Statistical Machine Learning (BE4M33SSU)
Lecture 3: Empirical Risk Minimization

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Learning

- The goal: Find a strategy $h\colon \mathcal{X} \to \mathcal{Y}$ minimizing $R(h)$ using the training set of examples

$$\mathcal{T}^m = \{(x^i, y^i) \in (\mathcal{X} \times \mathcal{Y}) \mid i = 1, \ldots, m\}$$

drawn from i.i.d. according to unknown $p(x, y)$.

- Hypothesis class (space):

$$\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}} = \{h\colon \mathcal{X} \to \mathcal{Y}\}$$

- Learning algorithm: a function

$$A\colon \cup_{m=1}^{\infty} (\mathcal{X} \times \mathcal{Y})^m \to \mathcal{H}$$

which returns a strategy $h_m = A(\mathcal{T}^m)$ for a training set $\mathcal{T}^m$

Learning: Empirical Risk Minimization approach

- The expected risk $R(h)$, i.e. the true but unknown objective, is replaced by the empirical risk computed from the training examples $\mathcal{T}^m$,

$$R_{\mathcal{T}^m}(h) = \frac{1}{m} \sum_{i=1}^{m} \ell(y^i, h(x^i))$$

- The ERM based algorithm returns h_m such that

$$h_m \in \operatorname*{Argmin}_{h \in \mathcal{H}} R_{\mathcal{T}^m}(h) \tag{1}$$

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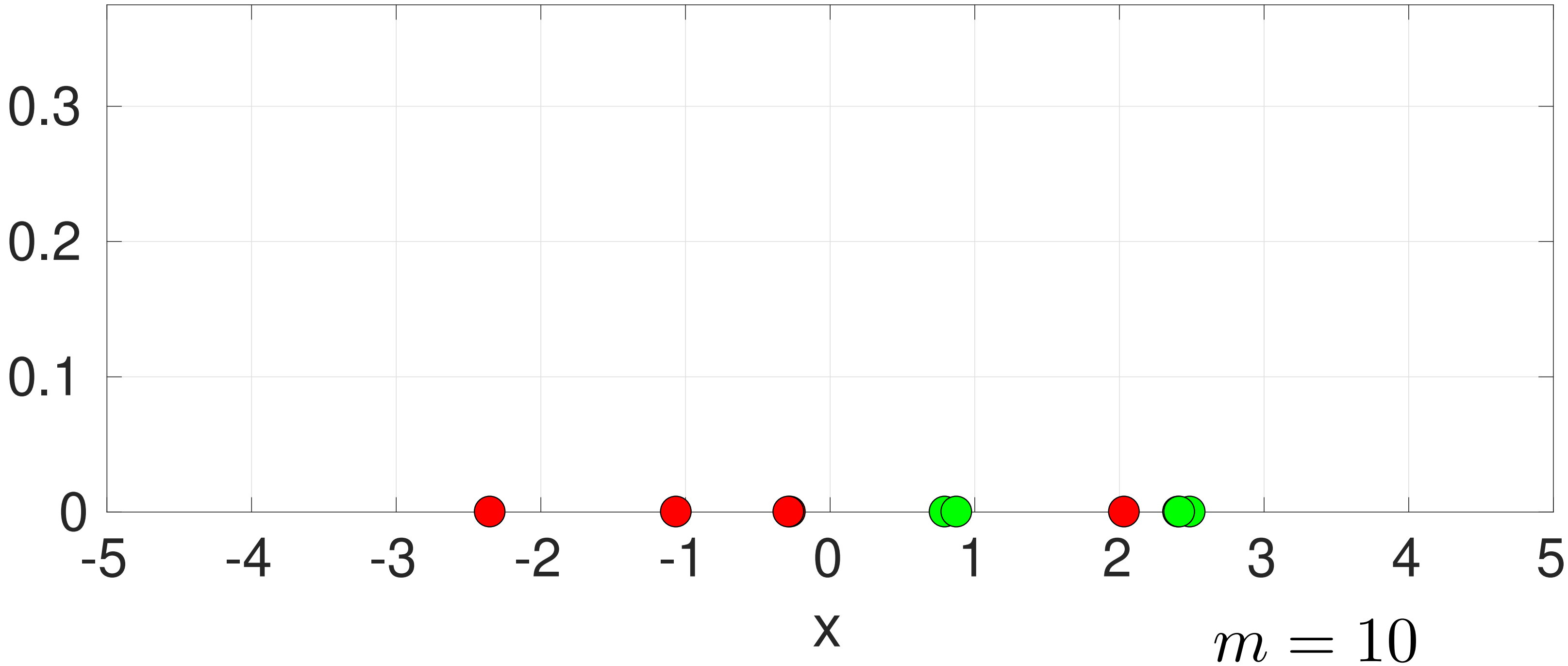
$$\mathcal{H} = \{h(x) = \mathrm{sign}(x - \theta) \mid \theta \in \mathbb{R}\}\ ,\ \ \ell(y, y') = [\![y \neq y']\!]$$



$m = 10$

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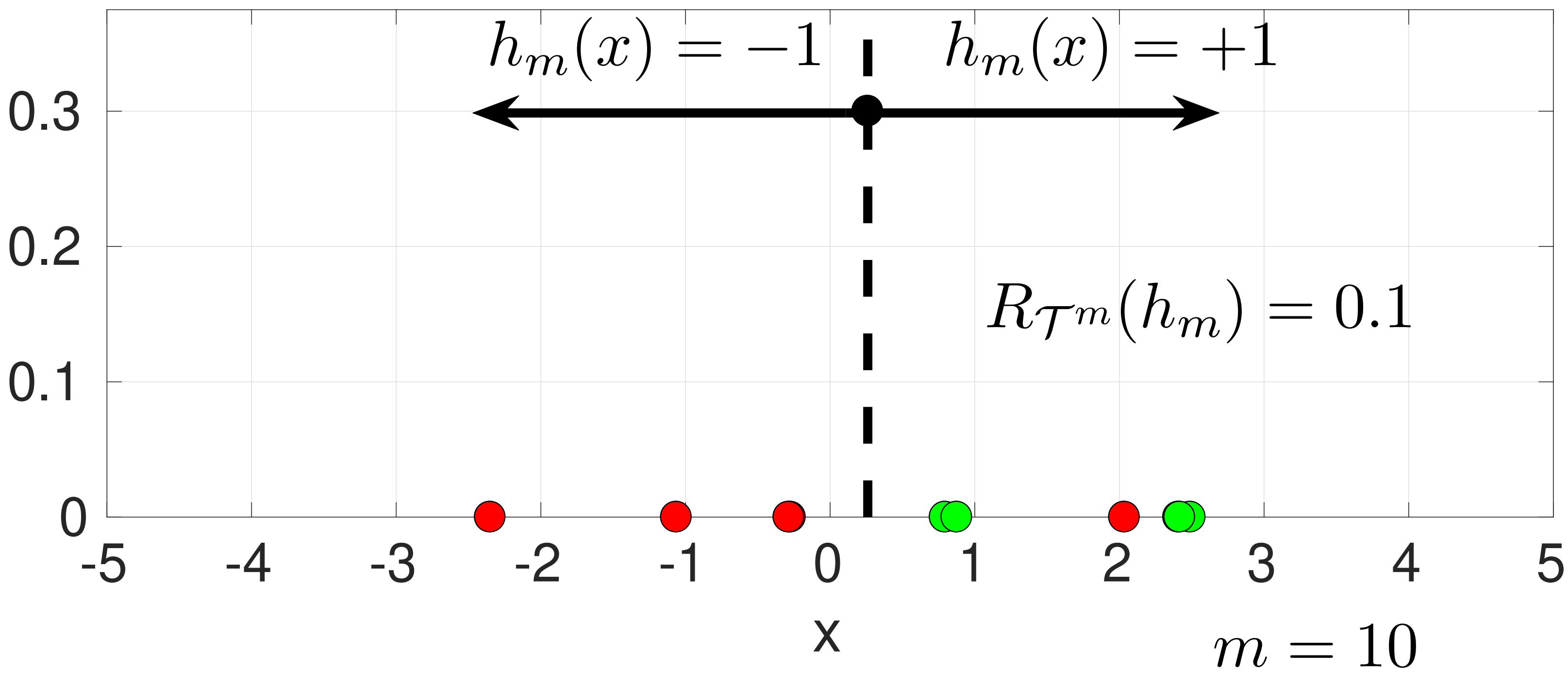

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$$h_m \in \operatorname*{Argmin}_{h\in\mathcal{H}} R_{\mathcal{T}^m}(h) \qquad (1)$$

- Depending on the choince of $\mathcal{H}$ and ℓ and algorithm solving (1) we get individual instances e.g. Support Vector Machines, Linear Regression, Logistic Regression, Neural Networks learned by back-propagation, AdaBoost, Gradient Boosted Trees, ...

Example of ERM failure

- Let $\mathcal{X} = [a, b] \subset \mathbb{R}$, $\mathcal{Y} = \{+1, -1\}$, $\ell(y, y') = [\![y \neq y']\!]$, $p(x \mid y = +1)$ and $p(x \mid y = -1)$ be uniform distributions on $\mathcal{X}$ and $p(y = +1) = 0.8$.

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- Consider learning algorithm which for a given training set $\mathcal{T}^m = \{(x^1, y^1), \ldots, (x^m, y^m)\}$ returns memorizing strategy

$$h_m(x) = \begin{cases} y^j & \text{if } \; x = x^j \; \text{ for some } \; j \in \{1, \ldots, m\} \\ -1 & \text{otherwise} \end{cases}$$

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- The empirical risk is $R_{\mathcal{T}^m}(h_m) = 0$ with probability 1 for any m.

- The expected risk is $R(h_m) = 0.8$ for any m.

Generalization error

- ERM may fail when $R_{\mathcal{T}^m}(h_m)$ is not a good proxy of $R(h_m)$, because $R_{\mathcal{T}^m}(h)$ is used as a guidance to select h_m.

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$$\forall\, \varepsilon > 0\colon\ \lim_{m\to\infty} \mathbb{P}\Big(\underbrace{\big|R_{\mathcal{T}^m}(h_m) - R(h_m)\big| \geq \varepsilon}_{\text{high generalization error}} \Big) = 0$$

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Plan for this lecture:

- Conditions on $\mathcal{H}$ which guarantee that the generalization error converges to zero with growing number of examples m.

What's wrong with Hoeffding ?

- Hoeffding inequality $\mathbb{P}(|\hat{\mu} - \mu| \geq \varepsilon) \leq 2e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}}$, $\hat{\mu} = \frac{1}{m}\sum_{i=1}^{m} z^i$, requires $\{z^1, \ldots, z^m\}$ to be sample from i.i.d. rv. with expeted value μ.

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Evaluation:

- h fixed independently on $\mathcal{T}^m$, $z^i = \ell(y^i, h(x^i))$ and $\{z^1, \dots, z^m\}$ is i.i.d.

- Therefore $\forall\, \varepsilon > 0$: $\lim_{m\to\infty} \mathbb{P}(|R_{\mathcal{T}^m}(h) - R(h)| \geq \varepsilon) = 0$

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Learning:

- $h_m = A(\mathcal{T}^m)$, $z^i = \ell(y^i, h_m(x^i))$ and thus $\{z^1,\ldots,z^m\}$ is not i.i.d.
- No guarantee that $\forall\,\varepsilon > 0\colon\ \lim_{m\to\infty} \mathbb{P}(|R_{\mathcal{T}^m}(h_m) - R(h_m)| \geq \varepsilon) = 0$

Uniform Law of Large Numbers

- Law of Large Numbers: for any $p(x,y)$ generating $\mathcal{T}^m$, and $h \in \mathcal{H}$ fixed without seeing $\mathcal{T}^m$ we have

$$\forall\, \varepsilon > 0\colon \lim_{m\to\infty} \mathbb{P}\Big(\underbrace{\big|R(h) - R_{\mathcal{T}^m}(h)\big| \geq \varepsilon}_{\text{high generalization error}} \Big) = 0$$

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- **Uniform Law of Large Numbers:** if for any $p(x,y)$ generating $\mathcal{T}^m$ it holds that

$$\forall \varepsilon > 0\colon \lim_{m\to\infty} \mathbb{P}\left(\begin{array}{l} \big|R(h_1) - R_{\mathcal{T}^m}(h_1)\big| \geq \varepsilon \quad \text{or} \\ \big|R(h_2) - R_{\mathcal{T}^m}(h_2)\big| \geq \varepsilon \quad \text{or} \\ \vdots \\ \underbrace{\big|R(h_{|\mathcal{H}|}) - R_{\mathcal{T}^m}(h_{|\mathcal{H}|})\big| \geq \varepsilon}_{\text{high generalization error at least for one strategy}} \end{array} \right) = 0$$

we say that ULLN applies for $\mathcal{H}$.

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- ULLN provides guarantees for all $h \in \mathcal{H}$ including $h_m = A(\mathcal{T}_m)$:

$$\mathbb{P}\Big(\big|R(h_m) - R_{\mathcal{T}^m}(h_m)\big| \geq \varepsilon \Big) \leq \mathbb{P}\Big(\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big| \geq \varepsilon \Big)$$

ULLN applies for finite hypothesis class

- Assume a finite hypothesis class $\mathcal{H} = \{h_1, \ldots, h_K\}$.
- Define the set of all "bad" training sets for a strategy $h \in \mathcal{H}$ as

$$\mathcal{B}(h) = \left\{ \mathcal{T}^m \in (\mathcal{X} \times \mathcal{Y})^m \,\middle|\, \left| R_{\mathcal{T}^m}(h) - R(h) \right| \geq \varepsilon \right\}$$

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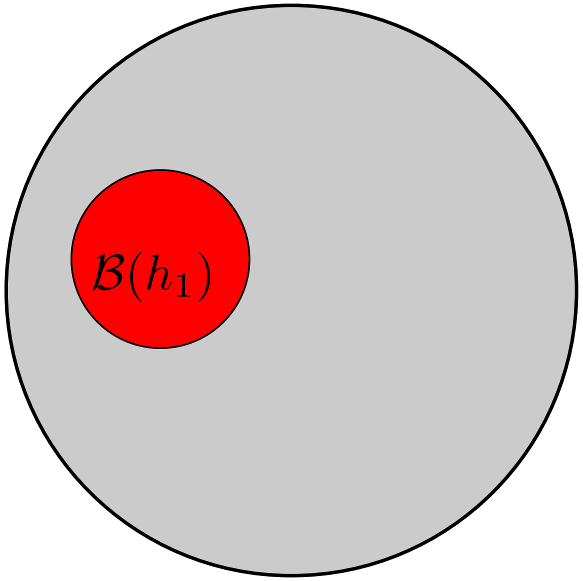

Single strategy

$$\mathbb{P}\Big(\left| R_{\mathcal{T}^m}(h_1) - R(h_1) \right| \geq \varepsilon \Big) = \mathbb{P}\Big(\mathcal{T}^m \in \mathcal{B}(h_1) \Big) \leq 2\, e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}}$$

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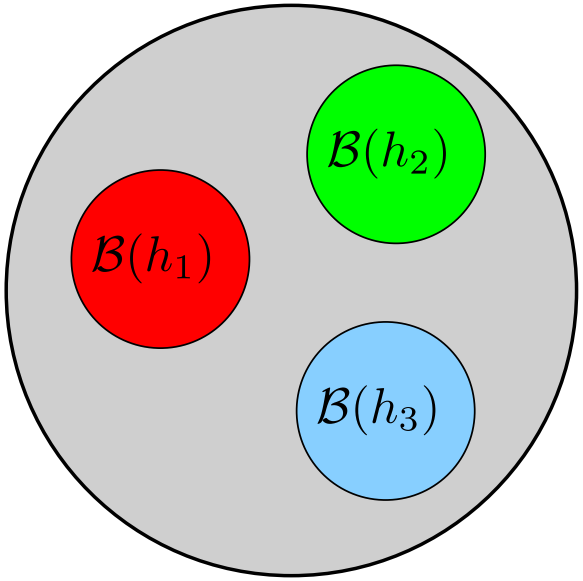

Three strategies

Events $\mathcal{T}^m \in \mathcal{B}(h)\,, h \in \mathcal{H}$

mutually exclusive

$$\mathbb{P}\Big(\max_{h \in \{h_1, h_2, h_3\}} \big| R_{\mathcal{T}^m}(h) - R(h) \big| \geq \varepsilon \Big) =$$

$$\mathbb{P}\Big(\mathcal{T}^m \in \mathcal{B}(h_1) \;\text{ or }\; \mathcal{T}^m \in \mathcal{B}(h_2) \;\text{ or }\; \mathcal{T}^m \in \mathcal{B}(h_3) \Big) =$$

$$\mathbb{P}\big(\mathcal{T}^m \in \mathcal{B}(h_1)\big) + \mathbb{P}\big(\mathcal{T}^m \in \mathcal{B}(h_2)\big) + \mathbb{P}\big(\mathcal{T}^m \in \mathcal{B}(h_3)\big)$$

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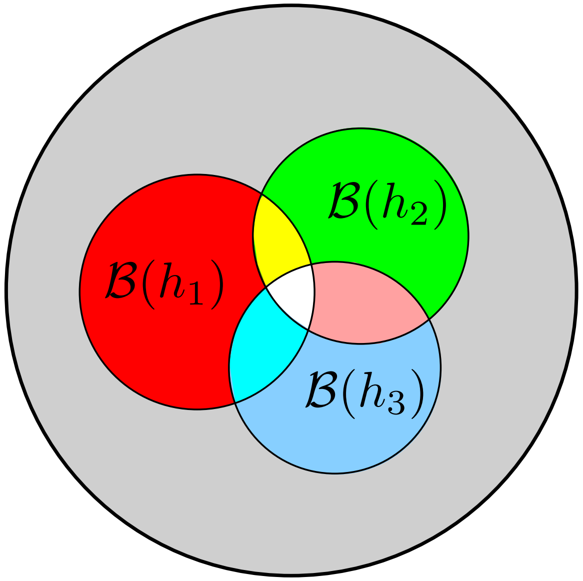

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- Hoeffding inequality generalized for finite hypothesis class $\mathcal{H}$:

$$\mathbb{P}\Big(\max_{h \in \mathcal{H}} \left| R_{\mathcal{T}^m}(h) - R(h) \right| \geq \varepsilon \Big) \leq \sum_{h \in \mathcal{H}} \mathbb{P}\big(\mathcal{T}^m \in \mathcal{B}(h) \big) = 2\, |\mathcal{H}|\, e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}}$$

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$$\forall\, \varepsilon > 0\colon \lim_{m \to \infty} \mathbb{P}\Big(\max_{h \in \mathcal{H}} \big|R_{\mathcal{T}^m}(h) - R(h)\big| \geq \varepsilon \Big) = 0$$

Generalization bound for finite hypothesis class

- Hoeffding inequality generalized for a finite hypothesis class $\mathcal{H}$:

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- Find an upper bound ε on the generalization error which holds uniformly for all $h \in \mathcal{H}$ with probability $1-\delta$ at least:

$$\begin{aligned}\mathbb{P}\Big(\max_{h\in\mathcal{H}} |R_{\mathcal{T}^m}(h) - R(h)| < \varepsilon \Big) &= 1 - \mathbb{P}\Big(\max_{h\in\mathcal{H}} |R_{\mathcal{T}^m}(h) - R(h)| \geq \varepsilon \Big) \\ &\geq 1 - 2|\mathcal{H}| e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}} = 1-\delta\end{aligned}$$

and solving the last equality for ε yields

$$\varepsilon = (b-a)\sqrt{\frac{\log 2|\mathcal{H}| + \log\frac{1}{\delta}}{2m}}$$

Generalization bound for finite hypothesis class

Theorem: Let $\mathcal{T}^m = \{(x^1, y^1), \ldots, (x^m, y^m)\} \in (\mathcal{X} \times \mathcal{Y})^m$ be draw from i.i.d. rv. with p.d.f. $p(x, y)$ and let $\mathcal{H}$ be a finite hypothesis class. Then, for any $0 < \delta < 1$, with probability at least $1 - \delta$ the inequality

$$R(h) \leq \underbrace{R_{\mathcal{T}^m}(h)}_{\text{empirical risk}} + \underbrace{(b - a)\sqrt{\frac{\log 2|\mathcal{H}| + \log \frac{1}{\delta}}{2m}}}_{\text{complexity term}}$$

holds for all $h \in \mathcal{H}$ simultaneously and any loss function $\ell \colon \mathcal{Y} \times \mathcal{Y} \to [a, b]$.

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Recommendations that follow from the bound:

- Minimize the empirical risk.
- More training examples the better.
- Select appropriate trade-off between $|\mathcal{H}|$ and m:

Structural Risk Minimization

- Learn $h\colon \mathcal{X} \to \mathcal{Y}$ by minimizing the generalization bound

$$R(h) \leq R_{\mathcal{T}^m}(h) + \underbrace{(b-a)\sqrt{\frac{\log 2|\mathcal{H}| + \log \frac{1}{\delta}}{2m}}}_{\epsilon(m,|\mathcal{H}|,\delta)}$$

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- Design a nested sequence of hypothesis classes

$$\mathcal{H}_1 \subset \mathcal{H}_2 \subset \cdots \subset \mathcal{H}_K$$

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- Minimize the generalization bound:

1. $h_i = \operatorname*{argmin}_{h \in \mathcal{H}_i} R_{\mathcal{T}^m}(h)\,, \quad \forall i \in \{1,\ldots,K\}$
2. $i^* = \operatorname*{argmin}_{i=1,\ldots,K} \Big(R_{\mathcal{T}^m}(h_i) + \epsilon(m, |\mathcal{H}_i|, \delta) \Big)$
3. Output h_{i^*}

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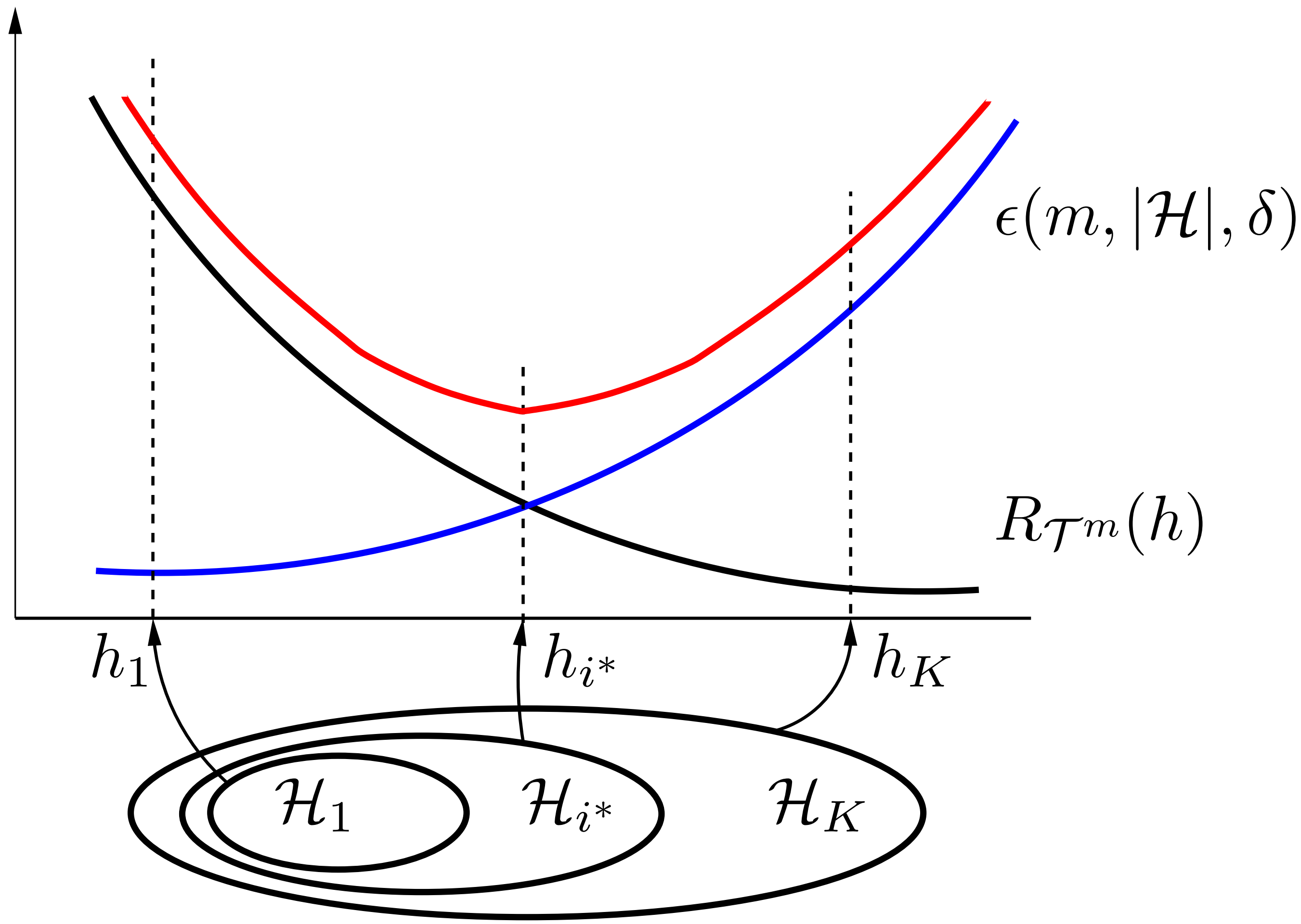

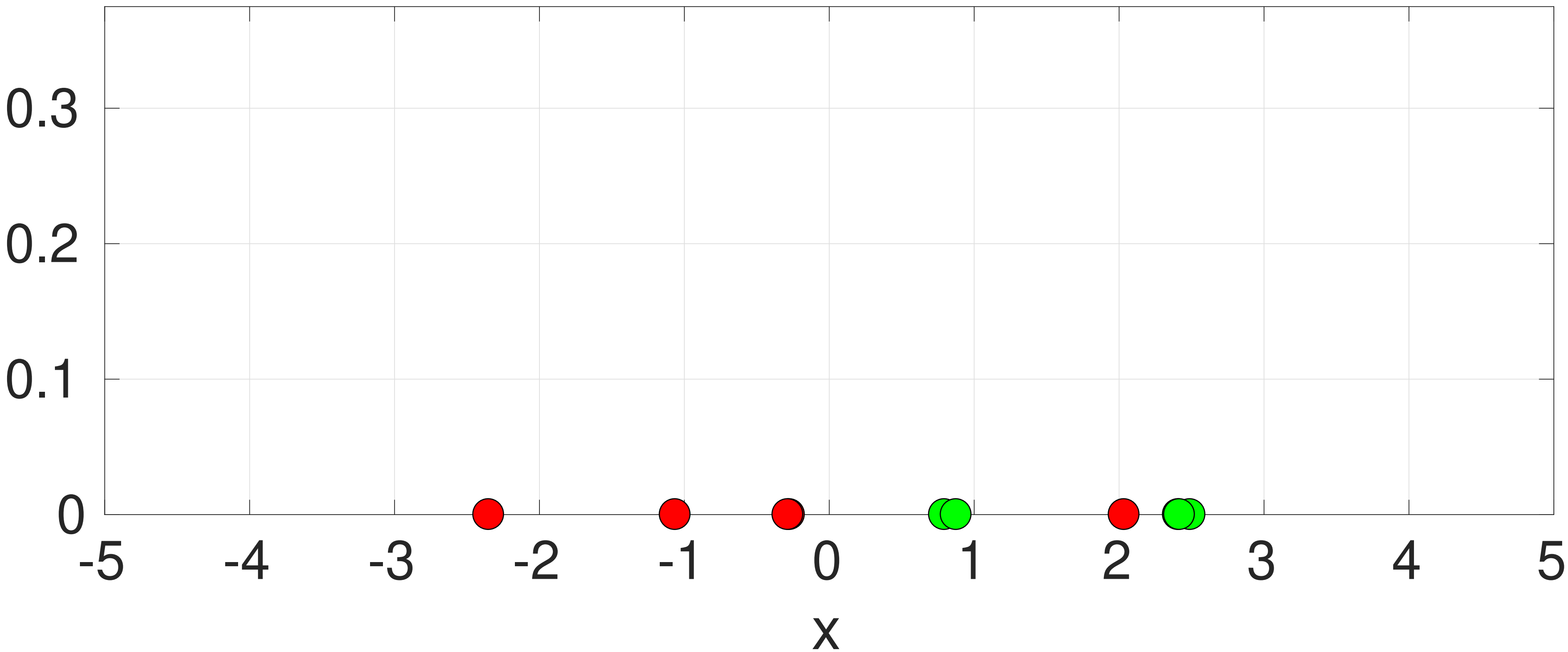
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0.2
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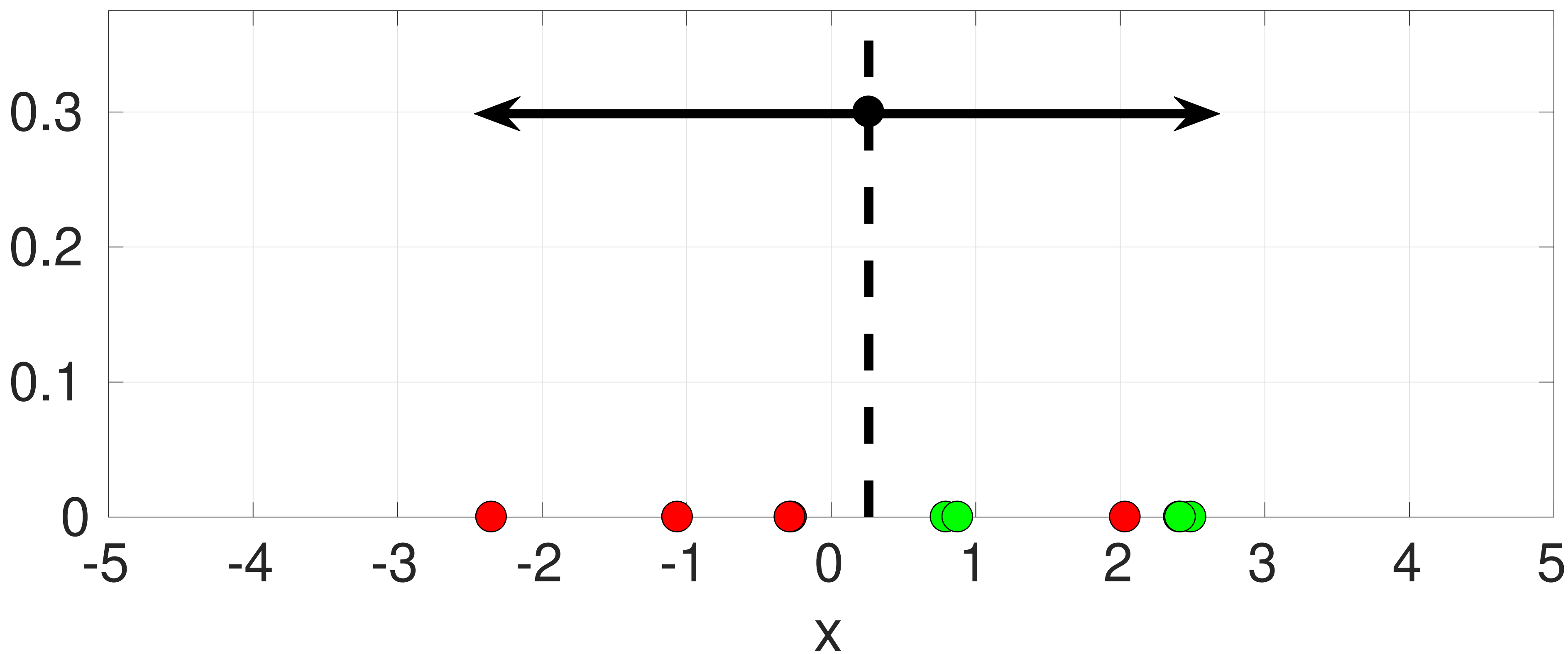
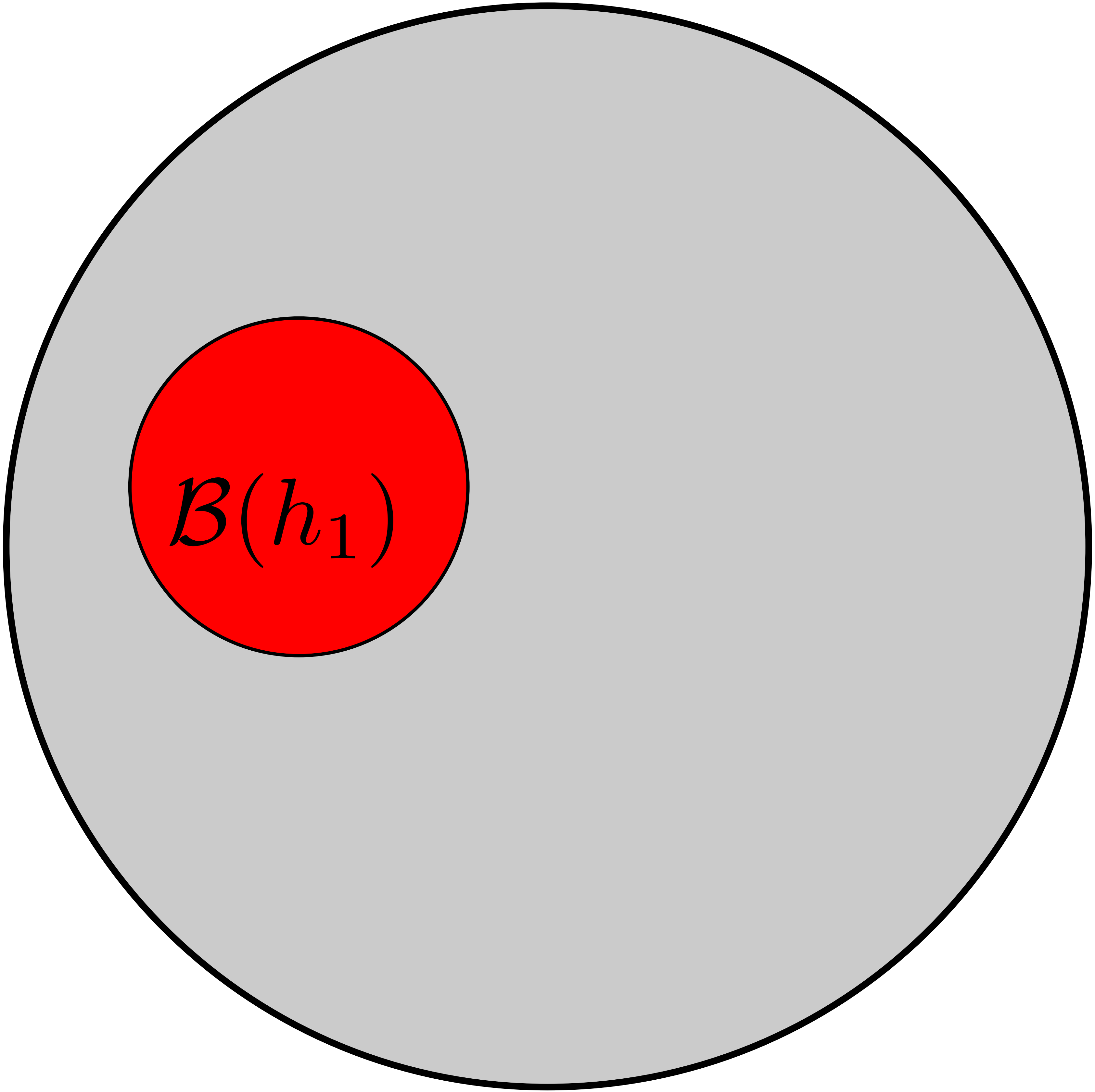
5
x


0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x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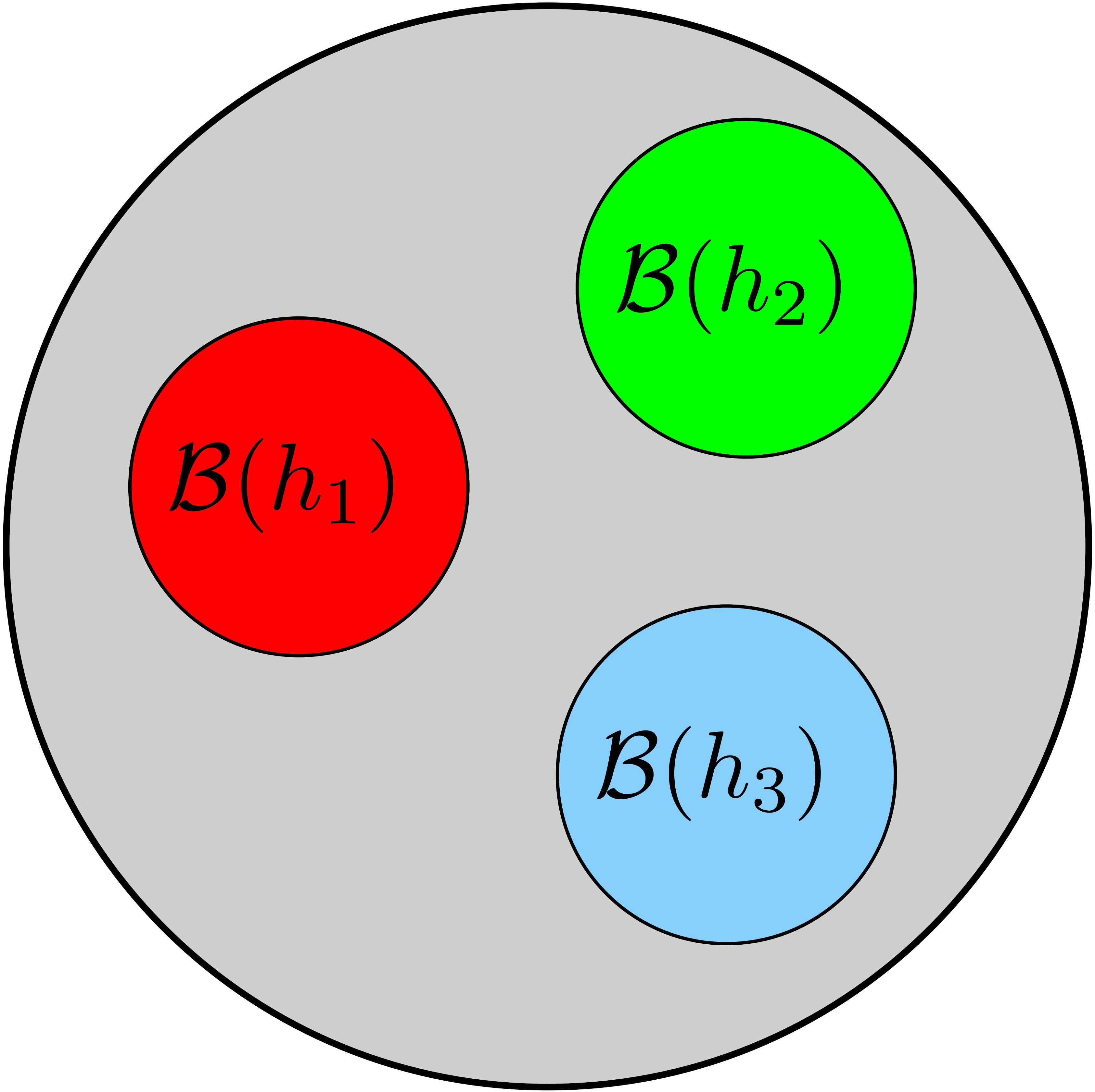
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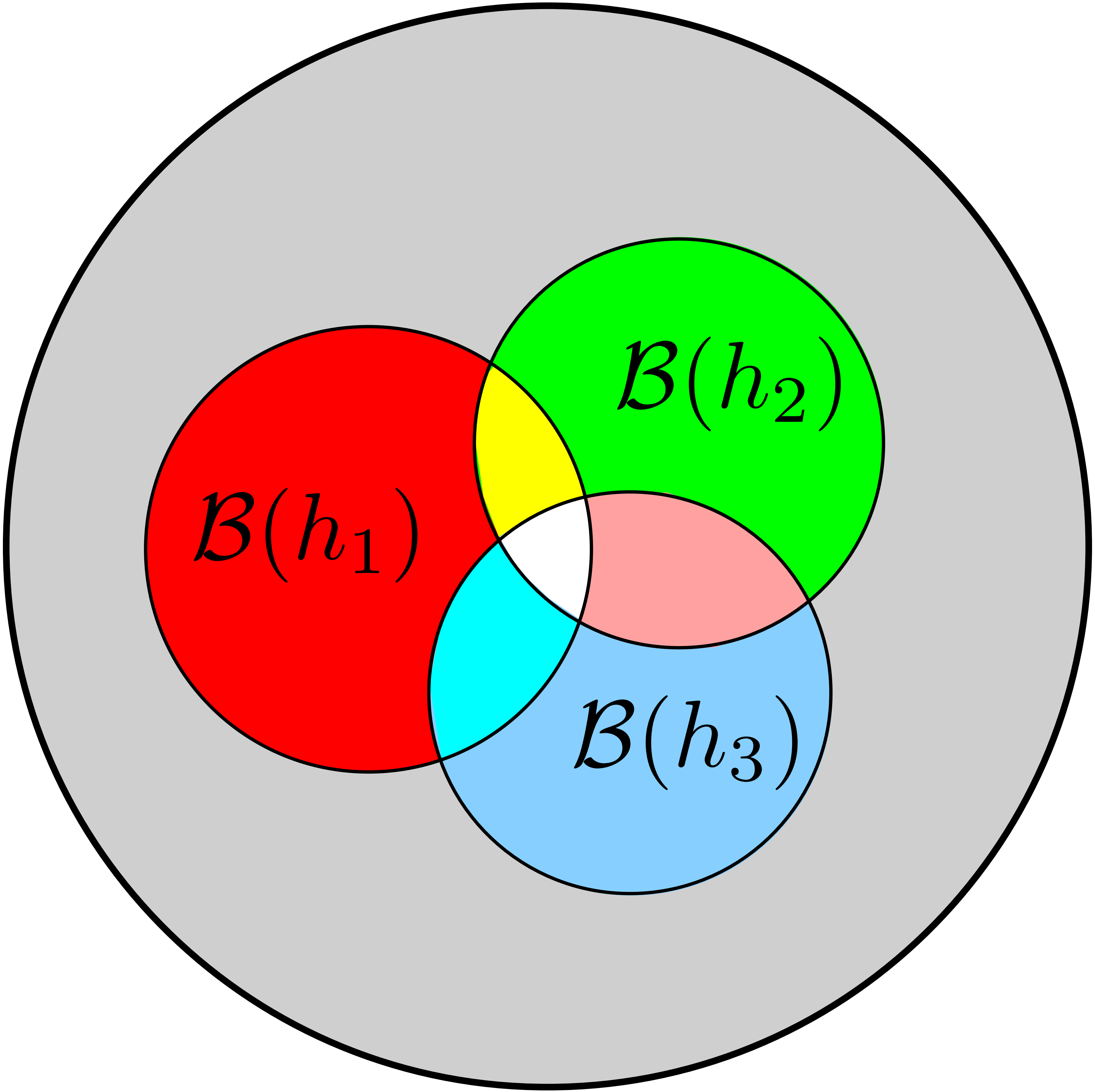
$\mathcal{B}(h_1)$
$\mathcal{B}(h_3)$


$\mathcal{B}(h_1)$
$\mathcal{B}(h_2)$
$\mathcal{B}(h_3)$