# Mathematics and numerics for data assimilation and 

 state estimation - Lecture 11Summer semester 2020

## Overview

1 Bayesian inversion and optimization

2 Entropy and Kullback-Leibler divergence

## Summary of lecture 10

■ Weak convergence of distributions $\mathbb{P}_{k} \Rightarrow \mathbb{P}$.

■ Bayesian inversion in the linear-Gaussian setting

$$
Y=A U+\eta, \quad \pi_{U}, \pi_{\eta} \quad \text { Gaussian pdfs. }
$$

■ Consistency of posterior $\pi(u \mid y)$ in small noise limit when $\eta$ "disappears", when $\mathbb{A}$ is overdetermined, determined and underdetermined. $A U=y$

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1 Bayesian inversion and optimization

## 2 Entropy and Kullback-Leibler divergence

## Problem setting

$$
\begin{equation*}
Y=G(U)+\eta \tag{1}
\end{equation*}
$$

with $G: \mathbb{R}^{d} \rightarrow \mathbb{R}^{k}, \eta \sim \pi_{\eta}, U \sim \pi_{U}$ and $\eta \perp U$.
For an observation $Y=y$, we obtained

$$
\pi(u \mid y) \propto \pi_{\eta}\left(y-\underline{Q}(u y) \pi_{u}(u)\right.
$$

And in the linear-Gaussian setting

$$
\pi(u \mid y) \propto \exp \left(-\frac{1}{2}|y-G(u)|_{\stackrel{ }{r}}^{2}-\frac{1}{2}|u-\hat{m}|_{\hat{C}}^{2}\right)=\exp (-J(u))
$$

where, decomposing into loss and regularization terms,

$$
\mathrm{L}(u):=-\log \left(\pi_{\eta}(y-G(u))\right) \quad \text { and } \quad \mathrm{R}(u):=-\log \left(\pi_{u}(u)\right)
$$

$$
\begin{equation*}
\text { and } \underbrace{\mathrm{J}(u)}_{\text {Objective fcn }}:=\mathrm{L}(u)+\mathrm{R}(u) \tag{2}
\end{equation*}
$$

Assuming $\pi_{\eta}, \pi_{U}>0$, we extend the notation (2) to general settings:

$$
\pi(u \mid y) \propto \pi_{\eta}(y-A u) \pi_{u}(u)=\exp (-\mathrm{J}(u))=\exp (-\mathrm{L}(u)-\mathrm{R}(u))
$$

## MAP estimators and Tikhonov regularization

Maximizing the posterior is equivalent to minimizing the objective function:

$$
\begin{aligned}
u_{M A P}[\pi(\cdot \mid y)]=\arg \max _{u \in \mathbb{R}^{d}} \pi(u \mid y)=\arg \max _{u \in \mathbb{R}^{d}} e^{-S(v)} & =\arg \min _{u \in \mathbb{R}^{d}} J(u) \\
\eta & \sim N(0, \Gamma)
\end{aligned}
$$

■ In Gaussian setting, with $U \mid Y=y \sim N(m, C)$ and $U \sim N\left(0, \lambda^{-1} l\right)$,

$$
u_{M A P}=m=\arg \min _{u \in \mathbb{R}^{d}} \frac{1}{2}|y-G(u)|_{\Gamma}^{2}+\frac{\lambda}{2}|u|^{2} .
$$

- This corresponds to Tikhonov regularization. Unique, closed form solution in linear setting $G(u)=A u$.


## Laplace-distributed prior and LASSO regression

- Alternatively, consider the prior with iid Laplace-distributed components

$$
\pi_{U}(u)=\prod_{i=1}^{d} \pi_{U_{i}}\left(u_{i}\right) \propto \prod_{i=1}^{d} e^{-\lambda\left|u_{i}\right|}=e^{-\lambda|u|_{1}}
$$

where

$$
|u|_{p}:=\left(\sum_{j=1}^{d}\left|u_{j}\right|^{p}\right)^{1 / p}
$$

■ This yields

$$
\mathrm{R}(u) \geq|u|_{1}+C \text { and } \quad u_{M A P}=\arg \min _{u \in \mathbb{R}^{d}} \frac{1}{2}|y-G(u)|_{\Gamma}^{2}+\lambda|u|_{1}
$$

which corresponds to lasso (least absolute shrinkage and slection operator) regression.
■ Generally, lasso has no closed-form solution, but a solution is typically attainable. It tends to produce more sparse solutions than Tikhonov.

Posterior setting with $R \gg L$ and regularizers so that approximately

$$
\pi_{1}(u \mid y) \propto \exp \left(-|u|^{2} / 2\right) \quad \text { and } \quad \pi_{2}(u \mid y) \propto \exp \left(-|u|_{1}\right)
$$




## Attainability of $u_{M A P}$

## $\pi(u \mid y) \propto e^{-\partial(u)}$

## Theorem 1

Assume that the objective fcn $J: \mathbb{R}^{d} \rightarrow \mathbb{R}$ is bounded from below, continuous and that $J(u) \rightarrow \infty$ as $|u| \rightarrow \infty$. Then J attains its infimum, which implies that

$$
u_{M A P}[\pi(\cdot \mid y)] \quad \text { is attained for } \pi(u \mid y) \propto \exp (-J(u))
$$

Sufficient conditions for attainable $u_{M A P}$ :
$\square G \in C\left(\mathbb{R}^{d}, \mathbb{R}^{k}\right)$ and $\eta \sim N(0, \Gamma), \pi\left(u(y) \in \pi_{\eta}\left(y-G_{Q}(u)\right) \Pi_{u}(u)\right.$

- $\mathrm{R}(u)=\lambda|u|_{p}^{p}$ for any $\lambda, p>0$
(as this implies $J(u) \rightarrow \infty$ as $|u| \rightarrow$ ).


## Examples of the MAP performing poorly

■ "All happy families are alike; each unhappy family is unhappy in its own way." Leo Tolstoy, in Anna Karenina

■ Paraphrasing: "All unimodal densities are alike; each multimodal density is multimodal in its own way"

In Lecture 7 we already saw that $u_{M A P}$ can be of limited value for bimodal densities:


## Slab-spike figure

For

$$
\pi(u \mid y)=\frac{\exp \left(-|u|^{2} / 0.02\right)+0.3 \exp \left(-|u-10|^{2} / 18\right)}{\sqrt{2 \pi}}
$$




## Low-regularity objective function

```
normalF = @(x) (x).^2/10;
objective = normalF(x)+1.5*(1-2*rand(size(x)));
posterior = exp(-objective);
posterior = exp(-objective)/(trapz(posterior)*dx);
```




And low-regularity in higher dimensions ...


Figure: Photo by Michel Royon / Wikimedia Commons

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## Low-rank approximations of posteriors

■ We have seen that one-parameter/vector compression of a posterior, like MAP or posterior mean, may provide little information.

■ Natural next step: Extend the compressed representations of posteriors to best fitting in a class of candidate densities:

$$
p^{*}=\arg \inf _{p \in \mathcal{A}} d(p, \pi(\cdot \mid y))
$$

for some $d: \mathcal{M} \times \mathcal{M} \rightarrow[0, \infty)$

- Here we will restrict ourselves to

$$
\mathcal{A}=\left\{p=P D F(N(\mu, C)) \mid \mu \in \mathbb{R}^{d} \text { and } C \in \mathbb{R}^{d \times d} \text { and pos definite }\right\}
$$

which can be viewed as a two-parameter (two-moment) compression of a posterior.

## Kullback-Leibler divergence

## Definition 2 (K-L divergence)

- For positive discrete measures: Let

$$
\mathcal{P}_{+}=\{\text {Probability measures on } A \mid \mathbb{P}(x)>0 \text { for all } x \in A\} .
$$

For all $\mathbb{P}, \mathbb{Q} \in \mathcal{P}_{+}$,

$$
d_{K L}(\mathbb{P} \| \mathbb{Q}):=\sum_{x \in A} \log \left(\frac{\mathbb{P}(x)}{\mathbb{Q}(x)}\right) \mathbb{P}(x)=E^{\mathbb{P}}\left[\log \left(\frac{\mathbb{P}(\mathbb{B})}{\mathbb{( Q}(x)}\right)\right]
$$

- For positive pdfs on $\mathbb{R}^{d}$ : Let

$$
\mathcal{M}_{+}:=\left\{\pi \in \mathcal{M} \mid \pi(x)>0 \quad \forall x \in \mathbb{R}^{d}\right\}
$$

For all $\pi, p \in \mathcal{M}_{+}$

$$
d_{K L}(\pi \| p):=\int_{\mathbb{R}^{d}} \log \left(\frac{\pi(x)}{p(x)}\right) \pi(x) d x=\mathbb{E}^{\pi}\left[\log \left(\frac{\pi}{p}\right)\right]
$$

## Properties of the K-L divergence

For all $\pi, p \in \mathcal{M}_{+}$, it holds that $d_{K L}(\pi \| p) \in[0, \infty]$ (similar result holds for prob measures).

Example of infinite K-L divergence:

$$
p(x) \propto e^{-|x|}, \quad \pi \propto(1+|x|)^{-2}, \quad x \in \mathbb{R}
$$

Then

$$
\int_{\mathbb{R}(1+|x|)^{2}} \frac{|x|}{(1 x}
$$

$$
\begin{aligned}
d_{K L}(\pi \| p) & =\int_{\mathbb{R}} \log \left(\frac{\pi(x)}{p(x)}\right) \pi(x) d x \\
& =C \int_{\mathbb{R}}(\log (\pi(x))-\log (p(x))) \pi(x) d x \\
& \left.=C \int_{\mathbb{R}} \frac{-2 \log ((1+|x|))+|x|}{(1+|x|)^{2}}\right) d x^{t} d x \\
& =\infty .
\end{aligned}
$$

## Properties of the K-L divergence

$d_{K L}$ is not a metric; neither does it saitisfy the triangle inequality nor is it symmetric in its arguments.

Example: Let $A=\{1,2,3\}$ and $\mathbb{P}(1)=\mathbb{P}(2)=\mathbb{P}(3)=1 / 3$ and $\mathbb{Q}(1)=1 / 2, \mathbb{Q}(2)=1 / 3, \mathbb{Q}(3)=1 / 6$. Then

$$
\begin{aligned}
d_{K L}(\mathbb{P} \| \mathbb{Q}) & =\sum_{x_{i} \in A} \log \left(\frac{\mathbb{P}\left(x_{i}\right)}{\mathbb{Q}\left(x_{i}\right)}\right) \mathbb{P}\left(x_{i}\right) \\
& =\frac{\log (2 / 3)+\log (1)+\log (2)}{3} \approx 0.0959
\end{aligned}
$$

while

$$
d_{K L}(\mathbb{Q} \| \mathbb{P})=\frac{3 \log (3 / 2)+2 \log (1)+\log (1 / 2)}{6} \approx 0.0872
$$

## Properties of the K-L divergence

■ K-L divergence has natural applications in information theory and thermodynamics.

- In Bayesian inference, for a prior $\pi_{U}$ and a posterior $\pi(\cdot \mid y)$, $d_{K L}\left(\pi(\cdot \mid y) \| \pi_{U}\right)$ is a measure of the information gain of replacing the prior by the posterior.
- The logarithm base in the definition of K-L divergence is flexible; use what is most suitable for the application (here, log denotes the natural logarithm).


## Lemma 3 (Lower bounds for K-L divergence, (SST 4.2))

For any $\backslash p i, p \in \mathcal{M}_{+}$it holds that

$$
d_{H}(\pi, p)^{2} \leq \frac{1}{2} d_{K L}(\pi \| p) \quad \text { and } \quad d_{T V}(\pi, p)^{2} \leq d_{K L}(\pi \| p)
$$

Proof of first inequality:

$$
\begin{aligned}
d_{H}(\pi, p)^{2} & =\frac{1}{2} \int_{\mathbb{R}^{d}}(\sqrt{\pi}-\sqrt{p})^{2} d x=\frac{1}{2} \int_{\mathbb{R ^ { d }}}^{\pi}+p-2 \sqrt{\pi p} d x \\
& =\frac{1}{2} \int_{\mathbb{R} \boldsymbol{d}^{d}} 2 \pi-2 \sqrt{\pi P^{\prime}} d x=\int_{\mathbb{R}}\left(\frac{\pi}{\pi}-\sqrt{\pi P}\right) d x \\
& = \\
& \equiv \int_{\mathbb{R}^{d}}\left(1-\sqrt{\frac{p}{\pi}}\right) \pi d x \leq-\frac{1}{2} \int_{\mathbb{R}^{d}} \log \left(\frac{p}{\pi}\right) \pi d x=\frac{1}{2} d_{K L}(\pi \| p) .
\end{aligned}
$$

where we used that

$$
1-\sqrt{x} \leq-\frac{1}{2} \log (x) \quad \forall x \in[0, \infty]
$$

## Comments

- Second inequality follows from $d_{T V}(\pi, p) \leq \sqrt{2} d_{H}(\pi, p)$.
- The lemma implies that K-L divergence is point/density separating: For all $\pi, p \in \mathcal{M}_{+}$,

$$
d_{K L}(\pi \| p) \geq 0
$$

and

$$
d_{K L}(\pi \| p)=0 \Longleftrightarrow p=\pi .
$$

(Similar for measures.)

## Entropy in information theory

Suppose you want to transmit a very long text encoded in some alphabet, e.g., $A=\{a, b, c, d, e\}$,

TEXT= "abbedeeeedcaababecbddaeedeccabe..." and that

- the data-transmission problem can to good approximation be viewed as transmitting a sequence iid characters drawn with relative frequencies $\mathbb{P}(a), \mathbb{P}(b)$ etc.
- you want to send the text over a digital communication channel with alphabet $\{0,1\}$. Hence, each letter in your original alphabet must be replaced with a codeword, e.g. $a=101, b=111$, and your want the digitally encoded text to be as short as possible.
- Core idea: assign shortest codeword to most frequent letter in the text, second shortest codeword to ... (then there is a subtle issue with uniqueness/reversibility of encoding).


## Huffman encoding

Input alphabet: $A=\{a 1, a 2, a 3, a 4\}$.


Letter frequency: $\mathbb{P}(a 1)=0.4, \mathbb{P}(a 2)=0.35$ etc
Digital codewords: $a 1=0, a 2=10$, etc
NB! A shorter encoding is possible: $a 1=0, a 2=1, a 3=10$ and $a 4=11$ but this encoding is, unlike Huffman's, not uniquely reversible, since it is not injective when applied to strings:

$$
a 4 \mapsto 11 \quad a 2 a 2 \mapsto 11
$$

## Shannon's approach

Shannon relates the text-frequency of a letter to the information content:

## Definition 4 (Information content of a character)

For an event/character a which occurs with probability $\mathbb{P}(a)$ we define its information content by

$$
I(a):=-\log _{2}(\mathbb{P}(a))
$$

Idealized motivation: if there are $1 / \mathbb{P}(a)$ many independent events, each occurring with probability $\mathbb{P}(a)$, how many bits do I need to distinguish all these events when encoded in $\{0,1\}$ ?

Example Alphabet $A=\{a, b, c, d, e\}$ with uniform letter probability $1 / 5$. Then at least $-\left\lceil\log _{2}(1 / 5)\right\rceil=3$ bits are needed to distinguish the letters/events.

## Shannon entropy

Generalization: Information content straightforwardly generalizes from a character to any text string $B$

$$
I(B):=-\log _{2}(\mathbb{P}(B))
$$

where we recall that letter sequences, e.g., $B=a b e b a$, are assumed to consist of iid characters,

$$
\mathbb{P}(a b e b a)=\mathbb{P}(a) \mathbb{P}(b) \mathbb{P}(e) \mathbb{P}(b) \mathbb{P}(a)
$$

## Lemma 5 (Information content of independent events)

Let $B$ and $C$ denote two independent events (i.e., text strings), then the information content of $B$ and $C$ is additive

$$
I(B C):=I(B)+I(C)
$$

Verification for two-character sequence: Consider basic events $B=a$ and $C=b$. Then $\left.=-\log _{2} \mathbb{P}(a)\right)^{2}-\log ^{(\mathbb{P}(b))}$

$$
I(a b)=-\log _{2}(\mathbb{P}(a b))=-\log _{2}(\mathbb{P}(a) \mathbb{P}(b))=I(a)+I(b)
$$

## Shannon entropy

Question: Given a text encoded in the alphabet $A=\left\{a_{1}, \ldots, a_{n}\right\}$ with relative frequencies $\left\{\mathbb{P}\left(a_{k}\right)\right\}_{k}$, and a digital encoding representing the letter $a_{k}$ by $I\left(a_{k}\right)$ bits (we allow fractional-bit encoding in this thought experiment) then if the original text consists of $N \gg 1$ characters, how long does the digitally encoded text become?

## Answer:

$N \times$ mean num of bits for single $A$-character $=N \sum_{k=1}^{n} I\left(a_{k}\right) \mathbb{P}\left(a_{k}\right)$
Introducing the information content rv

$$
\mathbb{I}_{\mathbb{P}}(a):=-\log _{2}(\mathbb{P}(a)), \quad\left(\mathscr{I}_{\mathbb{P}}: A \rightarrow[0, \infty], \text { and } \mathbb{P}_{\mathbb{P}}\left(I_{\mathbb{P}}(a)\right)=\mathbb{P}(a)\right)
$$

we may associate the above with the expected information content/Shannon entropy

$$
\mathbb{E}^{\mathbb{P}}\left[\mathscr{P}_{\mathbb{P}}\right]=\sum_{k=1}^{n} \mathscr{P}_{\mathbb{P}}\left(a_{k}\right) \mathbb{P}\left(a_{k}\right)=-\sum_{k=1}^{n} \log _{2}\left(\mathbb{P}\left(a_{k}\right)\right) \mathbb{P}\left(a_{k}\right)
$$

## Comparison of encoding methods

Assume that a text encoded in $A=\left\{a_{1}, \ldots, a_{n}\right\}$ has true relative frequencies $\left\{\mathbb{P}\left(a_{k}\right)\right\}$, but that

- you only have an approximation of the relative frequencies $\left\{\mathbb{Q}\left(a_{k}\right)\right\}$
- and that given $\mathbb{Q}$, your encoding in $\{0,1\}$ is optimal, meaning it uses $I_{\mathbb{Q}}\left(a_{k}\right)=-\log _{2}\left(\mathbb{Q}\left(a_{k}\right)\right)$ bits to encode the letter $a_{k}$.
$K-L$ divergence is a comparison of efficiency $\mathbb{Q}$ - vs $\mathbb{P}$-encoding:
[mean $\mathbb{Q}$-bits in encoded $A$-char] - [mean $\mathbb{P}$-bits in encoded $A$-char]

$$
\begin{aligned}
& =\sum_{k=1}^{n}\left(I_{\mathbb{Q}}\left(a_{k}\right)-I_{\mathbb{P}}\left(a_{k}\right)\right) \mathbb{P}\left(a_{k}\right) \\
& =\sum_{k=1}^{n}\left(\log _{2}\left(\mathbb{P}\left(a_{k}\right)\right)-\log _{2}\left(\mathbb{Q}\left(a_{k}\right)\right) \mathbb{P}\left(a_{k}\right)\right. \\
& =\sum_{k=1}^{n} \log _{2}\left(\frac{\mathbb{P}\left(a_{k}\right)}{\mathbb{Q}\left(a_{k}\right)}\right) \mathbb{P}\left(a_{k}\right)=d_{K L}(\mathbb{P} \| \mathbb{Q})
\end{aligned}
$$

## Best encoding in a set

Given a collection of encodings, a natural task is to find the most efficient one:

$$
\mathbb{Q}^{*}=\arg \min _{\mathbb{Q} \in \mathcal{A}} d_{K L}(\mathbb{P} \| \mathbb{Q})
$$

Example: Let $A=\{a, b, c, d, e\}$ and $\mathbb{P}(a)=\mathbb{P}(b)=\ldots=\mathbb{P}(\mathbb{\oplus})=1 / 5$, and $\mathcal{A}=\left\{\mathbb{Q}_{1}, \mathbb{Q}_{2}\right\}$ with

$$
\mathbb{Q}_{1}(a)=\mathbb{Q}_{1}(b)=\mathbb{Q}_{1}(c)=\mathbb{Q}_{1}(d)=2^{-4}, \quad \mathbb{Q}_{1}(e)=3 / 4
$$

and

$$
\mathbb{Q}_{2}(a)=\mathbb{Q}_{2}(b)=\mathbb{Q}_{2}(c)=\mathbb{Q}_{2}(d)=2^{-5}, \quad \mathbb{Q}_{2}(e)=7 / 8
$$

Result: $\mathbb{Q}^{*}=\mathbb{Q}_{1}$ as

$$
I_{Q_{1}}(x)=-\log _{2}\left(Q_{1}(x)\right)
$$

$$
d_{K L}\left(\mathbb{P} \| \mathbb{Q}_{1}\right)=\frac{4 \log _{2}(16 / 5)+\log _{2}(4 / 15)}{5} \approx 0.9611
$$

and

$$
d_{K L}\left(\mathbb{P} \| \mathbb{Q}_{2}\right)=\frac{4 \log _{2}(32 / 5)+\log _{2}(8 / 35)}{5} \approx 1.7166
$$

## Connecting information theory and random variables

 For discrete distributions $\mathbb{P}$ and $\mathbb{Q}$ on $A$ we defined the information content rv$$
I_{\mathbb{P}}(a)=-\log (\mathbb{P}(a)), \quad I_{\mathbb{Q}}(a)=-\log (\mathbb{Q}(a))
$$

and the K -L divergence from $\mathbb{Q}$ to $\mathbb{P}$ takes the form

$$
d_{K L}(\mathbb{P} \| \mathbb{Q})=\mathbb{E}^{\mathbb{P}}\left[I_{\mathbb{Q}}-I_{\mathbb{P}}\right]=\sum_{a \in A} \log \left(\frac{\mathbb{P}(a)}{\mathbb{Q}(a)}\right) \mathbb{P}(a)
$$

For continuous rv $X, Y$ with densities $\pi_{X}, \pi_{Y} \in \mathcal{M}_{+}$, we define the information content as

$$
I_{\pi_{X}}(x)=-\log \left(\pi_{X}(x)\right), \quad I_{\pi_{Y}}(x)=-\log \left(\pi_{Y}(x)\right)
$$

and

$$
d_{K L}\left(\pi_{X} \| \pi_{Y}\right)=\mathbb{E}^{\pi_{X}}\left[I_{\pi_{Y}}-I_{\pi_{X}}\right]=\int_{\mathbb{R}^{d}} \log \left(\frac{\pi_{X}(x)}{\pi_{Y}(x)}\right) \pi_{X}(x) d x
$$

## Expected information gain Bayesian inversion

For the addyive batustifity inverse problem

$$
\begin{equation*}
Y=G(U)+\eta \tag{3}
\end{equation*}
$$

with $\pi_{\eta}, \pi_{U} \in \mathcal{M}_{+}$and $U \perp \eta$, the posterior is also a strictly positive pdf

$$
\begin{equation*}
\pi(u \mid y)=\frac{\exp (-\mathrm{L}(u)) \pi_{u}(u)}{Z} \tag{4}
\end{equation*}
$$

Then

$$
d_{K L}\left(\pi(\cdot \mid y) \| \pi_{U}\right)=\mathbb{E}^{\pi(\cdot \mid y)}\left[I_{\pi_{U}}-I_{\pi(\cdot \mid y)}\right]
$$

is a measure of the information gained by revising the prior $\pi_{U}$ into the posterior $\operatorname{dg\pi L}(\pi(\cdot \mid y) \mid$ 有

Interpretation: wrt $\pi(\cdot \mid y), I_{\pi(\cdot \mid y)}$ yields the minimum expected information content, so, as we already know,

$$
\mathbb{E}^{\pi(\cdot \mid y)}\left[I_{\pi u}-I_{\pi(\cdot \mid y)}\right] \geq 0
$$

## Variational formulation of Bayes theorem

## Theorem 6 (SST Thm 4.9)

For the inverse problem (3) it holds that

$$
\pi(\cdot \mid y)=\arg \min _{p \in \mathcal{M}_{+}} d_{K L}\left(p \| \pi_{U}\right)+\mathbb{E}^{p}[L(u)]
$$

Verification: Recalling that $\pi(u \mid y)=\frac{\exp (-\mathrm{L}(u)) \pi_{u}(u)}{Z}$,

$$
\begin{aligned}
d_{K L}(p \| \pi(\cdot \mid y)) & =\int_{\mathbb{R}^{d}} \log \left(\frac{p \pi_{U}}{\pi(x \mid y) \pi_{U}}\right) p(x) d x \\
& =\int_{\mathbb{R}^{d}} \log \left(\frac{p Z \exp (\mathrm{~L}(u))}{\pi_{U}}\right) p(x) d x \\
& =\int_{\mathbb{R}^{d}}\left[\log \left(\frac{p}{\pi_{U}}\right)+\mathrm{L}(u) \$ p(x) d x+\log (Z)\right. \\
& =d_{K L}\left(p \| \pi_{U}\right)+\mathbb{E}^{p}[\mathrm{~L}]+\log (Z)
\end{aligned}
$$

and

$$
\pi(\cdot \mid y)=\arg \min _{p \in \mathcal{M}_{+}} d_{K L}(p \| \pi(\cdot \mid y))
$$

## Best Gaussian fit and K-L divergence

Consider again the posterior obtained from the inverse problem (3),

$$
\begin{equation*}
\pi(u \mid y)=\frac{\exp (-\mathrm{L}(u)) \pi u(u)}{Z} \tag{5}
\end{equation*}
$$

## Theorem 7

Assume that $L$ is non-negative, continuous, and globally bounded from above and that $U \sim N\left(0, \lambda^{-1} I\right)$ for some $\gamma>0$. Then there exists at least one $p d f p$ in

$$
\begin{equation*}
\mathcal{A}:=\left\{\rho=\operatorname{PDF}(N(\mu, C)) \mid \mu \in \mathbb{R}^{d} \text { and } C \in \mathbb{R}^{d \times d} \text { and pos definite }\right\} . \tag{6}
\end{equation*}
$$

which satisfies the best-Gaussian-fit-of-posterior condition

$$
d_{K L}(p \| \pi(\cdot \mid y))=\inf _{\rho \in \mathcal{A}} d_{K L}(\rho \| \pi(\cdot \mid y))
$$

Essential fitting idea:
make $\log \left(\frac{p(x)}{\pi(x \mid y)}\right) \quad$ small i.e., $\frac{p}{\pi(\cdot \mid y)} \lesssim 1$.

## Ideas in proof

For $p_{\mu, C}=\operatorname{PDF}(N(\mu, C))$ it is possible to show that for

$$
I(\mu, C):=d_{K L}\left(p_{\mu, C} \| \pi(\cdot \mid y)\right)
$$

it holds that

$$
I(0, I)<\infty, \quad \lim _{|\mu| \rightarrow \infty} I(\mu, C)=\infty
$$

and

$$
\lim _{\operatorname{trace}(C) \rightarrow 0} I(\mu, C)=\lim _{\operatorname{trace}(C) \rightarrow \infty} I(\mu, C)=\infty
$$

Consequently, there exists $R>r>0$ s.t.

$$
\arg \inf _{p \in \mathcal{A}} d_{K L}(p \| \pi) \in \tilde{\mathcal{A}}_{r, R}
$$

where

$$
\tilde{\mathcal{A}}_{r, R}=\left\{p_{\mu, C} \in \mathcal{A}| | \mu \mid<R, \quad \text { and } \quad r<\operatorname{trace}(C)<R\right\} .
$$

## Best Gaussian fit by moment matching

One may also fit $p$ to $\pi$ by minimizing $d_{K L}(\pi(\cdot \mid y) \| p)$

## Theorem 8 (SST Thm 4.5)

Let $\pi(\cdot \mid y)$ denote the posterior density of the inverse problem (3). If $\bar{\mu}=\mathbb{E}^{\pi(\cdot \mid y)}[u]$ is finite and $\bar{C}=\mathbb{E}^{\pi(\cdot \mid y)}\left[(u-\bar{\mu})(u-\bar{\mu})^{T}\right]$ is finite and positive definite then

$$
p_{\bar{\mu}, \bar{C}}=\arg \inf _{p \in \mathcal{A}} d_{K L}(\pi \| p)
$$

and the minimizer $p_{\bar{\mu}, \bar{C}}$ is unique.

Essential fitting idea:

$$
\text { make } \log \left(\frac{\pi(x \mid y)}{p(x)}\right) \quad \text { small, i.e., } \quad \frac{\pi(\cdot \mid y)}{p} \lesssim 1
$$

Comparison of the fitting approaches

- For $d_{K L}(p \| \pi(\cdot \mid y))$ : make $\frac{p}{\pi(\cdot \mid y)} \lesssim 1$
- For $d_{K L}(\pi(\cdot \mid y) \| p)$ : make $\frac{\pi(\cdot \mid y)}{p} \lesssim 1$



## Next time

- discrete time continuous state-space Markov chains

■ Markov chain Monte Carlo methods

■ introduction to smoothing and filtering in continuous state-space

