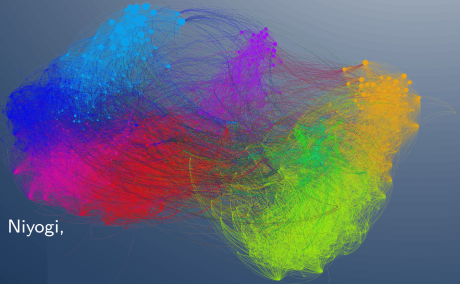
Graphs in Machine Learning

SSL with Graphs: Harmonic Functions

Gaussian Random Fields Solution

Michal Valko

Inria & ENS Paris-Saclay, MVA



Partially based on material by: Mikhail Belkin, Partha Niyogi, Olivier Chapelle, Bernhard Schölkopf

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Zhu/Ghahramani/Lafferty: Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions (ICML 2013)

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Idea 1: Look for a **unique** solution.

Idea 2: Find a smooth one.

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SSL with Graphs: Harmonic Functions

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$$s.t. \quad y_i = f(\mathbf{x}_i) \quad \forall i = 1, \ldots, n_l$$

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Properties of the relaxation from ± 1 to $\mathbb{R}$

- there is a closed form solution for $\mathbf{f}$
- this solution is unique
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- electric-network interpretation
- random-walk interpretation

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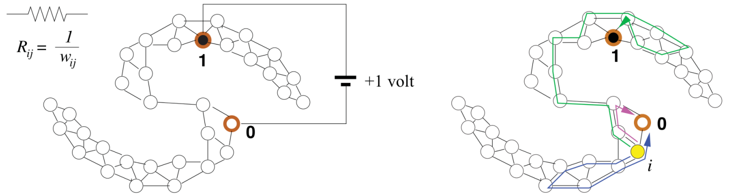

(a) The electric network interpretation (b) The random walk interpretation

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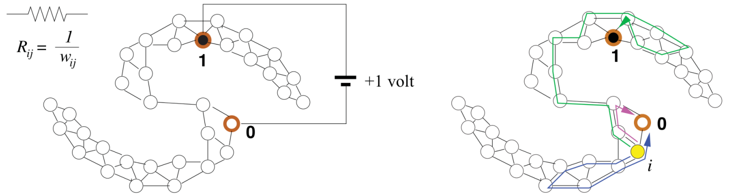

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Random walk interpretation:

1) start from the vertex you want to label and randomly walk

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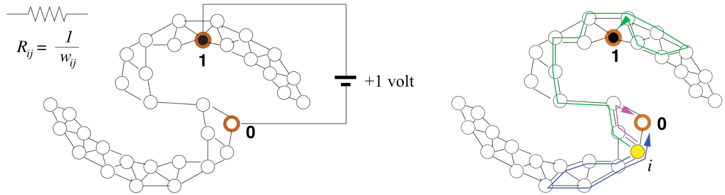

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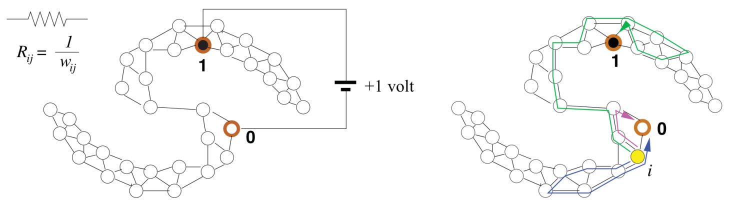

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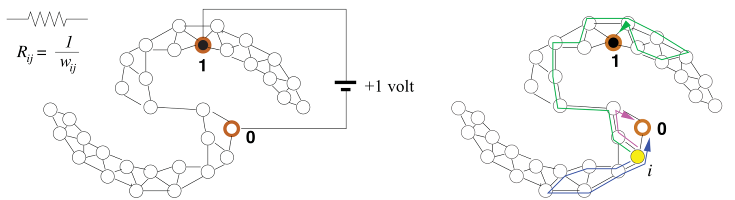

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3) finish when **a** labeled vertex is hit

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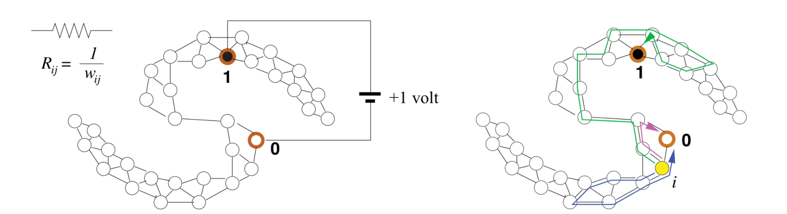

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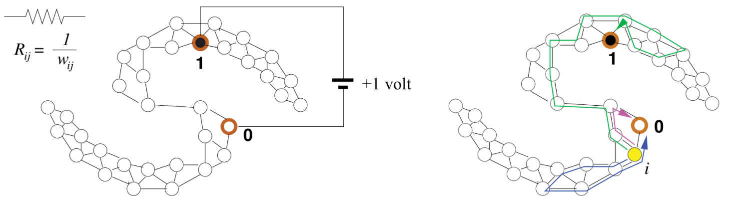

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absorbing random walk

f_i = probability of reaching a positive labeled vertex

SSL with Graphs: Harmonic Functions

How to compute HS?

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How to compute HS? **Option A:** iteration

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- an interesting option for large-scale data

SSL with Graphs: Harmonic Functions

How to compute HS? **Option B:** Closed form solution

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Yes, Lagrangian multipliers are an option, but . . .

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In matrix notation

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Note that $\mathbf{f}_u$ does not depend on $\mathbf{L}_{ll}$.

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Can we see that this calculates the probability of a random walk?

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SSL with Graphs: Harmonic Functions

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$$\mathbf{f}_u = \mathbf{L}_{uu}^{-1}(-\mathbf{L}_{ul}\mathbf{f}_l) = \mathbf{L}_{uu}^{-1}(\mathbf{W}_{ul}\mathbf{f}_l)$$

Note $\mathbf{P} = \mathbf{D}^{-1}\mathbf{W}$ and

$\mathbf{L}_{uu}^{-1} = (\mathbf{D}_{uu}(\mathbf{I} - \mathbf{P}_{uu}))^{-1} = (\mathbf{I} - \mathbf{P}_{uu})^{-1}\mathbf{D}_{uu}^{-1}$

$$\mathbf{f}_u = (\mathbf{I} - \mathbf{P}_{uu})^{-1}\mathbf{P}_{ul}\mathbf{f}_l.$$

Split the equation into +ve & -ve part:

$$f_i = (\mathbf{I} - \mathbf{P}_{uu})_{iu}^{-1}\mathbf{P}_{ul}\mathbf{f}_l$$

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Michal Valko

michal.valko@inria.fr

Inria & ENS Paris-Saclay, MVA

https://misovalko.github.io/mva-ml-graphs