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

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Learning

- **Goal:** Given a training set $\mathcal{T}^m \sim p^m$, find a strategy $h\colon \mathcal{X} \to \mathcal{Y}$ with minimizing the generalization error $R(h) = \mathbb{E}_{(x,y)\sim p}[\ell(y, h(x))]$.

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- Learning algorithm: a function

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

returns a strategy $h_m = A(\mathcal{T}^m)$ from $\mathcal{H}$ based on a training set $\mathcal{T}^m$

Empirical Risk Minimization learning

- The generalization error $R(h)$ is approximated by the empirical risk $R_{\mathcal{T}^m}(h)$ computed on the training examples $\mathcal{T}^m \sim p^m$:

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- The ERM based learning 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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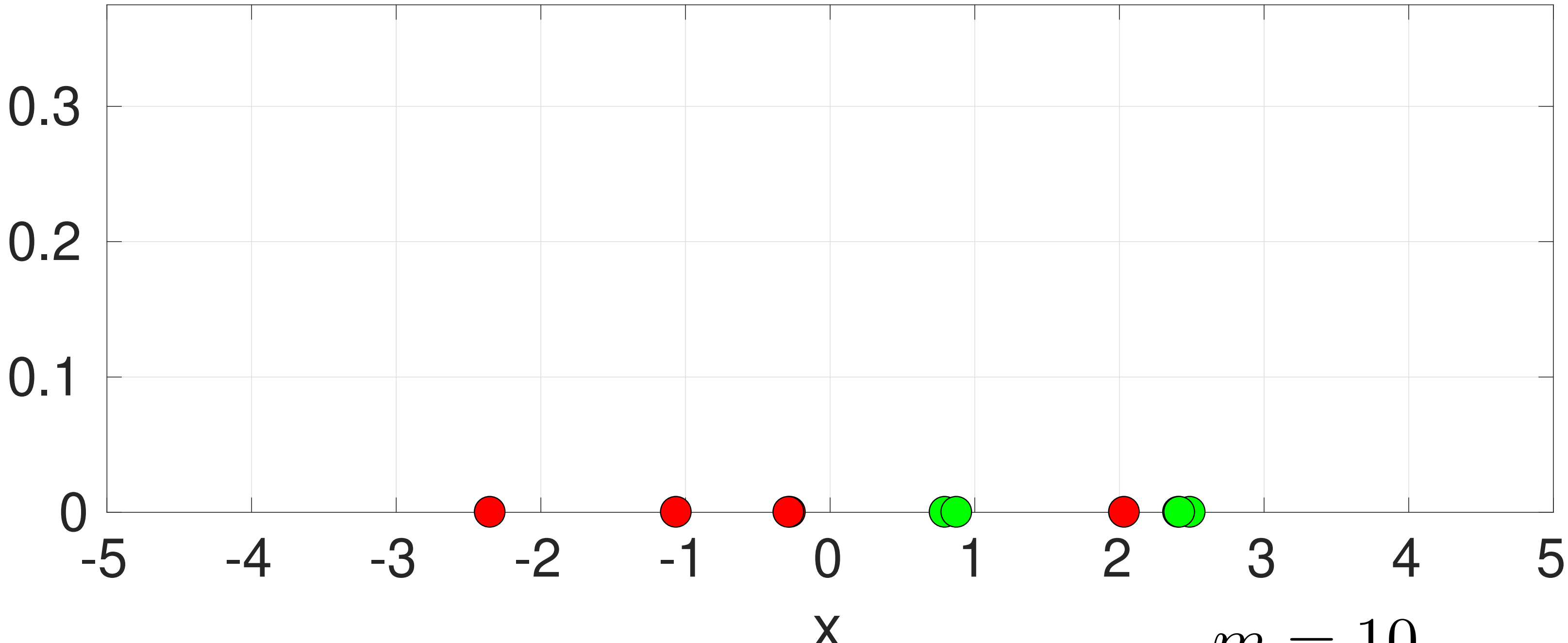

$m = 10$

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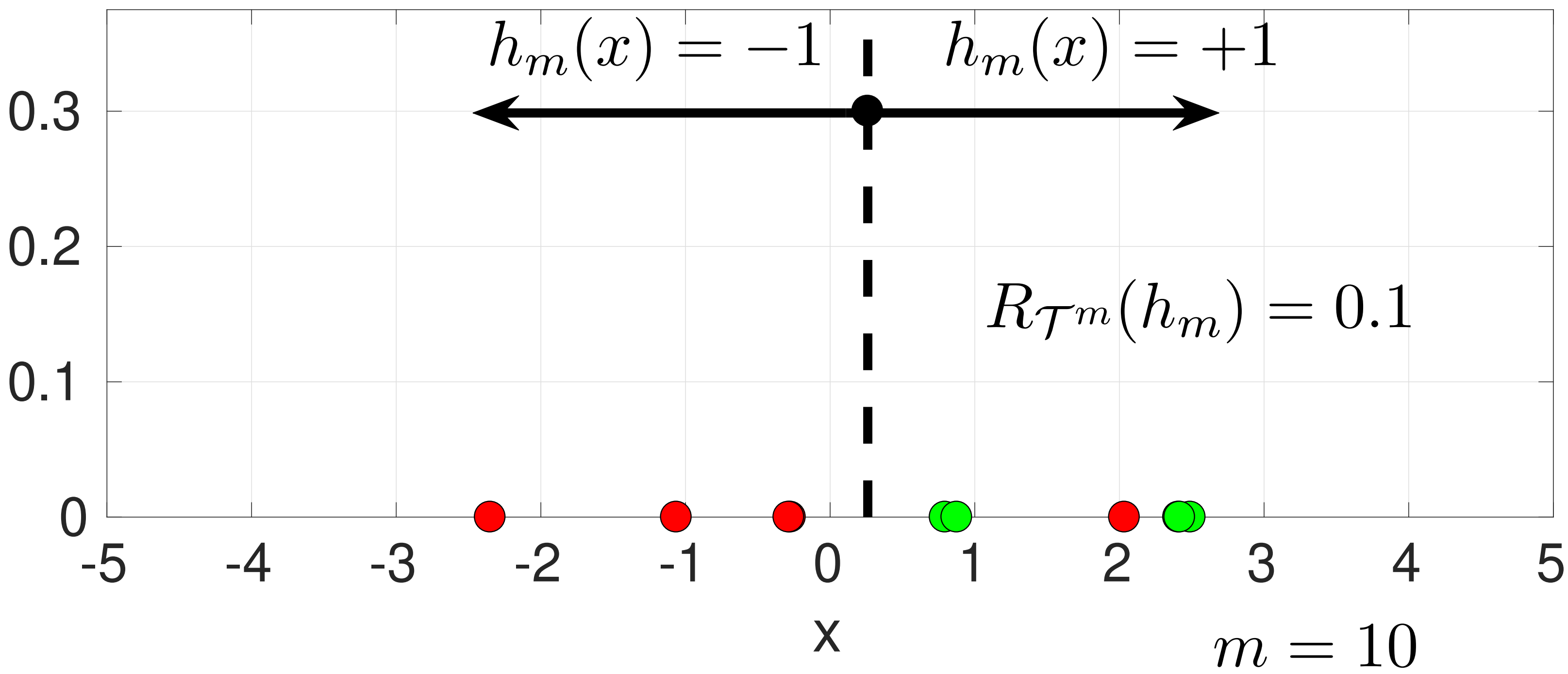

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- Depending on the choince of $\mathcal{H}$ and ℓ and algorithm solving (1) we get individual instances e.g. Support Vector Machines, Linear Regression, Logistic Regression, Neural Networks learned by back-propagation, AdaBoost, Gradient Boosted Trees,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

ERM can fail due to overfitting

- 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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- Learning algorithm "lookup table": given training set $\mathcal{T}^m$ it returns

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- Overfitting: the case when $h_m = A(\mathcal{T}^m)$ and the training error $R_{\mathcal{T}^k}(h_m)$ is low while the generalization error $R(h_m)$ is high.
- **Problem:** under which conditions the overfitting can be eliminated?

Why the law of large numbers does not apply for learning?

- 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 independent random variables with the expected value μ.

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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.

- We cannot apply Hoeffding to bound $\mathbb{P}(|R_{\mathcal{T}^m}(h_m) - R(h_m)| \geq \varepsilon)$

The overfitting can be eliminited in case of the finite hypothesis space

- Assume a finite hypothesis class $\mathcal{H} = \{h_1, \ldots, h_K\}$.
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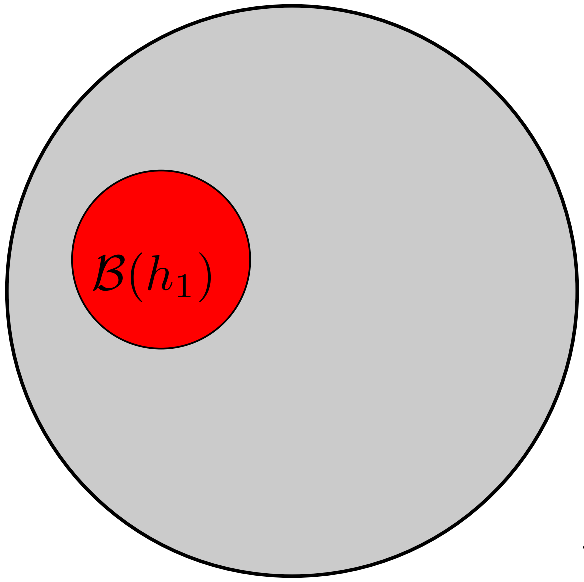

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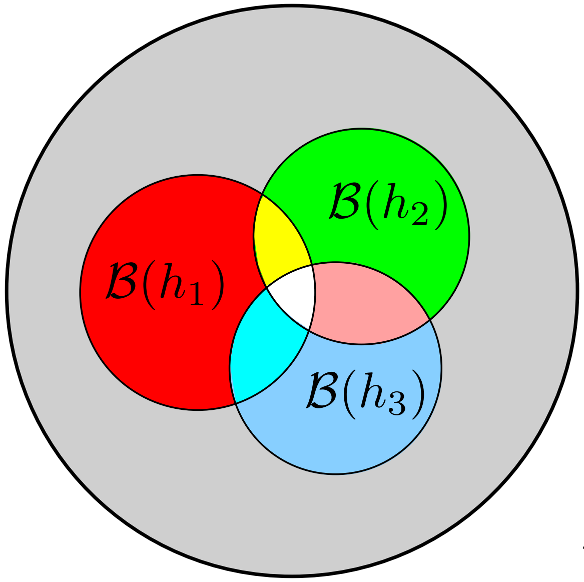

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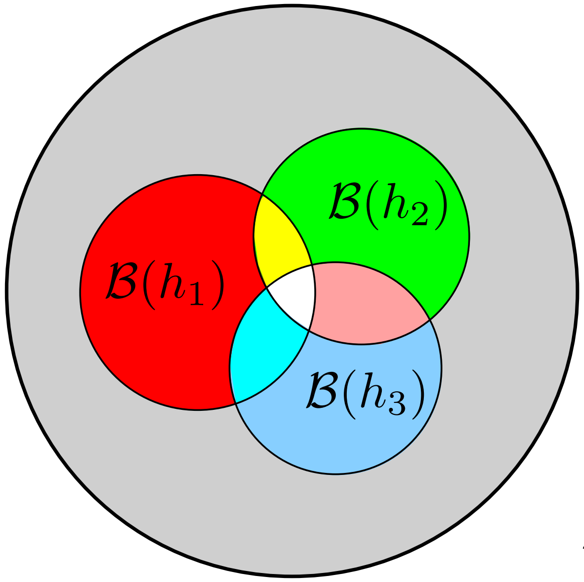

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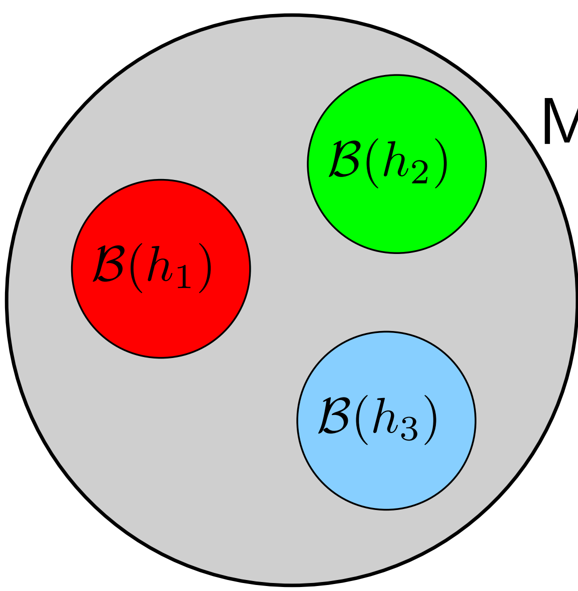

Mutually exclusive events: $\mathcal{B}(h_1) \cap \mathcal{B}(h_2) \cap \mathcal{B}(h_3) = \emptyset$

$$\mathbb{P}(\mathcal{B}(h_1) \cup \mathcal{B}(h_2) \cup \mathcal{B}(h_3)) = \mathbb{P}(\mathcal{B}(h_1)) + \mathbb{P}(\mathcal{B}(h_2)) + \mathbb{P}(\mathcal{B}(h_3))$$

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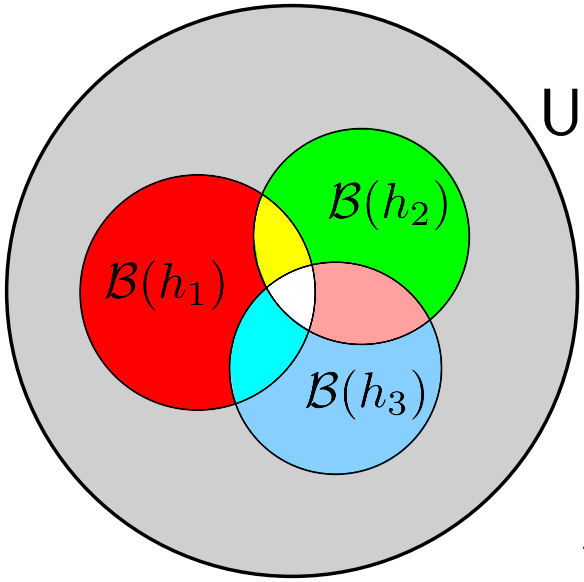

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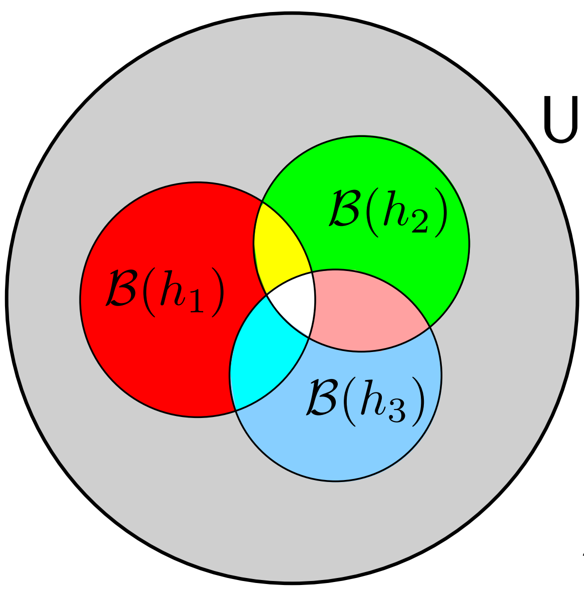

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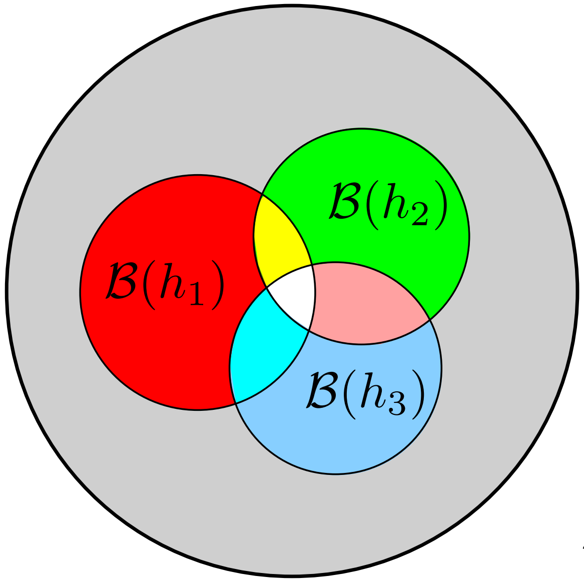

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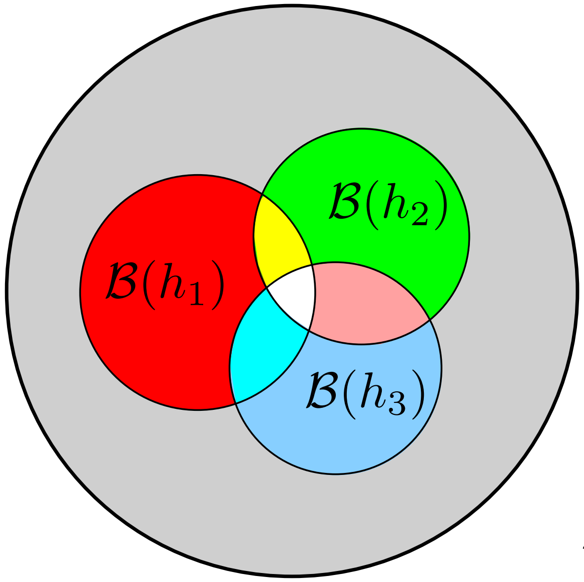

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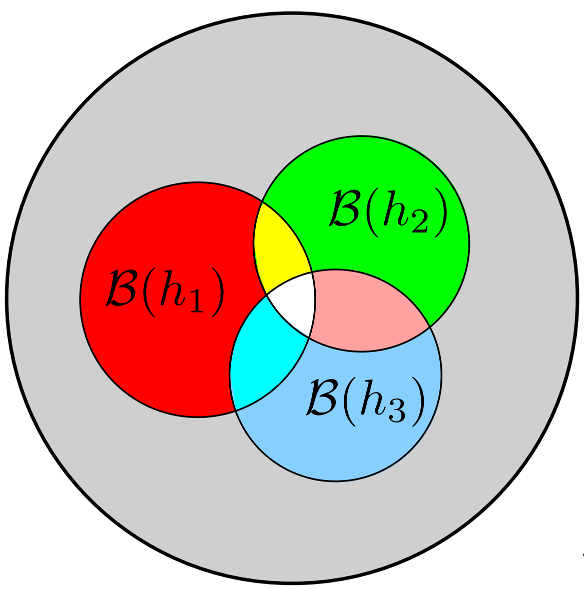

Hoeffding inequality:

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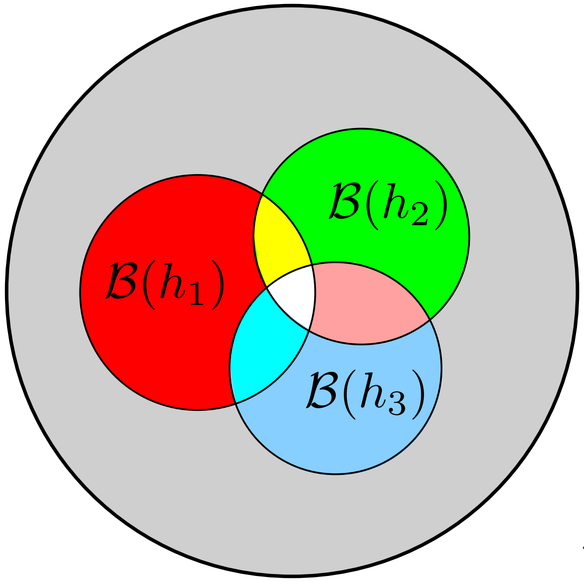
- Assume a finite hypothesis class $\mathcal{H} = \{h_1, \ldots, h_K\}$.
- ERM learning: $h_m \in \operatorname{Argmin}_{h \in \mathcal{H}} R_{\mathcal{T}^m}(h)$.

The probability that the empirical risk fails can be reduced to zero if we have anough examples:

$$\mathbb{P}\Big(\underbrace{\big|R(h_m) - R_{\mathcal{T}^m}(h_m)\big| \geq \varepsilon}_{\text{ER fails}}\Big) \leq \mathbb{P}\Big(\max_{h \in \mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big| \geq \varepsilon\Big)$$

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

$$\leq 2\,|\mathcal{H}|\, e^{-\frac{2m\,\varepsilon^2}{(\ell_{\max} - \ell_{\min})^2}}$$



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1. $\mathbb{P}\big($ ER fails for $h_m \in \mathcal{H}\big)$ is replaced by $\mathbb{P}\big($ ER can fail for some $h \in \mathcal{H}\big)$.
2. Union bound.
3. Hoeffding inequality.

Uniform Law of Large Numbers

We have shown for that for the finite hypothesis space, $\mathcal{H} = \{h_1, \ldots, h_K\}$, the Law of Large Numbers holds simultaneously (uniformly) for every $h \in \mathcal{H}$:

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Definition: We say that Uniform Law of Large Numbers applies for hypothesis space $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$ if there exists a function $m_{\mathcal{H}}\colon \mathbb{R}_{>0} \times (0,1) \to \mathbb{N}$ such that for every $\varepsilon > 0, \delta \in (0,1)$, every distribution $p(x,y)$ and every $m \geq m_{\mathcal{H}}(\varepsilon,\delta)$ the following inequality holds

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The next lecture:

- If ULLN applies then ERM learning is guaranteed to succeed.
- VC dimension as a tool to recognize that ULLN applies for given $\mathcal{H}$.

Generalization bound for finite hypothesis class

Theorem: Let $\mathcal{T}^m = \big((x^1, y^1), \ldots, (x^m, y^m)\big) \in (\mathcal{X} \times \mathcal{Y})^m$ 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

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

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- To decreases the complexity term: increase m or decrease $|\mathcal{H}|$.
- The generalization bound holds for any learning algorithm not just ERM.
- Recommendations for learning:
  1. Minimize the empirical risk.
  2. Use as much training examples m as you can.
  3. Limit the size of the hypothesis space $|\mathcal{H}|$, i.e. use prior knowledge.

Generalization bound for finite hypothesis class: the proof

- We have shown that ULLN holds for finite hypothesis class $\mathcal{H}$:

$$\mathbb{P}\Big(\max_{h\in\mathcal{H}} |R_{\mathcal{T}^m}(h) - R(h)| \geq \varepsilon\Big) \leq 2|\mathcal{H}|e^{-\frac{2m\,\varepsilon^2}{(\ell_{\max}-\ell_{\min})^2}}$$

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$$\begin{aligned}
\mathbb{P}\Big(|R_{\mathcal{T}^m}(h) - R(h)| < \varepsilon\,, \forall h \in \mathcal{H} \Big) &= \mathbb{P}\Big(\max_{h\in\mathcal{H}} |R_{\mathcal{T}^m}(h) - R(h)| < \varepsilon \Big) \\
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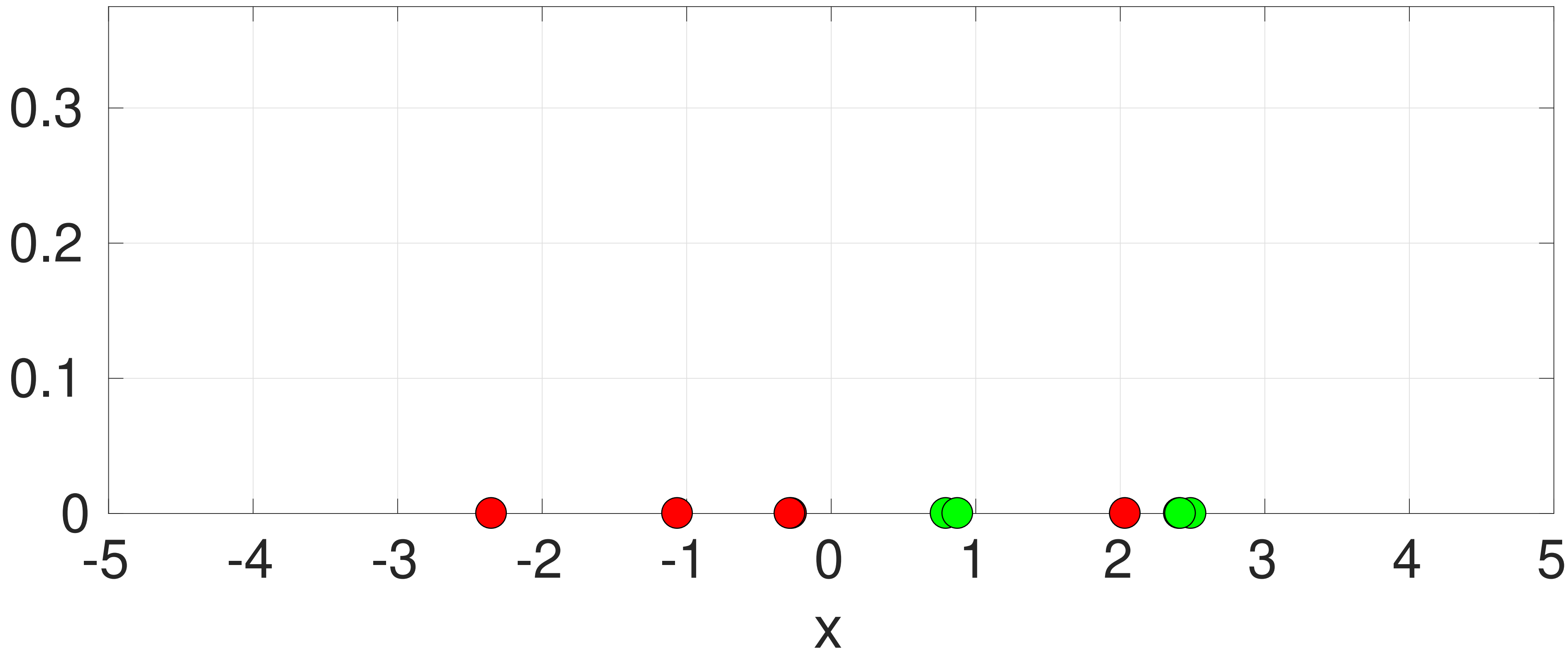
- Solving the last equality for ε yields $\varepsilon = L\sqrt{\frac{\log 2|\mathcal{H}| + \log\frac{1}{\delta}}{2m}}$ so that:

$$\mathbb{P}\left(|R_{\mathcal{T}^m}(h) - R(h)| < L\sqrt{\frac{\log 2|\mathcal{H}| + \log\frac{1}{\delta}}{2m}}\,,\, \forall h \in \mathcal{H}\right) \geq 1 - \delta$$

Summary

- Learning algorithm: the definition.
- Empirical Risk Minimization.
- Unrestricted hypothesis space: the ERM can overfit regardless the number of training examples.
- Finite hypothesis space: the chance of overfitting can be always eliminated.
- Uniform Law of Large Numbers.
- Generalization bound for finite hypothesis space.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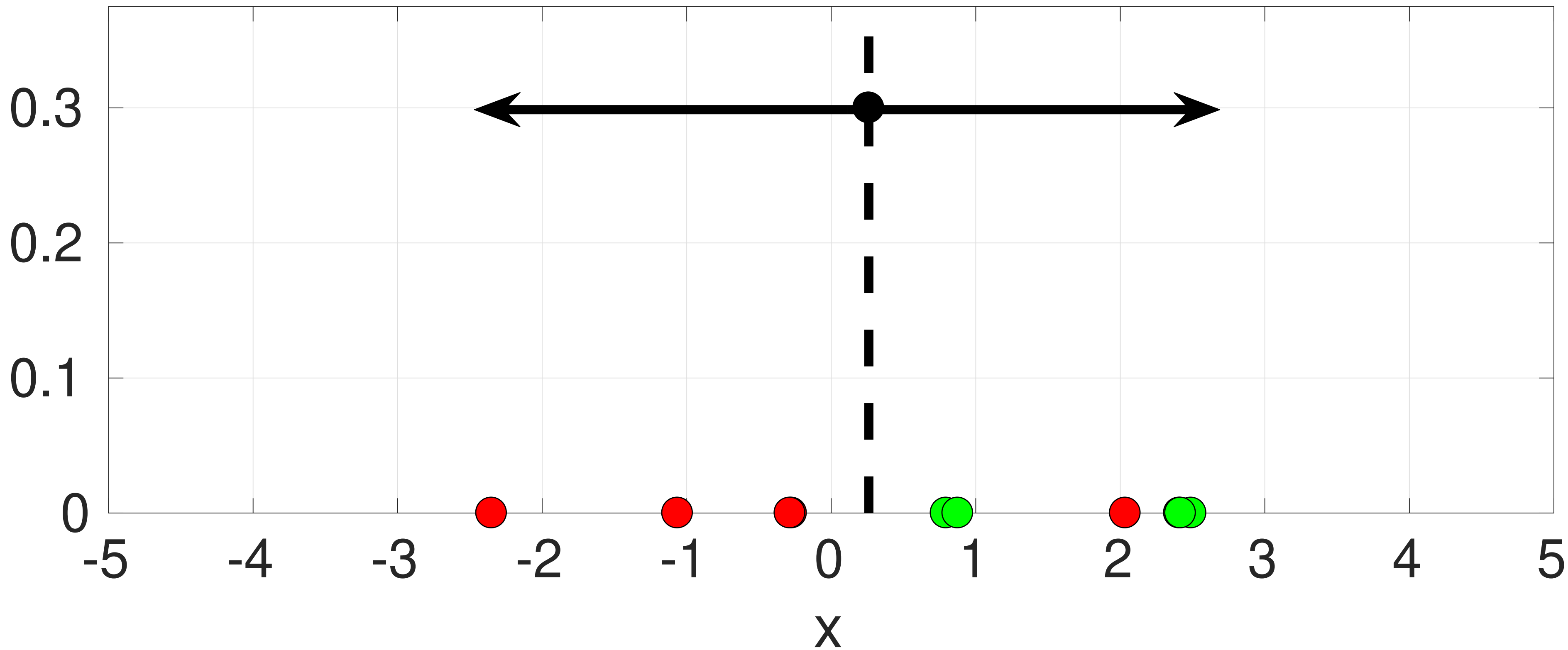
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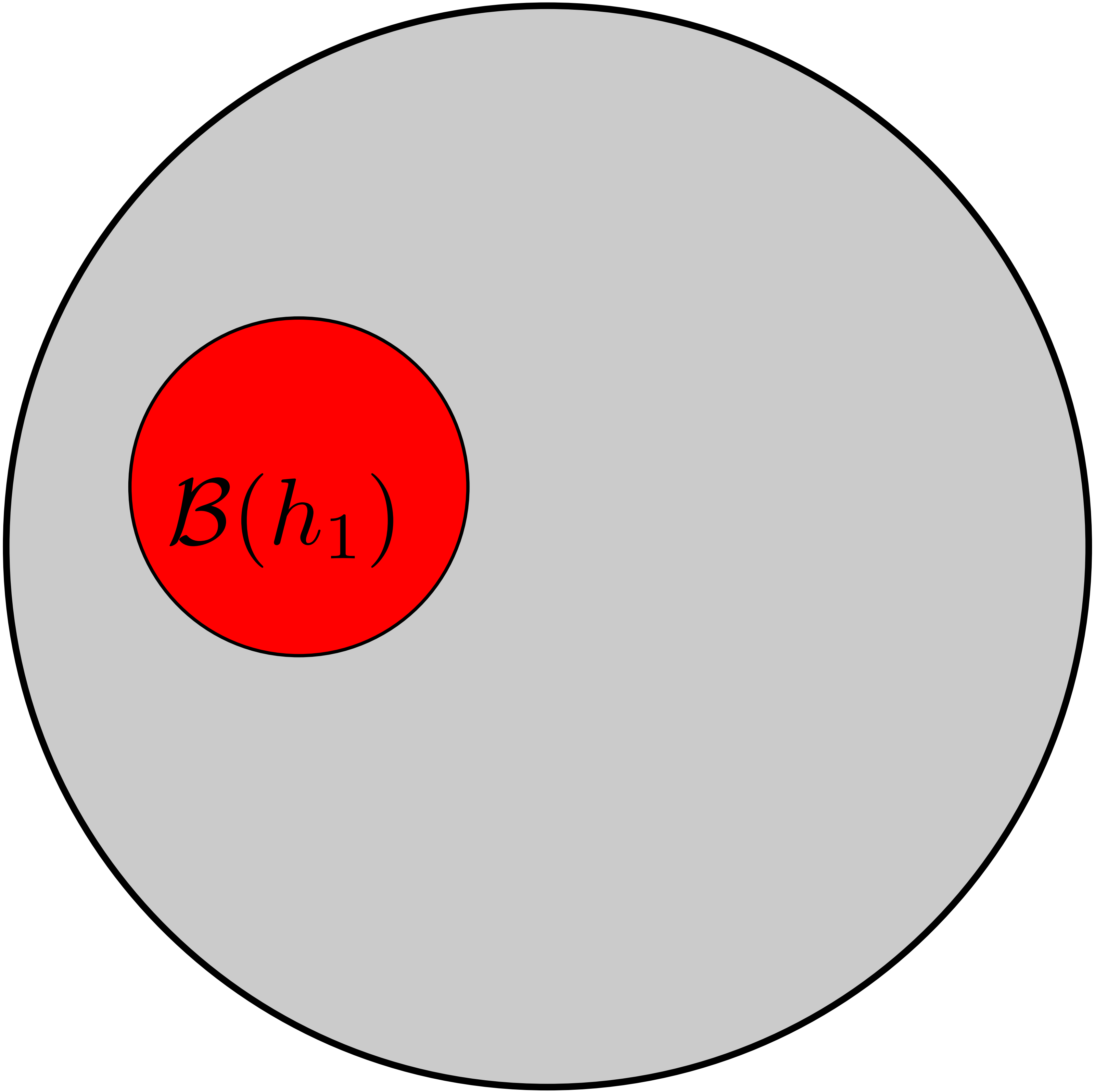
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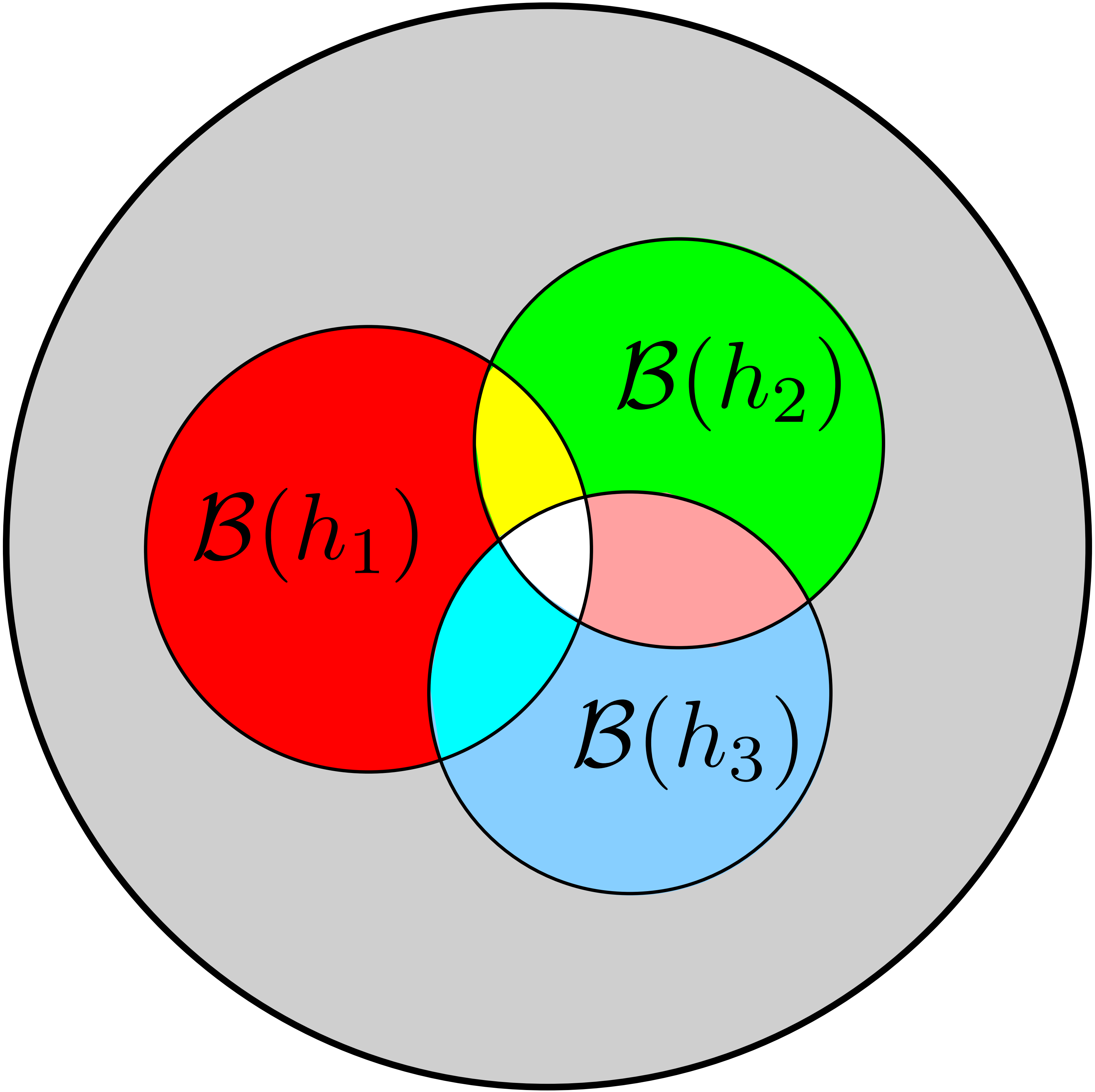

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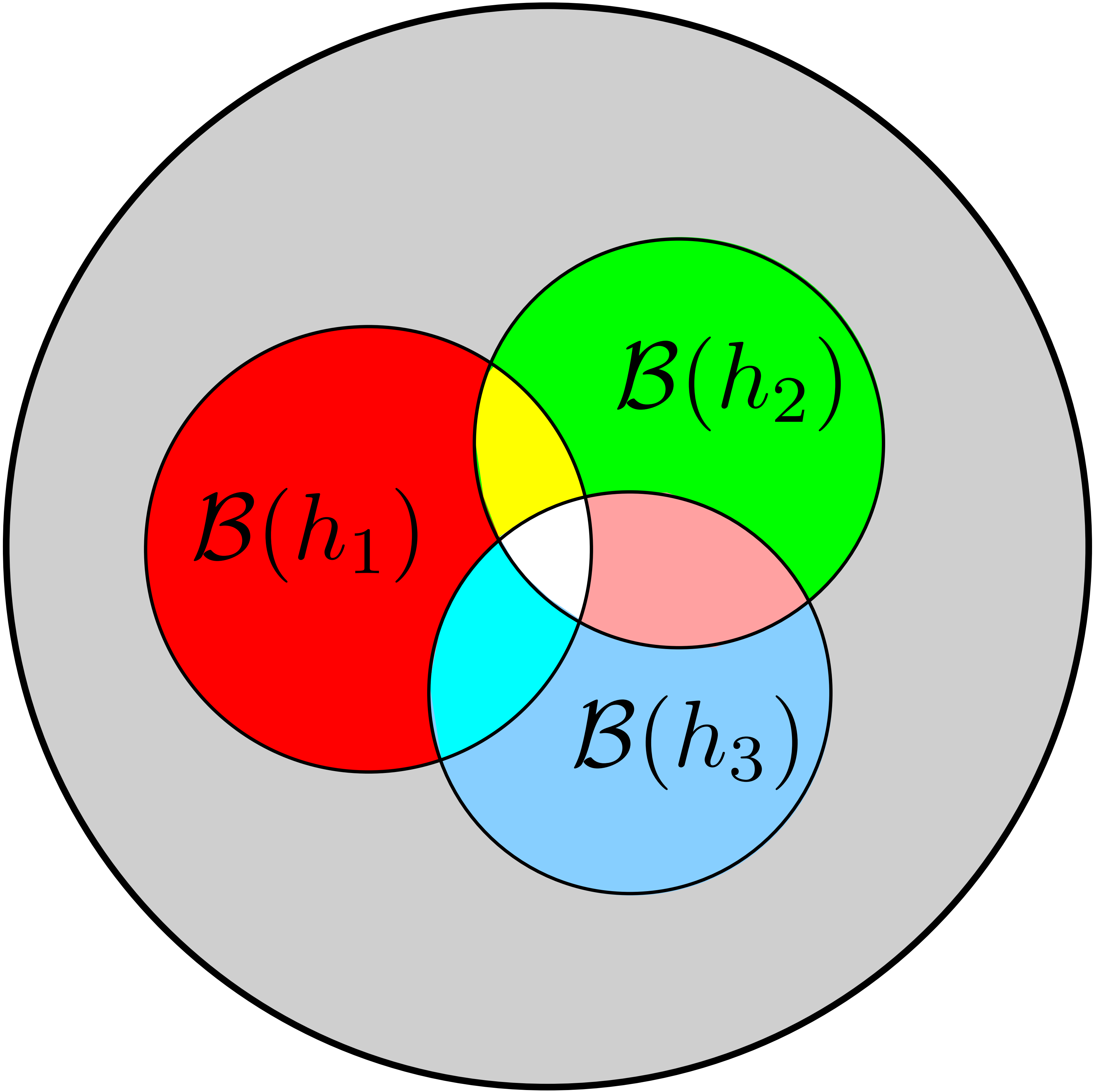
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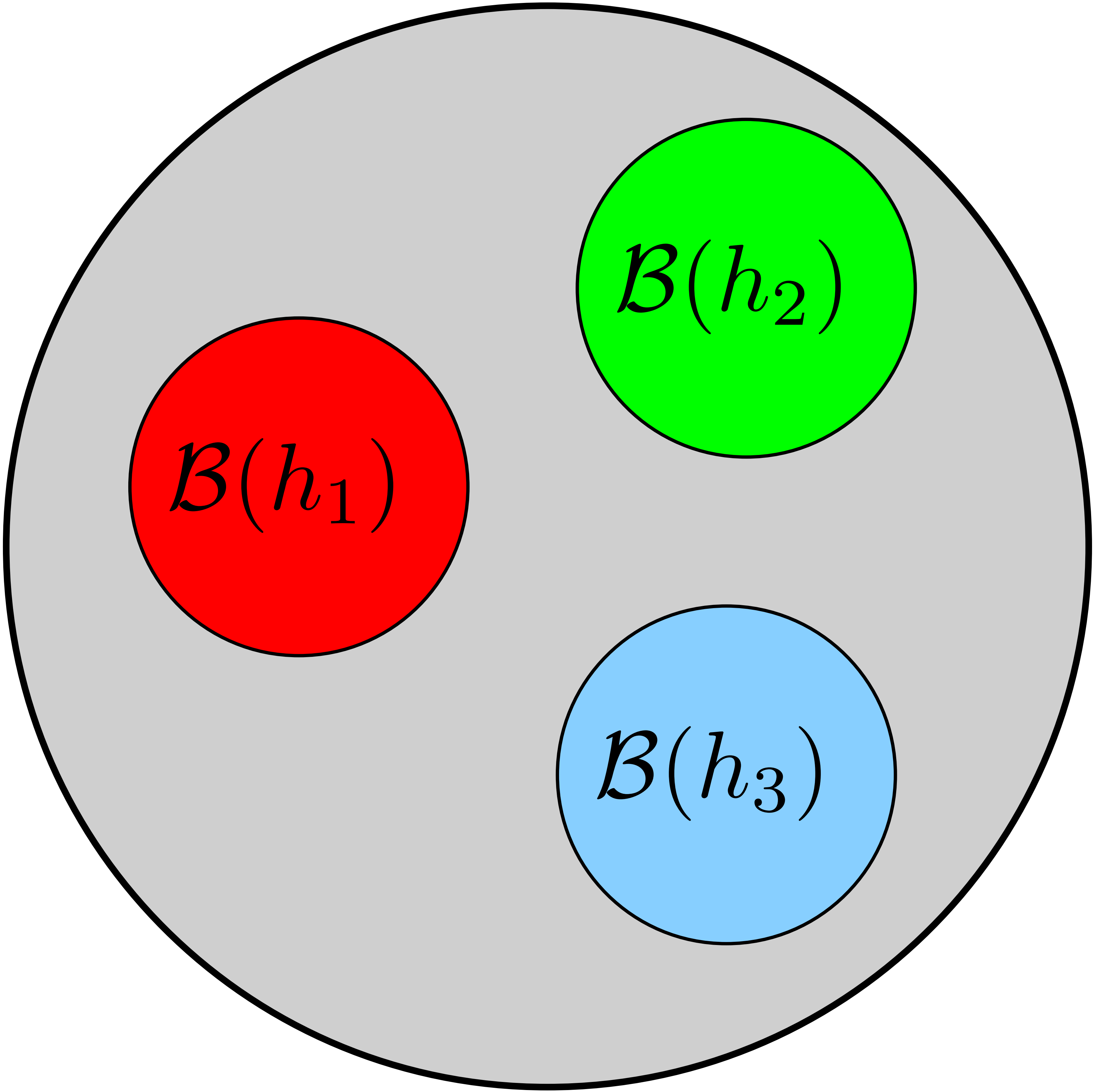
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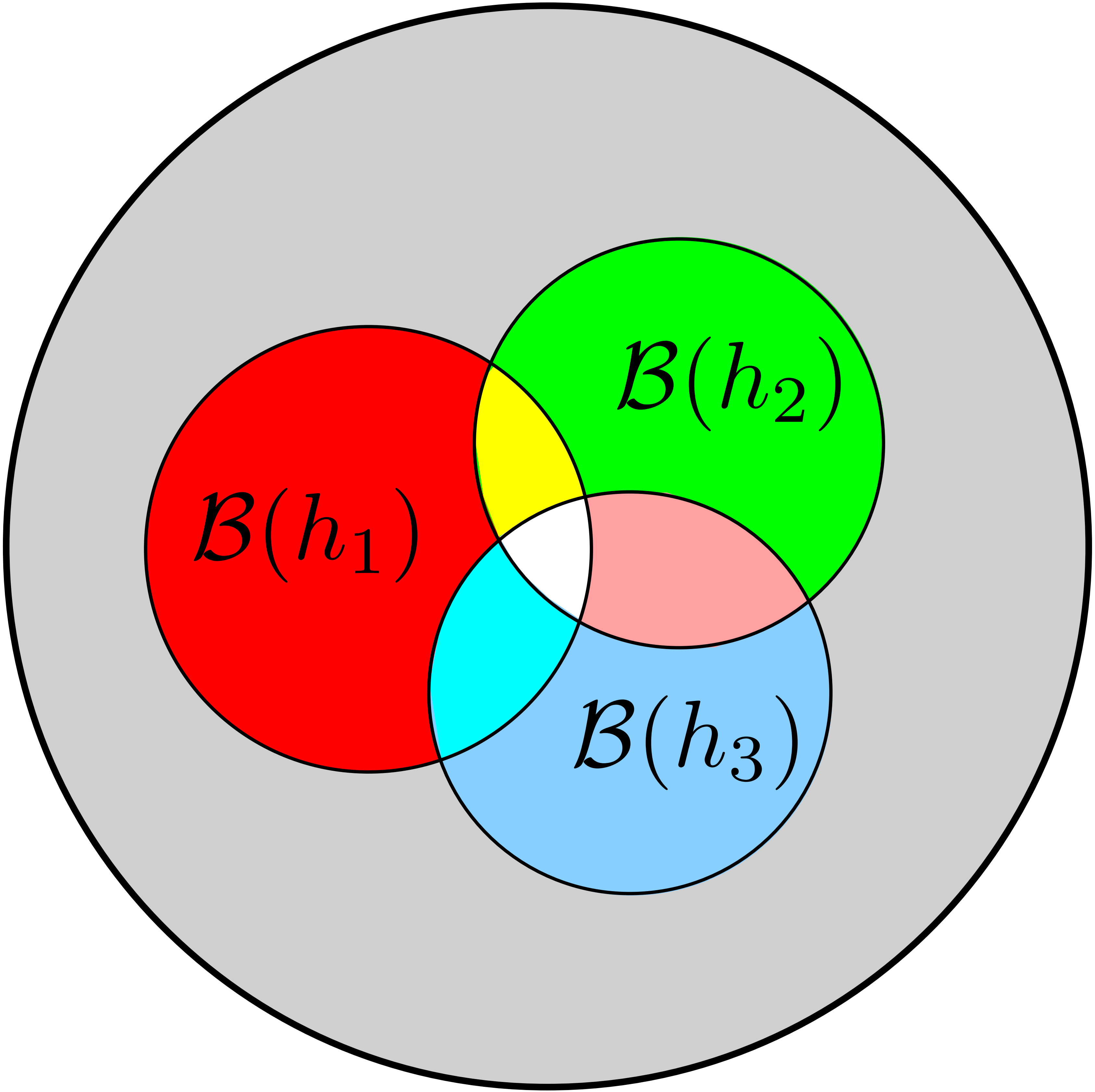
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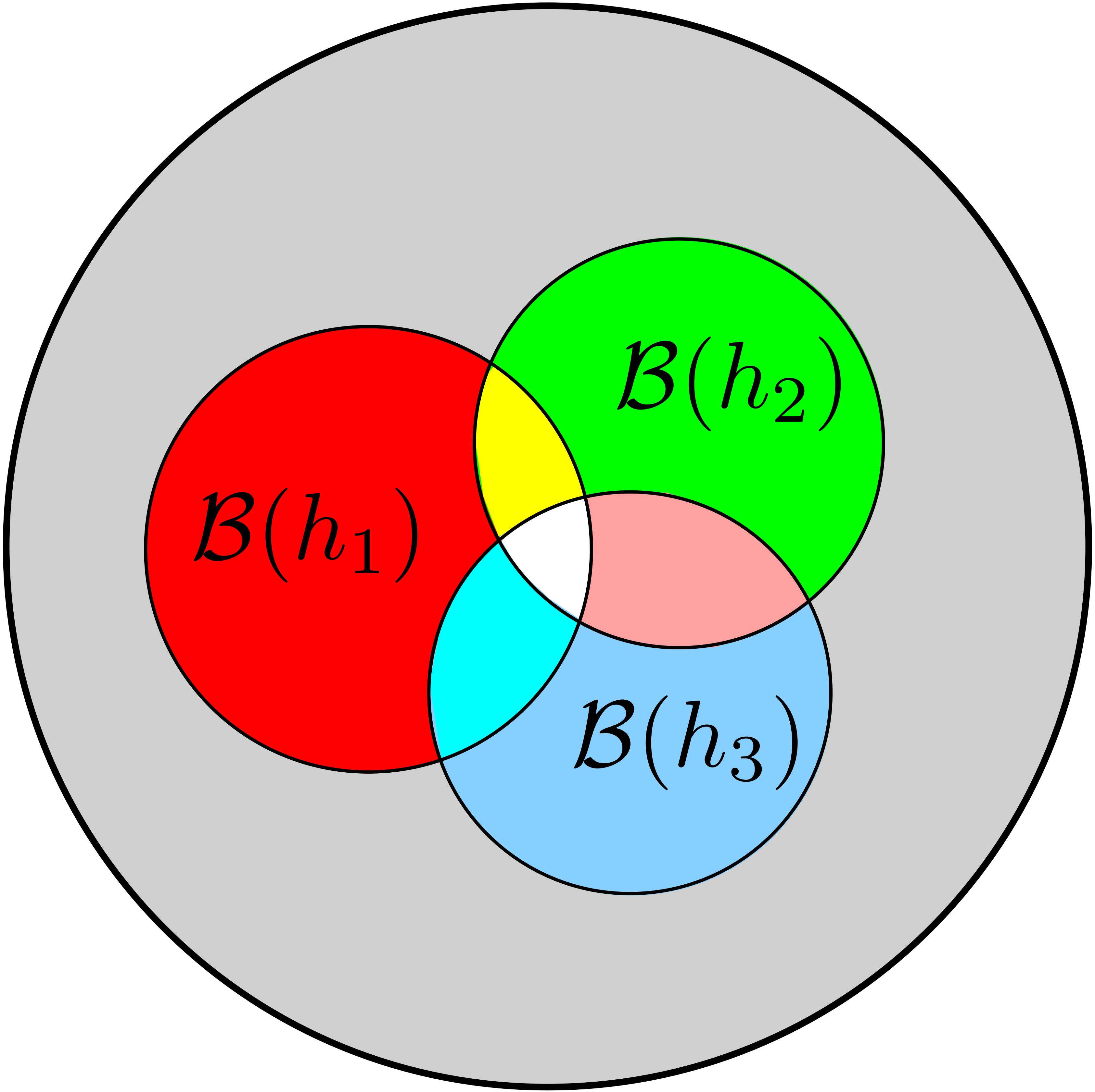

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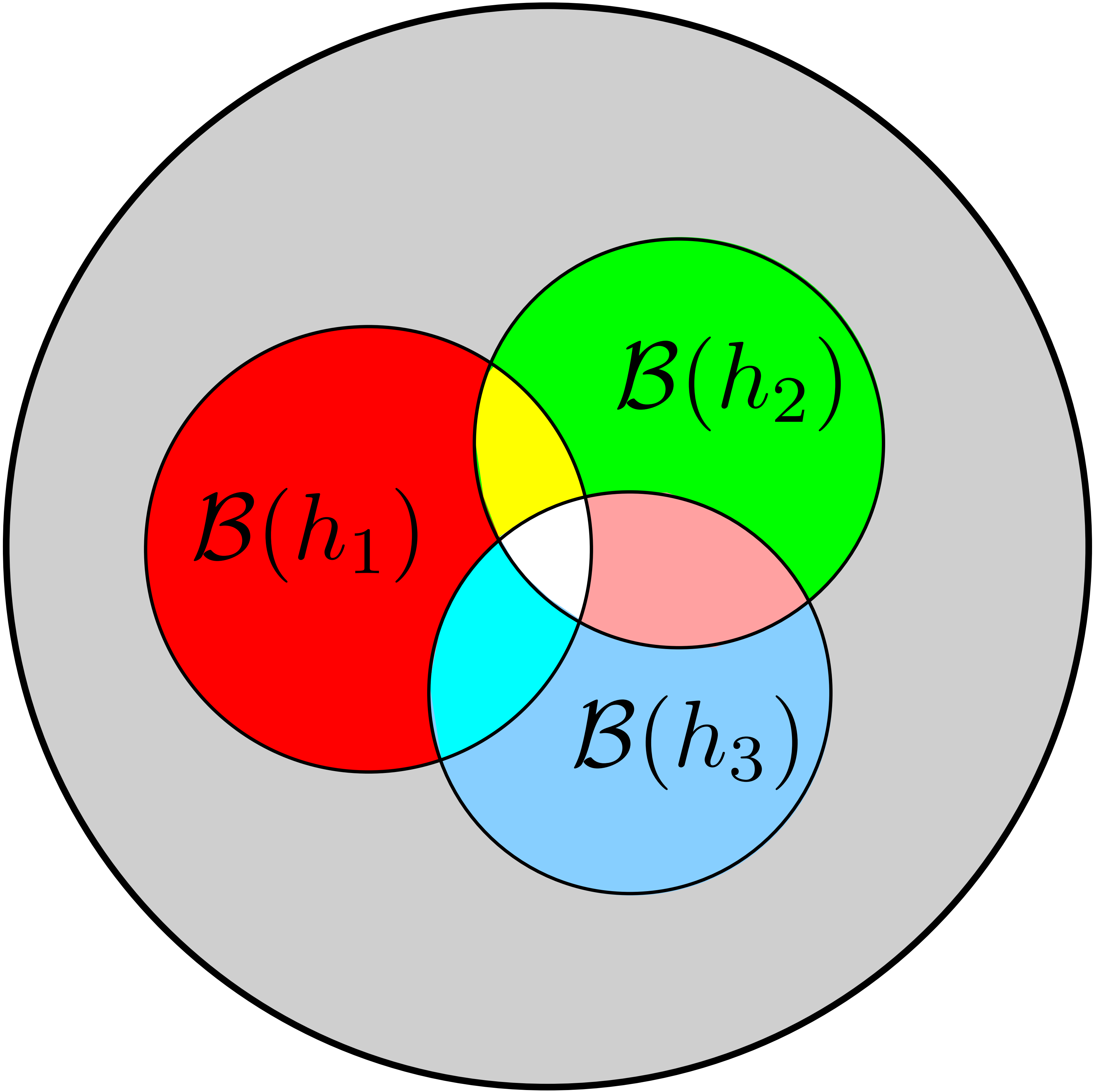
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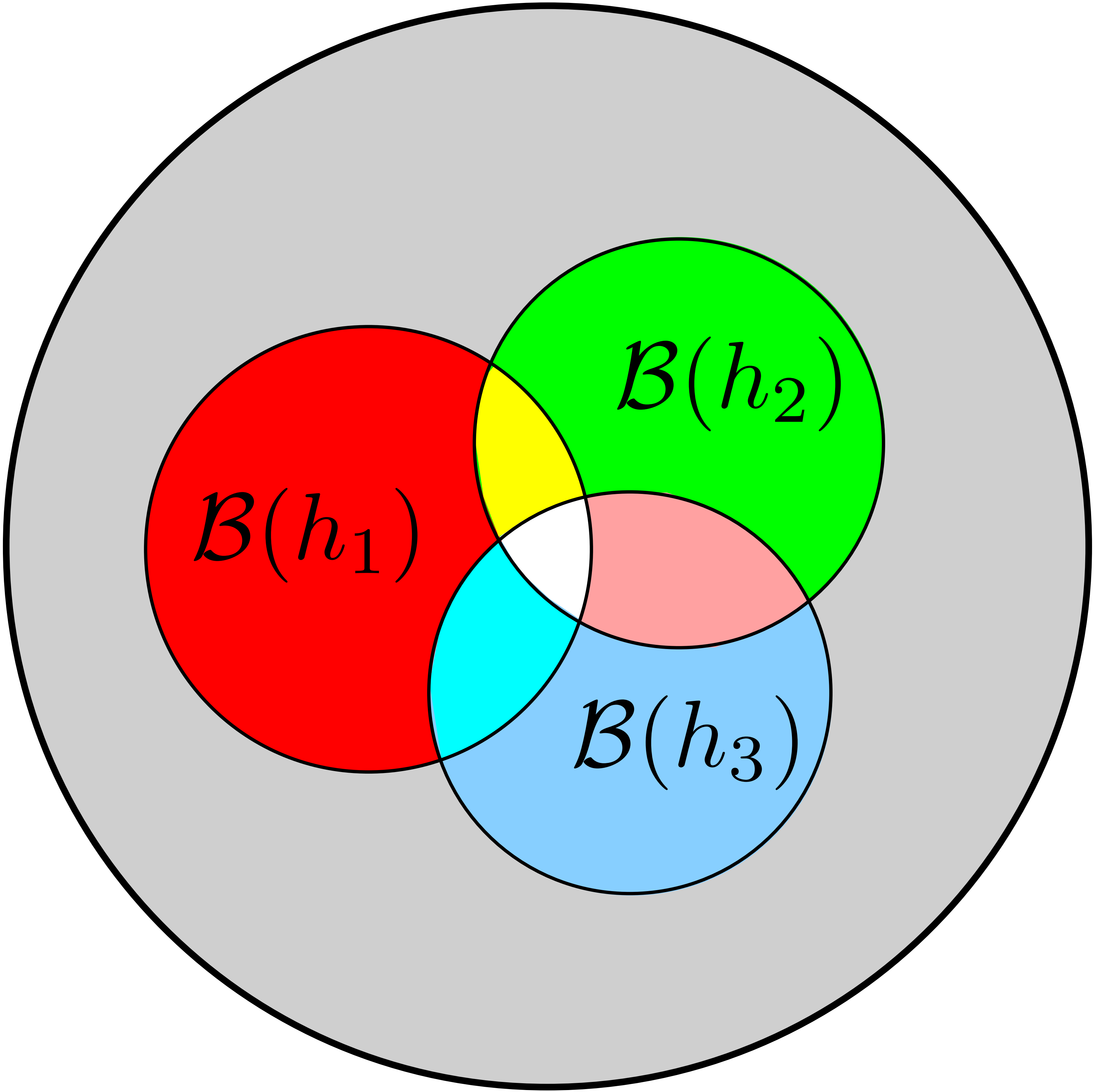
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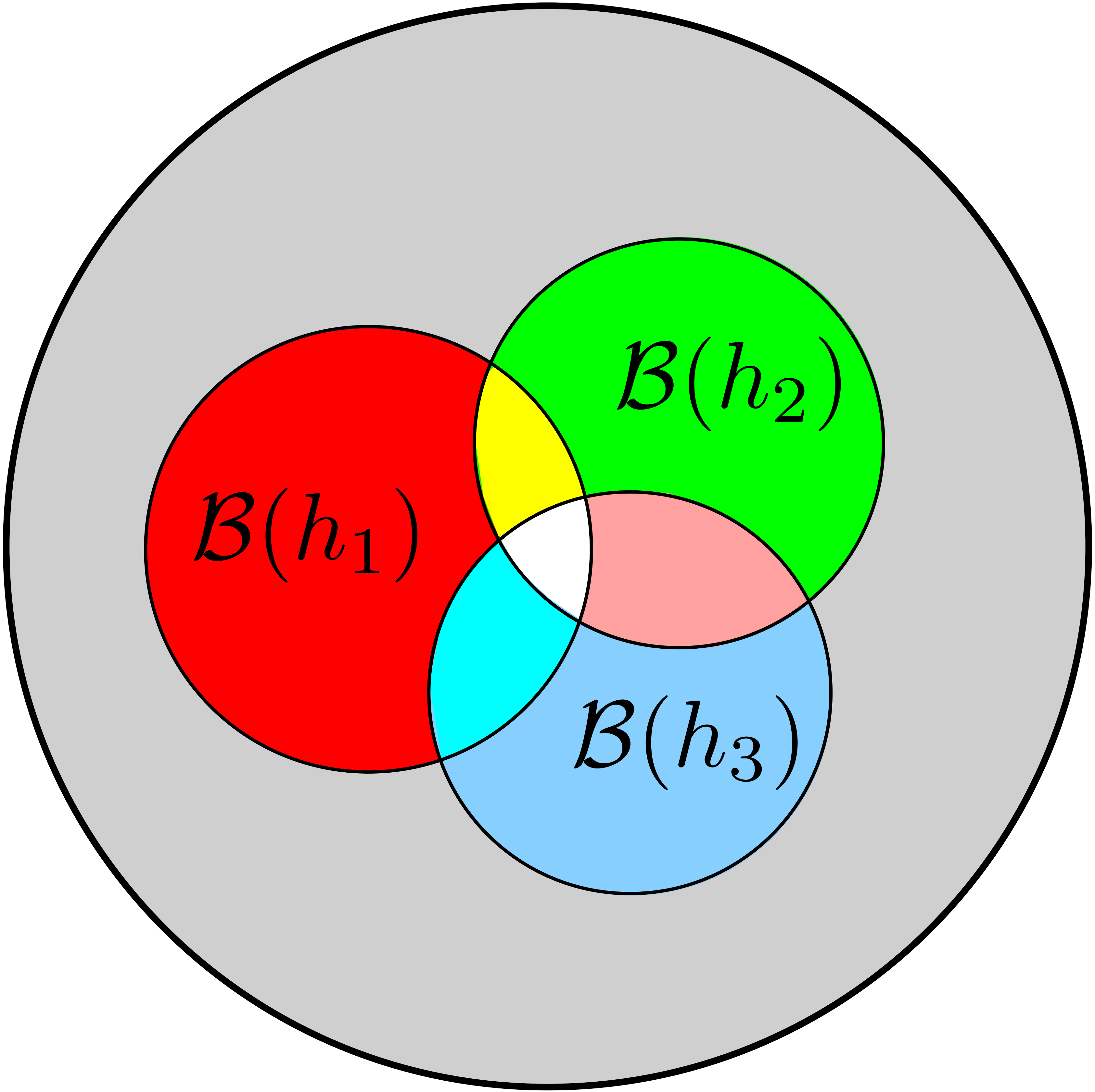
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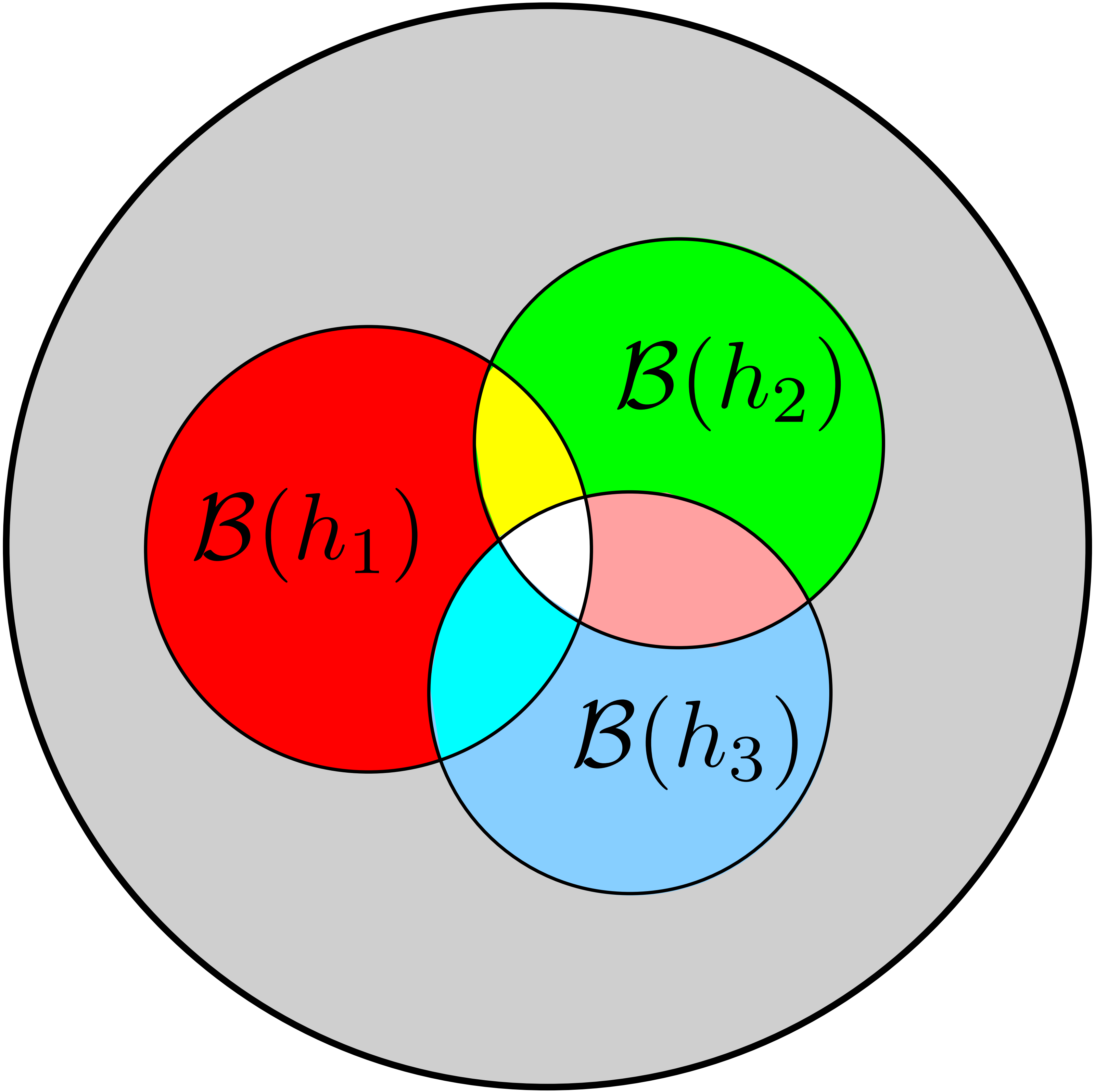
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