Landscape dynamics, interbasin kinetics and ultrametric diffusion

S.V. Kozyrev

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Abstract

We discuss the interbasin kinetics approximation for random walk on a complex landscape. We show that for a generic landscape the corresponding model of interbasin kinetics is equivalent to an ultrametric diffusion, generated by an ultrametric pseudodifferential operator on the ultrametric space related to the tree of basins. The simplest example of ultrametric diffusion of this kind is described by the $p$–adic heat equation.

1 Introduction

Dynamics of a broad class of complex systems (glasses, clusters, polymers) is described by a random walk on a complex landscape of energy [1], [2], [3], [4]. Landscape is a real valued function (energy) on a domain in $\mathbb{R}^N$. Complex landscape is a function which possesses many local minima. In particular, models of this kind are important for description of protein dynamics in the relaxation approach [5]. Therefore approximations of dynamics on complex landscapes are important for applications.

We discuss the random walk on the complex energy landscape, given by the real valued function $U(x)$ on $\mathbb{R}^N$, with the temperature $T$ and the inverse temperature $\beta = 1/kT$ ($k$ is the Boltzmann constant). This random walk is defined as follows: the transition probability rate for transitions between the two neighbor infinitesimal vicinities $O_1$, $O_2$ of the energy surface will be proportional to the Boltzmannian factor $\exp(-\beta \Delta U)$, where $\Delta U$ is the energy difference for the sets $O_1$ and $O_2$. This formula is valid for transitions which increase energy, for transitions which decrease energy we put the Boltzmannian factor equal to one.

For random walk under discussion the system will spend more time in the low energy areas of the energy landscape. Therefore we get the following picture — the system stays in the vicinities of local minima and performs transitions between local minima through the energy barriers. For a generic landscape local minima will be hierarchically clustered with respect to the energy barrier between the minima.

These arguments suggest the approach of interbasin kinetics, which is the approximation of a dynamics on a complex landscape, based on the description of the kinetics of transitions between the groups of states, called basins. The minimal basins correspond to local minima of energy, the larger basins are hierarchical unions of smaller basins.

The postulates of interbasin kinetics:
The space of states is separated into basins, basins are separated into subbasins in a hierarchical way.

The activation energy barrier between the two states depends only on basins, containing these states and does not depend on the choice of states in these basins.

Therefore the transitions between basins are described by the system of kinetic equations:

\[
\frac{d}{dt} f(i, t) = - \sum_j [T(i, j)f(i, t) - T(j, i)f(j, t)] \nu(j)
\]

Here the indices \(i, j\) enumerate the states of the system (which correspond to the minimal basins, or local energy minima), \(T(i, j) \geq 0\) is the probability rate for transitions from \(i\) to \(j\), \(\nu(j) > 0\) are positive numbers (volumes of the basins).

The described constraints of interbasin kinetics on the matrix \(T(i, j)\) imply that this matrix will be a block matrix with a large number of equal elements. The important example is the Parisi matrix \(T(i, j)\) (used in the theory of spin glasses, see [6]).

Various models of interbasin kinetics and hierarchical dynamics were studied in many papers, see [7], [8], [9], [10]. In papers [11], [12] \(p\)-adic diffusion was discussed in relation to the relaxation of spin glasses.

Protein dynamics was studied, with the help of the Mossbauer spectroscopy by H.Frauenfelder [1] and V.I.Goldansky [13]. Hierarchical approach to description of the space of state of a protein was proposed by H.Frauenfelder, see [1].

In [14] it was proposed the approach to describe the interbasin kinetics models with the help of ultrametric diffusion, generated by pseudodifferential operators. Namely, the postulates of interbasin kinetics are put into the form:

1. The space of states is ultrametric
2. Transition probability rate is locally constant

In the simplest case (when \(T(i, j)\) is the \(p\)-adic Parisi matrix of some simple form, all \(\nu(j)\) are equal) the system of equations of interbasin kinetics takes the form [15] of the \(p\)-adic heat equation

\[
\frac{\partial}{\partial t} f(x, t) + D_x^a f(x, t) = 0
\]

Initially this equation was introduced in [16] from purely mathematical motivations. Here \(D_x^a\) is the Vladimirov operator of \(p\)-adic fractional differentiation with respect to \(x\). This parameter describes the tree of basins for the complex energy landscape, in the system of equation of interbasin kinetics \(x\) corresponds to the index \(i\) of the local minima. For the models of protein dynamics \(x\) is the conformational parameter. \(p\)-Adic models of interbasin kinetics were discussed in [15], [14], [17].

Procedures of construction of the hierarchy of basins and of models of interbasin kinetics starting from the energy landscape were studied by Stilinger and Weber [18], [19], Becker and Karplus [20]. These models were applied to construction of hierarchy of basins for peptides [20] using the data of molecular dynamics. Complex landscape in this approach is approximated by the disconnectivity graph and the function of energy barriers on this graph.

In the present paper we construct the equation of ultrametric diffusion which describes the interbasin kinetics approximation for the dynamics on a complex landscape of a generic form.
This equation has the form of the following ultrametric pseudodifferential equation

\[ \frac{\partial}{\partial t} f(x, t) + \int_X e^{-\beta E(\sup(x, y))} \left[ e^{\beta E(x)} f(x, t) - e^{\beta E(y)} f(y, t) \right] d\nu(y) = 0 \]  

(3)

Here \( x, y \in X \) lie in the ultrametric space which describes the tree of basins for the landscape of energy, \( f(x, t) \) is the distribution of occupation. For a wide class of landscapes the above equations are exactly solvable. Thus the dynamics on complex landscapes in these cases can be investigated analytically. The important example of the above equation is the \( p \)-adic heat equation (2).

The exposition of the present paper is as follows.

In Section 2 we describe the procedure of construction of the tree of basins and the function of activation energy barriers for a generic landscape.

In Section 3 we construct the corresponding general model of interbasin kinetics.

In Section 4 we show the equivalence of the interbasin kinetics model of Section 3 and the model of ultrametric diffusion on the space corresponding to the tree of basins.

In Section 5 we discuss the clustering procedure.

In Section 6 we put some material on ultrametric analysis.

2 Energy landscape and the tree of basins

Let us describe the procedure which puts into correspondence to an energy landscape \( U \) (a smooth real valued function defined in a domain (or the configuration space) \( M \subset \mathbb{R}^N \)) the tree of basins, the function on this tree which describes the activation barriers for a random walk on the landscape, and the measure on the border of the tree of basins which describes volumes of the corresponding basins.

Let us consider the set of all local minima of \( U \). We assume that this set is finite. For the local minimum \( i \) consider the set \( R(i) \) in the configuration space \( M \) (the basin of attraction of \( i \)), which contains the points \( \xi \in M \), for which:

1) There exists a path (i.e. a continuous curve) in the configuration space, which connects \( \xi \) and \( i \), and the function \( U \) does not increase on the path from \( \xi \) to \( i \).

2) If there exist paths from \( \xi \) to several local minima, and the function \( U \) is non increasing along these paths, then the distance between \( \xi \) and \( i \) is less or equal than the distances between \( x \) and the other minima. Here the distance between \( \xi \) and \( i \) is understood as a distance along the surface of energy, i.e. the distance between two points of a landscape is the infimum of lengths of paths on the energy landscape, which connect the points.

The different \( R(i), R(j) \) can intersect on the sets of measure zero. The union of all \( R(i) \) gives the whole configuration space.

Put into correspondence to the basin \( R(i) \) the volume \( \#(i) \):

\[ \#(i) = \int_{R(i)} dx \]

Let us introduce the following notations.

1) Assume that the points \( a, b \) are connected by the path \( S \) in the configuration space \( M \). We say that the point \( a \) is separated from \( b \) by the energy barrier \( E \) at the path \( S \), if the following
supremum over the points $\xi \in S$ is equal to $E$:

$$\sup_{\xi \in S} U(\xi) = E$$

2) We say that the points $a, b$ in the configuration space are separated by the energy barrier (or the activation barrier) $E(a, b)$, if the infimum over the paths $S$ from $a$ to $b$ in the configuration space of the energy barriers at the path $S$ is equal to $E(a, b)$:

$$E(a, b) = \inf_S \sup_{\xi \in S} U(\xi)$$

Let $\beta$ be a positive number (the inverse temperature). Let us introduce on the set of local minima the metric

$$d(i, j) = e^{-\beta E(i, j)}$$

For a generic landscape $U$ this metric will satisfy the strong triangle inequality (i.e. will be an ultrametric).

Let us fix the energy scale — the increasing sequence of real numbers $\{E_k\}$, and the corresponding sequence of positive numbers $D = \{d_k\}, d_k = e^{-\beta E_k}$. Consider the corresponding clustering $C_D$ of the set of local minima with the distance $d(\cdot, \cdot)$ (see the Appendix 1).

The clusters from $C_D$ we will also call the basins. Let us call the directed tree $T$ for the clustering $C_D$ the disconnectivity graph of the landscape $U$. Using this tree we build the ultrametric space $X(T)$ (see the Appendix 2). The points of this space correspond to the local minima of the energy landscape, the balls (with respect to the ultrametric) correspond to the basins. One can say that a point $x$ corresponds to some local minimum $i$ together with the set of inclusions of the corresponding basins which contain $i$.

On the space $X$ there exists the natural measure $\nu$, such that the measure $\nu(x)$ of the point $x \in X$ (the space $X$ in the case under consideration consists of the finite number of points) is equal to the volume of the basin of attraction of the local minimum $\#(i)$.

3 Our ansatz of interbasin kinetics

Consider the tree of basins for the energy landscape, built with the help of the procedure of the previous section. Let us construct the system of equations of interbasin kinetics using the Arrhenius–Eyring formula, which gives the approximation for the velocity constant of reaction in chemical kinetics:

$$\kappa = A \exp(-\beta \Delta F)$$

where $\kappa$ is the velocity constant of reaction, $\Delta F$ is the free energy of activation, $A$ is some constant, $\beta$ is the inverse temperature. Let us remind that the free energy of the group of states (with the same energy) is defined as

$$F = E - \theta S$$

where $E$ is the energy of the group of states, $\theta = \beta^{-1}$ is the temperature, $S$ is the entropy (logarithm of the number of states in the group).

We consider the system of equations of interbasin kinetics of the form

$$\frac{dg(i, t)}{dt} = -\sum_{j \neq i} \left[ e^{\beta F(i) - G(\sup(i, j))} C(i, j) g(i, t) - e^{\beta F(j) - G(\sup(i, j))} C(j, i) g(j, t) \right]$$
Here $i, j$ are minimal basins (which correspond to local minima), $g(i)$ is the occupation of the minimal basin $i$, $F(i)$ is the free energy of the basin $i$, $\text{sup}(i, j)$ is the minimal superbasin which contains both the basins $i$ and $j$, $G(\text{sup}(i, j))$ is the free energy of the transition state for transitions between $i$ and $j$.

This system of equations is based on the Eyring formula and the assumption that the transition state for transitions between $i$ and $j$ is defined by the superbasin $\text{sup}(i, j)$.

We choose the coefficients $C(i, j)$ to be positive and symmetric. In this case the above system of kinetic equations satisfies the conditions of detailed balance. These coefficients describe the modification of the Eyring formula on the case of transitions between the groups of states with the unique intermediate transition state. Choice of the coefficients $C(i, j)$ fixes the model of interbasin kinetics. We propose the following ansatz for the coefficients:

$$C(i, j) = \frac{\#(i)#(j)}{\#^2(\text{sup}(i, j))}$$

(4)

Here $\#(i)$ is the number of states in the basin $i$ (i.e. the volume of this basin). This choice satisfies the scaling conditions — the coefficients $C(i, j)$ do not change with dilatations of the landscape.

With this choice of the coefficients the system of equations of interbasin kinetics takes the form

$$\frac{df(i, t)}{dt} = -\sum_{j \neq i} e^{-\beta G(\text{sup}(i, j))} \frac{\#(\text{sup}(i, j))}{\#^2(\text{sup}(i, j))} \left[ e^{\beta E(i)} f(i, t) - e^{\beta E(j)} f(j, t) \right] \#(j)$$

Here $f(i) = g(i)/\#(i)$ is the density of occupation of the basin $i$, $E(i)$ is the energy of the basin $i$ (i.e. $e^{\beta F(i)} = e^{\beta E}/\#(i)$). We choose the volumes of the transition states for basins $\text{sup}(i, j)$ to be proportional to the volumes of these basins:

$$e^{S(\text{sup}(i, j))} \sim \#(\text{sup}(i, j))$$

(5)

where $S(\text{sup}(i, j))$ is the entropy of the transition state. With this choice of entropy for transition states (we ignore the corresponding coefficient of proportionality) the system of equations of interbasin kinetics takes the form

$$\frac{df(i, t)}{dt} = -\sum_{j \neq i} e^{-\beta E(\text{sup}(i, j))} \frac{\#(\text{sup}(i, j))}{\#(\text{sup}(i, j))} \left[ e^{\beta E(i)} f(i, t) - e^{\beta E(j)} f(j, t) \right] \#(j)$$

(6)

Here $E(\text{sup}(i, j))$ is the energy of the transition state for the basin $\text{sup}(i, j)$, and this value coincides with the energy used in the clustering procedure of construction of the tree of basins.

Therefore the introduced here ansatz of interbasin kinetics is based on the clustering procedure of construction of the tree of basins, the Arrhenius–Eyring formula and conditions (4), (5), and generates the system of equations (6).

### 4 Ultrametric diffusion

In the present section we show that the system of equations of interbasin kinetics is equivalent to the dynamics on the ultrametric space $X$ corresponding to the tree of basins.

We have the following theorem.
Theorem 1  The system of equations of interbasin kinetics (6) is equivalent to the ultrametric pseudodifferential equation

\[
\frac{\partial}{\partial t} f(x, t) + \int_X e^{-\beta E(\sup(x, y))} \left[ e^{\beta E(x)} f(x, t) - e^{\beta E(y)} f(y, t) \right] d\nu(y) = 0
\]  

(7)

where the ultrametric space \( X \) corresponds to the tree of basins of the energy landscape, the points \( x \) of the ultrametric space correspond to the minimal basins \( i \) (basins of attraction of local minima), the measure \( \nu \) describes volumes of the basins (i.e. for the minimal basin \( i \) corresponding to the minimal ball \( x \) we have \( \nu(x) = \#(i) \)).

We will not restrict the consideration of the dynamics on energy landscapes to ultrametric spaces containing finite number of points, but instead we will consider the general case of equations of the form (7). Finite trees of basins are obtained because we consider smooth energy landscapes. In reality energy landscapes can be complex and rugged. For a rugged energy landscape the described procedure is not directly applicable. Instead we can consider the inductive limit of directed trees and related spaces of functions. We investigate the pseudodifferential equation of the form (7) on the ultrametric space corresponding to the limiting infinite tree, and interpret this equation as describing dynamics on a rugged landscape.

Example  Consider the case when \( X = Q_p \), the measure \( \nu \) is the Haar measure \( \mu \), and the activation energy is chosen as follows:

\[
E(|x - y|_p) = k \ln |x - y|_p, \quad k > 0,
\]

The potential of the minimal basins (point in \( Q_p \)) is equal to zero. In the notation \( |x - y|_p = p^\gamma \), the activation energy is linear with respect to \( \gamma \). We get for the transition probability rate the expression

\[
\frac{e^{-\beta E(\sup(x, y))}}{\nu(\sup(x, y))} = \frac{e^{-\beta k \ln |x - y|_p}}{|x - y|_p} = \frac{1}{|x - y|_p^{1+\beta k}}
\]

Equation of interbasin kinetics takes the form of the \( p \)-adic heat equation

\[
\frac{\partial}{\partial t} f(x, t) + D_x^\alpha f(x, t) = 0
\]

where the parameter \( \alpha \) of the Vladimirov operator of the \( p \)-adic fractional differentiation

\[
D_x^\alpha f(x, t) = \Gamma_p^{-1}(-\alpha) \int_{Q_p} \frac{f(x, t) - f(y, t)}{|x - y|_p^{1+\alpha}} d\mu(x)
\]

is proportional to the inverse temperature: \( \alpha = \beta k \).

Remark  Cauchy problem for the \( p \)-adic heat equation is exactly solvable. Analogously, Cauchy problem for equation (7) is exactly solvable (with the help of the ultrametric wavelet transform) if the energies of local minima are equal: \( E(x) = \text{const} \). Therefore in the interbasin kinetics approximation the dynamics for a wide class of complex energy landscapes possesses analytical investigation.
Example: Mb–CO rebinding  

One of the most important applications of the dynamics on energy landscapes and interbasin kinetics is the application to conformational dynamics of proteins. In this case the ultrametric parameter $x$ describes the conformational coordinate for the protein.

In paper [14] it was shown that the obtained with the help of $p$–adic methods results on protein dynamics coincide with the data of spectroscopic experiments for Mb–CO rebinding. Mb–CO rebinding is a fundamental model in the physics of proteins and plays the role of "the hydrogen atom of biology" [2].

Let us describe the approach of [14]. Myoglobin can bind CO only when myoglobin is in some particular subset of the space of conformations (when the path to the active center of the molecule is opened). Consider the model of Mb–CO rebinding described by the equation of interbasin kinetics

$$\frac{\partial}{\partial t} + D_\alpha x + \Omega(|x|_p) f(x, t) = 0 \quad (8)$$

Here $\alpha$ is proportional to the inverse temperature $\beta$, the conformational coordinate is parameterized by the field of $p$–adic numbers. The function $f(x,t)$ is the density of occupation of the space of conformations for molecules of myoglobin (not bound to CO). The Mb–CO binding takes place on the subset of the space of conformations described by the unit ball in $Q_p$.

Equation (8) is a model of ultrametric diffusion with a sink.

Remark  

In the model of Mb–CO rebinding (8) we get the generator of diffusion with a sink in the form of the $p$–adic Schrödinger operator

$$D_\alpha x + \Omega(|x|_p).$$

The term with positive potential describes a sink (negative potential will describe a source). The Vladimirov operator $D_\alpha x$ plays the role of a $p$–adic Laplacian.

The operator in the RHS of the equation (17) have the form of the product of operators

$$Df(x) = \int_X e^{-\beta E(\text{sup}(x,y))} \left[ e^{\beta E(x)} f(x) - e^{\beta E(y)} f(y) \right] d\nu(y) = TXf(x),$$

where

$$TF(x) = \int_X \frac{e^{-\beta E(\text{sup}(x,y))}}{\nu(\text{sup}(x,y))} [f(x) - f(y)] d\nu(y),$$

is the ultrametric pseudodifferential operator and

$$Xf(x) = e^{\beta E(x)} f(x)$$

is the operator of multiplication by the exponent of the potential.

Therefore in applications of ultrametric analysis to models of interbasin kinetics we get the Schrödinger operator (a sum of a pseudodifferential operator and an operator of multiplication by a function), and a product of a pseudodifferential operator and an operator of multiplication by a positive function.
5 Appendix 1: Clustering

In the present section we discuss the clustering procedure for metric spaces. Denote \((M, \rho)\) the metric space \(M\) with metric \(\rho\).

**Definition 2** A sequence of points \(a = x_0, x_1, \ldots, x_{n-1}, x_n = b\) in the metric space \((M, \rho)\) is called an \(\varepsilon\)-chain connecting \(a\) and \(b\), if \(\rho(x_k, x_{k+1}) \leq \varepsilon\) for all \(0 \leq k < n\). If there exists an \(\varepsilon\)-chain connecting \(a\) and \(b\), we say that \(a\) and \(b\) are \(\varepsilon\)-connected.

In an ultrametric space any two points \(a, b\) are not \(\varepsilon\)-connected for \(\varepsilon < \rho(a, b)\).

**Definition 3** Let \((M, \rho)\) be an arbitrary metric space. Let us define the chain distance

\[
d(a, b) = \inf (\varepsilon : a, b \text{ are } \varepsilon\text{-connected}).
\]

The chain distance \(d(a, b)\) between the points \(a\) and \(b\) satisfies all the properties of ultrametric except for nondegeneracy, i.e.

\[
d(a, b) = d(b, a) \quad \forall a, b,
\]

\[
d(a, b) \leq \max (d(a, c), d(c, b)) \quad \forall a, b, c,
\]

but it is possible that \(d(a, b) = 0\) for some \(a \neq b\).

If the space \(M\) is ultrametric (i.e. \(\rho\) satisfies the strong triangle inequality), then the chain distance \(d(\cdot, \cdot)\) will coincide with the ultrametric \(\rho(\cdot, \cdot)\).

**Definition 4** Let us call the cluster \(C(i, R)\) in the metric space \((M, \rho)\) the ball with respect to the chain distance with the center in \(i\) and the radius \(R\), i.e. the set \(\{j \in M : d(i, j) \leq R\}\). The clustering of the space \(M\) is the set of clusters in \(M\), such that any element of \(M\) lies in some cluster.

By this definition the set of clusterings is partially ordered: assume we have two clusterings \(\mathcal{A}\) and \(\mathcal{B}\) of the set \(S\), then \(\mathcal{A} > \mathcal{B}\), if all clusters of \(\mathcal{B}\) are subsets of clusters of \(\mathcal{A}\).

Since the chain distance satisfies the strong triangle inequality, any clustering \(\mathcal{C}\) generates a directed tree of clusters \(\mathcal{T} = \mathcal{T}[M]\) and an ultrametric on this tree (the chain distance between clusters). Then using the standard procedure (see the Appendix 2) we construct the ultrametric space \(X = X(\mathcal{T})\) (the chain space of the clustering \(\mathcal{C}\)), which can be identified with the border of the tree \(\mathcal{T}\). Clusters in the metric space \(M\) correspond to balls in the ultrametric space \(X\).

**Example** Consider the important example of clustering. Let \(D = \{d_i\}\) be a finite or countable set of positive numbers without positive accumulation points. Consider the clustering \(\mathcal{C}_D\) of the metric space \((M, \rho)\) which contains all clusters of chain radii \(d_i \in D\) and arbitrary centers.

6 Appendix 2: Ultrametric analysis

In this Section we discuss some results on ultrametric analysis, which can be found in [21], [22], [23].
**Definition 5** An ultrametric space is a metric space with the ultrametric \(d(x, y)\) (where \(d(x, y)\) is called the distance between \(x\) and \(y\)), i.e. a function of two variables, satisfying the properties of positivity and non degeneracy

\[
d(x, y) \geq 0, \quad d(x, y) = 0 \implies x = y;
\]

symmetricity

\[
d(x, y) = d(y, x);
\]

and the strong triangle inequality

\[
d(x, y) \leq \max(d(x, z), d(y, z)), \quad \forall x, y, z.
\]

We say that an ultrametric space \(X\) is regular, if this space satisfies the following properties:

1) The set of all the balls of nonzero diameter in \(X\) is finite or countable;

2) For any decreasing sequence of balls \(\{D^{(k)}\}\), \(D^{(k)} \supset D^{(k+1)}\), the diameters of the balls tend to zero;

3) Any ball of non–zero diameter is a finite union of maximal subballs.

Ultrametric spaces are dual to directed trees. Below we describe some part of the duality construction.

For a regular ultrametric space \(X\) consider the set \(\mathcal{T}(X)\), which contains all the balls in \(X\) of nonzero diameters, and the balls of zero diameter which are maximal subbals in balls of nonzero diameters. This set possesses a natural structure of a directed tree. Two vertices \(I\) and \(J\) in \(\mathcal{T}(X)\) are connected by an edge if the corresponding balls are ordered by inclusion, say \(I \supset J\) (i.e. one of the balls contain the other), and there are no intermediate balls between \(I\) and \(J\).

The partial order in \(\mathcal{T}(X)\) is defined by inclusion of balls, this partial order is a direction. We recall that a partially ordered set is a directed set (and a partial order is a direction), if for any pair of elements there exists the unique supremum with respect to the partial order.

On the directed tree \(\mathcal{T}(X)\) we have the natural increasing positive function which puts into correspondence to any vertex the diameter of the corresponding ball.

Assume now we have a directed tree \(\mathcal{T}\) with the positive increasing function \(F\) on this tree. Then we define the ultrametric on the set of vertices of the tree as follows: \(d(I, J) = F(\text{sup}(I, J))\) where \(\text{sup}(I, J)\) is the supremum of vertices \(I, J\) with respect to the direction.

Then we take completion of the set of vertices with respect to the defined ultrametric and eliminate from the completion all the inner points of the tree (a vertex of the tree is inner if it does not belong to the border of the tree). We denote the obtained space \(X(\mathcal{T})\), this space is ultrametric.

An ultrametric pseudodifferential operator is defined in the following way. Consider a \(\sigma–\)additive Borel measure \(\nu\) with countable or finite basis on a regular ultrametric space \(X\). Consider the pseudodifferential operator

\[
Tf(x) = \int T(\text{sup}(x, y))(f(x) - f(y))d\nu(y)
\]

Here \(T(I)\) is some complex valued function on the tree \(\mathcal{T}(X)\). The supremum

\[
\text{sup}(x, y) = I
\]
of the points \( x, y \in X \) is the minimal ball \( I \) in \( X \), containing both points.

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