

Definition. An X -tree $\mathcal{T} = (T, \varphi)$ is an ordered pair where $T = (V, E)$ is a tree and $\varphi : X \rightarrow V$ is a labeling map such that $\varphi(X)$ contains all vertices of T with degree ≤ 2 .

Definition. A phylogenetic X -tree $\mathcal{T} = (T, \varphi)$ is an X -tree where φ is a bijection (1-to-1) from X to the leaves of T .

Definition. A dissimilarity map on X is a function $\delta : X \times X \rightarrow \mathbb{R}$ with $\delta(x, x) = 0$ and $\delta(x, y) = \delta(y, x)$ for all $x, y \in X$.

Definition. A dissimilarity map δ on X is a tree metric if there exists an X -tree $\mathcal{T} = (T, \varphi)$ and edge weight function $w : E \rightarrow \mathbb{R}_+$ such that the induced metric $d_{(\mathcal{T}, w)}$ is equal to δ .

Definition. A dissimilarity map δ on X satisfies the 4 point condition (4PC) if for all $w, x, y, z \in X$, $\delta(w, x) + \delta(y, z) \leq \max\{\delta(w, y) + \delta(x, z), \delta(w, z) + \delta(x, y)\}$.

Definition. A dissimilarity map δ on X is an ultrametric if for distinct $x, y, z \in X$, $\delta(x, y) \leq \max\{\delta(x, z), \delta(y, z)\}$.

Definition. An equidistant X -tree is a phylogenetic X -tree $\mathcal{T} = (T, \varphi)$ rooted at ρ , and an edge weight function $w : E \rightarrow \mathbb{R}$ such that for all $x, y \in X$, $d_{(\mathcal{T}, w)}(\rho, \varphi(x)) = d_{(\mathcal{T}, w)}(\rho, \varphi(y))$, and $w(e) \geq 0$ for all $e \in E$.

Definition. Given a dissimilarity map δ on X and some $r \in X$, the Gromov product is a function $\delta_r : X \setminus \{r\} \rightarrow \mathbb{R}$ defined

$$\delta_r(x, y) = \begin{cases} \frac{1}{2}(\delta(x, y) - \delta(x, r) - \delta(y, r)), & \text{if } x \neq y, \\ 0, & \text{if } x = y. \end{cases}$$

Lemma. If δ is an ultrametric, then there exists an equidistant X -tree (\mathcal{T}, w) with $\delta = d_{(\mathcal{T}, w)}$.

Lemma. A dissimilarity map δ satisfies the 4PC if and only if for all $r \in X$, the Gromov product δ_r is an ultrametric on $X \setminus \{r\}$.

Theorem. A nonnegative dissimilarity map δ satisfies the 4PC if and only if it is a tree metric.