Uncertainty Quantification and Data Fusion

Johannes O. Royset
Visiting Professor, Mathematics, University of California, Davis
Associate Professor, OR, Naval Postgraduate School, Monterey

with R. Wets (Mathematics, UC Davis)

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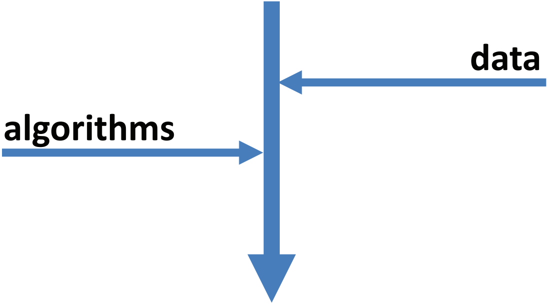
Components of deterministic optimization practice

modeling

- objective function
- constraints

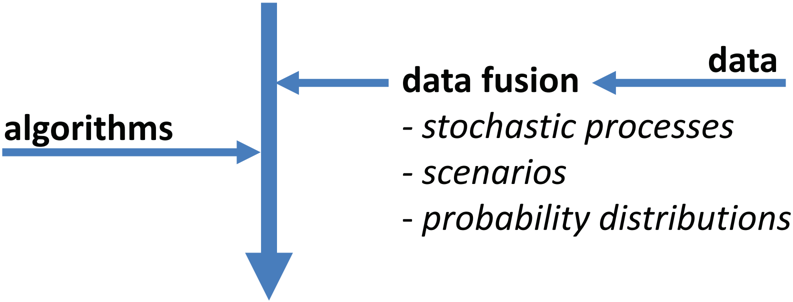


solutions (with guarantees)
recommended decisions

Components of stochastic optimization practice

modeling

- objective and constraint functions
- *decision stages, uncertainty model*



solutions (with guarantees)

recommended decisions

Components of stochastic optimization practice

modeling

- objective and constraint functions
- *decision stages, uncertainty model*

algorithms

data fusion

- *stochastic processes*
- *scenarios*
- *probability densities*

data

solutions (with guarantees)

recommended decisions

Example: 100 observations of demand

Possibilities: Use the 100 scenarios; fit to assumed parametric form; Bayesian update; nonparametric estimation

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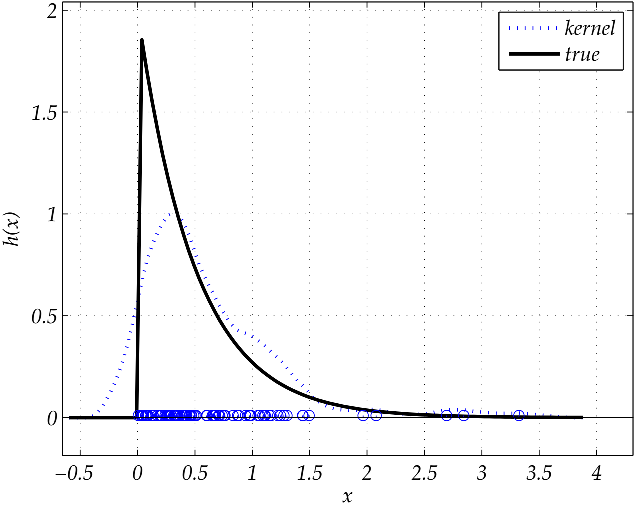
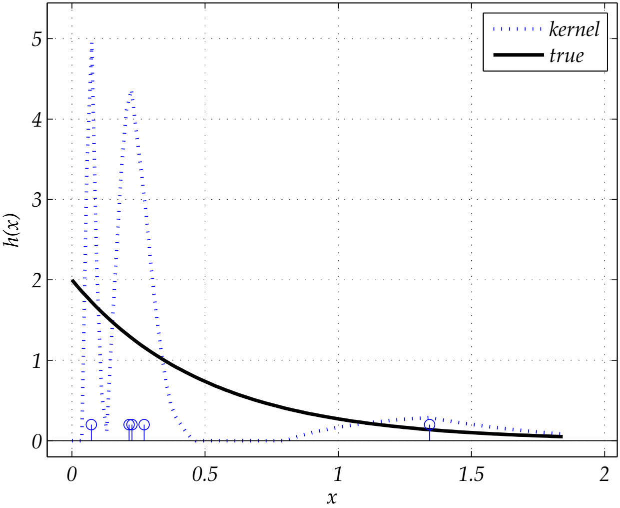


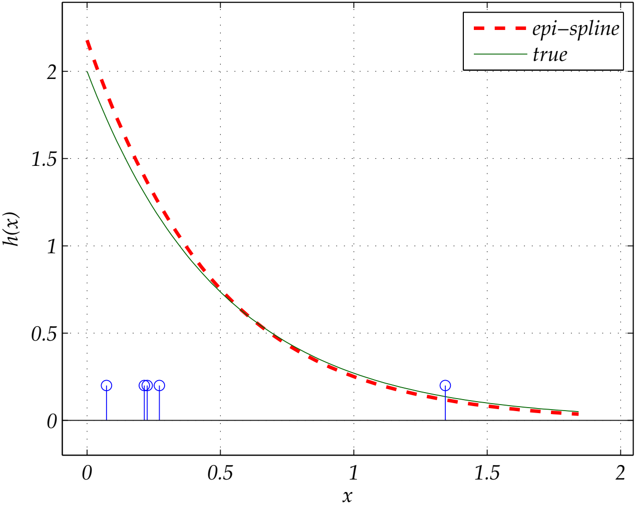
...but with only 5 observations



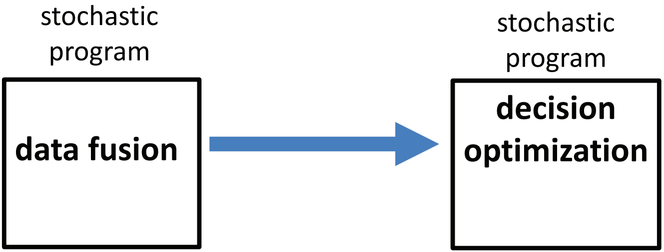
Almost always soft information available

Use stochastic programming!

Same 5 points, but with epi-splines and soft info. (nonnegativity, continuous differentiable, and decreasing)



Two roles for stochastic programming



Independent value in data fusion and uncertainty quant.

Engineering, biological, physical systems

- Input: random V ("known" distribution)
- System function G; implicitly defined e.g. by simulation
- Output: random variable

$$X = G(V)$$

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$$X = G(V)$$

Given observations (data) $x^1 = G(v^1), ..., x^\nu = G(v^\nu)$, we seek a description of X:

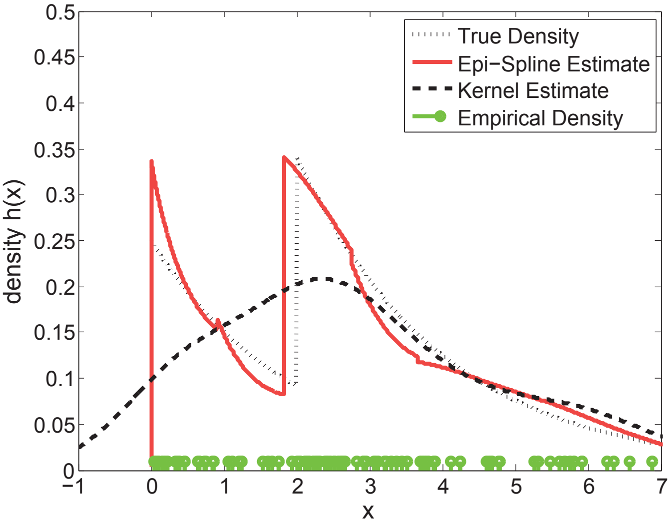
- mean, standard deviation
- quantile, superquantile
- distribution, density (pdf)

Main challenge: few data points; little relevant data
But soft information might be available

Example: M/M/1; 50% of customers delayed for fixed time

X = customer time-in-service; 100 observations

Soft info: lsc, $X \geq 0$, pointwise Fisher, unimodal upper tail



Outline

- Density estimation as a stochastic program
- Epi-splines: pliable approximation tools
- Consistency and asymptotics
- Fusion of hard and soft information
- Numerical examples

Formulation of density estimation problem

Kullback-Leibler divergence from density h to density g on $\boldsymbol{R}$

$$d_{KL}(h||g) = \int_{-\infty}^{\infty} h(x) \log \frac{h(x)}{g(x)} dx$$

Facts:

$$d_{KL}(h||g) \geq 0 \text{ for all densities } h, g$$

$$d_{KL}(h||g) = 0 \iff h(x) = g(x) \text{ (Lebesgue) almost every } x \in \boldsymbol{R}$$

Formulation (cont.)

Consequently, for density $h^0 \in \mathcal{H}$:
If

$$\begin{aligned} \tilde{h} \in \operatorname*{argmin}_h d_{KL}(h^0 || h) & \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x)dx &= 1 \\ h &\geq 0 \\ h &\in \mathcal{H} \end{aligned}$$

then

$$\tilde{h} = h^0 \text{ a.e.}$$

Formulation (cont.)

Let X^0 be a random variable with density h^0

Then,

$$d_{KL}(h^0||h) = \int_{-\infty}^{\infty} h^0(x) \log \frac{h^0(x)}{h(x)} dx = E\{\log h^0(X^0)\} - E\{\log h(X^0)\}$$

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So minimizing $d_{KL}(h^0||h)$ is equivalent to

$$\begin{aligned} \tilde{h} \in \underset{h}{\operatorname{argmax}}\, & E\{\log h(X^0)\} \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x)dx &= 1 \\ h &\geq 0, \; h \in \mathcal{H} \end{aligned}$$

Of course, expectation is with respect to the true distribution

Formulation (cont.)

Data (sample) $X^1, X^2, ..., X^\nu$ available

$$\begin{aligned} h^\nu \in \operatorname*{argmax}_h \frac{1}{\nu}\sum_{i=1}^{\nu} \log h(X^i) &= \log\left(\prod_{i=1}^{\nu} h(X^i)\right)^{1/\nu} \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x)dx &= 1 \\ h &\geq 0,\ h \in \mathcal{H} \end{aligned}$$

Formulation (cont.)

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approximates

$$\begin{array}{rcl} \tilde{h} \in \operatorname*{argmax}_h E\{\log h(X^0)\} & & \\ \text{s.t.} \qquad \int_{-\infty}^{\infty} h(x)dx & = & 1 \\ h & \geq & 0, \;\; h \in \mathcal{H} \end{array}$$

Approximation is a max log-likelihood problem

Incorporating soft information

$$\begin{aligned} h^\nu \in \operatorname*{argmax}_h \frac{1}{\nu}\sum_{i=1}^{\nu} \log h(X^i) &= \log\left(\prod_{i=1}^{\nu} h(X^i)\right)^{1/\nu} \\ \text{s.t.} \qquad \int_{-\infty}^{\infty} h(x)dx &= 1 \\ h &\geq 0,\ h \in H^\nu \subset \mathcal{H} \end{aligned}$$

where H^ν includes essentially any soft information about h^0:

- support bounds
- density continuity, smoothness
- density shape (unimodal, decreasing, etc.)
- moments
- proximity to known density
- system knowledge (convex G, gradient of G)

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Challenge: infinite-dimensional problems

$$
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\text{s.t.} \qquad \int_{-\infty}^{\infty} h(x)dx &= 1 \\
h &\geq 0,\ h \in H^\nu \subset \mathcal{H}
\end{aligned}
$$

Need approximation of $\mathcal{H}$ by set of flexible functions given by finite number of parameters

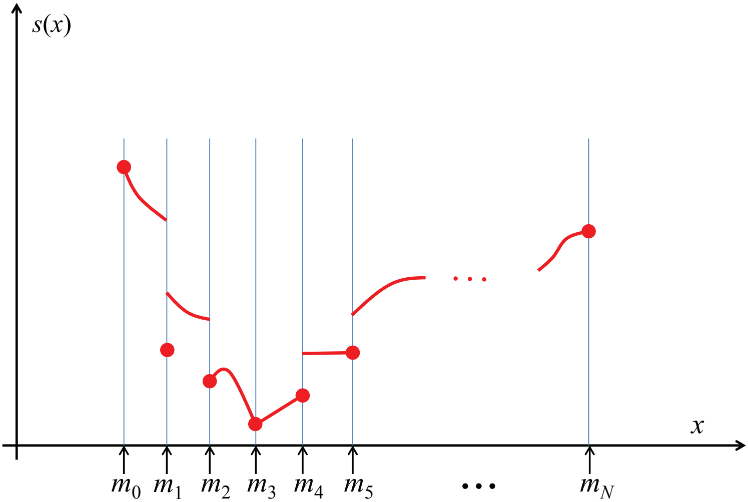
Exponential epi-spline estimator

Given sample $X^1, ..., X^\nu$, the exponential epi-spline estimator of the true density is

$$h^\nu = e^{-s^\nu},$$

where s^ν is an epi-spline

Epi-splines: piecewise polynomial functions



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Main features:

- finite number of parameters; powerful optimization technology available
- approximates to arbitrary accuracy essentially any function
- easily includes soft information
- substantially more flexible and pliable than 'classical' splines
- nonnegativity achieved automatically

Epi-splines

- *Number of partitions N*
- *Mesh* $m = \{m_k\}_{k=0}^{N}$, where $m_{k-1} < m_k,\ k = 1, 2, ..., N$
- Estimation on $[m_0, m_N]$
- *Order p*

Epi-splines

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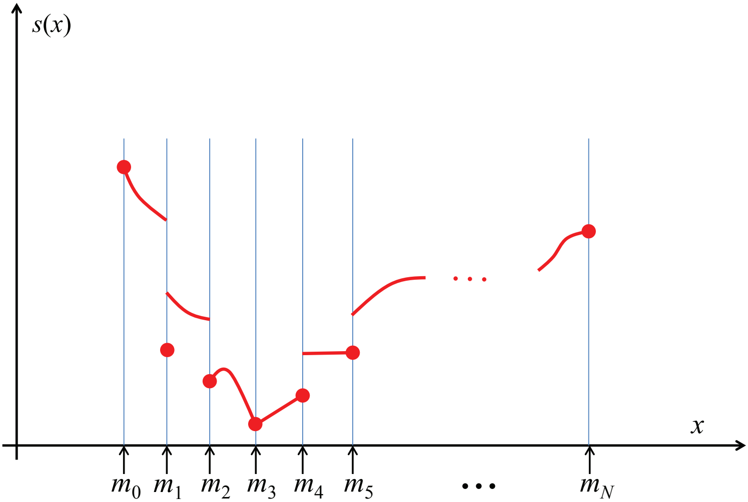
Definition

$\text{e-spl}^p(m)$= family of (basic) epi-splines of order p, with mesh $m = \{m_k\}_{k=0}^N$, consists of:

- functions $s : [m_0, m_N] \to \boldsymbol{R}$
- that are polynomials of degree p in each segment (m_{k-1}, m_k), $k = 1, 2, ..., N$, and
- that are finite valued at m_0, m_1, ..., m_N

Representation of epi-spline



Representation of epi-spline

Every $s \in \mathrm{e\text{-}spl}^p(m)$, with $m = \{m_k\}_{k=0}^N$, is uniquely represented by

$$r = (s_0, s_1, ..., s_N, a_1, a_2, ..., a_N), \quad s_k \in \boldsymbol{R}, \ a_k \in \boldsymbol{R}^{p+1},$$

such that

$$s(x) = \langle c(x), r \rangle, \quad x \in [m_0, m_N],$$

where

$$c(x) = \begin{cases} (0, ..., 0, 1, x - m_{k-1}, \ ..., & (x - m_{k-1})^p, 0, ..., 0) \\ & \text{if } x \in (m_{k-1}, m_k), k = 1, ..., N \\ (0, ..., 0, 1, 0, ..., 0) & \text{if } x = m_k, k = 0, 1, ..., N. \end{cases}$$

Approximation of functions by epi-splines

$\text{lsc-fcns}([l, u]) =$
lower semicontinuous functions (lsc) on $[l, u]$ not $\not\equiv \infty$

Adopt metric topology induced by the epi-distance

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Adopt metric topology induced by the epi-distance

Need to allow for

- jumps (discontinuous densities)
- infinity (due to e^{-s})
- pointwise constraints (soft information)
- mixtures with probability mass functions
- subsequent maximization of densities (find modes)

Epi-distance

point-to-set distance $= d(x, S) = \inf_{y \in S} \|x - y\|$ for $S \subset \boldsymbol{R}^2$

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epi-graph of $f = \mathrm{epi}\ f = \{(x, \beta) \in \boldsymbol{R}^2 \mid f(x) \leq \beta\}$

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epi-graph of $f = \mathrm{epi}\ f = \{(x,\beta) \in \boldsymbol{R}^2 \mid f(x) \le \beta\}$

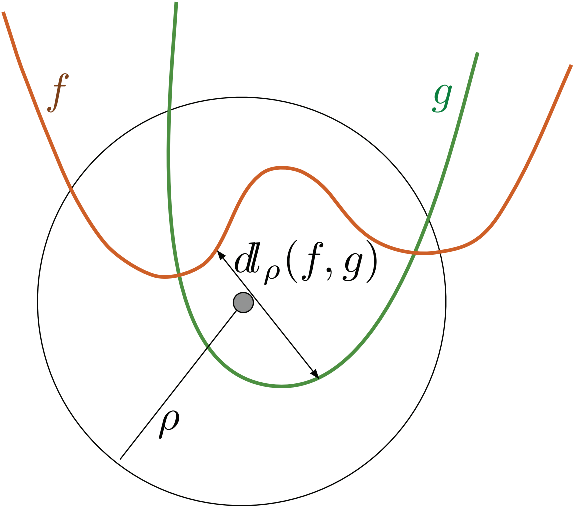
$$\text{Epi-distance } = dl(f,g) = \int_0^\infty dl_\rho(f,g)e^{-\rho}d\rho$$

where for $\rho \ge 0$

$$dl_\rho(f,g) = \max_{\|x\|\le\rho} |d(x,\mathrm{epi}\ f) - d(x,\mathrm{epi}\ g)|$$

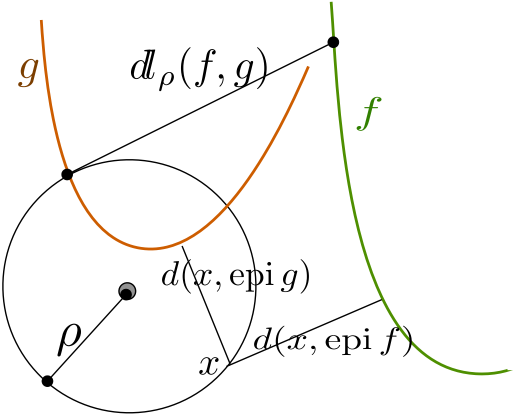
Epi-distance (cont.)

$$d\!l_\rho(f, g) = \max_{\|x\| \le \rho} |d(x, \mathrm{epi}\ f) - d(x, \mathrm{epi}\ g)|$$



Epi-distance (cont.)

$$dl_\rho(f,g) = \max_{\|x\|\leq\rho} |d(x, \text{epi } f) - d(x, \text{epi } g)|$$



Characterization of convergence

For any $\bar{\rho} \geq 0$:

$$dl(f^\nu, f) \to 0 \iff dl_\rho(f^\nu, f) \to 0 \text{ for all } \rho \geq \bar{\rho}$$

$(\text{lsc-fcns}([l, u]), dl)$ complete separable metric space

Convergence of exponential epi-splines

exponential epi-splines $= \text{x-spl}^p(m) = \{e^{-s} \mid s \in \text{e-spl}^p(m)\}$
hypo-distance $dl_{\text{hypo}}(f, g) = dl(-f, -g)$

$h^\nu, h^0 \in \text{x-spl}^p(m)$, $h^\nu = e^{-s^\nu} = e^{-\langle c(\cdot), r^\nu \rangle}$, $h^0 = e^{-s^0} = e^{-\langle c(\cdot), r^0 \rangle}$
Then, the following hold:

$$r^\nu \to r^0 \Longleftrightarrow h^\nu \to h^0 \text{ uniformly on } [m_0, m_N]$$
$$\Longrightarrow dl_{\text{hypo}}(h^\nu, h^0) \to 0 \Longleftrightarrow dl(s^\nu, s^0) \to 0$$

Moreover, if h^ν, h^0 are usc, then also

$$h^\nu \to h^0 \text{ uniformly on } [m_0, m_N] \Longleftarrow dl_{\text{hypo}}(h^\nu, h^0) \to 0$$

Properties of (exponential) epi-splines

If $\{m^\nu\}_{\nu=1}^\infty$ are refining meshes, then

- lsc $\{\text{e-spl}^p(m^\nu)\}_{\nu=1}^\infty$ dense in $\text{lsc-fcns}([l,u])$
- usc $\{\text{x-spl}^p(m^\nu)\}_{\nu=1}^\infty$ dense in $\{e^{-s} \mid s \in \text{lsc-fcns}([l,u])\}$

Examples

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Examples

- most densities approximated to arbitrary accuracy
- normal density represented by $\text{e-spl}^2(m)$ on $[m_0, m_N]$ for any m
- exponential density represented by $\text{e-spl}^1(m)$ on $[m_0, m_N]$ for any choice of m with $m_0 = 0$
- lognormal and Pareto also exactly represented after transformation

Recall: maximize log-likelihood

$$
\begin{aligned}
h^{\nu} \in \operatorname*{argmax}_{h} \frac{1}{\nu} \sum_{i=1}^{\nu} \log h(X^i) \\
\text{s.t.} \qquad \int_{-\infty}^{\infty} h(x)dx &= 1 \\
h &\geq 0 \\
h &\in H^{\nu} \subset \mathcal{H}
\end{aligned}
$$

Now $h = e^{-\langle c(\cdot), r \rangle}$ and optimize over $r \in \boldsymbol{R}^{(p+2)N+1}$ instead

Resulting optimization problem

$$
\begin{aligned}
&\min_r \frac{1}{\nu}\sum_{i=1}^{\nu}\langle c(X^i), r\rangle \\
\text{s.t.} \quad &\int_{m_0}^{m_N} e^{-\langle c(x),r\rangle}\,dx \;=\; 1 \\
&r \in R^\nu \;=\; \left\{ r \in \boldsymbol{R}^{(p+2)N+1} \;\middle|\; e^{-\langle c(\cdot),r\rangle} \in H^\nu \right\}
\end{aligned}
$$

R^ν often convex; $\leq$ often replaces $=$

$\Longrightarrow$ convex problem

Estimator unique under additional assumptions

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- Density estimation as a stochastic program
- Epi-splines: pliable approximation tools
- Consistency and asymptotics
- Fusion of hard and soft information
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Consistency

Kullback-Leibler projection of density h on $\text{e-spl}^p(m)$ is the set

$$\mathcal{P}_{p,m}(h) = \underset{s \in \text{e-spl}^p(m)}{\text{argmin}} \, d_{KL}(h || e^{-s}) \text{ s.t. } \int_{m_0}^{m_N} e^{-s(x)} dx = 1$$

$\mathcal{P}^S_{p,m}(h)$ = KL-projection relative to $S \subset \text{e-spl}^p(m)$

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$\mathcal{P}^S_{p,m}(h)$ = KL-projection relative to $S \subset \text{e-spl}^p(m)$

$$P^\nu_{p,m}: \quad s^\nu \in \underset{s \in S^\nu}{\text{argmin}} \frac{1}{\nu} \sum_{i=1}^{\nu} s(X^i) \;\; \text{s.t.} \quad \int_{m_0}^{m_N} e^{-s(x)} dx = 1$$

$$S^\nu = \left\{ s \in \text{e-spl}^p(m) \;\middle|\; e^{-s} \in H^\nu \right\}$$

Consistency (cont.)

True density $h^0 = e^{-s^0}$, with $s^0 = \langle c(\cdot), r^0 \rangle \in \text{e-spl}^p(m)$
Independent sample from h^0
$\{s^\nu\}_{\nu=1}^\infty$ sequence of optimal solutions of $P_{p,m}^\nu$, with $\{r^\nu\}_{\nu=1}^\infty$

Consistency (cont.)

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Independent sample from h^0
$\{s^\nu\}_{\nu=1}^\infty$ sequence of optimal solutions of $P_{p,m}^\nu$, with $\{r^\nu\}_{\nu=1}^\infty$

If $\lim R^\nu$ exists almost surely and is deterministic, then every accumulation point r^∞ of $\{r^\nu\}_{\nu=1}^\infty$ satisfies

$$\langle c(\cdot), r^\infty \rangle \in \mathcal{P}_{p,m}^{S^\infty}(h^0) \text{ almost surely,}$$

where $S^\infty = \{s \in \mathrm{e\text{-}spl}^p(m) \mid s = \langle c(\cdot), r \rangle, r \in \lim R^\nu\}$

Consistency (cont.)

Regardless of whether R^ν has a limit, if there exists $\{\hat{r}^\nu\}_{\nu=1}^\infty$, $\hat{r}^\nu \in R^\nu$, such that $\hat{r}^\nu \to r^0$ a.s., then a.s.:

(i) $\langle c(\cdot), r^\infty \rangle \in \mathcal{P}_{p,m}(h^0)$

(ii) $r^\infty_{\text{ess}} = r^0_{\text{ess}}$ ('essential' part: $r^0 = (r^0_{\text{mesh}}, r^0_{\text{ess}})$)

(iii) If $r^\nu \to^K r^\infty$ along a subsequence K, then

$$\langle c(\cdot), r^\nu \rangle \to^K s^0 \text{ and } e^{-\langle c(\cdot), r^\nu \rangle} \to^K h^0$$

uniformly on $[m_0, m_N]$, possibly except on m

Proof of consistency

- Let X^0 have density h^0.
- Since $X^0 \in [m_0, m_N]$ almost surely, $c(X^0)$ is a random vector with finite moments
- Law of large number $(1/\nu)\sum_{i=1}^{\nu} c(X^i) \to E\{c(X^0)\}$ a.s.
- Epi-convergence of (effective) objective functions follow

Stability of Kullback-Leibler projection

Densities h^ν, h^0 on $[l, u]$ satisfy $dl_{\rm hypo}\,(h^\nu, h^0) \to 0$

If r^ν is such that

$$\langle c(\cdot), r^\nu \rangle \in \mathcal{P}_{p,m}(h^\nu) \text{ for } m = \{m_k\}_{k=0}^N, m_0 = l, m_N = u,$$

then every accumulation point of $\{r^\nu\}_{\nu=1}^\infty$ is the epi-spline parameter of some $s^0 \in \mathcal{P}_{p,m}(h^0)$

Connections between modes of convergence

Densities $h^\nu, h^0 \in \text{x-spl}^p(m)$, with $h^\nu = e^{-\langle c(\cdot), r^\nu \rangle}$, $h^0 = e^{-\langle c(\cdot), r^0 \rangle}$

Then,

$$r^\nu \to r^0 \Longrightarrow d_{KL}(h^0||h^\nu) \to 0 \Longleftrightarrow d_{KL}(h^\nu||h^0) \to 0 \Longrightarrow r^\nu_{\text{ess}} \to r^0_{\text{ess}}$$

Asymptotic normality

True density $h^0 = e^{-s^0} \in \mathrm{x\text{-}spl}^p(m)$, $s^0 = \langle c(\cdot), r^0 \rangle$
r^0 in the interior of $\liminf R^\nu$ a.s.
Independent sample from h^0
$\{s^\nu\}_{\nu=1}^\infty$ optimal solutions of $P^\nu_{p,m}$, with $\{r^\nu\}_{\nu=1}^\infty$, $h^\nu = e^{-\langle c(\cdot), r^\nu \rangle}$

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Then:

$$\nu^{1/2}(r^\nu_{\text{ess}} - r^0_{\text{ess}}) \to^d \mathcal{N}(0, \Sigma(r^0_{\text{ess}}))$$

$$\nu^{1/2}(h^\nu(x) - h^0(x)) \to^d \mathcal{N}\left(0, \Sigma_x(r^0_{\text{ess}}\right), \ x \in (m_{k-1}, m_k), k = 1, ..., N$$

Moment estimator $\mu^\nu_j = \int_{m_0}^{m_N} x^j e^{-\langle c(x), r^\nu \rangle} dx$ satisfies

$$\nu^{1/2}(\mu^\nu_j - \mu^0_j) \to^d \mathcal{N}(0, \langle w, \Sigma(r^0_{\text{ess}}) w \rangle)$$

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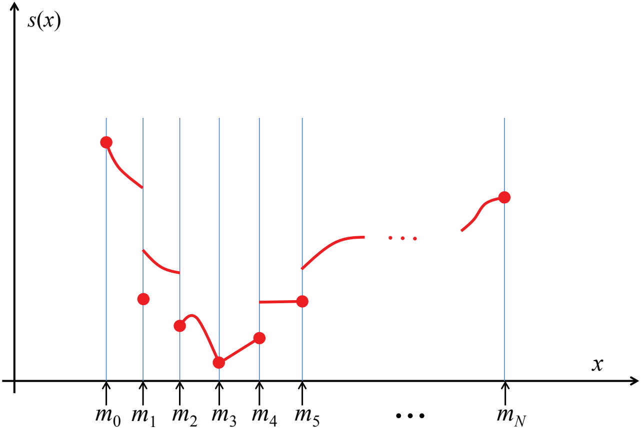
Formulation of soft information

Easy to ensure bounds on domain, continuity, smoothness, monotonicity



Continuity

Epi-spline parameter

$r =$

$(s_0, ..., s_N, a_{1,0}, a_{1,1}, ..., a_{1,p}, a_{2,0}, a_{2,1}, ..., a_{2,p}, ..., a_{N,0}, a_{N,1}, ..., a_{N,p})$

$$s_{k-1} = a_{k,0}, \quad s_k = \sum_{i=0}^{p} a_{k,i}(m_k - m_{k-1})^i, \quad k = 1, 2, ..., N$$

Kullback-Leibler constraint

Recall: Kullback-Leibler divergence from density h to density g

$$d_{KL}(h||g) = \int_{-\infty}^{\infty} h(x) \log \frac{h(x)}{g(x)} dx$$

If $s \in \text{e-spl}^p(m)$ and r its epi-spline parameter, then

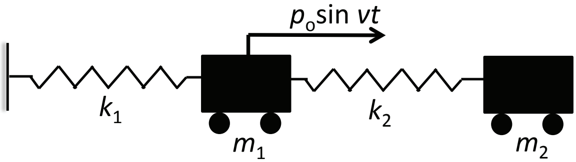
$$d_{KL}(h||e^{-s}) = \left\langle \int_{m_0}^{m_N} c(x)h(x)dx, r \right\rangle + \int_{-\infty}^{\infty} (\log h(x))h(x)dx,$$

So $\kappa_1 \leq d_{KL}(h||e^{-s}) \leq \kappa_2$ are linear constraints

Outline

- Density estimation as a stochastic program
- Epi-splines: pliable approximation tools
- Consistency and asymptotics
- Fusion of hard and soft information
- Numerical examples

Example: 2-dof dynamical system



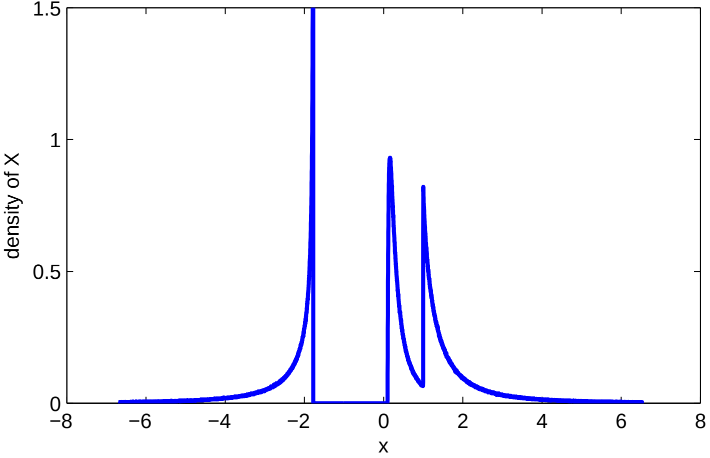
$$m_1 \ddot{u}_1(t) + (k_1 + k_2) u_1(t) - k_2 u_2(t) = p_o \sin vt$$
$$m_2 \ddot{u}_2(t) - k_2 u_1(t) + k_2 u_2(t) = 0$$

For choices of k_i, m_i, steady-state displacement at node 2:

$$u_2(t) = u_{2o} \sin vt \text{ with amplitude } u_{2o} = \frac{1}{(1 - v^2)(1 - v^2/4)}$$

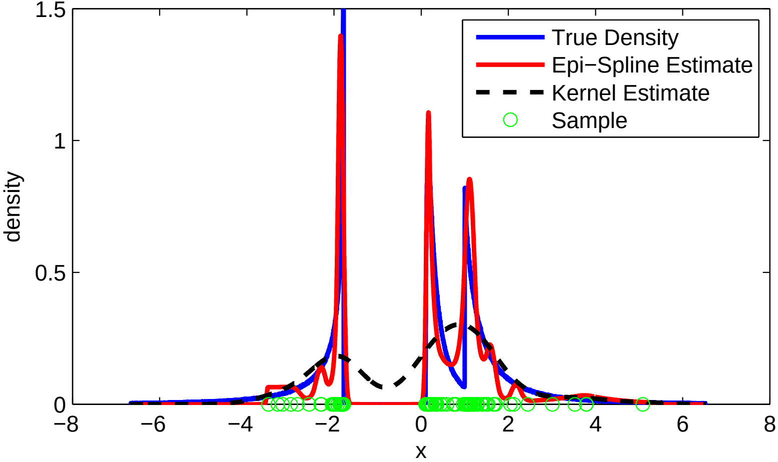
Example: Density of response amplitude

V mix of beta densities gives density for amplitude X:



Example: Density of response amplitude (cont.)

Sample size 100; continuously differentiable; "unimodal" tails



Gradient information

Gradient information for bijective $G : \boldsymbol{R} \to \boldsymbol{R}$
Recall: If $X = G(V)$, then

$$h_X(x) = h_V(G^{-1}(x))/|G'(G^{-1}(x))|$$

Present context *without* a bijection and data $x^i = G(v^i), G'(v^i)$:

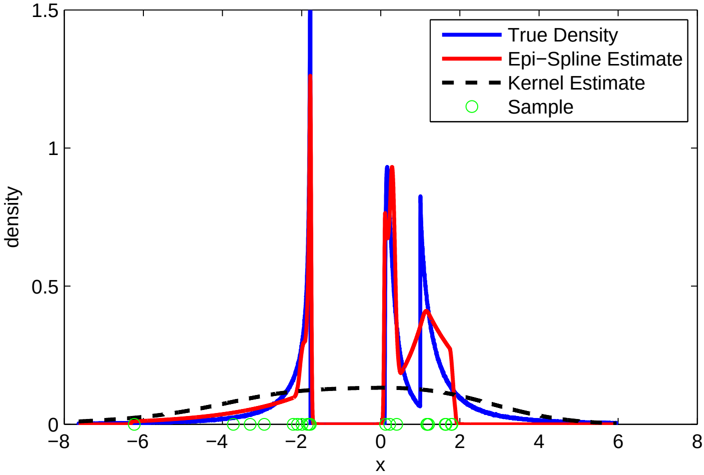
$$h^\nu(x^i) = e^{-\langle c(x^i), r\rangle} \geq \frac{h_V(v^i)}{|G'(v^i)|}$$

$$\langle c(x^i), r\rangle \leq -\log \frac{h_V(v^i)}{|G'(v^i)|}$$

Value of pdf bounded from below at x^i

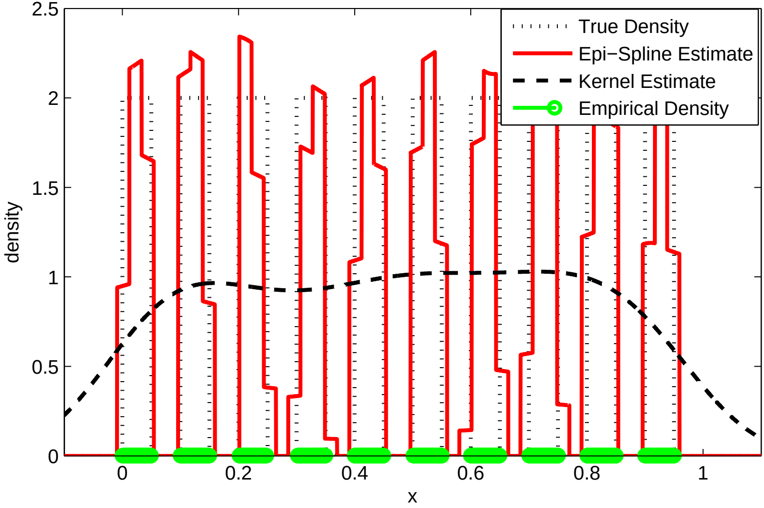
Back to example

Sample size 20; gradient information



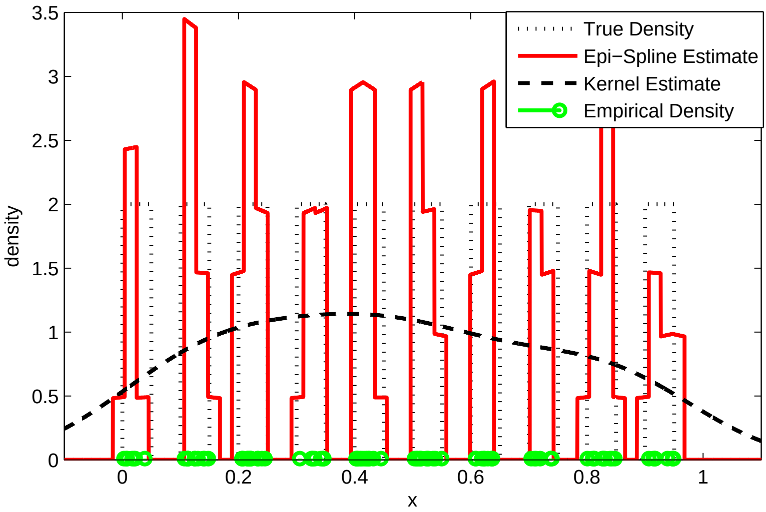
Example: Uniform mixture density

sample size 1000; lsc



Example: Uniform mixture density (cont.)

sample size just 100; lsc



Summary

- Density estimation problems as stochastic programs
- Exponential epi-splines offer a tractable class of density estimators
- Incorporate soft information by means of constraints
- Extensions to response surface, regression curve, multivariate density estimation, and many other curve fitting problems

References

- Royset & Wets, "Nonparametric density estimation via exponential epi-splines: fusion of soft and hard information"
- Royset & Wets, "Epi-splines and exponential epi-splines: Pliable approximation tools"
- Singham, Royset, & Wets, "Density estimation of simulation output using exponential epi-splines," *Proc. WSC*, 2013
- Royset, Sukumar, & Wets "Uncertainty quantification using exponential epi-splines," *Proc. ICOSSAR*, 2013

- More examples: https://www.math.ucdavis.edu/~prop01/
- Matlab implementations available