Generalization bounds for learning under graph-dependence

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ML & VL Seminar

The content is based upon

- *McDiarmid-type inequalities for graph-dependent variables and stability bounds* (with Xingwu Liu, Yuyi Wang, Liwei Wang) Spotlight in Advances in Neural Information Processing Systems 32 (NeurIPS 2019).
- *When Janson meets McDiarmid: Bounded difference inequalities under graph-dependence* Statistics & Probability Letters, 2022.
- *Generalization bounds for learning under graph-dependence: A survey* (with Massih-Reza Amini, arXiv:2203.13534).

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- The goal is to establish generalisation error bounds

$$R(f) \leqslant \widehat{R}(f) + ?$$

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The ways to establish generalisation error (also called generalization gap) bounds is by

- Measuring of the complexity of the output hypothesis space.
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Most of them assume that samples are i.i.d., which is not the case in many settings.

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They are basic tools to establish generalization theory, in which

$$g(\boldsymbol{x}) = \mathbb{E}[\ell(y, f(x))] - \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i))$$

is the difference of expected error and empirical error.

Bounded difference inequality

c-Lipschitz

Given $\boldsymbol{c} = (c_1, \ldots, c_n) \in \mathbb{R}_+^n$, a function g is $\boldsymbol{c}$-Lipschitz if

$$\left| g(x_1, \ldots, x_i, \ldots, x_n) - g(x_1, \ldots, x_i', \ldots, x_n) \right| \leq c_i.$$

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then for $t > 0$,

$$\mathbb{P}(g(\boldsymbol{X}) - \mathbb{E}[g(\boldsymbol{X})] \geqslant t) \leqslant \exp\left(-\frac{2t^2}{\|\boldsymbol{c}\|_2^2} \right).$$

This is also called Azuma-Hoeffding inequality.

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- If all $c_i = c$, then for any fixed $\delta \in (0,1)$, with probability at least $1 - \delta$, we have

$$f - \mathbb{E}[f] \leqslant \|\boldsymbol{c}\|_2 \sqrt{\frac{1}{2} \log\left(\frac{1}{\delta}\right)} = c\sqrt{\frac{n}{2} \log\left(\frac{1}{\delta}\right)}.$$

Dependent random variables

- Mixing coefficients: α, β, ϕ-mixing, etc.
  - quantitatively measure the dependencies, and widely used in probability, statistics, e.g.,

$$\alpha(s) = \sup\left\{\left|\mathbb{P}(A \cap B) - \mathbb{P}(A)\mathbb{P}(B)\right| : A \in \sigma\left(\{X_i\}_{-\infty}^{t}\right), B \in \sigma\left(\{X_i\}_{t+s}^{\infty}\right)\right\}$$

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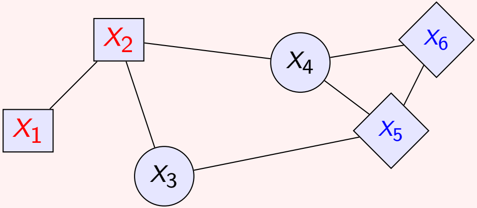
- Copula, graphical models (random field, Bayesian network, etc.), time series, etc.

Dependency Graphs

Definition

Graph G is a dependency graph for random variables $\boldsymbol{X} = (X_1, \ldots, X_n)$ if

- *Vertex set $V(G) = [n] = \{1, \ldots, n\}$.*



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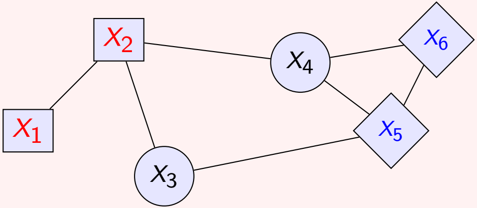

- *If disjoint subsets $I, J \subset [n]$ are non-adjacent in G, then $\{X_i\}_{i \in I}$ and $\{X_j\}_{j \in J}$ are independent.*
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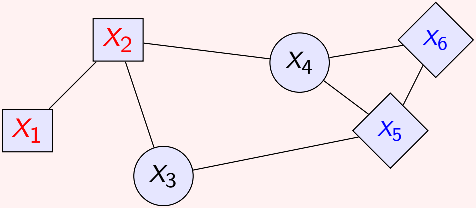

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- The dependency graph for a set of random variables is not necessarily unique.

Idea: to utilise independence among variables

Given a graph G with n vertices, a fractional vertex covering $\{(I_j, w_j)\}_j$ of G satisfies

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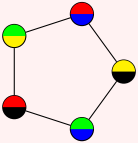

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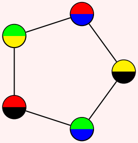

A function g is *decomposable* $\boldsymbol{c}$*-Lipschitz* with respect to graph G if there exist $(c_i)_{i \in I_j}$-Lipschitz functions $\{g_j\}_j$ such that

$$g(\boldsymbol{x}) = \sum_j w_j g_j(\mathrm{x}_{I_j}),$$

for all $\mathrm{x} = (x_1, \ldots, x_n)$, and for all fractional vertex covers $\{(I_j, w_j)\}_j$ of G.

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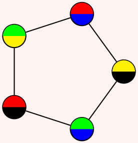

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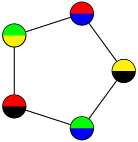

Theorem (Usunier et al. NIPS05; Z 2022; Z. and Amini 2022+)

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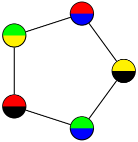

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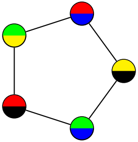

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where $\chi^\star(G) = \sum_j w_j \leqslant \Delta(G) + 1$.

- In the above example, $\chi^\star(G) = 5/2$.

Forest-dependent random variables

Theorem (Z. et al. NeurIPS19, Z. 2022)

If we have that

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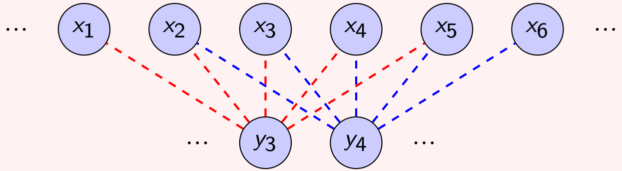
- General graphs are handled via tree-partitions (transforming a graph to a forest by merging vertices).

Applications

Stability bound for learning m-dependent data

Example

- y_i: observation at location i, e.g., house price
- x_i: random variable modelling influential factors at location i



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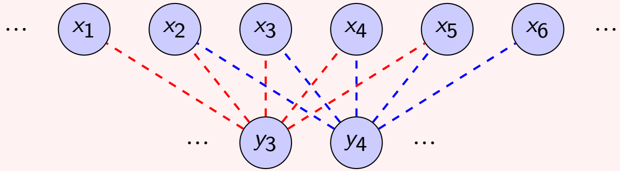

- Given training data: $\mathrm{S} = \{\ldots, ((x_1, x_2, x_3, x_4, x_5), y_3), ((x_2, x_3, x_4, x_5, x_6), y_4), \ldots\}$.
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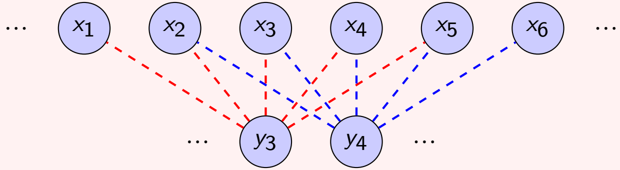

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Definition (Hoeffding and Robbins 1948)

A sequence of random variables $(X_i)_{i=1}^n$ is m-dependent for some $m \geqslant 1$ if $(X_j)_{j=1}^i$ and $(X_j)_{j=i+m+1}^n$ are independent for all $i > 0$.

Stability bound for learning m-dependent data

Given a sample S, a learning algorithm $\mathscr{A} : \mathsf{S} \mapsto f_{\mathsf{S}}^{\mathscr{A}}$ outputs $f_{\mathsf{S}}^{\mathscr{A}}$.

Uniform stability (Bousquet and Elisseeff 2002)

A learning algorithm $\mathscr{A}$ is β_n-uniformly stable if

$$\max_{i \in [n]} \left| \ell(y, f_{\mathsf{S}}^{\mathscr{A}}(x)) - \ell(y, f_{\mathsf{S}^{\setminus i}}^{\mathscr{A}}(x)) \right| \leqslant \beta_n,$$

where $\mathsf{S}^{\setminus i}$ is by deleting i-th data point from S.

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We have

$$R(f_{\mathrm{S}}^{\mathscr{A}}) \leqslant \widehat{R}(f_{\mathrm{S}}^{\mathscr{A}}) + 2\beta_{n,2m}(2m+1) + (4n\beta_n + M)\sqrt{\frac{2m}{n} \log\left(\frac{1}{\delta}\right)},$$

which introduces a factor $4m$ comparing with the independent case (Bousquet and Elisseeff 2002)

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Bipartite ranking

- Training set: $T = (x_i, y_i)_{i=1}^m$ with $y_i \in \{-1, +1\}$.
- The goal: to find a scoring function h that gives higher scores to instances of the positive class than the ones of the negative class.

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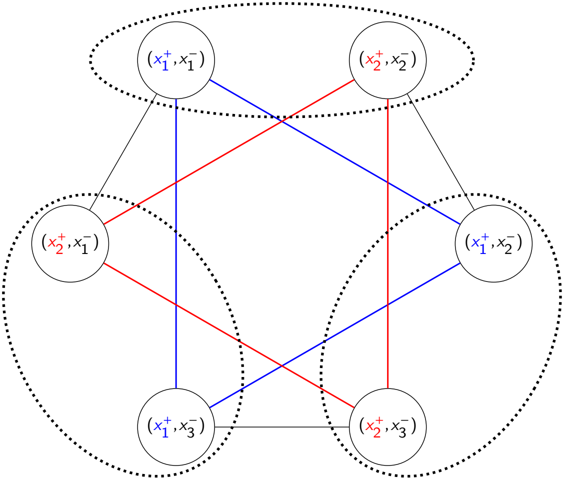
- For $(x, y), (x', y')$ with $y \neq y'$, we consider unordered pairs of examples (x, x').



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- The empirical loss of a scoring function h over T can be written as a summation over the pairs of instances of different classes:

$$\widehat{R}(h) = \frac{1}{|\mathsf{S}|} \sum_{(x,x') \in \mathsf{S}} \mathbb{1}_{\{z_{x,x'}(h(x) - h(x')) \leqslant 0\}},$$

where $z_{x,x'} = 2\mathbb{1}_{\{y - y' > 0\}} - 1$.

  - If $y = 1$ and $y' = -1$, then $z_{x,x'}(h(x) - h(x')) = h(x) - h(x')$.

Bipartite ranking

An approach based on fractional Rademacher complexity gives the following.

Corollary (Z. and Amini 2022+)

Let T be a training set composed of m_+ positive instances and m_- negative ones. Then for any scoring functions in $\{h : (x, x') \mapsto \langle \mathrm{w}, \phi(x) - \phi(x') \rangle ; \|\mathrm{w}\| \leqslant B\}$, where ϕ is a feature mapping with bounded norm, such that $\forall (x, x'), \|\phi(x) - \phi(x')\| \leqslant \Gamma$, and for any $\delta \in (0, 1)$ with probability at least $1 - \delta$, we have

$$R(f) \leqslant \widehat{R}(f) + \frac{4B\Gamma}{\sqrt{m}} + 3\sqrt{\frac{1}{2m} \log\left(\frac{2}{\delta}\right)},$$

where $m = \min(m_-, m_+)$.

Thanks for your attention!