Advances in kernel exponential families

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Outline

Motivating application:

- Fast estimation of complex multivariate densities

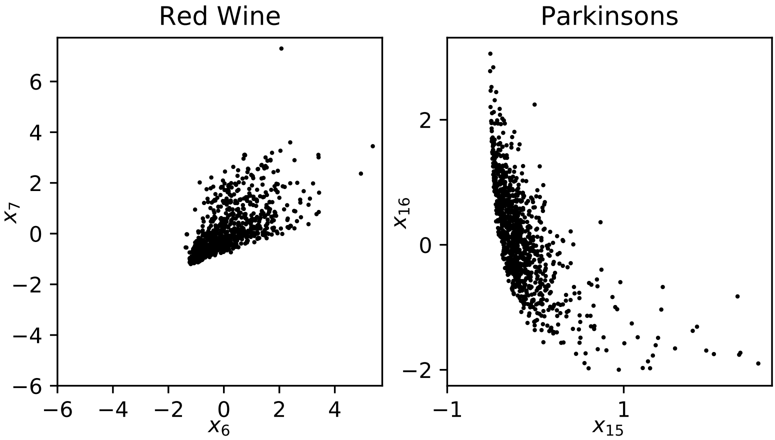
The infinite exponential family:

- Multivariate Gaussian $\rightarrow$ Gaussian process
- Finite mixture model $\rightarrow$ Dirichlet process mixture model
- Finite exponential family $\rightarrow$???

In this talk:

- Guaranteed speed improvements by Nystrom
- Conditional models

Goal: learn high dimensional, complex densities



We want:

- Efficient computation and representation
- Statistical guarantees

The exponential family

The exponential family in in $\mathbb{R}^d$

$$p(x) = \exp\left(\left\langle \underbrace{\eta}_{\substack{\text{natural}\\\text{parameter}}}, \underbrace{T(x)}_{\substack{\text{sufficient}\\\text{startistic}}} \right\rangle - \underbrace{A(\eta)}_{\substack{\text{log}\\\text{normaliser}}} \right) \underbrace{q_0(x)}_{\substack{\text{base}\\\text{measure}}}$$

Examples:

- Gaussian density: $T(x) = \begin{bmatrix} x & x^2 \end{bmatrix}$
- Gamma density: $T(x) = \begin{bmatrix} \ln x & x \end{bmatrix}$

Can we extend this to infinite dimensions?

Infinitely many features using kernels

Kernels: dot products of features

Feature map $\varphi(x) \in \mathcal{H}$,

$$\varphi(x) = [\ldots \varphi_i(x) \ldots] \in \ell_2$$

For positive definite k,

$$\begin{aligned} k(x, x') &= \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}} \\ &= \langle k(x, \cdot), k(x', \cdot) \rangle_{\mathcal{H}} \end{aligned}$$

Infinitely many features $\varphi(x)$, dot product in closed form!

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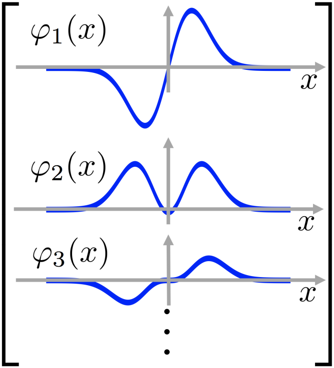
Exponentiated quadratic kernel

$$k(x, x') = \exp\left(-\gamma \left\|x - x'\right\|^2\right)$$

$$\varphi(x) =$$

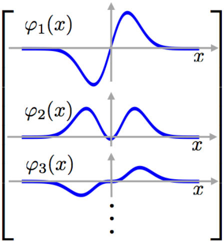


Features: Gaussian Processes for Machine learning, Rasmussen and Williams, Ch. 4.

Functions of infinitely many features

Functions are linear combinations of features:

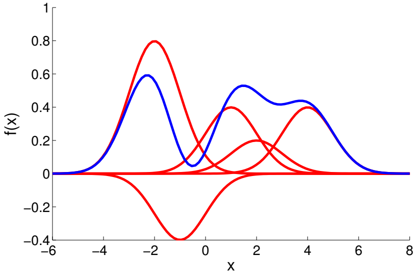
$$f(x) = \langle f, \varphi(x) \rangle_{\mathcal{H}} = \sum_{\ell=1}^{\infty} f_\ell \varphi_\ell(x) = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix}^\top$$



How to represent functions?

Function with exponentiated quadratic kernel:

$$
\begin{aligned}
f(x) :&= \sum_{i=1}^{m} \alpha_i k(x_i, x) \\
&= \sum_{i=1}^{m} \alpha_i \left\langle \varphi(x_i), \varphi(x) \right\rangle_{\mathcal{H}} \\
&= \left\langle \sum_{i=1}^{m} \alpha_i \varphi(x_i), \varphi(x) \right\rangle_{\mathcal{H}} \\
&= \sum_{\ell=1}^{\infty} f_\ell \varphi_\ell(x)
\end{aligned}
$$



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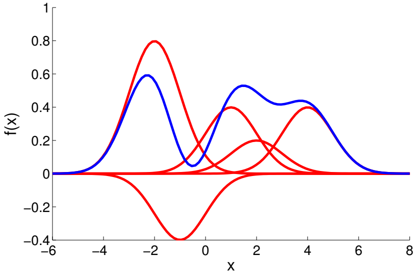

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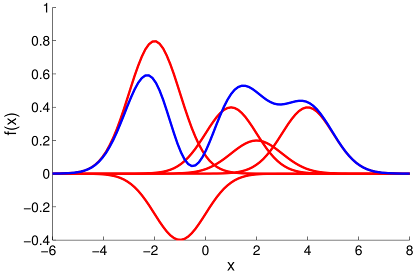

$f_\ell = \sum_{i=1}^{m} \alpha_i \varphi_\ell(x_i)$

The kernel exponential family

Kernel exponential families [Canu and Smola (2006), Fukumizu (2009)] and their GP counterparts [Adams, Murray, MacKay (2009), Rasmussen(2003)]

$$\mathcal{P} = \left\{ p_f(x) = e^{\langle f, \varphi(x) \rangle_{\mathcal{H}} - A(f)} q_0(x), \;\; x \in \Omega, f \in \mathcal{F} \right\}$$

where

$$\mathcal{F} = \left\{ f \in \mathcal{H} \; : \; A(f) = \log \int e^{f(x)} q_0(x) \, dx < \infty \right\}$$

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Finite dimensional RKHS: one-to-one correspondence between finite dimensional exponential family and RKHS.

- Example: Gaussian kernel, $T(x) = \begin{bmatrix} x & x^2 \end{bmatrix} = \varphi(x)$ and $k(x, y) = xy + x^2 y^2$

Fitting an infinite dimensional exponential family

Given random samples, $X_1, \ldots, X_n$ drawn i.i.d. from an unknown density, $p_0 := p_{f_0} \in \mathcal{P}$, estimate p_0

How not to do it: maximum likelihood

Maximum likelihood:

$$f_{ML} = \arg\max_{f\in\mathcal{F}} \sum_{i=1}^{n} \log p_f(X_i)$$
$$= \arg\max_{f\in\mathcal{F}} \sum_{i=1}^{n} f(X_i) - n \log \int e^{f(x)} q_0(x)\, dx.$$

Solving the above yields that f_{ML} satisfies

$$\frac{1}{n}\sum_{i=1}^{n} \varphi(x_i) = \int \varphi(x) p_{f_{ML}}(x)\, dx$$

where $p_{f_{ML}} = \frac{d\mathbb{P}_{\mathrm{ML}}}{dx}$.

Ill posed for infinite dimensional $\varphi(x)$!

Score matching

Journal of Machine Learning Research 6 (2005) 695–708 Submitted 11/04; Revised 3/05; Published 4/05

Estimation of Non-Normalized Statistical Models by Score Matching

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Helsinki Institute for Information Technology (BRU)
Department of Computer Science
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Editor: Peter Dayan

Loss is Fisher Score:

$$D_F(p_0, p_f) := \frac{1}{2} \int p_0(x) \left\| \nabla_x \log p_0(x) - \nabla_x \log p_f(x) \right\|^2 \, dx$$

Score matching (general version)

Assuming p_f to be differentiable (w.r.t. x) and $\int p_0(x) \|\nabla_x \log p_f(x)\|^2 \, dx < \infty, \forall \theta \in \Theta$

$$D_F(p_0, p_f) := \frac{1}{2} \int p_0(x) \, \|\nabla_x \log p_0(x) - \nabla_x \log p_f(x)\|^2 \, dx$$

$$\overset{(a)}{=} \int p_0(x) \sum_{i=1}^{d} \left(\frac{1}{2} \left(\frac{\partial \log p_f(x)}{\partial x_i} \right)^2 + \frac{\partial^2 \log p_f(x)}{\partial x_i^2} \right) \, dx$$

$$+ \frac{1}{2} \int p_0(x) \left\| \frac{\partial \log p_0(x)}{\partial x} \right\|^2 \, dx$$

where partial integration is used in (a) under the condition that

$$p_0(x) \frac{\partial \log p_f(x)}{\partial x_i} \to 0 \text{ as } x_i \to \pm\infty, \; \forall \, i = 1, \ldots, d$$

Empirical score matching

p_n represents n i.i.d. samples from P_0

$$D_F(p_n, p_f) := \frac{1}{n} \sum_{a=1}^{n} \sum_{i=1}^{d} \left(\frac{1}{2} \left(\frac{\partial \log p_f(X_a)}{\partial x_i} \right)^2 + \frac{\partial^2 \log p_f(X_a)}{\partial x_i^2} \right) + C$$

Since $D_F(p_n, p_f)$ is independent of $A(f)$,

$$f_n^* = \arg\min_{f \in \mathcal{F}} D_F(p_n, p_f)$$

should be easily computable, unlike the MLE.

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Add extra term $\lambda\|f\|_{\mathcal{H}}^2$ to regularize.

A kernel solution

Infinite exponential family:

$$p_f(x) = e^{\langle f, \varphi(x) \rangle_{\mathcal{H}} - A(f)} q_0(x)$$

Thus

$$\frac{\partial}{\partial x} \log p_f(x) = \frac{\partial}{\partial x} \langle f, \varphi(x) \rangle_{\mathcal{H}} + \frac{\partial}{\partial x} \log q_0(x).$$

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Kernel trick for derivatives:

$$\frac{\partial}{\partial x_i} f(X) = \left\langle f, \frac{\partial}{\partial x_i} \varphi(X) \right\rangle_{\mathcal{H}}$$

Dot product between feature derivatives:

$$\left\langle \frac{\partial}{\partial x_i} \varphi(X), \frac{\partial}{\partial x_j} \varphi(X') \right\rangle_{\mathcal{H}} = \frac{\partial^2}{\partial x_i \partial x_{d+j}} k(X, X')$$

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By representer theorem:

$$f_n^* = \alpha \hat{\xi} + \sum_{\ell=1}^{n} \sum_{j=1}^{d} \beta_{\ell j} \frac{\partial \varphi(X_\ell)}{\partial x_j}$$

An RKHS solution

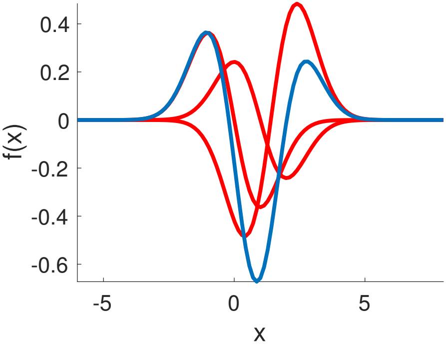
The RKHS solution

$$f_n^* = \alpha\hat{\xi} + \sum_{\ell=1}^{n}\sum_{j=1}^{d}\beta_{\ell j}\frac{\partial\varphi(X_\ell)}{\partial x_j}$$

Need to solve a linear system

$$\beta_n^* = -\frac{1}{\lambda}\left(\underbrace{G_{XX}}_{nd\times nd} + n\lambda I\right)^{-1} h_X$$

Very costly in high dimensions!



The Nystrom approximation

Nystrom approach for efficient solution

- Find best estimator $f^*_{n,m}$ in $\mathcal{H}_Y := \text{span}\{\partial_i k(y_a, \cdot)\}_{a \in [m], i \in [d]}$, where $y_a \in \{x_i\}_{i=1}^n$ chosen at random.
- Nystrom solution:

$$\beta^*_{n,m} = -\left(\frac{1}{n} B_{XY}^\top \underbrace{B_{XY}}_{md \times nd} + \lambda \underbrace{G_{YY}}_{md \times md}\right)^\dagger h_Y$$

Solve in time $\mathcal{O}(nm^2 d^3)$, evaluate in time $\mathcal{O}(md)$.

- Sill cubic in d, but similar results if we take a random dimension per datapoint.

Consistency: original solution

Define C as the covariance between feature derivatives. Then from

[Sriperumbudur et al. JMLR (2017)]

- Rates of convergence: Suppose
  - $f_0 \in \mathcal{R}(C^\beta)$ for some $\beta > 0$.
  - $\lambda = n^{-\max\left\{\frac{1}{3}, \frac{1}{2(\beta+1)}\right\}}$ as $n \to \infty$.

Then

$$D_F(p_0, p_{f_n}) = O_{p_0}\left(n^{-\min\left\{\frac{2}{3}, \frac{\beta}{2(\beta+1)}\right\}}\right)$$

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- Convergence in other metrics: KL, Hellinger, $L_r, 1 < r < \infty$.

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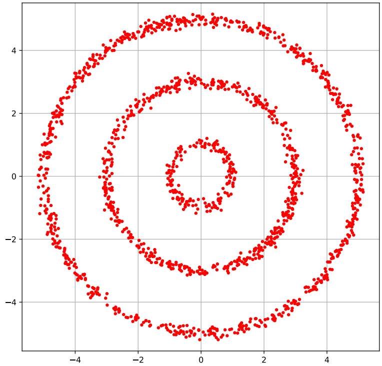
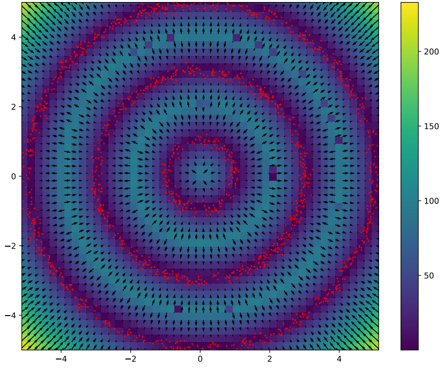
- Convergence in other metrics: KL, Hellinger, $L_r, 1 < r < \infty$. Same rate but saturates sooner.
  - Full KL original saturates at $O_{p_0}\left(n^{-\frac{1}{2}}\right)$
  - Nystrom saturates at $O_{p_0}\left(n^{-\frac{1}{3}}\right)$

Experimental results: ring

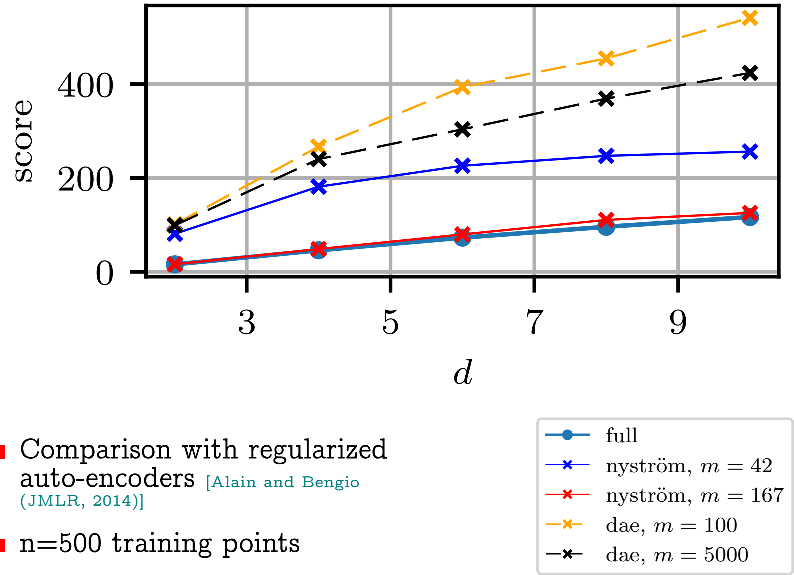
Sample:



Score:



Experimental results: comparison with autoencoder



- Comparison with regularized auto-encoders [Alain and Bengio (JMLR, 2014)]
- n=500 training points

Experimental results: grid of Gaussians

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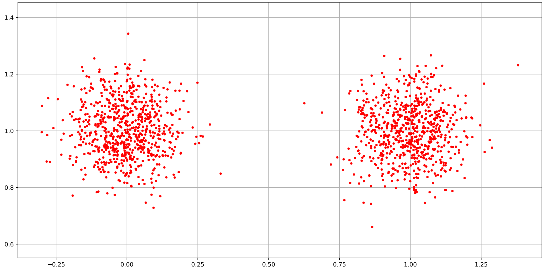

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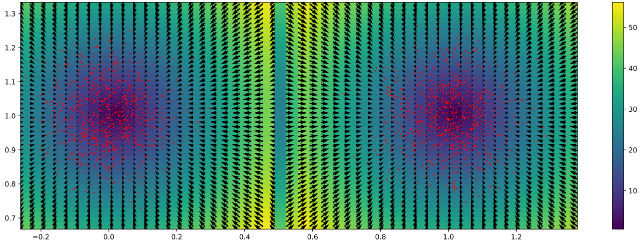

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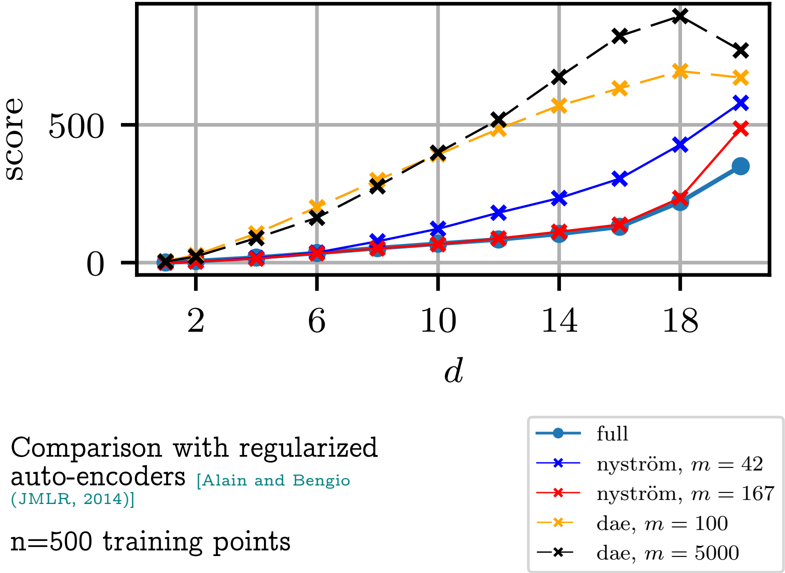

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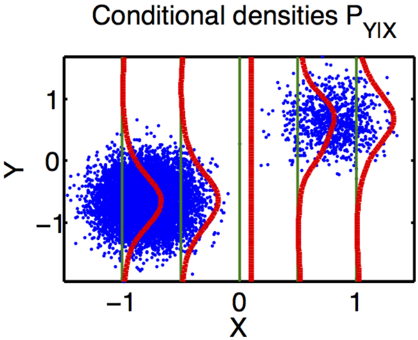
The kernel conditional exponential family

The kernel conditional exponential family

- Can we take advantage of the graphical structure of $(X_1, ..., X_d)$?
- Start from a general factorization of P

$$P(X_1, ..., X_d) = \prod_i P(X_i | \underbrace{X_{\pi(i)}}_{\text{parents of } X_i})$$



- Estimate each factor independently

Kernel conditional exponential family

General definition, kernel conditional exponential family

[Smola and Canu, 2006]

$$p_f(y|x) = e^{\langle f, \psi(x,y) \rangle_{\mathcal{H}} - A(f,x)} q_0(y) \qquad A(f,x) = \log \int q_o(y) e^{\langle f, \psi(x,y) \rangle_{\mathcal{H}}} dy$$

(joint feature map $\psi(x, y)$)

Kernel conditional exponential family

Our kernel conditional exponential family:

$$p_f(x) = e^{\langle f_x, \phi(y) \rangle_{\mathcal{G}} - A(f,x)} q_0(y) \qquad A(f,x) = \log \int q_o(y) e^{\langle f_x, \phi(y) \rangle_{\mathcal{G}}}$$

linear in the sufficient statistic $\phi(y) \in \mathcal{G}$.

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What does this RKHS look like?

[Micchelli and Pontil, (2005)]

$$\begin{aligned} &\langle f_x, \phi(y) \rangle_{\mathcal{G}} \\ &= \langle \Gamma_x^* f, \phi(y) \rangle_{\mathcal{G}} \\ &= \langle f, \Gamma_x \phi(y) \rangle_{\mathcal{H}} \end{aligned}$$

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- $\Gamma_x : \mathcal{G} \to \mathcal{H}$ is a linear operator.
- The feature map $\psi(x,y) := \Gamma_x \phi(y)$

What is our loss function?

The obvious approach: minimise

$$D_F\left[p_0(x)p_0(y|x) \| p_f(x)p_f(y|x)\right]$$

Problem: the expression still contains $\int p_0(y|x)\,dy$.

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Our loss function:

$$\widetilde{D}_F(p_0, p_f) := \int D_F(p_0(y|x)||p_f(y|x))\pi(x)dx$$

for some $\pi(x)$ that includes the support of $p(x)$.

Finite sample estimate of the conditional density

Use the simplest operator-valued RKHS $\Gamma_x = I_{\mathcal{G}} k(x, \cdot)$.

$$\begin{aligned} \Gamma_x &: \mathcal{G} \to \mathcal{H} \\ \Gamma_x \phi(y) &\mapsto \phi(y) k(x, \cdot) \end{aligned}$$

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Solution:

$$f_n^*(y|x) = \sum_{b=1}^{n} \sum_{i=1}^{d} \beta_{(b,i)} k(X_b, x) \partial_i \mathfrak{K}(Y_b, y) + \alpha \hat{\xi}$$

where

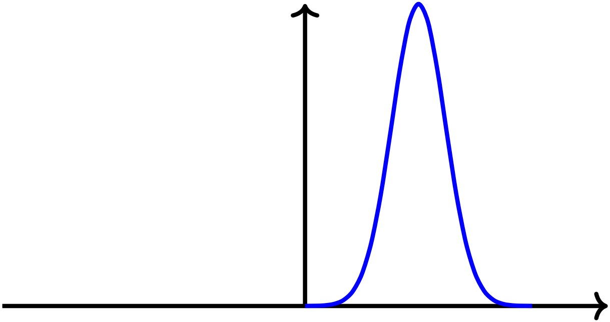
$$\beta_n^* = -\frac{1}{\lambda} (G + n\lambda I)^{-1} h$$

$$(G)_{(a,i),(b,j)} = k(X_a, X_b) \partial_i \partial_{j+d} \mathfrak{K}(Y_a, Y_b),$$

and $\langle \phi(y), \phi(y') \rangle_{\mathcal{G}} = \mathfrak{K}(y, y')$.

Expected conditional score: a failure case

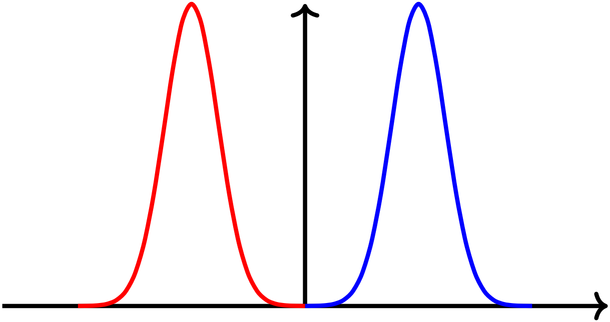
- $P(Y|X=1)$
- $P(Y|X=-1)$
- $P(Y) = \frac{1}{2}(P(Y|X=1) + P(Y|X=-1))$



$$\widetilde{D}_F(\underbrace{p(y|x)}_{\text{target}}, \underbrace{p(y)}_{\text{model}}) = 0$$

Expected conditional score: a failure case

- $P(Y|X=1)$
- $P(Y|X=-1)$
- $P(Y) = \frac{1}{2}(P(Y|X=1) + P(Y|X=-1))$



$$\widetilde{D}_F(\underbrace{p(y|x)}_{\text{target}}, \underbrace{p(y)}_{\text{model}}) = 0$$

Expected conditional score: a failure case

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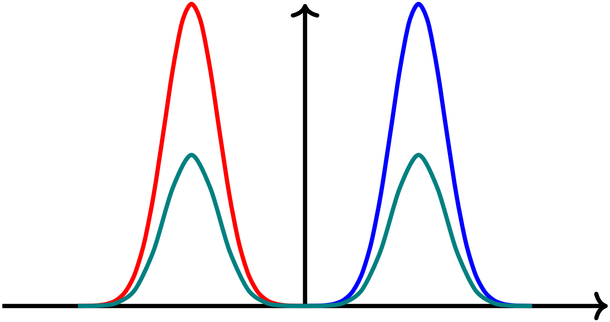

$$\widetilde{D}_F(\underbrace{p(y|x)}_{\text{target}}, \underbrace{p(y)}_{\text{model}}) = 0$$

Expected conditional score: a failure case

- $P(Y|X=1)$
- $P(Y|X=-1)$
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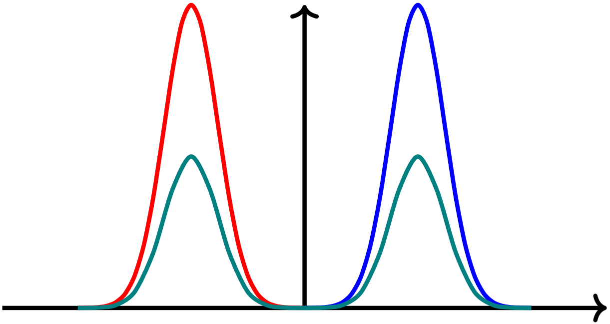

$$\widetilde{D}_F(\underbrace{p(y|x)}_{\text{target}}, \underbrace{p(y)}_{\text{model}}) = 0$$

Expected conditional score: a failure case

Why does it fail? Recall

$$\widetilde{D}_F(p_0(y|x), p_f(y|x)) := \int \pi(x) D_F(p_0(y|x), p_f(y|x)) dx$$

Note that

$$D_F(\underbrace{p(y|x=1)}_{\text{target}}, \underbrace{p(y)}_{\text{model}}) = \int p(y|1) \left\| \nabla_x \log p(y|1) - \nabla_x \log p(y) \right\|^2 \, dy$$

Model $p(y)$ puts mass where target conditional $p(y|1)$ has no support.

- Care needed when this failure mode approached!

Unconditional vs conditional model in practice

- Red Wine: Physiochemical measurements on wine samples.
- Parkinsons: Biomedical voice measurements from patients with early stage Parkinson's disease.

	Parkinsons	Red Wine
Dimension	15	11
Samples	5875	1599

Unconditional vs conditional model in practice

- Red Wine: Physiochemical measurements on wine samples.
- Parkinsons: Biomedical voice measurements from patients with early stage Parkinson's disease.

Comparison with

- LSCDE model: with consistency guarantees [Sugiyama et al., (2010)]
- RNADE model: mixture models with deep features of parents, no guarantees [Uria et al. (2016)]

Unconditional vs conditional model in practice

- Red Wine: Physiochemical measurements on wine samples.
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Comparison with

- LSCDE model: with consistency guarantees [Sugiyama et al., (2010)]
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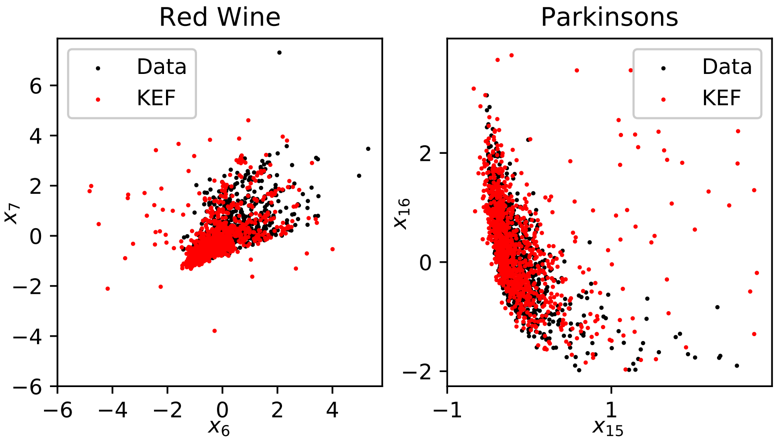
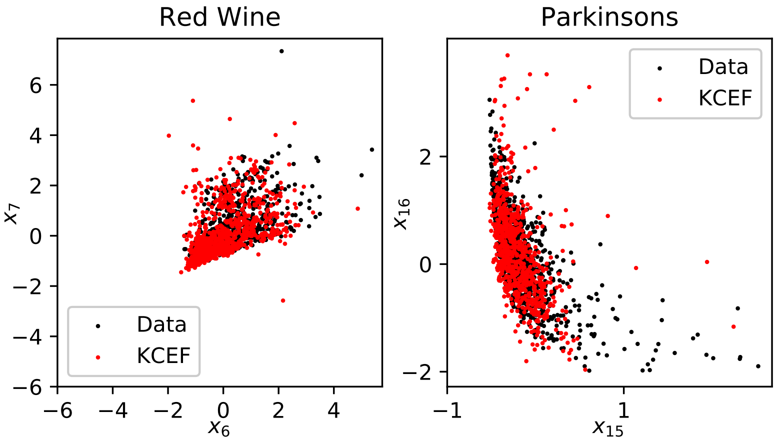
Negative log likelihoods (smaller is better, average over 5 test/train splits)

	Parkinsons	Red wine
KCEF	$\mathbf{2.86 \pm 0.77}$	11.8 ± 0.93
LSCDE	15.89 ± 1.48	14.43 ± 1.5
NADE	3.63 ± 0.0	$\mathbf{9.98 \pm 0.0}$

Results: unconditional model



Results: conditional model



Co-authors

From Gatsby:

- Michael Arbel
- Heiko Strathmann
- Dougal Sutherland

External collaborators:

- Kenji Fukumizu
- Bharath Sriperumbudur

Questions?

Score matching: 1-D proof

$$
\begin{aligned}
&D_F(p_0, p_f) \\
&= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx} - \frac{d\log p_f(x)}{dx}\right)^2 dx
\end{aligned}
$$

Score matching: 1-D proof

$$
\begin{aligned}
&D_F(p_0, p_f) \\
&= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx} - \frac{d\log p_f(x)}{dx}\right)^2 dx \\
&= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx}\right)^2 dx + \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)^2 dx \\
&\quad - \int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx
\end{aligned}
$$

Score matching: 1-D proof

$$D_F(p_0, p_f)$$

$$= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx} - \frac{d\log p_f(x)}{dx}\right)^2 dx$$

$$= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx}\right)^2 dx + \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)^2 dx$$

$$-\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx$$

Final term:

$$\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx$$

$$= \int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{1}{p_0(x)}\frac{dp_0(x)}{dx}\right) dx$$

$$= \left[\left(\frac{d\log p_f(x)}{dx}\right) p_0(x)\right]_a^b - \int_a^b p_0(x)\frac{d^2\log p_f(x)}{dx^2}.$$

Score matching: 1-D proof

$$D_F(p_0, p_f)$$

$$= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx} - \frac{d\log p_f(x)}{dx}\right)^2 dx$$

$$= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx}\right)^2 dx + \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)^2 dx$$

$$- \int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx$$

Final term:

$$\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx$$

$$= \int_a^b \cancel{p_0(x)}\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{1}{\cancel{p_0(x)}}\frac{dp_0(x)}{dx}\right) dx$$

$$= \left[\left(\frac{d\log p_f(x)}{dx}\right)p_0(x)\right]_a^b - \int_a^b p_0(x)\frac{d^2\log p_f(x)}{dx^2}.$$

Score matching: 1-D proof

$$
\begin{aligned}
&D_F(p_0, p_f) \\
&= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx} - \frac{d\log p_f(x)}{dx}\right)^2 dx \\
&= \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_0(x)}{dx}\right)^2 dx + \frac{1}{2}\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)^2 dx \\
&\quad - \int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx
\end{aligned}
$$

Final term:

$$
\begin{aligned}
&\int_a^b p_0(x)\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{d\log p_0(x)}{dx}\right) dx \\
&= \int_a^b \cancel{p_0(x)}\left(\frac{d\log p_f(x)}{dx}\right)\left(\frac{1}{\cancel{p_0(x)}}\frac{dp_0(x)}{dx}\right) dx \\
&= \left[\left(\frac{d\log p_f(x)}{dx}\right)p_0(x)\right]_a^b - \int_a^b p_0(x)\frac{d^2\log p_f(x)}{dx^2}.
\end{aligned}
$$