Talk: Systematic approaches
to generate reversiblizations
of non-reversible Markov chains

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Setting: Given target distribution π on $\mathcal{X}$
and an infinitesimal Markov generator L,
what are the different ways to
reversiblize L?

· **Today**: Geometric projection approach.

· **Known reversiblizations**:

1. (Additive) $\frac{L+L_\pi}{2} =: P_1$
2. (Metropolis-Hastings):
   For $x \neq y \in \mathcal{X}$,
   $$P_{-\infty}(x,y) = \min\left(L(x,y), L_\pi(x,y)\right)$$
3. (Choi):
   $$P_{+\infty}(x,y) = \max\left(L(x,y), L_\pi(x,y)\right)$$
4. (Barker proposal):
   $$P_{-1}(x,y) = \frac{2L(x,y)L_\pi(x,y)}{L(x,y)+L_\pi(x}$$

$$L_\pi(x,y) \triangleq \frac{\pi(y)}{\pi(x)} L(y,x)$$

$f : \mathbb{R}_+ \to \mathbb{R}_+$ convex with $f(1) = 0$ and
$f'(1) = 0$.

$\mathcal{L} \triangleq$ set of Markov infinitesimal generator on $\mathcal{X}$

$\mathcal{L}(\pi) \triangleq$ set of π-reversible Markov generator on $\mathcal{X}$.

<u>Def^{n}</u> (f-divergence): For $M, L \in \mathcal{L}$,

$$D_f(M \| L) \triangleq \sum_{x \in \mathcal{X}} \pi(x) \sum_{y \in \mathcal{X} \setminus \{x\}} L(x,y) f\left(\frac{M(x,y)}{L(x,y)}\right)$$

with the conventions of $0 f\left(\frac{0}{0}\right) = 0$ and $0 f\left(\frac{a}{0}\right) = 0$
for $a > 0$.

f^*: convex $*$-conjugate

$$f^*(t) \triangleq \begin{cases} t f\left(\frac{1}{t}\right), & t > 0 \\ [illegible], & t = 0 \end{cases}$$

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<u>Def</u>

Def^{n} (f-projection, f^*-projection):

$$M^f = M^f(L,\pi) \triangleq \underset{M \in \mathcal{L}(\pi)}{\operatorname{argmin}} D_f(M \| L)$$

$$M^{f^*} = M^{f^*}(L,\pi) \triangleq \underset{M \in \mathcal{L}(\pi)}{\operatorname{argmin}} D_f(L \| M)$$

Def^{n} (Power mean reversiblization)
For $x \neq y \in \mathcal{X}$, $p \in \mathbb{R} \setminus \{0\}$,

$$P_p(x,y) \triangleq \left(\frac{L(x,y)^p + L_\pi(x,y)^p}{2} \right)^{\frac{1}{p}}$$

Detailed balance: $$\pi(x) P_p(x,y) = \left(\frac{(\pi(x) L(x,y))^p + (\pi(x) L_\pi(x,y))^p}{2} \right)^{\frac{1}{p}}$$

$$= \left(\frac{(\pi(y) L_\pi(y,x))^p + (\pi(y) L(y,x))^p}{2} \right)^{\frac{1}{p}}$$

$$= \pi(y) P_p(y,x).$$

$$P_0(x,y) \triangleq \lim_{p \to 0} P_p(x,y) = \sqrt{L(x,y) L_\pi(x,y)}$$ (geometric mean reversibliza[tion])

$$P_{+\infty}(x,y) \triangleq \lim_{p \to \infty} P_p(x,y) = \max\{L(x,y), L_\pi(x,y)\}$$

$$P_{-\infty}(x,y) \triangleq \lim_{p \to -\infty} P_p(x,y) = \min\{L(x,y), L_\pi(x,y)\}.$$

Thm (Diaconis and Miclo '09, Wolfer and Watanabe '21):

Let $f(t) = t\ln t - t + 1$ (KL divergence),

$$M^f = P_0$$

$$M^{f^*} = P_1$$

Thm

- $f(t) = (\sqrt{t}-1)^2$ (Squared Hellinger distance), $f = f^*$

(i). $$M^f = P_{\frac{1}{2}}$$
$$M^{f^*} = P_{\frac{1}{2}}$$

(ii). (Bisection) $D_f(L\|M) = D_f(L_\pi\|M)$ $M \in \mathcal{L}(\pi)$, $L \in \mathcal{L}$
$$D_f(M\|L) = D_f(M\|L_\pi)$$

(iii). (Pythagorean identity) $\overline{M} \in \mathcal{L}(\pi)$
$$D_f(L\|\overline{M}) = D_f(L\|M^{f^*}) + D_f(M^{f^*}\|\overline{M})$$
$$D_f(\overline{M}\|L) = D_f(\overline{M}\|M^f) + D_f(M^f\|L)$$

- $f(t) = (t-1)^2$, $f^*(t) = t\left(\frac{1}{t}-1\right)^2$
  (χ^2-divergence) (Reverse χ^2-divergence)

(i). • $M^f = P_1$ (Harmonic mean / Barker proposal)

• $M^{f^*} = P_2$

(ii). (Bisection) $M \in \mathcal{L}(\pi)$, $L \in \mathcal{L}$

$$D_f(L \| M) = D_f(L_\pi \| M)$$

$$D_f(M \| L) = D_f(M \| L_\pi)$$

(iii). (Pythagorean identity) "

- $f(t) = \dfrac{t^\alpha - \alpha t - (1-\alpha)}{\alpha(\alpha-1)}$, $\alpha \in \mathbb{R} \setminus \{0,1\}$

$f^*(t) = t f\left(\frac{1}{t}\right)$.

(i). $M^f = P_{1-\alpha}$

$M^{f^*} = P_\alpha$

(ii). (Bisection)

(iii). (Pythagorean identity)

~~For f,g~~ For $g, h : \mathcal{X} \to \mathbb{R}$, $L \in \mathcal{L}$

$$\langle g, h \rangle_\pi \triangleq \sum_{x \in \mathcal{X}} g(x) h(x) \pi(x)$$

$$\langle -Lg, g \rangle_\pi \triangleq \frac{1}{2} \sum_{x,y \in \mathcal{X}} \pi(x) L(x,y) \left(g(x) - g(y)\right)^2$$

<u>Def^{n}</u> (Peskun ordering) For $L_1, L_2 \in \mathcal{L}(\pi)$,

we write $L_1 \succeq L_2$ if $L_1(x,y) \geq L_2(x,y) \ \forall x \neq y$

$$\Rightarrow \langle -L_1 g, g \rangle_\pi \geq \langle -L_2 g, g \rangle_\pi .$$

<u>Thm</u> (Markov chain AM-GM-HM inequality):

$$P_1 \succeq P_0 \succeq P_{-1}$$

and equality holds iff L is π-reversible
$(L \in \mathcal{L}(\pi))$

Def^{n} (f-projection and f^*-projection centroid)

Given $L_1, L_2, \dots L_n \in \mathcal{L}$,

$$M_n^f = M_n^f(L_1, \dots, L_n, \pi) \triangleq \underset{M \in \mathcal{L}(\pi)}{\operatorname{argmin}} \sum_{i=1}^{n} D_f(M \| L_i)$$

$$M_n^{f^*} = M_n^{f^*}(L_1, \dots L_n, \pi) \triangleq \underset{M \in \mathcal{L}(\pi)}{\operatorname{argmin}} \sum_{i=1}^{n} D_f(L_i \| M).$$

Thm : M_n^f and $M_n^{f^*}$ exist and are unique under strictly convex f.

Examples of centroids :

- $f(t) = t\ln t - t + 1$, $x \neq y \in \mathcal{X}$

(i) $M_n^f(x,y) = \left(\prod_{i=1}^{n} M^f(L_i, \pi)(x,y) \right)^{\frac{1}{n}} = \left(\sqrt{L_1(x,y) L_{1,\pi}(x,y)} \cdots \right)$

(ii) $M_n^{f^*}(x,y) = \frac{1}{n} \sum_{i=1}^{n} M^{f^*}(L_i, \pi)(x,y)$

(iii) (AM $\geq$ GM) : $M_n^{f^*}(x,y) \geq M_n^f(x,y)$

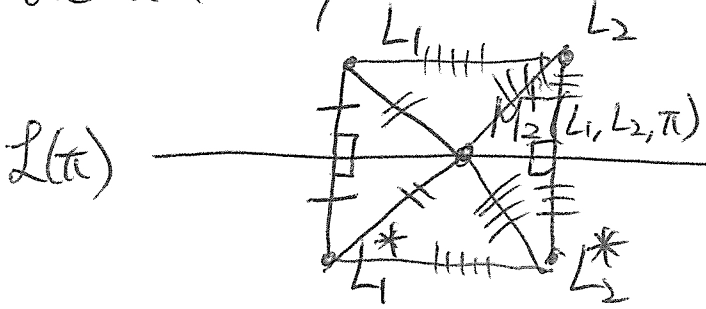
$$M_n^{f^*} \gtrsim M_n^f$$

equality holds iff $L_1, \dots L_n$ are all π-reve

- $f(t) = (\sqrt{t}-1)^2$ (squared Hellinger)
  $= f^*(t)$

- $M_n^f(x,y) = M_n^{f^*}(x,y)$
  $= \left(\frac{1}{n} \sum_{i=1}^{n} \sqrt{M^{\#}(L_i,\pi)(x,y)} \right)^2$

L_1, L_2 are π-stationary



L_1, L_2, L_3, L_4 are π-stationary