Methods for Model Approximation and Optimization in the Presence of Model Uncertainty Using Information Divergences

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Outflow species A	$\kappa_2 X_A$	$X_A \to X_A - 1$
Inflow species B	κ_3	$X_B \to X_B + 1$
Outflow species B	$\kappa_4 X_B$	$X_B \to X_B - 1$
Reaction $A + 2B \to 3B$	$\kappa_5 X_A X_B (X_B - 1)$	$X_A \to X_A - 1$ $X_B \to X_B + 1$

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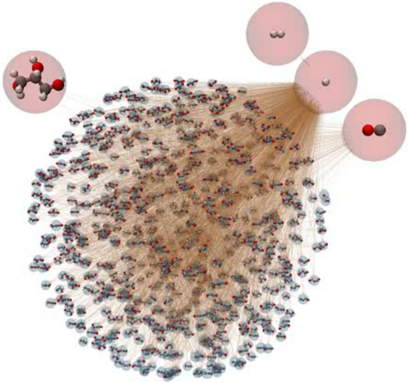
Model determined by reaction rates κ_i. Generator

$$\mathcal{L} f(x) = \sum_{i=1}^{5} r_i(x) \left[f(x + v_i) - f(x) \right]$$

Example

Glycerol reforming CRN. Network visualization:



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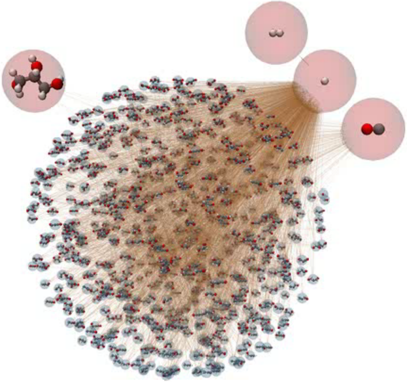

780 species, 3898 reactions. Quantities of interest (performance measures) are functionals of stationary distribution (ergodic averages).

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- *Optimization and control for uncertain systems*: optimize a performance measure for a family of models, a min/max problem
- *Model reduction* (e.g., course graining).

Abstract formulation

Elements of the framework

- *Probability models*, on space $\mathcal{S}$, often a path space

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  Here f may combine a cost with dynamics that take random variables under Q (or P) into the system state:

$$f(w) = \int_0^T c(\mathcal{G}[w](t))dt,$$

$$\mathcal{G} : W \to X, \quad dX(t) = b(X(t))dt + dW(t).$$

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Ingredients in the framework

- *Divergence or distance* between nominal and true models. Most important (but not only) example is relative entropy, aka Kullback-Leibler divergence:

$$R(Q \| P) = \begin{cases} E_Q\left[\log \frac{dQ}{dP}\right] & \text{if } Q \ll P \\ \infty & \text{else.} \end{cases}$$

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$$\log E_P\left[e^{cf}\right] = \sup_{Q \ll P}\left[cE_Q[f] - R(Q \| P)\right],$$

  hence whenever $Q \ll P$,

$$cE_Q[f] \leq R(Q \| P) + \log E_P\left[e^{cf}\right].$$

  Minimizing Q^* is $dQ^* = e^{cf}dP / \int e^{cf}dP$.

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Then using Lagrange multipliers ($\lambda = 1/c$)

$$\begin{aligned}
&\min_{\alpha \in A} \left[\max_{Q} \min_{c>0} \left(E_Q[f_\alpha] + \frac{1}{c}[r - R(Q \| P)] \right) \right] \\
&\quad = \min_{\alpha \in A} \left[\min_{c>0} \max_{Q} \left(E_Q[f_\alpha] - \frac{1}{c} R(Q \| P) \right) + \frac{1}{c} r \right] \\
&\quad = \min_{\alpha \in A} \min_{c>0} \frac{1}{c} \left(r + \log E_P \left[e^{c f_\alpha} \right] \right).
\end{aligned}$$

Final problem phrased purely in terms of the design model.

Important properties of a good divergence

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- Good scaling properties, e.g.:
  - the bounds remain meaningful for systems over long times, ergodic QoI
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- Good computational properties of the divergence and the dual functional under the design P.
- Bounds should not depend on the underlying probability space (e.g., for $dX = b(X)dt + dW$ can have P is Wiener measure vs P measure induced by X).

A little history

First applications of relative entropy/exponential integral duality in problems of model uncertainty:

- Robust properties of risk–sensitive control (D, James and Petersen), *Math. of Control, Signals and Systems*, **13,** (2000), pp. 318–332.

This paper introduces the general framework in the setting of diffusions with uncertain drift, and makes connections with H^∞ control.

- Minimax optimal control of stochastic uncertain systems with relative entropy constraints (Petersen, James and D), *IEEE Trans. on Auto. Control.,* **45,** (2000), pp. 398–412.

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Ideas had substantial impact in economics:

- Robust control and model uncertainty (Hansen and Sargent), *The American Economic Review*, **91**, (2001), pp. 60-66.
- *Robustness*, (Hansen and Sargent), Wiley, 2008.
- Many subsequent papers.

Outline

- Uses of KL divergence and standard QoI
    - Why bounds do not depend on how system is represented
    - Performance bounds for static problem
    - Chain rule for KL divergence
    - Performance bounds for large time (ergodic) problem
    - Sensitivity bounds for ergodic problem
    - Robust optimization for ergodic problem

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- Uses of KL divergence and standard QoI
  - Why bounds do not depend on how system is represented
  - Performance bounds for static problem
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  - Performance bounds for large time (ergodic) problem
  - Sensitivity bounds for ergodic problem
  - Robust optimization for ergodic problem
- Nonstandard QoI and other distance/variational representation pairs
  - Situations that require new ideas/open problems
  - Rare event performance measures and Rényi divergence

Why bounds do not depend on how system is represented

Relative entropy under mapping. Suppose $\psi : \mathcal{S} \to \mathcal{T}$ and

$$\lambda(A) = P(\{x : \psi(x) \in A\}), \quad \sigma(A) = Q(\{x : \psi(x) \in A\}).$$

Then $R(Q \| P) \geq R(\sigma \| \lambda)$. Given feasible σ there is always a Q^* such that $\psi \sim \sigma$ under Q^*, and $R(Q^* \| P) = R(\sigma \| \lambda)$. In particular, take

$$\frac{dQ^*}{dP}(x) = \frac{d\sigma}{d\lambda}(y) \text{ on } \{x : \psi(x) = y\}.$$

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Now suppose view $f(y)$ under σ or $f(\psi(x))$ under Q. Performance bounds on f are *same* for a given allowed relative entropy distance:

$$\sup_{Q:R(Q\|P)\leq r} E_Q[f \circ \psi] = \sup_{\sigma:R(\sigma\|\lambda)\leq r} E_\sigma[f].$$

Performance bounds for static problem

For a given QoI f, define centered cumulant generating function

$$\tilde{\Lambda}_{P,f}(c) = \log \int_{\mathcal{S}} e^{c(f(x) - E_P[f])} P(dx).$$

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Also if $c > 0$ then

$$-cE_Q[f] \leq R\left(Q \,\|\, P\right) + \log E_P\left[e^{-cf}\right]$$

so for any $c > 0$

$$-\frac{1}{c}\tilde{\Lambda}_{P,f}(-c) - \frac{1}{c} R\left(Q \,\|\, P\right) \leq E_Q[f] - E_P[f] \leq \frac{1}{c}\tilde{\Lambda}_{P,f}(c) + \frac{1}{c} R\left(Q \,\|\, P\right).$$

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Optimizing the two bounds gives

$$\sup_{c>0}\left\{-\frac{1}{c}\tilde{\Lambda}_{P,f}(-c)-\frac{1}{c}R\left(Q\,\|P\right)\right\} \leq E_Q[f]-E_P[f]$$
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If f is not a constant the quantities

$$\Xi_{\pm}(Q\,\|P\,;f)=\inf_{c>0}\left\{\frac{R\left(Q\,\|P\right)+\tilde{\Lambda}_{P,f}(\pm c)}{c}\right\}$$

behave themselves like divergences: $\Xi_{\pm}(Q\,\|P\,;f)\geq 0$ and $\Xi_{\pm}(Q\,\|P\,;f)=0$ iff $Q=P$. Optimization problem has good properties.

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How to scale up to ergodic problem?

Properties of relative entropy/KL divergence

Chain rule and Markov models. For the bounds to be useful, the quantities involved should scale and take concrete form. For Markov systems, done (in discrete time) via the *chain rule*. (In continuous time, for systems driven by Brownian and Poisson noise, see*.)

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$$\begin{aligned} Q(dx_0 \times dx_1) &= \nu(dx_0) q(x_0, dx_1), \\ P(dx_0 \times dx_1) &= \mu(dx_0) p(x_0, dx_1). \end{aligned}$$

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Then relative entropy decomposes as

$$\begin{aligned} R\left(Q \,\|P\right) &= \int_{\mathcal{X}^2} \left[\log\left(\frac{d\nu}{d\mu}(x_0)\right) + \log\left(\frac{dq(x_0,\cdot)}{dp(x_0,\cdot)}(x_1)\right)\right] \nu(dx_0)q(x_0, dx_1) \\ &= R\left(\nu \,\|\mu\right) + \int_{\mathcal{X}} R\left(q(x_0,\cdot) \,\|p(x_0,\cdot)\right) \nu(dx_0) \\ &= R\left(\nu \,\|\mu\right) + E_Q R\left(q(X_0,\cdot) \,\|p(X_0,\cdot)\right) \end{aligned}$$

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Properties of relative entropy/KL divergence

Chain rule and Markov models. Now let P_T be a Markov measure on $\{0, 1, \ldots, T\}$ with initial measure μ and transition kernel $p(x, dy)$, and similarly for Q_T with ν and $q(x, dy)$. Then repeated use of chain rule gives

$$R\left(Q_T \,\|P_T\right) = R\left(\nu \,\|\mu\right) + \sum_{t=0}^{T-1} E_{Q_T} R\left(q(X_t, \cdot) \,\|p(X_t, \cdot)\right),$$

where E_{Q_T} means expectation where $(X_0, X_1, \ldots, X_T)$ has distribution Q_T.

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where E_{Q_T} means expectation where $(X_0, X_1, \ldots, X_T)$ has distribution Q_T. If $p(x, dy)$ is ergodic with stationary distribution π_p and $q(x, dy)$ with π_q, then

$$r(q \,\|\, p) = \lim_{T \to \infty} \frac{1}{T} R\left(Q_T \,\|\, P_T\right) = \int_{\mathcal{X}} R\left(q(x, \cdot) \,\|\, p(x, \cdot)\right) \pi_q(dx)$$

is called the *relative entropy rate (RER)*.

Performance bounds for large time (ergodic) problem

Suppose the QoI is a functional of the empirical measure, e.g.,

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Then

$$\begin{aligned} -\frac{1}{c}\frac{1}{T}\tilde{\Lambda}_{P_T,f}(-c) - \frac{1}{c}\frac{1}{T}R\left(Q_T \,\|\, P_T\right) &\leq \frac{1}{T}E_{Q_T}\sum_{t=0}^{T-1} g(X_t) - \frac{1}{T}E_{P_T}\sum_{t=0}^{T-1} g(X_t) \\ &\leq \frac{1}{c}\frac{1}{T}\tilde{\Lambda}_{P_T,f}(c) + \frac{1}{c}\frac{1}{T}R\left(Q_T \,\|\, P_T\right). \end{aligned}$$

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\end{aligned}$$

By chain rule all terms scale $\propto T$. Send $T \to \infty$ to get

$$-\frac{1}{c}\Lambda(-c) - \frac{1}{c}r(q\,\|\,p) \leq E_{\pi_q}[g] - E_{\pi_p}[g] \leq \frac{1}{c}\Lambda(c) + \frac{1}{c}r(q\,\|\,p),$$

$$\Lambda(c) = \lim_{T\to\infty}\frac{1}{T}\log E_{P_T}\left[e^{c\sum_{t=0}^{T-1} g(X_t) - E_{\pi_p}[g]}\right]$$

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"Small model error" version of bounds useful and frequently tractable.
Optimizing bounds over $c > 0$ (separately LHS and RHS) in

$$-\frac{1}{c}\Lambda(-c) - \frac{1}{c} r(q \,\|\, p) \leq E_{\pi_q}[g] - E_{\pi_p}[g] \leq \frac{1}{c}\Lambda(c) + \frac{1}{c} r(q \,\|\, p)$$

gives

$$\left| E_{\pi_q}[g] - E_{\pi_p}[g] \right| \leq \sqrt{v_p[g] 2 r(q \,\|\, p)} + O(r(q \,\|\, p))$$

$$v_p[g] = 2 \sum_{t=0}^{\infty} E_p[\left(g(X_t) - E_{\pi_p}[g]\right)\left(g(X_0) - E_{\pi_p}[g]\right)].$$

Sensitivity bounds for ergodic problem

For sensitivity bounds we assume q is a small perturbation of p. Thus

$$p(x, dy) = p(x, dy; \theta) \text{ and } q(x, dy) = p(x, dy; \theta + \varepsilon v),$$

where the parameter θ takes values in a subset of some Euclidean space.

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where the parameter θ takes values in a subset of some Euclidean space. Assume reference measure so

$$p(x, dy; \theta) = p(x, y; \theta) R(dy).$$

Then one can expand the relative entropy rate:

$$\begin{aligned} r(q \,\|\, p) &= \int_{\mathcal{X}} R\left(q(x, \cdot) \,\|\, p(x, \cdot)\right) \pi_q(dx) \\ &= \int_{\mathcal{X}} \int_{\mathcal{X}} \log \frac{p(x, y; \theta + \varepsilon v)}{p(x, y; \theta)} p(x, y; \theta + \varepsilon v) R(dy) \pi_q(dx) \\ &= \frac{|\varepsilon|}{2} \langle v, \mathcal{I}(p(\theta)) v \rangle + O(\varepsilon^2), \end{aligned}$$

where

$$\mathcal{I}(p(\theta)) = \int_{\mathcal{X}^2} \nabla_\theta \log p(x, y; \theta) [\nabla_\theta \log p(x, y; \theta)]^T p(x, y; \theta) R(dy) \pi_p(dx)$$

Sensitivity bounds for ergodic problem

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is called a *path Fisher Information Matrix*. From

$$\left| E_{\pi_q}[g] - E_{\pi_p}[g] \right| \leq \sqrt{v_p[g] 2 r(q \,\|\, p)} + O(r(q \,\|\, p)),$$

and expansion of RER, for any QoI g one has bounds

$$\frac{1}{|\varepsilon|} \left| E_{\pi_{p(\theta+\varepsilon v)}}[g] - E_{\pi_{p(\theta)}}[g] \right| \leq \sqrt{v_{p(\theta)}[g]} \sqrt{\langle v, \mathcal{I}(p(\theta)) v \rangle} + O(\varepsilon)$$

Sensitivity bounds for ergodic problem

The sensitivity bound

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allows for sensitivity screening: which parameters are less important.

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allows for sensitivity screening: which parameters are less important. The path FIM

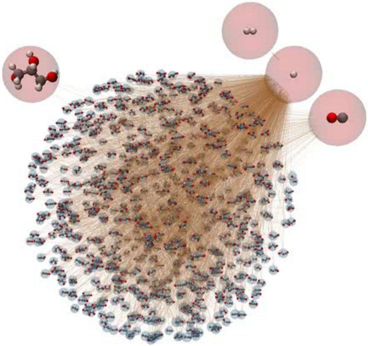
$$\mathcal{I}(p(\theta))=\int_{\mathcal{X}^2}\nabla_\theta\log p(x,y;\theta)[\nabla_\theta\log p(x,y;\theta)]^T p(x,y;\theta)R(dy)\pi_p(dx)$$

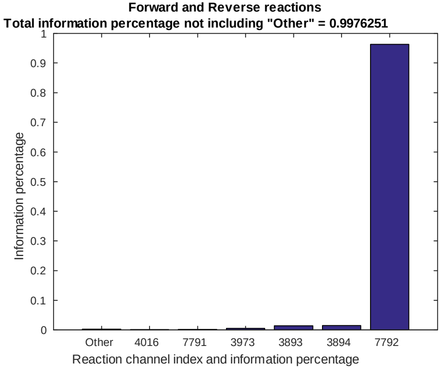
can be obtained via Monte Carlo since by ergodic theorem, with $\{X_t\}\sim p(x,dy;\theta)$

$$\frac{1}{T}\sum_{t=0}^{T-1}\delta_{(X_t,X_{t+1})}(dx\,dy)\Rightarrow\pi_p(dx)p(x,y;\theta)R(dy)$$

Sensitivity bounds for ergodic problem

Example: glycerol reforming. With $\theta =$ vector of rate parameters, and "information percentage" is fraction of trace of $\mathcal{I}(p(\theta))$ associated with given parameter[†]





[†] Computations courtesy Pedro Vilanova

Other uses

Optimally robust for ergodic cost. Suppose $g = g_\alpha$ with $\alpha \in A$. Now to solve

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Then choose α according to

$$\begin{aligned}
&\min_{\alpha \in A} \left[\max_{q} \min_{c>0} \left(E_{\pi_q}[g_\alpha] + \frac{1}{c}[r - r(q \| p)] \right) \right] \\
&\quad = \min_{\alpha \in A} \left[\min_{c>0} \max_{q} \left(E_{\pi_q}[g_\alpha] - \frac{1}{c} r(q \| p) \right) + \frac{1}{c} r \right] \\
&\quad = \min_{\alpha \in A} \min_{c>0} \frac{1}{c} \left(r + \Lambda_\alpha(c) \right).
\end{aligned}$$

Situations that require new ideas/open problems

- **Issue:** Want alternative measures that are not absolutely continuous w.r.t. design. **Possible solution:** Distances not limited to divergences, e.g., Wasserstein. However chain rule only for product measures, and in general there is dependence on probability space.

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- Multi-scale problems, e.g., models of form

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\begin{aligned}
dX^{\varepsilon} &= b(X^{\varepsilon}, Y^{\varepsilon})dt + \sigma(X^{\varepsilon}, Y^{\varepsilon})dW_t \\
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  Issue: relative entropy counts fast process more heavily. **Possible solution:** "multi-level" exponential integral and corresponding variational inequalities.
- **Issue:** QoI is itself risk-sensitive (i.e., depends of rare events). KL divergence is not suitable for robust bounds.

Rare event performance measures and Rényi divergence

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Recently derived variational formula relates risk-sensitive QoI and Rényi divergence. Let $0 < \beta < \gamma$. Then

$$\frac{1}{\gamma} \log E_P\left[e^{\gamma f}\right] = \sup_{Q \ll P} \left[\frac{1}{\beta} \log E_Q\left[e^{\beta f}\right] - \frac{1}{\gamma - \beta} R_{\frac{\gamma}{\gamma-\beta}}(Q \,\|\, P)\right],$$

where for mutually absolutely continuous P, Q and $\alpha > 1$

$$R_\alpha(Q \,\|\, P) = \frac{1}{\alpha(\alpha-1)} \log \int_S \left(\frac{dQ}{dP}\right)^{\alpha-1} dQ.$$

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As $\beta \downarrow 0$ recover Kullback-Leibler formula. Bounds on risk-sensitive QoI for various Q at level β in terms of one at level γ in terms of design:

$$\frac{1}{\beta}\log E_Q\left[e^{\beta f}\right] \le \frac{1}{\gamma}\log E_P\left[e^{\gamma f}\right] + \frac{1}{\gamma-\beta} R_{\frac{\gamma}{\gamma-\beta}}(Q\,\|\,P).$$

Example use: sensitivity bounds

Rare event performance measures and Rényi divergence

Let $P = P^{\theta}, Q = P^{\theta+\varepsilon v}$, where $P^{\theta}(dx) = p(x;\theta)R(dx)$.

Rare event performance measures and Rényi divergence

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$$\frac{d}{d\varepsilon}\frac{1}{\beta}\log E_{P^{\theta}}\left[e^{\beta f}\right] \leq \frac{1}{\beta^2}\inf_{c>0}\left[\frac{R(P^{\theta}_{\beta}\,\|P^{\theta}) + \log\int e^{c\beta v^T\nabla_{\theta}p(\cdot;\theta)}dP^{\theta}}{c}\right],$$

where

$$dP^{\theta}_{\beta} = \frac{e^{\beta f}\,dP^{\theta}}{\int e^{\beta f}\,dP^{\theta}},$$

and corresponding lower bound.

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where

$$dP^{\theta}_{\beta} = \frac{e^{\beta f}\,dP^{\theta}}{\int e^{\beta f}\,dP^{\theta}},$$

and corresponding lower bound. Again decomposes into term depending on g and term plays role of Fisher information matrix. With $f = -\infty 1_{A^c}$,

$$\frac{d}{d\varepsilon}\frac{1}{\beta}\log P^{\theta}(A) \leq \frac{1}{\beta^2}\inf_{c>0}\left[\frac{-\log P^{\theta}(A) + \log\int e^{c\beta v^T\nabla_{\theta}p(\cdot;\theta)}dP^{\theta}}{c}\right],$$

with bounds uniform w.r.t. events A with uniformly bounded $-\log P^{\theta}(A)$.

Rare event performance measures and Rényi divergence

Negatives of Rényi:

- A chain rule for product measures, but not for Markov measures
- Quantity one would optimize over in robust design (here γ) appears also in $R_{\frac{\gamma}{\gamma-\beta}}(Q \,\|\, P)$. Complicates formulation of robust optimization

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- A chain rule for product measures, but not for Markov measures
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Positives of Rényi:

- Bounds still scale with meaningful limits large time/system size, even for Markov measures
- Bounds independent of underlying probability space

Summary

- Variational formulas relating QoI and information divergences/distances provide a natural way to quantitatively deal with model uncertainty and robust design
- Can treat various issues such as sensitivity bounds, optimal robust design, etc.
- Important properties are (i) preservation of bounds under scalings, (ii) computationally tractable, (iii) bounds should not depend on underlying probabilistic formulation
- Variational formula with nicest properties seems to be that of Kullback-Leibler divergence and ordinary QoI
- However for some problems this framework is not appropriate, and for these alternatives are being (or need to be) investigated

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