

Generative Modeling

Distances and metrics

Denis Derkach, Artem Ryzhikov, Sergei Popov

Laboratory for methods of big data analysis



LAMBDA • HSE

Spring 2023

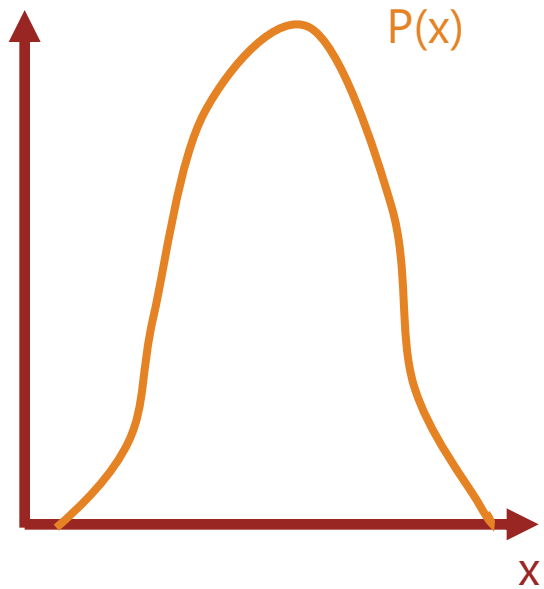
In this Lecture

- ▶ f -divergences
 - total Variation Distance;
 - Kullback-Leibler Divergence;
 - Jensen-Shannon Divergence;
 - divergence inequalities;
 - variational lower bound.
- ▶ Metrics (seminar)

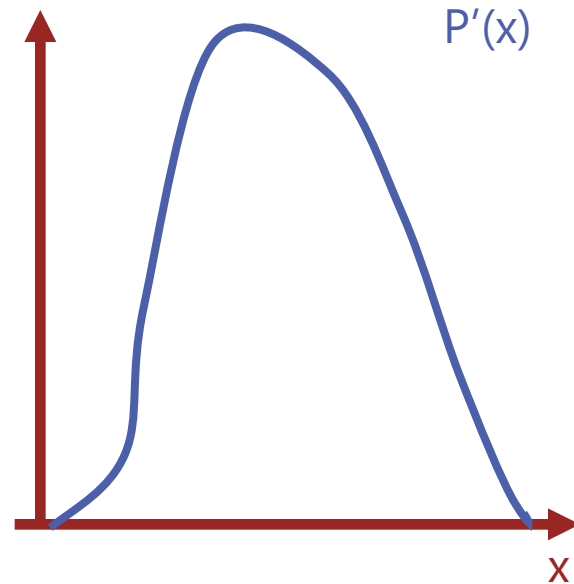
Total Variation Distance



What we measure



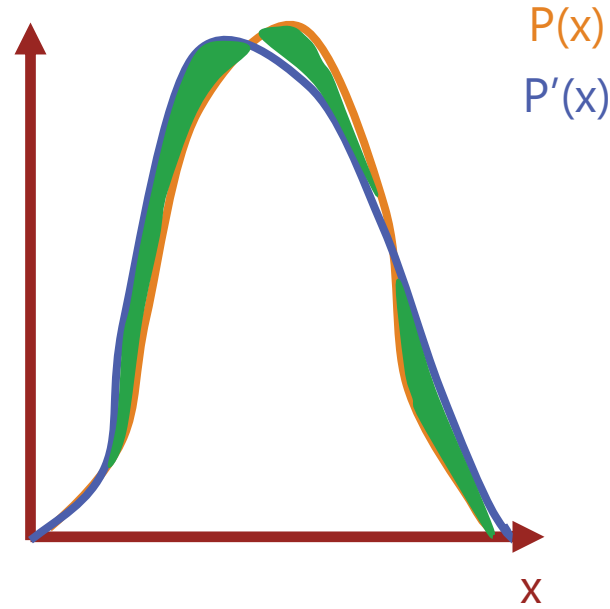
True Probability Density



Fitted Probability Density

$P'(x)$ is similar to $P(x)$?

First idea: absolute difference



$$\int |P(x) - P'(x)| dx$$

Total Variation Distance

For $p(x)$ and $q_\theta(x)$ being PDFs:

$$D(p(x), q_\theta(x)) = \frac{1}{2} \int |p(x) - q_\theta(x)| dx$$

This can be rewritten using Scheffe's theorem

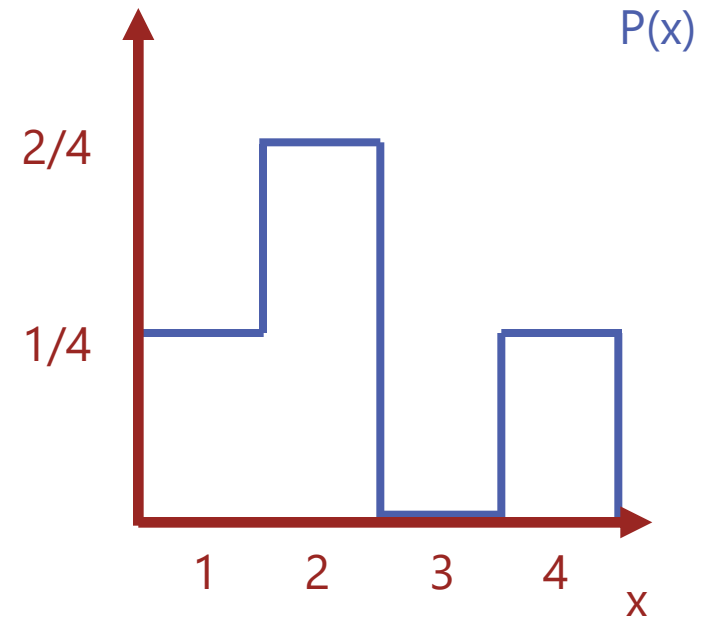
$$D(p(x), q_\theta(x)) = \sup_A \left| \int_A p(x) dx - \int_A q_\theta(x) dx \right|$$

Where A is any measurable set.

A. B. Tsybakov, Introduction to Nonparametric Estimation, sec 2.4

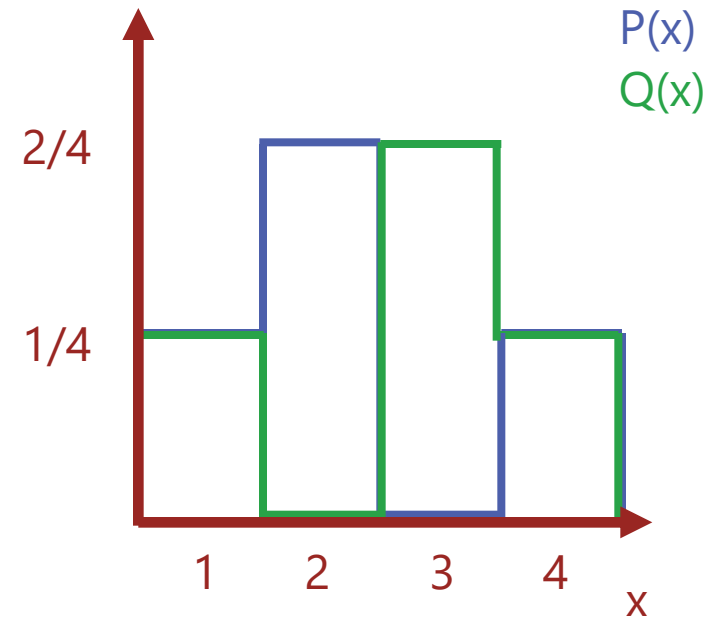
Total Variation Distance: example 1D

- discrete case for two PDFs



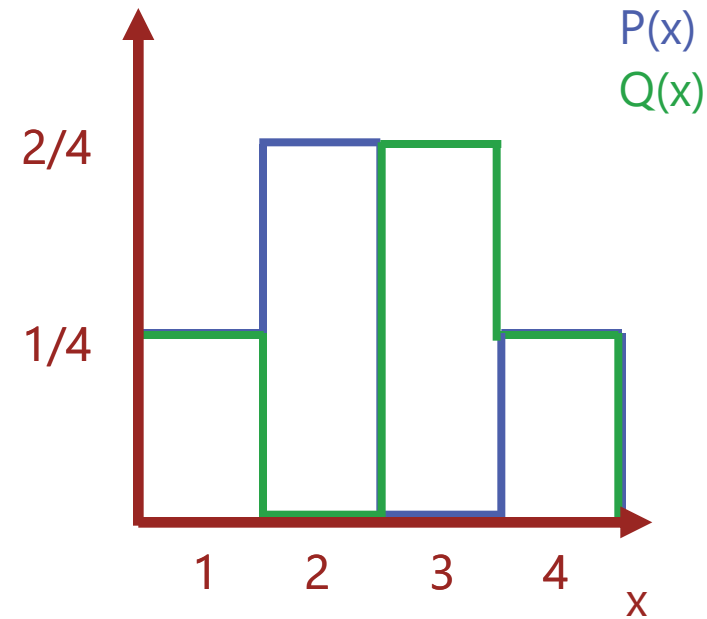
Total Variation Distance: example 1D

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Total Variation Distance: example 1D

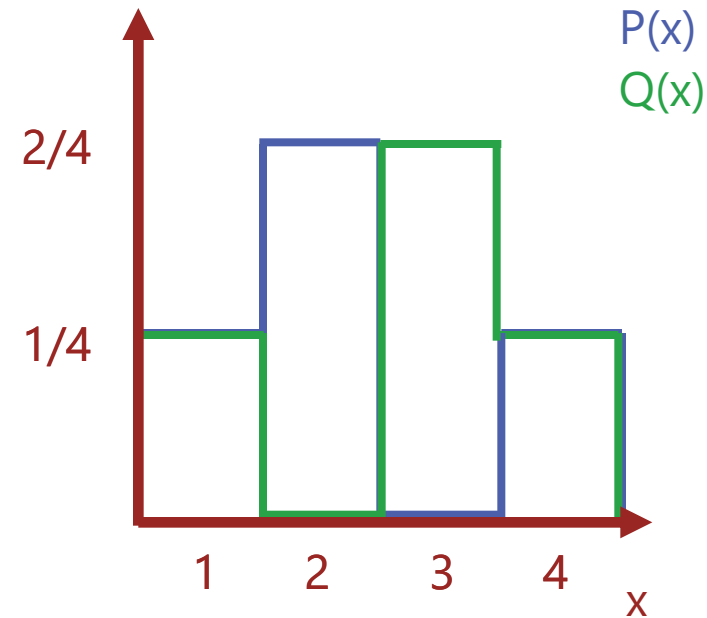
- discrete case for two PDFs
- calculate in two ways:



Total Variation Distance: example 1D

- discrete case for two PDFs
- calculate in two ways:
 - construct all possible subsets:

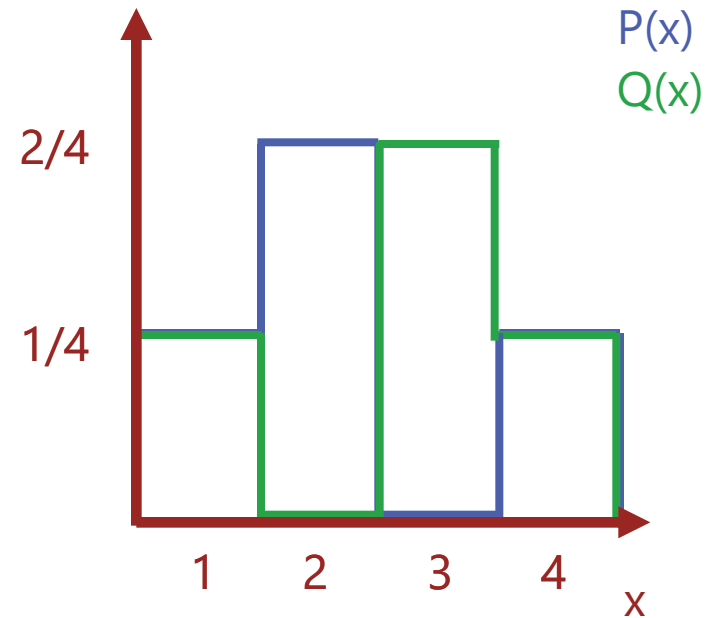
$\{1\}, \{2\}, \{3\}, \{4\}, \{1;2\}, \{1;3\}, \{1;4\},$
 $\{2;3\}, \{2;4\}, \{3;4\}, \{1;2;3\}, \{1;2;4\},$
 $\{1;3;4\}, \{1,2,3,4\}.$



Total Variation Distance: example 1D

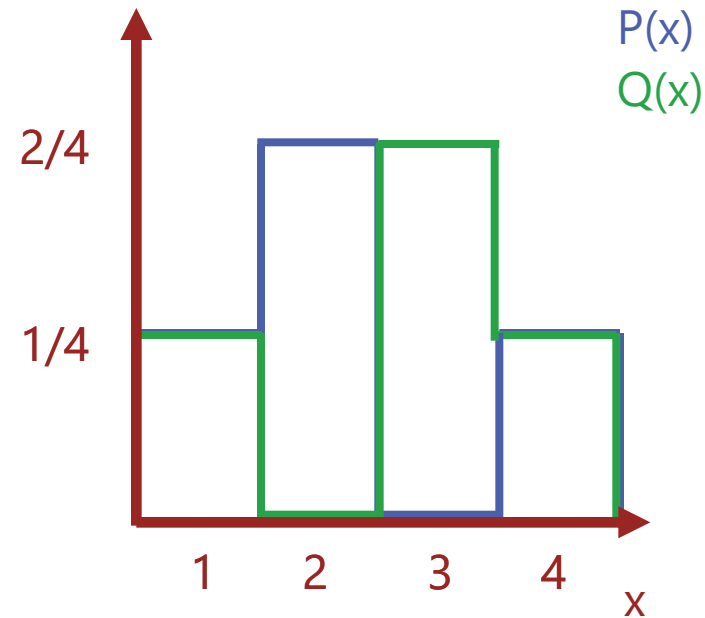
- discrete case for two PDFs
- calculate in two ways:
 - construct all possible subsets:

$$D(p,q) = 0.5$$



Total Variation Distance: example 1D

- discrete case for two PDFs
- calculate in two ways:
 - construct all possible subsets:
$$D(p,q) = 0.5$$
 - integrate over full range:
$$D(p,q) = 0.5$$



Total Variation Distance: observations

- Symmetric $D(p, q) = D(q, p)$
- Interpretable (using Scheffe lemma)
- Connected to hypothesis testing (D is the sum of errors)

Total Variation Distance: observations

- Symmetric $D(p, q) = D(q, p)$
- Interpretable (using Scheffe's theorem)
- Connected to hypothesis testing (D is the sum of errors)
- Too strong:

The distance might ignore the growing number of trials.

$$X_1, \dots, X_n \sim \pm 1, S_n = \sum_n X_i. \text{ Then}$$
$$S_n / \sqrt{n} \rightarrow \mathcal{N}(0, 1),$$

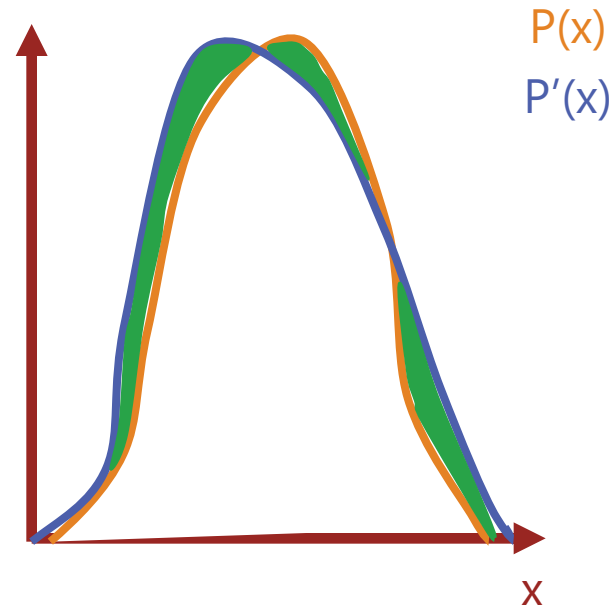
but $D(S_n, \mathcal{N}(0, 1)) = 1$ for any n .

A. L. Gibbs, F. E. Su On Choosing and Bounding Probability Metrics
F Pollard, Total variation distance between measures

Kullback-Leibler Divergence



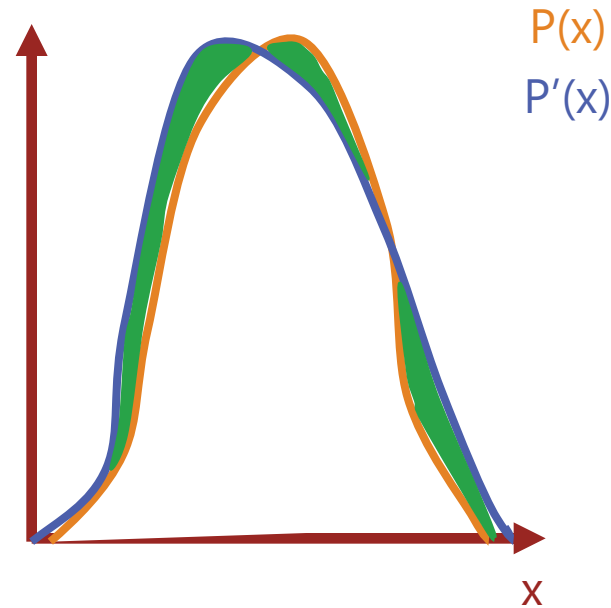
Kullback-Leibler divergence: ideas



Previously:

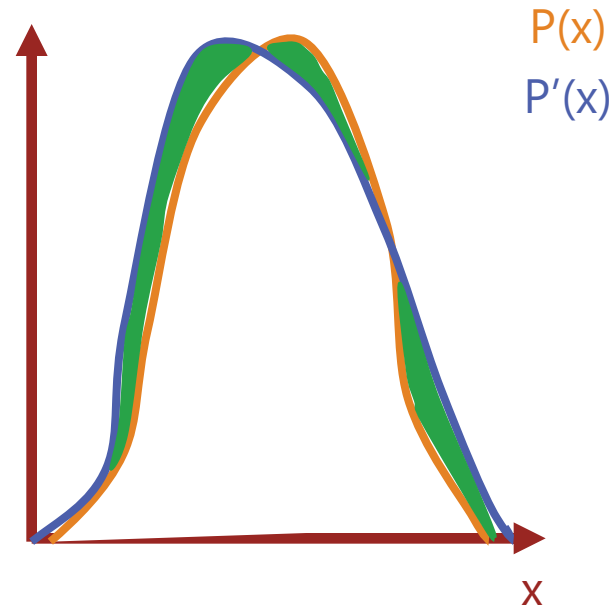
$$\int |P(x) - P'(x)| dx$$

Kullback-Leibler divergence: ideas



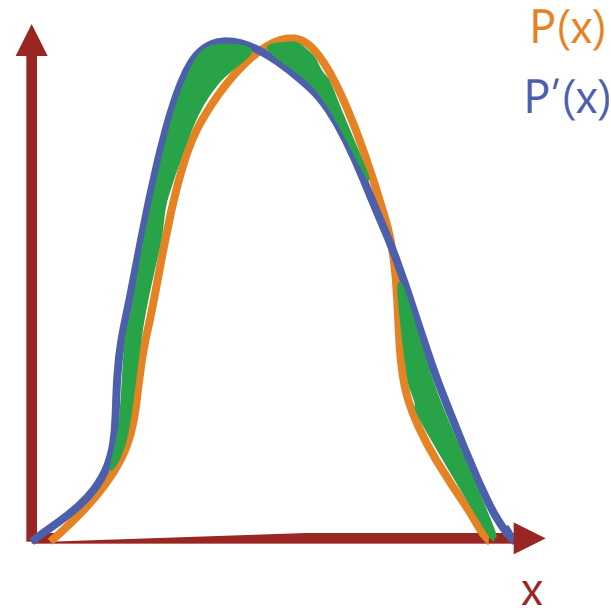
$$\frac{P(x)}{P'(x)}$$

Kullback-Leibler divergence: ideas



$$\ln \frac{P(x)}{P'(x)}$$

Kullback-Leibler divergence: ideas



$$\int P(x) \ln \frac{P(x)}{P'(x)} dx$$

Kullback-Leibler divergence: definition

For $p(x)$ and $q(x)$, two probability distributions,

$$KL(p||q_\theta) = \int p(x) \log \left(\frac{p(x)}{q_\theta(x)} \right) dx$$

Kullback-Leibler divergence: definition

For $p(x)$ and $q(x)$, two probability distributions,

$$KL(p||q_\theta) = \int p(x) \log \left(\frac{p(x)}{q_\theta(x)} \right) dx$$

- not symmetric $KL(P||Q) \neq KL(Q||P)$
- invariant under change of variables
- additive for independent variables
- Nonnegative (Gibbs inequality)

Kullback-Leibler divergence: observations

- **KL divergence is connected to cross-entropy:**

$$KL(p||q) = H(p) + H(p, q),$$

where $H(p, q) = \mathbb{E}_p(\log q)$.

KL and Maximum Likelihood

Find the optimal parameter, θ^* :

$$\theta^* = \operatorname{argmin}_{\theta} KL(p(x) || q_{\theta}(x))$$

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KL and Maximum Likelihood

Find the optimal parameter, θ^* :

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$$= \operatorname{argmin}_{\theta} (\mathbb{E}_{x \sim p} [\log p(x)] - \mathbb{E}_{x \sim p} [\log q_{\theta}(x)])$$

$$= -\operatorname{argmin}_{\theta} \mathbb{E}_{x \sim p} [\log q_{\theta}(x)]$$

KL divergence: observations

- **KL divergence is connected to cross-entropy:**

$$KL(p||q) = H(p) + H(p, q),$$

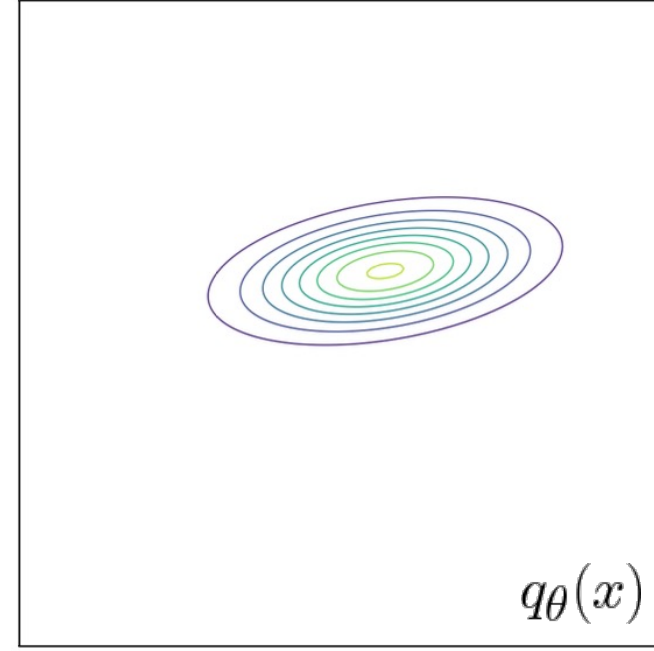
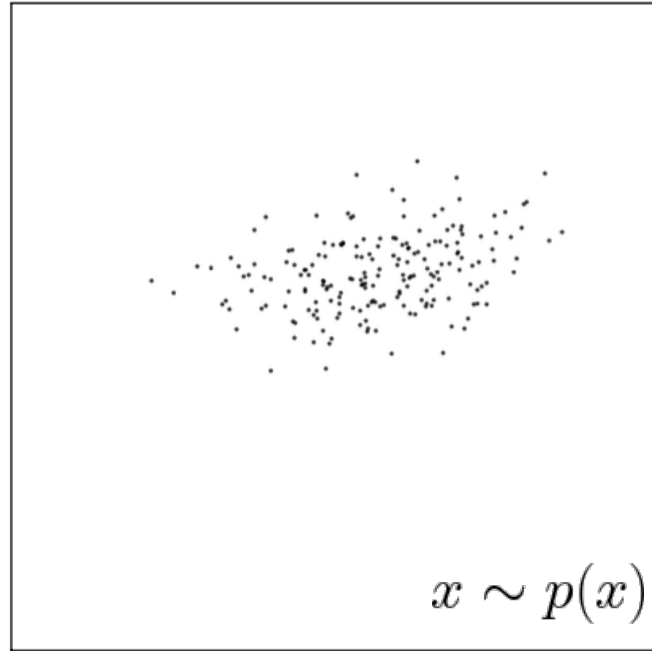
where $H(p, q) = \mathbb{E}_p(\log q)$.

- **Minimizing KL divergence is equivalent to maximizing the likelihood.**

$$\theta^* = \operatorname{argmin}_{\theta} KL(p(x)||q_{\theta}(x)) = \operatorname{argmax}_{\theta} \mathcal{L}(q_{\theta}(x); x)$$

Using in fits

Fit data points from 2D Gaussian function

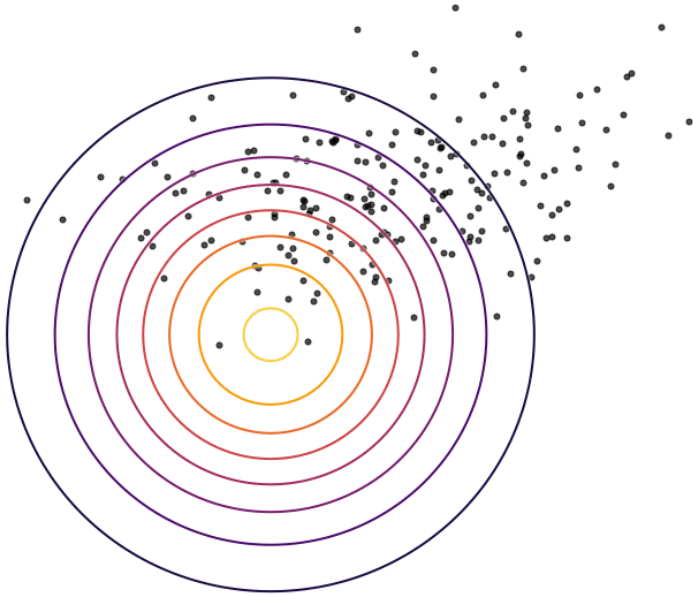


...with 2D Gaussian function

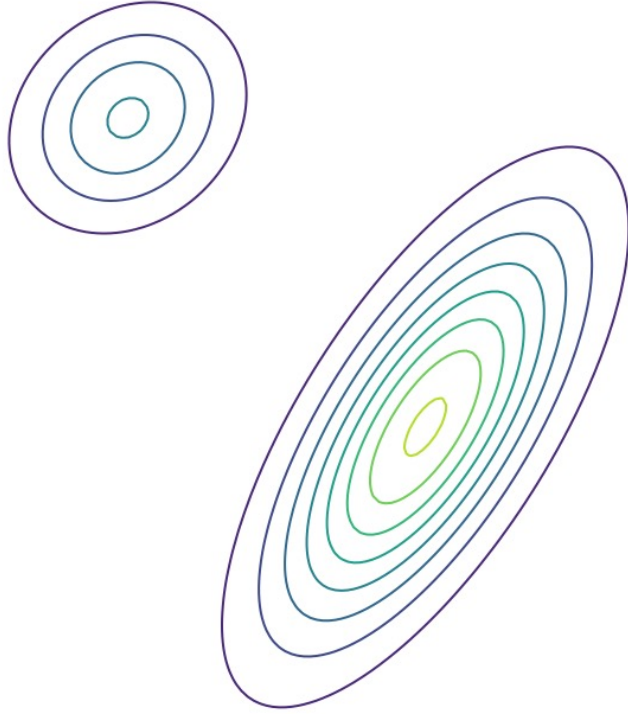
[Here and Later: Colin Raffel's blog](#)

Using in fits

- Runs smoothly for simple data

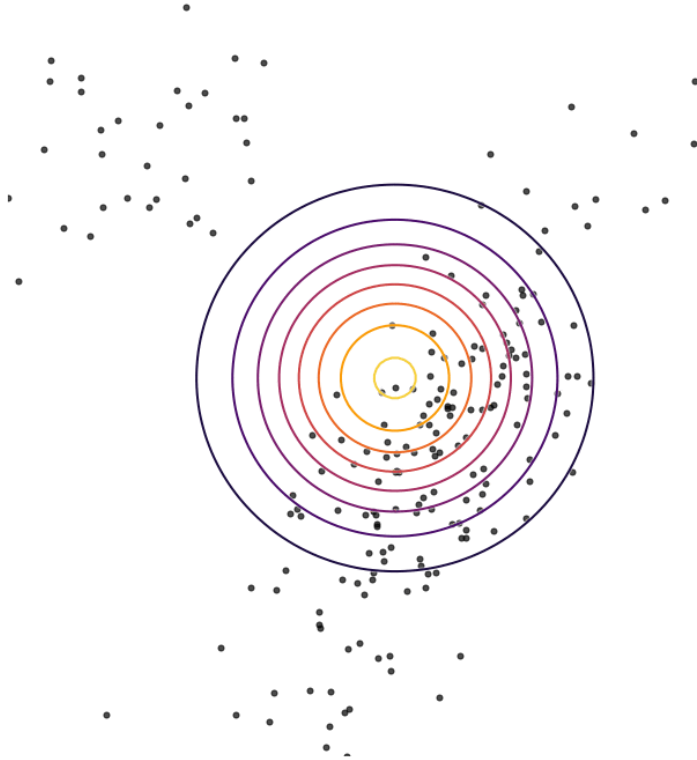


Using in fits: Multimodal data



- Runs smoothly for simple data

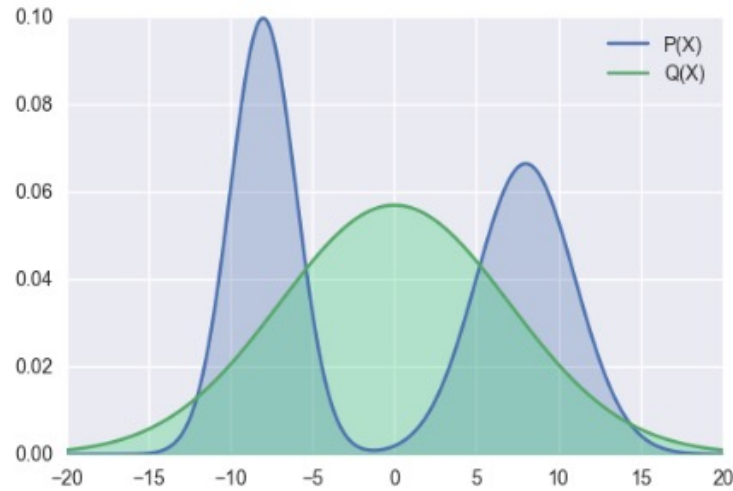
Using in fits: Multimodal data



- Runs smoothly for simple data
- Problems for multimodal data
- Covers significant amount of empty spaces

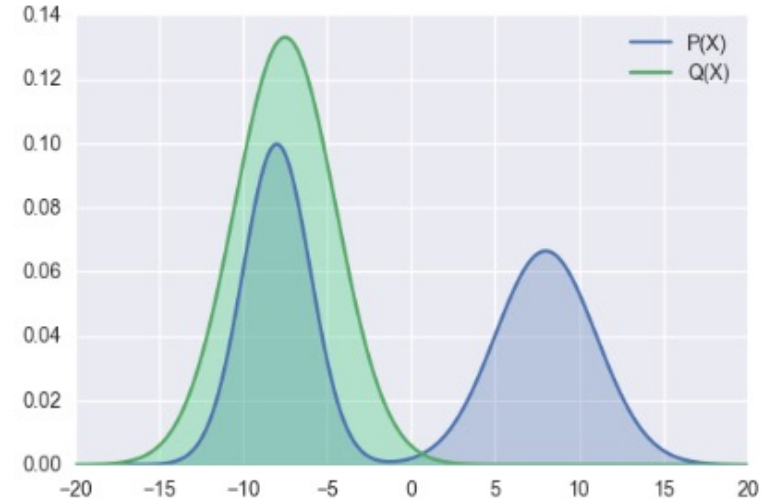
KL divergence: study

$$KL(p||q_\theta) = \int p(x) \log \left(\frac{p(x)}{q_\theta(x)} \right) dx$$



KL is zero avoiding, as it is avoiding $q(x) = 0$ whenever $p(x) > 0$

$$KL(q_\theta||p) = \int q_\theta(x) \log \left(\frac{q_\theta(x)}{p(x)} \right) dx$$



Reverse KL is zero forcing, as it forces $q(X)$ to be 0 on some areas, even if $p(X) > 0$

Reverse KL divergence: fits

Find the optimal parameter, θ^* :

$$\theta^* = \operatorname{argmin}_{\theta} KL(q_{\theta}(x) || p(x))$$

Reverse KL divergence: fits

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Reverse KL divergence: fits

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$$= \operatorname{argmax}_{\theta} (-\mathbb{E}_{\tilde{x} \sim q_{\theta}} [\log q_{\theta}(x)] + \mathbb{E}_{\tilde{x} \sim q_{\theta}} [\log p(x)])$$


Reverse KL divergence: fits

Find the optimal parameter, θ^* :

$$\theta^* = \operatorname{argmin}_{\theta} KL(q_{\theta}(x) || p(x))$$

entropy for the
fitted model

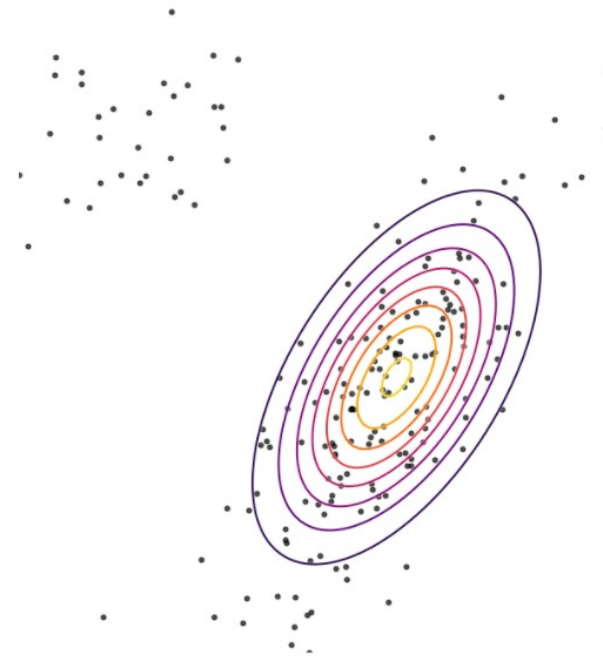

$$= \operatorname{argmax}_{\theta} (-\mathbb{E}_{\tilde{x} \sim q_{\theta}}[\log q_{\theta}(x)] + \mathbb{E}_{\tilde{x} \sim q_{\theta}}[\log p(x)])$$



relation between
fitted and generated

Reverse KL divergence: fits

- $q_{\theta}(x)$ covers only regions with data
- reasonable in multi-modal data for one solution



Critical: we do not have direct access to $p(x)$.

Jensen-Shannon Divergence



Jensen-Shannon Divergence: idea

- KL divergence is asymmetric

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$$KL(p||q) + KL(q||p)$$

Jensen-Shannon Divergence: idea

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- KL can become infinite

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Jensen-Shannon Divergence: idea

- KL divergence is asymmetric
- KL can become infinite

$$KL(p(x) || \frac{p(x) + q_{\theta}(x)}{2}) + KL(q_{\theta}(x) || \frac{p(x) + q_{\theta}(x)}{2})$$

Jensen-Shannon Divergence: Definition

For $p(x)$ and $q(x)$, two probability distributions,

$$JS(p, q) = \frac{1}{2} \left(KL(p(x) || \frac{p(x) + q(x)}{2}) + KL(q(x) || \frac{p(x) + q(x)}{2}) \right)$$

- symmetric
- nonnegative $0 \leq JS(P, Q) \leq \ln(2)$
- can be transformed to a true distance $\sqrt{JS(p, q)}$

J. Lin Divergence measures based on the Shannon entropy

f -divergences



Definition

- ▶ Let $f: (0; \infty) \rightarrow \mathbb{R}$ be a convex function with $f(1) = 0$.
- ▶ P and Q - two probability distributions on a measurable space $(\mathcal{X}, \mathcal{F})$.
- ▶ p and q - absolutely continuous with respect to a base measure dx defined on \mathcal{X} .
- ▶ f -divergence is defined:

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx$$

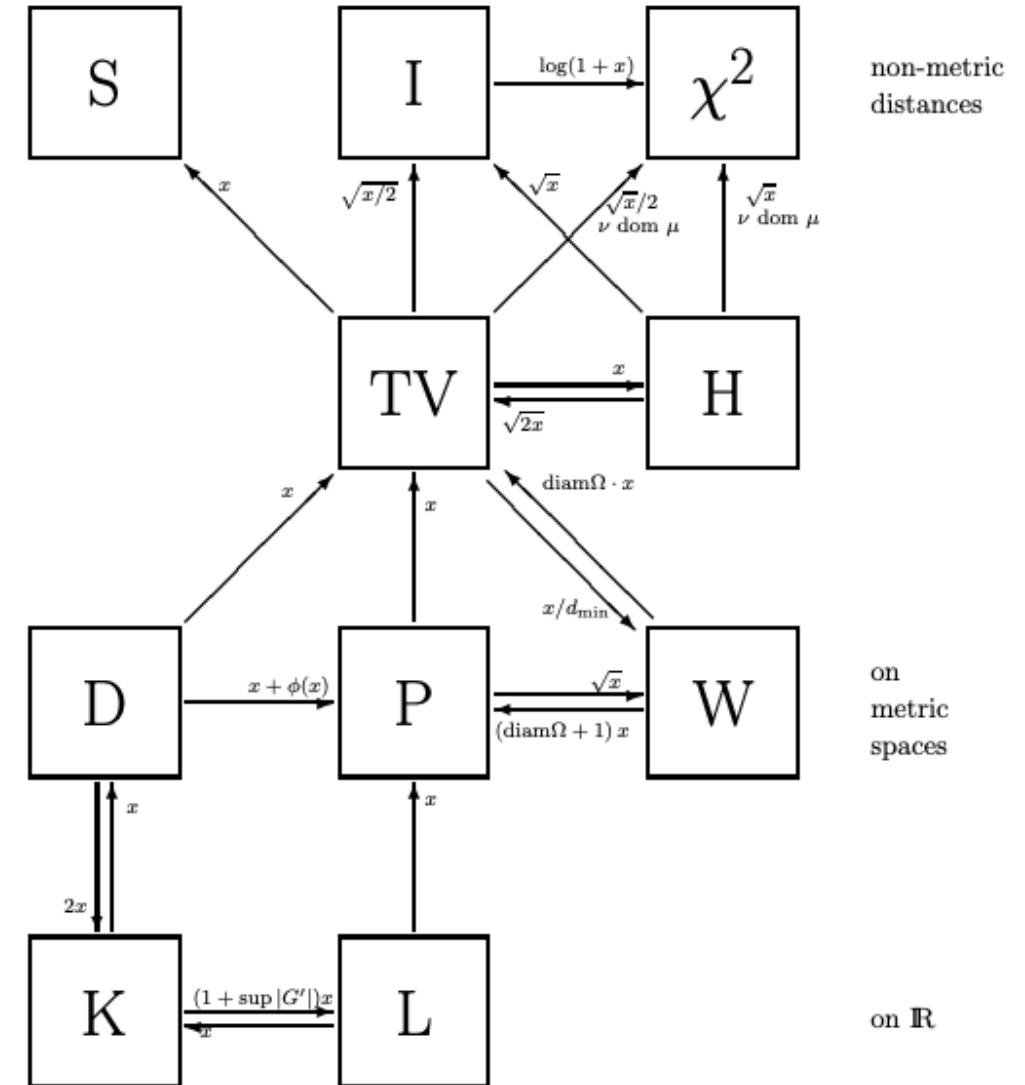
- ▶ f is called generator.

Examples

Name	$D_f(P\ Q)$	Generator $f(u)$
Total variation	$\frac{1}{2} \int p(x) - q(x) \, dx$	$\frac{1}{2} u - 1 $
Kullback-Leibler	$\int p(x) \log \frac{p(x)}{q(x)} \, dx$	$u \log u$
Reverse Kullback-Leibler	$\int q(x) \log \frac{q(x)}{p(x)} \, dx$	$-\log u$
Pearson χ^2	$\int \frac{(q(x) - p(x))^2}{p(x)} \, dx$	$(u - 1)^2$
Neyman χ^2	$\int \frac{(p(x) - q(x))^2}{q(x)} \, dx$	$\frac{(1-u)^2}{u}$
Squared Hellinger	$\int \left(\sqrt{p(x)} - \sqrt{q(x)} \right)^2 \, dx$	$(\sqrt{u} - 1)^2$
Jeffrey	$\int (p(x) - q(x)) \log \left(\frac{p(x)}{q(x)} \right) \, dx$	$(u - 1) \log u$
Jensen-Shannon	$\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} \, dx$	$-(u + 1) \log \frac{1+u}{2} + u \log u$
Jensen-Shannon-weighted	$\int p(x) \pi \log \frac{p(x)}{\pi p(x) + (1-\pi)q(x)} + (1 - \pi)q(x) \log \frac{q(x)}{\pi p(x) + (1-\pi)q(x)} \, dx$	$\pi u \log u - (1 - \pi + \pi u) \log(1 - \pi + \pi u)$

f -divergence inequalities

Abbreviation	Metric
D	Discrepancy
H	Hellinger distance
I	Relative entropy (or Kullback-Leibler divergence)
K	Kolmogorov (or Uniform) metric
L	Lévy metric
P	Prokhorov metric
S	Separation distance
TV	Total variation distance
W	Wasserstein (or Kantorovich) metric
χ^2	χ^2 distance



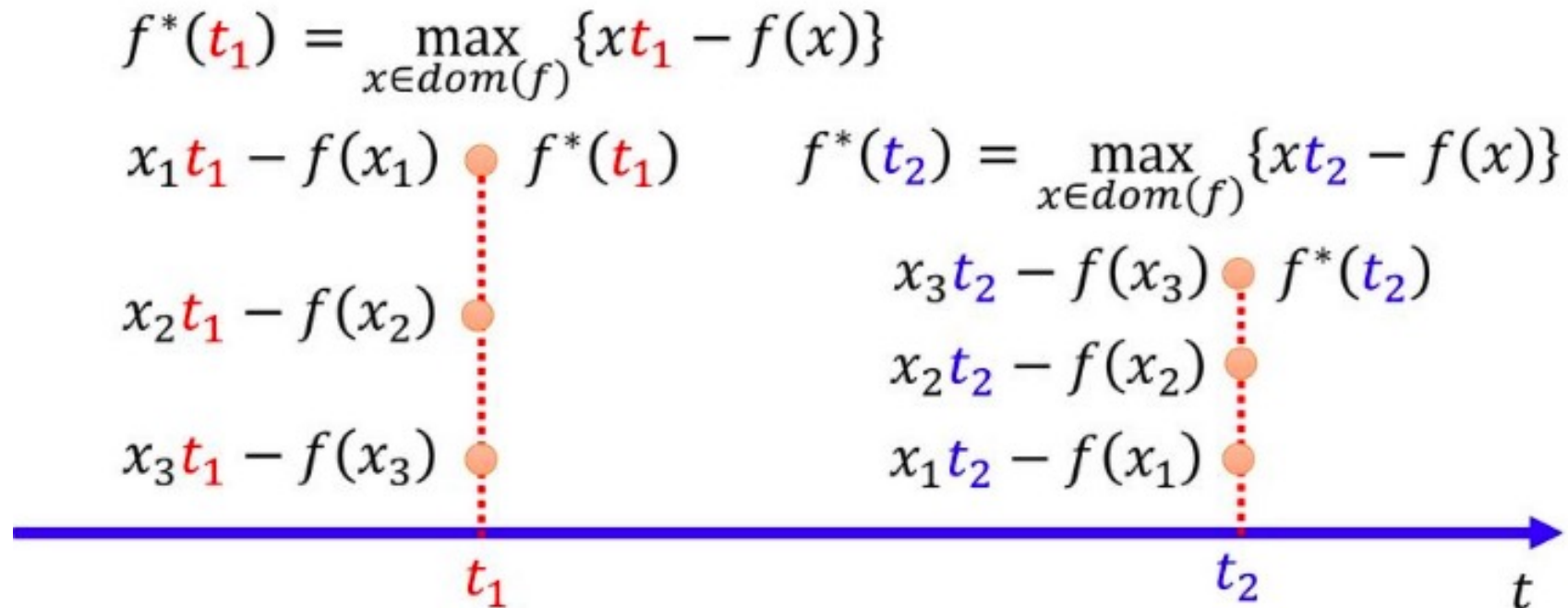
A. L. Gibbs, F. E. Su On Choosing and Bounding Probability Metrics

Fenchel conjugate

- ▶ Each generator has a **Fenchel conjugate** function:

$$f^*(t) = \sup_x (xt - f(x))$$

if f is convex, then $(f^*)^* = f$.

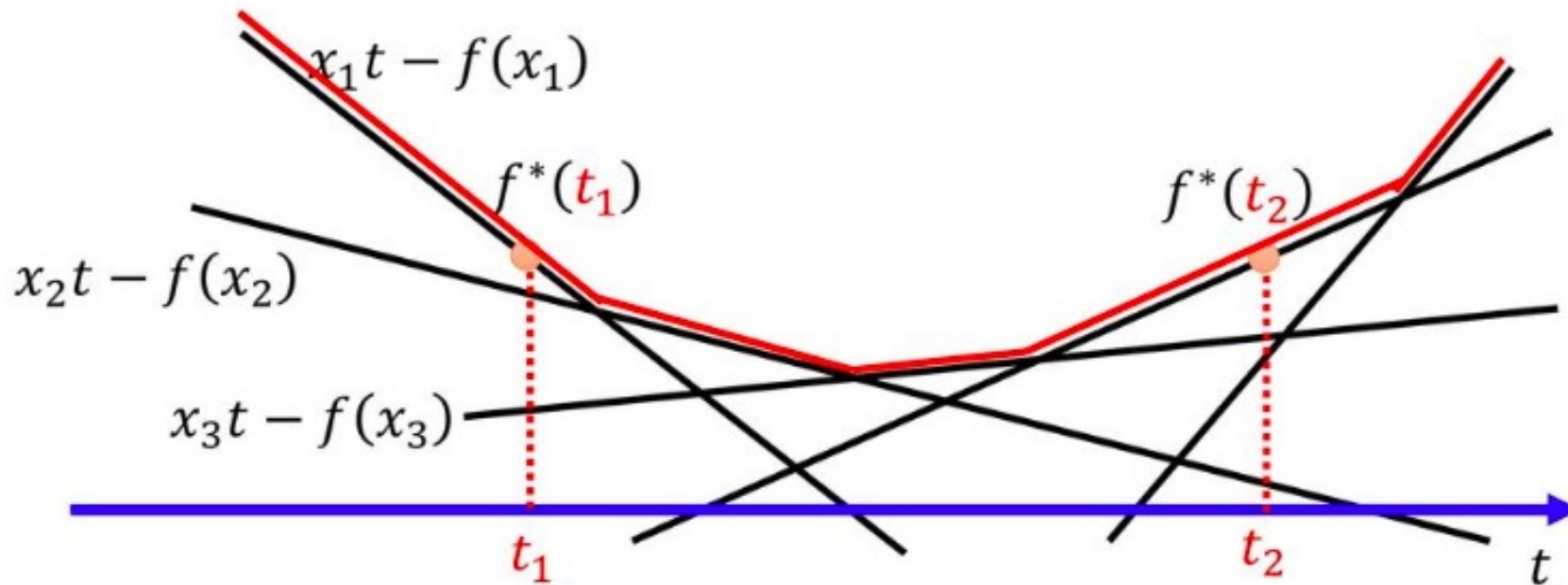


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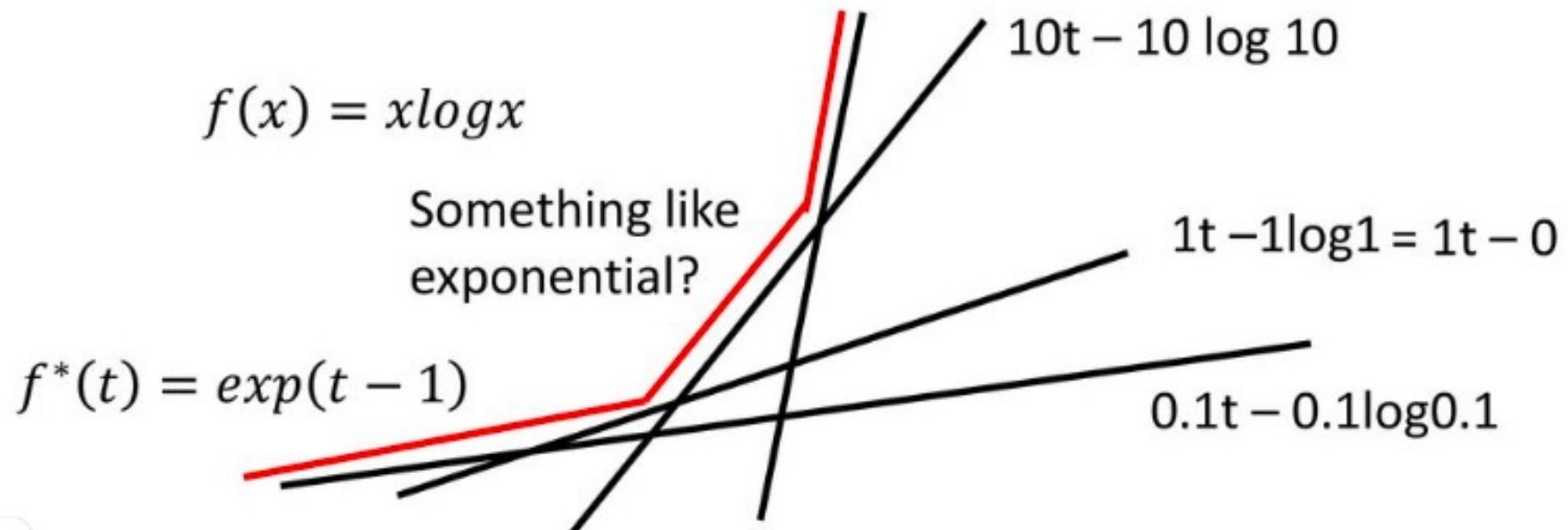


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Fenchel conjugate

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx$$

- ▶ Each generator has a **Fenchel conjugate** function:

$$f^*(t) = \sup_x (xt - f(x))$$

if f is convex, then $(f^*)^* = f$.

$$f(x) = (f^*)^*(x) = \sup_t (xt - f^*(t))$$

$$D_f(P||Q) = \int_{\mathcal{X}} q(x) \sup_{t \in \text{dom}_{f^*}} \left\{ t \frac{p(x)}{q(x)} - f^*(t) \right\} dx$$

$$\geq \sup_{T \in \mathcal{T}} \left(\int_{\mathcal{X}} p(x) T(x) dx - \int_{\mathcal{X}} q(x) f^*(T(x)) dx \right)$$

$$= \sup_{T \in \mathcal{T}} (\mathbb{E}_{x \sim P} [T(x)] - \mathbb{E}_{x \sim Q} [f^*(T(x))]) ,$$

Optimal Variational Function $T(x)$

- ▶ We can choose $T^*(x)$, an optimal variational function, that makes inequality tightest:

$$T^*(x) = f'\left(\frac{p(x)}{q(x)}\right).$$

X. Nguyen et al. Estimating divergence functionals and the likelihood ratio by convex risk minimization

Name	$D_f(P\ Q)$	Generator $f(u)$	$T^*(x)$
Kullback-Leibler	$\int p(x) \log \frac{p(x)}{q(x)} dx$	$u \log u$	$1 + \log \frac{p(x)}{q(x)}$
Reverse KL	$\int q(x) \log \frac{q(x)}{p(x)} dx$	$-\log u$	$-\frac{q(x)}{p(x)}$
Pearson χ^2	$\int \frac{(q(x)-p(x))^2}{p(x)} dx$	$(u-1)^2$	$2\left(\frac{p(x)}{q(x)} - 1\right)$
Squared Hellinger	$\int \left(\sqrt{p(x)} - \sqrt{q(x)}\right)^2 dx$	$(\sqrt{u} - 1)^2$	$\left(\sqrt{\frac{p(x)}{q(x)}} - 1\right) \cdot \sqrt{\frac{q(x)}{p(x)}}$
Jensen-Shannon	$\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} dx$	$-(u+1) \log \frac{1+u}{2} + u \log u$	$\log \frac{2p(x)}{p(x)+q(x)}$

Conclusions

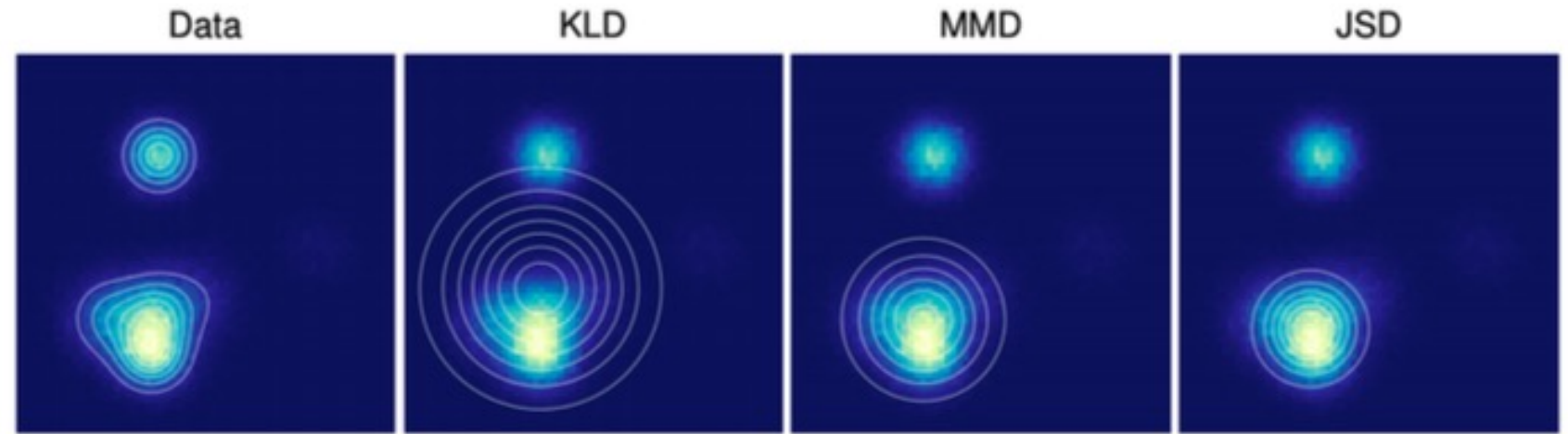


Figure 1: An isotropic Gaussian distribution was fit to data drawn from a mixture of Gaussians by either minimizing Kullback-Leibler divergence (KLD), maximum mean discrepancy (MMD), or Jensen-Shannon divergence (JSD). The different fits demonstrate different tradeoffs made by the three measures of distance between distributions.

Problems:

- ▶ need to use metrics different from optimised;
- ▶ difficulties in case of high dimension problem;
- ▶ not evident choice of a good metric.

<https://arxiv.org/abs/1506.05751>

Conclusions

- ▶ f -divergences quantify dissimilarities between probability densities.
- ▶ Direct optimization of popular divergence requires the knowledge of true function.
- ▶ Special metrics should be developed to quantify quality of generative models (see seminar).