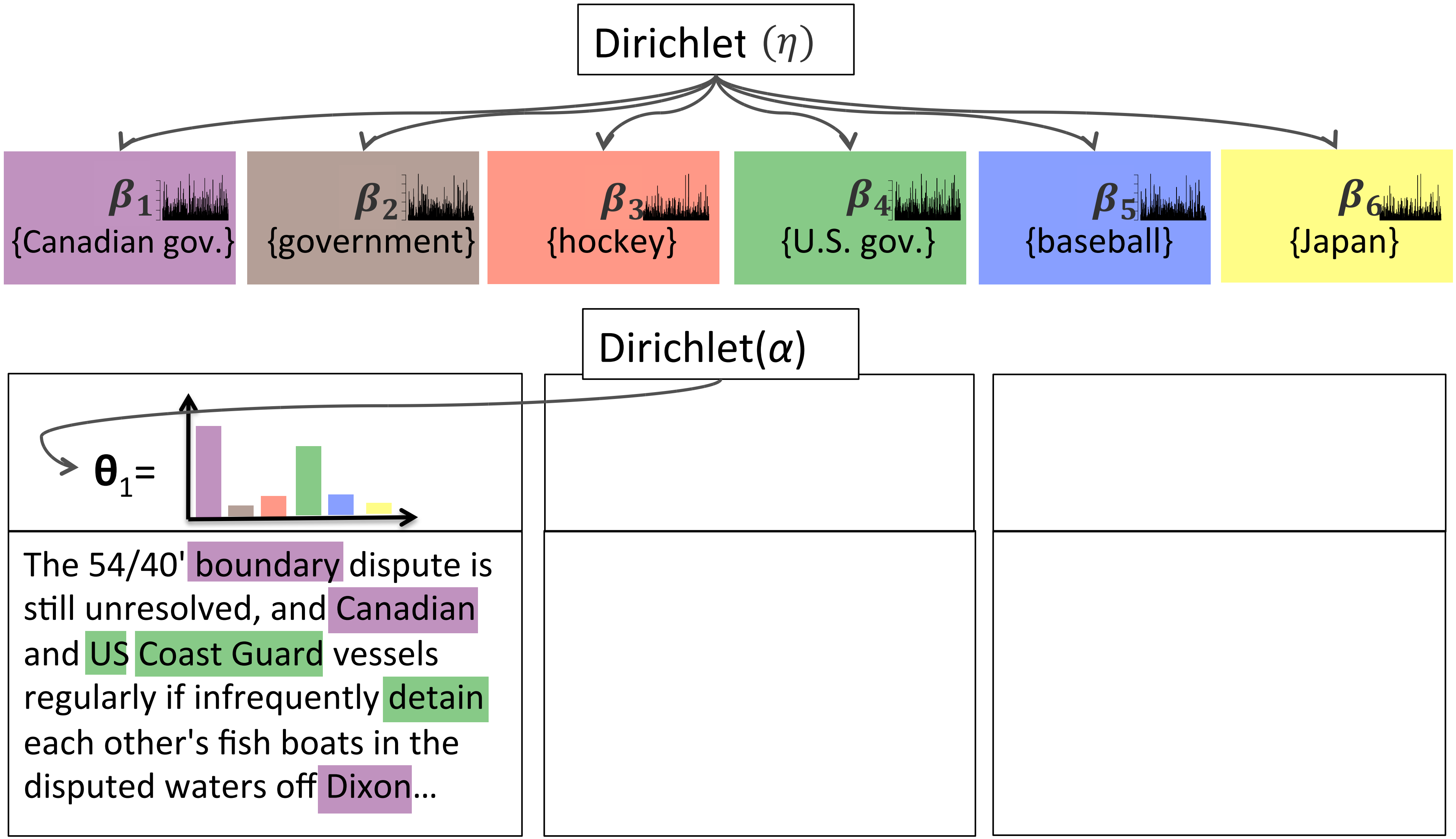

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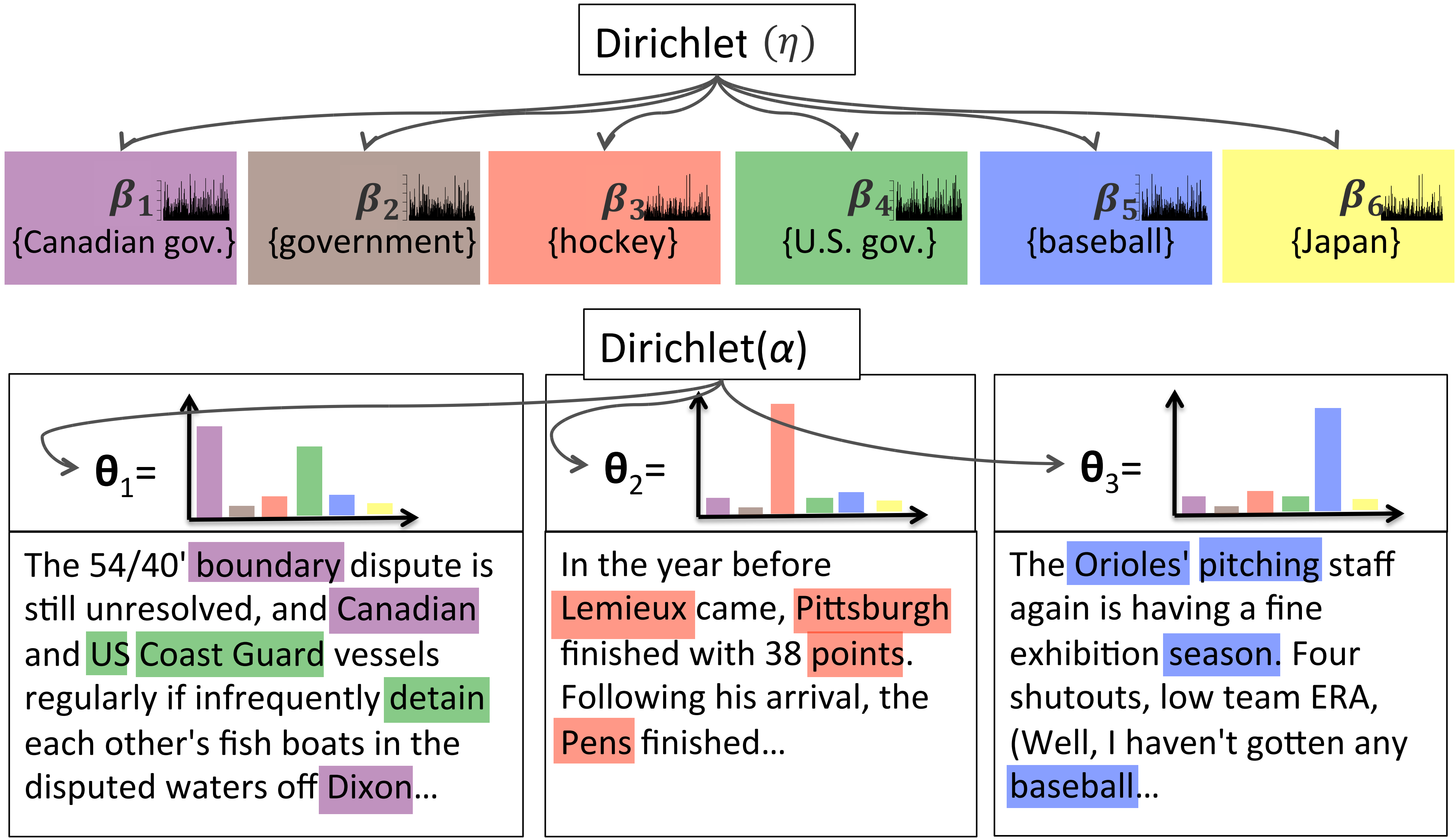

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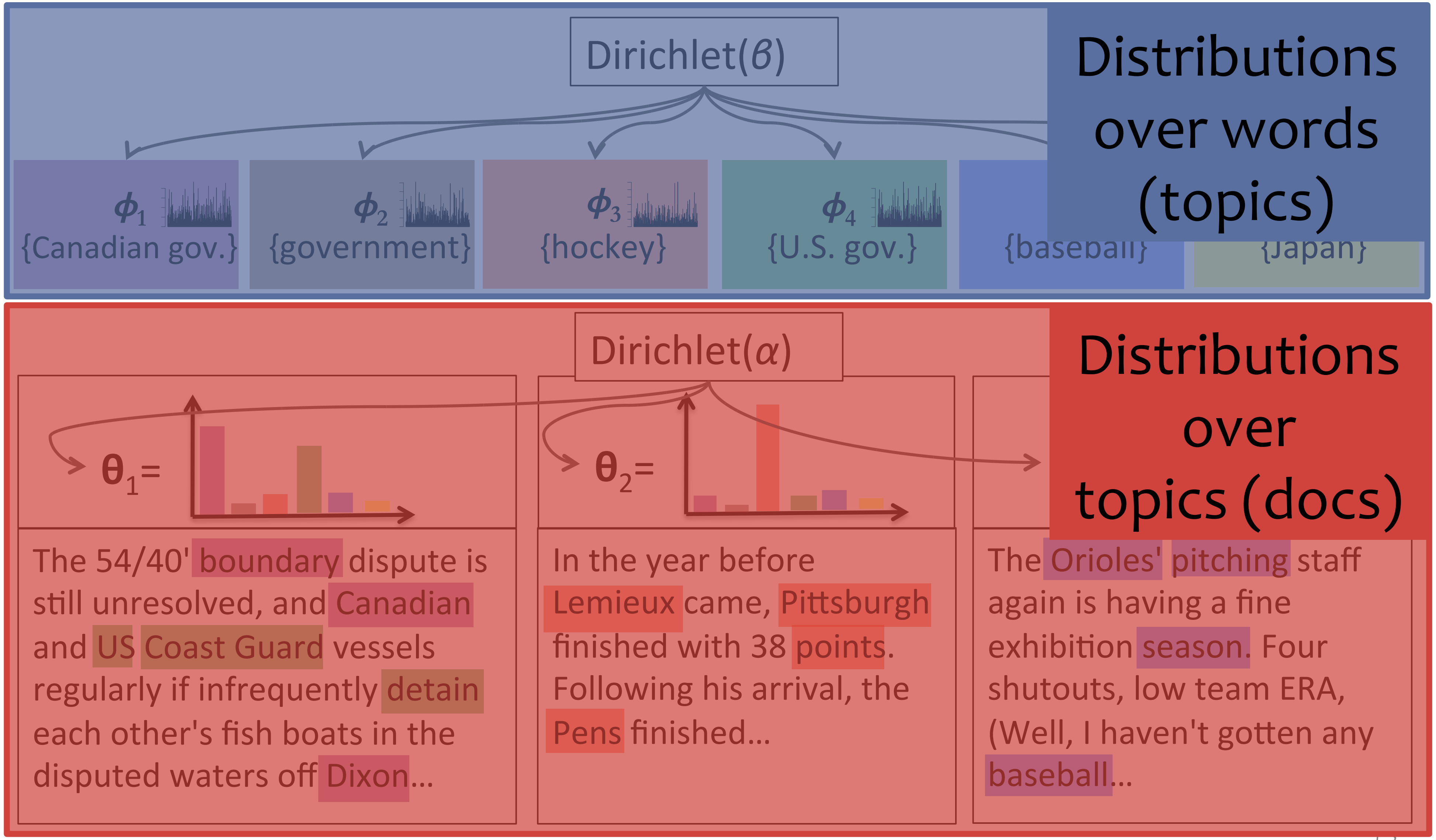
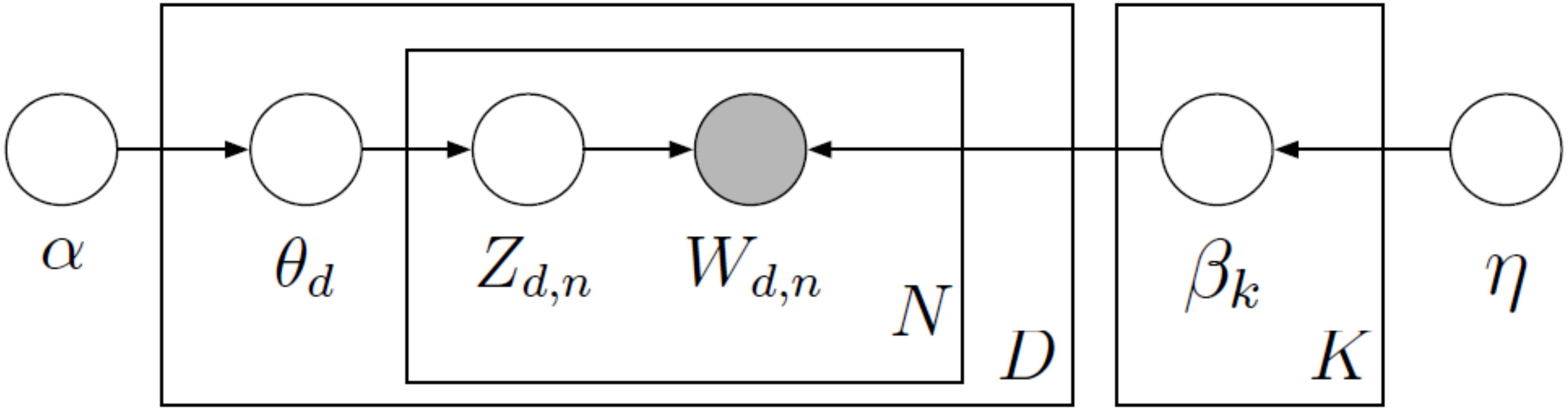


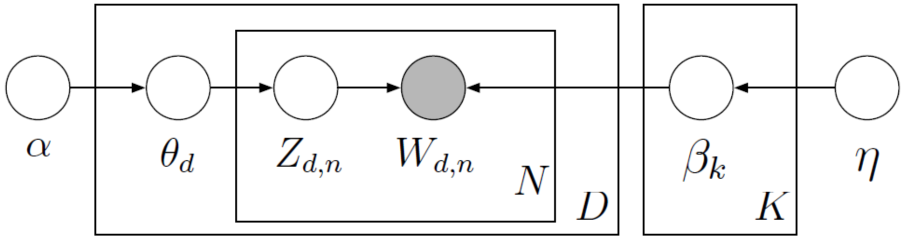
Joint Distribution for LDA



- Joint distribution of latent variables and documents is:
  $p(\boldsymbol{\beta}_{1:K}, \boldsymbol{z}_{1:D}, \boldsymbol{\theta}_{1:D}, \boldsymbol{w}_{1:D} | \alpha, \eta) =$

$$\prod_{i=1}^{K} p(\beta_i | \eta) \prod_{d=1}^{D} p(\theta_d | \alpha) \left(\prod_{n=1}^{N} p(z_{d,n} | \theta_d) p(w_{d,n} | \beta_{1:K}, z_{d,n}) \right)$$

Likelihood Function for LDA



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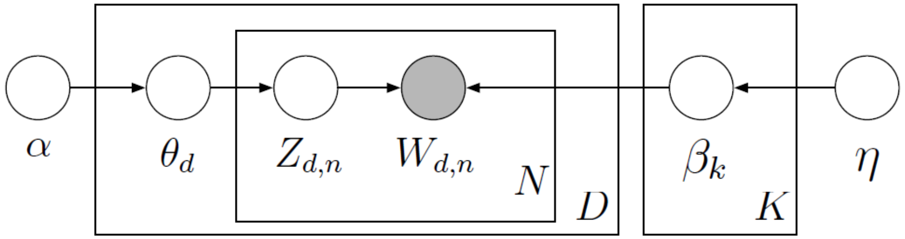
Likelihood Function for LDA



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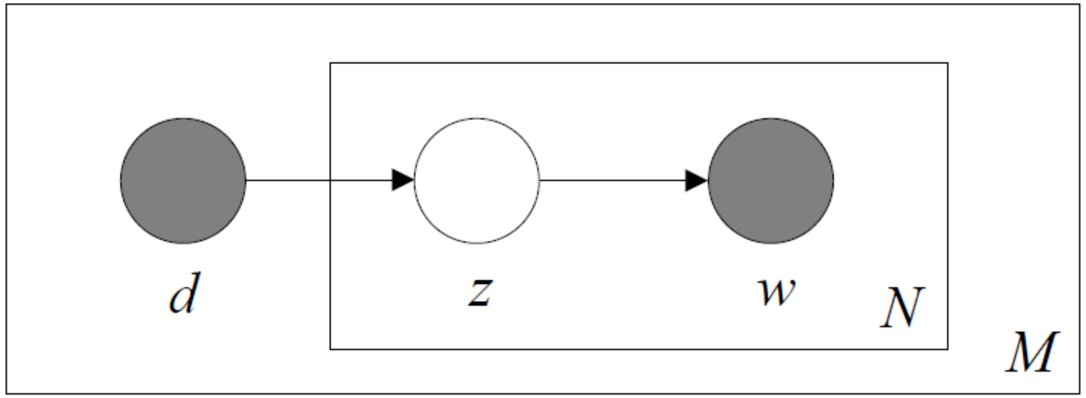
Learning of Topic Models

Recap: pLSA Topic Model



- Observed variables:
- Latent variables:
- Parameters:

The General Unsupervised Learning Problem

- Each data instance is partitioned into two parts:
  - observed variables $\boldsymbol{x}$
  - latent (unobserved) variables $\boldsymbol{z}$
- Want to learn a model $p_\theta(\boldsymbol{x}, \boldsymbol{z})$

[Content adapted from CMU 10-708]

Latent (unobserved) variables

- A variable can be unobserved (latent) because:
  - imaginary quantity: meant to provide some simplified and abstractive view of the data generation process
    - e.g., topic model, speech recognition models, …

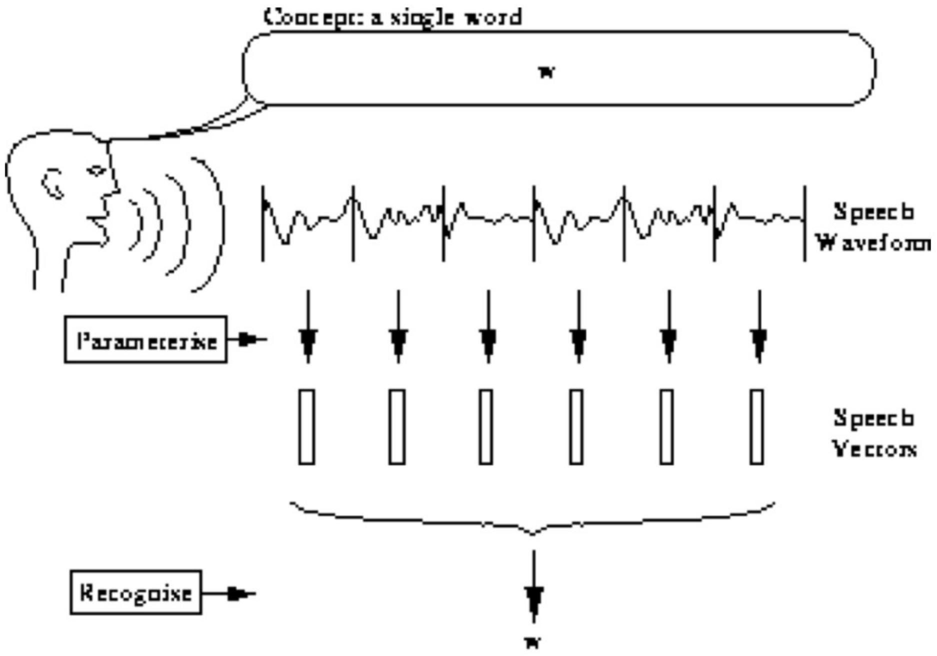
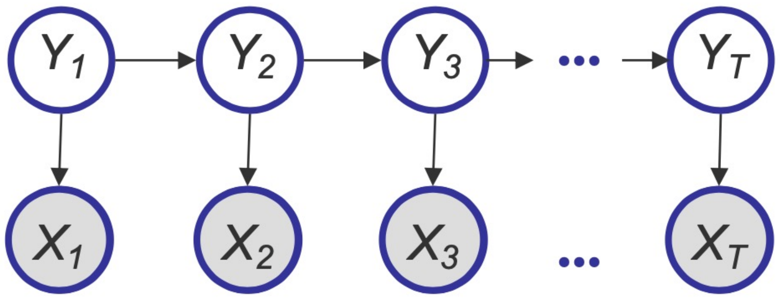


Fig. 1.2 Isolated Word Problem



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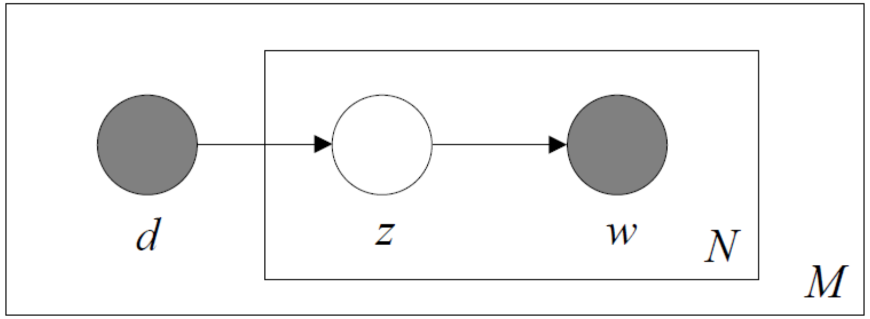
- A variable can be unobserved (latent) because:
  - imaginary quantity: meant to provide some simplified and abstractive view of the data generation process
    - e.g., topic model, speech recognition models, ...
  - a real-world object (and/or phenomena), but difficult or impossible to measure
    - e.g., the temperature of a star, causes of a disease, evolutionary ancestors ...
  - a real-world object (and/or phenomena), but sometimes wasn't measured, because of faulty sensors, etc.
- Discrete latent variables can be used to partition/cluster data into sub-groups
- Continuous latent variables (factors) can be used for dimensionality reduction (e.g., factor analysis, etc.)

Recap: pLSA Topic Model

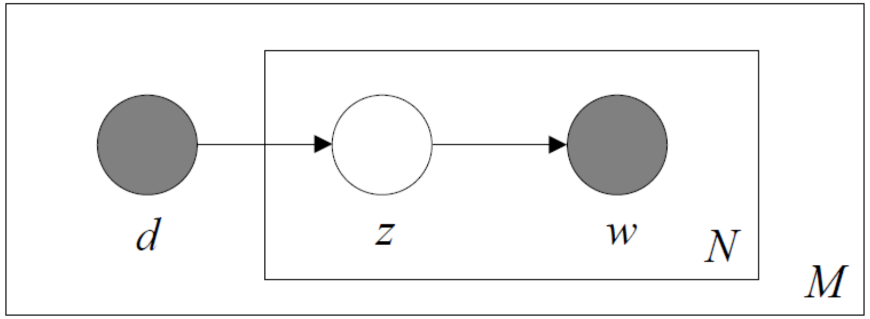


- Likelihood function of a word w:

$$p(w|d,\theta,\beta) = \sum_k p(w, z = k|d,\theta,\beta)$$

$$= \sum_k p(w|z = k, d, \theta, \beta) p(z = k|d,\theta,\beta) = \sum_k \beta_{kw}\theta_{dk}$$

Recap: pLSA Topic Model



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- Learning by maximizing the log likelihood:

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- Complete log likelihood: if both $\boldsymbol{x}$ and $\boldsymbol{z}$ can be observed, then

$$\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z}) = \log p(\boldsymbol{x}, \boldsymbol{z}|\theta) = \log p(\boldsymbol{z}|\theta_z) + \log p(\boldsymbol{x}|\boldsymbol{z}, \theta_x)$$

  - Decomposes into a sum of factors, the parameter for each factor can be estimated separately
- But given that $\boldsymbol{z}$ is not observed, $\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})$ is a random quantity, cannot be maximized directly

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  - Decomposes into a sum of factors, the parameter for each factor can be estimated separately
- But given that $\boldsymbol{z}$ is not observed, $\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})$ is a random quantity, cannot be maximized directly
- Incomplete (or marginal) log likelihood: with $\boldsymbol{z}$ unobserved, our objective becomes the log of a marginal probability:

$$\ell(\theta; \boldsymbol{x}) = \log p(\boldsymbol{x}|\theta) = \log \sum_{z} p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

  - All parameters become coupled together
  - In other models when $\boldsymbol{z}$ is complex (continuous) variables, marginalization over $\boldsymbol{z}$ is intractable.

Expectation Maximization (EM)

- For any distribution $q(\boldsymbol{z}|\boldsymbol{x})$, define expected complete log likelihood:

$$\mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] = \sum_z q(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

  - A deterministic function of θ
  - Inherit the factorizability of $\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})$
- Use this as the surrogate objective

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- Use this as the surrogate objective
- Does maximizing this surrogate yield a maximizer of the likelihood?

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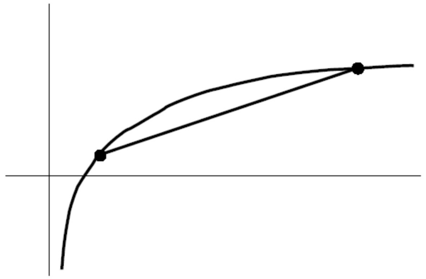
- Jensen's inequality

$$\begin{aligned} \ell(\theta; x) &= \log p(x \mid \theta) \\ &= \log \sum_z p(x, z \mid \theta) \\ &= \log \sum_z q(z \mid x) \frac{p(x, z \mid \theta)}{q(z \mid x)} \\ &\geq \sum_z q(z \mid x) \log \frac{p(x, z \mid \theta)}{q(z \mid x)} \end{aligned}$$



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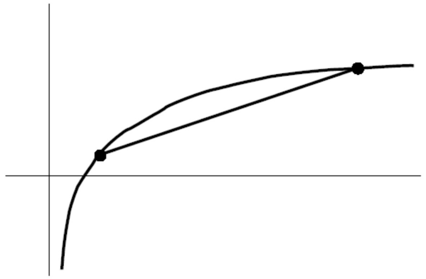

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Evidence Lower Bound (ELBO)

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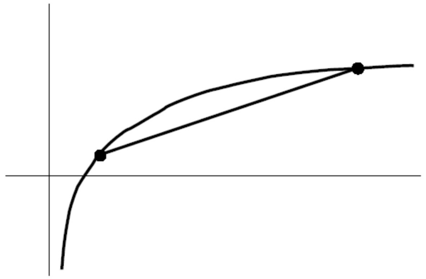

$$\begin{aligned}
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&\geq \sum_z q(z \mid x) \log \frac{p(x, z \mid \theta)}{q(z \mid x)} \quad \text{Evidence Lower Bound (ELBO)} \\
&= \sum_z q(z \mid x) \log p(x, z \mid \theta) - \sum_z q(z \mid x) \log q(z \mid x) \\
&= \mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] + H(q)
\end{aligned}$$

Expectation Maximization (EM)

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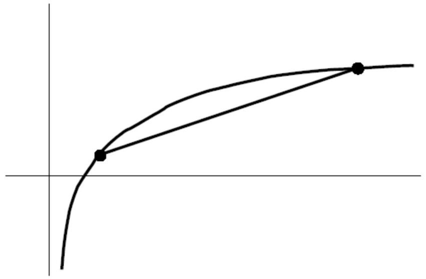


- Indeed we have

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

Lower Bound and Free Energy

- For fixed data $\boldsymbol{x}$, define a functional called the (variational) free energy:

$$F(q,\theta) = -\mathbb{E}_q[\ell_c(\theta;\boldsymbol{x},\boldsymbol{z})] - H(q) \geq \ell(\theta;\boldsymbol{x})$$

- The EM algorithm is coordinate-decent on F
  - At each step t:
    - E-step: $$q^{t+1} = \arg\min_q F\left(q, \theta^t\right)$$
    - M-step: $$\theta^{t+1} = \arg\min_\theta F\left(q^{t+1}, \theta^t\right)$$

E-step: minimization of $F(q, \theta)$ w.r.t q

- Claim:

$$q^{t+1} = \operatorname{argmin}_q F(q, \theta^t) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$$

  - This is the posterior distribution over the latent variables given the data and the current parameters.

- Proof (easy): recall

$$\underbrace{\ell(\theta^t; \boldsymbol{x})}_{\text{Independent of } q} = \underbrace{\mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta^t)}{q(\boldsymbol{z}|\boldsymbol{x})}\right]}_{-F(q,\theta^t)} + \underbrace{\mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)\big)}_{\geq 0}$$

  - $F(q, \theta^t)$ is minimized when $\mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)\big) = 0$, which is achieved only when $q(\boldsymbol{z}|\boldsymbol{x}) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$

M-step: minimization of $F(q, \theta)$ w.r.t $\boldsymbol{\theta}$

- Note that the free energy breaks into two terms:

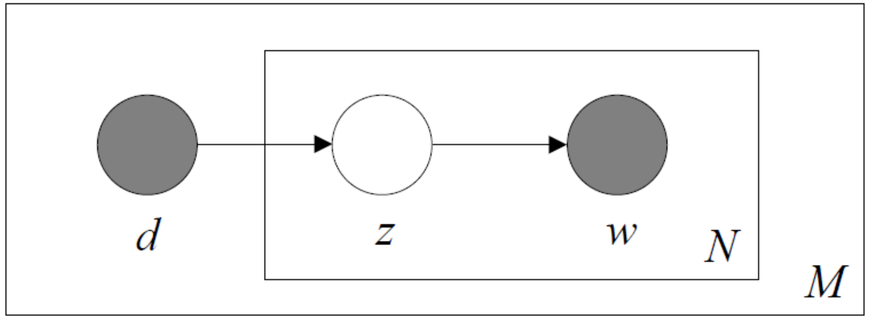
$$F(q, \theta) = -\mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] - H(q) \geq \ell(\theta; \boldsymbol{x})$$

  - The first term is the expected complete log likelihood and the second term, which does not depend on q, is the entropy.
- Thus, in the M-step, maximizing with respect to θ for fixed q we only need to consider the first term:

$$\theta^{t+1} = \mathrm{argmax}_\theta\, \mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] = \mathrm{argmax}_\theta \sum_z q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

  - Under optimal q^{t+1}, this is equivalent to solving a standard MLE of fully observed model $p(\boldsymbol{x}, \boldsymbol{z}|\theta)$, with z replaced by its expectation w.r.t $p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$

Learning pLSA with EM



- E-step:

$$p(z|w,d,\theta^t,\beta^t) = \frac{p(w|z,d,\beta^t)p(z|d,\theta^t)}{\sum_{z'} p(w|z',d,\beta^t)p(z'|d,\theta^t)} = \frac{\beta^t_{zw}\theta^t_{dz}}{\sum_{z'}\beta^t_{z'w}\theta^t_{dz'}}$$

$\hookrightarrow p(z|x)$

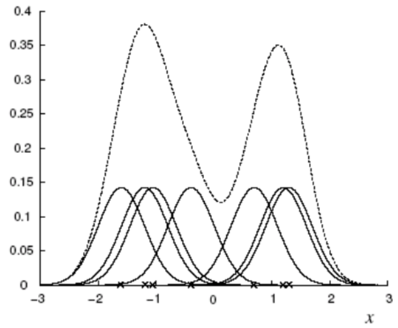
- M-step:

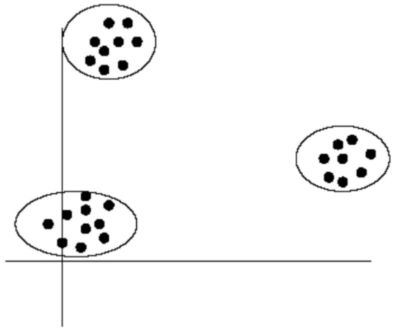
Another Example: Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components:

$$p(x_n|\mu,\Sigma)=\sum_k \pi_k N(x_i|\mu_k,\Sigma_k)$$

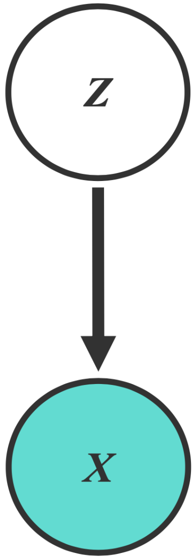
mixture proportion   mixture component





- This model can be used for unsupervised clustering.
  - This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

Example: Gaussian Mixture Models (GMMs)



- Consider a mixture of K Gaussian components:
  - Z is a latent class indicator vector:

$$p(z_n) = \mathrm{multi}(z_n : \pi) = \prod_k (\pi_k)^{z_n^k}$$

  - X is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n \mid z_n^k = 1, \mu, \Sigma) = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{ -\tfrac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right\}$$

Parameters to be learned:

  - The likelihood of a sample:

mixture component

mixture proportion

$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z^k = 1 \mid \pi) p(x, \mid z^k = 1, \mu, \Sigma) \\ &= \sum_{z_n} \prod_k \left((\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, \mid \mu_k, \Sigma_k) \end{aligned}$$

Example: Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components
- The expected complete log likelihood

$$\mathbb{E}_q\left[\ell_c(\boldsymbol{\theta}; x, z)\right] = \sum_n \mathbb{E}_q\left[\log p\left(z_n \mid \pi\right)\right] + \sum_n \mathbb{E}_q\left[\log p\left(x_n \mid z_n, \mu, \Sigma\right)\right]$$

$$= \sum_n \sum_k \mathbb{E}_q\left[z_n^k\right] \log \pi_k - \frac{1}{2} \sum_n \sum_k \mathbb{E}_q\left[z_n^k\right] \left(\left(x_n - \mu_k\right)^T \Sigma_k^{-1} \left(x_n - \mu_k\right) + \log\left|\Sigma_k\right| + C\right)$$

- E-step: computing the posterior of z_n given the current estimate of the parameters (i.e., π , μ, Σ)

$$p(z_n^k = 1 \mid x, \mu^{(t)}, \Sigma^{(t)}) = \frac{\pi_k^{(t)} N(x_n, \mid \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_i \pi_i^{(t)} N(x_n, \mid \mu_i^{(t)}, \Sigma_i^{(t)})}$$

$p(z_n^k = 1, x, \mu^{(t)}, \Sigma^{(t)})$

$p(x, \mu^{(t)}, \Sigma^{(t)})$

Example: Gaussian Mixture Models (GMMs)

- M-step: computing the parameters given the current estimate of z_n

$$\pi_k^* = \arg\max \langle l_c(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \frac{\partial}{\partial \pi_k} \langle l_c(\boldsymbol{\theta}) \rangle = 0, \forall k, \quad \text{s.t.} \sum_{\text{k}} \pi_k = 1$$

$$\Rightarrow \quad \pi_k^* = \sum_n \langle z_n^k \rangle_{q^{(t)}} \Big/ N = \sum_n \tau_n^{k(t)} \Big/ N = \langle n_k \rangle \Big/ N$$

$$\mu_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \quad \mu_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} x_n}{\sum_n \tau_n^{k(t)}}$$

$$\Sigma_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \quad \Sigma_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \tau_n^{k(t)}}$$

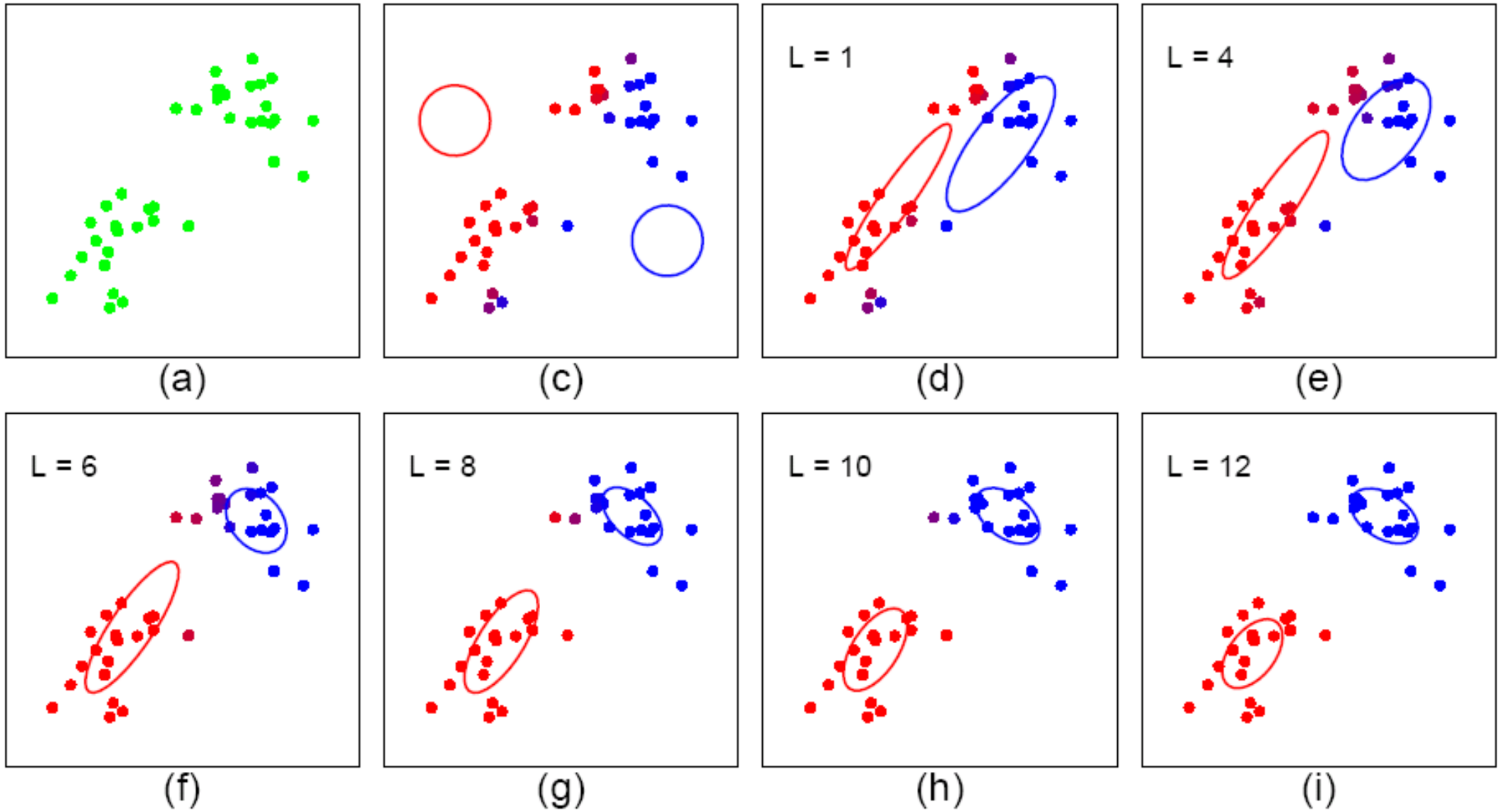
Fact:

$$\frac{\partial \log |\mathrm{A}^{-1}|}{\partial \mathrm{A}^{-1}} = \mathrm{A}^T$$

$$\frac{\partial \mathbf{x}^T \mathrm{A} \mathbf{x}}{\partial \mathrm{A}} = \mathbf{x}\mathbf{x}^T$$

Example: Gaussian Mixture Models (GMMs)

- Start: "guess" the centroid μ_k and covariance Σ_k of each of the K clusters
- Loop:



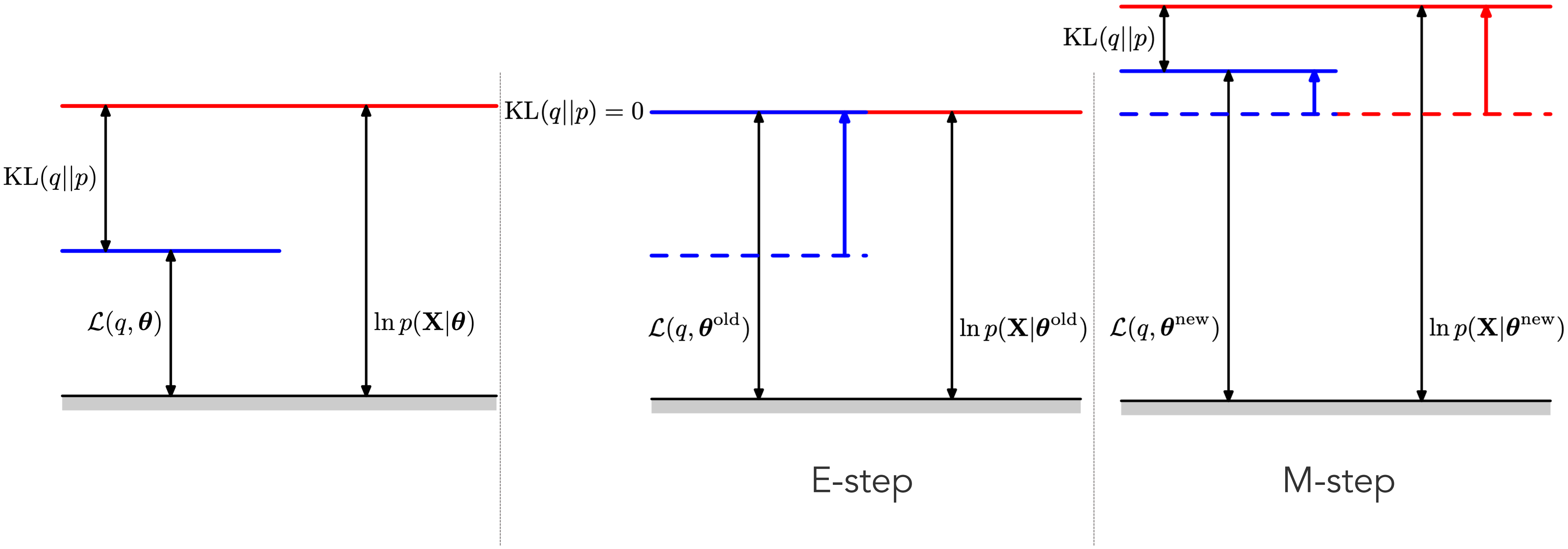
Summary: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces
  - Estimate some "missing" or "unobserved" data from observed data and current parameters.
  - Using this "complete" data, find the maximum likelihood parameter estimates.

- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:
  - E-step: $q^{t+1} = \arg\min_{q} F\left(q, \theta^{t}\right)$
  - M-step: $\theta^{t+1} = \arg\min_{\theta} F\left(q^{t+1}, \theta^{t}\right)$

Each EM iteration guarantees to improve the likelihood

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$



[PRML, Chap 9.4]

EM Variants

- Sparse EM
  - Do not re-compute exactly the posterior probability on each data point under all models, because it is almost zero.
  - Instead keep an "active list" which you update every once in a while.

- Generalized (Incomplete) EM:
  - It might be hard to find the ML parameters in the M-step, even given the completed data. We can still make progress by doing an M-step that improves the likelihood a bit (e.g. gradient step).

Questions?