### PROBABILISTIC MACHINE LEARNING Lecture 19 Example: Topic Models

Philipp Hennig 28 June 2021

### EBERHARD KARLS UNIVERSITÄT TÜBINGEN



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The Toolbox



#### Framework:

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

#### 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



#### the goal for (most of) the rest of the course: Build a Model of History

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# The State of the Union

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[The President] shall from time to time give to the Congress Information of the State of the Union, and recommend to their Consideration such Measures as he shall judge necessary and expedient.

- Delivered annually since 1790
- Summarizes affairs of the US federal government
- historically delivered in writing, generally spoken since 1982,
- on radio since 1923, TV since 1947, in the evenings since 1965, webcast since 2002
- the inaugural SotU of a new president typically has a different tone

Article II, §3 of the US Constitution



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#### Article II, §3 of the US Constitution





The SotU Addresses are not a perfect reflection of US history, but they are ...

- ▶ available in their entirety online
- ▶ available without interruption for over 200 years
- ▶ topical
- given in a reasonably similar setting, annually

Our task: Find topics of US history over time.

This is an **unsupervised dimensionality reduction** task.



#### Disclaimer:

- ► This is not a course in natural language processing!
- There is an entire toolbox of models for text analysis that will not be discussed here. Some of them have probabilistic interpretation, others don't.
- ► The point of this exercise is to try out the tools developed in this course on a practical problem. There is no claim that this is the "best" thing to do

However, the model ultimately developed here is likely unusually expressive in its structure, and more flexible than the standard tools. Key takeaway: It does pay to spend time developing your model!

Our Goal: Build *craftware*: customized, effective and efficient solution to the learning task. Use toolboxes where they help, be willing to write our own solution where necessary.

- ▶ D = 231 documents (1790 2019; 2 in 1961 (Eisenhower & JFK))
- individual documents of length  $I_d \sim 10^3$  words
- >  $V \sim 10\,000$  words in vocabulary
- A few first simplifications
  - ► there are many redundant **stop words** required for human understanding but carrying only negligible semantic information
  - since we are looking to *reduce* complexity, we necessarily have to throw out a bit of structure
  - e.g., usage of word is significant, but its position in the text is not crucial. We will model the texts as Bags of Words

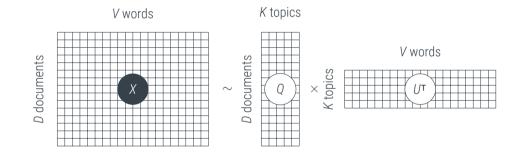


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### A Reduced Representation

low-rank decomposition







Consider a dataset  $X \in \mathbb{R}^{D \times V}$ . Dimensionality Reduction aims to find an encoding  $\phi : \mathbb{R}^V \to \mathbb{R}^K$  and a decoding  $\psi : \mathbb{R}^K \to \mathbb{R}^V$  with  $K \ll V$  such that the encoded representation

 $Z := \phi(X) \in \mathbb{R}^{D \times K}$ 

is a good approximation of X in the sense that some reconstruction loss of  $\tilde{X} = \psi(Z)$ ,

 $\mathcal{L}(X,\psi(Z)) = \mathcal{L}(X,\psi\circ\phi(X))$ 

is minimized or small. This may be done, e.g., to

► save memory

► construct a low-dimensional visualization

▶ "find structure"

## Linear dimensionality reduction

The classic derivation of PCA



Data: 
$$X \in \mathbb{R}^{D \times V} = [\mathbf{x}_1; \ldots; \mathbf{x}_D].$$

► Consider an orthonormal basis  $\{u_i\}_{i=1,...,V}$ ,  $u_i^{\mathsf{T}}u_j = \delta_{ij}$ . Then

$$\mathbf{x}_{d} = \sum_{i=1}^{V} (\mathbf{x}_{d}^{\mathsf{T}} \mathbf{u}_{i}) \mathbf{u}_{i} =: \sum_{i=1}^{V} \alpha_{di} \mathbf{u}_{i} \qquad \qquad \mathbf{X} = (\mathbf{X} U) U^{\mathsf{T}}$$

An *approximation* in K < D degrees of freedom is given by any set (A, b, U) as

$$\tilde{\mathbf{x}}_d := \sum_{k=1}^{K} a_{dk} \mathbf{u}_k + \sum_{\ell=K+1}^{V} b_\ell \mathbf{u}_\ell$$

What is the *best* approximation?



### The *best* approximation

Empirical Risk Minimization derivation of PCA

Let's find (A, b, U) to minimize the square empirical risk

$$J = \frac{1}{D} \sum_{d=1}^{D} \|\mathbf{x}_{d} - \tilde{\mathbf{x}}_{d}\|^{2} = \frac{1}{D} \sum_{d=1}^{D} \sum_{v=1}^{V} \left[\mathbf{x}_{d} - \sum_{k=1}^{K} a_{dk} \mathbf{u}_{k} - \sum_{j=K+1}^{V} b_{j} \mathbf{u}_{j}\right]_{v}^{2}$$

First, let's find  $a_{dk}$  and  $b_j$ : Recall  $\sum_j u_{ij}u_{kj} = \delta_{ik}$ , use  $\bar{\mathbf{x}} := \frac{1}{D} \sum_d \mathbf{x}_d$ , to find

$$\frac{\partial J}{\partial a_{d\ell}} = \frac{2}{D} \sum_{\nu=1}^{V} \left[ \mathbf{x}_d - \sum_{k=1}^{K} a_{dk} \mathbf{u}_k - \sum_{j=K+1}^{V} b_j \mathbf{u}_j \right]_{\nu} (-u_{\ell\nu}) = \frac{2}{D} (-\mathbf{x}_d^{\mathsf{T}} \mathbf{u}_\ell) + \frac{2}{D} a_{d\ell} \stackrel{!}{=} 0$$
$$\frac{\partial J}{\partial b_\ell} = \frac{2}{D} \sum_{d=1}^{D} \sum_{\nu=1}^{V} \left[ \mathbf{x}_d - \sum_{k=1}^{K} a_{dk} \mathbf{u}_k - \sum_{j=K+1}^{V} b_j \mathbf{u}_j \right]_{\nu} (-u_{\ell\nu}) = \frac{2}{D} \sum_{d=1}^{D} (-\mathbf{x}_d^{\mathsf{T}} \mathbf{u}_\ell) + 2b_\ell \stackrel{!}{=} 0$$

Thus  $a_{dk} = \mathbf{x}_d^{\mathsf{T}} \mathbf{u}_k$ , and  $b_j = \bar{\mathbf{x}}^{\mathsf{T}} \mathbf{u}_j$ .

### The best approximation

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Empirical Risk Minimization derivation of PCA

With  $a_{dk} = \mathbf{x}_d^{\mathsf{T}} \mathbf{u}_k$ ,  $b_i = \bar{\mathbf{x}}^{\mathsf{T}} \mathbf{u}_i$ , things simplify:  $\mathbf{x}_d - \tilde{\mathbf{x}}_d = \mathbf{x}_d - \sum_{k=1}^{K} a_{dk} \mathbf{u}_k - \sum_{k=1}^{V} b_j \mathbf{u}_j = \sum_{k=1}^{V} (\mathbf{x}_d^{\mathsf{T}} \mathbf{u}_\ell) \mathbf{u}_\ell - \sum_{k=1}^{K} (\mathbf{x}_d^{\mathsf{T}} \mathbf{u}_k) \mathbf{u}_k - \sum_{k=1}^{V} (\mathbf{x}_d^{\mathsf{T}} \mathbf{u}_k) \mathbf{u}_j$  $i = K \pm 1$   $\ell = 1$  $=\sum_{k=1}^{K}(\mathbf{x}_{d}^{\mathsf{T}}\mathbf{u}_{\ell})\mathbf{u}_{\ell}-\sum_{k=1}^{K}(\mathbf{x}_{d}^{\mathsf{T}}\mathbf{u}_{k})\mathbf{u}_{k}+\sum_{k=1}^{V}(\mathbf{x}_{d}^{\mathsf{T}}\mathbf{u}_{\ell})\mathbf{u}_{\ell}-\sum_{k=1}^{V}(\bar{\mathbf{x}}^{\mathsf{T}}\mathbf{u}_{j})\mathbf{u}_{j}$  $=\sum_{i=1}^{\nu} ((\mathbf{x}_d - \bar{\mathbf{x}})^{\mathsf{T}} \mathbf{u}_j) \mathbf{u}_j$ , so, with the sample covariance matrix  $S := \frac{1}{D} \sum_{i=1}^{\nu} (\mathbf{x}_d - \bar{\mathbf{x}}) (\mathbf{x}_d - \bar{\mathbf{x}})^{\mathsf{T}}$ i=K+i $J = \frac{1}{D} \sum_{j=1}^{D} \| \mathbf{x}_{d} - \tilde{\mathbf{x}}_{d} \|^{2} = \frac{1}{D} \sum_{j=1}^{D} \sum_{j=1}^{V} ((\mathbf{x}_{d} - \bar{\mathbf{x}})^{\mathsf{T}} \mathbf{u}_{j})^{2} = \frac{1}{D} \sum_{j=1}^{V} \sum_{j=1}^{D} u_{j}^{\mathsf{T}} (\mathbf{x}_{d} - \bar{\mathbf{x}}) (\mathbf{x}_{d} - \bar{\mathbf{x}})^{\mathsf{T}} \mathbf{u}_{j}$  $=\sum u_i^{\mathsf{T}} S u_i$ i=K+i

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### Maybe we can get away with linear algebra?

Principal Component Analysis

Beltrami, 1873, Jordan, 1874, Pearson, 1901, Schmidt, 1907, Hotelling, 1933, Lanczos, 195

To find a set of *orthonormal* vectors  $u_i$  to minimize the square reconstruction error

$$J = \frac{1}{D} \sum_{d=1}^{D} \|\mathbf{x}_d - \tilde{\mathbf{x}}_d\|^2 = \sum_{j=K+1}^{V} u_j^{\mathsf{T}} S u_j$$

Choose *U* as the eigenvectors of the sample covariance  $S := \frac{1}{D} \sum_{d=1}^{D} (\mathbf{x}_d - \bar{\mathbf{x}}) (\mathbf{x}_d - \bar{\mathbf{x}})^{\mathsf{T}}$ , and get the *best* 

rank K reconstruction  $\tilde{x}_d$  by setting

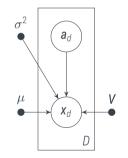
$$\tilde{x}_{d} := \sum_{k=1}^{K} a_{dk} u_{k} + \sum_{j=K+1}^{V} b_{j} u_{j} = \sum_{i=1}^{M} (x_{d}^{\mathsf{T}} u_{i}) u_{i} + \sum_{i=M+1}^{D} (\bar{x}^{\mathsf{T}} u_{i}) u_{i}$$

This yields  $J = \sum_{j=K+1}^{V} \lambda_j$  (where  $\lambda_j$  are the eigenvalues of *S*, sorted descendingly). If we first center the data  $\hat{X} = X - \mathbf{1}\bar{\mathbf{x}}^{\mathsf{T}}$ , so  $\mathbf{b} = 0$ , the *U* are the (right) **singular vectors** of  $\hat{X} = Q\Sigma U^{\mathsf{T}}$ .

Treat the loss, up to scaling, as a non-normalised negative log likelihood:

$$J = -c \cdot \log p(X \mid \tilde{X}) + \log Z = \frac{1}{D} \sum_{d=1}^{D} ||\mathbf{x}_d - \tilde{\mathbf{x}}_d||^2$$
$$\Rightarrow p(X \mid \tilde{X}) = \prod_{d=1}^{D} \mathcal{N}(\mathbf{x}_d; \tilde{\mathbf{x}}_d, \sigma^2 I)$$

We also need to encode that we want a *low-dimensional, linear* embedding, and that the embedding should be in terms of *independent* (orthogonal) dimensions.

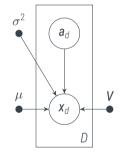


Thus, consider

$$\mathbf{x}_d = \mathbf{V}\mathbf{a}_d + \mathbf{\mu} + \varepsilon$$
 with  $p(\mathbf{a}_d) = \mathcal{N}(0; I_K), \mathbf{V} \in \mathbb{R}^{V \times K}$  and  $p(\varepsilon) = \mathcal{N}(0; \sigma^2)$ 

with marginal likelihood (where  $C := VV^{T} + \sigma^{2} l$ )

$$p(X) = \int \prod_{d=1}^{D} p(\mathbf{x}_d \mid \mathbf{a}_d) p(\mathbf{a}_d) d\mathbf{a}_d = \prod_d \mathcal{N}(\mathbf{x}_d; \boldsymbol{\mu}, C)$$
$$\log p(X) = -\frac{DV}{2} \log(2\pi) - \frac{D}{2} \log|C| - \frac{1}{2} \sum_{d=1}^{D} (\mathbf{x}_d - \boldsymbol{\mu})^{\mathsf{T}} C^{-1} (\mathbf{x}_d - \boldsymbol{\mu})$$
$$\bar{\mathbf{x}} = \arg\max \log p(X), \quad \text{thus the max. lik. can be written as}$$
$$\log p(X) = -\frac{D}{2} \left( V \log(2\pi) + \log|C| + \operatorname{tr}(C^{-1}S) \right)$$







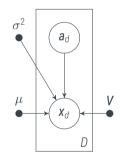
$$\log p(X) = -\frac{D}{2} \left( V \log(2\pi) - \log |C| + \operatorname{tr}(C^{-1}S) \right)$$

yields max. lik. for  $V, \sigma^2$  at [Tipping & Bishop, 1999], with  $RR^{\intercal} = I_K$  and  $S = U\Lambda U^{\intercal}$ 

$$\mathbf{V}_{ML} = U_{1:K} (\Lambda_K - \sigma^2 I)^{1/2} R$$
 and  $\sigma_{ML}^2 = \frac{1}{V - K} \sum_{j=K+1}^V \lambda_j$ 

setting  $\sigma^2$ ,  $\mu$ , U this way, and R = I w.l.o.g., gives posterior

$$p(\mathbf{a}_d \mid \mathbf{x}_d) = \mathcal{N}(\mathbf{a}_d; (\mathbf{V}^{\mathsf{T}}\mathbf{V} + \sigma^2 l)^{-1}\mathbf{V}^{\mathsf{T}}(\mathbf{x}_d - \bar{\mathbf{x}}), \sigma^2(\mathbf{V}^{\mathsf{T}}\mathbf{V} + \sigma^2 l)^{-1})$$
  
=  $\mathcal{N}(\mathbf{a}_d; \Lambda_K^{-1}(\Lambda_K - \sigma^2 l_K)^{1/2} U_{1:K}(\mathbf{x}_d - \bar{\mathbf{x}}), \sigma^2 \Lambda^{-1})$ 





So, does it work?

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# Latent Semantic Indexing / Principal Component Analysis

a first result on our dataset

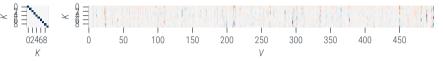
50

100 -

150 -

200

02468 *K* 



- 1. tonight fight taxis faith century today enemy fellow
- 2. year program world new work need help america
- 3. dollar war program fiscal year expenditure million united
- 4. man law dollar business national corporation legislation labor
- 5. administration policy energy program continue development provide effort
- 6. war nation power man mexico world peace public
- 7. united war states american world mexico man nation
- 8. government people states world free shall dollar constitution
- 9. year free nation world increase report subject great
- 10. world free gold government bank note american treasury

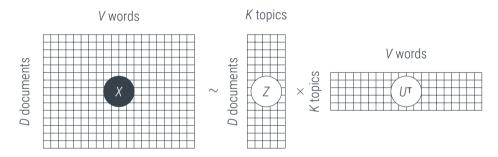


- ► The singular value decomposition (SVD) minimizes  $||X Q\Sigma U'||_F^2$  for orthonormal matrices  $Q \in \mathbb{R}^{D \times K}$  and  $U \in \mathbb{R}^{V \times K}$ , and a diagonal  $\Sigma \in \mathbb{R}^{K \times K}$  with positive diagonal entries (the *singular values*).
- We might naïvely think of Q as a mapping from documents to topics, U' from topics to words, and  $\Sigma$  as the relative strength of topics.
- ► However, there are several problems:
  - ▶ the matrices *Q*, *U* returned by the SVD are in general *dense*: Every document contains contributions from *every* topic, and *every* topic involves *all* words.
  - ▶ the entries in  $Q, U, \Sigma$  are hard to interpret: They do not correspond to probabilities
  - ▶ the entries of *Q*, *U* can be *negative*! What does it mean to have a negative topic?

We need Sparsity

How about one topic per document?

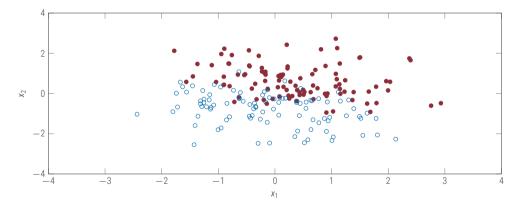




For PCA, we allowed  $Z \in \mathbb{R}^{D \times K}$ . Maybe we need  $Z \in \{0, 1\}^{D \times K}$  and  $Z\mathbf{1}_{K} = \mathbf{1}_{D}$ ?

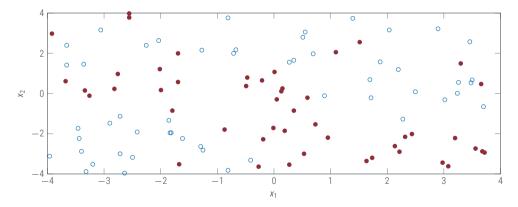


#### a supervised problem that can be solved discriminatively in a linear fashion



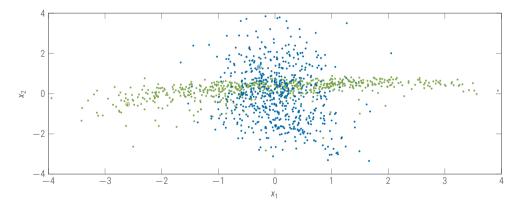


#### a supervised problem that can be solved discriminatively in a nonlinear fashion





#### a supervised problem that can be solved generatively (in a Gaussian fashion?)



### Mixture Models

100

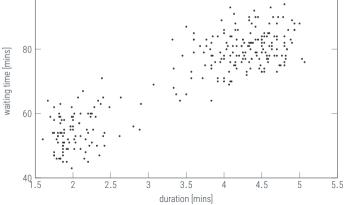
#### generative modelling with discrete classes



an **unsupervised** problem

https://www.stat.cmu.edu/ larry/all-of-statistics/=data/faithful.dat

Azzalini, A. and Bowman, A. W. (1990). A look at some data on the Old Faithful geyser. Applied Statistics 39, 357-365.



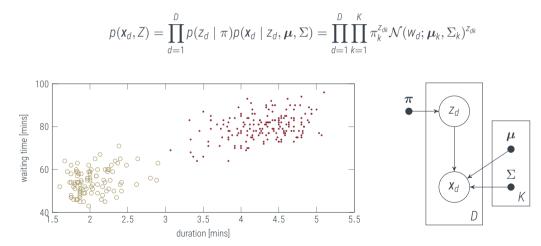


### Mixture Models

#### generative modelling with discrete classes



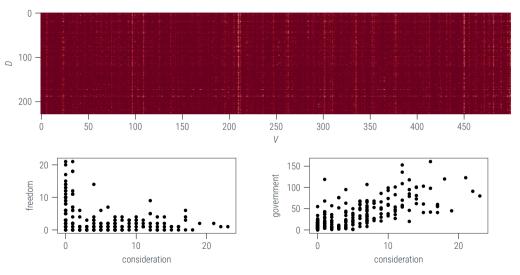
a Gaussian mixture



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### A Gaussian Mixture isn't quite right yet

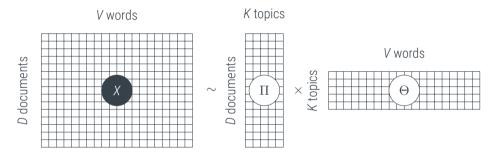
word counts aren't real-valued





Desiderata





► topics should be probabilities:  $p(\mathbf{x}_d \mid k) = \prod_{v=1}^{V} \theta_{kv}^{\mathbf{x}_{dv}}$ 

but documents should have several topics! Let  $\pi_{dk}$  be the probability to draw a word from topic k