Tension tensors of harmonic nets

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Net

We consider an infinite graph $X = (V, E)$ periodically embedded in $\mathbb{R}^N$.

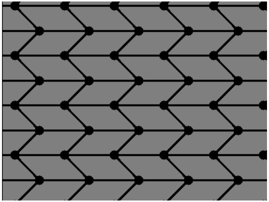

Figure: Yabane pattern

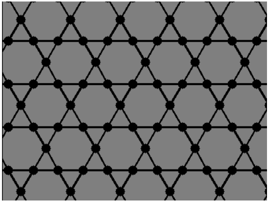

Figure: Kagome pattern

Let $L \subset \mathbb{R}^N$ be a period of the embedded graph X.
L is called a period lattice for X.
We assume that the quotient graph $X/L = (V/L, E/L)$ is finite.
Then X is called a net.

Harmonic net

The net $\boldsymbol{X}$ is called harmonic iff for any $\boldsymbol{v} \in \boldsymbol{V}$,

$$\sum_{(\boldsymbol{v},\boldsymbol{w})\in \boldsymbol{E}} (\boldsymbol{w} - \boldsymbol{v}) = \boldsymbol{0}.$$

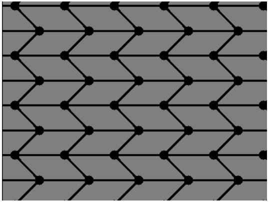

Figure: Yabane is not harmonic

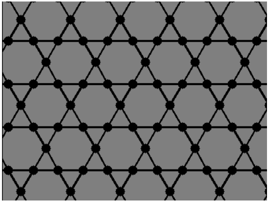

Figure: Kagome is harmonic

In other words, suppose that
(*) Every edge is an identical spring with original length zero and the same spring constant.
Then the net $\boldsymbol{X}$ is harmonic iff the sum of the spring's forces is balanced at any vertex.

Background – TPE (thermoplastic elastomer)

We are working on a project to research on TPE, which is polymeric material with the rubber elasticity.
We model the structure of TPE by an embedded graph.

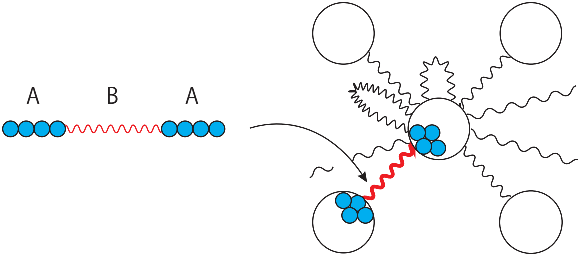

Figure: Structure of TPE (Figure by Ken'ichi Yoshida)

Tension Tensor (TT for short)

For a net $\boldsymbol{X} = (\boldsymbol{V}, \boldsymbol{E})$ with a period $\boldsymbol{L}$, we define the tension tensor (per period) $\mathcal{T}(\boldsymbol{X})$ by

$$\mathcal{T}(\boldsymbol{X}) := \sum_{\boldsymbol{e} \in \boldsymbol{E}/\boldsymbol{L}} \boldsymbol{e} \otimes \boldsymbol{e},$$

where

$$\begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} \otimes \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} (x_1, \dots, x_N) = \begin{pmatrix} x_1^2 & \cdots & x_1 x_N \\ \vdots & \ddots & \vdots \\ x_N x_1 & \cdots & x_N^2 \end{pmatrix}.$$

Remark that the trace of the tension tensor

$$\mathcal{E}(\boldsymbol{X}) = \operatorname{tr} \mathcal{T}(\boldsymbol{X}) = \sum_{\boldsymbol{e} \in \boldsymbol{E}/\boldsymbol{L}} \|\boldsymbol{e}\|^2$$

has been known as the energy of the net.

TT per edge / TT per volume

Remind that tension tensor per period

$$\mathcal{T}(X) := \sum_{e \in E/L} e \otimes e$$

depends on the choice of L.

To avoid such an ambiguity, we also use tension tensor per edge

$$\mathcal{T}_E(X) := \frac{\mathcal{T}(X)}{\#(E/L)}$$

or tension tensor per volume

$$\mathcal{T}_V(X) := \frac{\mathcal{T}(X)}{\mathrm{vol}(\mathbb{R}^N/L)}.$$

A volume preserving linear tranformation $A \in \mathrm{SL}(N, \mathbb{R})$ deforms a harmonic net X into $A(X)$. Remark that $A(X)$ is also a harmonic net. However the energy $\mathcal{E}(A(X))$ may differ from $\mathcal{E}(X)$.
A harmonic net X is said to be a standard net
if $\mathcal{E}(X)$ is the minimum among $\{\mathcal{E}(A(X)) \mid A \in \mathrm{SL}(N, \mathbb{R})\}$.

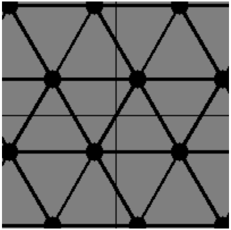

Figure: standard net

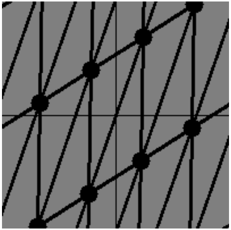

Figure: not standard net

Th. A harmonic net X is standard iff the tension tensor $\mathcal{T}(X)$ is a constant multiple of the identity matrix.

Visualisation of TT

To visualize the tension tensor, we define an ellipsoid by

$$\mathrm{Ell}(X) = \{x \in \mathbb{R}^N \mid x^{\mathsf{T}} \mathcal{T}_E(X)^{-1} x = 1\}.$$

It is easy to check that $A(\mathrm{Ell}(X)) = \mathrm{Ell}(A(X))$.
A harmonic net X is standard iff $\mathrm{Ell}(X)$ is a true sphere.

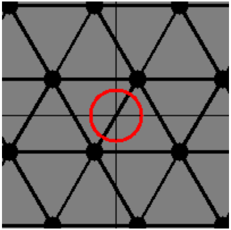

Figure: standard net

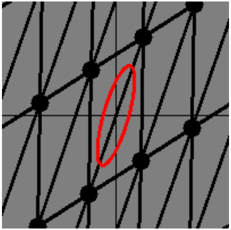

Figure: not standard net

TT as Cauchy stress tensor

Th. [K.-Yoshida]
We assume the condition
(*) Every edge is an identical spring with original length zero and the same spring constant.
Then the Cauchy stress tensor $\mathbf{\Sigma}$ of the whole structure is

$$\mathbf{\Sigma} = 2\mathcal{T}_{\mathcal{V}}(X).$$

Suppose X is a harmonic net in $\mathbb{R}^N$ and the origin of $\mathbb{R}^N$ is a vertex of X. Consider the random walk on the net X starting from the origin. Here, the random walk indicates that the random walker at a vertex $v \in V$ chooses an edge e originating from v with probability $1/\deg(v)$.

We denote by $(\xi_k^1, \ldots, \xi_k^N) \in \mathbb{R}^N$ the coordinates of the random walk after k steps. Note that for any k and i, the expected value $E[\xi_k^i]$ is equal to zero since X is harmonic.

Let Σ_k denote the k-th variance–covariance matrix of the random walk. In other words, the (i, j)-entry of Σ_k is $E[\xi_k^i \xi_k^j]$.

Prop. It holds that

$$\lim_{k\to\infty} \frac{1}{k}\Sigma_k = \mathcal{T}_E(X).$$

Proof. We use the well-known lemma for Cesàro means:
if $\lim_{k\to\infty} a_k = a$, then we have $\lim_{k\to\infty}(a_1 + \cdots + a_k)/k = a$.

Let $V_l^i = \xi_l^i - \xi_{l-1}^i$ for $l = 1, \ldots, k$. Then $\xi_k^i = V_1^i + \cdots + V_k^i$.
Set $\Delta_k = \Sigma_k - \Sigma_{k-1}$ for $k \geq 1$.

Thanks to Cesàro means' lemma, it is sufficient to show that

$$\lim_{k\to\infty} \Delta_k = \mathcal{T}_E(X).$$

Characterization of TT by a random walk (3/4)

Proof. (Cont.) The (i,j)-entry of Δ_k is equal to

$$\begin{aligned} E[\xi_k^i \xi_k^j] - E[\xi_{k-1}^i \xi_{k-1}^j] &= E[(V_k^i + \xi_{k-1}^i)(V_k^j + \xi_{k-1,}^j)] - E[\xi_{k-1}^i \xi_{k-1}^j] \\ &= E[V_k^i V_k^j] + E[V_k^i \xi_{k-1}^j] + E[\xi_{k-1}^i V_k^j] \\ &= E[V_k^i V_k^j]. \end{aligned}$$

Here, $E[V_k^i \xi_{k-1}^j] = E[\xi_{k-1}^i V_k^j] = 0$ since X is harmonic.
For each edge $\hat{e} \in E/L$, the probability that $\hat{e}$ is chosen as the k-th step converges to $1/\#(E/L)$ as $k \to \infty$. Therefore,

$$\lim_{k \to \infty} E[V_k^i V_k^j] = \frac{\sum_{e \in E/L} e^i e^j}{\#(E/L)},$$

where e^i and e^j are the i-th and j-th coordinates of e, respectively.
This limit coincides with the (i,j)-entry of $\mathcal{T}_E(X)$. □

Prop. (Restatement)

$$\lim_{k\to\infty} \frac{1}{k}\Sigma_k = \mathcal{T}_E(X).$$

Cor. The $1/\sqrt{k}$-rescaled random walk on X converges (in distribution) to the multivariate normal distribution with the variance–covariance matrix $\mathcal{T}_E(X)$.

proof. In the case of a standard net, the central limit theorem by Kotani and Sunada implies convergence to the spherical normal distribution.
For a general harmonic case, a linear transformation induces a multivariate normal distribution.
The variance–covariance matrix is given by the **Prop**. □