Concentration and generalization for learning under graph-dependence

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- Generalisation error bounds bound expected error using empirical error:

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

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and are the basic tools to establish generalization theory, in which

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

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

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

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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

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

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 fields, Bayesian networks, etc.), time series, etc.

Dependency Graphs

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

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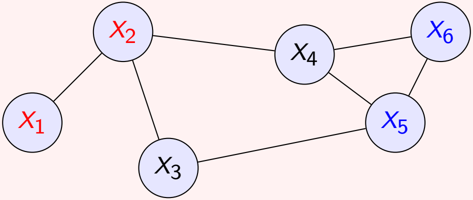

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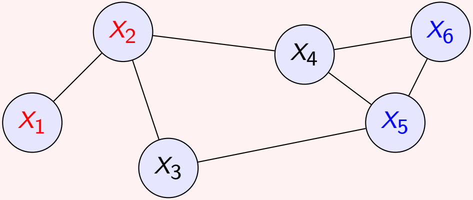

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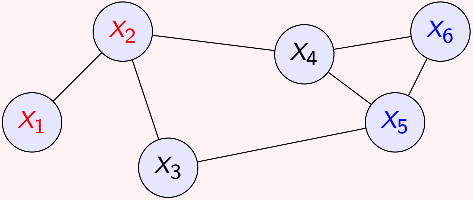

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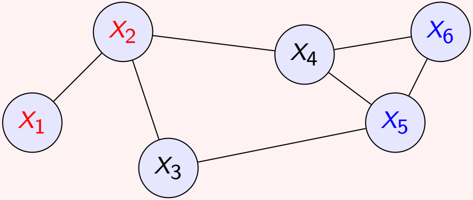

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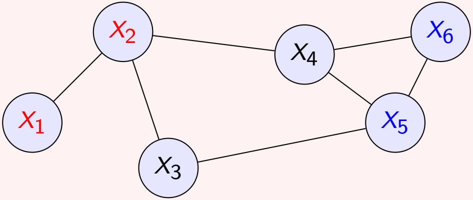

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This model has deep connections to cumulant, cluster expansion, Stein's method, etc.

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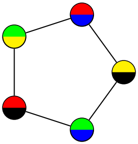

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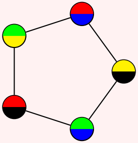

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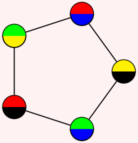

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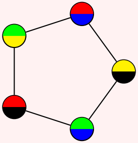

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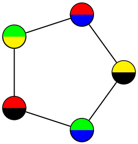

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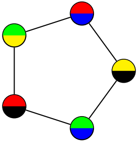

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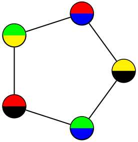

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If we have that

1. *g is decomposable $\boldsymbol{c}$-Lipschitz,*
2. *$\boldsymbol{X} = (X_1, \ldots, X_n)$ is G-dependent,*

then for $t > 0$,

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

Forest-dependent random variables

Theorem (Z. Liu, Wang, Wang 2019)

If we have that

1. g *is* $\boldsymbol{c}$*-Lipschitz,*
2. F *is a dependency graph for* $\boldsymbol{X}$*, where* $F = \{T_i\}_{i=1}^{k}$ *is a forest,*

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

Cramér-Chernoff method

c-Lipschitz + independence

Cramér-Chernoff method

$$\begin{aligned} & \boldsymbol{c}\text{-Lipschitz} + \text{independence} \\ \Rightarrow \quad & \sup_{\alpha \in \Omega_i} \mathbb{E}\left[g \,\middle|\, \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \alpha \right] - \inf_{\beta \in \Omega_i} \mathbb{E}\left[g \,\middle|\, \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \beta \right] \leqslant c_i \end{aligned}$$

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\end{aligned}
$$

Proof Sketch

- Choose c_{min} as root, expose vertices via topological ordering, i.e., child i before parent $p(i)$. We will show that

$$\sup_{\alpha \in \Omega_i} \mathbb{E}\left[g(\boldsymbol{X}) \middle| \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \alpha\right] - \inf_{\beta \in \Omega_i} \mathbb{E}\left[g(\boldsymbol{X}) \middle| \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \beta\right] \leqslant c_i + c_{p(i)},$$

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- by choosing a suitable coupling of conditional distributions , i.e., a joint distribution $\mathbb{P}$ of $(\boldsymbol{X}_{[i+1:n]}, \widetilde{\boldsymbol{X}}_{[i+1:n]})$ with desirable marginal distributions and with few different bits

$$\mathbb{P}(\boldsymbol{X}_{[i+1:n]}) = \mathbb{P}\left(\boldsymbol{X}_{[i+1:n]} \middle| \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \alpha\right)$$
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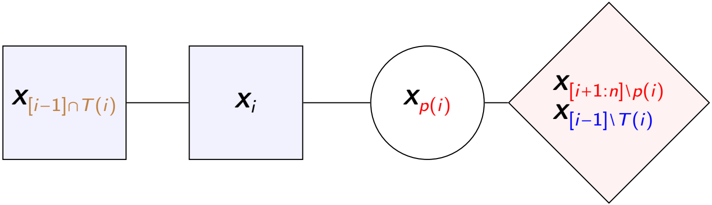

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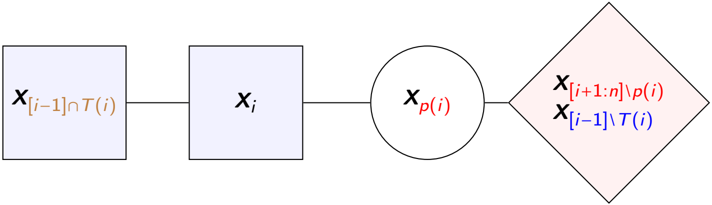

$$\begin{aligned}\mathbb{P}\left(\boldsymbol{X}_{[i+1:n]\setminus p(i)}\middle|\boldsymbol{X}_{[i-1]},\boldsymbol{X}_i\right) &= \mathbb{P}\left(\boldsymbol{X}_{[i+1:n]\setminus p(i)}\middle|\boldsymbol{X}_{[i-1]\setminus T(i)},\boldsymbol{X}_{[i-1]\cap T(i)},\boldsymbol{X}_i\right)\\ &= \mathbb{P}\left(\boldsymbol{X}_{[i+1:n]\setminus p(i)}\middle|\boldsymbol{X}_{[i-1]\setminus T(i)}\right)\end{aligned}$$

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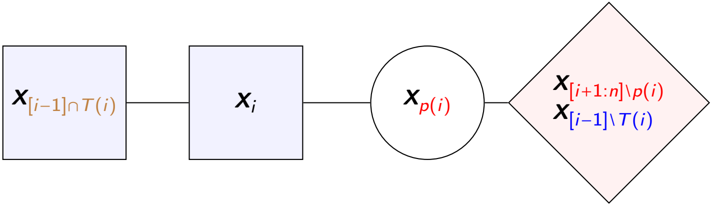

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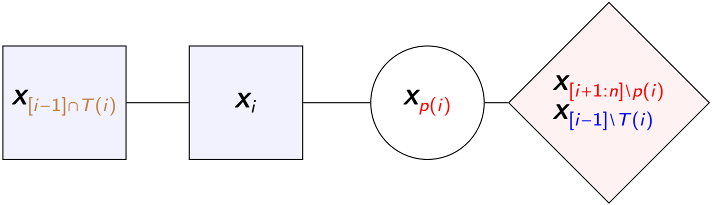

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- If we set the conditional distribution of $\boldsymbol{X}_{[i+1:n]\setminus p(i)}$ to be the same,
- then the change of $\boldsymbol{X}_i$ only influences $\left\{\boldsymbol{X}_i, \boldsymbol{X}_{p(i)}\right\}$, which is bounded by $c_i + c_{p(i)}$.

Proof Sketch

$\boldsymbol{c}$-Lipschitz + tree-dependence

$$\Rightarrow \quad \sup_{\alpha \in \Omega_i} \mathbb{E}\left[g \,\middle|\, \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \alpha\right] - \inf_{\beta \in \Omega_i} \mathbb{E}\left[g \,\middle|\, \boldsymbol{X}_{[i-1]} = \mathrm{x}_{[i-1]}, \boldsymbol{X}_i = \beta\right] \leqslant c_i + c_{p(i)}$$

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\Rightarrow \quad & \mathbb{E}\left[\exp\left(s(g - \mathbb{E}[g])\right)\right] \leqslant \exp\left(\frac{s^2}{8} \left(c_n^2 + \sum_{i \in V(G) \setminus n} \left(c_i + c_{p(i)}\right)^2 \right) \right) \\
\Rightarrow \quad & \mathbb{P}\left(g - \mathbb{E}[g] \geqslant t\right) \leqslant \exp\left(-\frac{2t^2}{c_{\min}^2 + \sum_{\{i,j\} \in E(T)} (c_i + c_j)^2} \right)
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Janson, 2004

If we have that

1. $\boldsymbol{X} = (X_1, \ldots, X_n)$ is G-dependent, and every X_i is in an interval of length $c_i \geqslant 0$,
2. and the function is a summation,

then, for every $t > 0$,

$$\mathbb{P}\left(\sum_{i \in V(G)} X_i - \mathbb{E}\left[\sum_{i \in V(G)} X_i\right] \geqslant t\right) \leqslant \exp\left(-\frac{2t^2}{\chi_f(G) \sum_{i \in V(G)} c_i^2}\right),$$

where $\chi_f(G)$ is the fractional chromatic number of G.

Z., 2022

Under the same setting,

$$\mathbb{P}\left(\sum_{i \in V(G)} X_i - \mathbb{E}\left[\sum_{i \in V(G)} X_i\right] \geqslant t\right) \leqslant \exp\left(-\frac{2t^2}{D}\right),$$

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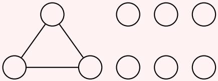
- It is no worse than Janson's, better when G is sparse.
- It generalises to certain forest-decomposable functions, extending McDiarmid's.

Example

Let $\{X_i\}_{i\in[9]}$ be random indicators with the dependency graph G, and $X = \sum_{i\in[9]} X_i$.



$$\mathbb{P}(X - \mathbb{E}[X] \geqslant t) \leqslant ?$$

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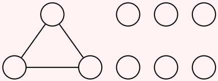

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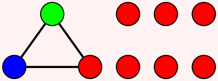
- Janson's idea: to fractionally cover vertices with weighted independent sets such that the sum of weights for each vertex equals 1



$$\mathbb{P}(X - \mathbb{E}[X] \geqslant t) \leqslant \exp\left(-\frac{2t^2}{3\times 9}\right)$$

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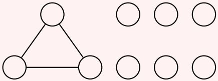

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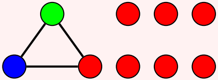
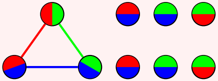


$$\mathbb{P}(X - \mathbb{E}[X] \geqslant t) \leqslant \exp\left(-\frac{2t^2}{3\times 9}\right)$$

- New idea: to fractionally cover vertices with weighted induced forests such that the sum of weights for each vertex equals 1

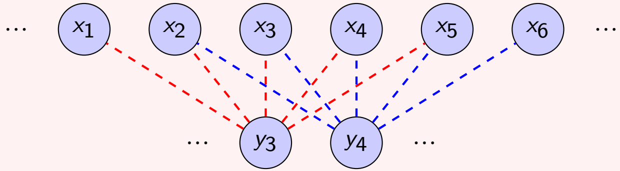


$$\mathbb{P}(X - \mathbb{E}[X] \geqslant t) \leqslant \exp\left(-\frac{8t^2}{81}\right)$$

Applications in statistics

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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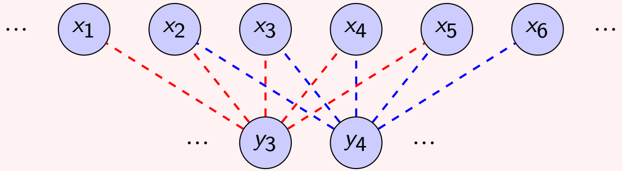

- Given training data: $\boldsymbol{S} = \{\ldots,((x_1,x_2,x_3,x_4,x_5),y_3),((x_2,x_3,x_4,x_5,x_6),y_4),\ldots\}$.
- To find $f : (x_{i-2},x_{i-1},x_i,x_{i+1},x_{i+2}) \mapsto y_i$.

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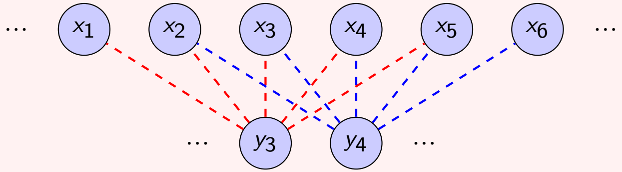

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Question: is this realistic?

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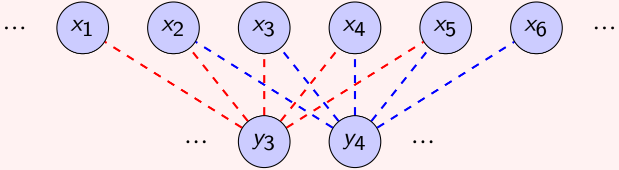

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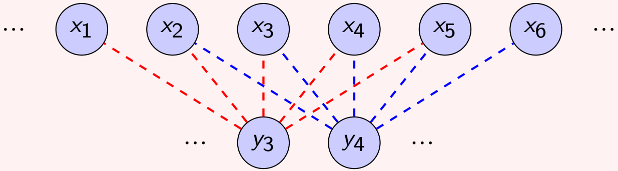

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- To find $f : (x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}) \mapsto y_i$.

Question: is this realistic? Ask property agents or statisticians!

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

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Uniform stability (Bousquet and Elisseeff 2002)

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

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

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

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Z. Liu, Wang, Wang 2019

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

which introduces some multiplicative factor of order m,
comparing with the independent case (Bousquet and Elisseeff 2002):

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Z. 2022 contains slightly improved concentration results for m-dependent case.

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.

Bipartite ranking

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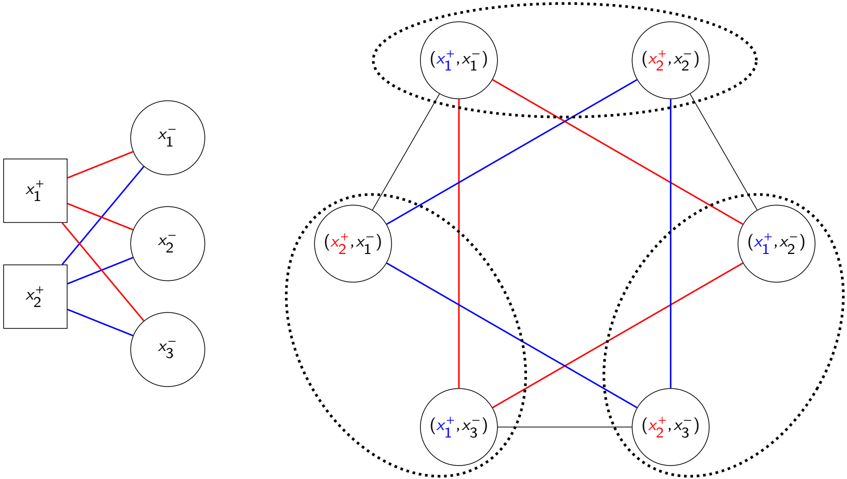
- The goal: to find a scoring function h that gives higher scores to instances of the positive class than the ones of the negative class.
- For $(x,y),(x',y')$ with $y \neq y'$, we consider unordered pairs of examples (x,x').



Bipartite ranking

- Let $\boldsymbol{S} = \{(x, x') \in T \times T : y \neq y'\}$ be the set of unordered pairs of examples from different classes in T.

Bipartite ranking

- Let $\boldsymbol{S} = \{(x, x') \in T \times T : y \neq y'\}$ be the set of unordered pairs of examples from different classes in T.
- The empirical loss of a scoring function h over T can be written as a summation over the pairs of instances of different classes:

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

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 2023+)

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

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**
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Thanks for your attention!
Question: how to compress it into a 5-min talk at ICSDS?