Probabilistic Machine Learning
Lecture 23
Tuning Inference Algorithms

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Designing a probabilistic machine learning method:

1. get the **data**
   1.1 try to collect as much meta-data as possible
2. build the **model**
   2.1 identify quantities and datastructures; assign names
   2.2 design a generative process (graphical model)
   2.3 assign (conditional) distributions to factors/arrows (use exponential families!)
3. design the **algorithm**
   3.1 consider conditional independence
   3.2 try standard methods for early experiments
   3.3 run unit-tests and sanity-checks
   3.4 identify bottlenecks, find customized approximations and refinements

The Toolbox

Framework:

$$\int p(x_1, x_2)\, dx_2 = p(x_1) \qquad p(x_1, x_2) = p(x_1 \mid x_2) p(x_2) \qquad p(x \mid y) = \frac{p(y \mid x) p(x)}{p(y)}$$

Modelling:

- graphical models
- Gaussian distributions
- (deep) learnt representations
- Kernels
- Markov Chains
- Exponential Families / Conjugate Priors
- Factor Graphs & Message Passing

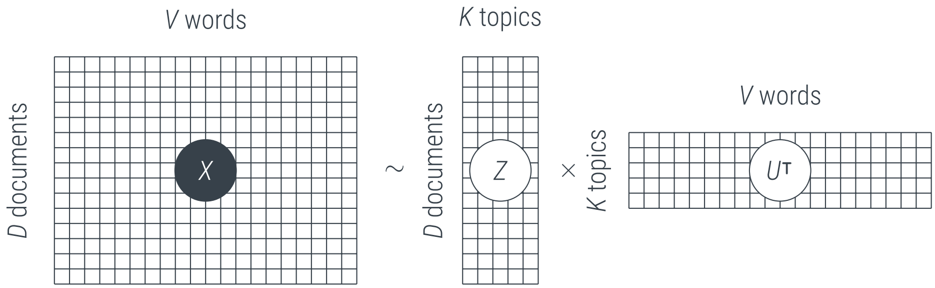
Computation:

- Monte Carlo
- Linear algebra / Gaussian inference
- maximum likelihood / MAP
- Laplace approximations
- EM / variational approximations

The Data
and an idea for a model

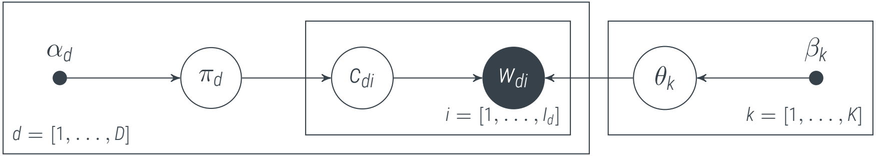
Making Assumptions

Our Data, our model



- a corpus of D documents
- each containing I_d words from a vocabulary of V words
- assumed to consist of K topics

The Model

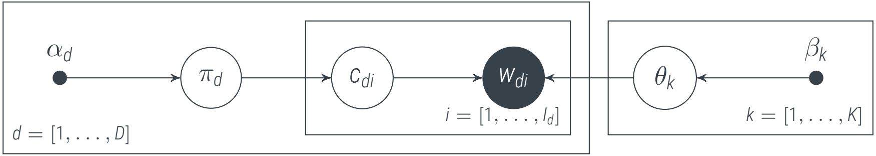


To draw I_d words $w_{di} \in [1, \dots, V]$ of document $d \in [1, \dots, D]$:

- Draw K topic distributions θ_k over V words from $\quad p(\Theta \mid \boldsymbol{\beta}) = \prod_{k=1}^{K} \mathcal{D}(\theta_k; \beta_k)$
- Draw D document distributions over K topics from $\quad p(\Pi \mid \boldsymbol{\alpha}) = \prod_{d=1}^{D} \mathcal{D}(\pi_d; \alpha_d)$
- Draw topic assignments c_{dik} of word w_{di} from $\quad p(C \mid \Pi) = \prod_{i,d,k} \pi_{dk}^{c_{dik}}$
- Draw word w_{di} from $\quad p(w_{di} = v \mid c_{di}, \Theta) = \prod_k \theta_{kv}^{c_{dik}}$

Useful notation: $n_{dkv} = \#\{i : w_{di} = v, c_{dik} = 1\}$. Write $n_{dk:} := [n_{dk1}, \dots, n_{dkV}]$ and $n_{dk\cdot} = \sum_v n_{dkv}$, etc.

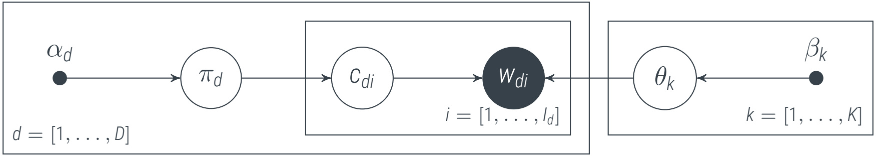
[Blei, D. M., Ng, A. Y. & Jordan, M. I. (2003) JMLR 3, 993–1022]



$$p(C, \Pi, \Theta, W) = \underbrace{\left(\prod_{d=1}^{D} \mathcal{D}(\boldsymbol{\pi}_d; \boldsymbol{\alpha}_d)\right)}_{p(\Pi|\boldsymbol{\alpha})} \cdot \underbrace{\left(\prod_{d=1}^{D} \prod_{i=1}^{I_d} \left(\prod_{k=1}^{K} \pi_{dk}^{c_{dik}}\right)\right)}_{p(C|\Pi)} \cdot \underbrace{\left(\prod_{d=1}^{D} \prod_{i=1}^{I_d} \left(\prod_{k=1}^{K} \theta_{kw_{di}}^{c_{dik}}\right)\right)}_{p(W|C,\Theta)} \cdot \underbrace{\left(\prod_{k=1}^{K} \mathcal{D}(\boldsymbol{\theta}_k; \boldsymbol{\beta}_k)\right)}_{p(\Theta|\boldsymbol{\beta})}$$

$$= \underbrace{\left(\prod_{d=1}^{D} \mathcal{D}(\boldsymbol{\pi}_d; \boldsymbol{\alpha}_d)\right)}_{p(\Pi|\boldsymbol{\alpha})} \cdot \underbrace{\left(\prod_{d=1}^{D} \prod_{i=1}^{I_d} \left(\prod_{k=1}^{K} (\pi_{dk}\theta_{kw_{di}})^{c_{dik}}\right)\right)}_{p(W,C|\Theta,\Pi)} \cdot \underbrace{\left(\prod_{k=1}^{K} \mathcal{D}(\boldsymbol{\theta}_k; \boldsymbol{\beta}_k)\right)}_{p(\Theta|\boldsymbol{\beta})}$$

$$= \left(\prod_{d=1}^{D} \frac{\Gamma(\sum_k \alpha_{dk})}{\prod_k \Gamma(\alpha_{dk})} \prod_{k=1}^{K} \pi_{dk}^{\alpha_{dk}-1+n_{dk\cdot}}\right) \cdot \left(\prod_{k=1}^{K} \frac{\Gamma(\sum_v \beta_{kv})}{\prod_v \Gamma(\beta_{kv})} \prod_{v=1}^{V} \theta_{kv}^{\beta_{kv}-1+n_{\cdot kv}}\right)$$



$$p(C, \Pi, \Theta, W) = \left(\prod_{d=1}^{D} \mathcal{D}(\boldsymbol{\pi}_d; \boldsymbol{\alpha}_d)\right) \cdot \left(\prod_{d=1}^{D} \prod_{i=1}^{I_d} \left(\prod_{k=1}^{K} \pi_{dk}^{c_{dik}}\right)\right) \cdot \left(\prod_{d=1}^{D} \prod_{i=1}^{I_d} \left(\prod_{k=1}^{K} \theta_{kw_{di}}^{c_{dik}}\right)\right) \cdot \left(\prod_{k=1}^{K} \mathcal{D}(\boldsymbol{\theta}_k; \boldsymbol{\beta}_k)\right)$$

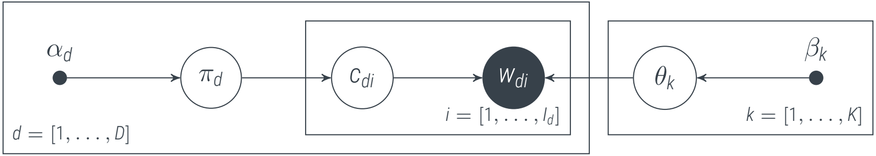
- If we had Π, Θ (which we don't), then the posterior $p(C \mid \Theta, \Pi, W)$ would be easy:

$$p(C \mid \Theta, \Pi, W) = \frac{p(W, C, \Theta, \Pi)}{\sum_C p(W, C, \Theta, \Pi)} = \prod_{d=1}^{D} \prod_{i=1}^{I_d} \frac{\prod_{k=1}^{K} (\pi_{dk} \theta_{kw_{di}})^{c_{dik}}}{\sum_{k'} (\pi_{dk'} \theta_{k' w_{di}})}$$

- note that this conditional independence can easily be read off from the above graph!

Posteriors

Latent Dirichlet Allocation



$$p(C, \Pi, \Theta, W) = \left(\prod_{d=1}^{D} \frac{\Gamma(\sum_k \alpha_{dk})}{\prod_k \Gamma(\alpha_{dk})} \prod_{k=1}^{K} \pi_{dk}^{\alpha_{dk}-1+n_{dk\cdot}} \right) \cdot \left(\prod_{k=1}^{K} \frac{\Gamma(\sum_v \beta_{kv})}{\prod_v \Gamma(\beta_{kv})} \prod_{v=1}^{V} \theta_{kv}^{\beta_{kv}-1+n_{\cdot kv}} \right)$$

- If we had C (which we don't), then the posterior $p(\Theta, \Pi \mid C, W)$ would be easy:

$$p(\Theta, \Pi \mid C, W) = \frac{p(C, W, \Pi, \Theta)}{\int p(\Theta, \Pi, C, W)\, d\Theta\, d\Pi} = \frac{\left(\prod_d \mathcal{D}(\pi_d; \alpha_d) \left(\prod_k \pi_{dk}^{n_{dk\cdot}}\right)\right) \left(\prod_k \mathcal{D}(\theta_k; \beta_k) \left(\prod_v \theta_{kv}^{n_{\cdot kv}}\right)\right)}{p(C, W)}$$

$$= \left(\prod_d \mathcal{D}(\pi_d; \alpha_{d:} + n_{d:\cdot}) \right) \left(\prod_k \mathcal{D}(\theta_k; \beta_{k:} + n_{\cdot k:}) \right)$$

- note that this conditional independence **can not** easily be read off from the above graph!

The Algorithms

A Gibbs Sampler

Simple Markov Chain Monte Carlo inference

Iterate between (recall $n_{dkv} = \#\{i : w_{di} = v, c_{ijk} = 1\}$)

$$\Theta \sim p(\Theta \mid C, W) = \prod_k \mathcal{D}(\theta_k; \beta_{k:} + n_{\cdot k:})$$

$$\Pi \sim p(\Pi \mid C, W) = \prod_d \mathcal{D}(\pi_d; \alpha_{d:} + n_{d:\cdot})$$

$$C \sim p(C \mid \Theta, \Pi, W) = \prod_{d=1}^{D} \prod_{i=1}^{I_d} \frac{\prod_{k=1}^{K} (\pi_{dk}\theta_{kw_{di}})^{c_{dik}}}{\sum_{k'} (\pi_{dk'}\theta_{k'w_{di}})}$$

- This is *comparably* easy to implement because there are libraries for sampling from Dirichlet's, and discrete sampling is trivial. All we have to keep around are the counts n (which are sparse!) and Θ, Π (which are comparably small). Thanks to factorization, much can also be done in parallel!
- Unfortunately, this sampling scheme is relatively slow to move out of initialization, because z depends strongly on θ, π and vice versa.
- properly vectorizing the code is important for speed

Expectation Maximization

Iterative maximum likelihood (or maximum a posteriori)

To maximize $p(\Theta, \Pi \mid W)$, consider (where $\gamma_{dik} := \pi_{dk}\theta_{kw_{di}}$ and $\tilde{\gamma}_{dik} := \gamma_{dik} / \sum_{k'} \gamma_{dik'}$)

$$p(C \mid \Theta, \Pi, W) = \prod_{d=1}^{D} \prod_{i=1}^{I_d} \frac{\prod_{k=1}^{K} (\pi_{dk}\theta_{kw_{di}})^{c_{dik}}}{\sum_{k'} (\pi_{dk'}\theta_{k'w_{di}})} = \prod_{d=1}^{D} \prod_{i=1}^{I_d} \prod_{k=1}^{K} \tilde{\gamma}_{dik}^{c_{dik}}$$

And **M**aximize the **E**xpected complete log posterior

$$\mathbb{E}_{p(C|\gamma)}[\log p(\Theta, \Pi \mid W, C)] = \sum_{d}^{D} \sum_{k}^{K} (\tilde{\gamma}_{d\cdot k} + \alpha_{dk}) \cdot \log \pi_{dk} + \sum_{k}^{K} \sum_{v}^{V} \left(\beta_{kv} + \sum_{d}^{D} \sum_{i}^{I_d} \mathbb{I}(w_{di} = v)\tilde{\gamma}_{dik} \right) \log \theta_{kv}$$

at

$$\pi_{dk} = \frac{\tilde{\gamma}_{d\cdot k} + \alpha_{dk}}{\tilde{\gamma}_{d\cdot\cdot} + \alpha_{d\cdot}} \quad \text{and} \quad \theta_{kv} = \frac{\beta_{kv} + \sum_{d,i} \mathbb{I}(w_{di} = v)\tilde{\gamma}_{dik}}{\beta_{k\cdot} + \sum_{v'} \sum_{d,i} \mathbb{I}(w_{di} = v')\tilde{\gamma}_{dik}}$$

and repeat.

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To find the distribution q the minimizes, subject to $q(\Pi, \Theta, C) = q(\Pi, \Theta) \cdot q(C)$

$$D_{\mathrm{KL}}(q(\Pi, \Theta, C) \| p(\Pi, \Theta, C \mid W)) = \int q \log \frac{q}{p}\, dq$$

or, equivalently, maximizes the ELBO

$$\mathcal{L}(q) = \int q(C, \Pi, \Theta) \log \left(\frac{p(C, \Pi, \Theta, W)}{q(C, \Pi, \Theta)}\, dC\, d\Pi\, d\Theta \right)$$

set $\log q(C) = \mathbb{E}_{q(\Pi,\Theta)}(\log p(C, \Pi, \Theta, W)$ and vice versa, to get…

Variational Inference

iterative minimum KL divergence

[Blei, D. M., Ng, A. Y. & Jordan, M. I. (2003) JMLR 3, 993–1022]

$$q(\boldsymbol{\pi}_d) = \mathcal{D}\left(\boldsymbol{\pi}_d; \tilde{\alpha}_{dk} := \left[\alpha_{dk} + \sum_{i=1}^{I_d} \tilde{\gamma}_{dik}\right]_{k=1,\dots,K}\right) \qquad \forall d = 1, \dots, D$$

$$q(\boldsymbol{\theta}_k) = \mathcal{D}\left(\boldsymbol{\theta}_k; \tilde{\beta}_{kv} := \left[\beta_{kv} + \sum_{d}^{D} \sum_{i=1}^{I_d} \tilde{\gamma}_{dik}\mathbb{I}(w_{di} = v)\right]_{v=1,\dots,V}\right) \qquad \forall k = 1, \dots, K$$

$$q(\mathbf{c}_{di}) = \prod_k \tilde{\gamma}_{dik}^{c_{dik}}, \qquad \forall d \quad i = 1, \dots, I_d$$

where $\tilde{\gamma}_{dik} = \gamma_{dik} / \sum_k \gamma_{dik}$ and (note that $\sum_k \tilde{\alpha}_{dk} = \text{const.}$)

$$\gamma_{dik} = \exp\left(\mathbb{E}_{q(\pi_{dk})}(\log \pi_{dk}) + \mathbb{E}_{q(\theta_{di})}(\log \theta_{kw_{di}})\right) = \exp\left(\digamma(\tilde{\alpha}_{jk}) + \digamma(\tilde{\beta}_{kw_{di}}) - \digamma\left(\sum_v \tilde{\beta}_{kv}\right)\right)$$

and repeat

An idea.

- Consider the exponential family $p_w(x \mid w) = \exp\left[\phi(x)^\intercal w - \log Z(w)\right]$
- its conjugate prior is the exponential family $F(\alpha, \nu) = \int \exp(\alpha^\intercal w - \nu^\intercal \log Z(w))\, dw$

$$p_\alpha(w \mid \alpha, \nu) = \exp\left[\begin{pmatrix} w \\ -\log Z(w) \end{pmatrix}^\intercal \begin{pmatrix} \alpha \\ \nu \end{pmatrix} - \log F(\alpha, \nu)\right]$$

because $p_\alpha(w \mid \alpha, \nu) \prod_{i=1}^{n} p_w(x_i \mid w) \propto p_\alpha\left(w \,\middle|\, \alpha + \sum_i \phi(x_i), \nu + n\right)$

- and the predictive is

$$p(x) = \int p_w(x \mid w) p_\alpha(w \mid \alpha, \nu)\, dw = \int e^{(\phi(x)+\alpha)^\intercal w - (\nu+1)\log Z(w) - \log F(\alpha,\nu)}\, dw$$
$$= \frac{F(\phi(x) + \alpha, \nu + 1)}{F(\alpha, \nu)}$$

Exponential Families, among other things (see also last lecture) provide **conjugate priors** for standard distributions (Lectures 2,15)

- Consider the exponential family $p(c \mid \pi) = \exp\left[c^\intercal(\log \pi) - \log \sum_k \pi_k\right]$
- its conjugate prior is the exponential family $B(\alpha) = \int \exp(\alpha^\intercal \log \pi - \nu \cdot 0)\, d\pi$

$$\mathcal{D}(\pi \mid \alpha) = \exp\left[\log \pi^\intercal \alpha - \log B(\alpha)\right]$$

$$\text{because } \mathcal{D}(\pi \mid \alpha) \prod_{i=1}^{n} \pi^{c_i} \propto \mathcal{D}\left(\pi \mid \alpha + \sum_i c_i\right)$$

- and the predictive is

$$p(c) = \int p(c \mid \pi)\mathcal{D}(\pi \mid \alpha)\, d\pi = \int e^{(c+\alpha)^\intercal(\log \pi) + \log B(\alpha)}\, d\pi = \frac{B(c+\alpha)}{B(\alpha)}$$

Exponential Families, among other things (see also last lecture) provide **conjugate priors** for standard distributions (Lectures 2,15)

Recall $\Gamma(x+1) = x \cdot \Gamma(x) \ \forall x \in \mathbb{R}_+$

$$p(C, \Pi, \Theta, W) = \left(\prod_{d=1}^{D} \frac{\Gamma(\sum_k \alpha_{dk})}{\prod_k \Gamma(\alpha_{dk})} \prod_{k=1}^{K} \pi_{dk}^{\alpha_{dk}-1+n_{dk\cdot}} \right) \cdot \left(\prod_{k=1}^{K} \frac{\Gamma(\sum_v \beta_{kv})}{\prod_v \Gamma(\beta_{kv})} \prod_{v=1}^{V} \theta_{kv}^{\beta_{kv}-1+n_{\cdot kv}} \right)$$

$$= \left(\prod_{d=1}^{D} \frac{B(\alpha_d + n_{d:\cdot})}{B(\alpha_d)} \mathcal{D}(\pi_d; \alpha_d + n_{d:\cdot}) \right) \cdot \left(\prod_{k=1}^{K} \frac{B(\beta_k + n_{\cdot k:})}{B(\beta_k)} \mathcal{D}(\theta_k; \beta_k + n_{\cdot k:}) \right)$$

$$p(C, W) = \left(\prod_{d=1}^{D} \frac{B(\alpha_d + n_{d:\cdot})}{B(\alpha_d)} \right) \cdot \left(\prod_{k=1}^{K} \frac{B(\beta_k + n_{\cdot k:})}{B(\beta_k)} \right)$$

$$= \left(\prod_{d} \frac{\Gamma(\sum_{k'} \alpha_{dk'})}{\Gamma(\sum_{k'} \alpha_{dk'} + n_{dk'\cdot})} \prod_k \frac{\Gamma(\alpha_{dk} + n_{dk\cdot})}{\Gamma(\alpha_{dk})} \right) \left(\prod_{k} \frac{\Gamma(\sum_v \beta_{kv})}{\Gamma(\sum_v \beta_{kv} + n_{\cdot kv})} \prod_v \frac{\Gamma(\beta_{kv} + n_{\cdot kv})}{\Gamma(\beta_{kv})} \right)$$

$$p(c_{dik} = 1 \mid C^{\setminus di}, W) = \frac{(\alpha_{dk} + n_{dk\cdot}^{\setminus di})(\beta_{kw_{di}} + n_{\cdot kw_{di}}^{\setminus di})(\sum_v \beta_{kv} + n_{\cdot kv}^{\setminus di})^{-1}}{\sum_{k'} (\alpha_{dk'} + n_{dk'\cdot}^{\setminus di}) \cdot \sum_{w'} (\beta_{kw'} + n_{\cdot kw'}^{\setminus di}) \cdot \sum_{v'} (\beta_{kv'} + n_{\cdot kv'}^{\setminus di})^{-1}}$$

A Collapsed Gibbs Sampler for LDA

It pays off to look closely at the math!

T. L. Griffiths & M. Steyvers, *Finding scientific topics*, PNAS **101**/1 (4/2004), 5228–5235

$$p(C, W) = \left(\prod_d \frac{\Gamma(\sum_k \alpha_{dk})}{\Gamma(\sum_k \alpha_{dk} + n_{dk\cdot})} \prod_k \frac{\Gamma(\alpha_{dk} + n_{dk\cdot})}{\Gamma(\alpha_{dk})} \right) \left(\prod_k \frac{\Gamma(\sum_v \beta_{kv})}{\Gamma(\sum_v \beta_{kv} + n_{\cdot kv})} \prod_v \frac{\Gamma(\beta_{kv} + n_{\cdot kv})}{\Gamma(\beta_{kv})} \right)$$

A **collapsed** sampling method can converge much faster by eliminating the latent variables that mediate between individual data.

procedure LDA(W, α, β)
- $\gamma_{dkv} \leftarrow 0 \;\forall d, k, v$ // initialize counts
- **while** true **do**
  - **for** $d = 1, \dots, D; i = 1, \dots, I_d$ **do** // can be parallelized
    - $c_{di} \propto (\alpha_{dk} + n_{dk\cdot}^{\backslash di})(\beta_{kw_{di}} + n_{\cdot kw_{di}}^{\backslash di})(\sum_v \beta_{kv} + n_{\cdot kv}^{\backslash di})^{-1}$ // sample assignment
    - $n \leftarrow \textsc{UpdateCounts}(c_{di})$ // update counts (check whether first pass or repeat)
  - **end for**
- **end while**

end procedure

Collapsed Sampling is quite efficient

The Mean Field argument [figure: T. L. Griffiths & M. Steyvers, *Finding scientific topics*, PNAS **101**/1 (4/2004), 5228–5235]

Thomas Griffiths

image: Princeton U

Mark Steyvers

image: UC Irvine

The collapsed sampler operates on the **mean field**

$$p(C \mid W) = \int p(C \mid \Theta, \Pi, W) p(\Theta, \Pi \mid W) \, d\Theta \, d\Pi$$

The *expected* value of the variables Θ, Π that mediate between the "particles" (words). This works well because each word's topic is approximately independent of all individual other words' topics (but together they create the whole thing).

- Deriving our variational bound, we previously imposed the factorization

$$q(\Pi, \Theta, C) = q(\Pi, \Theta) \cdot q(C), \quad \text{but can we get away with less? Like,}$$
$$q(\Pi, \Theta, C) = q(\Theta, \Pi \mid C) \cdot q(C)$$

- Note $p(C, \Theta, \Pi \mid W) = p(\Theta, \Pi \mid C, W)p(C \mid W)$. So when we minimize

$$\begin{aligned}
D_{\mathrm{KL}}(q(\Pi, \Theta, C) \| p(\Pi, \Theta, C \mid W)) &= \int q(\Pi, \Theta \mid C)q(C) \log\left(\frac{q(\Pi, \Theta | C)q(C)}{p(\Pi, \Theta \mid C, W)p(C \mid W)}\right) dC \, d\Pi \, d\Theta \\
&= \int q(\Pi, \Theta \mid C)q(C) \left[\log\left(\frac{q(\Pi, \Theta \mid C)}{p(\Pi, \Theta \mid C, W)}\right) + \log\left(\frac{q(C)}{p(C \mid W)}\right)\right] dC \, d\Pi \, d\Theta \\
&= D_{\mathrm{KL}}(q(\Pi, \Theta \mid C) \| p(\Pi, \Theta \mid C, W)) + D_{\mathrm{KL}}(q(C) \| p(C \mid W))
\end{aligned}$$

we will just get $q(\Theta, \Pi) = p(\Theta, \Pi \mid C, W)$ and the bound will be *tight* in Π, Θ.

A Collapsed Variational Bound

Why don't we use the mean field in our variational bound?

Yee Whye Teh, David Newman & Max Welling, NeurIPS 2007

$$p(C,W) = \left(\prod_d \frac{\Gamma(\sum_k \alpha_{dk})}{\Gamma(\sum_k \alpha_{dk} + n_{dk\cdot})} \prod_k \frac{\Gamma(\alpha_{dk} + n_{dk\cdot})}{\Gamma(\alpha_{dk})}\right) \left(\prod_k \frac{\Gamma(\sum_v \beta_{kv})}{\Gamma(\sum_v \beta_{kv} + n_{\cdot kv})} \prod_v \frac{\Gamma(\beta_{kv} + n_{\cdot kv})}{\Gamma(\beta_{kv})}\right)$$

- The remaining **collapsed variational bound** (ELBO) becomes

$$\mathcal{L}(q) = \int q(C) \log p(C,W)\, dC + \mathbb{H}(q(C))$$

- because we make strictly less assumptions about q than before, we will get a strictly better approximation to the true posterior!
- The bound is maximized for c_{di} if

$$\log q(c_{di}) = \mathbb{E}_{q(C^{\setminus di})}(\log p(C,W)) + \text{const.}$$

Constructing the Algorithm

Why didn't we do this earlier?

- Note that $c_{di} \in \{0;1\}^K$ and $\sum_k c_{dik} = 1$. So $q(c_{di}) = \prod_k \gamma_{dik}$ with $\sum_k \gamma_{dik} = 1$
- Also: $\Gamma(\alpha + n) = \prod_{\ell=0}^{n-1}(\alpha + \ell)$, thus $\log \Gamma(\alpha + n) = \sum_{\ell=0}^{n-1} \log(\alpha + \ell)$

$$p(C, W) = \left(\prod_d \frac{\Gamma(\sum_k \alpha_{dk})}{\Gamma(\sum_k \alpha_{dk} + n_{dk\cdot})} \prod_k \frac{\Gamma(\alpha_{dk} + n_{dk\cdot})}{\Gamma(\alpha_{dk})}\right) \left(\prod_k \frac{\Gamma(\sum_v \beta_{kv})}{\Gamma(\sum_v \beta_{kv} + n_{\cdot kv})} \prod_v \frac{\Gamma(\beta_{kv} + n_{\cdot kv})}{\Gamma(\beta_{kv})}\right)$$

$$\begin{aligned}
\log q(c_{di}) &= \mathbb{E}_{q(C^{\setminus di})}(\log p(C, W)) + \text{const.} \\
\log \gamma_{dik} &= \log q(c_{dik} = 1) \\
&= \mathbb{E}_{q(C^{\setminus di})}\left[\log \Gamma(\alpha_{dk} + n_{dk\cdot}) + \log \Gamma(\beta_{kw_{di}} + n_{\cdot kw_{di}}) - \log \Gamma\left(\sum_v \beta_{kv} + n_{\cdot kv}\right)\right] + \text{const.} \\
&= \mathbb{E}_{q(C^{\setminus di})}\left[\log(\alpha_{dk} + n_{dk\cdot}^{\setminus di}) + \log(\beta_{kw_{di}} + n_{\cdot kw_{di}}^{\setminus di}) - \log\left(\sum_v \beta_{kv} + n_{\cdot kv}^{\setminus di}\right)\right] + \text{const.}
\end{aligned}$$

(note all terms in $p(C, W)$ that don't involve c_{dik} can be moved into the constant, as can all sums over k. We can also *add* terms to const., such as $\sum_{\ell=0}^{n^{\setminus di}-1} \log(\alpha + \ell)$, effectively cancelling terms in $\log \Gamma$)

A Complication

Ah, that's why!

$$\gamma_{dik} \propto \exp\left(\mathbb{E}_{q(C^{\setminus di})}\left[\log(\alpha_{dk} + n_{dk\cdot}^{\setminus di}) + \log(\beta_{kw_{di}} + n_{\cdot kw_{di}}^{\setminus di}) - \log\left(\sum_v \beta_{kv} + n_{\cdot kv}^{\setminus di}\right)\right]\right)$$

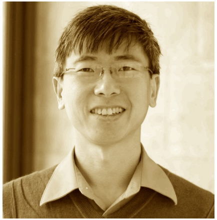
- Under $q(C) = \prod_{di} c_{di}$, the counts $n_{dk\cdot}$ are sums of independent Bernoulli variables (i.e. they have a **multinomial** distribution). Computing their expected logarithm is tricky ($\mathcal{O}(n_{d\cdot\cdot}^2)$):

$$\mathbb{H}(q(n_{dk\cdot})) = \mathbb{E}[\log n_{dk\cdot}] = -\log(I_d!) - I_d \sum_k^K \gamma_{dk\cdot} \log(\gamma_{dk\cdot}) + \sum_{k=1}^K \sum_{n_{dk\cdot}=1}^{I_d} \binom{I_d}{n_{dk\cdot}} \gamma_{dk\cdot}^{n_{dk\cdot}} (1 - \gamma_{dk\cdot})^{I_d - n_{dk\cdot}} \log(n_{dk\cdot}!)$$

- That's likely why the original paper (and `scikit-learn`) don't do this.

If arithmetic doesn't work, try creativity!

Yee Whye Teh, David Newman & Max Welling, NeurIPS 2007



Yee Whye Teh

image: Oxford U

Max Welling

image: U v Amsterdam

$$\gamma_{dik} \propto \exp\left(\mathbb{E}_{q(c^{\setminus di})}\left[\log(\alpha_{dk} + n_{dk\cdot}^{\setminus di}) + \log(\beta_{kw_{di}} + n_{\cdot kw_{di}}^{\setminus di}) - \log\left(\sum_v \beta_{kv} + n_{\cdot kv}^{\setminus di}\right)\right]\right)$$

Statistics for the rescue

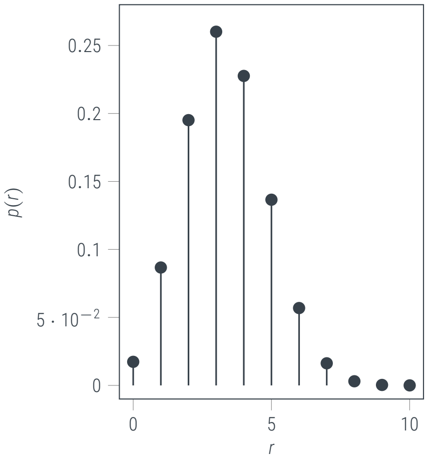
recall Lecture 3

Yee Whye Teh, David Newman & Max Welling, NeurIPS 2007

The probability measure of $R = \sum_i^N x_i$ with discrete x_i of probablity f is

$$
\begin{aligned}
P(R = r \mid f, N) &= \frac{N!}{(N-r)! \cdot r!} \cdot f^r \cdot (1-f)^{N-r} \\
&= \binom{N}{r} \cdot f^r \cdot (1-f)^{N-r} \\
&\approx \mathcal{N}(r; Nr, Nr(1-r))
\end{aligned}
$$

$f = 1/3, N = 10$



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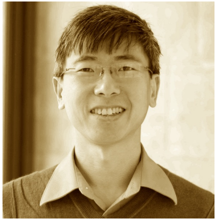

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but the CLT applies! So a Gaussian approximation should be good:

$$p(n_{dk\cdot}^{\setminus di}) \approx \mathcal{N}(n_{dk\cdot}^{\setminus di}; \mathbb{E}_q[n_{dk\cdot}^{\setminus di}], \operatorname{var}_q[n_{dk\cdot}^{\setminus di}]) \quad \text{with} \quad \mathbb{E}_q[n_{dk\cdot}^{\setminus di}] = \sum_{j \neq i} \gamma_{dkj}, \quad \operatorname{var}_q[n_{dk\cdot}^{\setminus di}] = \sum_{j \neq i} \gamma_{dkj}(1 - \gamma_{dkj})$$

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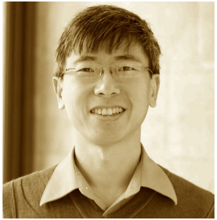
Yee Whye Teh, David Newman & Max Welling, NeurIPS 2007



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$$\mathbb{E}_q[\log(\alpha_{dk} + n_{dk\cdot}^{\backslash di})] \approx \log(\alpha_{dk} + \mathbb{E}_q[n_{dk\cdot}^{\backslash di}]) - \frac{\operatorname{var}_q[n_{dk\cdot}^{\backslash di}]}{2(\alpha_{dk} + \mathbb{E}_q[n_{dk\cdot}^{\backslash di}])^2}$$

$$\gamma_{dik} \propto \exp\left(\mathbb{E}_{q(C^{\setminus di})}\left[\log(\alpha_{dk} + n_{dk\cdot}^{\setminus di}) + \log(\beta_{kw_{di}} + n_{\cdot kw_{di}}^{\setminus di}) - \log\left(\sum_v \beta_{kv} + n_{\cdot kv}^{\setminus di}\right)\right]\right)$$

$$\mathbb{E}_q[\log(\alpha_{dk} + n_{dk\cdot}^{\setminus di})] \approx \log(\alpha_{dk} + \mathbb{E}_q[n_{dk\cdot}^{\setminus di}]) - \frac{\mathrm{var}_q[n_{dk\cdot}^{\setminus di}]}{2(\alpha_{dk} + \mathbb{E}_q[n_{dk\cdot}^{\setminus di}])^2}$$

$$\gamma_{dik} \propto (\alpha_{dk} + \mathbb{E}[n_{dk\cdot}^{\setminus di}])(\beta_{kw_{di}} + \mathbb{E}[n_{\cdot kw_{di}}^{\setminus di}])\left(\sum_v \beta_{kv} + \mathbb{E}[n_{\cdot kv}^{\setminus di}]\right)^{-1}$$

$$\cdot \exp\left(-\frac{\mathrm{var}_q[n_{dk\cdot}^{\setminus di}]}{2(\alpha_{dk} + \mathbb{E}_q[n_{dk\cdot}^{\setminus di}])^2} - \frac{\mathrm{var}_q[n_{\cdot kw_{di}}^{\setminus di}]}{2(\beta_{kw_{di}} + \mathbb{E}_q[n_{\cdot kw_{di}}^{\setminus di}])^2} + \frac{\mathrm{var}_q[n_{\cdot k\cdot}^{\setminus di}]}{2(\sum_v \beta_{kv} + \mathbb{E}_q[n_{\cdot kv}^{\setminus di}])^2}\right)$$

Complexity

The algorithm

$$\gamma_{dik} \propto (\alpha_{dk} + \mathbb{E}[n_{dk\cdot}^{\setminus di}])(\beta_{kw_{di}} + \mathbb{E}[n_{\cdot kw_{di}}^{\setminus di}]) \left(\sum_v \beta_{kv} + \mathbb{E}[n_{\cdot kv}^{\setminus di}]\right)^{-1}$$

$$\cdot \exp\left(-\frac{\mathrm{var}_q[n_{dk\cdot}^{\setminus di}]}{2(\alpha_{dk} + \mathbb{E}_q[n_{dk\cdot}^{\setminus di}])^2} - \frac{\mathrm{var}_q[n_{\cdot kw_{di}}^{\setminus di}]}{2(\beta_{kw_{di}} + \mathbb{E}_q[n_{\cdot kw_{di}}^{\setminus di}])^2} + \frac{\mathrm{var}_q[n_{\cdot k\cdot}^{\setminus di}]}{2(\sum_v \beta_{kv} + \mathbb{E}_q[n_{\cdot kv}^{\setminus di}])^2}\right)$$

Note that γ_{dik} doesn't depend on $i \in 1, \dots, I_d$, it's the same for all w_{di} in d with $w_{di} = v$!

- memory requirement: $\mathcal{O}(DKV)$, since we have to store γ_{dik} for each value of $i \in 1, \dots, V$ and
  - $\mathbb{E}[n_{dk\cdot}], \mathrm{var}[n_{dk\cdot}] \in \mathbb{R}^{D \times K}$
  - $\mathbb{E}[n_{\cdot kv}], \mathrm{var}[n_{\cdot kv}] \in \mathbb{R}^{K \times V}$
  - $\mathbb{E}[n_{\cdot k\cdot}], \mathrm{var}[n_{\cdot k\cdot}] \in \mathbb{R}^{K}$
- computational complexity: $\mathcal{O}(DKV)$ We can loop over V rather than I_d (good for long documents!) Often, a document will be sparse in V, so iteration cost can be much lower.

Designing a probabilistic machine learning method:

1. get the **data**
   1.1 try to collect as much meta-data as possible
2. build the **model**
   2.1 identify quantities and datastructures; assign names
   2.2 design a generative process (graphical model)
   2.3 assign (conditional) distributions to factors/arrows (use exponential families!)
3. design the **algorithm**
   3.1 consider conditional independence
   3.2 try standard methods for early experiments
   3.3 run unit-tests and sanity-checks
   3.4 identify bottlenecks, find customized approximations and refinements

Simple, generic algorithms or toolboxes can give an idea of a model's efficacy.
To make an efficient product, you might have to build your own approximation, and tune it.