Energy for Markov chains

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UNDER CONSTRUCTION
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The Dirichlet Principle

Lemma. Let P be the transition matrix for a Markov chain with stationary measure α. Let

$$\langle g, h \rangle = \sum_{ij} \alpha_i g_i (I_{ij} - P_{ij}) h_j.$$

Then

$$\langle g, g \rangle \geq 0.$$

If P is ergodic, then equality holds only if $g = 0$.

Proof. (See Kemeny, Snell, and Knapp, Lemmas 9-121 and 8-54.)

$$\begin{aligned}
\langle g, g \rangle &= \sum_{ij} \alpha_i g_i (I_{ij} - P_{ij}) g_j \\
&= \frac{1}{2}[\sum_i \alpha_i g_i^2 + \sum_{ij} (-2\alpha_i g_i P_{ij} g_j) + \sum_j \alpha_j g_j^2] \\
&= \frac{1}{2} \sum_{ij} (\alpha_i P_{ij} g_i^2 - 2\alpha_i P_{ij} g_i g_j + \alpha_i P_{ij} g_j^2)
\end{aligned}$$

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$$
\begin{aligned}
&= \frac{1}{2}\sum_{ij}\alpha_i P_{ij}(g_i - g_j)^2 \\
&\geq 0. \clubsuit
\end{aligned}
$$

The previous lemma is stated for a general (not necessarily ergodic) chain because at one point later on we will need the result in this generality. However, from now on we will be assuming that P is nice and ergodic.

Theorem (Dirichlet Principle). Given a set of states E (the boundary) and a real-valued function f on E (telling the boundary values), let ϕ be the unique P-harmonic function with $\phi|E = f$, and let $\hat{\phi}$ be the unique $\hat{P}$-harmonic function with $\hat{\phi}|E = f$. Let

$$
D_E(f) = \min_{v|E=f} I_E(v),
$$

where

$$
\begin{aligned}
I_E(v) &= \max_{u|E=v,\hat{u}|E=v,(u+\hat{u})/2=v} \langle \hat{u}, u\rangle \\
&= \max_{w|E=0} \langle v-w, v+w\rangle.
\end{aligned}
$$

Then

$$
D_E(f) = \langle \hat{\phi}, \phi\rangle,
$$

and this minimax is attained when and only when $u = v + w = \phi$ and $\hat{u} = v - w = \hat{\phi}$.

Proof. For any functions g, h with $g|E = h|E = 0$,

$$
\langle g, \phi\rangle = \langle \hat{\phi}, h\rangle = 0
$$

since $(I-P)\phi$ and $(I-\hat{P})\hat{\phi}$ vanish on the complement of E. Hence

$$
\begin{aligned}
\langle \hat{\phi}+g, \phi+h\rangle &= \langle \hat{\phi}, \phi\rangle + \langle g, \phi\rangle + \langle \hat{\phi}, h\rangle + \langle g, h\rangle \\
&= \langle \hat{\phi}, \phi\rangle + \langle g, h\rangle.
\end{aligned}
$$

In particular,

$$
\begin{aligned}
\langle \hat{\phi}+g, \phi+g\rangle &= \langle \hat{\phi}, \phi\rangle + \langle g, g\rangle \\
&\geq \langle \hat{\phi}, \phi\rangle
\end{aligned}
$$

and

$$\begin{aligned} \langle \hat{\phi} - g, \phi + g \rangle &= \langle \hat{\phi}, \phi \rangle - \langle g, g \rangle \\ &\leq \langle \hat{\phi}, \phi \rangle. \end{aligned}$$

The rest is standard minimax: Let $v_0 = (\phi + \hat{\phi})/2$ and $w_0 = (\phi - \hat{\phi})/2$, so that $\phi = v_0 + w_0$ and $\hat{\phi} = v_0 - w_0$. For any v with $v|E = f$ let $g = v - v_0$, so that $v = v_0 + g$. Then

$$\begin{aligned} \langle v - w_0, v + w_0 \rangle &= \langle v_0 - w_0 + g, v_0 + w_0 + g \rangle \\ &= \langle \hat{\phi} + g, \phi + g \rangle \\ &\geq \langle \hat{\phi}, \phi \rangle. \end{aligned}$$

Hence

$$\begin{aligned} I_E(v) &= \max_w \langle v - w, v + w \rangle \\ &\geq \langle v - w_0, v + w_0 \rangle \\ &\geq \langle \hat{\phi}, \phi \rangle. \end{aligned}$$

Since this holds for any v with $v|E = f$,

$$\begin{aligned} D_E(f) &= min_v I_E(v) \\ &\geq \langle \hat{\phi}, \phi \rangle. \end{aligned}$$

By the same token, for any w with $w|E = 0$ let $g = w - w_0$, so that $w = w_0 + g$. Then

$$\begin{aligned} \langle v_0 - w, v_0 + w \rangle &= \langle v_0 - w_0 - g, v_0 + w_0 + g \rangle \\ &= \langle \hat{\phi} - g, \phi + g \rangle \\ &\leq \langle \hat{\phi}, \phi \rangle. \end{aligned}$$

Since this holds for any w with $w|E = 0$,

$$\begin{aligned} I_E(v_0) &= \max_w \langle v_0 - w, v_0 + w \rangle \\ &\leq \langle \hat{\phi}, \phi \rangle. \end{aligned}$$

Thus

$$\begin{aligned} D_E(f) &= \min_v I_E(v) \\ &\leq I_E(v_0) \\ &\leq \langle \hat{\phi}, \phi \rangle. \quad \clubsuit \end{aligned}$$

The classical Dirichlet Principle

In the reversible case, we can turn the minimax into an honest minimum, because we can explicitly evaluate the maximum that appears in the expression for $I_E(v)$.

Lemma. If P is reversible,

$$\begin{aligned} I_E(v) &= \langle v, v \rangle \\ &= \sum_{ij} \alpha_i P_{ij} (v_i - v_j)^2. \end{aligned}$$

Proof. If $\hat{P} = P$ then $\langle g, h \rangle = \langle h, g \rangle$, so

$$\begin{aligned} \langle v - w, v + w \rangle &= \langle v, v \rangle + \langle v, w \rangle - \langle w, v \rangle - \langle w, w \rangle \\ &= \langle v, v \rangle - \langle w, w \rangle \leq \langle v, v \rangle. \end{aligned}$$

Since this hold for any w,

$$\begin{aligned} I_E(v) &= \max_w \langle v - w, v + w \rangle \\ &\leq \langle v, v \rangle. \end{aligned}$$

Taking $w = 0$ shows that in fact

$$I_E(v) = \langle v, v \rangle. \ \clubsuit$$

Theorem (Classical Dirichlet Principle). If P is reversible,

$$D_E(f) = \min_{v|E=f} \langle v, v \rangle = \langle \phi, \phi \rangle,$$

where ϕ is the unique P-harmonic function with $\phi|E = f$, and this minimum is attained only when $v = \phi$. *qed*

Escape probabilities and commuting time

As an example of the Dirichlet Principle, take $E = \{a, b\}$, $f(a) = 1$, $f(b) = 0$. Then

$$\begin{aligned} D_E(f) &= \alpha_a P(\text{escape from } a \text{ to } b) \\ &= \alpha_a P(\text{escape from } a \text{ to } b \text{ backwards in time}) \\ &= \alpha_b P(\text{escape from } b \text{ to } a) \\ &= \alpha_b P(\text{escape from } b \text{ to } a \text{ backwards in time}) \\ &= 1/E(\text{commuting time between } a \text{ and } b). \end{aligned}$$

In the reversible case,

$$\begin{aligned} D_E(f) &= 1/E(\text{commuting time between } a \text{ and } b) \\ &= 1/(CR_{\text{eff}}) \\ &= C_{\text{eff}}/C, \end{aligned}$$

where R_{eff} is the effective resistance between a and b, and C_{eff} the effective conductance.

The Monotonicity Law

Given two matrices P and P', say that $P \leq P'$ if

$$P_{ij} \leq P'_{ij}$$

for all $i \neq j$.

Theorem (Monotonicity Law). Let P and P' be two Markov chains with the same equilibrium measure α. If $P \leq P'$ and P is reversible, then

$$D_E(f) \leq D'_E(f)$$

for any set E and real-valued function f on E.

Proof. Write

$$P' = P + R,$$

and let

$$P'' = I + R.$$

Then P'' is the transition matrix of a Markov chain with stationary measure α, and hence for any v,

$$\langle v, v\rangle' \;=\; \langle v, v\rangle + \langle v, v\rangle'' \geq \langle v, v\rangle.$$

Since P is reversible, $I_E(v) = \langle v, v\rangle$, and

$$\begin{aligned} I'_E(v) &= \max_w \langle v - w, v + w\rangle' \\ &\geq \langle v, v\rangle' \\ &\geq \langle v, v\rangle \\ &= I_E(v). \end{aligned}$$

Thus

$$D'_E(f) \geq D_E(f). \ \clubsuit$$

In the particular case where $E = \{a, b\}$, $f(a) = 1$, and $f(b) = 0$, the Monotonicity Law states that under the assumptions above, passing from P to P' increases the escape probability. From this it follows that if you perturb a transient reversible process by adding to it a drift that doesn't change the equilibrium measure of the process, the perturbed process is even more transient than the original. This result is due to Ross Pinsky, who proved it using his own theory of energy for non-reversible processes.

Note. Actually, I seem to recall that there is a question whether Pinsky's results do actually follow using this approach to energy, as claimed in the paragraph above. This has got to be looked into.

Probabilistic interpretation of energy

Theorem (Probabilistic interpretation of energy). Given E and f, let the process run for a long time N, and make a list of the values of f at all the times when the process is *in a state of* E. Add up the squares of the differences of consecutive entries in this list. Divide by N. You get $D_E(f)$. $\clubsuit$