Taming numerical imprecision by adapting the KL divergence to negative probabilities[a]

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Slides: **pfahler.online**

[a]Pfahler et al. in *Stat. Comput.* **34** (2024)

Introduction

Introduction - Example

- Consider the SVD of a matrix:

$$\mathrm{p} \sim \begin{pmatrix} 1 & 2 & 2 \\ 2 & 2 & 1 \\ 2 & 1 & 0.01 \end{pmatrix} \approx \begin{pmatrix} -0.62 & 0.68 & 0.40 \\ -0.66 & -0.18 & -0.73 \\ -0.42 & -0.72 & 0.56 \end{pmatrix} \begin{pmatrix} 4.51 & 0 & 0 \\ 0 & 1.63 & 0 \\ 0 & 0 & 0.14 \end{pmatrix} \begin{pmatrix} -0.62 & -0.66 & -0.42 \\ -0.68 & 0.18 & 0.72 \\ 0.40 & -0.73 & 0.56 \end{pmatrix}$$

- Truncating the smallest singular value, we get the approximation

$$\tilde{\mathrm{p}} \sim \begin{pmatrix} 0.98 & 2.04 & 1.97 \\ 2.04 & 1.93 & 1.06 \\ 1.97 & 1.06 & \text{-0.03} \end{pmatrix} \approx \begin{pmatrix} -0.62 & 0.68 \\ -0.66 & -0.18 \\ -0.42 & -0.72 \end{pmatrix} \begin{pmatrix} 4.51 & 0 \\ 0 & 1.63 \end{pmatrix} \begin{pmatrix} -0.62 & -0.66 & -0.42 \\ -0.68 & 0.18 & 0.72 \end{pmatrix}$$

- $\tilde{\mathrm{p}}$ can not be used to calculate a KL divergence, even though it is an approximation of a probability distribution

Introduction - Approach

$$D_{\mathrm{KL}}(\mathrm{p}\|\mathrm{q}) = \sum_{i=1}^{n} p_i \log \frac{p_i}{q_i}$$

- we consider the case where p is our data and q is our model
- negative entries can occur in q due to various reasons:
  1. approximations
  2. assumptions of a theory
  3. rounding errors
- if a KL-like divergence is needed, we can
  (a) give up
  (b) reformulate
  (c) devise a workaround
- this talk follows approach (c)

shifted KL divergence

sKL divergence - Idea

$$D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q}) = \sum_{i=1}^{n} (p_i + \varepsilon_i) \log \frac{p_i + \varepsilon_i}{q_i + \varepsilon_i}$$

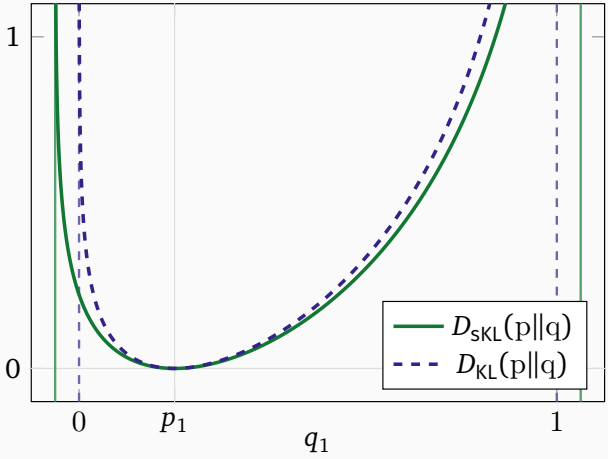
- Negative entries cause a problem because $\log x$ is only well-defined for $x > 0$
- How can we adapt the KL divergence so we can use it as an objective function in an optimization task?
- Can we just shift the negative entries? → Almost!
- In order to retain important properties of the KL divergence, p also has to be shifted

sKL divergence - Properties

$$D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q}) = \sum_{i=1}^{n} (p_i + \varepsilon_i) \log \frac{p_i + \varepsilon_i}{q_i + \varepsilon_i}$$

The sKL divergence retains many properties of the KL divergence:

- The sKL divergence is a statistical divergence, i.e.
  (1) $D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q}) \geq 0$
  (2) $D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q}) = 0 \iff \mathrm{p} = \mathrm{q}$
  (3) $\frac{\mathrm{d}^2 D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q})}{\mathrm{d}q_i \mathrm{d}q_j}|_{\mathrm{q}=\mathrm{p}}$ is a positive definite matrix
- The sKL divergence is convex in the pair of its arguments

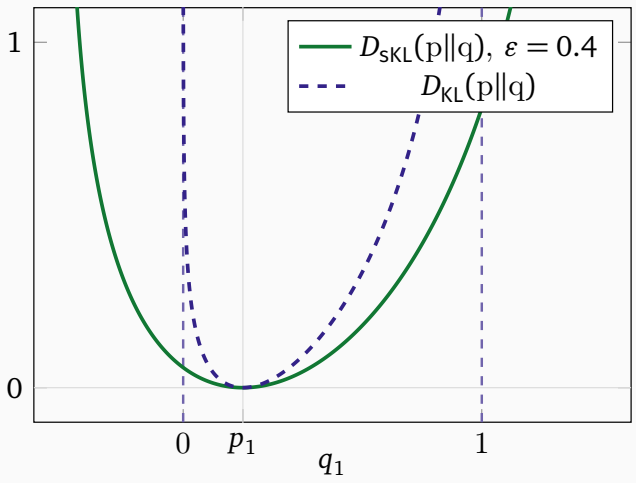


2D example with $\mathrm{p} = (0.2, 0.8)$, $\mathrm{q} = (q_1, 1 - q_1)$ and $\varepsilon = (0.05, 0.05)$

Parameter choice

Parameter choice - General observations

$D_{\mathrm{SKL}}(\mathrm{p}\|\mathrm{q}) = \sum_{i=1}^{n}(p_i+\varepsilon_i)\log\frac{p_i+\varepsilon_i}{q_i+\varepsilon_i}$



- Especially in high-dimensional data, often many entries of the data distribution p are zero → choose $\varepsilon_i = 0$ if $p_i = 0$
- The gradient with respect to q_i is

$$\frac{\partial D_{\mathrm{SKL}}(\mathrm{p}\|\mathrm{q})}{\partial q_i} = -\frac{p_i+\varepsilon_i}{q_i+\varepsilon_i} \xrightarrow{\varepsilon_i\to\infty} -1$$

→ large ε_i lead to a loss of gradient information

Simplest idea: $\varepsilon_i = \begin{cases} 0\,, & p_i = 0\,, \\ \varepsilon\,, & \text{else} \end{cases}$

⊕ Pros:

- ε does not depend on q, so the sKL divergence is the same function for any q
- Use in higher-order optimizers is possible

⊖ Cons:

- A reasonable value for ε has to be determined before the sKL divergence can be used
- Negative values $q_i < -\varepsilon$ still render the sKL divergence undefined

$$\text{Dynamic choice: } \varepsilon_i = \begin{cases} 0, & p_i = 0 \text{ or } q_i > 0, \\ |q_i| + f(|q_i|), & \text{else} \end{cases}$$

with $f : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$, e.g. $f(x) = \delta \cdot x$ with $\delta > 0$

⊕ Pros:
- No prior knowledge about q is needed
- Less gradient information is lost
- Average of the sKL divergence under Gaussian noise is controlled → next slide

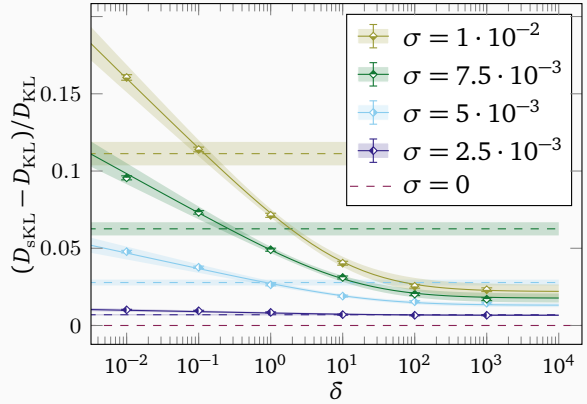
⊖ Cons:
- The sKL divergence is a different function for every q
- Only first-order optimizers can be used

Parameter choice - Gaussian noise

$D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q}) = \sum_{i=1}^{n}(p_i+\varepsilon_i)\log\frac{p_i+\varepsilon_i}{q_i+\varepsilon_i}$

Consider a vector x of i.i.d. Gaussian random variables with mean 0 and standard deviation σ.
With the dynamic choice of ε, we get

$$\langle D_{\mathrm{sKL}}(\mathrm{p}\|\mathrm{q}+\mathrm{x})\rangle_{\mathrm{x}} = D_{\mathrm{KL}}(\mathrm{p}\|\mathrm{q}) + \sigma^2\sum_i \frac{p_i}{2q_i^2} + \mathcal{O}(\sigma^4)$$



example for $\mathrm{p},\mathrm{q}\in\mathbb{R}^{10}$

numerical result σ^2-term

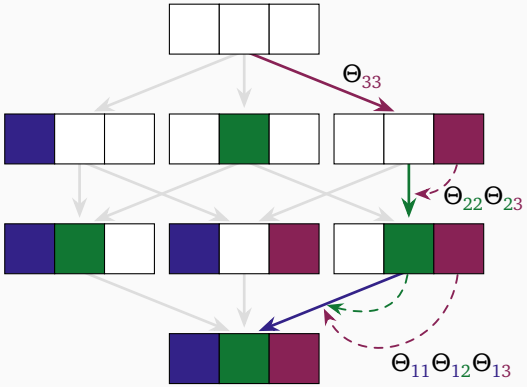
Application

Application - Mutual Hazard Networks[b]

- Modeling tumor progression as a Markov chain
- d binary events (mutations, CNAs) → 
- Tumors start healthy and accumulate events one by one with transition rate

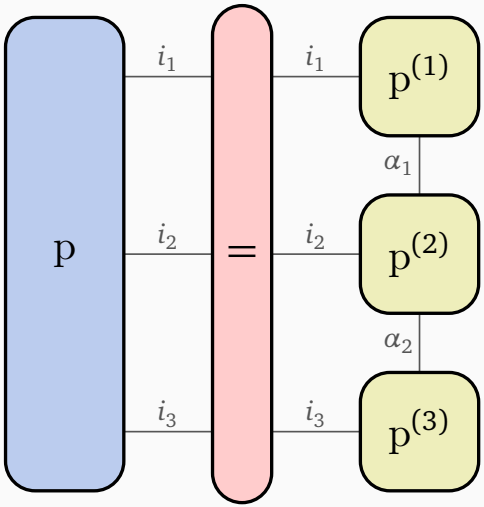
$$Q_{x^{+i},x} = \Theta_{ii} \prod_{x_j=1} \Theta_{ij}$$

- The model is parameterized by $\Theta \in \mathbb{R}^{d \times d}$, which we can learn from patient data



[b] Schill et al. in *Bioinformatics* **36** (2020)

Application - Mutual Hazard Networks



- The model parameters Θ are optimized by minimizing the KL divergence of

$$p_\Theta = (I - Q_\Theta)^{-1} p(t = 0)$$

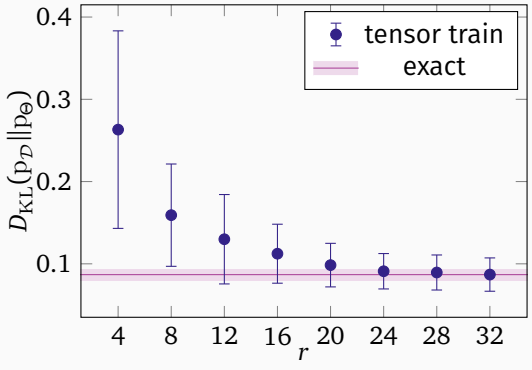
  from a given patient data distribution $p_{\mathcal{D}}$
- The size of $Q_\Theta \in \mathbb{R}^{2^d \times 2^d}$ and $p_\Theta \in \mathbb{R}^{2^d}$ grows exponentially with d → Efficient format needed!
- We use the tensor train format[c], which approximates the probability distribution using d 3D tensors

[c] Oseledets in *SIAM J. Sci. Comput.* **33** (2011)

Application - Results

- Tests on datasets with 20 events, so we can compare to the exact result
- Tensor train rank r is used to control the approximation quality (tensor trains would be exact for $r = 1024$)

$\Rightarrow$ Results quickly converge when increasing the approximation quality



Summary

Summary

- The sKL divergence provides a statistical divergence measure which
  1. shares important theoretical properties with the KL divergence
  2. is compatible with approximations of probability vectors, even if negative values occur
  3. is applicable to a wide range of problems
- Optimization tasks on high-dimensional data can be performed using the sKL divergence as an objective function
- Mutual Hazard Networks with up to ~ 40 events (compared to ~ 25 before) can be learned using tensor trains
  $\rightarrow$ for more events, we are working on another approach

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