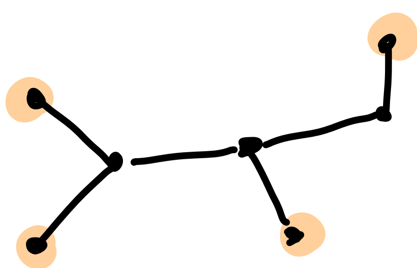
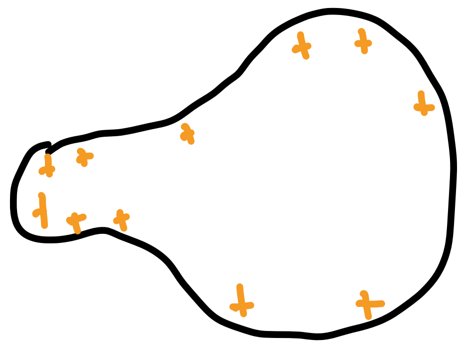
Distance matrices & equilibrium measures on trees



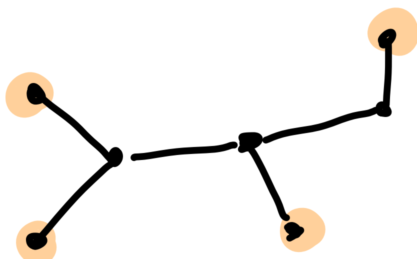


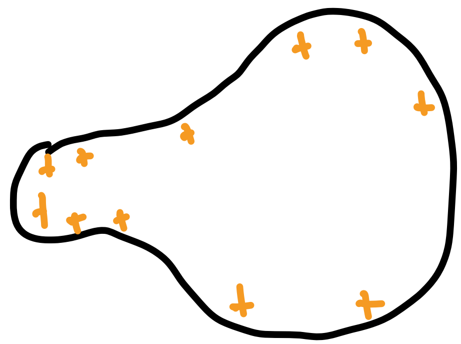
Harry Richman

7 December 2022

Matsen Lab, Fred Hutch

Distance matrices & equilibrium measures on trees

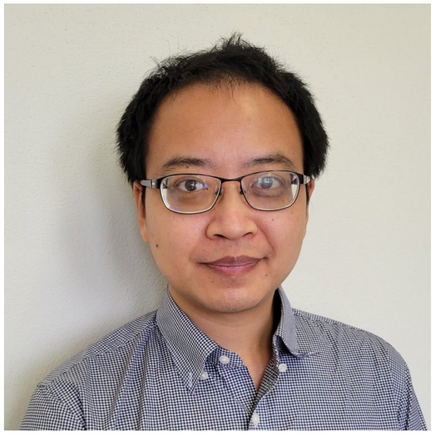




joint work w/

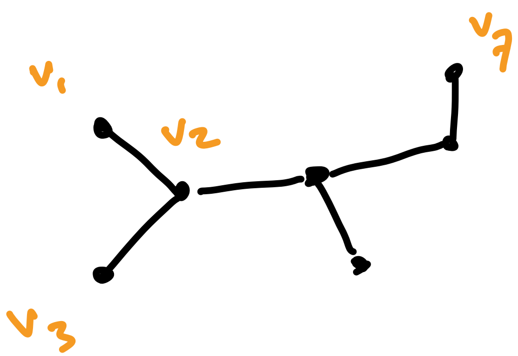
Farbod Shokrieh, Chenxi Wu

U. Washington U. Wisconsin



Distance matrices

Problem What does the determinant of a distance matrix tell us "combinatorially"?



tree

$$D = \begin{array}{cc} & \begin{array}{ccccccc} v_1 & v_2 & v_3 & & \cdots & & v_7 \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ \\ \vdots \\ \\ v_7 \end{array} & \begin{bmatrix} 0 & 1 & 2 & 2 & 3 & 3 & 4 \\ 1 & 0 & 1 & 1 & 2 & 2 & 3 \\ 2 & 1 & 0 & 2 & 3 & 3 & 4 \\ 2 & 1 & 2 & 0 & 1 & 1 & 2 \\ 3 & 2 & 3 & 1 & 0 & 2 & 3 \\ 3 & 2 & 3 & 1 & 2 & 0 & 1 \\ 4 & 3 & 4 & 2 & 3 & 1 & 0 \end{bmatrix} \end{array}$$

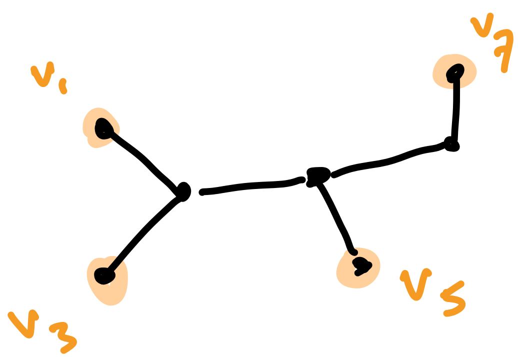
distance matrix

all nodes, internal included

Distance matrices

Problem What does the determinant of a distance submatrix tell us "combinatorially"?

$$D = \begin{bmatrix} 0 & 1 & 2 & 2 & 3 & 3 & 4 \\ 1 & 0 & 1 & 1 & 2 & 2 & 3 \\ 2 & 1 & 0 & 2 & 3 & 3 & 4 \\ 2 & 1 & 2 & 0 & 1 & 1 & 2 \\ 3 & 2 & 3 & 1 & 0 & 2 & 3 \\ 3 & 2 & 3 & 1 & 2 & 0 & 1 \\ 4 & 3 & 4 & 2 & 3 & 1 & 0 \end{bmatrix}$$



tree

$$D[S] = \begin{bmatrix} 0 & 2 & 3 & 4 \\ 2 & 0 & 3 & 4 \\ 3 & 3 & 0 & 3 \\ 4 & 4 & 3 & 0 \end{bmatrix}$$

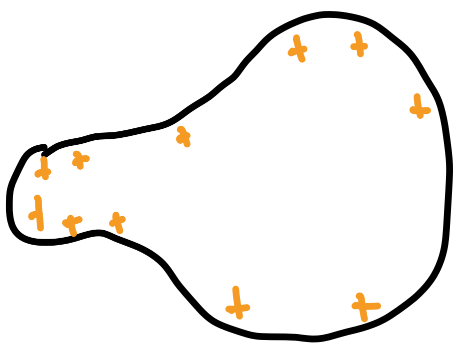
e.g. only leaf nodes

distance submatrix

Equilibrium measures $\rightsquigarrow$ "Potential theory"

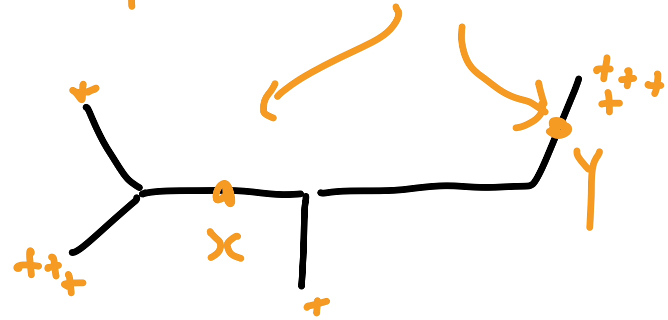
Problem How do particles "distribute" along a region, given repulsive potential $U(x,y)$?

$U(x,y) = -\ln|x-y|$



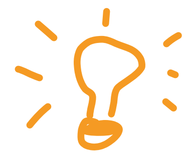
2-dim region

$U(x,y) = -\operatorname{dist}(x,y)$



1-dim tree

Problem What does the determinant of a distance matrix tell us "combinatorially"?



Problem How do particles "distribute" along a tree, given repulsion function $U(x,y)$?

Distance matrices

__Problem__ What does the determinant of a distance matrix tell us "combinatorially"?

What do we mean?

__Ex.__ Matrix tree theorem:

Laplacian matrix $\rightsquigarrow$ number of spanning trees

Aside:

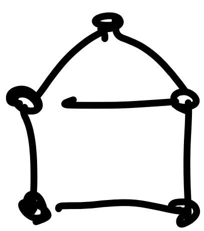
Spanning trees

A spanning tree is a subgraph which

"spanning" • contains all vertices

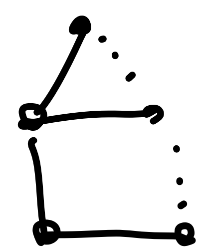
"tree"
• contains no cycles
• is connected

Ex.



G

⇝ spanning trees



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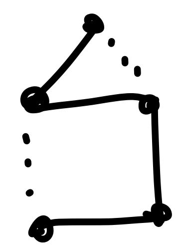


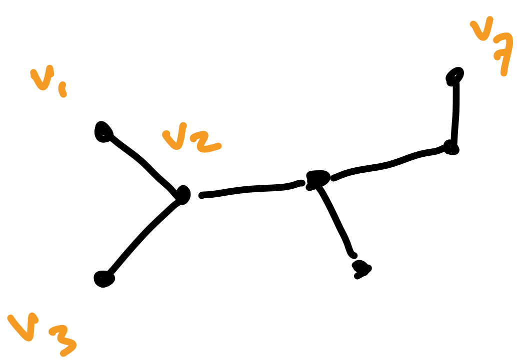
, . . .

How many?

Aside: Laplacian matrices

$L = (\text{degree}) - \left(\begin{smallmatrix}\text{adjacency} \\ \text{matrix}\end{smallmatrix}\right)$

Problem What does the determinant of a Laplacian matrix tell us "combinatorially"?



tree

$$L = \begin{array}{c|ccccccc}
 & v_1 & v_2 & v_3 & \cdots & & & v_7 \\
\hline
v_1 & 1 & -1 & & & & & \\
v_2 & -1 & 3 & -1 & -1 & & & \\
v_3 & & -1 & 1 & & & & \\
\vdots & & -1 & & 3 & -1 & -1 & \\
 & & & & -1 & 1 & & \\
 & & & & -1 & & 2 & -1 \\
v_7 & & & & & & -1 & 1
\end{array}$$

Laplacian matrix

Aside: Laplacian matrices

Problem What does the determinant of a Laplacian matrix tell us "combinatorially"?

Note: $\det L = 0$:(

Theorem (Kirchhoff 1847, "Matrix-tree theorem")

Given graph G, Laplacian matrix L

$$\det L[\bar{q}] = \#\{\text{spanning trees of } G\}$$

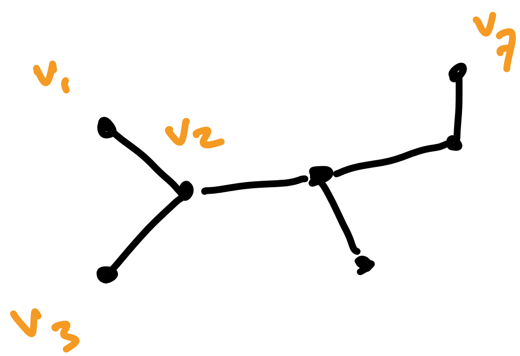
"q-reduced Laplacian", any $q \in V$

Aside: Laplacian matrices

Theorem (Kirchhoff) $\quad \det L[\bar{q}] = \#\{\text{spanning trees of } G\}$

"reduced Laplacian"

Ex.



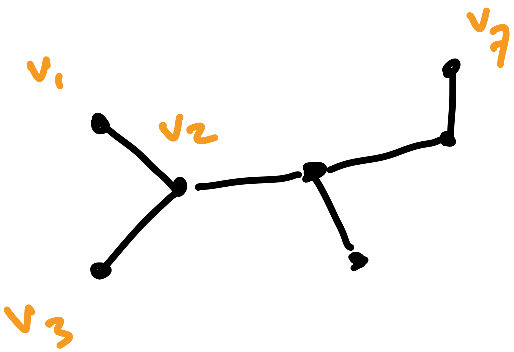
tree

$$L = \begin{array}{c|ccccccc} & v_1 & v_2 & v_3 & & \cdots & & v_7 \\ \hline v_1 & 1 & -1 & & & & & \\ v_2 & -1 & 3 & -1 & -1 & & & \\ v_3 & & -1 & 1 & & & & \\ & & -1 & & 3 & -1 & -1 & \\ \vdots & & & & -1 & 1 & & \\ & & & & -1 & & 2 & -1 \\ v_7 & & & & & & -1 & 1 \end{array}$$

$$\Rightarrow \quad \det L[\bar{v}_1] = 1$$

Distance matrices

Problem What does the determinant tell us ?



tree

$$D = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ \\ \\ v_7 \end{array} \begin{array}{c} \begin{array}{ccccccc} v_1 & v_2 & v_3 & & \cdots & & v_7 \end{array} \\ \begin{bmatrix} 0 & 1 & 2 & 2 & 3 & 3 & 4 \\ 1 & 0 & 1 & 1 & 2 & 2 & 3 \\ 2 & 1 & 0 & 2 & 3 & 3 & 4 \\ 2 & 1 & 2 & 0 & 1 & 1 & 2 \\ 3 & 2 & 3 & 1 & 0 & 2 & 3 \\ 3 & 2 & 3 & 1 & 2 & 0 & 1 \\ 4 & 3 & 4 & 2 & 3 & 1 & 0 \end{bmatrix} \end{array}$$

distance matrix

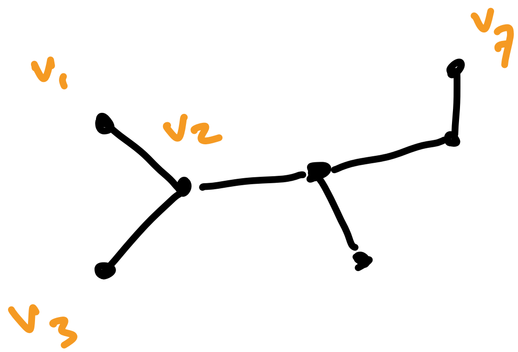
all nodes, internal included

$\Rightarrow \det D = 192$

Combinatorial info ?

Distance matrices

Problem What does the determinant tell us ?



tree

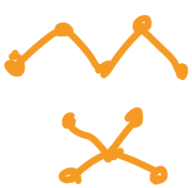
$$D = \begin{array}{c c} & \begin{array}{ccccccc} v_1 & v_2 & v_3 & & \cdots & & v_7 \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ \\ \vdots \\ \\ v_7 \end{array} & \begin{bmatrix} 0 & 1 & 2 & 2 & 3 & 3 & 4 \\ 1 & 0 & 1 & 1 & 2 & 2 & 3 \\ 2 & 1 & 0 & 2 & 3 & 3 & 4 \\ 2 & 1 & 2 & 0 & 1 & 1 & 2 \\ 3 & 2 & 3 & 1 & 0 & 2 & 3 \\ 3 & 2 & 3 & 1 & 2 & 0 & 1 \\ 4 & 3 & 4 & 2 & 3 & 1 & 0 \end{bmatrix} \end{array}$$

distance matrix

all nodes,
internal included

Theorem (Graham – Pollak, 1971)

$$\det D = (-1)^{n-1} 2^{n-2} (n-1)$$

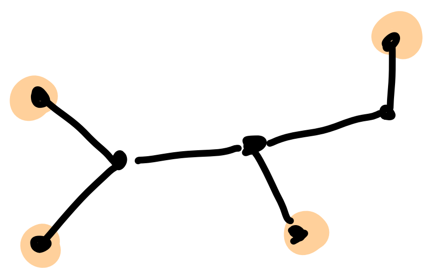


where n = # of vertices

no
combinatorics

Distance matrices

<u>Problem</u> What does the determinant tell us ?



tree

$$D[S] = \begin{bmatrix} 0 & 2 & 3 & 4 \\ 2 & 0 & 3 & 4 \\ 3 & 3 & 0 & 3 \\ 4 & 4 & 3 & 0 \end{bmatrix}$$

e.g. only leaf nodes

distance submatrix

$\rightsquigarrow \det D[S] = -252$??

⚠ No previously known combinatorial interpretation, to my knowledge ...

Distance matrices

Thm (Graham-Pollak)

$\det D = (-1)^{n-1} 2^{n-2} (n-1)$

Theorem (R - Shokrieh - Wu)

Given a tree $G = (V, E)$

a vertex subset $S \subset V$

corresponding distance submatrix $D[S]$,

then

$$\det D[S] = (-1)^{|S|-1} 2^{|S|-2} \left((n-1)\, \kappa_1(G;S) - \sum_{F \in \mathcal{F}_2(G;S)} \left(\deg^{\circ}(F,*)-2\right)^2 \right)$$

where n = # vertices

$\kappa_1(G;S)$ = # S-rooted spanning forests

$\mathcal{F}_2(G;S)$ = $(S,*)$ - rooted spanning forests

$\deg^{\circ}(F,*)$ = out-degree of floating component

Rmk: $\mathcal{F}_1(G;S) \leftrightarrow$ spanning tree G/S

Distance matrices: spanning forests

Given graph $G := (V, E)$

vertex subset $S \subset V$

$K_1(G;S) := \# \mathcal{F}_1(G;S)$

$\downarrow$

How many?

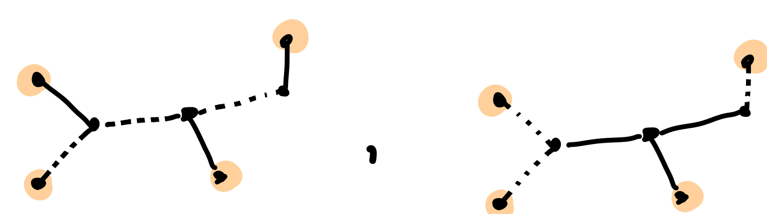
Def'n An S-rooted spanning forest of G is a subgraph which

"spanning" • contains all vertices of G

"forest" • contains no cycles

"S-rooted" • each connected component contains exactly one vertex of S

S = leaf set "∂G"

Ex. $\mathcal{F}_1(G;\underline{S}) = \Big\{$  $, \ldots \Big\}$

Distance matrices: spanning forests

$\# \mathcal{F}_2(G;S) = ?$

$\mathcal{F}_2(G;S) \leftrightarrow$ 2-comp. forests G/S

Given graph $G = (V, E)$

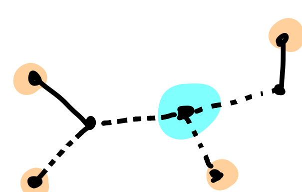
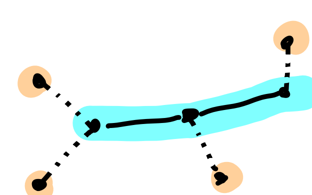
vertex subset $S \subset V$

Def'n An $(S,*)$-rooted spanning forest of G is a subgraph which

"spanning" • contains all vertices of G

"forest" • contains no cycles

"$(S,*)$-rooted" • each connected component contains one vertex of S, PLUS a "floating" component $=: F(*)$

Ex. $\mathcal{F}_2(G;S) = \{$  ,  , $\ldots \}$

Distance matrices: spanning forests

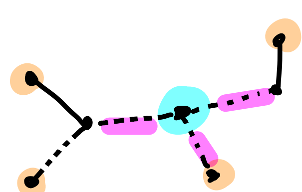
Given graph $G = (V, E)$

vertex subset $S \subset V$

$(S, *)$-rooted spanning forest $F \in \mathcal{F}_2(G; S)$

Def'n The out-degree $\deg^o(F, *)$ of the floating component is $\#\{\text{edges from } F(*) \text{ to outside}\} =: \#\partial F(*)$

Ex.



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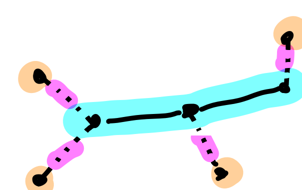
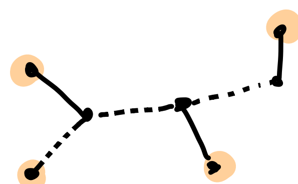
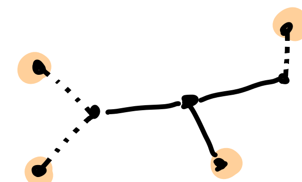
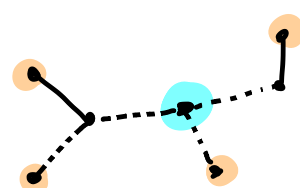
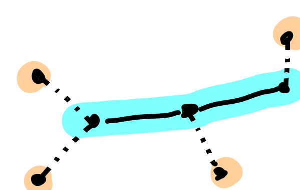


$\deg^o(F, *) = 3$ $\qquad\qquad$ $\deg^o(F, *) = 4$

Aside: Transitions between $\mathcal{F}_1(G;S)$ and $\mathcal{F}_2(G;S)$ form interesting "Dynamical system"

$\mathcal{F}_1(G;S) = \{$  ,  $\}$

delete edge $e \in T$ $\downarrow$ $\uparrow$ add edge $e \in \partial F(*)$

$\mathcal{F}_2(G;S) = \{$  ,  $\}$

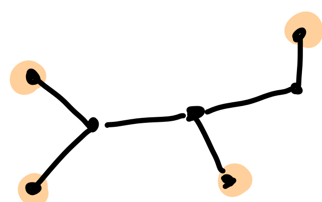
★ Fields Medal: June Huh

Distance matrices

Theorem (R - Shokrieh - Wu)

$$\det D[S] = (-1)^{|S|-1}\, 2^{|S|-2} \left((n-1)\, \kappa(G;S) - \sum_{F \in \mathcal{F}_2(G;S)} \left(\deg^{o}(F,*)-2\right)^2 \right)$$

Ex.



tree

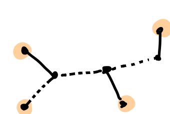
$$D[S] = \begin{bmatrix} 0 & 2 & 3 & 4 \\ 2 & 0 & 3 & 4 \\ 3 & 3 & 0 & 3 \\ 4 & 4 & 3 & 0 \end{bmatrix}$$

distance submatrix

$$\Rightarrow \quad \det D[S] = -252$$

$$= (-1)^3\, 2^2 \Big(\overbrace{(7-1)\cdot 13 \;-\; \left(5\cdot 0^2 + 7\cdot 1^2 + 2\cdot 2^2\right)}^{63} \Big)$$

{



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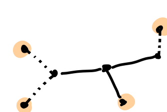

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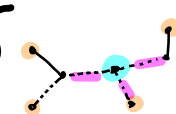

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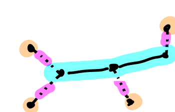

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Distance matrices

<u>Theorem</u> (R - Shokrieh - Wu)

$$\det D[S] = (-1)^{|S|-1} \, 2^{|S|-2} \left((n-1)\, \kappa(G;S) - \sum_{F \in \mathcal{F}_2(G;S)} \left(\deg^\circ(F,*) - 2\right)^2 \right)$$

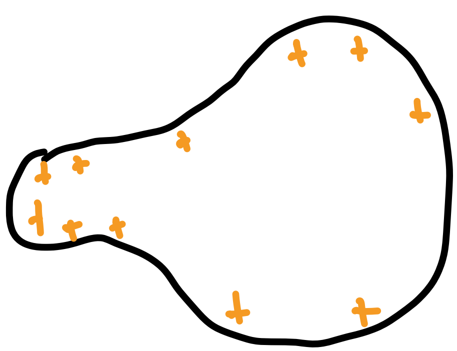
How to prove?

Equilibrium measures & potential theory on trees

Equilibrium measures ⇝ "Potential theory"

<u>Problem</u> How do particles "distribute" along a planar region, given repulsive potential $U(x,y)$?

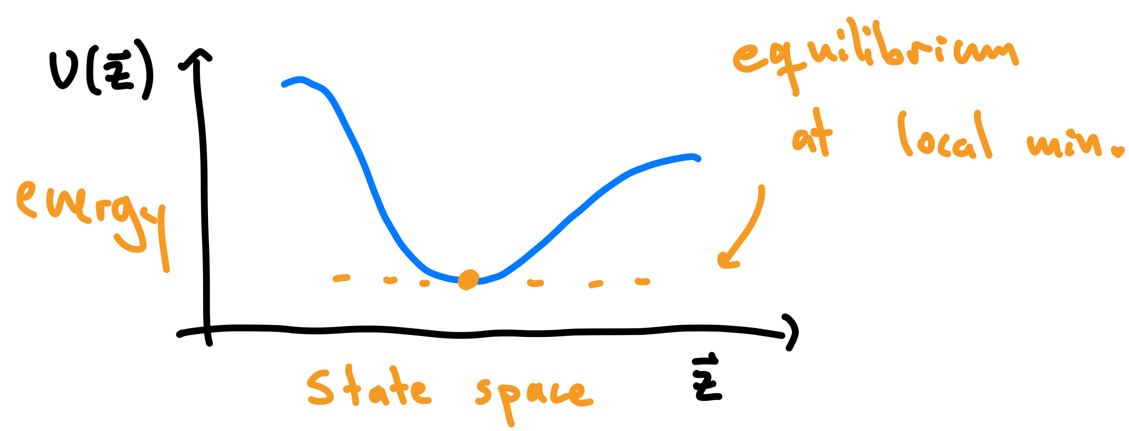
$U(x,y) = -\ln|x-y|$



2-dim region

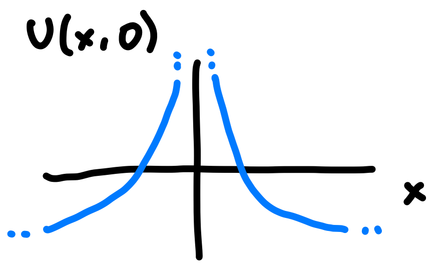
[<u>Physics view</u>:

A system changes over time to lower its "potential energy"]



Equilibrium measures: planar case

For a planar region $R \subset \mathbb{R}^2$,

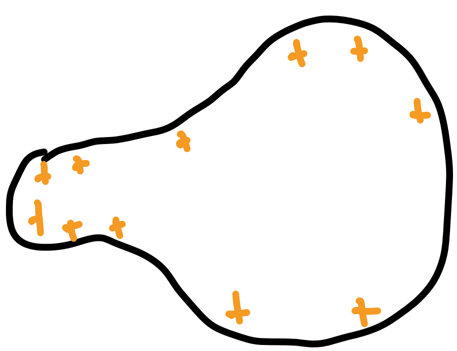


① Two-point potential

$$U(x,y) = -\ln|x-y|$$

② Linearity of potential

$$U\left(\sum_i a_i x_i, \sum_j b_j y_j\right) = -\sum_i \sum_j a_i b_j \ln|x_i - y_j|$$



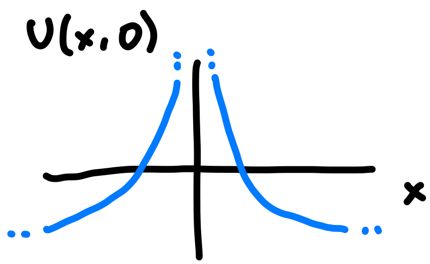
2-dim region

②' Continuous limit

$$U(\mu,\nu) = -\iint \ln|x-y| \, d\mu(x) \, d\nu(y)$$

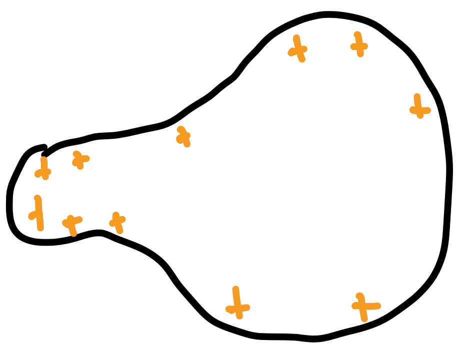
Equilibrium measures: planar case

Physics Fact: On region $R \subset \mathbb{R}^2$, equilibrium is unique measure $\mu = \mu_R$ on ∂R such that



- $\mu(\partial R) = 1$ → conservation of mass
- $\mathcal{E}(\mu) := -\iint \log|x-y| \, d\mu(y) \, d\mu(x)$ is minimized

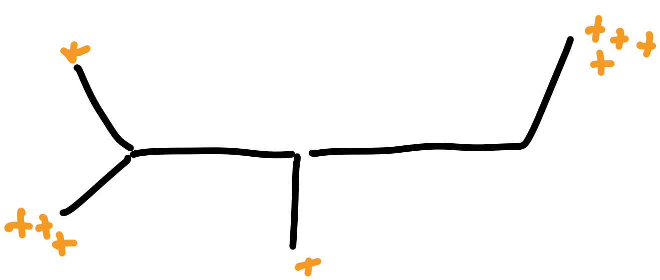
$U(\mu, \mu)$ self-repulsion potential



2-dim region

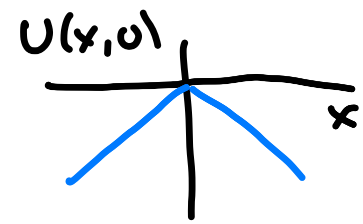
Equilibrium measures: trees

Problem How do particles "distribute" along a tree, given repulsive potential $U(x,y)$?



① Two-point potential

$$U(x,y) = -\,\mathrm{dist}(x,y)$$



② Linearity of potential

$$U\Big(\sum_i a_i v_i, \sum_j b_j v_j\Big) = -\sum_i \sum_j a_i b_j \,\mathrm{dist}(v_i, v_j)$$

$$= -\left([a_1 \cdots a_n] \begin{bmatrix} D \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} \right)$$

distance matrix!

Equilibrium measures: trees

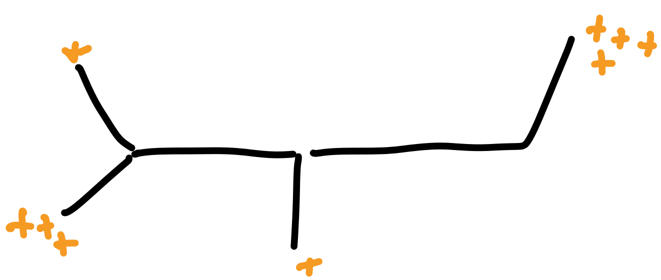
$G, \quad S \subset V$

(Math Def'n)
Physics Fact: The equilibrium vector is the (unique) vector $\vec{\mu} \in \mathbb{R}^S$ satisfying

- $\vec{1} \cdot \vec{\mu} = 1$

→ "conservation of mass"

- $\mathcal{E}(\vec{\mu}) = -\vec{\mu}^T D[S] \vec{\mu}$ is minimized



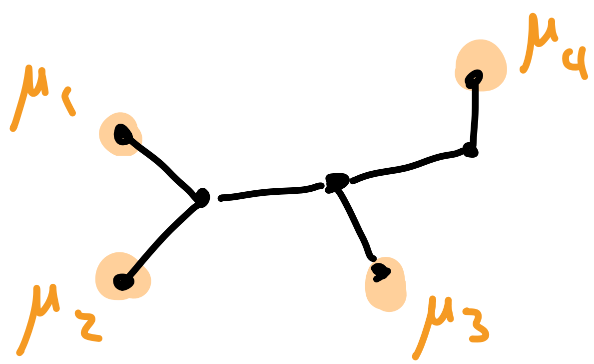
1-dim tree

Equilibrium measures

<u>Physics Fact</u>: The equilibrium is the unique vector $\vec{\mu} \in \mathbb{R}^S$ satisfying

- $\vec{\mathbb{1}} \cdot \vec{\mu} = 1$
- $\mathcal{E}(\vec{\mu}) = -\vec{\mu}^T D[S] \vec{\mu}$ is minimized

Ex. What happens in pactice?



tree

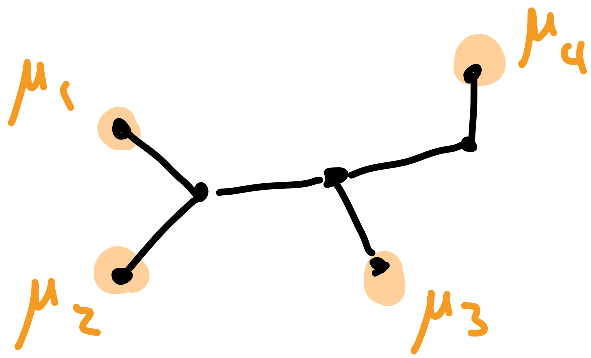
$$D[S] = \begin{bmatrix} 0 & 2 & 3 & 4 \\ 2 & 0 & 3 & 4 \\ 3 & 3 & 0 & 3 \\ 4 & 4 & 3 & 0 \end{bmatrix}$$

distance submatrix

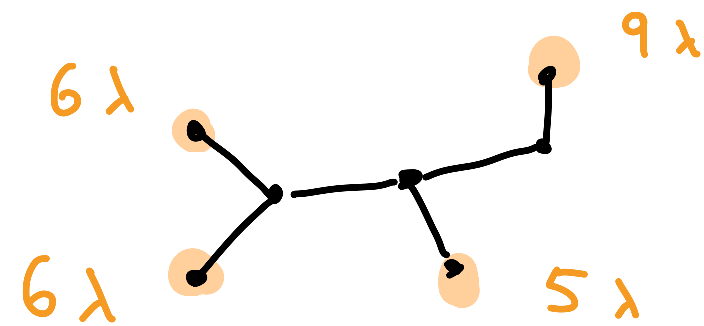
$\Rightarrow$ Computational demo, gradient descent

Equilibrium measures

Ex.



Equilibrium



equilibrium ratio

$$\underbrace{D[S]}_{\text{distance submatrix}}\vec{\mu}^* = \begin{bmatrix} 0 & 2 & 3 & 4 \\ 2 & 0 & 3 & 4 \\ 3 & 3 & 0 & 3 \\ 4 & 4 & 3 & 0 \end{bmatrix} \begin{bmatrix} 6 \\ 6 \\ 5 \\ 9 \end{bmatrix} = \begin{bmatrix} 63 \\ 63 \\ 63 \\ 63 \end{bmatrix}$$

Recall:

$$\det D[S] = -252$$
$$= -4(63)$$

Equilibrium measures

* Technical detail:
$D[S]$ has signature $(1, |S|-1)$

Theorem (Lagrange multipliers + linear algebra*)

Suppose $\vec{\mu}^*$ is the unique vector in $\mathbb{R}^S$ satisfying

- $\vec{1} \cdot \vec{\mu} = 1$
- $\mathcal{E}(\vec{\mu}) = -\vec{\mu}^T D[S] \vec{\mu}$ is minimized

Then

$$\mathcal{E}(\vec{\mu}^*) = -\frac{\det D[S]}{\operatorname{cof} D[S]}$$

$$\operatorname{cof} A = \sum_{i,j} (-1)^{i+j} \det A_{i,j}$$

where cof = "sum of cofactors"

$\rightsquigarrow$ **Goal**: Compute $\det D[S] = -(\operatorname{cof} D[S]) \cdot \mathcal{E}(\vec{\mu}^*)$

Equilibrium measures

Goal: Compute $\det D[S] = -(\mathrm{cof}\ D[S]) \cdot \mathcal{E}(\vec{\mu}^*)$

Theorem (Bapat - Sivasubramanian, et al.?)

The equilibrium vector $\vec{\mu}^* = \sum_i \mu_i^* v_i$

is

$$\mu_i^* = \frac{\sum_{T \in \mathcal{F}_1} (2 - \deg^{o}(T, i))}{2 \cdot \kappa_1(G; S)}$$

Equilibrium vector

- $\vec{\mathbb{1}} \cdot \vec{\mu} = 1$
- $\mathcal{E}(\vec{\mu}) = -\vec{\mu}^T D[S] \vec{\mu}$ is minimized

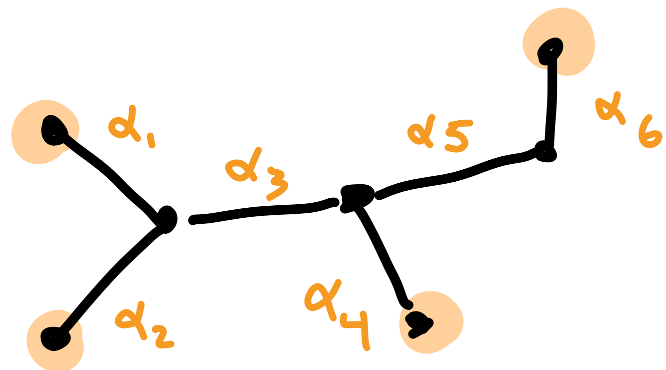
Theorem (Bapat - Sivasubramanian, 2011)

$$\mathrm{cof}\ D[S] = (-2)^{|S|-1} \kappa_1(G; S)$$

Generalizations : edge weights

Assign positive weight α_e to each edge $e \in E$

Ex.



edge-weighted tree

$$D = \begin{bmatrix} 0 & \alpha_1 & \alpha_1 + \alpha_2 & \cdots \\ \alpha_1 & 0 & \alpha_2 & \\ \alpha_1 + \alpha_2 & \alpha_2 & 0 & \\ \vdots & \vdots & & \ddots \end{bmatrix}$$

weighted distance matrix

Theorem (Bapat – Kirkland – Neumann, 2005)

$$\det D = (-1)^{n-1} 2^{n-2} \left(\sum_E \alpha_e \prod_E \alpha_e \right)$$

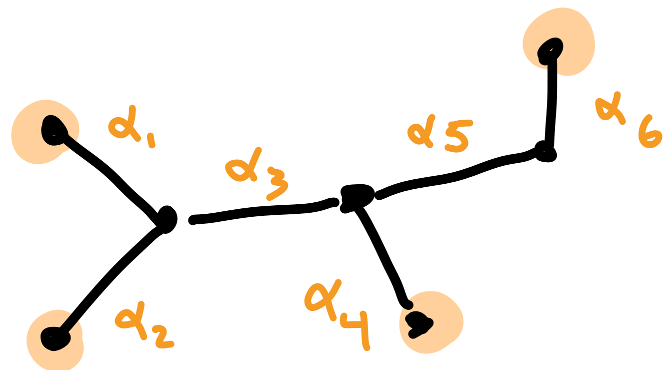
Thm (Graham – Pollak)

$$\det D = (-1)^{n-1} 2^{n-2} (n-1)$$

Generalizations : edge weights

Assign positive weight α_e to each edge $e \in E$

Ex.



edge-weighted tree

$$D = \begin{bmatrix} 0 & \alpha_1 & \alpha_1 + \alpha_2 & \cdots \\ \alpha_1 & 0 & \alpha_2 & \\ \alpha_1 + \alpha_2 & \alpha_2 & 0 & \\ \vdots & \vdots & & \ddots \end{bmatrix}$$

weighted distance matrix

edge weights

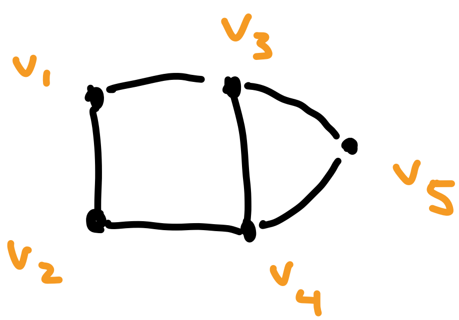
Theorem (R - Shokrieh - Wu)

$$\det D[S] = (-1)^{|S|-1} \, 2^{|S|-2} \left(\sum_{E} \alpha_e \sum_{T \in \mathcal{F}_1} w(T) - \sum_{F \in \mathcal{F}_2} \left(\deg^{o}(F,*) - 2 \right)^2 w(F) \right)$$

Generalizations : graphs w/ cycles

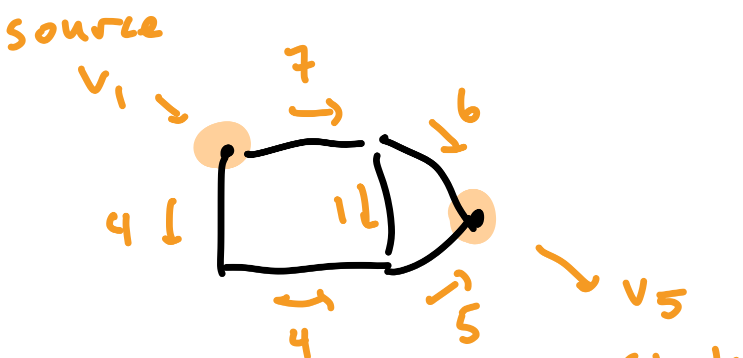
$$\cancel{D} = \begin{bmatrix} 0 & 1 & 1 & 2 & 2 \\ 1 & 0 & 2 & 1 & 2 \\ 1 & 2 & 0 & 1 & 1 \\ 2 & 1 & 1 & 0 & 1 \\ 2 & 2 & 1 & 1 & 0 \end{bmatrix}$$

Ex.



graph

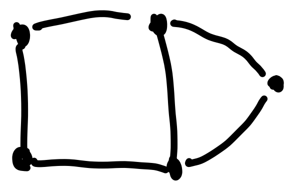
effective resistance matrix



$$R = \begin{bmatrix} 0 & 8/11 & 8/11 & 10/11 & 13/11 \\ 8/11 & 0 & 10/11 & 8/11 & 13/11 \\ 8/11 & 10/11 & 0 & 6/11 & 7/11 \\ 10/11 & 8/11 & 6/11 & 0 & 7/11 \\ 13/11 & 13/11 & 7/11 & 7/11 & 0 \end{bmatrix}$$

Generalizations : "continuous" graphs

Ex.



graph G

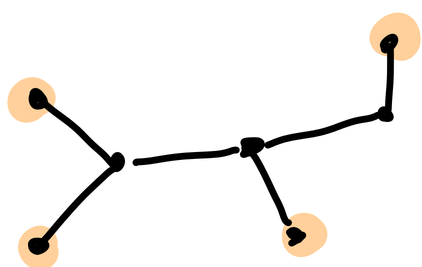
$\rightsquigarrow$

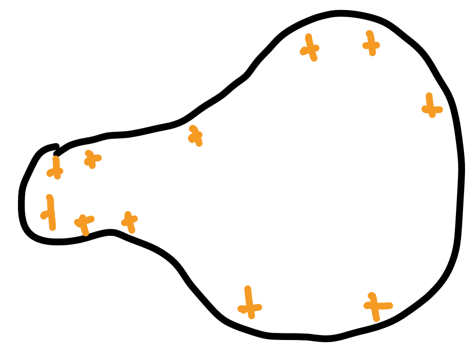
metric graph Γ

Theorem (R-S-W) Calculate equilibrium measure μ^* on Γ and "resistance energy"

$$\mathcal{E}(\mu^*) := -\int_\Gamma \int_\Gamma r(x,y)\, d\mu^*(x)\, d\mu^*(y)$$

Thank you!





Harry Richman

7 December 2022

Matsen Lab, Fred Hutch

Remark Flavors of discretization

$$X \xrightarrow{f} Y$$

	continuous mass $n_i \in \mathbb{R} = Y$	discrete mass $m_i \in \mathbb{Z} = Y$
continuous space $X = \mathbb{R}$ or Γ	"classical" physics, potential theory	algebraic curves & divisors, tropical geometry, divisor theory
discrete space $X = G$	linear algebra $\mathrm{Mat}_{n\times n}(\mathbb{R})$, $\mathbb{R}^n$	$\mathrm{Mat}_{n\times n}(\mathbb{Z})$, $\mathbb{Z}^n$, critical group, sandpile group