Statistical Machine Learning (BE4M33SSU)
Lecture 4: Empirical Risk Minimization II

Czech Technical University in Prague
V. Franc

Recap of the previous lecture

- We bounded the probability that empirical risk $R_{\mathcal{T}^m}(h_m)$ is not a good proxy of true risk $R(h_m)$ where $h_m = A(\mathcal{T}^m)$ is a learned from $\mathcal{T}^m$:

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

$$\underbrace{\leq}_{\text{union bound}} \sum_{h\in\mathcal{H}} \mathbb{P}\Big(\Big|R(h) - R_{\mathcal{T}^m}(h)\Big| \geq \varepsilon\Big) \underbrace{\leq}_{\text{Hoeffding inequality}} 2|\mathcal{H}|e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}} = B(m, |\mathcal{H}|, \varepsilon)$$

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- We derived a generalization bound:

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

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- This lecture answers the following quations:
  - How to deal with infinite hypothesis space $\mathcal{H}$?
  - How to define a good learning algorithm? Is ERM good?

Linear classifier minimizing classification error

- $\mathcal{X}$ is a set of observations and $\mathcal{Y} = \{+1, -1\}$ a set of hidden labels
- $\phi\colon \mathcal{X} \to \mathbb{R}^n$ is fixed feature map embedding $\mathcal{X}$ to $\mathbb{R}^n$
- Task: find linear classification strategy $h\colon \mathcal{X} \to \mathcal{Y}$

$$h(x; \boldsymbol{w}, b) = \text{sign}(\langle \boldsymbol{w}, \boldsymbol{\phi}(x)\rangle + b) = \begin{cases} +1 & \text{if} \quad \langle \boldsymbol{w}, \boldsymbol{\phi}(x)\rangle + b \geq 0 \\ -1 & \text{if} \quad \langle \boldsymbol{w}, \boldsymbol{\phi}(x)\rangle + b < 0 \end{cases}$$

with minimal expected risk

$$R^{0/1}(h) = \mathbb{E}_{(x,y)\sim p}\Big(\ell^{0/1}(y, h(x))\Big) \quad \text{where} \quad \ell^{0/1}(y, y') = [\![y \neq y']\!]$$

- We are given a set of training examples

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

drawn from i.i.d. with the distribution $p(x, y)$.

ERM learning for linear classifiers

- ERM for $\mathcal{H} = \{h(x;\boldsymbol{w},b) = \mathrm{sign}(\langle \boldsymbol{w}, \boldsymbol{\phi}(x)\rangle + b) \mid (\boldsymbol{w},b) \in \mathbb{R}^{n+1}\}$ leads to

$$(\boldsymbol{w}^*, b^*) \in \operatorname*{Argmin}_{h\in\mathcal{H}} R^{0/1}_{\mathcal{T}^m}(h) = \operatorname*{Argmin}_{(\boldsymbol{w},b)\in(\mathbb{R}^n\times\mathbb{R})} R^{0/1}_{\mathcal{T}^m}(h(\cdot;\boldsymbol{w},b)) \qquad (1)$$

where the empirical risk is

$$R^{0/1}_{\mathcal{T}^m}(h(\cdot;\boldsymbol{w},b)) = \frac{1}{m}\sum_{i=1}^{m} [\![y^i \neq h(x^i;\boldsymbol{w},b)]\!]$$

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- Algorithmic issues (next lecture): in general, there is no known algorithm solving the task (1) in time polynomial in m.
- Does ULLN applies for the class of two-class linear classifiers? Recall that ULLN $\forall\, \varepsilon > 0\colon \mathbb{P}\Big(\sup_{h\in\mathcal{H}} \Big| R^{0/1}(h) - R^{0/1}_{\mathcal{T}^m}(h) \Big| \geq \varepsilon \Big) = 0$

Vapnik-Chervonenkis (VC) dimension

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Definition: Let $\mathcal{H} \subseteq \{-1,+1\}^{\mathcal{X}}$. The Vapnik-Chervonenkis dimension of $\mathcal{H}$ is the cardinality of the largest set of points from $\mathcal{X}$ which can be shattered by $\mathcal{H}$.

VC dimension of class of two-class linear classifiers

Theorem: The VC-dimension of the hypothesis class of all two-class linear classifiers operating in n-dimensional feature space
$\mathcal{H} = \{h(x; \boldsymbol{w}, b) = \text{sign}(\langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b) \mid (\boldsymbol{w}, b) \in (\mathbb{R}^n \times \mathbb{R})\}$ is $n + 1$.

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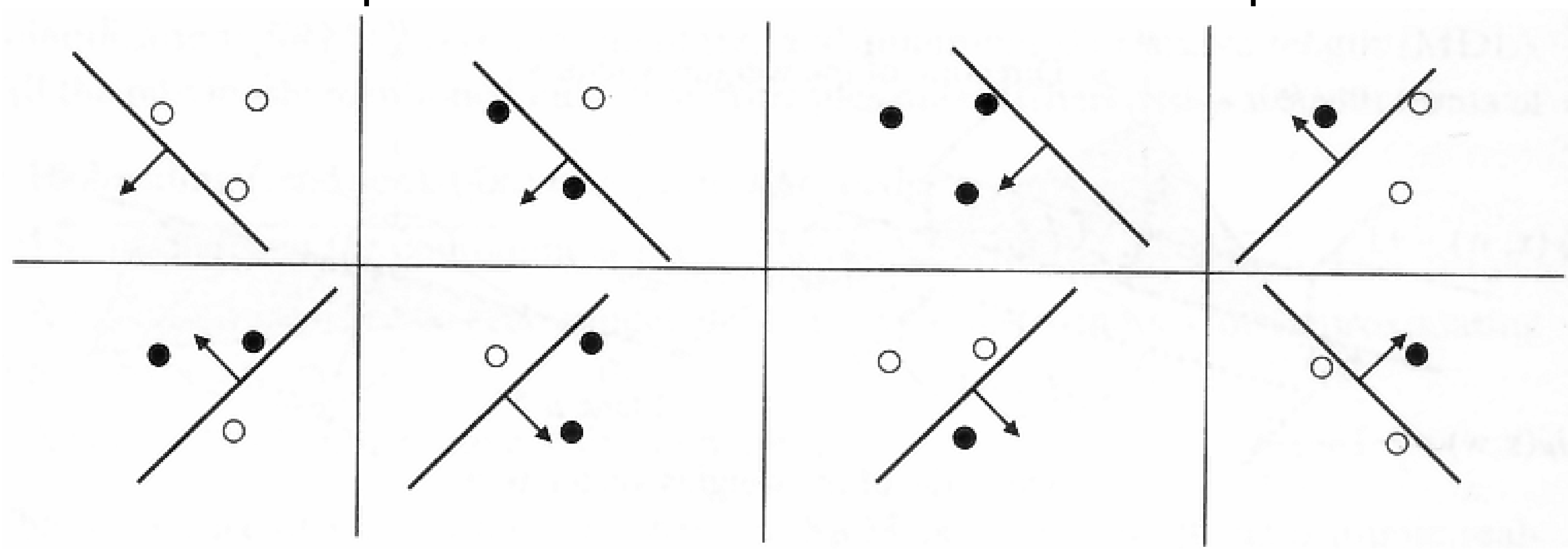
Example for $n = 2$-dimensional feature space



ULLN for two class predictors and $0/1$-loss

Theorem: Let $\mathcal{H} \subseteq \{+1,-1\}^{\mathcal{X}}$ be a hypothesis class with VC dimension $d < \infty$ and $\mathcal{T}^m = \{(x^1,y^1),\ldots,(x^m,y^m)\} \in (\mathcal{X}\times\mathcal{Y})^m$ a training set draw from i.i.d. rand vars with distribution $p(x,y)$. Then

$$\forall\, \varepsilon > 0\colon \mathbb{P}\left(\sup_{h\in\mathcal{H}} \left| R^{0/1}(h) - R^{0/1}_{\mathcal{T}^m}(h) \right| \geq \varepsilon \right) \leq 4 \left(\frac{2\,e\,m}{d} \right)^d e^{-\frac{m\,\varepsilon^2}{8}}$$

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Corollary: Let $\mathcal{H} \subseteq \{+1, -1\}^{\mathcal{X}}$ be a hypothesis class with VC dimension $d < \infty$. Then ULLN applies.

Summary: uniform law of large numbers

- We learned how to bound deviation between the empirical and the true risk uniformly for:
  - Finite hypothesis class $\mathcal{H} = \{h_1, \ldots, h_K\}$:

$$\mathbb{P}\Big(\max_{h \in \mathcal{H}} |R_{\mathcal{T}^m}(h) - R(h)| \geq \varepsilon \Big) \leq 2|\mathcal{H}| e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}} = B_1(m, |\mathcal{H}|, \varepsilon)$$

  - Two-class classifiers $\mathcal{H} \subseteq \{+1, -1\}^{\mathcal{X}}$ a finite VC-dimensions d:

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In both cases the bound goes to zero, i.e., ULLN applies.

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- Does ERM algorithm $h_m \in \operatorname*{Argmin}_{h\in\mathcal{H}} R_{\mathcal{T}^m}(h)$ finds strategy with the minimal risk $R(h)$?

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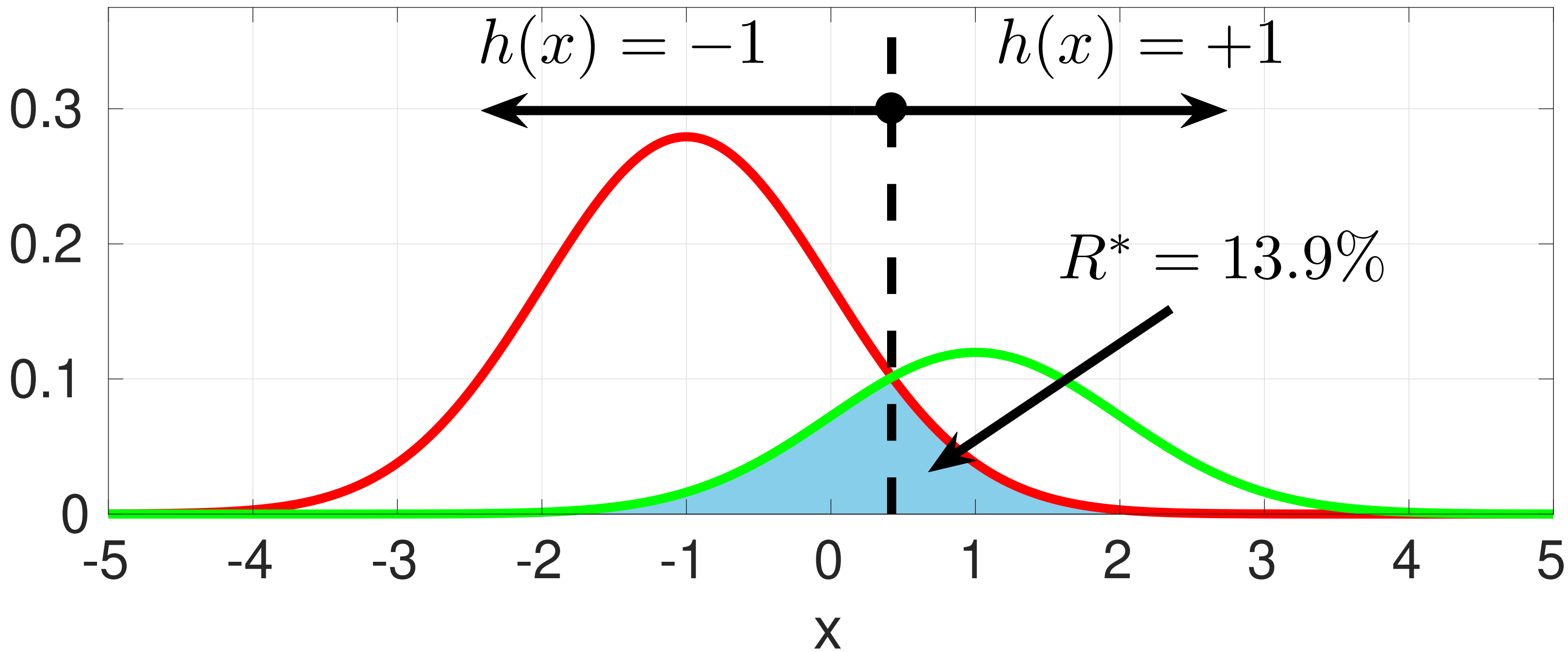

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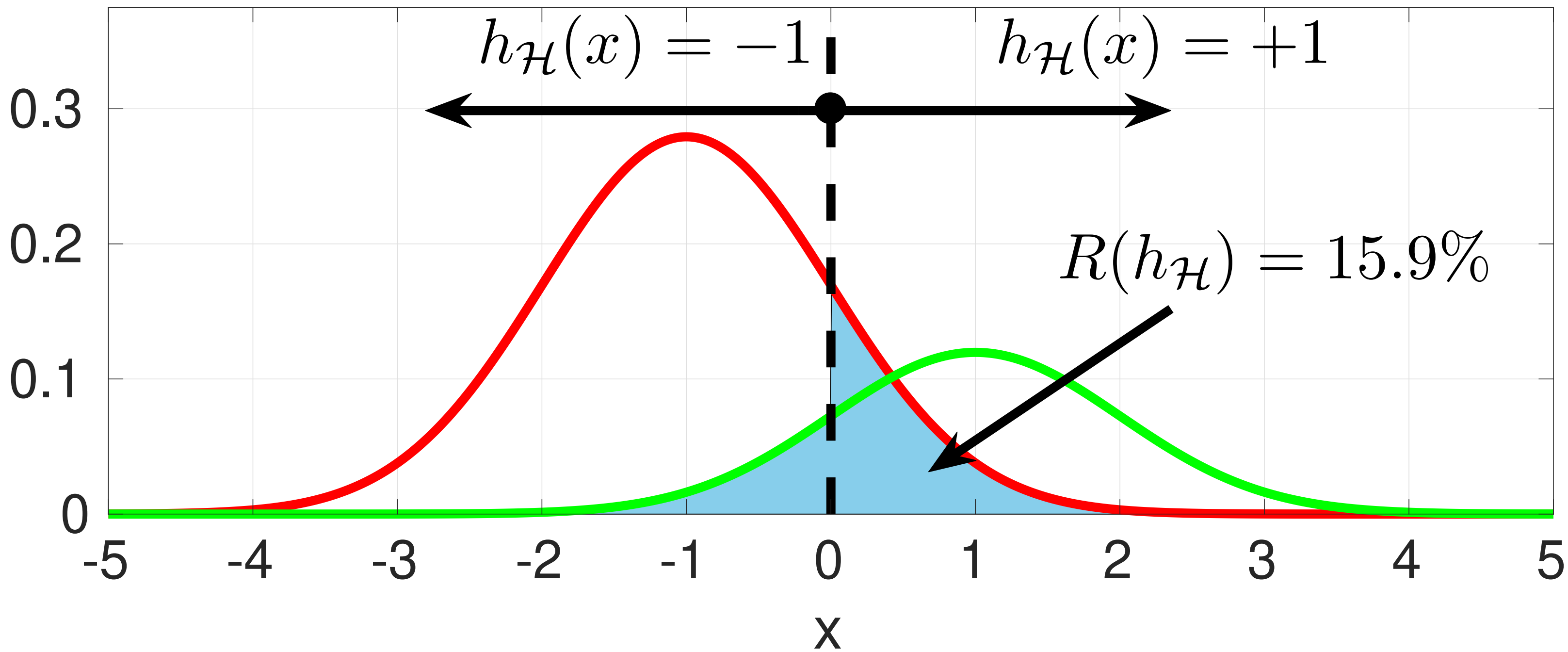

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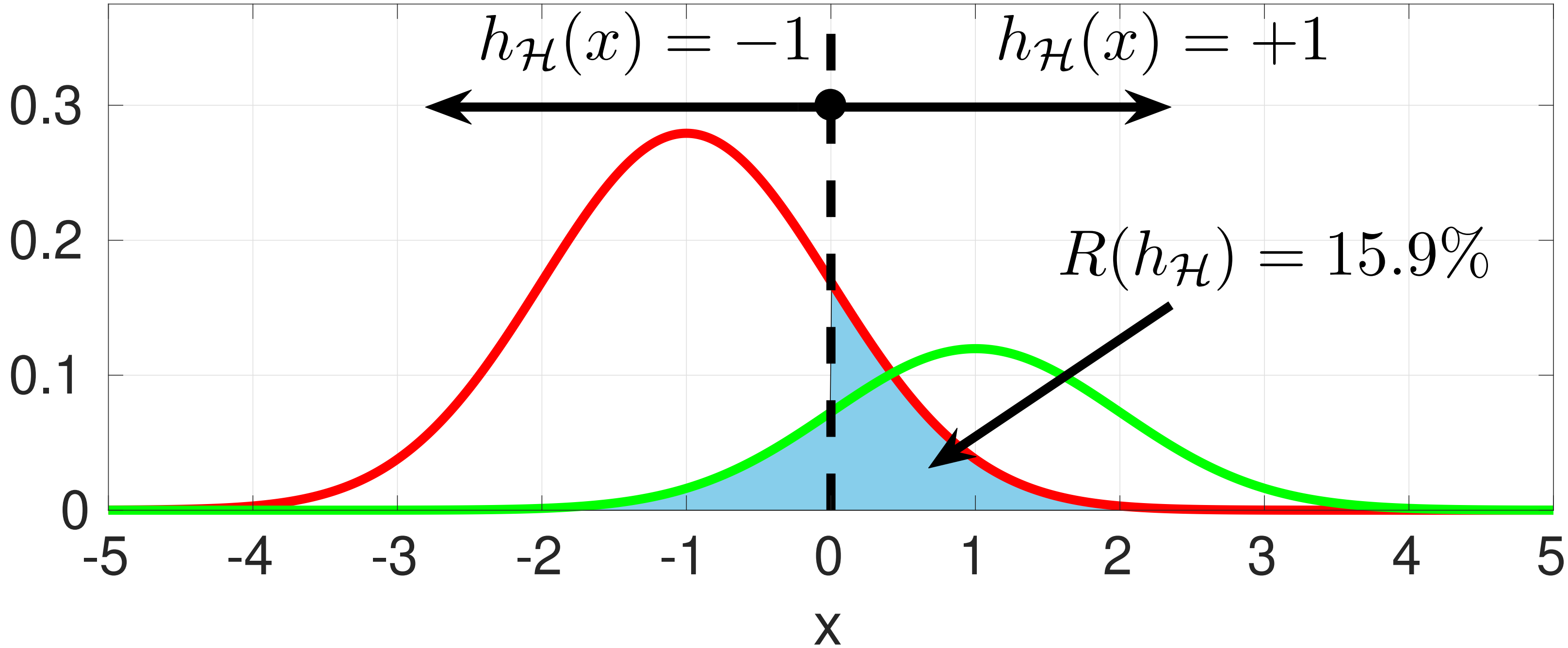

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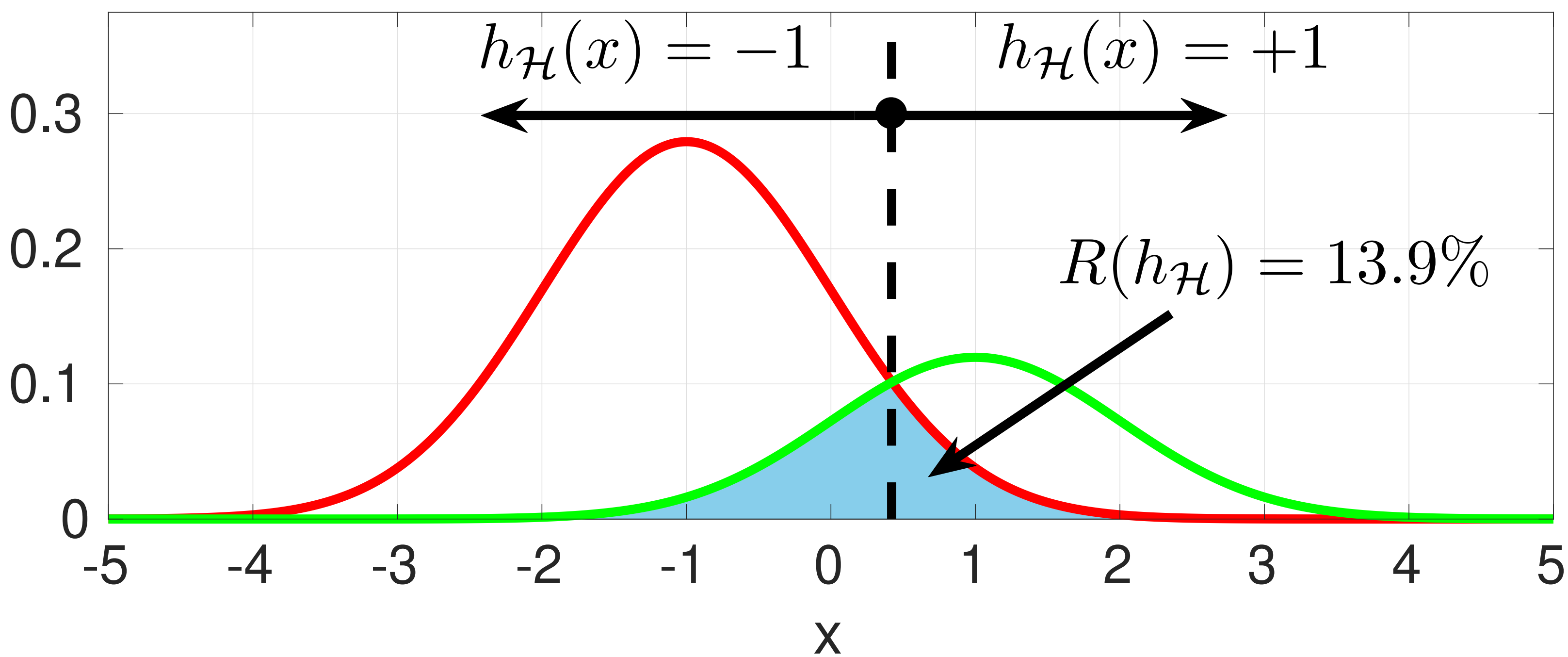

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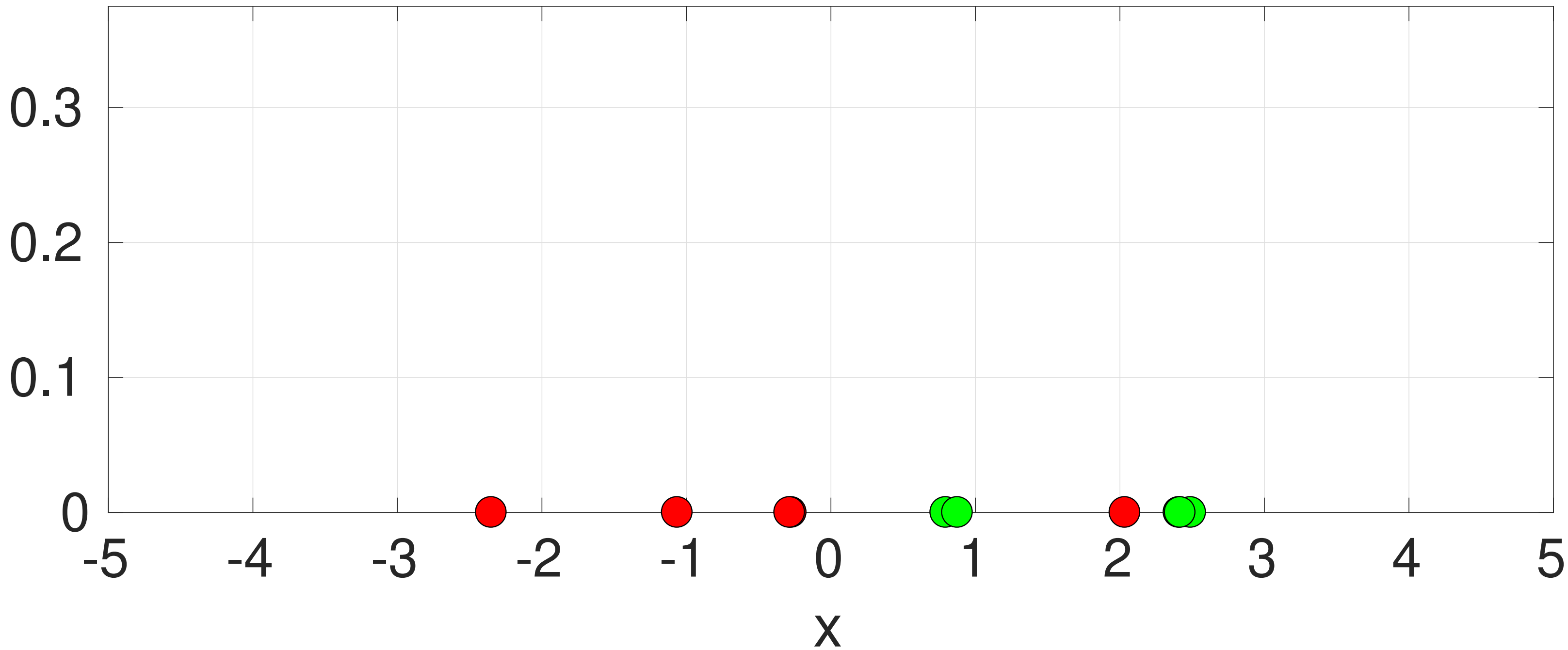

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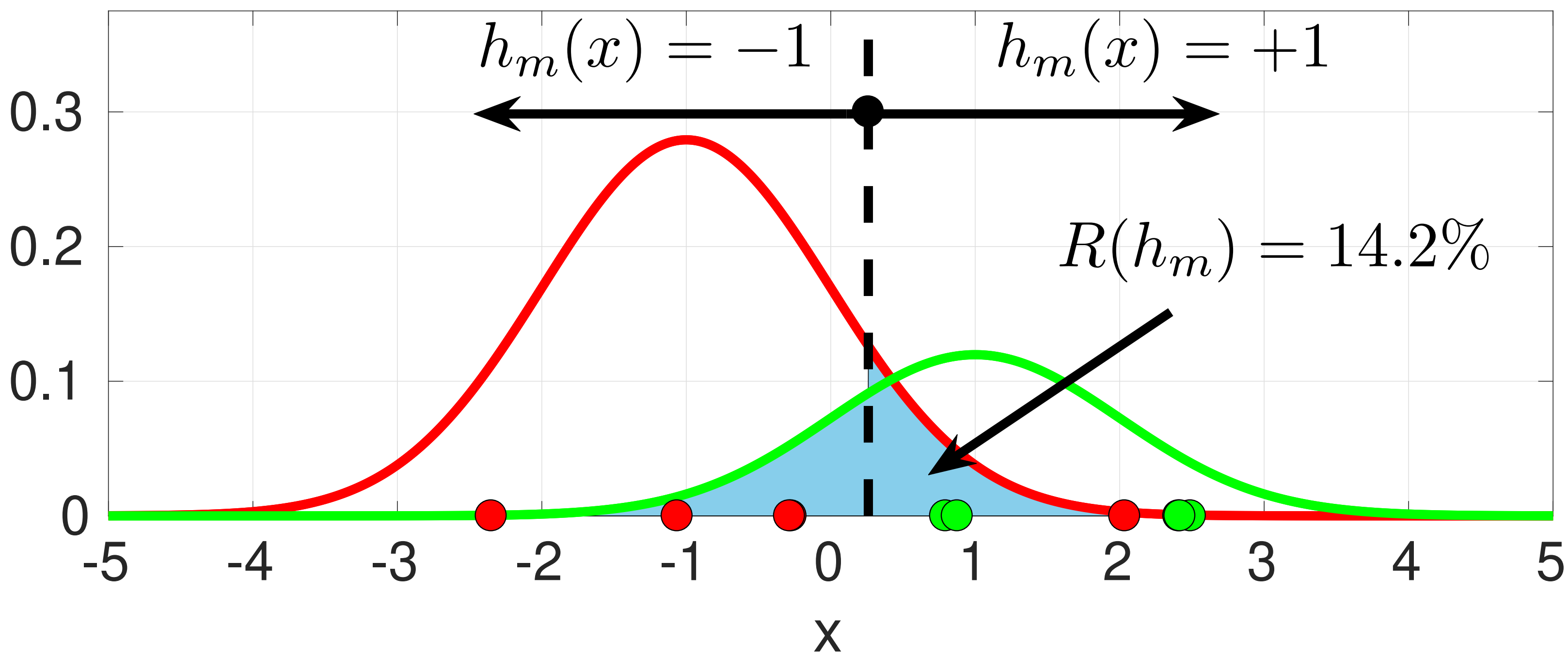

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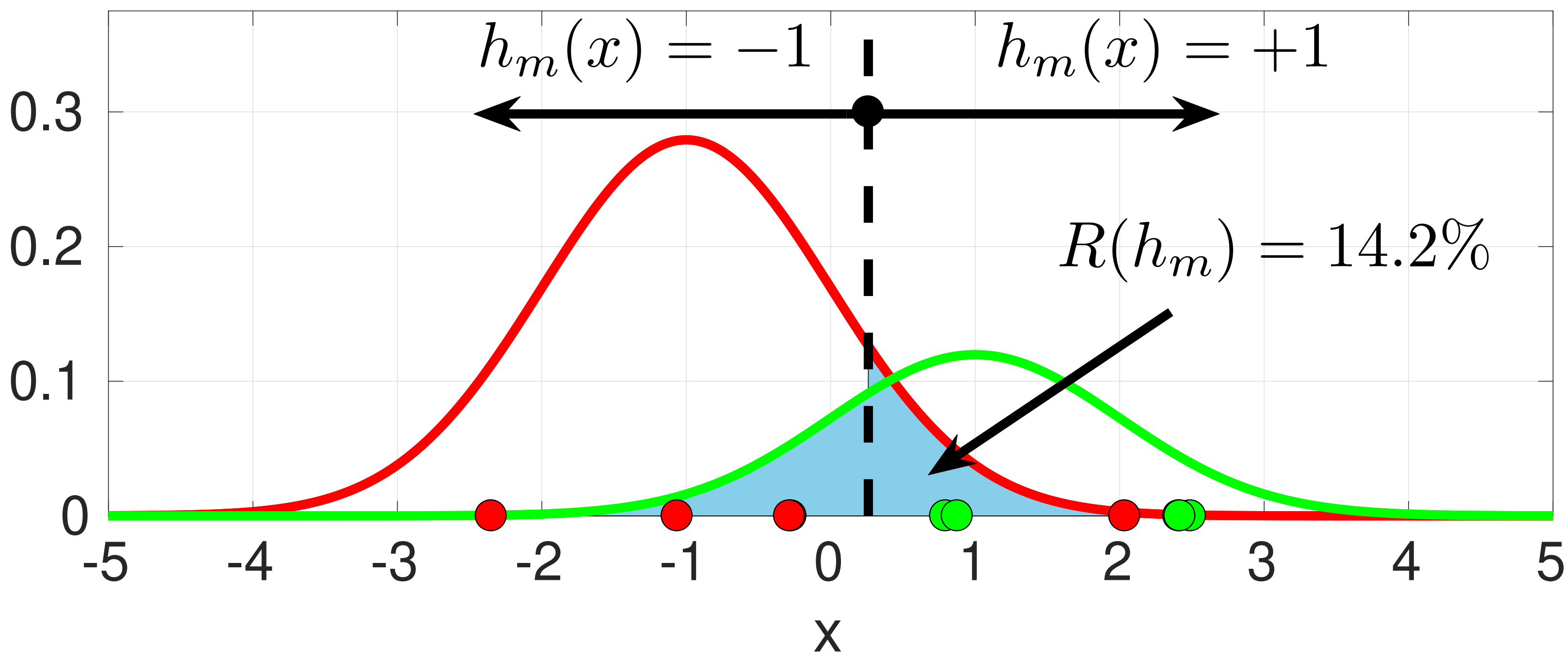
estimation error: $R(h_m) - R(h_\mathcal{H}) = 14.2 - 13.9 = 0.3\%$



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Excess error: the quantity we want to minimize

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Note that:

- The approximation error depends on $\mathcal{H}$.
- The estimation error is random and depends on $\mathcal{H}$, m and A.

Universally statistically consistent learning algorithm

- A good algorihtm $h_m = A(\mathcal{T}^m)$ for $\mathcal{H}$ can make the estimation error $R(h_m) - R(h_{\mathcal{H}})$ arbitrarily small if it has enough examples m.

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- When is ERM based algorithm universally statistically consistent?

ULLN implies universal consistency of ERM

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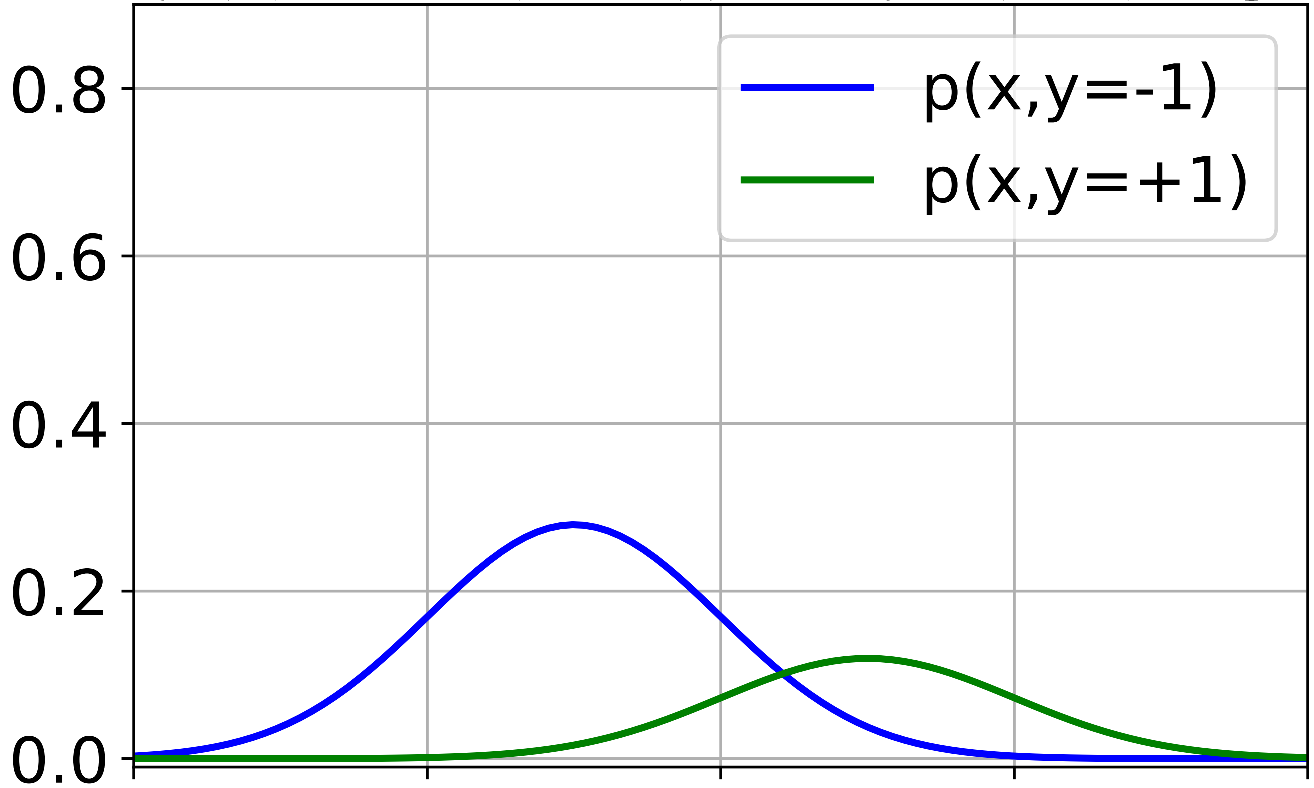

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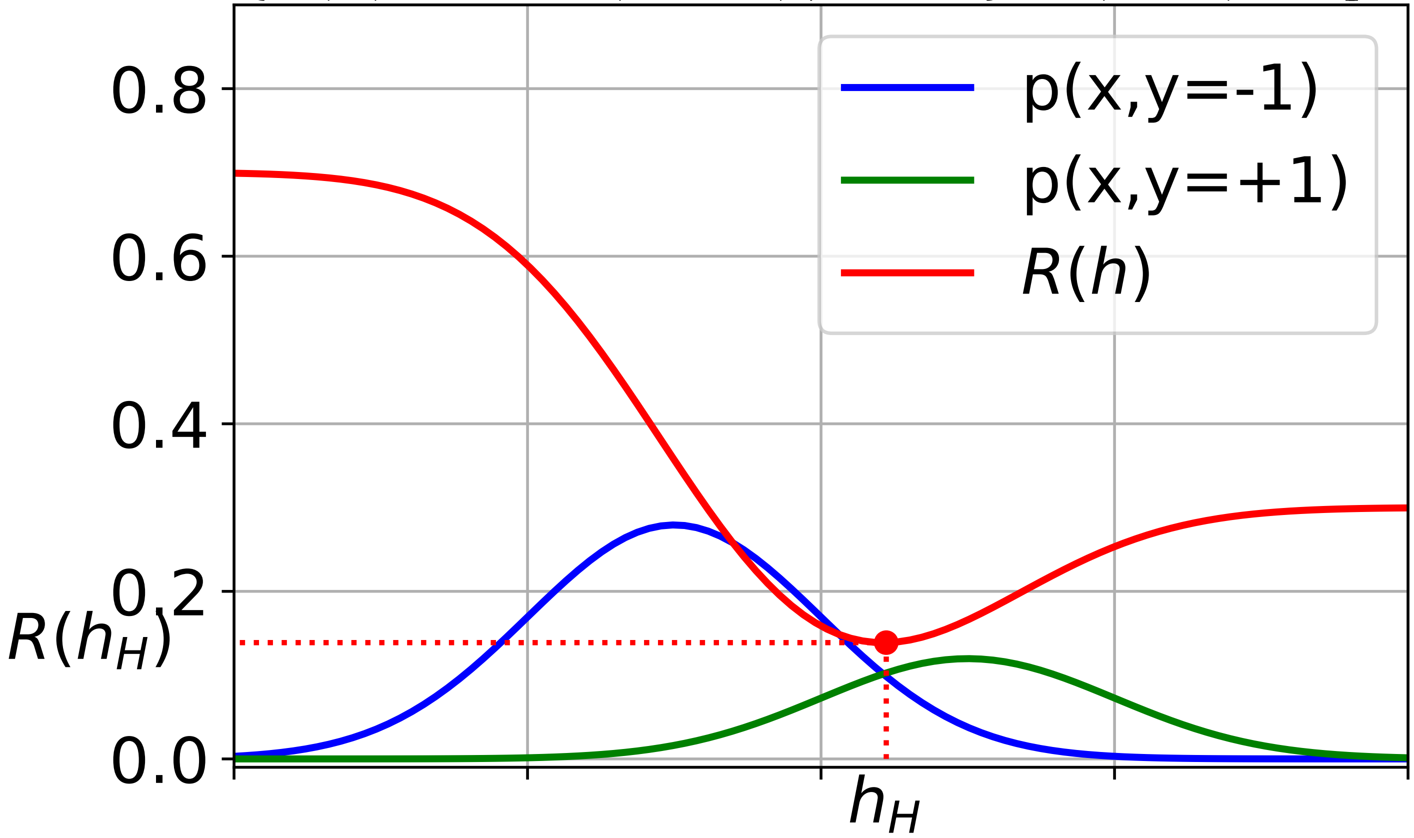

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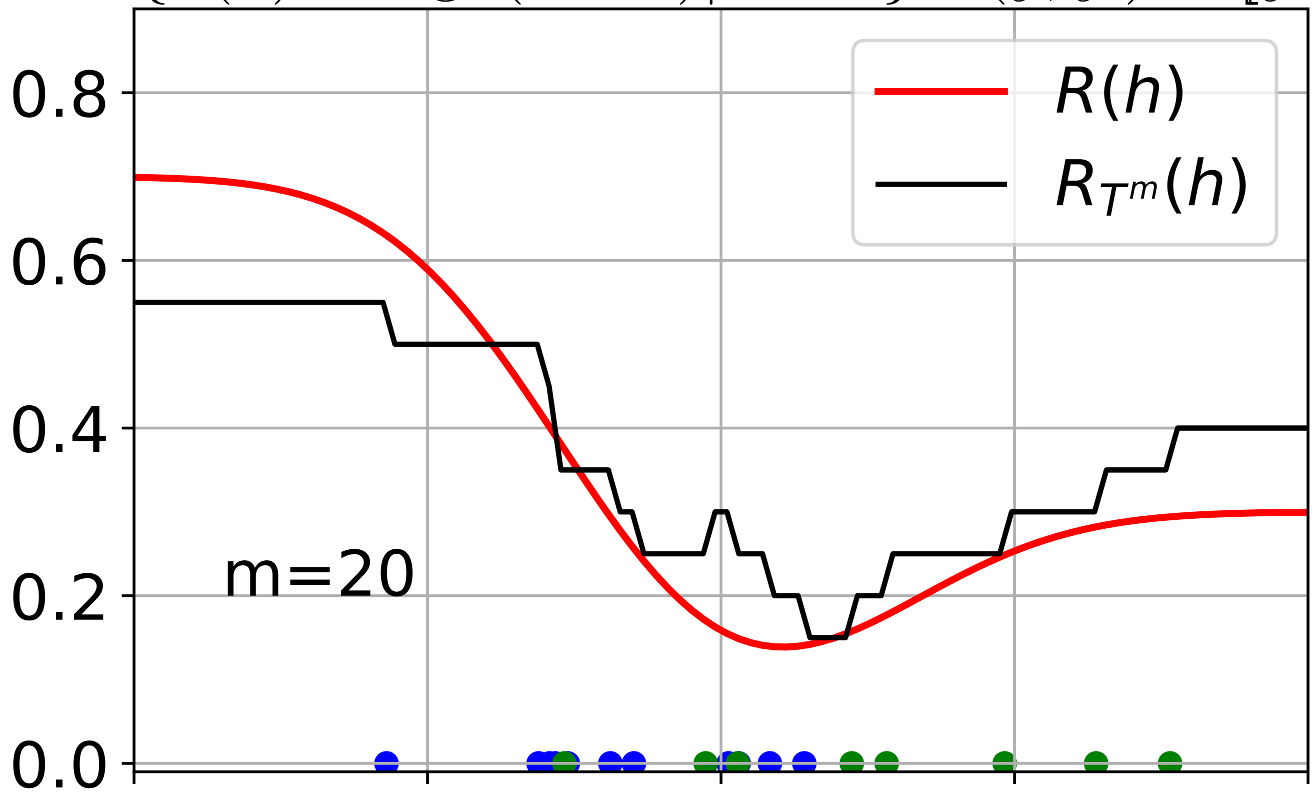
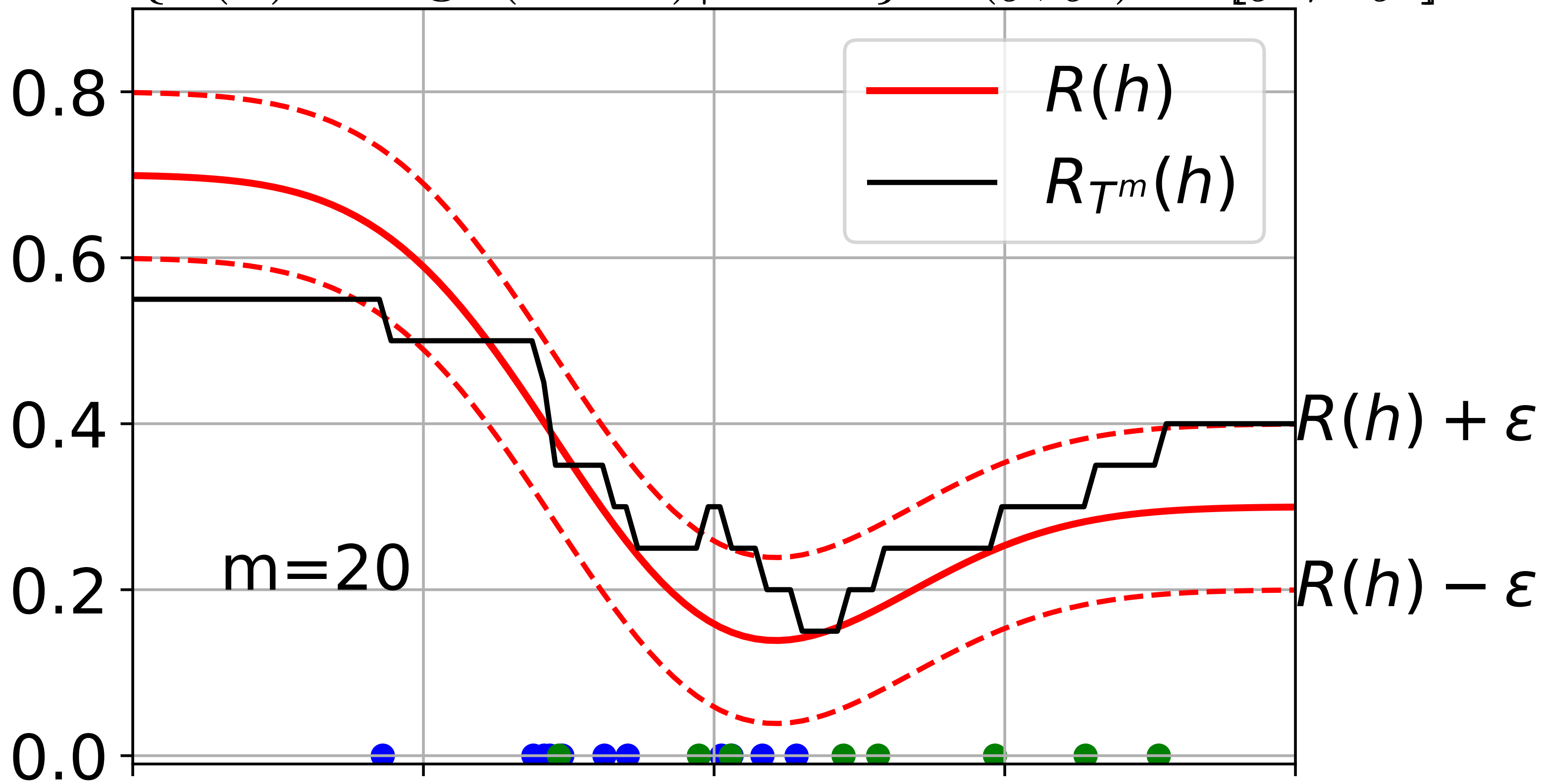


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m, \mathcal{H}, \varepsilon)$$

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



ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m, \mathcal{H}, \varepsilon)$$

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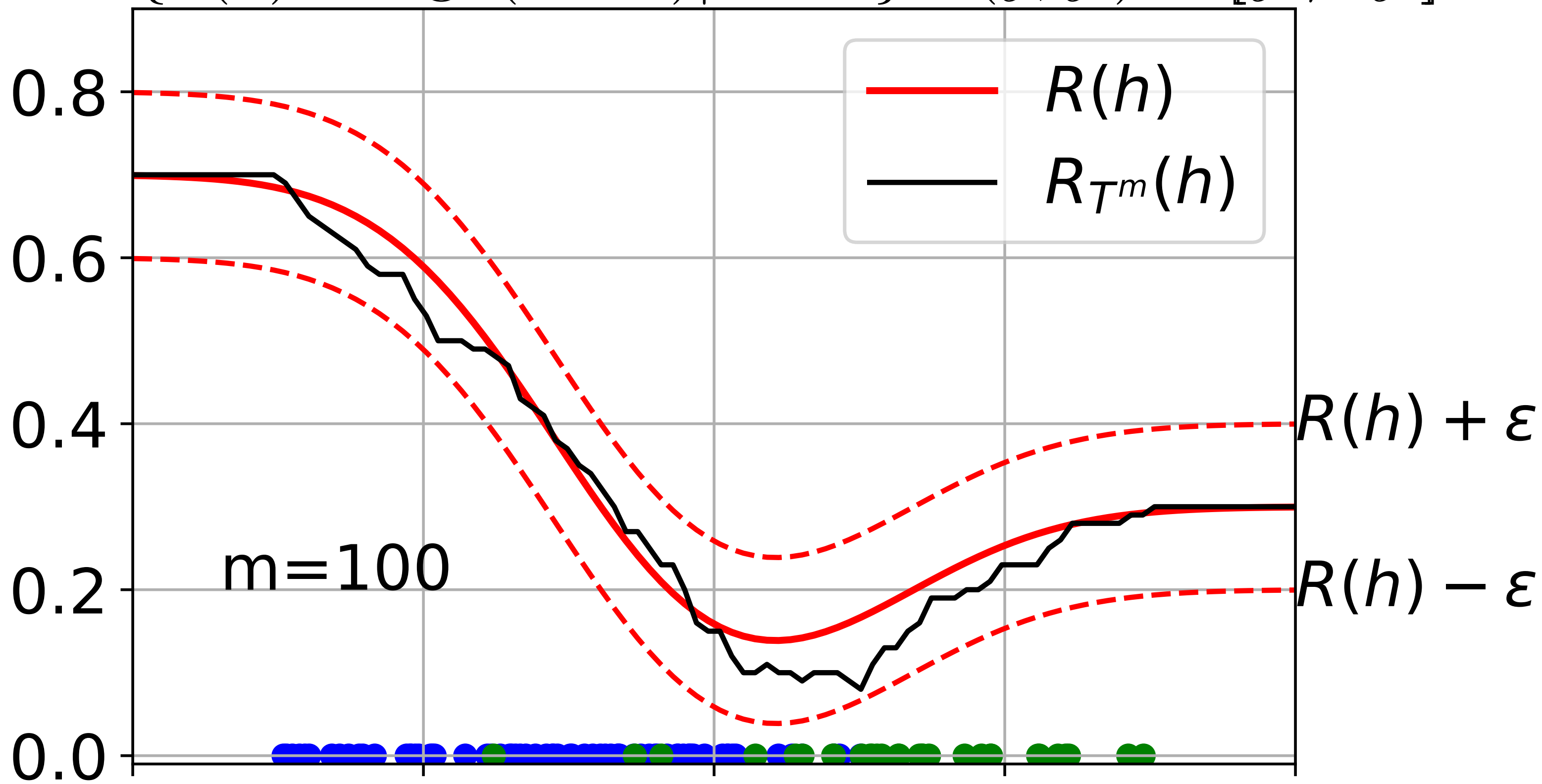
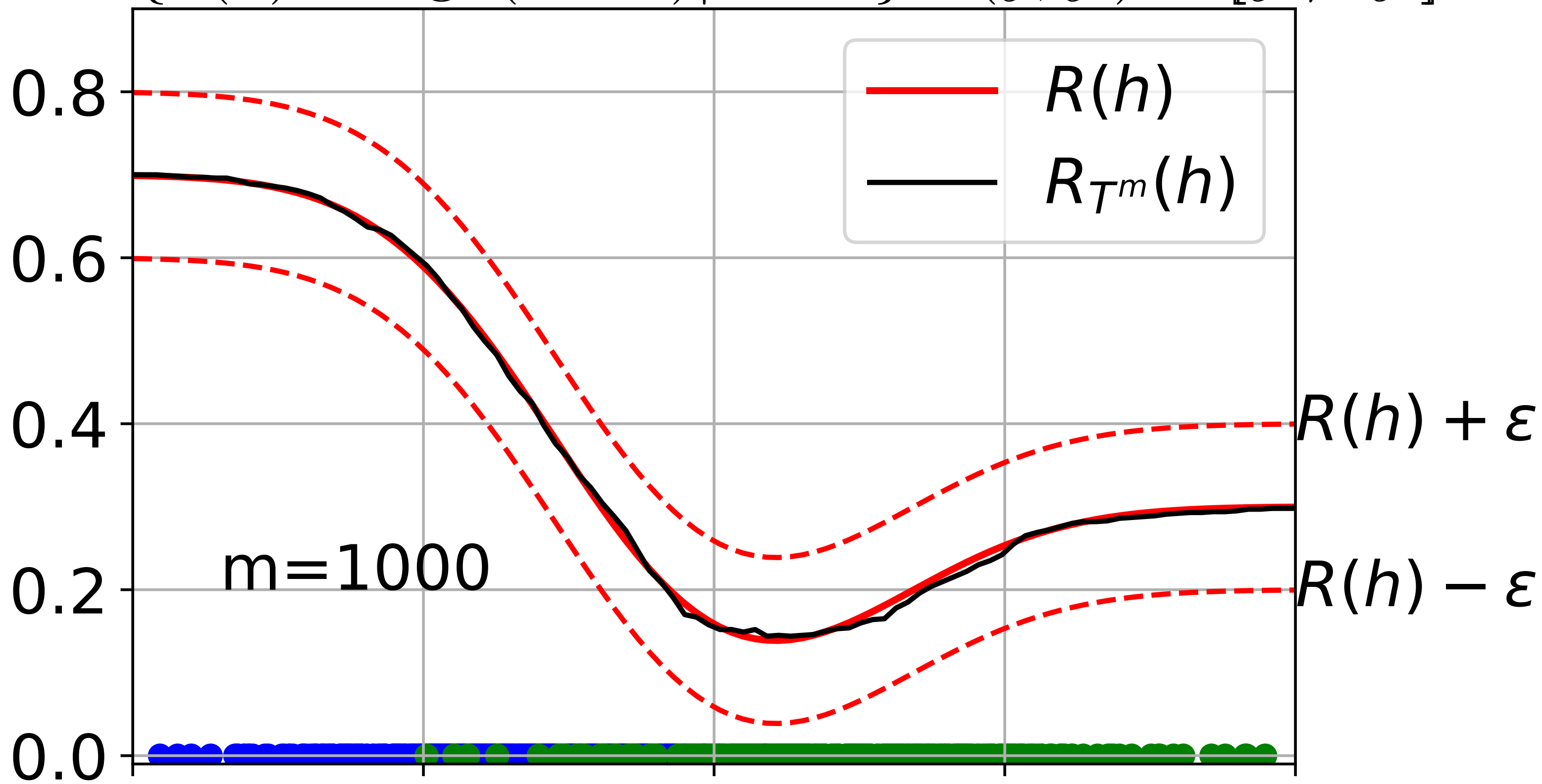


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m,\mathcal{H},\varepsilon)$$

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



ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m,\mathcal{H},\varepsilon)$$

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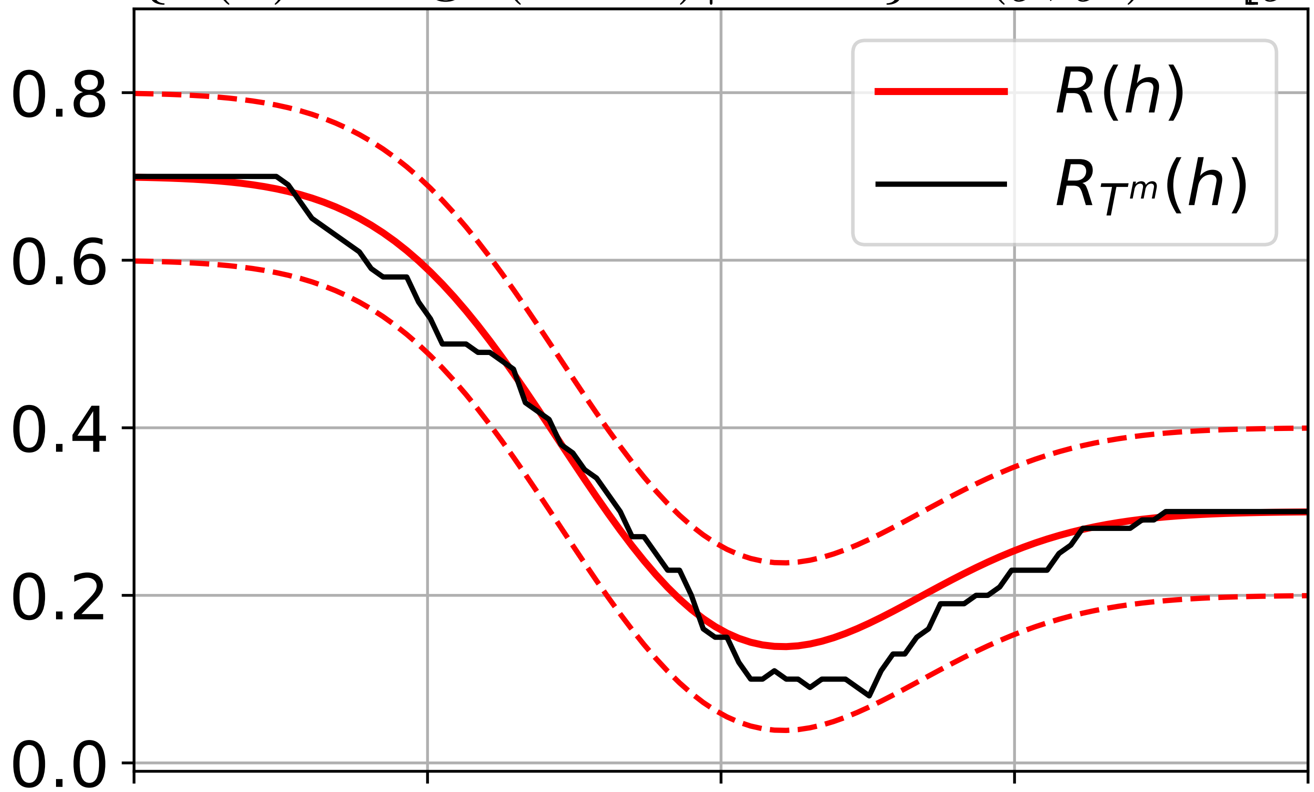
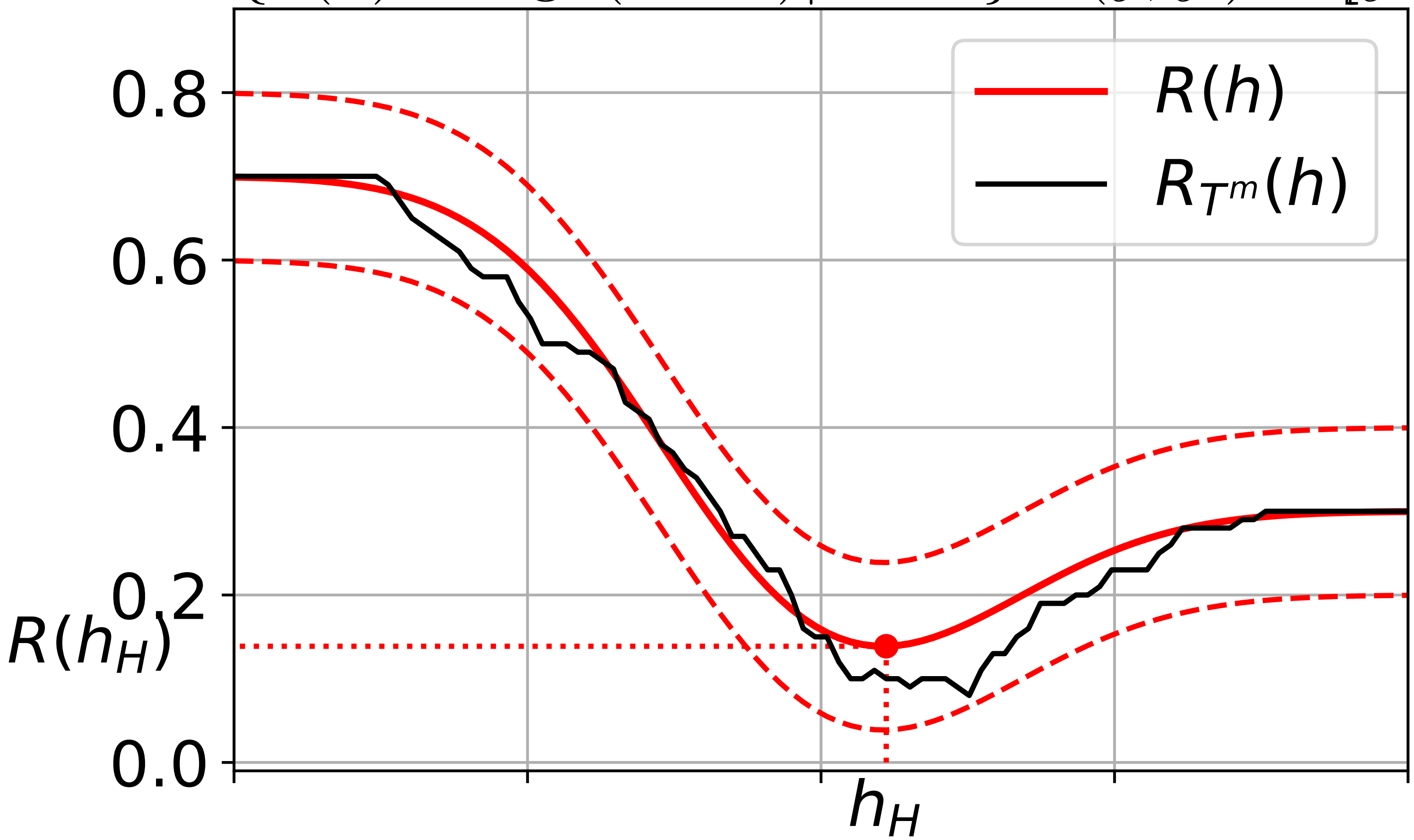


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m, \mathcal{H}, \varepsilon)$$

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

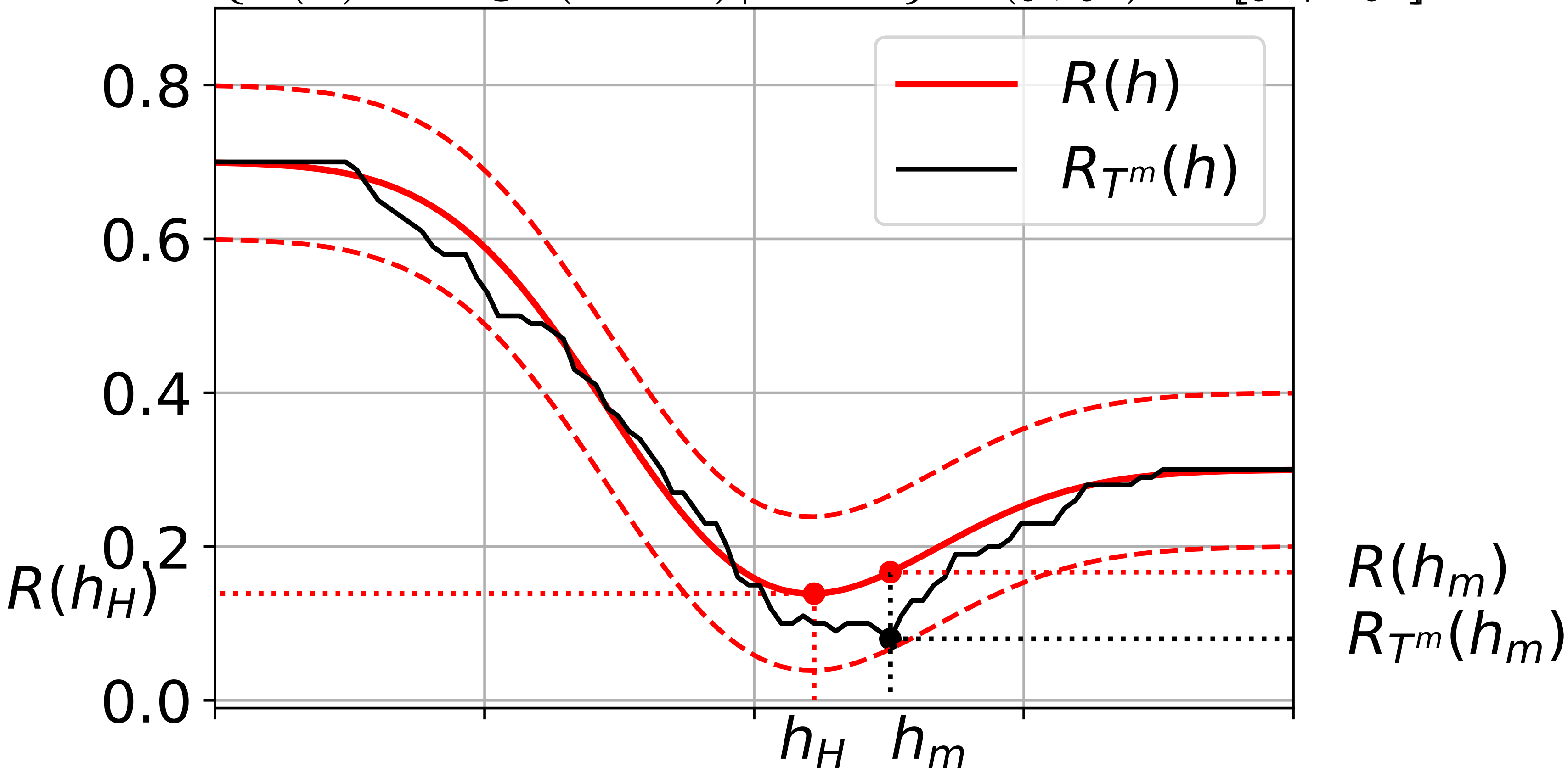


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m,\mathcal{H},\varepsilon)$$

$$\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}}$$

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

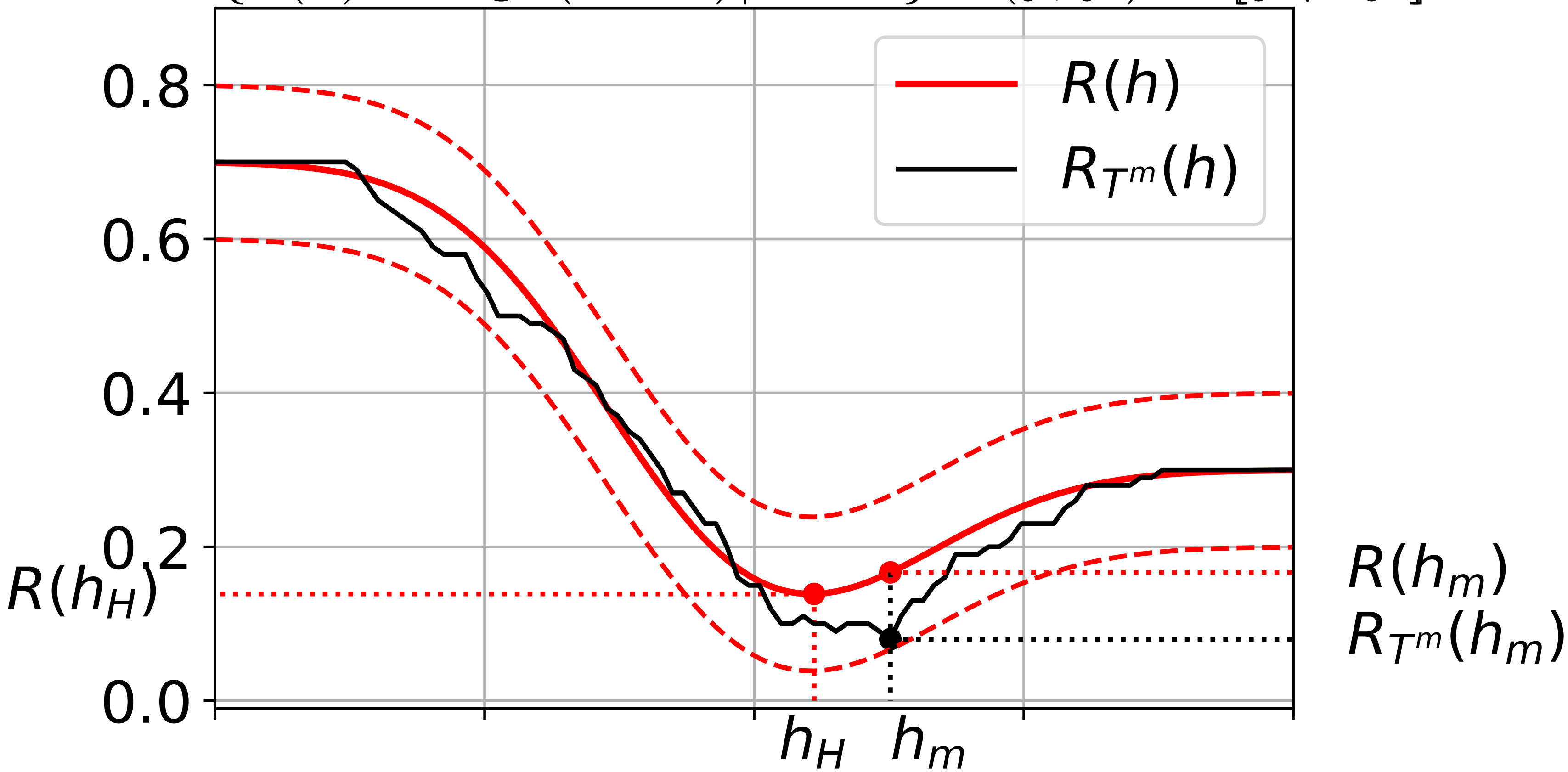


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m, \mathcal{H}, \varepsilon)$$

$$\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} \leq 2 \underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}}$$

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

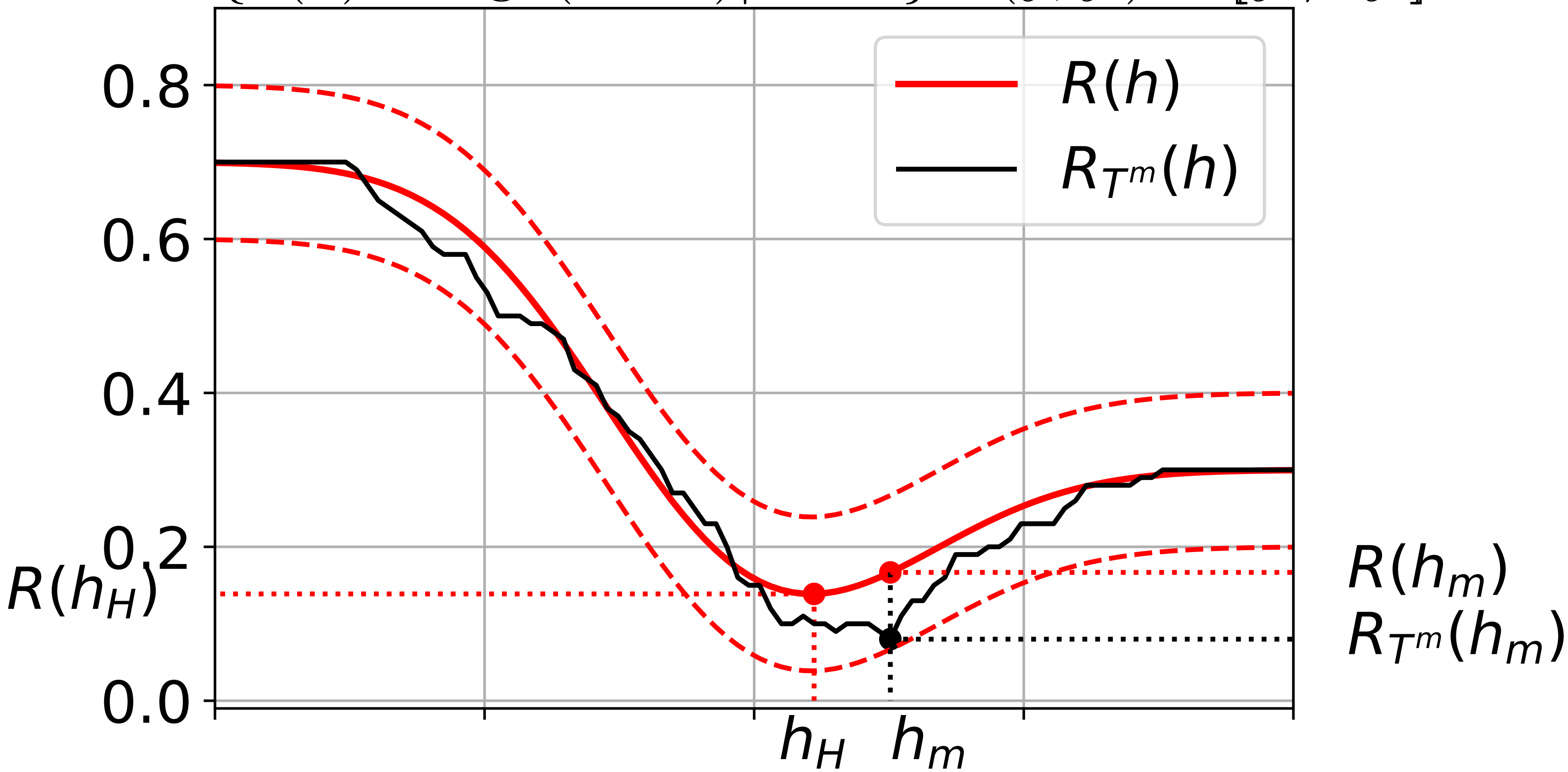


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m,\mathcal{H},\varepsilon)$$

$$\mathbb{P}\Big(\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} \geq \varepsilon \Big) \leq \mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \frac{\varepsilon}{2} \Big)$$

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

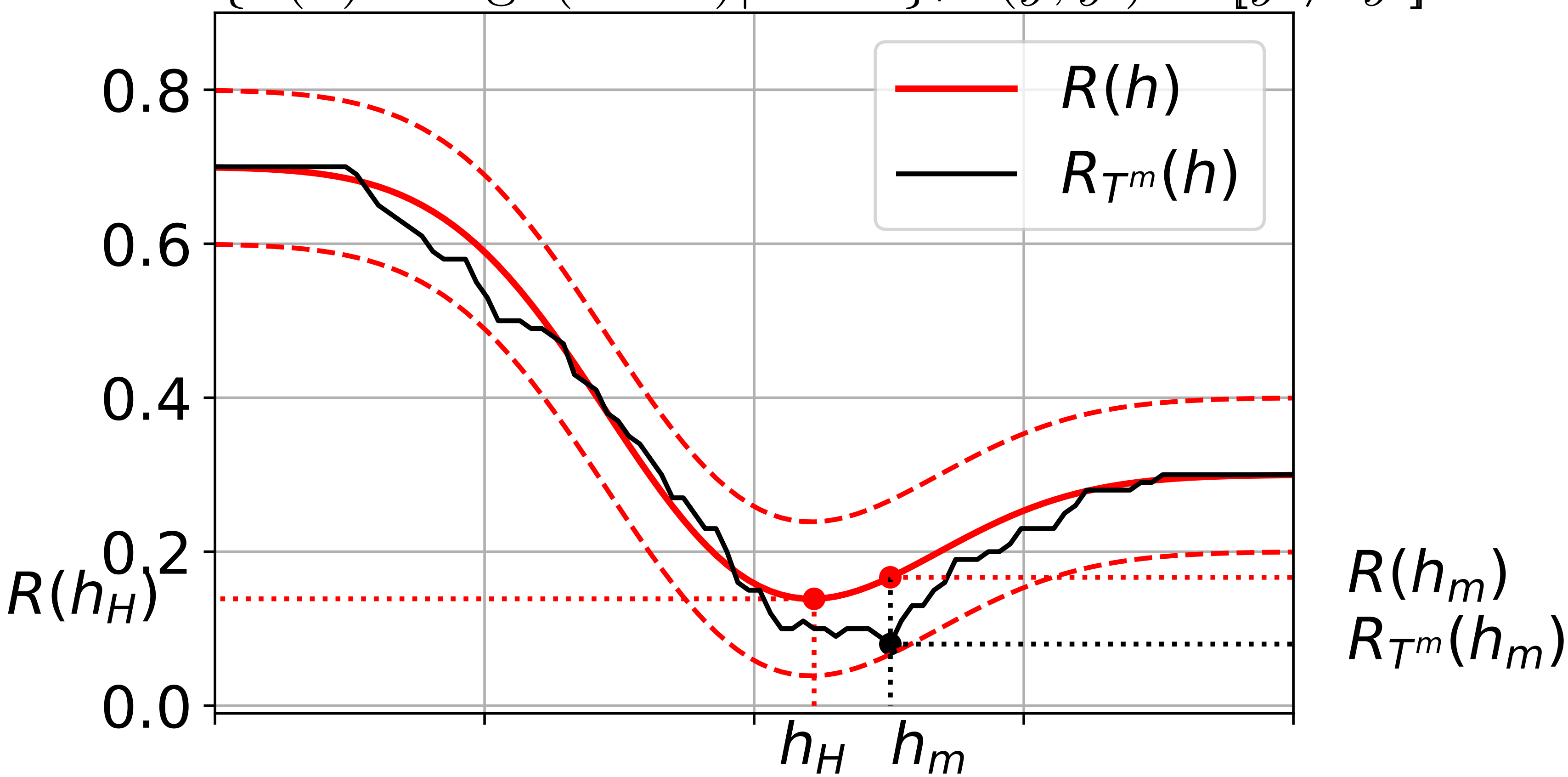


ULLN implies universal consistency of ERM

$$\mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \varepsilon \Big) \leq B(m,\mathcal{H},\varepsilon)$$

$$\mathbb{P}\Big(\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} \geq \varepsilon \Big) \leq \mathbb{P}\Big(\underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{empirical risk fails for some h}\in\mathcal{H}} \geq \tfrac{\varepsilon}{2} \Big) \leq B(m,H,\tfrac{\varepsilon}{2})$$

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



Theorem: ULLN implies universal consistency of ERM

For fixed $\mathcal{T}^m$ and $h_m \in \operatorname{Argmin}_{h\in\mathcal{H}} R_{\mathcal{T}^m}(h)$ we have:

$$\begin{aligned} R(h_m) - R(h_{\mathcal{H}}) &= \Big(R(h_m) - R_{\mathcal{T}^m}(h_m)\Big) + \Big(R_{\mathcal{T}^m}(h_m) - R(h_{\mathcal{H}})\Big) \\ &\le \Big(R(h_m) - R_{\mathcal{T}^m}(h_m)\Big) + \Big(R_{\mathcal{T}^m}(h_{\mathcal{H}}) - R(h_{\mathcal{H}})\Big) \\ &\le 2 \sup_{h\in\mathcal{H}} \Big|R(h) - R_{\mathcal{T}^m}(h)\Big| \end{aligned}$$

Therefore $\varepsilon \le R(h_m) - R(h_{\mathcal{H}})$ implies $\frac{\varepsilon}{2} \le \sup_{h\in\mathcal{H}} \Big|R(h) - R_{\mathcal{T}^m}(h)\Big|$ and

$$\mathbb{P}\Big(R(h_m) - R(h_{\mathcal{H}}) \ge \varepsilon\Big) \le \mathbb{P}\Big(\sup_{h\in\mathcal{H}} \Big|R(h) - R_{\mathcal{T}^m}(h)\Big| \ge \frac{\varepsilon}{2}\Big)$$

so if converges the RHS to zero (ULLN) so does the LHS (estimation error).

Universal consistency for ERM algorithms

- We have shown relation between the estimation error and the uniform bound on the empirical risk:

$$\mathbb{P}\Big(R(h_m) - R(h_{\mathcal{H}}) \geq \varepsilon\Big) \leq \mathbb{P}\Big(\sup_{h\in\mathcal{H}} \Big|R(h) - R_{\mathcal{T}^m}(h)\Big| \geq \frac{\varepsilon}{2}\Big)$$

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- We have shown ULLN for:
  - Finite hypothesis class $\mathcal{H} = \{h_1,\ldots,h_K\}$:

$$\mathbb{P}\Big(\max_{h\in\mathcal{H}}|R_{\mathcal{T}^m}(h) - R(h)| \geq \varepsilon\Big) \leq 2|\mathcal{H}|e^{-\frac{2m\,\varepsilon^2}{(b-a)^2}} = B_1(m, |\mathcal{H}|, \varepsilon)$$

  - Two-class classifiers $\mathcal{H} \subseteq \{+1,-1\}^{\mathcal{X}}$ a finite VC-dimensions d:

$$\mathbb{P}\Big(\sup_{h\in\mathcal{H}}\Big|R^{0/1}(h) - R^{0/1}_{\mathcal{T}^m}(h)\Big| \geq \varepsilon\Big) \leq 4\Big(\frac{2\,e\,m}{d}\Big)^d e^{-\frac{m\,\varepsilon^2}{8}} = B_2(m, d, \varepsilon)$$

Universal consistency for ERM algorithms

- We have shown relation between the estimation error and the uniform bound on the empirical risk:

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$$\mathbb{P}\Big(\sup_{h\in\mathcal{H}} \Big|R^{0/1}(h) - R^{0/1}_{\mathcal{T}^m}(h)\Big| \geq \varepsilon\Big) \leq 4\Big(\frac{2\,e\,m}{d}\Big)^d e^{-\frac{m\,\varepsilon^2}{8}} = B_2(m, d, \varepsilon)$$

Corollary: If $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ is finite or $\mathcal{H} \subseteq \{-1, +1\}^{\mathcal{X}}$ has finite VC-dimension, then ERM algorithm is universally consistent in $\mathcal{H}$.

Bound on the number of training examples for finite hypothesis space

- For finite hypothesis space we derived that

$$\mathbb{P}\Big(R(h_m) - R(h_{\mathcal{H}}) \geq \varepsilon\Big) \leq \mathbb{P}\Big(\sup_{h \in \mathcal{H}} \Big|R(h) - R_{\mathcal{T}^m}(h)\Big| \geq \frac{\varepsilon}{2}\Big) \leq 2|\mathcal{H}|e^{-\frac{m\,\varepsilon^2}{2(b-a)^2}}$$

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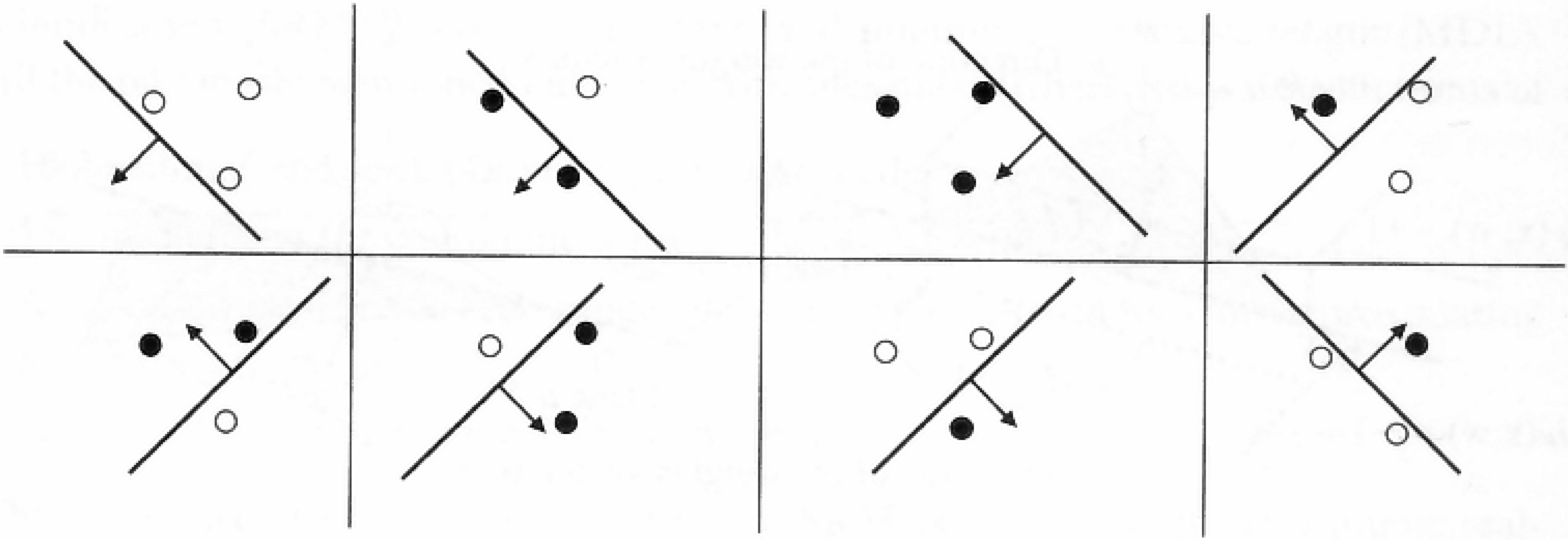
$$\mathbb{P}\Big(R(h_m)-R(h_{\mathcal{H}}) \geq \varepsilon\Big) \leq \mathbb{P}\Big(\sup_{h\in\mathcal{H}}\Big|R(h)-R_{\mathcal{T}^m}(h)\Big| \geq \frac{\varepsilon}{2}\Big) \leq 2|\mathcal{H}|e^{-\frac{m\,\varepsilon^2}{2(b-a)^2}}$$

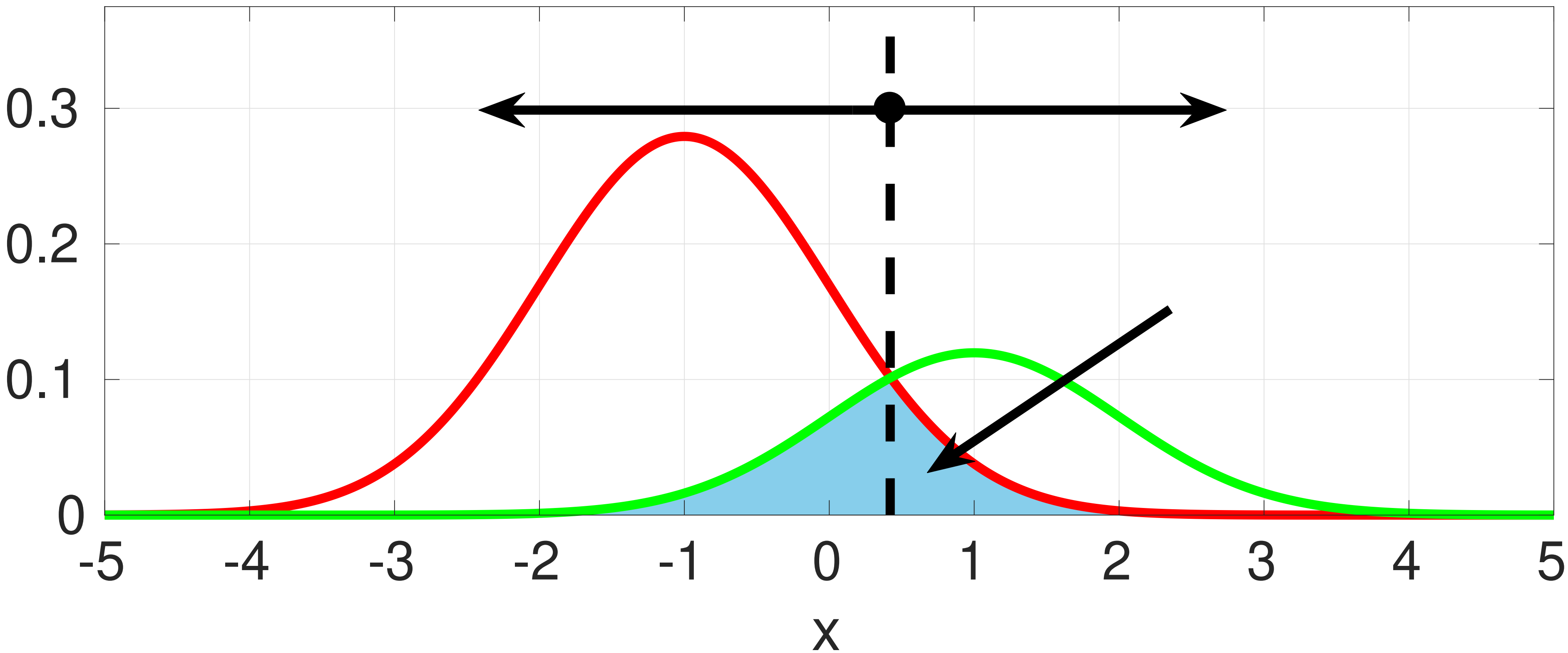
Corollary: Let $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ be a finite hypothesis space and $h_{\mathcal{H}} \in \mathrm{Argmin}_{h\in\mathcal{H}} R(h)$ the best strategy in $\mathcal{H}$. For very $\varepsilon, \delta \in (0,1)$, let us define $m_{\mathcal{H}}\colon (0,1)^2 \to \mathbb{N}$ such that

$$m_{\mathcal{H}}(\varepsilon,\delta) = \frac{2(\log 2|\mathcal{H}| - \log\delta)}{\varepsilon^2}(\ell_{max} - \ell_{min})^2 \,.$$

Let $h_m \in \mathrm{Argmin}_{h\in\mathcal{H}} R_{\mathcal{T}^m}(h)$ be a strategy learned by ERM algorithm from $m \geq m_{\mathcal{H}}(\varepsilon,\delta)$ training examples $\mathcal{T}^m$ generated i.i.d. from some $p(x,y)$. Then, with probability $1-\delta$ at least it holds that

$$R(h_m) - R(h_{\mathcal{H}}) \leq \varepsilon \;\;.$$





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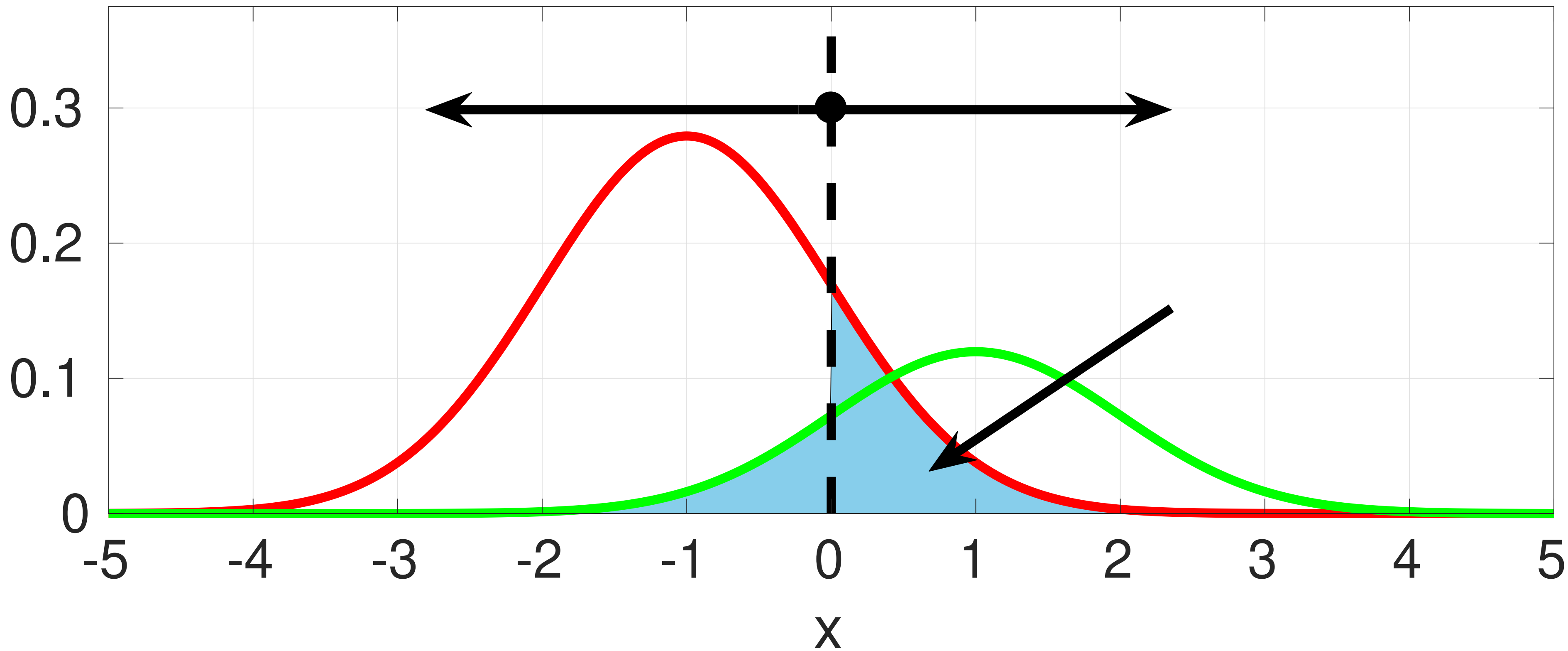

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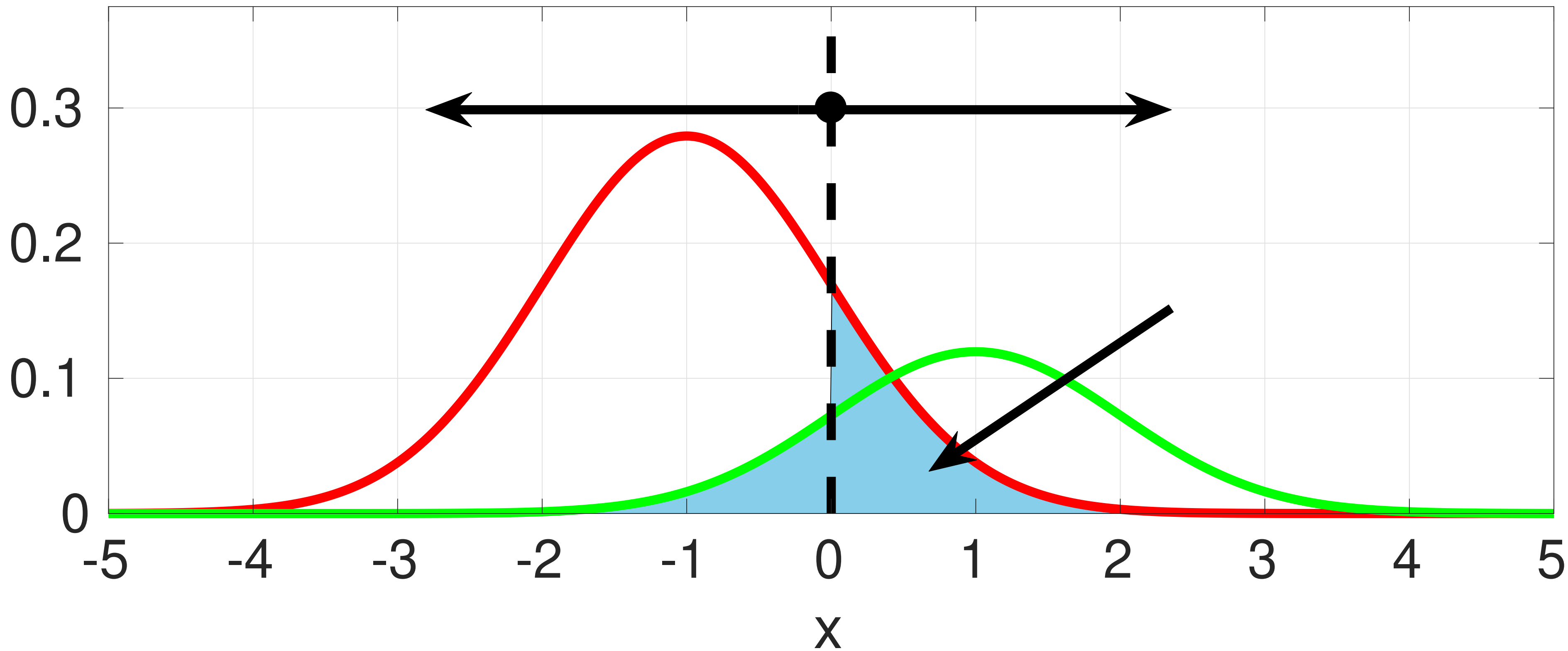

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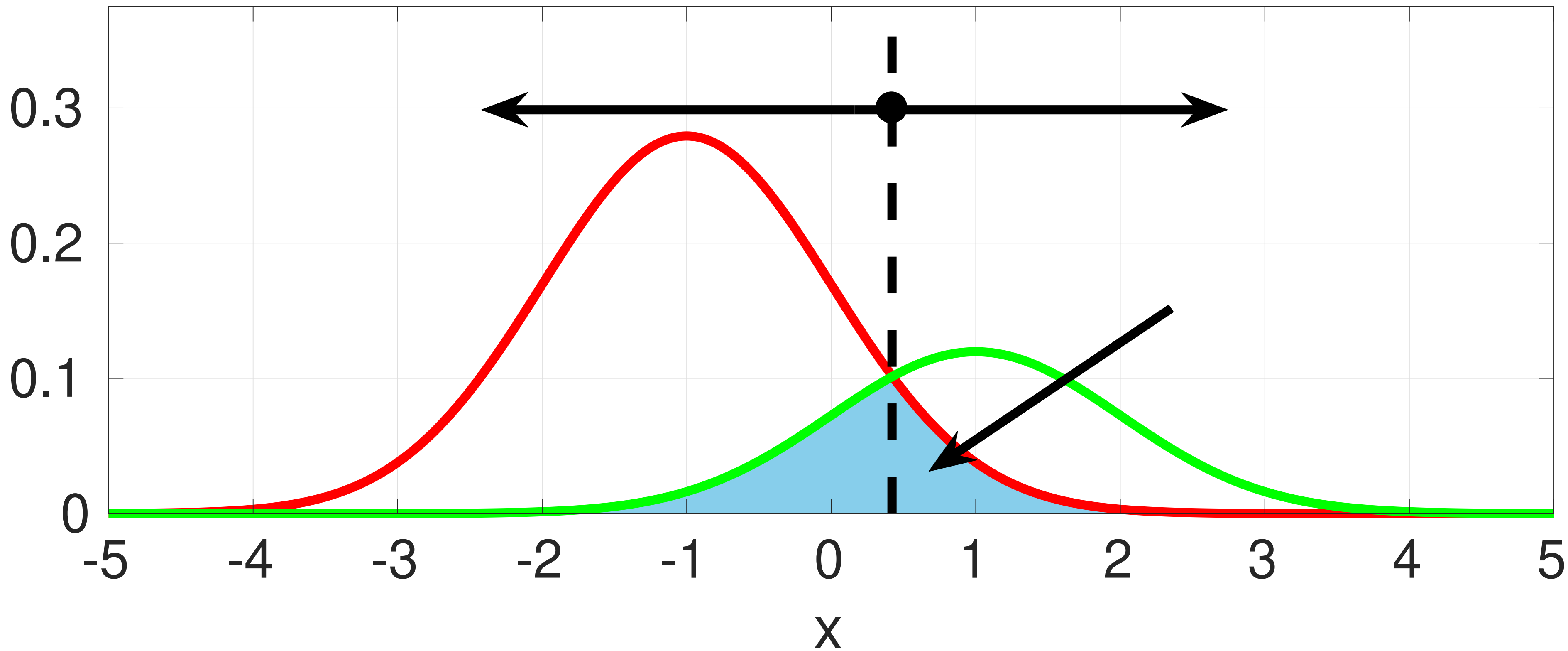
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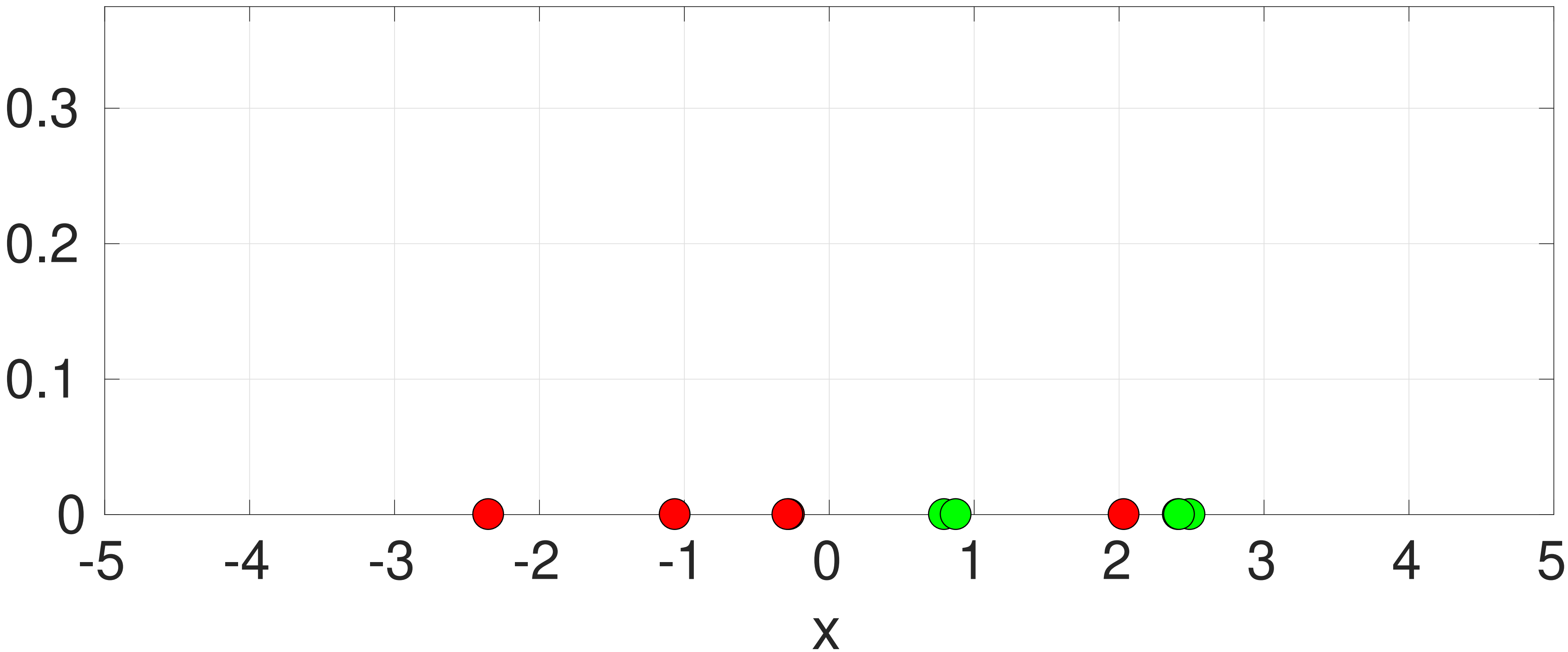

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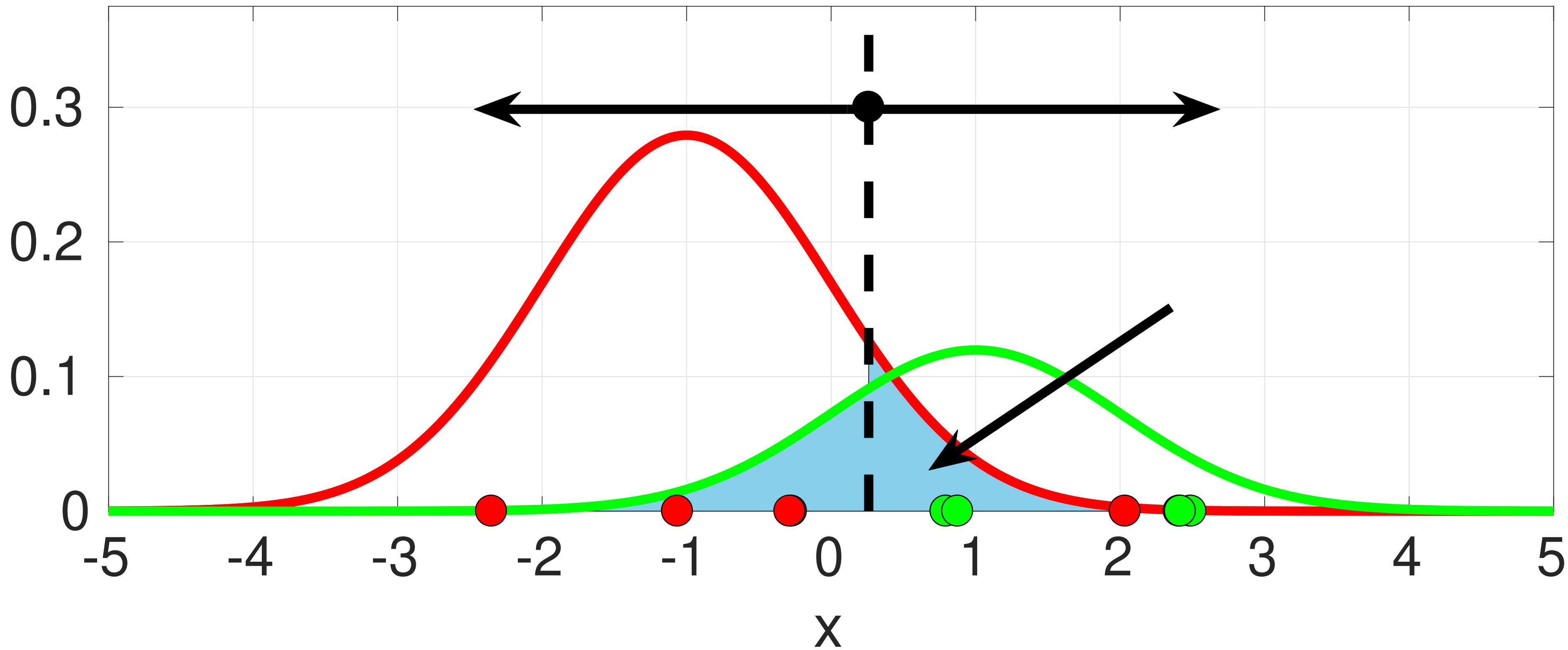
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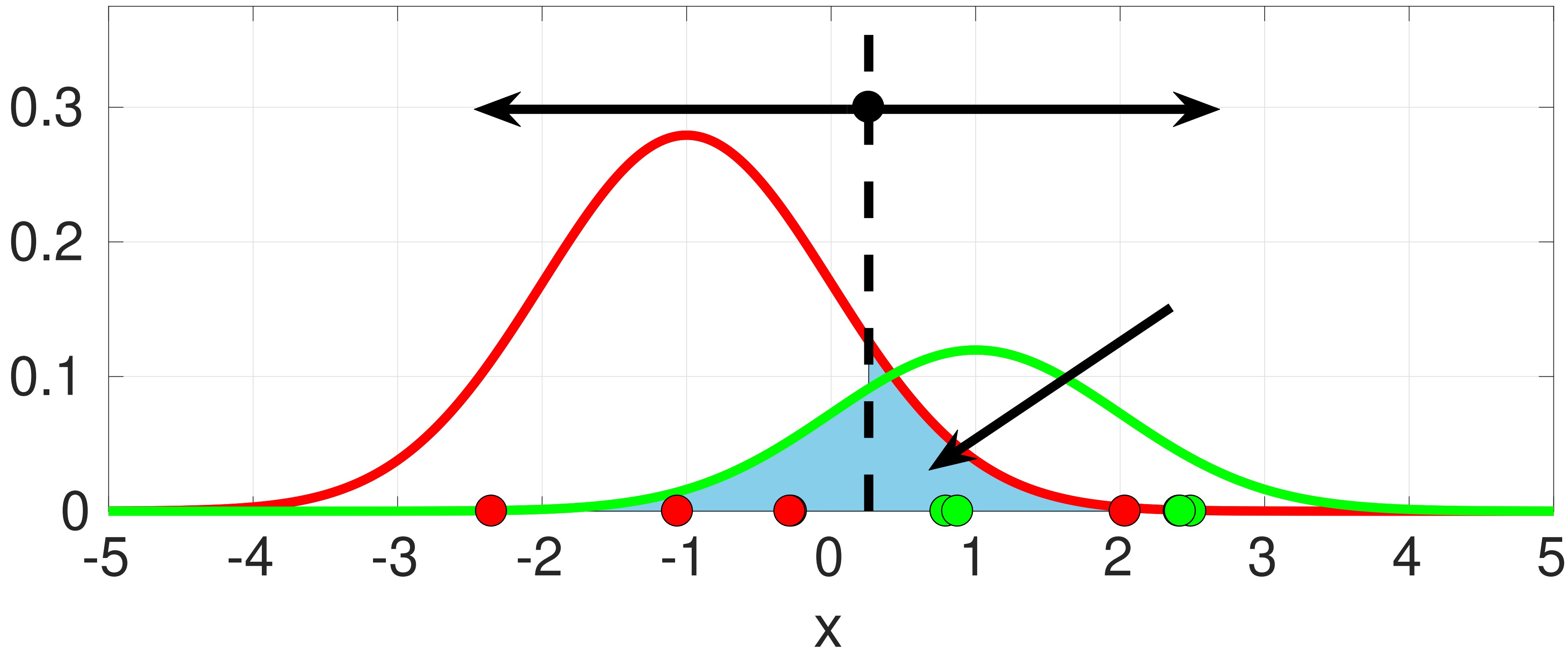
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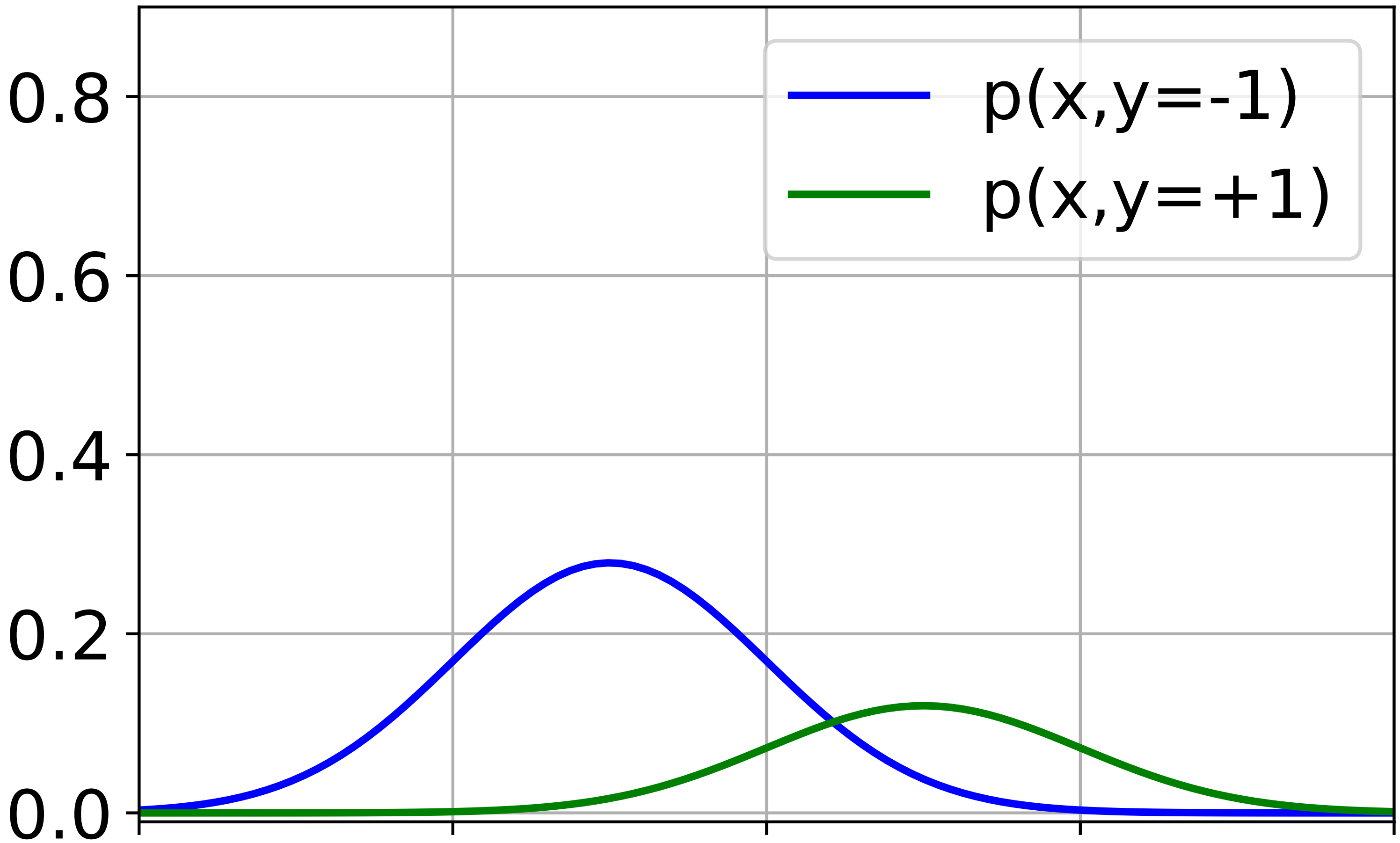
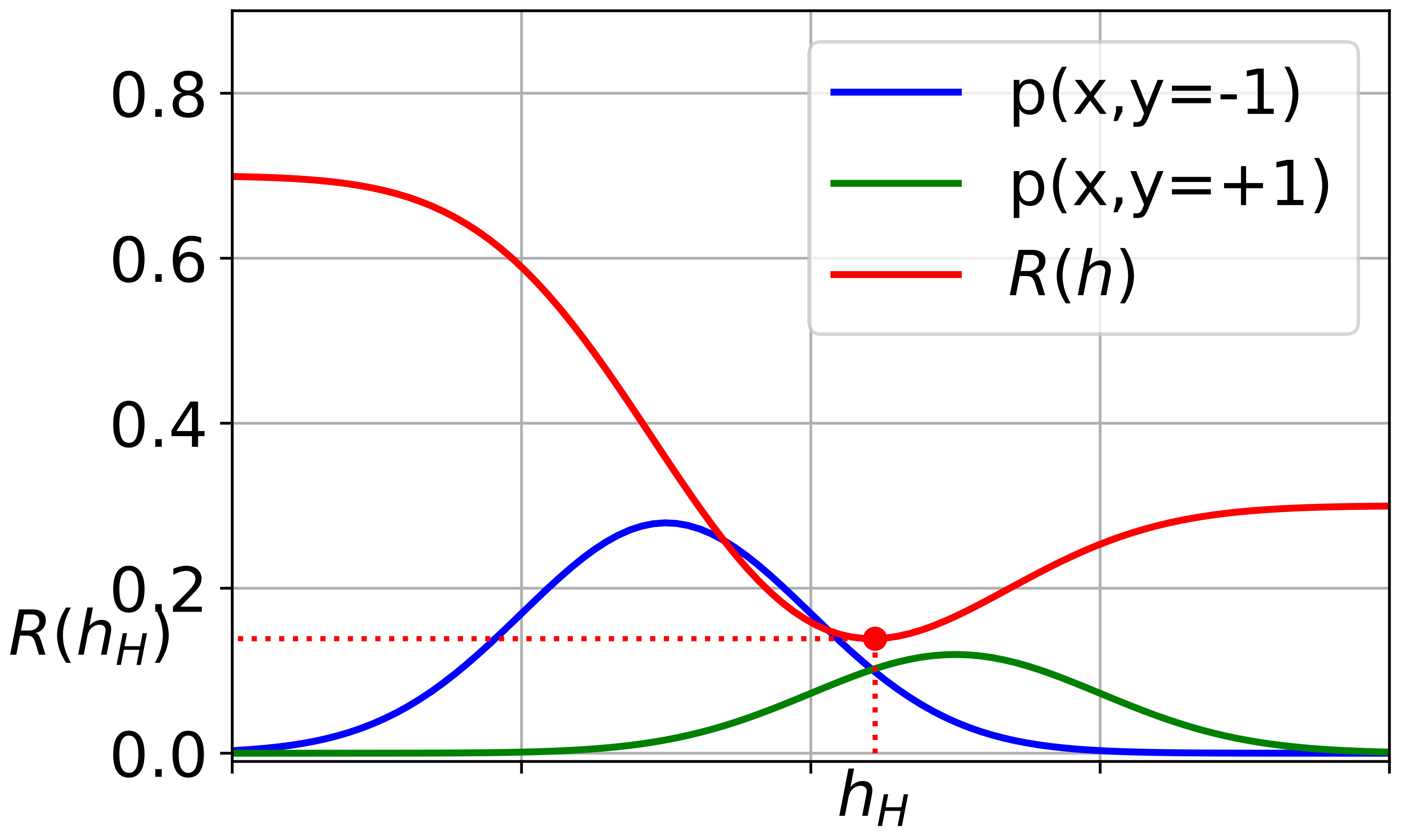

0.8
0.6
0.4
0.2
0.0
p(x,y=-1)
p(x,y=+1)


0.8
0.6
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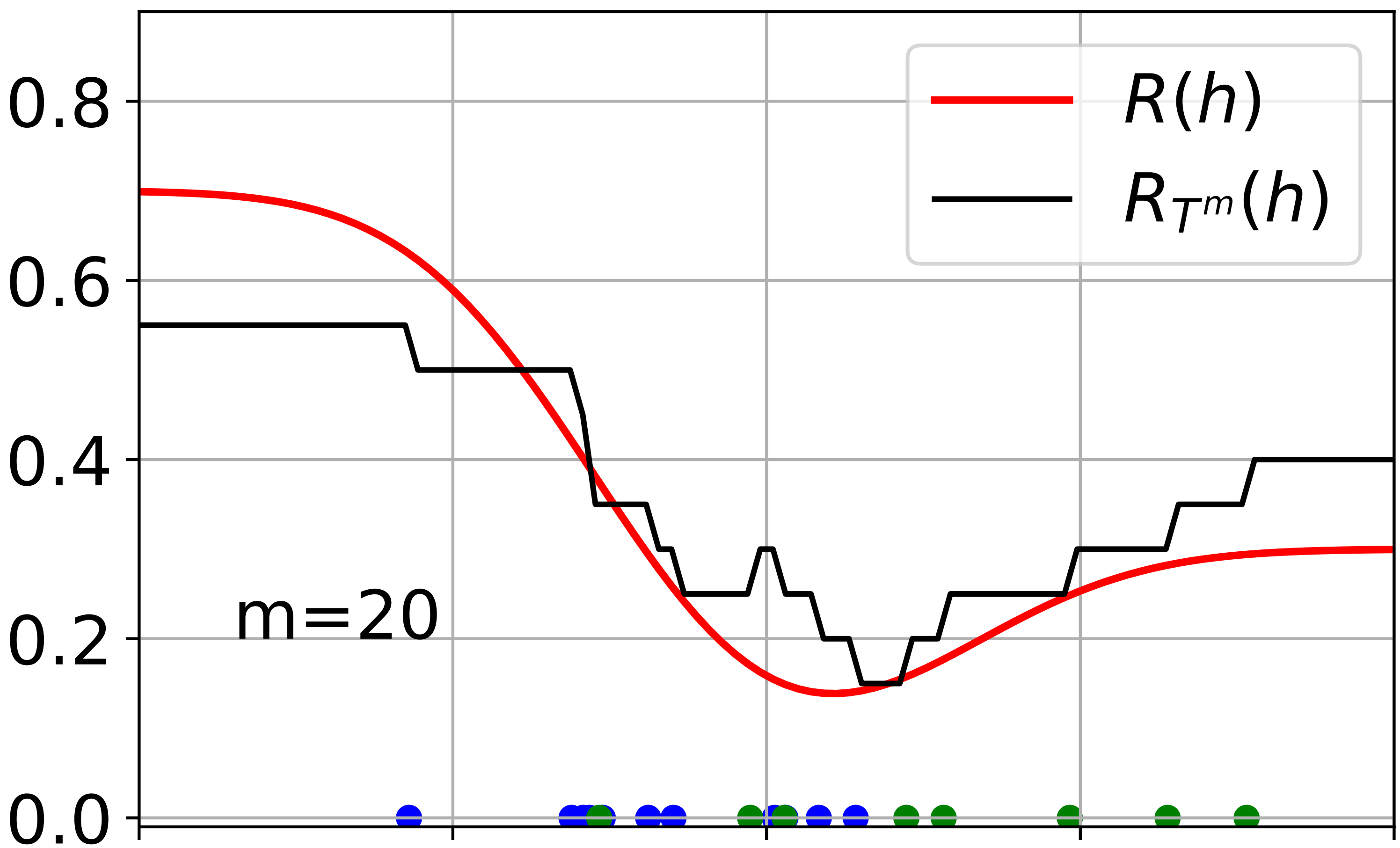
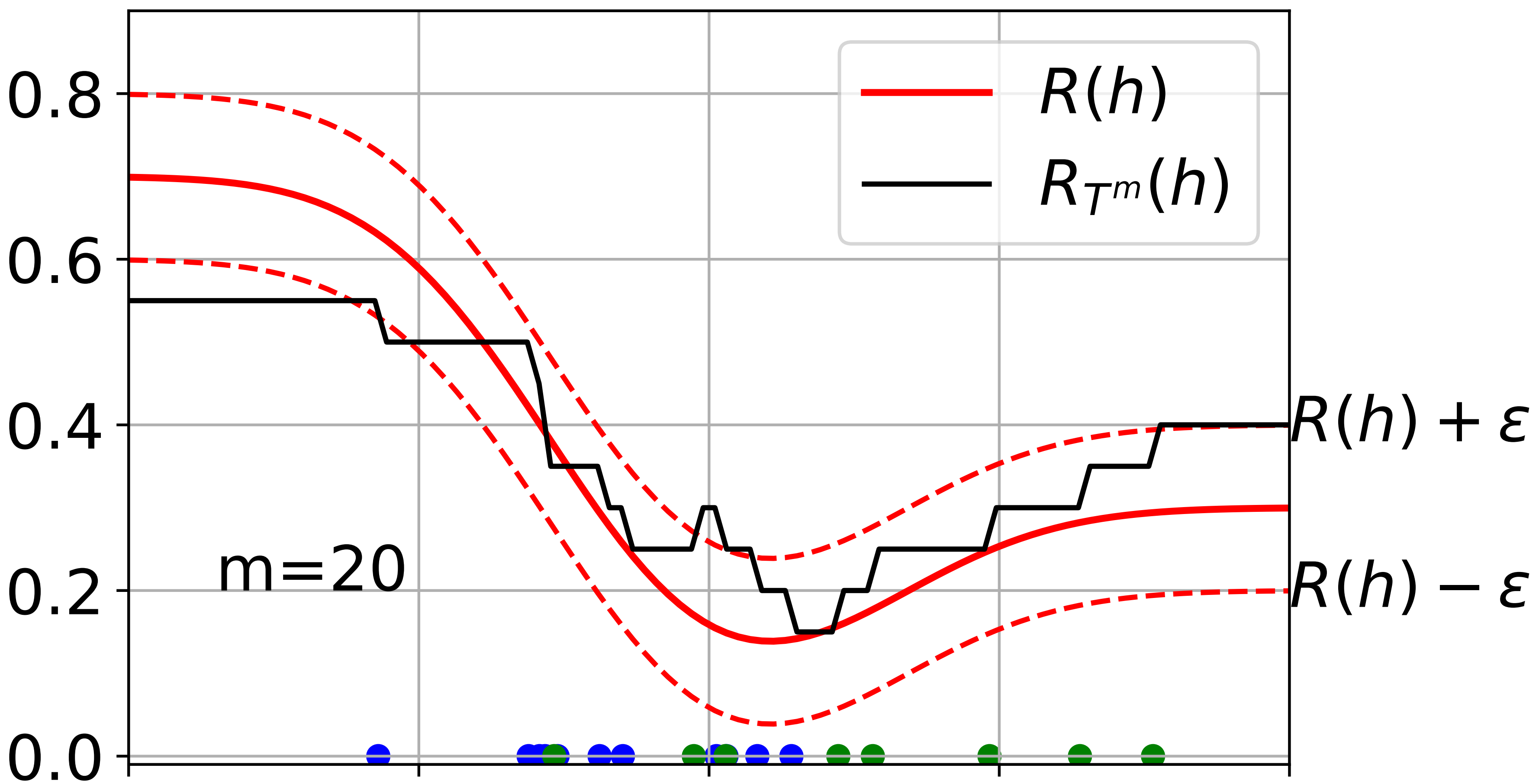
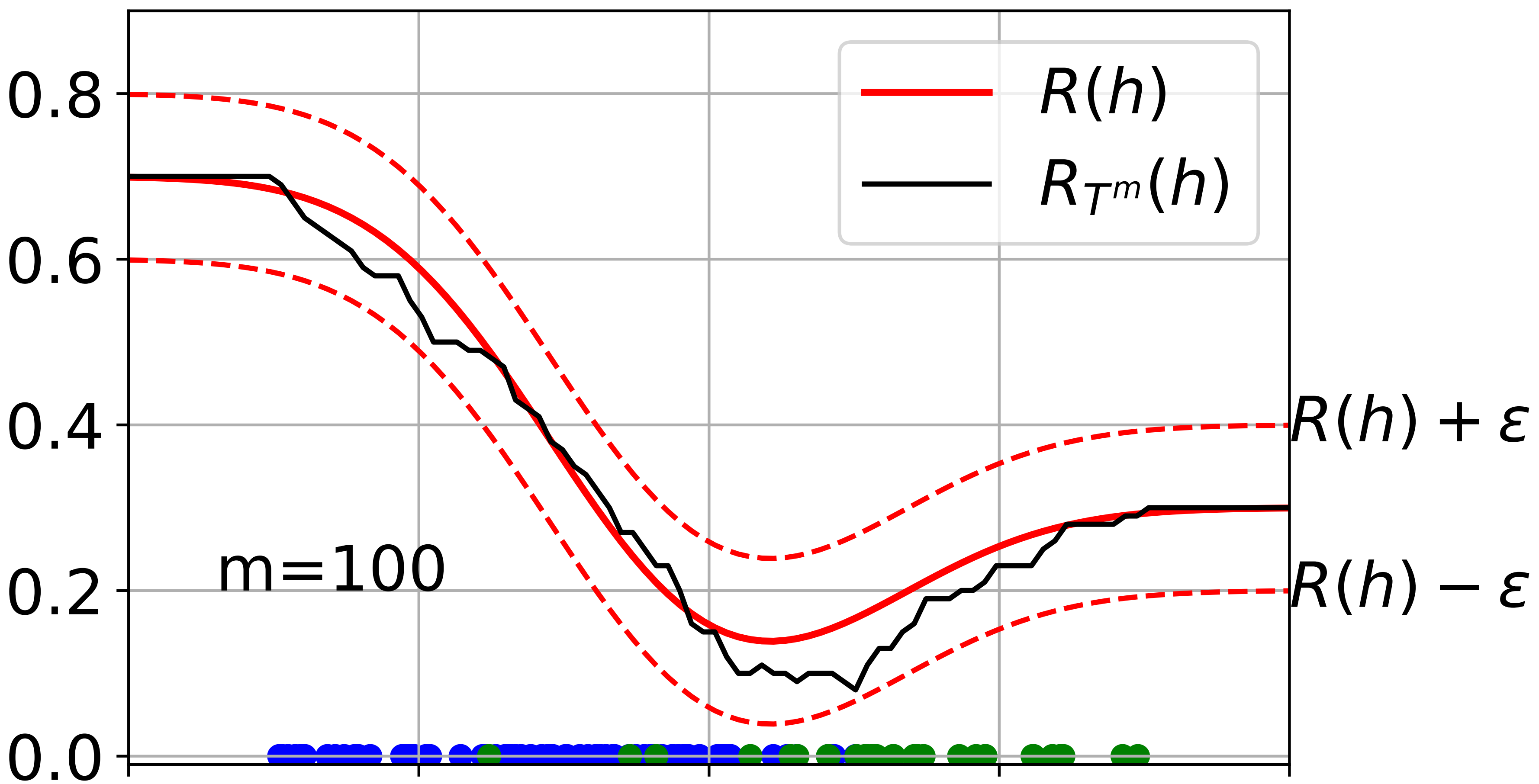
0.2
0.0
$R(h_H)$
h_H
p(x,y=-1)
p(x,y=+1)
$R(h)$



0.8
0.6
0.4
0.2
0.0
m=20
$R(h)$
$R_{T^m}(h)$



0.8
0.6
0.4
0.2
0.0
m=20
$R(h)$
$R_{T^m}(h)$
$R(h) + \varepsilon$
$R(h) - \varepsilon$


0.8
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0.4
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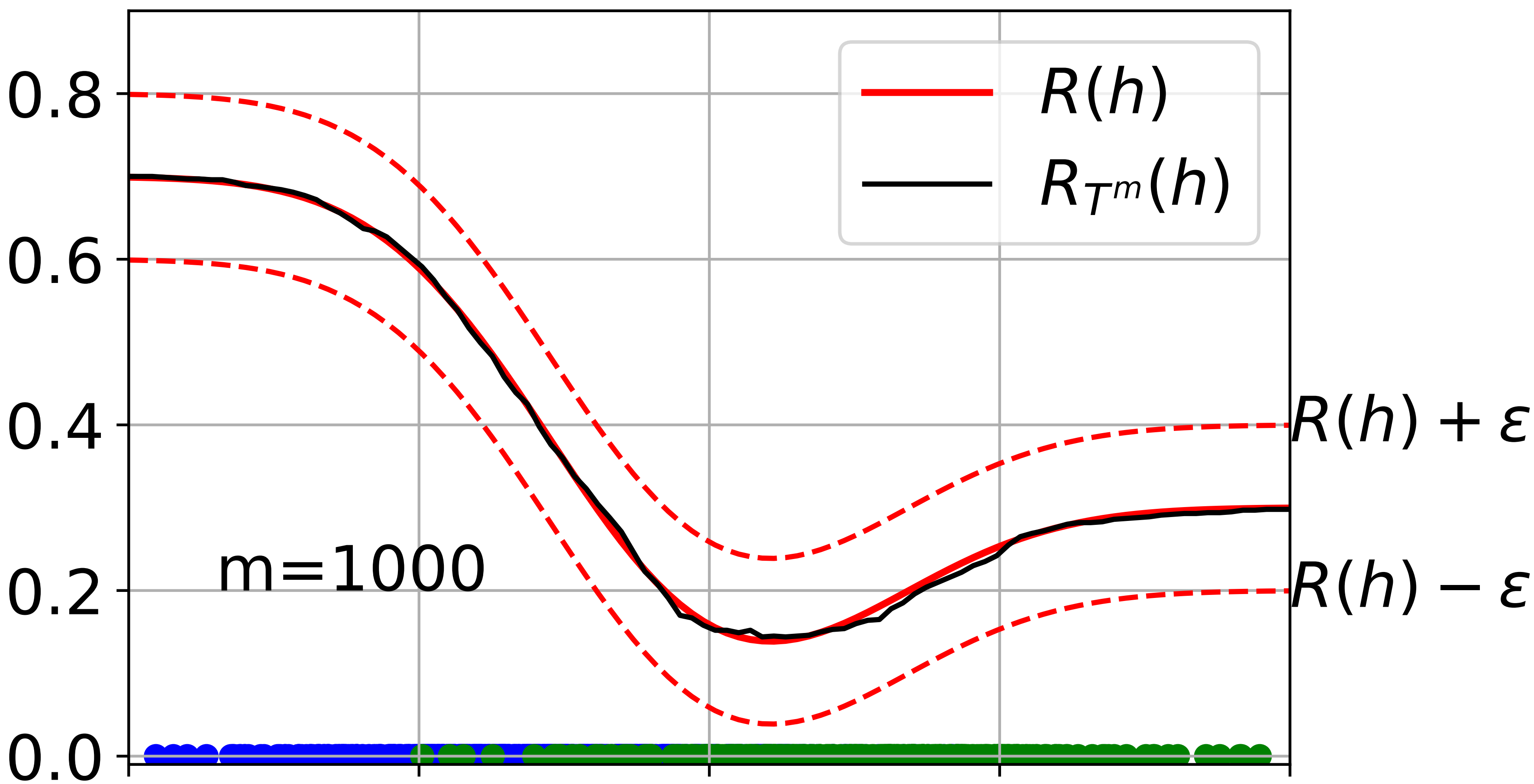
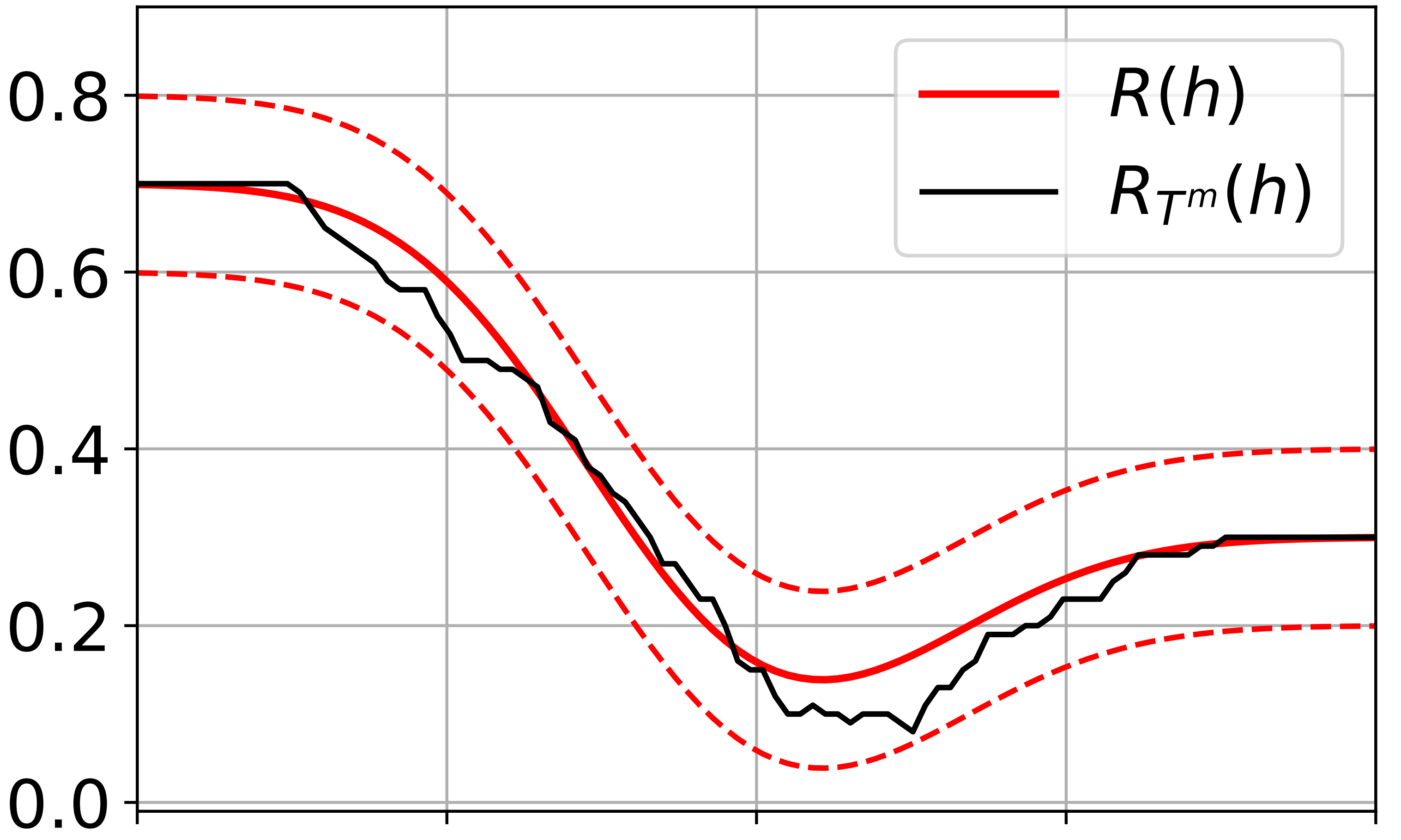
0.0
$R(h)$
$R_{T^m}(h)$
$R(h)+\varepsilon$
$R(h)-\varepsilon$
m=100



0.8
0.6
0.4
0.2
0.0
R(h)
R_{T^m}(h)
R(h) + ε
R(h) − ε
m=1000



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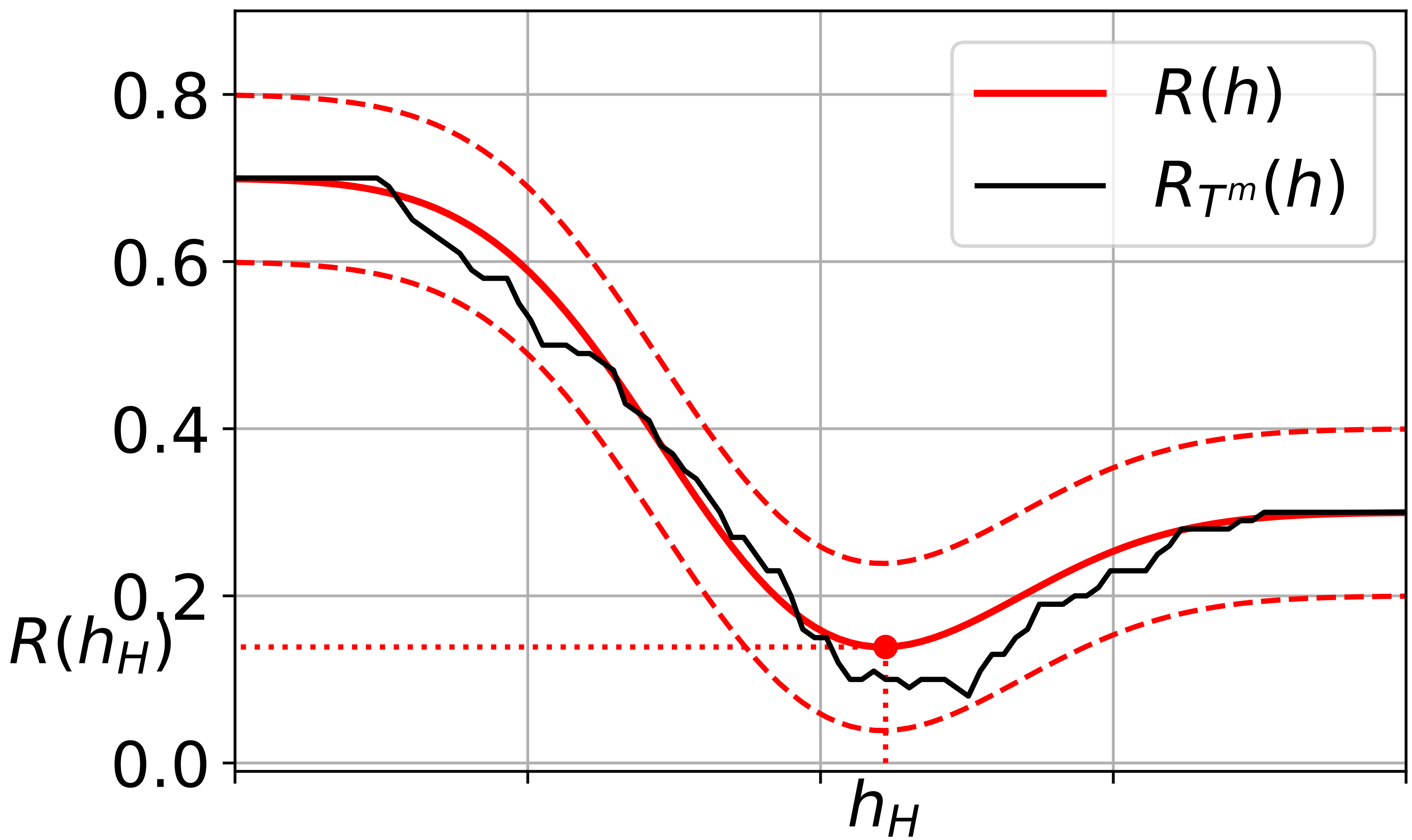
$R(h)$
$R_{T^m}(h)$



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$R(h_H)$
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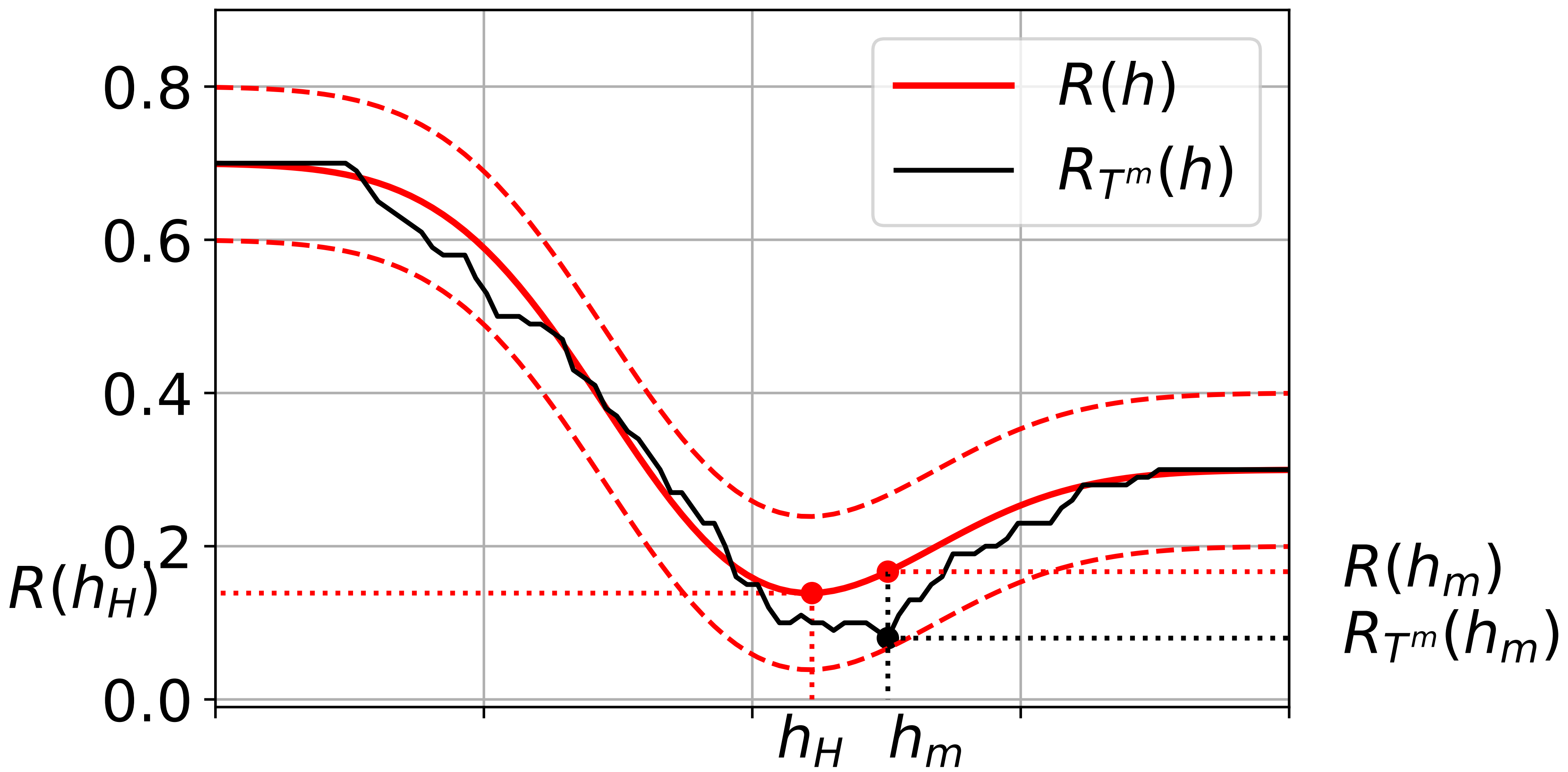
$R(h)$
$R_{T^m}(h)$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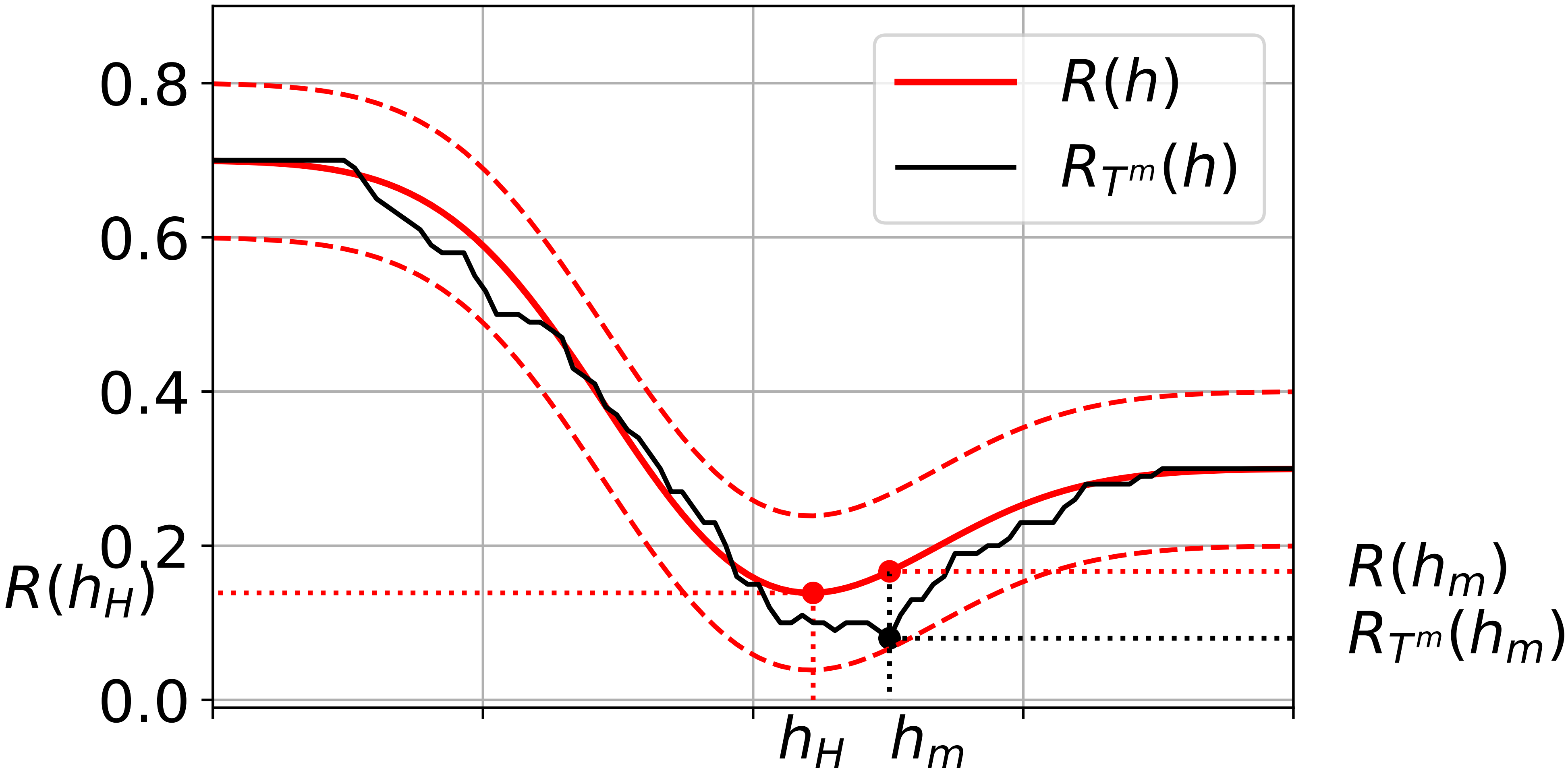
$R(h_m)$
$R_{T^m}(h_m)$
h_H
h_m



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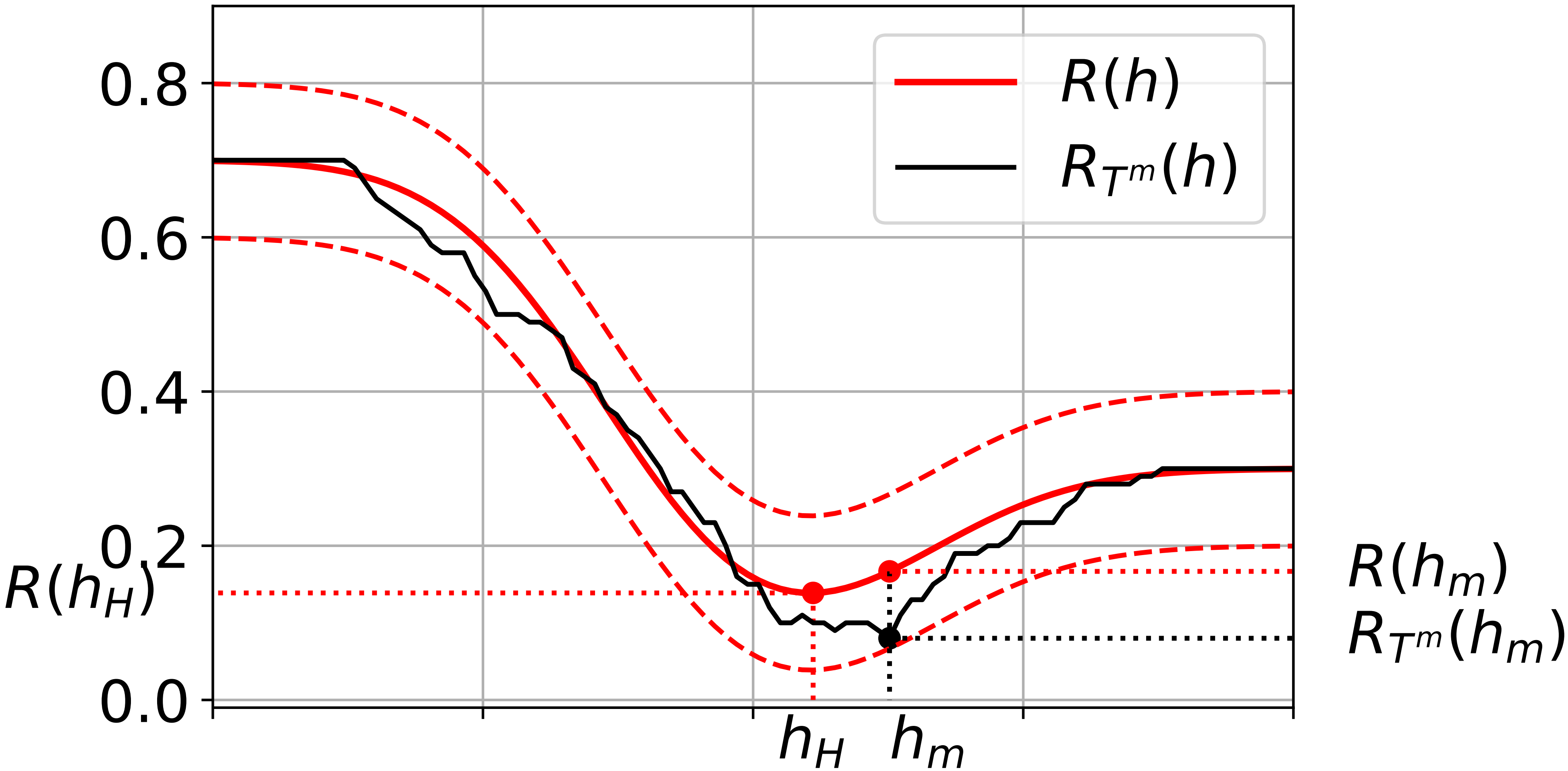
h_H
h_m



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$R_{T^m}(h_m)$
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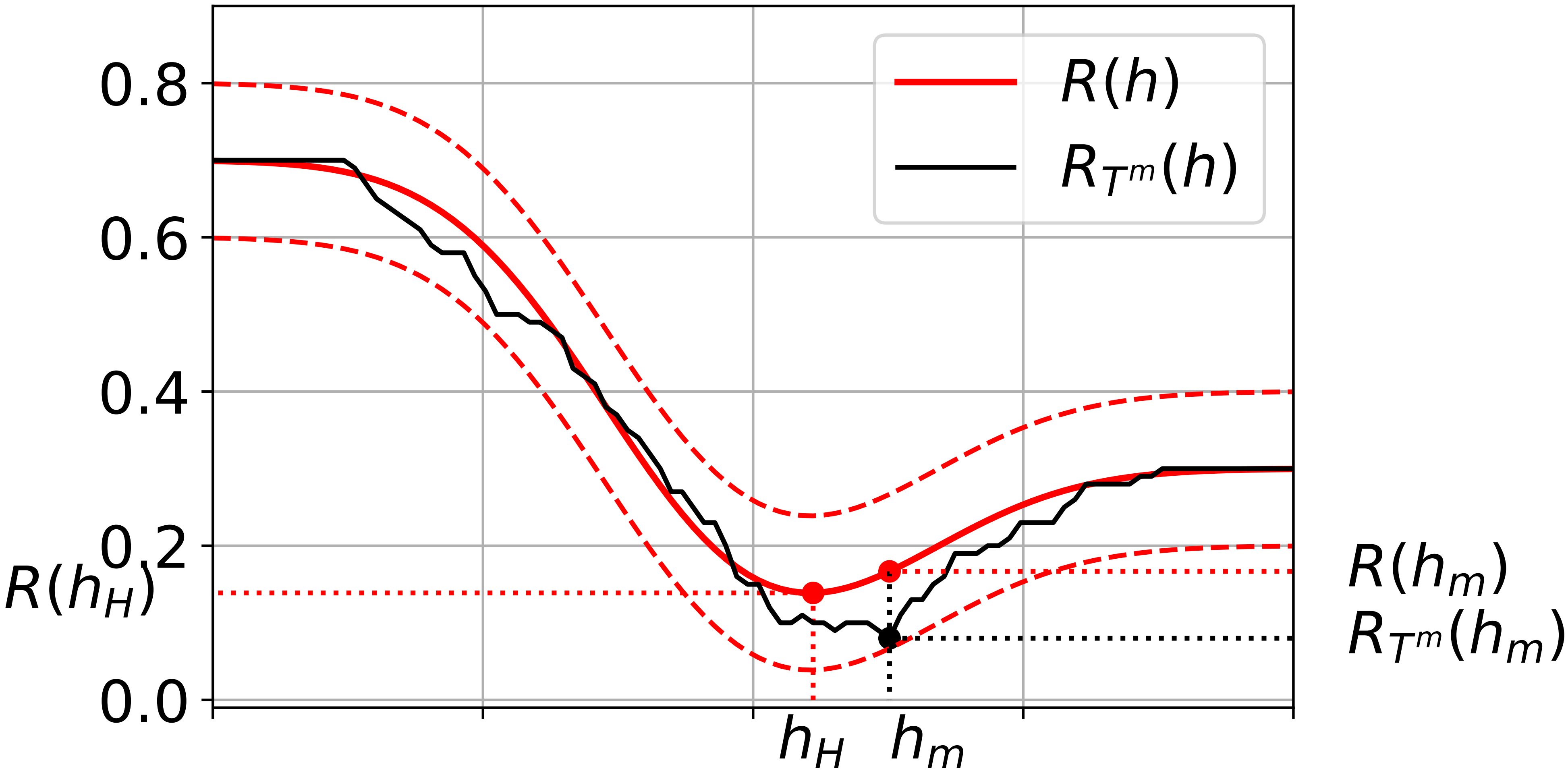
h_m



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$R(h)$
$R_{T^m}(h)$
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$R(h_m)$
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h_H
h_m