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Machine learning – Block 7

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Assignment 6: Evaluation

- ?

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This week's lectures

- Variational autoencoders
- Probabilistic Topic Models

Section 2

Introduction

Why variational autoencoders and topic models?

- Popular approaches in industry and academia
- Probabilistic methods for unsupervised learning

Why variational autoencoders and topic models?

- Popular approaches in industry and academia
- Probabilistic methods for unsupervised learning
- Aim of this lecture:
  - Describe the models
  - How to estimate these models
  - Explain what they are used for

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Use Cases

- Variational autoencoders: Unsupervised modeling of images
- Topic models: Unsupervised modeling of documents

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  - Visualize/analyze data
  - Compression
  - Feature construction
  - Analyze underlying patterns

Use Cases: Examples

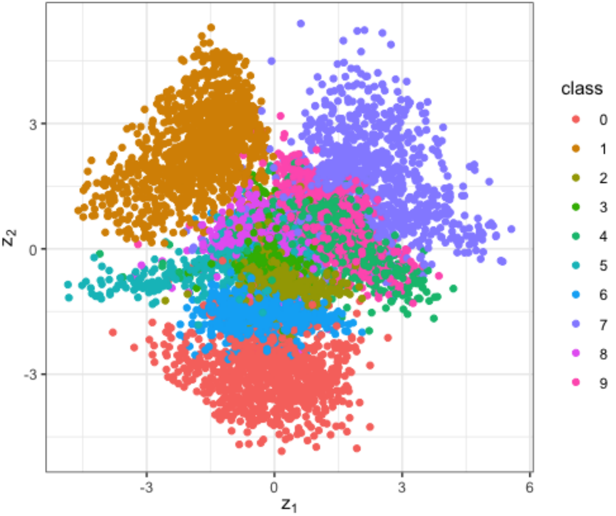

Figure: The latent state of MNIST using an Variational Autoencoder

Section 3

Autoencoders

Autoencoder

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- Three parts:
  - encoder $f(x)$ (or $e(x)$)
  - code h
  - decoder $g(h)$ (or $d(z)$)

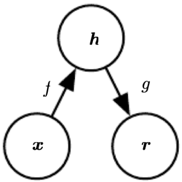

Figure: A Neural Autoencoder (Goodfellow et al, 2018)

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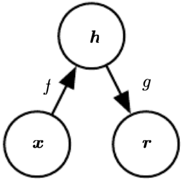

Figure: A Neural Autoencoder (Goodfellow et al, 2018)

- Loss function (reconstruction error):

$$L(\phi, \theta) = (x - d_\phi(e_\theta(x)))^2$$

The Undercomplete Autoencoder

- More interesting: an undercomplete autoencoder: Dimension of code is lower than that of x

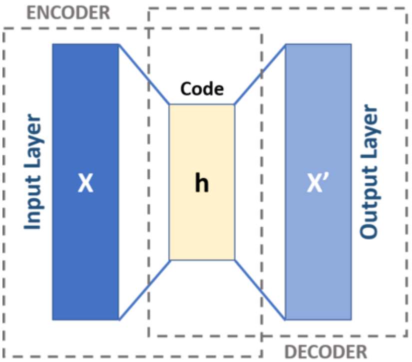

Figure: A Neural Autoencoder (Wikipedia)

PCA and autoencoders

- A linear autoencoder: $e_\theta(x) = W_\phi$, and $d_\theta(x) = W_\phi$
- We want to minimize the loss (ignoring b/the mean):

$$L(\phi, \theta) = \sum_{i=1}^{N} (x_i - W_\theta W_\phi x_i)^2$$

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- Remember PCA loss:

$$L(P) = \sum_{i=1}^{N} (x_i - P_q P_q^T x_i)^2 \,,$$

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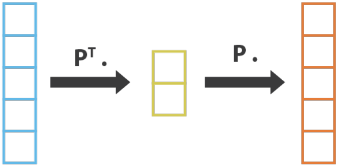
- Hence: PCA can be seen as an autoencoder



Deep Autoencoders

- Deep Autoencoder: An autoencoder with multilayer neural networks as encoder and decoder
  - can be seen as a non-linear PCA
  - learn nonlinear representations

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- Deep Autoencoder: An autoencoder with multilayer neural networks as encoder and decoder
  - can be seen as a non-linear PCA
  - learn nonlinear representations
- Problem: Deep autoencoders needs to be regularized to not overfit the latent state

probabilistic PCA as an decoder

- Problem: Autoencoders (as PCA) are not probabilistic models:
  - cannot generate data.
  - no notion of uncertainty

probabilistic PCA as an decoder

- Problem: Autoencoders (as PCA) are not probabilistic models:
  - cannot generate data.
  - no notion of uncertainty
- We would like something like probabilistic PCA for (deep) autoencoders

probabilistic PCA as an decoder

- Remember the pPCA model (with z as latent variable):

$$x_i \sim N(b + W z_i^T, \sigma I)$$

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- Another example is the Variational Autoencoder

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Section 4

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  1. The (probabilistic) encoder $q(z|\phi, x)$: inference model
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- VAEs get their name from variational inference (used in training)

The Variational Autoencoder

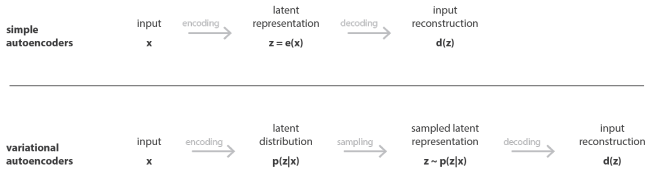

Figure: Autoencoder vs. the Variational Autoencoder (Rocca, 2019)

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The Variational Autoencoder

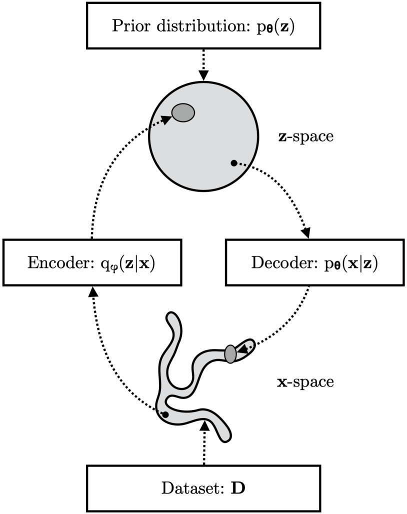

Figure: The Variational Autoencoder (Kingma and Welling, 2018, Fig. 2.1)

The probabilistic decoder

- The probabilistic decoder $p(x|\theta, z)$ (observation model)
- Usually a Normal distribution:

$$x_i \sim N(\text{NeuralNetwork}(z, \theta), cI)$$

- x_i for observation i depends non-linearly on z_i
- A probabilistic linear decoder: pPCA

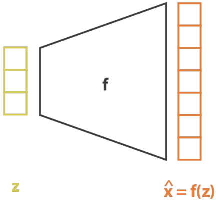

Figure: The Decoder (Rocca, 2019)

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- We assume that $q_\phi(z|x)$ follows a specific distribution. Commonly:

$$z \sim N(\mu, \Sigma)$$

- A neural network learns the parameters μ and Σ

$$\mu = \text{NeuralNetwork}(x, \phi_\mu)\,, \Sigma = \text{NeuralNetwork}(x, \phi_\Sigma)\,,$$

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$$\mu = \text{NeuralNetwork}(x, \phi_\mu)\,, \Sigma = \text{NeuralNetwork}(x, \phi_\Sigma)\,,$$

  where $\phi = (\phi_\mu, \phi_\Sigma)$
- One common assumption is that Σ is a diagonal matrix.
- Result: z_i for observation i depends non-linearly on x_i

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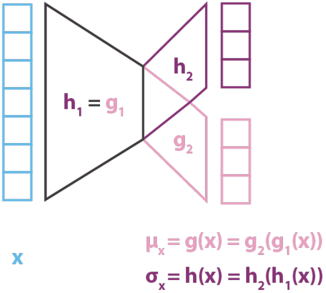

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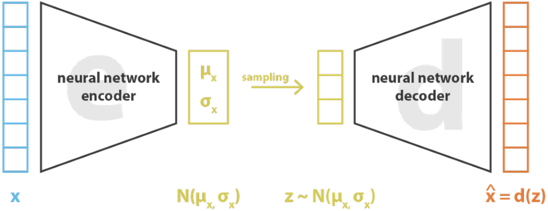

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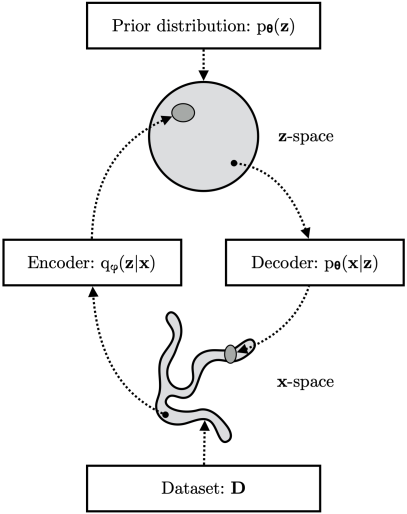

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Training a VAE

- Goal: estimating ϕ, θ (and z_i)
- The encoder and decoder are (usually) complicated (no close form solution)
- Need to estimate ϕ and θ using gradient ascent
- Target:
  - Maximize $\log p(x)$
    (Explain the data as well as possible)

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- Target:
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    (Explain the data as well as possible)
- Optimization target:
  Maximize the variational lower bound or evidence lower bound (ELBO)

The marginal log-likelihood

$$
\begin{aligned}
\log p_\theta(x) &= \int q_\phi(z|x) \log p_\theta(x) dz \\
&= \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x)] \\
&= \mathbb{E}_{q_\phi(z|x)}\left[\log\left(\frac{p_\theta(x,z)}{p_\theta(z|x)}\right)\right] \text{, using } p(z|x) = \frac{p(x,z)}{p(x)} \\
&= \mathbb{E}_{q_\phi(z|x)}\left[\log\left(\frac{p_\theta(x,z)}{q_\phi(z|x)}\frac{q_\phi(z|x)}{p_\theta(z|x)}\right)\right] \\
&= \mathbb{E}_{q_\phi(z|x)}\left[\log\left(\frac{p_\theta(x,z)}{q_\phi(z|x)}\right)\right] + \mathbb{E}_{q_\phi(z|x)}\left[\log\left(\frac{q_\phi(z|x)}{p_\theta(z|x)}\right)\right] \\
&= \underbrace{\mathcal{L}_{\theta,\phi}(x)}_{\text{ELBO}} + D_{KL}(q_\phi(z|x)||p_\theta(z|x))
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The Kullback-Leibler divergence

- The Kulback-Leibler divergence: a way of measuring the distance between probability distributions (although, not a metric)

$$D_{KL}(q_\phi(z|x)||p_\theta(z|x)) = \mathbb{E}_{q_\phi(z|x)}\left[\log\left(\frac{q_\phi(z|x)}{p_\theta(z|x)}\right)\right]$$

$$D_{KL}(q_\phi(z|x)||p_\theta(z|x)) \geq 0$$

Training target

- Optimization target: Maximize the ELBO

$$\mathcal{L}_{\theta,\phi}(x) = \log p_\theta(x) - D_{KL}(q_\phi(z|x)||p_\theta(z|x))$$

- ELBO is a lower bound for the marginal log-likelihood (similar to the EM algorithm)

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- ELBO is a lower bound for the marginal log-likelihood (similar to the EM algorithm)
- Maximizing the ELBO will do two things:
  - Maximize the marginal log-likelihood $\log p_\theta(x)$: Better generative model/decoder
  - Minimize the KL-divergence between $q_\phi(z|x)$ and $p_\theta(z|x)$: Better approximation of the latent space/encoder

Optimizing the ELBO

- Stochastic Gradient *Ascent* to maximize:

$$\mathcal{L}_{\theta,\phi}(x) = \sum_{i}^{N} \mathcal{L}_{\theta,\phi}(x_i)$$
$$= \sum_{i}^{N} \mathbb{E}_{q_\phi(z_i|x_i)} \left[\log\left(p_\theta(x_i, z_i)\right) - \log(q_\phi(z_i|x_i))\right]$$

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- Two problems:
  1. How do we compute the expectation?
     Solution: Monte Carlo Approximation
  2. How compute the gradient wrt ϕ?
     Solution: Change of variables: $z = g(\epsilon, \phi, x)$
     This is called the reparametrization trick

Optimizing the ELBO

- Using the reparametrization trick and Monte Carlo approximation, we get:

$$
\begin{aligned}
\mathcal{L}_{\theta,\phi}(x) =& \mathbb{E}_{q_\phi(z|x)}\left[\log\left(p_\theta(x,z)\right) - \log(q_\phi(z|x))\right] \\
=& \mathbb{E}_{p(\epsilon)}\left[\log\left(p_\theta(x, g(\epsilon,\phi,x))\right) - \log(q_\phi(g(\epsilon,\phi,x)|x))\right] \\
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- We approximate both $\mathcal{L}_{\theta,\phi}(x)$ and $\nabla\mathcal{L}_{\theta,\phi}(x)$
- Sometimes called a doubly stochastic algorithm.

The Autoencoding Variational Bayes Algorithm

Algorithm 1: Stochastic optimization of the ELBO. Since noise originates from both the minibatch sampling and sampling of $p(\boldsymbol{\epsilon})$, this is a doubly stochastic optimization procedure. We also refer to this procedure as the *Auto-Encoding Variational Bayes* (AEVB) algorithm.

Data:
- $\mathcal{D}$: Dataset
- $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$: Inference model
- $p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})$: Generative model

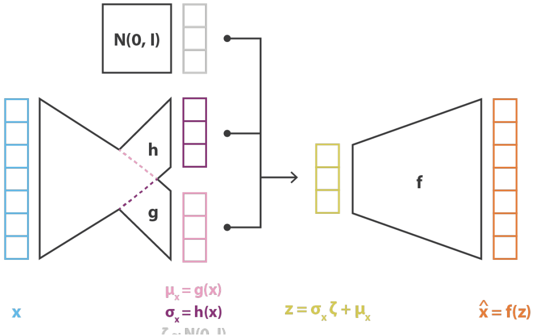
Result:
- $\boldsymbol{\theta}, \boldsymbol{\phi}$: Learned parameters

$(\boldsymbol{\theta}, \boldsymbol{\phi}) \leftarrow$ Initialize parameters
while *SGD not converged* **do**
- $\mathcal{M} \sim \mathcal{D}$ (Random minibatch of data)
- $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$ (Random noise for every datapoint in $\mathcal{M}$)
- Compute $\tilde{\mathcal{L}}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathcal{M}, \boldsymbol{\epsilon})$ and its gradients $\nabla_{\boldsymbol{\theta},\boldsymbol{\phi}} \tilde{\mathcal{L}}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathcal{M}, \boldsymbol{\epsilon})$
- Update $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ using SGD optimizer

end

Figure: The Autoencoding Variational Bayes Algorithm (Kingma and Welling, 2018, Algo. 1)

The Autoencoding Variational Bayes Algorithm



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Summary

- Benefits of VAE:
  - Get a more interpretable latent state
  - We can estimate uncertainty
  - We can inject knowledge in our latent state
- Problems:
  - The blurry image problem
- Still much ongoing research:

Figure: Examples of images generated with a deep hierarchical Variational Autoencoder (Vahdat and Kautz, 2020)

Section 5

Probabilistic Topic Models

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  - Create features for supervised models
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  - Visualize document collections

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- A mixed membership model (a mixture of multinomial mixtures model)
- Topic model builds on the the distributional hypothesis
- Use cases:
  - Create features for supervised models
  - Integrated in neural networks for model efficient learning
  - Visualize document collections
  - Analyzing large corpora using statistical methods

Probabilistic Topic Models

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- Example: All ears media monitoring of speech data

The Dirichlet Distribution

- Probability distribution over the simplex with K categories:

$$f(\mathbf{x}|\boldsymbol{\alpha}) = \frac{1}{\mathrm{B}(\boldsymbol{\alpha})} \prod_{i=1}^{K} x_i^{\alpha_i - 1}$$

where

$$\mathrm{B}(\boldsymbol{\alpha}) = \frac{\prod_{i=1}^{K} \Gamma(\alpha_i)}{\Gamma\left(\sum_{i=1}^{K} \alpha_i\right)},$$

and where

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- The parameters $\boldsymbol{\alpha}$ can be seen as pseudo-counts

The Dirichlet Distribution

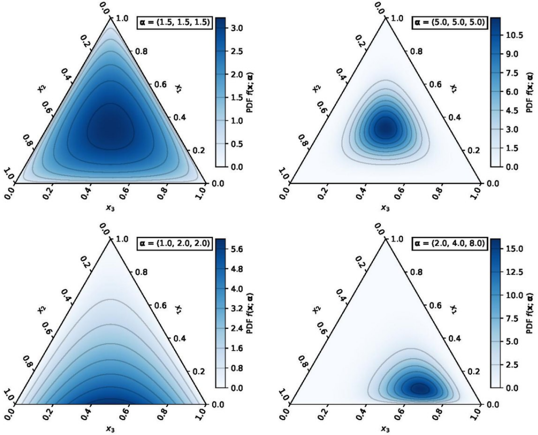

Figure: The Dirichlet Distribution (Wikipedia)

The distributional hypothesis

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  "Word is characterized by the company it keeps"

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- Rough definition: word windows of different sizes
- Different window sizes, different semantic content:
  - Word embeddings (context: word windows)
  - Topic models (context: documents)

Example

1. "A friend in need is a friend indeed."
2. "She is my friend indeed."

Latent Dirichlet Allocation

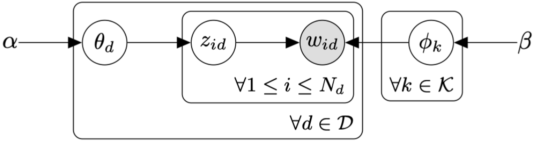

Figure: The Latent Dirichlet Allocation Model

where ϕ_k is the kth row in Φ (of dimension $K \times V$) and θ_d is the dth row in Θ (of dimension $D \times K$).

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Generative model for LDA

Relies on the bag-of-word assumption

1. For each component k to K:
   1.1 $\phi_k \sim \text{Dirichlet}(\beta)$
2. For each document d:
   2.1 $\theta_d \sim \text{Dirichlet}(\alpha)$
   2.2 For each token i:
      2.2.1 $z_{id} \sim \text{Categorical}(\theta_d)$
      2.2.2 $w_{id} \sim \text{Categorical}(\phi_{z_{id}})$

Example of parameters $\mathbf{z}$, Θ and Φ

$\mathbf{w}_1$	boat	shore	bank		
$\mathbf{z}_1$	1	1	1		
$\mathbf{w}_2$	Zlatan	boat	shore	money	bank
$\mathbf{z}_2$	2	1	1	3	3
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$\Phi =$

	boat	shore	soccer	Zlatan	bank	money
Topic 1	0.35	0.35	0.05	0.05	0.15	0.05
Topic 2	0.025	0.025	0.45	0.45	0.025	0.025
Topic 3	0.025	0.025	0.025	0.025	0.45	0.45

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$\Theta =$

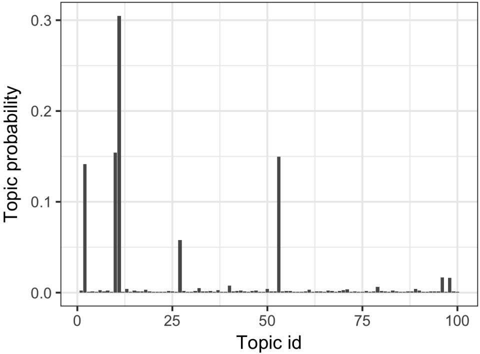
	Topic 1	Topic 2	Topic 3
doc 1	0.96	0.02	0.02
doc 2	0.3	0.2	0.5
doc 3	0.05	0.35	0.6

Closing arguments were heard yesterday in the Federal bankruptcy fraud trial of Stephen J. Sabbeth, whose legal problems have raised doubts about his ability to continue as leader of the Nassau County Democratic Party.

Mr. Sabbeth is charged with trying to conceal $750,000 from his bank creditors by hiding the money in a secret account in his wife's maiden name, rather than use it to pay creditors when his lumber business went into bankruptcy 10 years ago.

– The New York Times 25th of Febuary 1999

The estimated topic proportion ($\hat{\theta}_d$)



Topic top words

Topic	Top words (by ϕ_{kv})
2	party election voters campaign democratic
10	bank banks loans loan insurance savings
11	trial prison jury prosecutors convicted guilty
53	investigation inquiry documents investigators

Table: The words with highest probability ($p(w|k)$) for topic 2, 10, 11 and 53.

The Latent Dirichlet Allocation Model

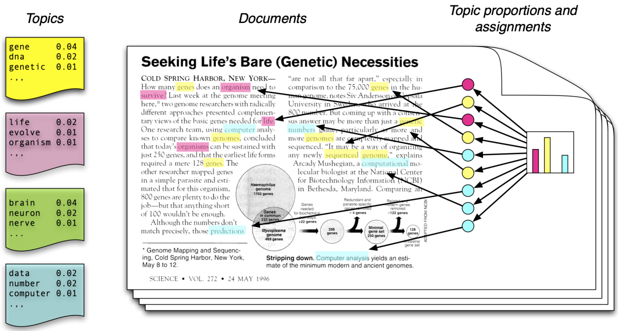


Figure: The Latent Dirichlet Allocation Model (Blei 2012, Fig. 1)

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Inference

- Common inference approaches
  1. Variational inference
  2. Markov Chain Monte Carlo (MCMC)

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  1. Variational inference
  2. Markov Chain Monte Carlo (MCMC)
- The Gibbs sampler is usually prefered
- Similar to (Stochastic) EM

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Gibbs sampler for LDA

The basic Gibbs sampler:

1. We want to estimate z, Φ, Θ:

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$$p(z = k|\Phi, \Theta) \propto \phi_{v,k}\theta_{k,d}$$

3. Sample model parameters

$$\theta_d|\mathbf{z} \sim Dir(\mathbf{n}^{(d)} + \alpha)$$

$$\phi_k|\mathbf{z} \sim Dir(\mathbf{n}^{(v)} + \beta)$$

where $\mathbf{n}^{(d)}$ is the number of tokens by topic in document d and $\mathbf{n}^{(v)}$ is the number of tokens by topic for word type v.

Gibbs sampler for LDA

Integrating out (collapsing) Θ and Φ

$$p(\mathbf{z}|\mathbf{w}) = \int\int p(\mathbf{z}, \Theta, \Phi|\mathbf{w}) \cdot p(\mathbf{z}, \Theta, \Phi) d\Phi d\Theta$$

will result in the following Gibbs sampler:

$$p(z_i = k|w_i, \mathbf{z}_{\neg i}) \propto \underbrace{\frac{n_k^{(v)} + \beta}{n_k^{(v)} + V\beta}}_{type-topic\ (\Phi)} \cdot \underbrace{(n_k^{(d)} + \alpha)}_{topic-doc\ (\Theta)}$$

where $n^{(v)}$ and $n^{(d)}$ are count matrices of size $D \times K$ and $K \times V$.

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Example of $n^{(v)}$ and $n^{(d)}$

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$$n^{(v)} = \begin{array}{cccccc} \text{boat} & \text{shore} & \text{soccer} & \text{Zlatan} & \text{bank} & \text{money} \\ 2 & 2 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 2 \end{array}$$

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$$n^{(d)} = \begin{bmatrix} 3 & 0 & 0 \\ 2 & 1 & 3 \\ 0 & 2 & 3 \end{bmatrix}$$

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Topic Models as non-negative matrix factorization

$$\begin{bmatrix} \\ n_{dv} \\ (D \times V) \\ \\ \end{bmatrix} \approx \begin{bmatrix} \\ \Theta \\ (D \times K) \\ \\ \end{bmatrix} \times \begin{bmatrix} \Phi \\ (K \times V \end{bmatrix}$$

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Practicalities

- Setting K, α and β

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- Setting K, α and β
- Reducing the vocabulary: stopwords, rare words, stemming
- "Junk" topics
- We can analyze the topic indicators z directly

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- Practicalities
- Introduction
- Autoencoders
- The Variational Autoencoder
  - The probabilistic decoder
  - The probabilistic encoder
  - Traing a variational autoencoder
- Probabilistic Topic Models
  - Latent Dirichlet Allocation
  - Estimating the LDA model

Research Example: Swedish Immigration Discourse

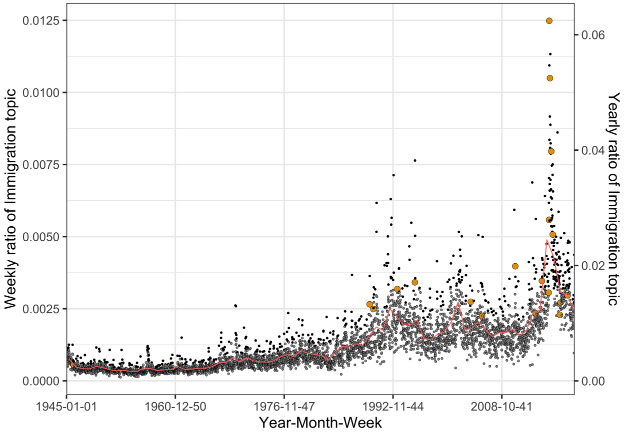

Figure: The Immigration topic in Swedish Newspapers (Hurtado Bodell et al, not in print)

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- The Latent Dirichlet Allocation is a popular model
- A mixed membership model (a mixture of multinomial mixtures model)
- Usually use Gibbs samplers for estimation