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

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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 $h\colon \mathcal{X} \to \mathcal{Y}$

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

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

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

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

ERM learning for linear classifiers

- The Empirical Risk Minimization principle leads to solving

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

where the empirical risk is

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

- Algorithmic issues (next lecture): in general, there is no known algorithm solving the task (1) in time polynomial in m.
- The uniform bound on the generalization error (this lecture):

$$\mathbb{P}\left(\sup_{h\in\mathcal{H}}\left|R^{0/1}(h) - R^{0/1}_{\mathcal{T}^m}(h)\right| \geq \varepsilon\right) \leq B(m,\mathcal{H},\varepsilon)$$

Vapnik-Chervonenkis (VC) dimension

Definition: Let $\mathcal{H} \subseteq \{-1,+1\}^{\mathcal{X}}$ and $\{x^1,\ldots,x^m\} \in \mathcal{X}^m$ be a set of m input observations. The set $\{x^1,\ldots,x^m\}$ is said to be shattered by $\mathcal{H}$ if for all $\boldsymbol{y} \in \{+1,-1\}^m$ there exists $h \in \mathcal{H}$ such that $h(x^i) = y^i$, $i \in \{1,\ldots,m\}$.

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 $\mathcal{H} = \{h(x; \boldsymbol{w}, b) = \mathrm{sign}(\langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b) \mid (\boldsymbol{w}, b) \in (\mathbb{R}^n \times \mathbb{R})\}$ is $n + 1$.

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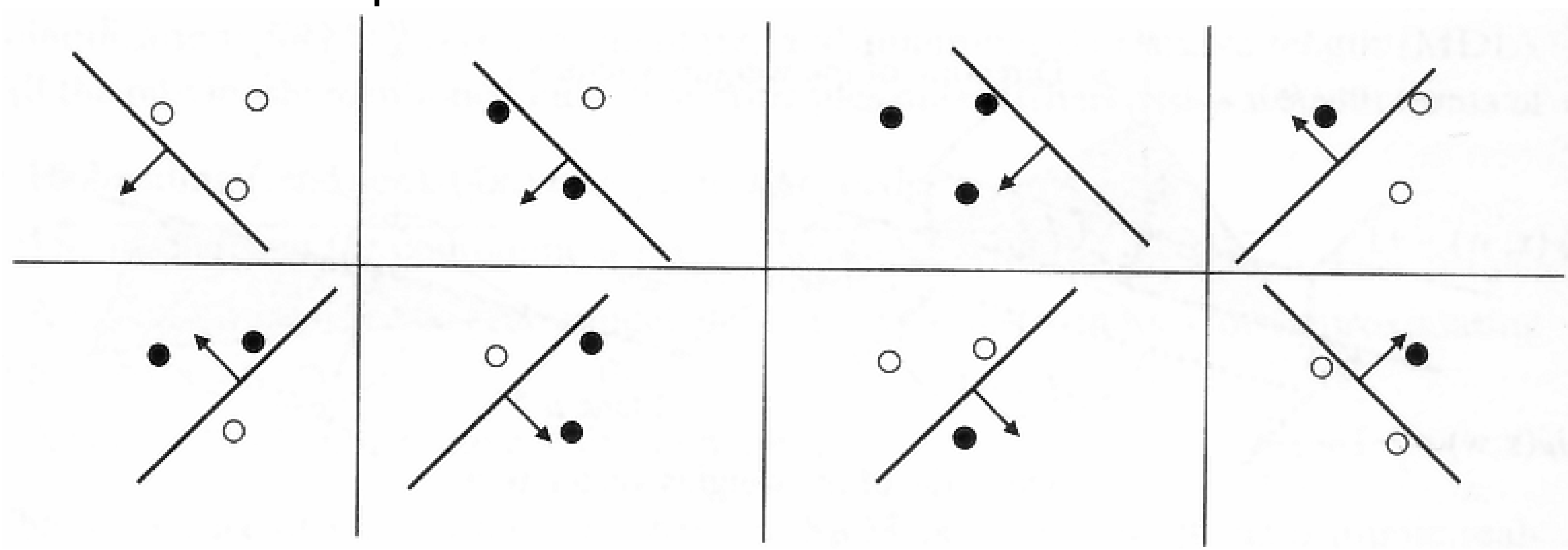
Example for $n = 2$-dimensional feature class



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, for any $\varepsilon > 0$ it holds

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

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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 bounds on the generalization error

- We learned how to bound the generalization error uniformly for:
  - Finite hypothesis class $\mathcal{H} = \{h_1, \ldots, h_K\}$:

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

  - 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 $R(h)$?

Statistically consistent learning algorithm

- $h_{\mathcal{H}} \in \mathrm{Argmin}_{h \in \mathcal{H}} R(h)$ the best strategy in $\mathcal{H}$ has the risk $R(h_{\mathcal{H}})$
- $h_m = A(\mathcal{T}_m)$ strategy learned from $\mathcal{T}_m$ with has risk $R(h_m)$
- $R(h_m) - R(h_{\mathcal{H}})$ is the estimation error
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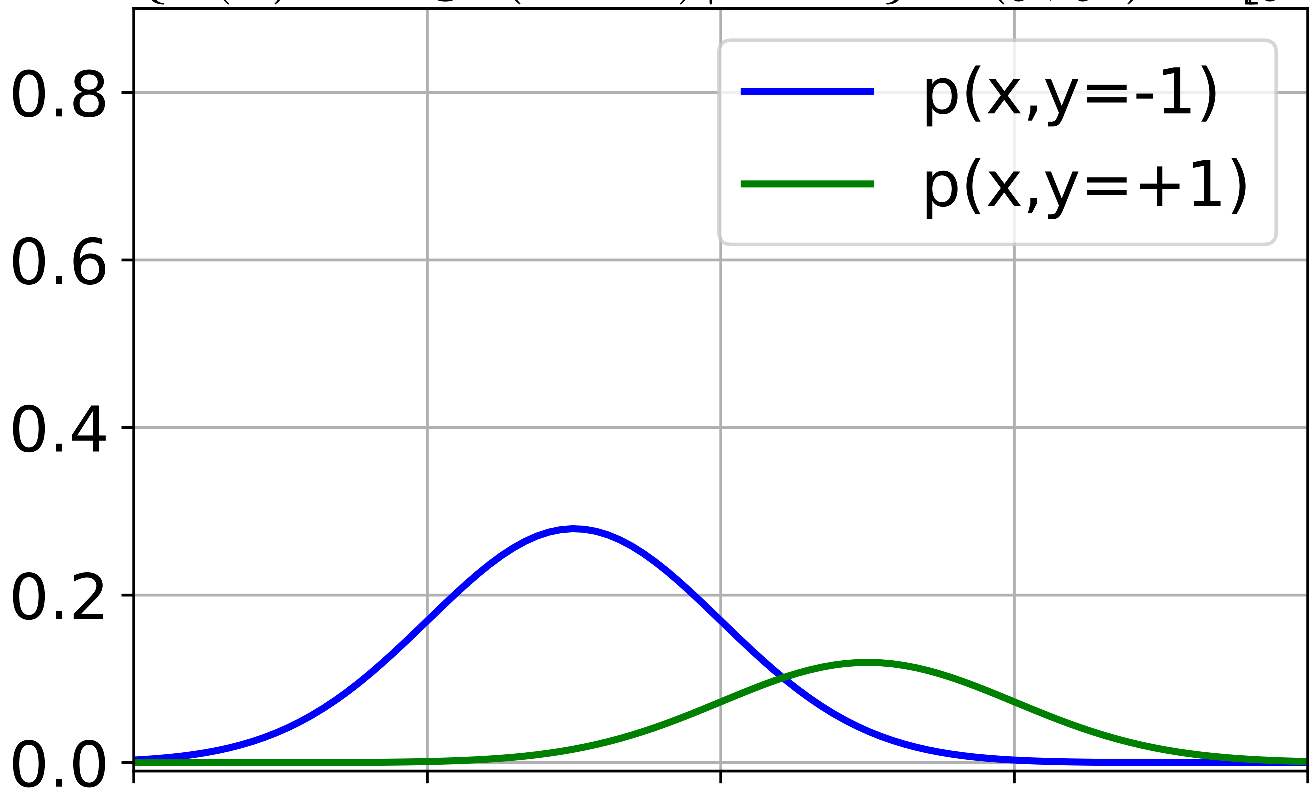
Definition: The algorithm $A\colon \cup_{m=1}^{\infty} (\mathcal{X} \times \mathcal{Y})^m \to \mathcal{H}$ is statistically consistent in $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ if for any $p(x,y)$ it holds that

$$\forall\, \varepsilon > 0\colon \lim_{m \to \infty} \mathbb{P}\Bigg(\underbrace{R(h_m) - R(h_{\mathcal{H}}) \geq \varepsilon}_{\text{high estimation error}} \Bigg) = 0$$

where $h_m = A(\mathcal{T}^m)$ is learned by A for $\mathcal{T}^m$ generated from $p(x,y)$.

Example: generalization error and estimation error

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



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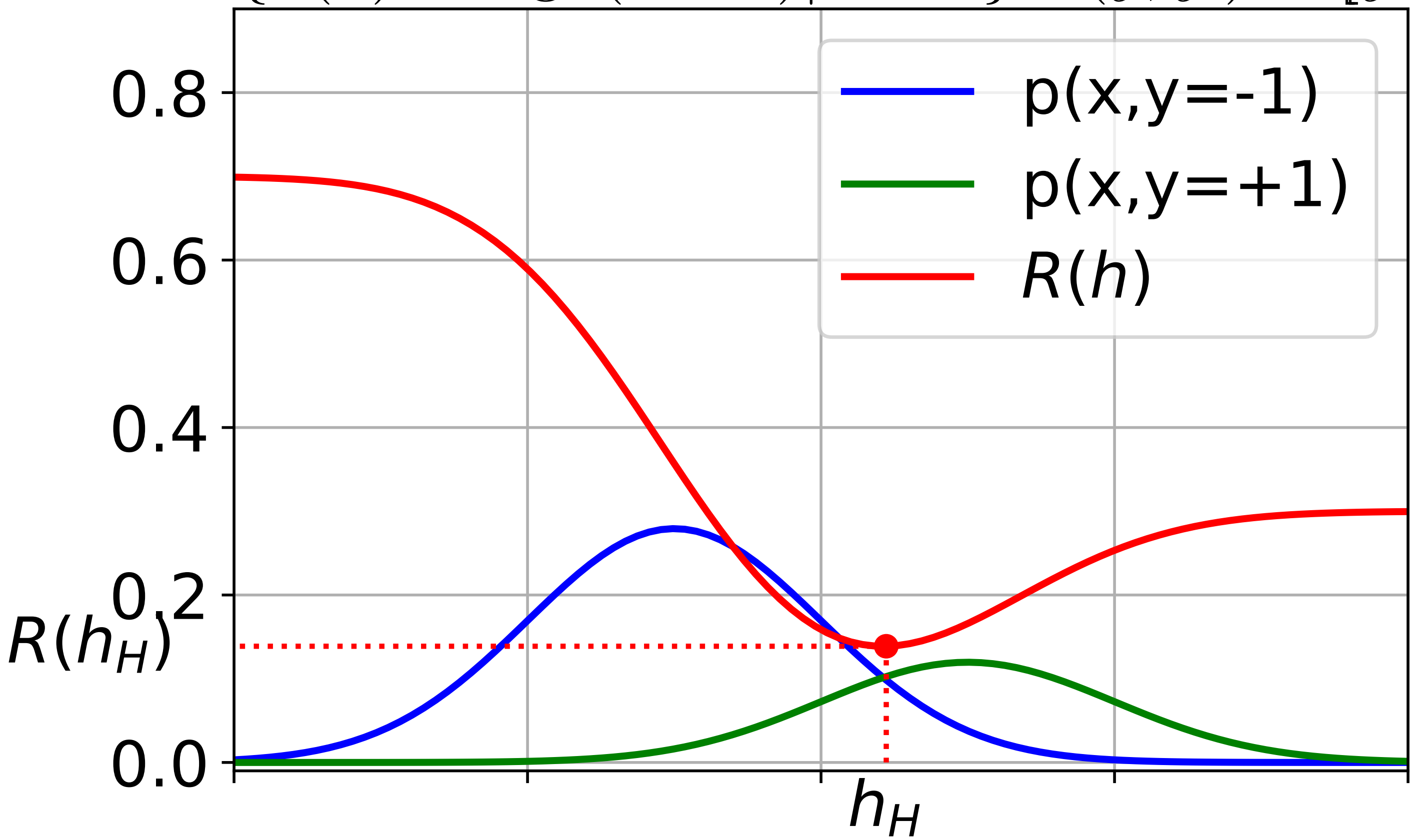

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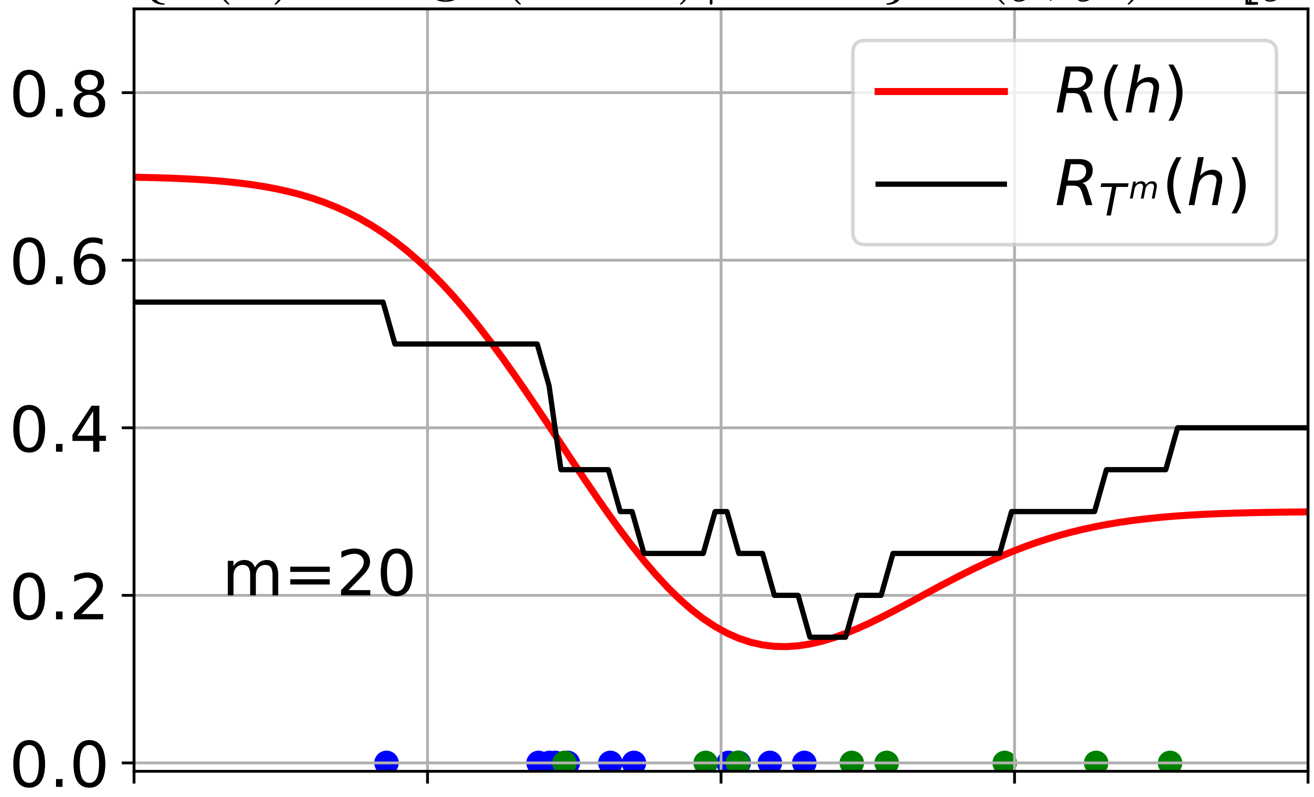

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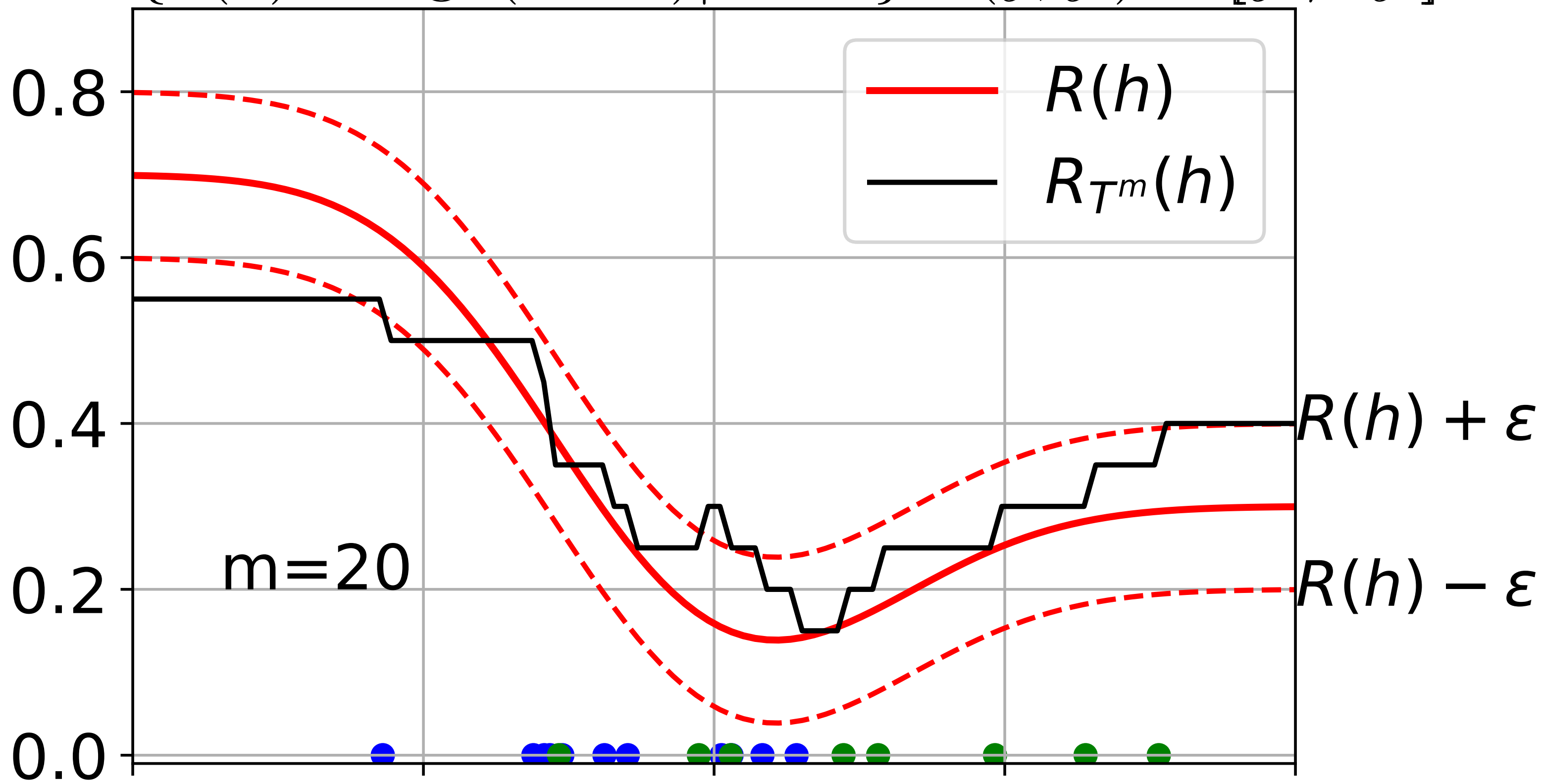

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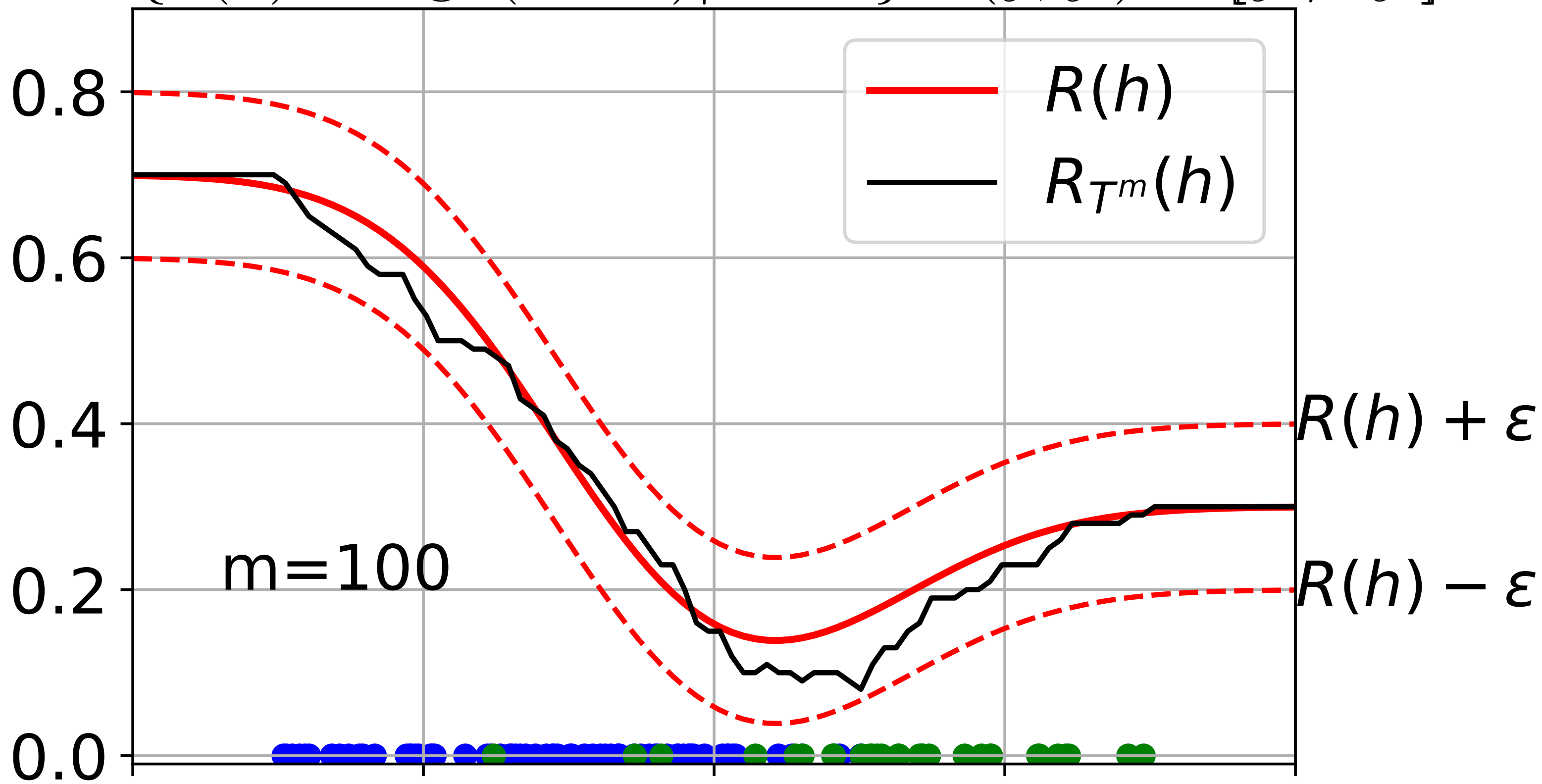

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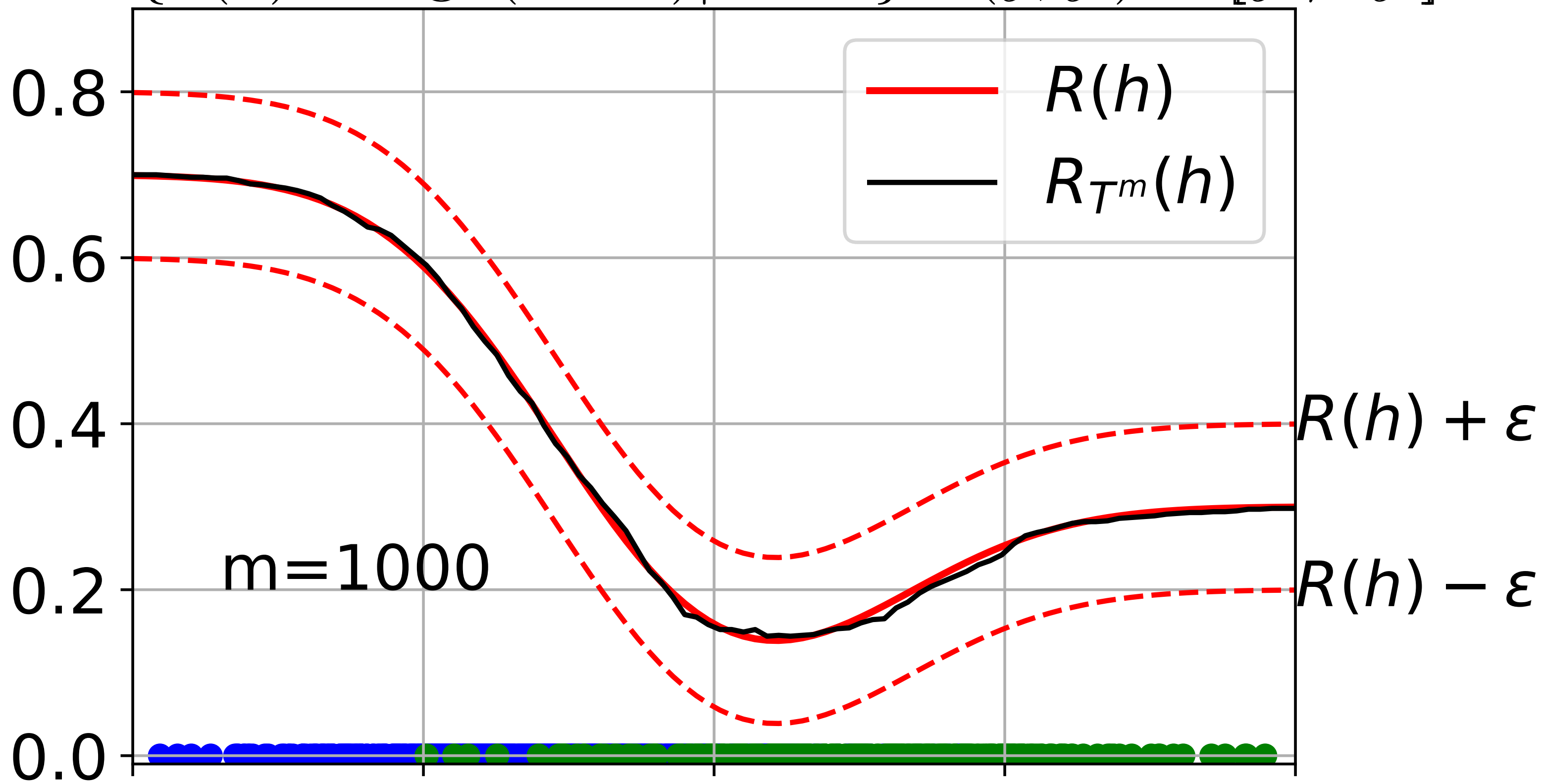

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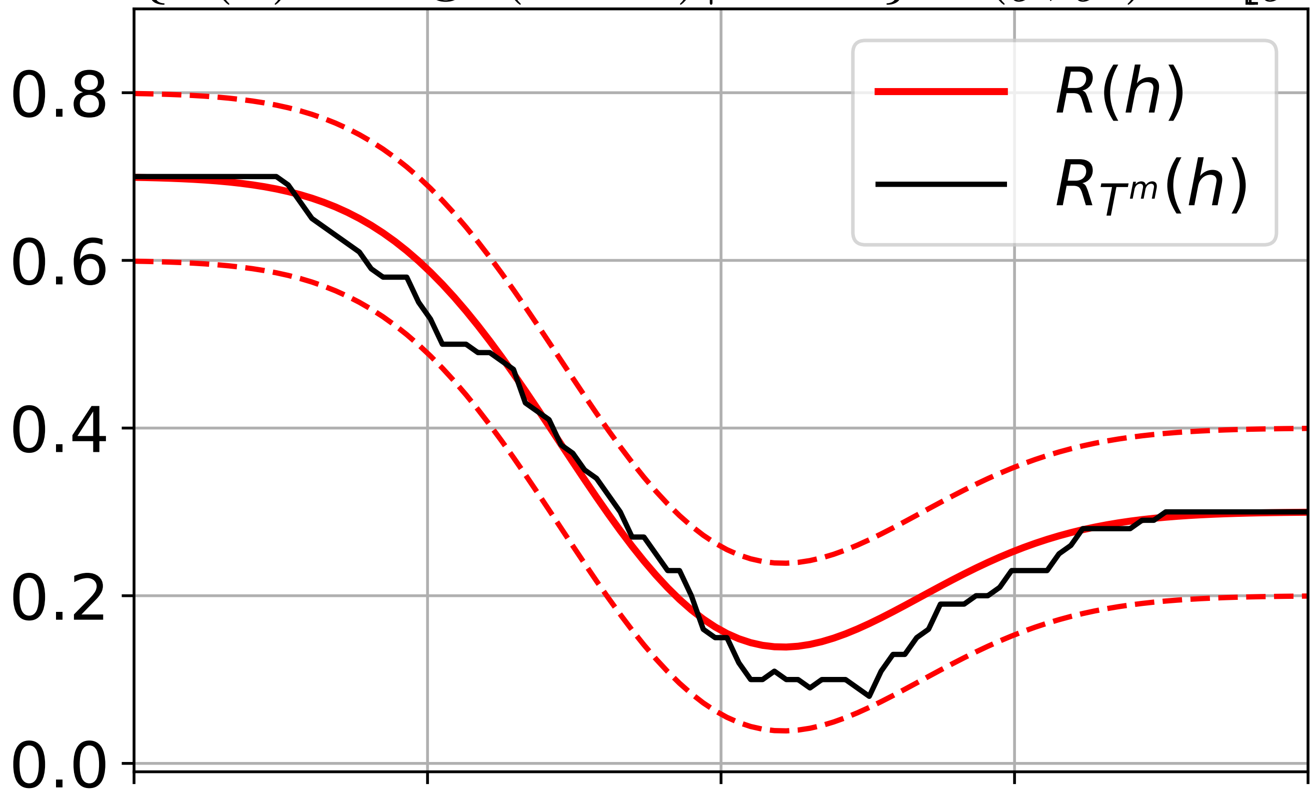

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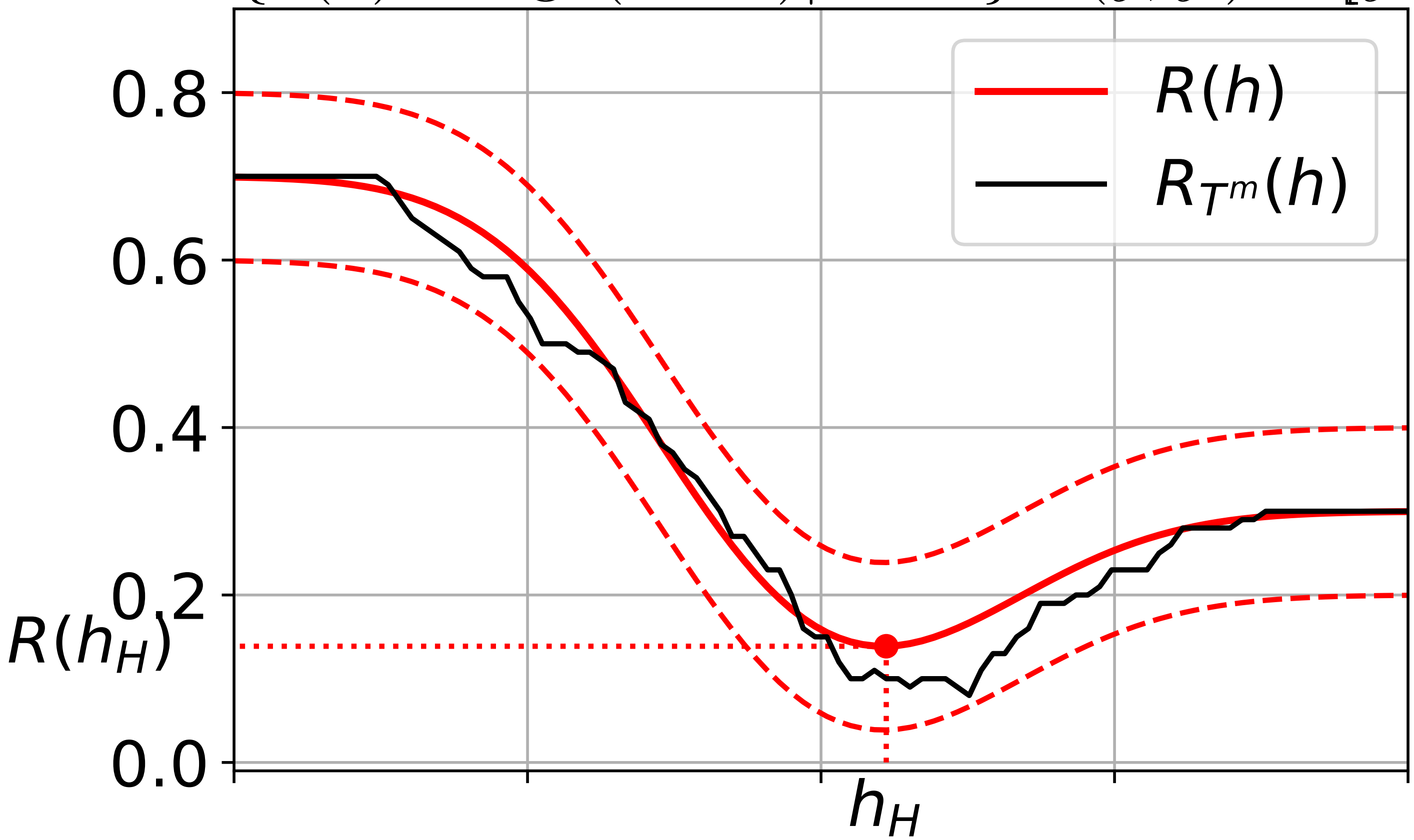

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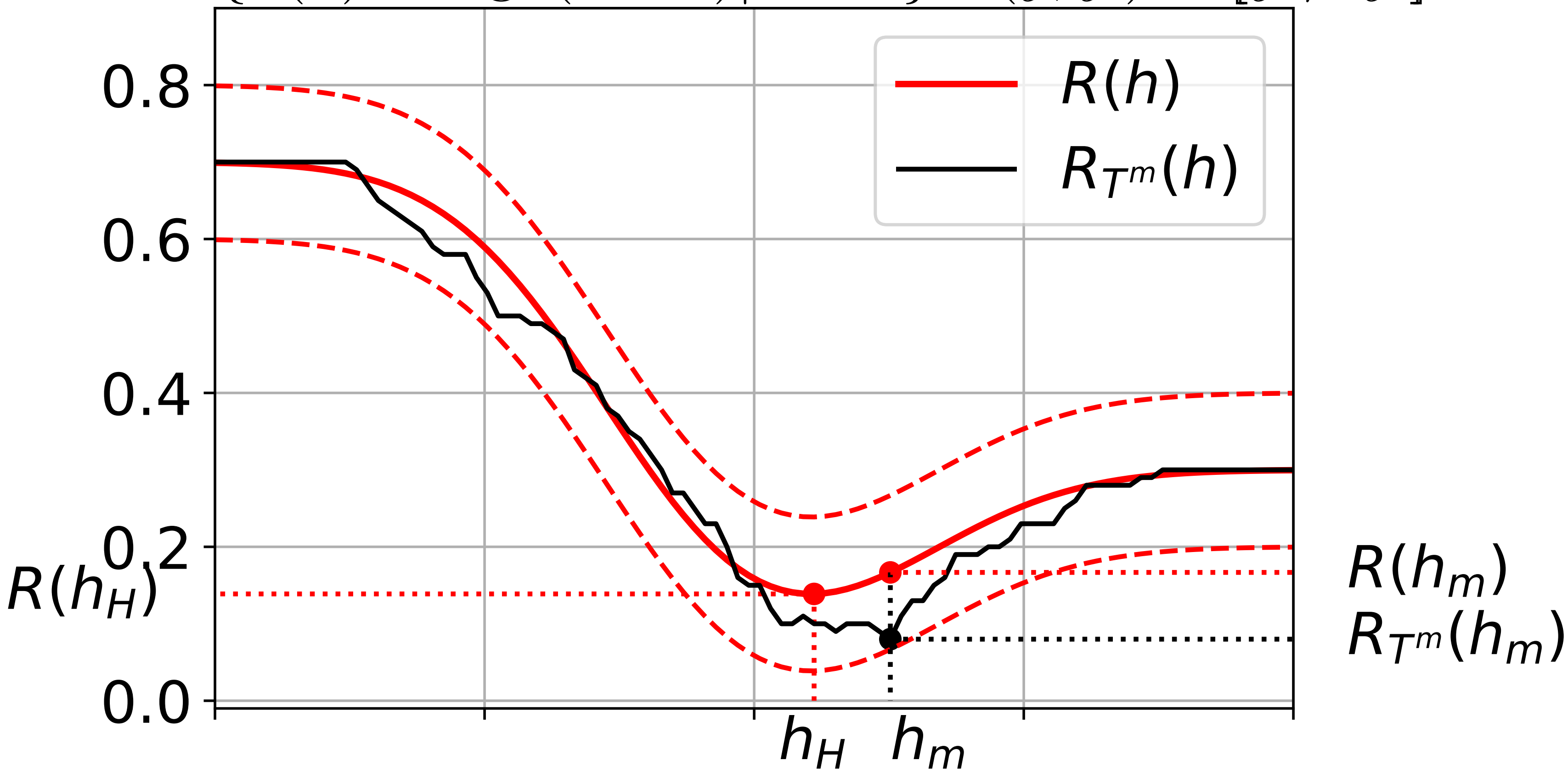

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$$\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} \leq 2 \underbrace{\sup_{h\in\mathcal{H}} \big|R(h) - R_{\mathcal{T}^m}(h)\big|}_{\text{highest generalizaton error}}$$

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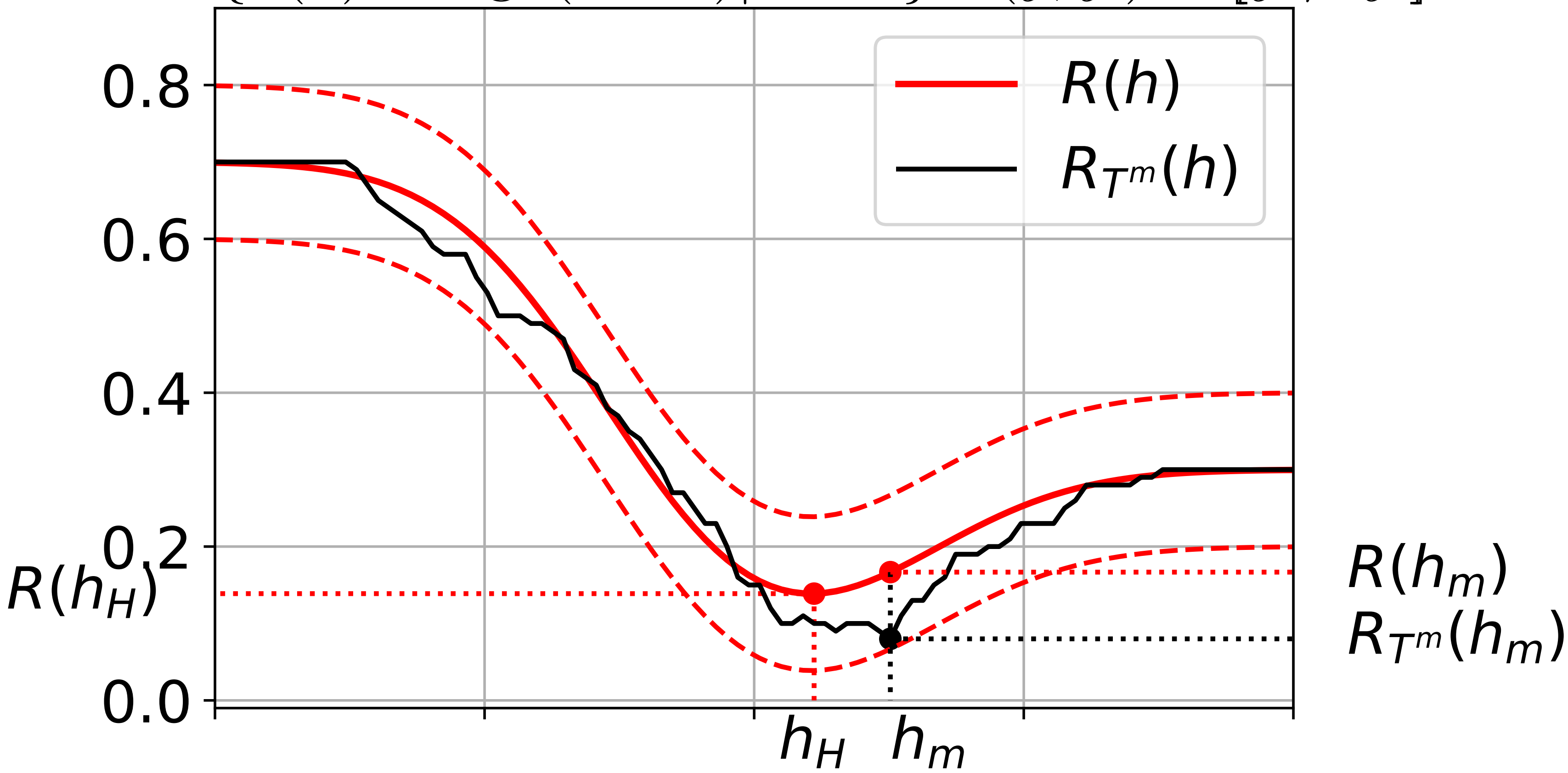

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$$\mathbb{P}\Big(\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} \geq \varepsilon \Big) \leq \mathbb{P}\Big(\underbrace{\sup_{h \in \mathcal{H}} \big| R(h) - R_{\mathcal{T}^m}(h) \big| \geq \tfrac{\varepsilon}{2}}_{\text{highest generalizaton error}} \Big)$$

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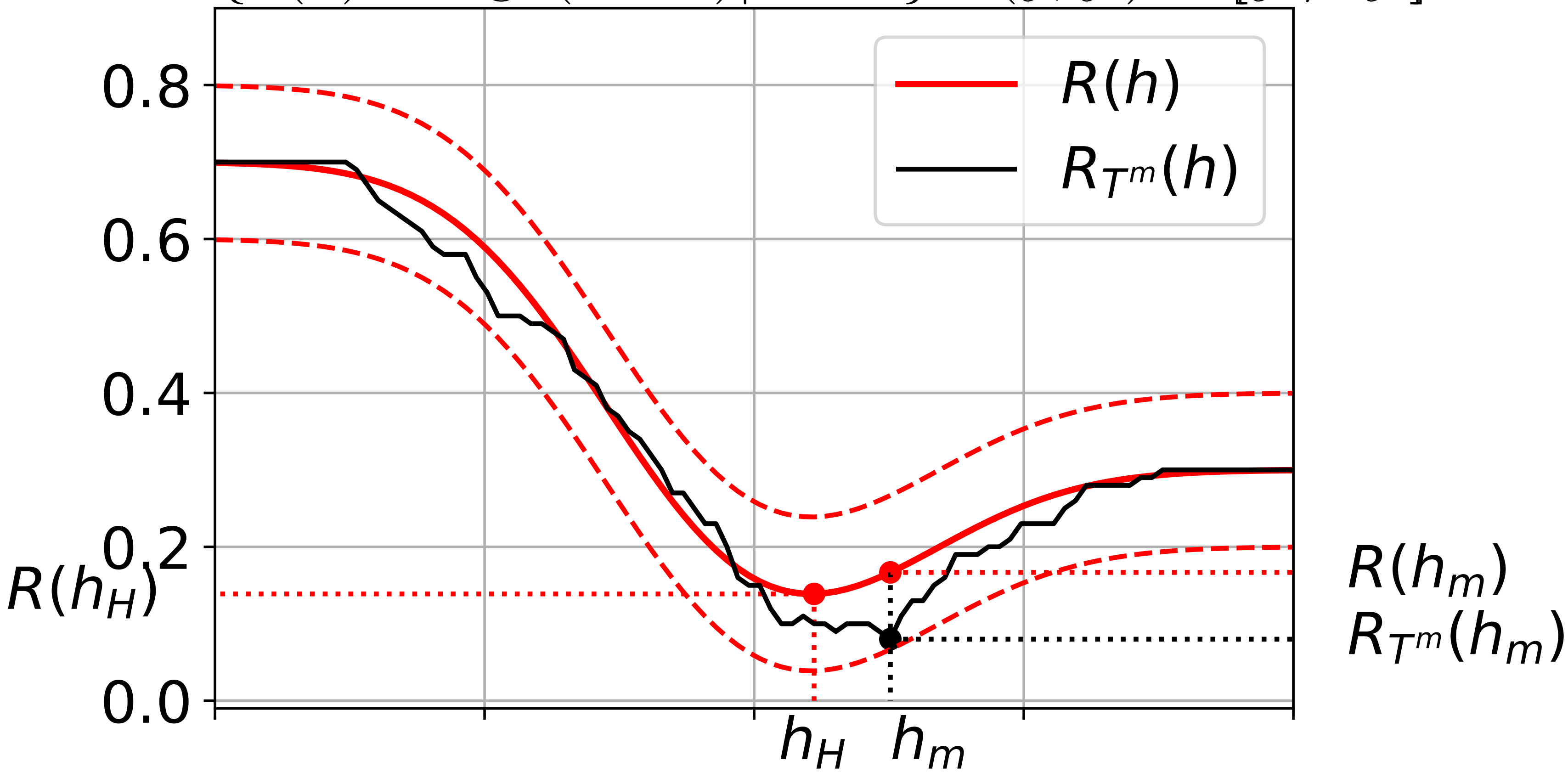

Theorem: ULLN implies consistency of ERM

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

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

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

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

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

Finite sample bound on the estimation error

- Let $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ be the hypothesis class with the best predictor

$$h_{\mathcal{H}} \in \operatorname*{Argmin}_{h \in \mathcal{H}} R(h)$$

- We learn h_m from $\mathcal{T}^m \sim p(x, y)$ with the ERM algorithm

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

- Assume we have for $\mathcal{H}$ the uniform bound on the generalization error

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

- Then, for any $\varepsilon > 0$ the inequality

$$R(h_m) \leq R(h_{\mathcal{H}}) + \varepsilon$$

holds with the probability $1 - B(m, \mathcal{H}, \varepsilon/2)$ at least.

Excess error = Estimation error + Approximation errors

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The characters of the play:

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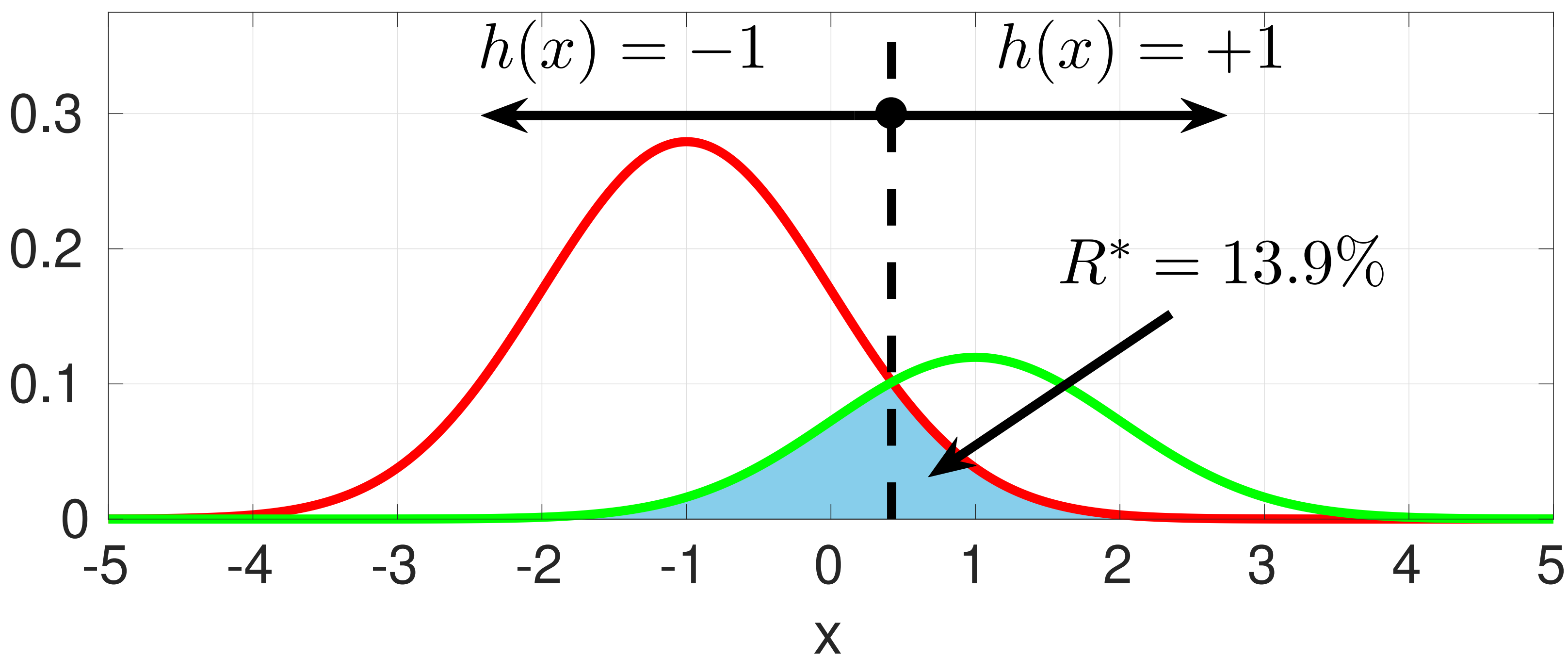

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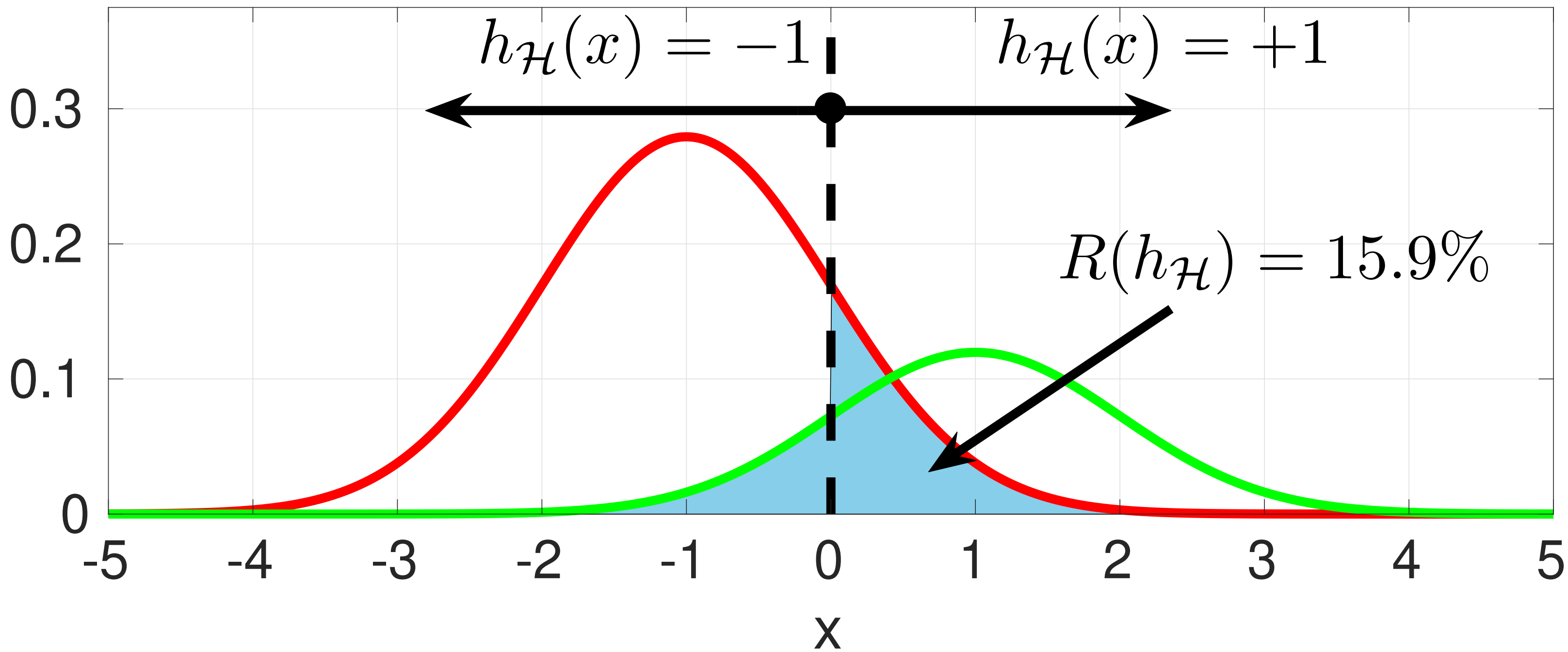

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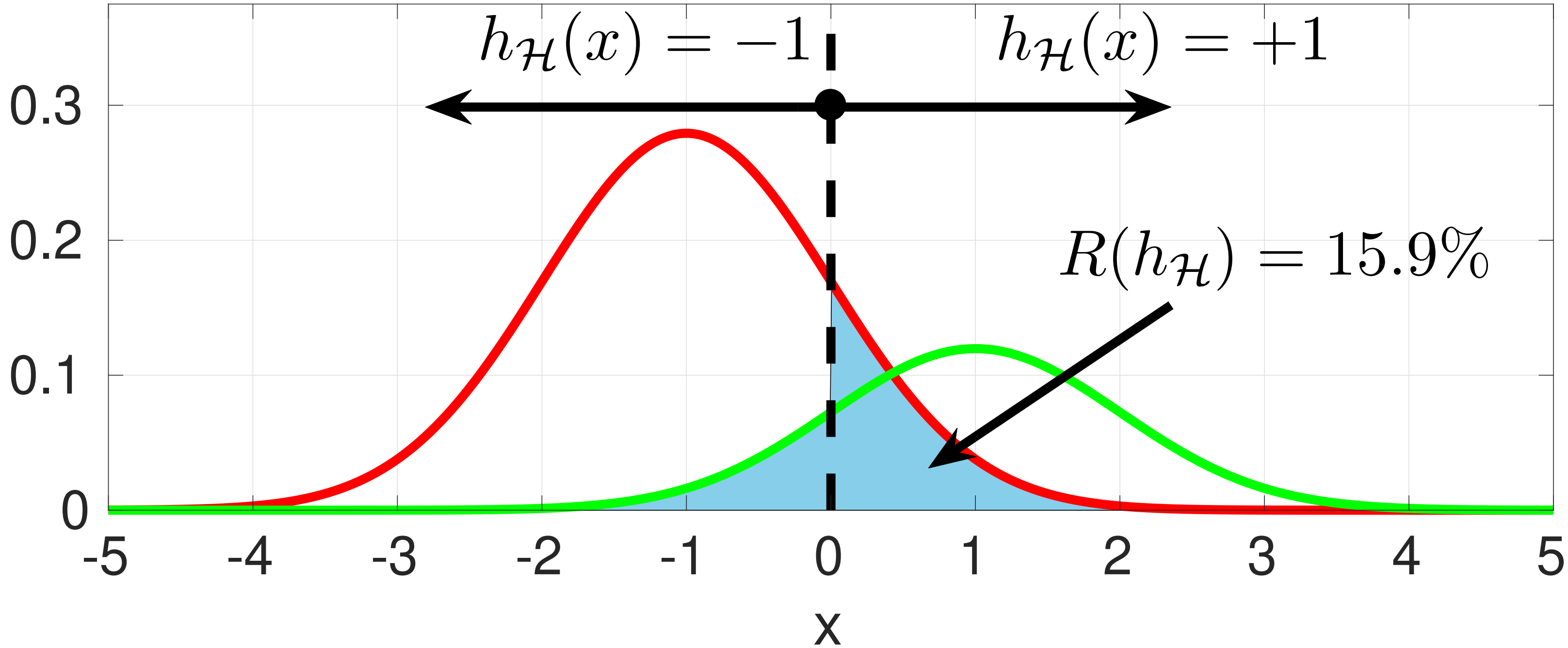
approximation error: $R(h_\mathcal{H}) - R^* = 15.9 - 13.9 = 2.0\%$



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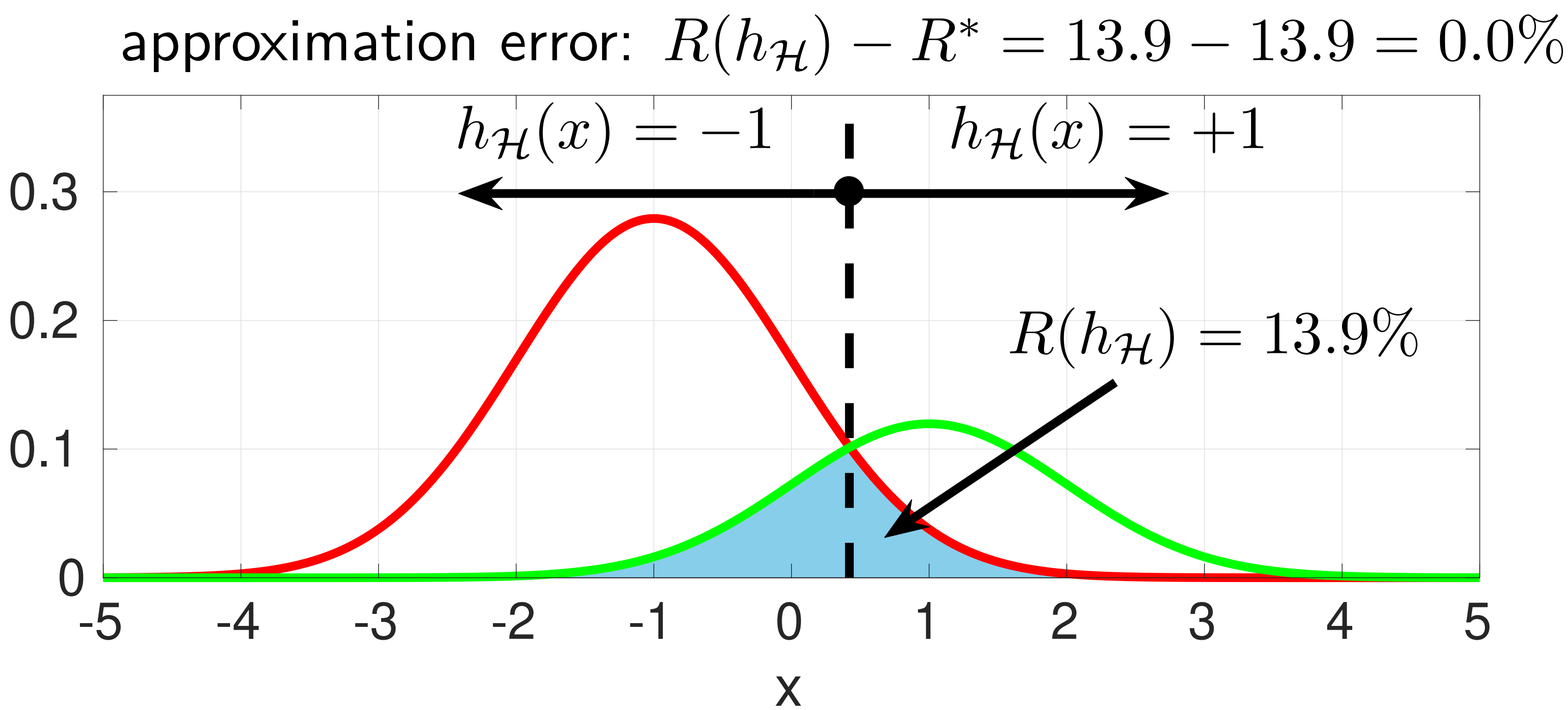

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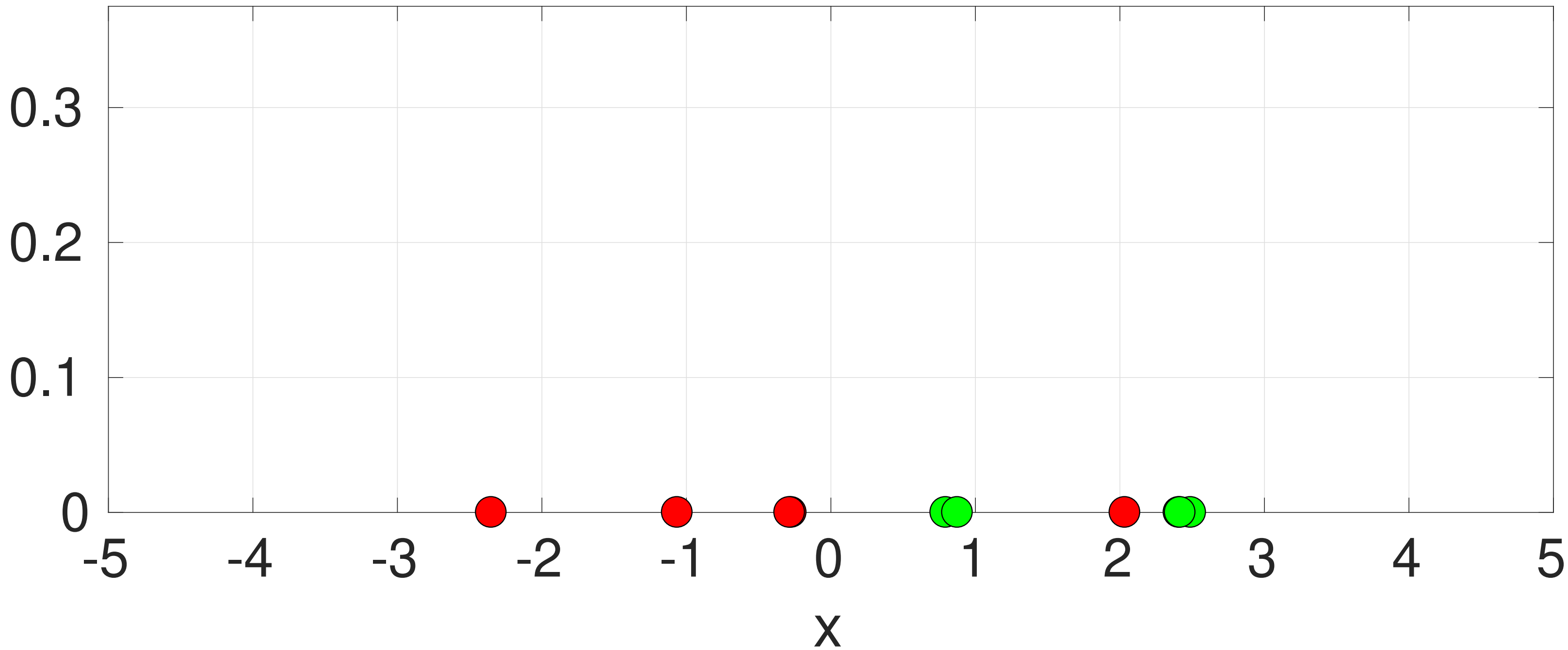

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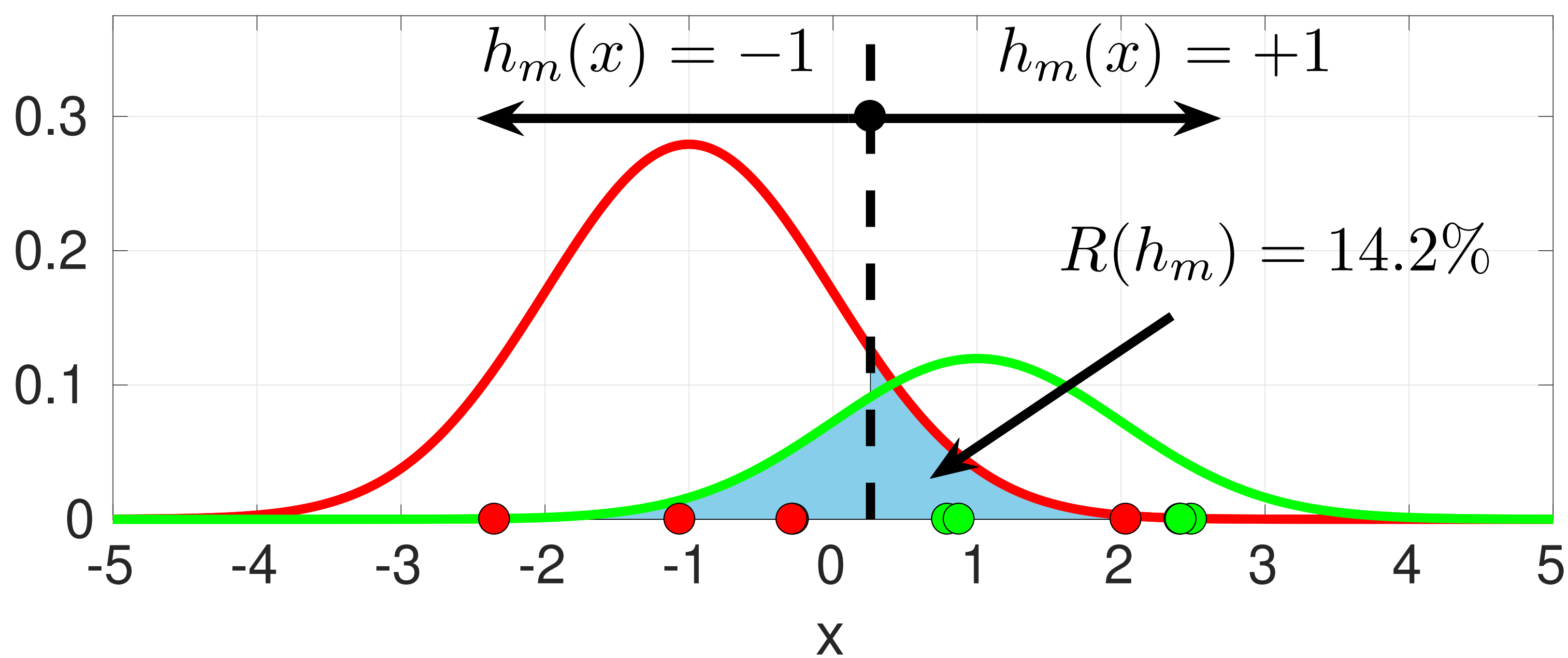

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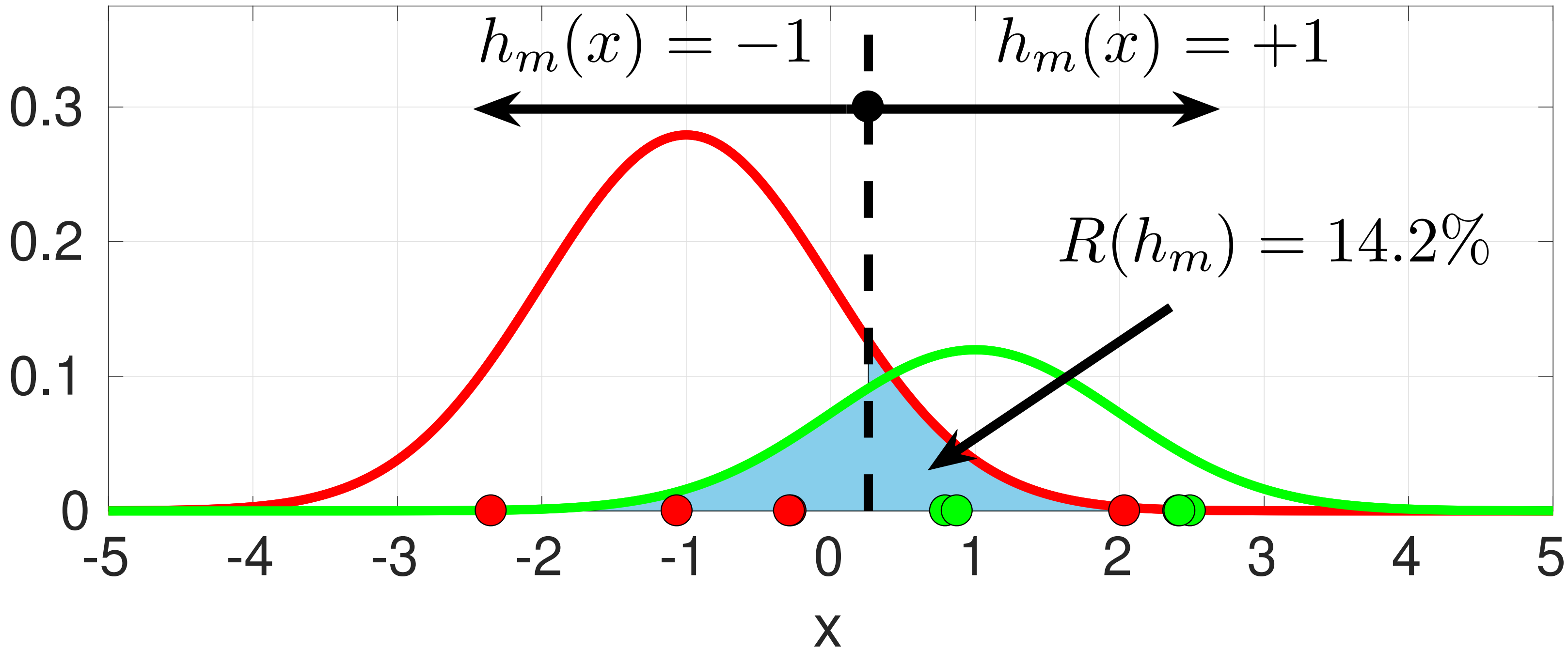
estimation error: $R(h_m) - R(h_\mathcal{H}) = 14.2 - 13.9 = 0.3\%$



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- $R(h_m)$ risk of $h_m = A(\mathcal{T}_m)$ learned from $\mathcal{T}^m$

Excess error: the quantity we want to minimize

$$\underbrace{\left(R(h_m) - R^*\right)}_{\text{excess error}} = \underbrace{\left(R(h_m) - R(h_\mathcal{H})\right)}_{\text{estimation error}} + \underbrace{\left(R(h_\mathcal{H}) - R^*\right)}_{\text{approximation error}}$$

Excess error = Estimation error + Approximation errors

The characters of the play:

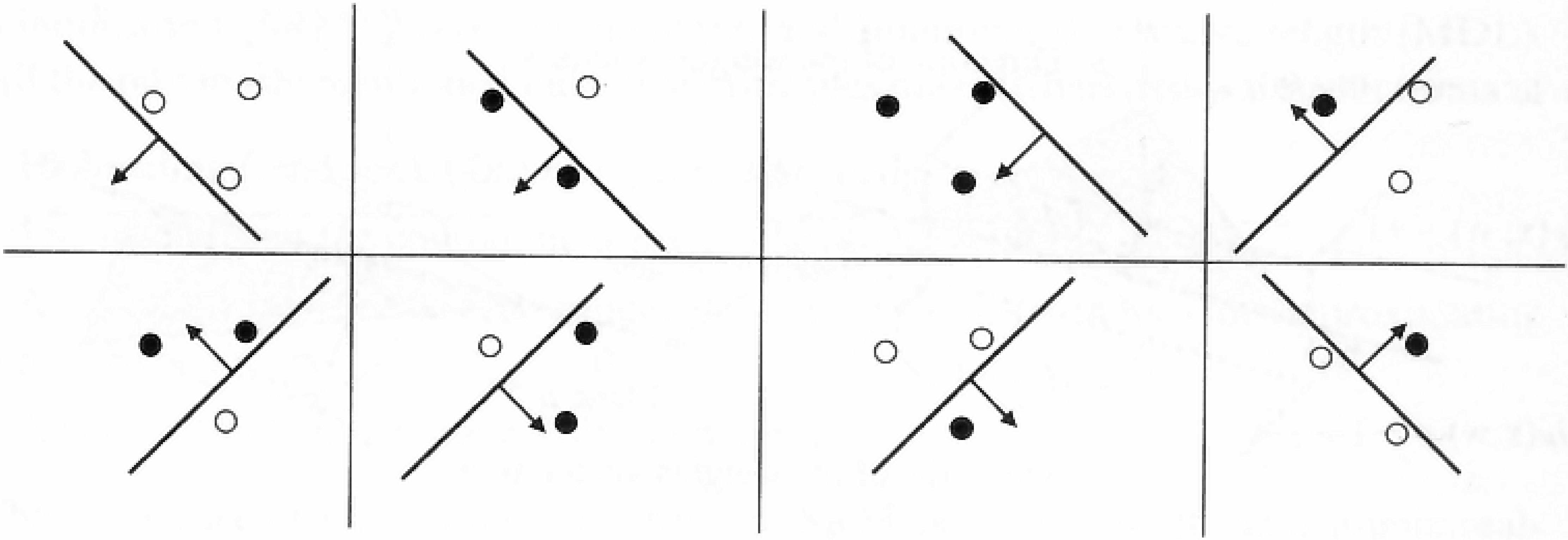
- $R^* = \inf_{h \in \mathcal{Y}^\mathcal{X}} R(h)$ best attainable true risk
- $R(h_\mathcal{H})$ best risk in $\mathcal{H}$ where $h_\mathcal{H} \in \mathrm{Argmin}_{h \in \mathcal{H}} R(h)$
- $R(h_m)$ risk of $h_m = A(\mathcal{T}_m)$ learned from $\mathcal{T}^m$

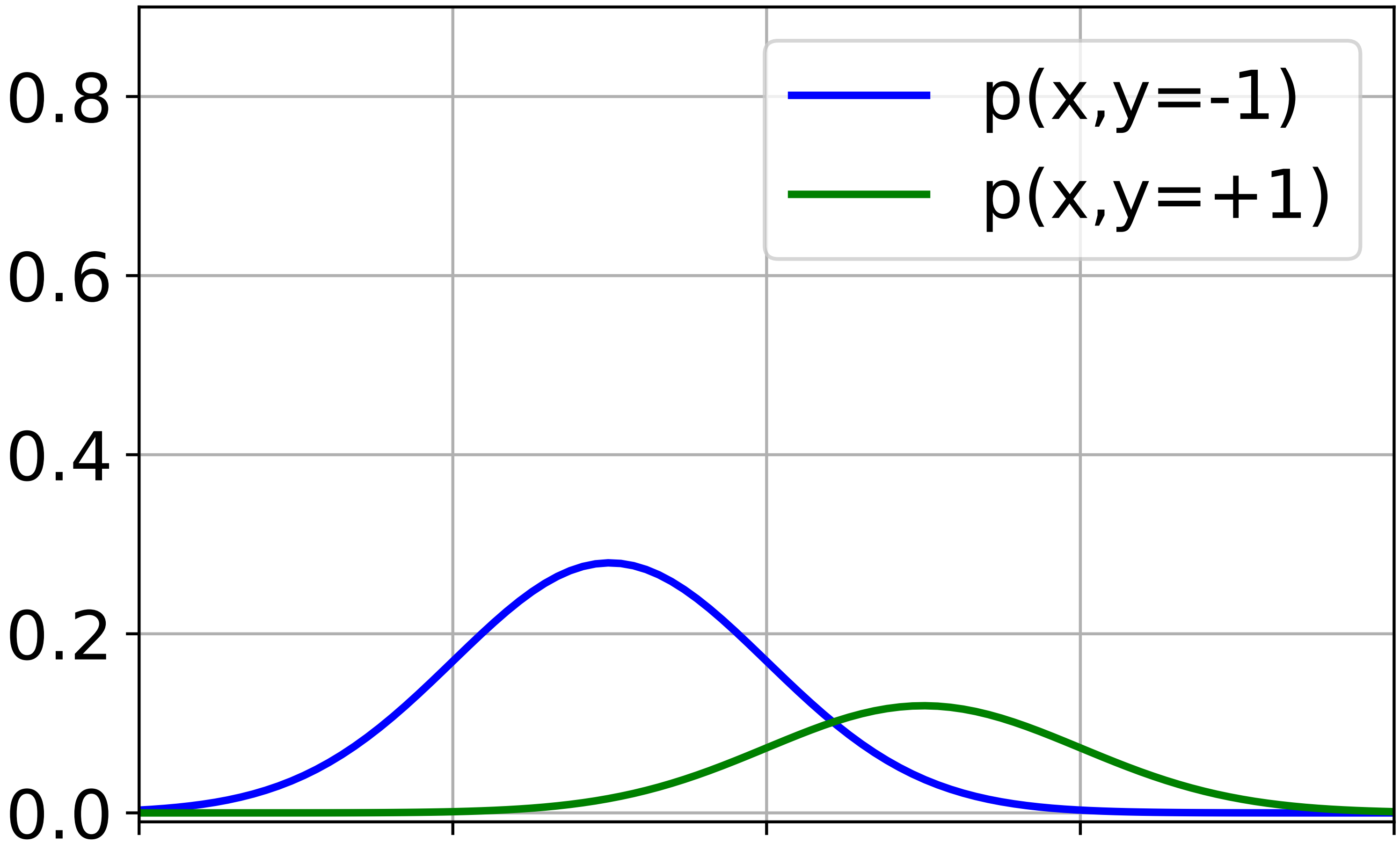
Excess error: the quantity we want to minimize

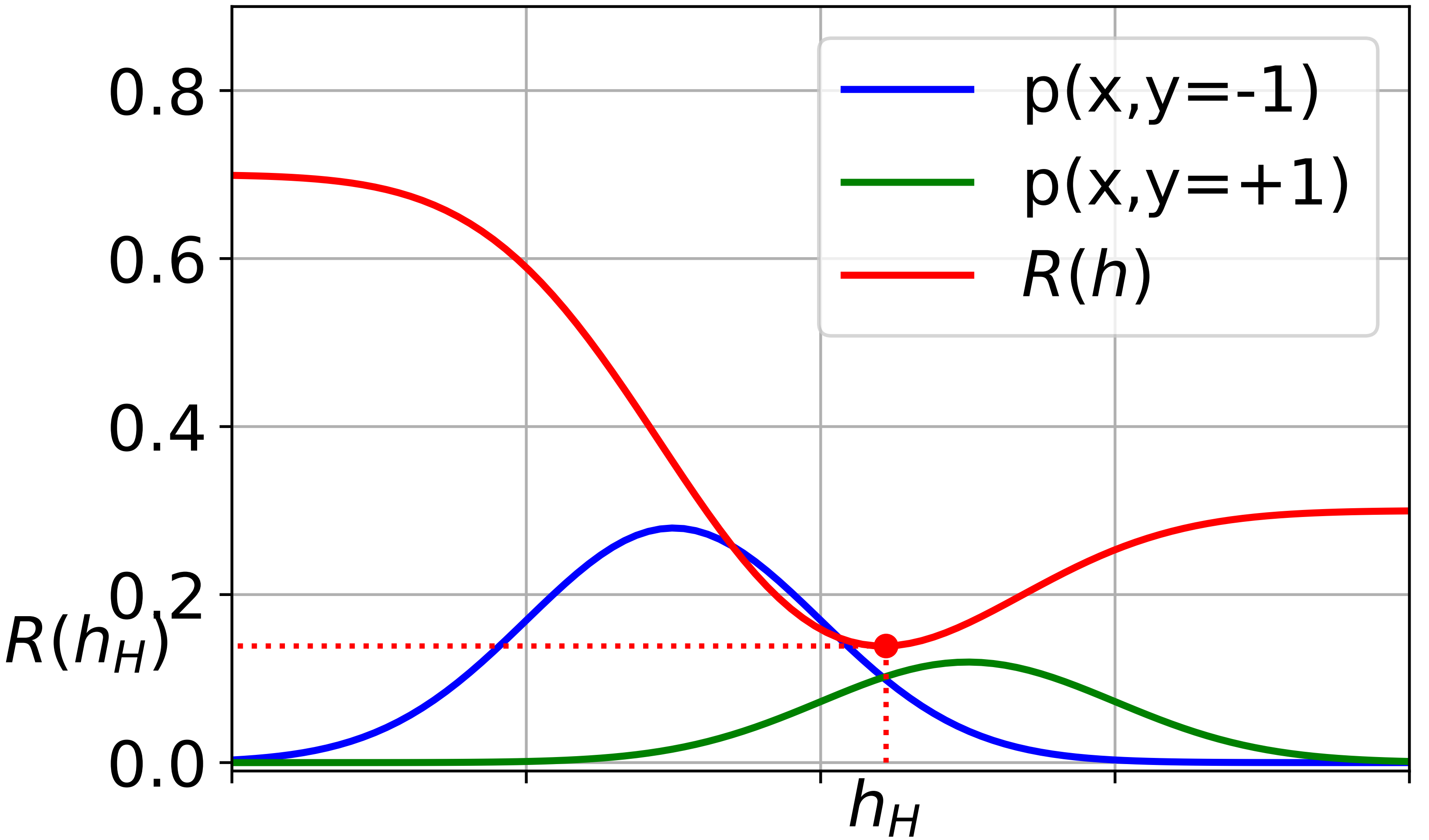
$$\underbrace{\left(R(h_m) - R^*\right)}_{\text{excess error}} = \underbrace{\left(R(h_m) - R(h_\mathcal{H})\right)}_{\text{estimation error}} + \underbrace{\left(R(h_\mathcal{H}) - R^*\right)}_{\text{approximation error}}$$

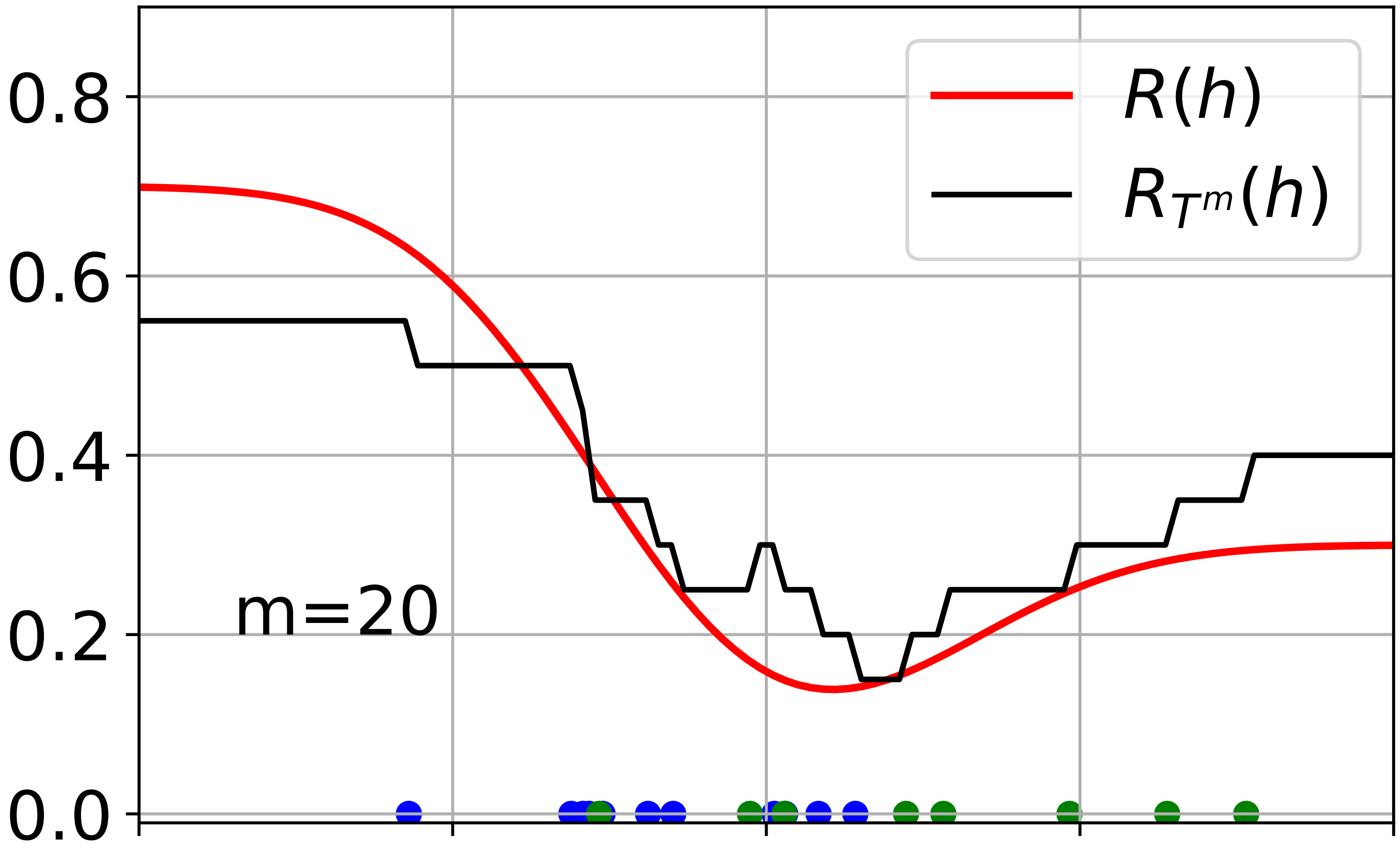
Questions:

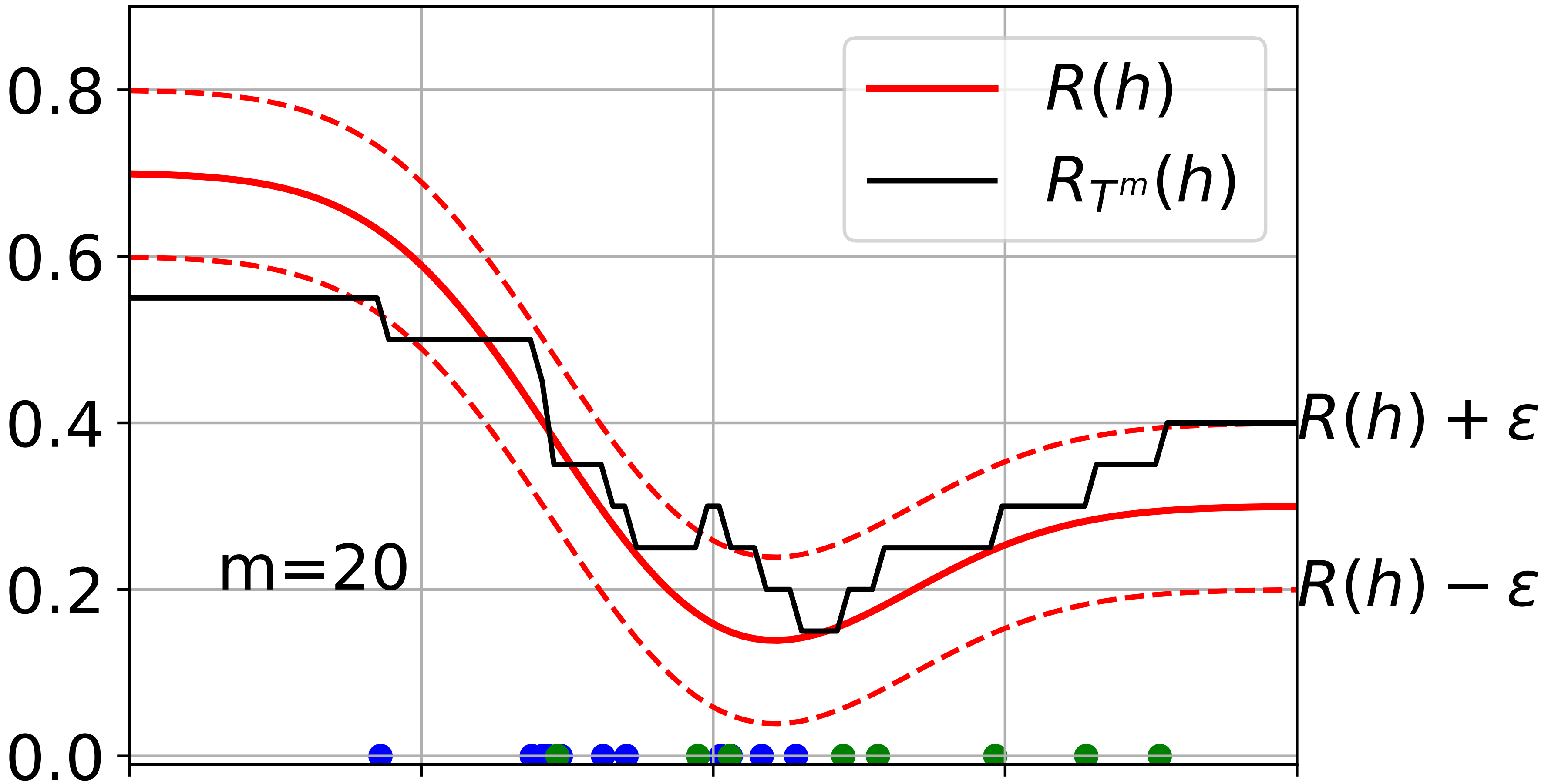
- What causes individual errors ?
- How do the errors depend on $\mathcal{H}$ and m?



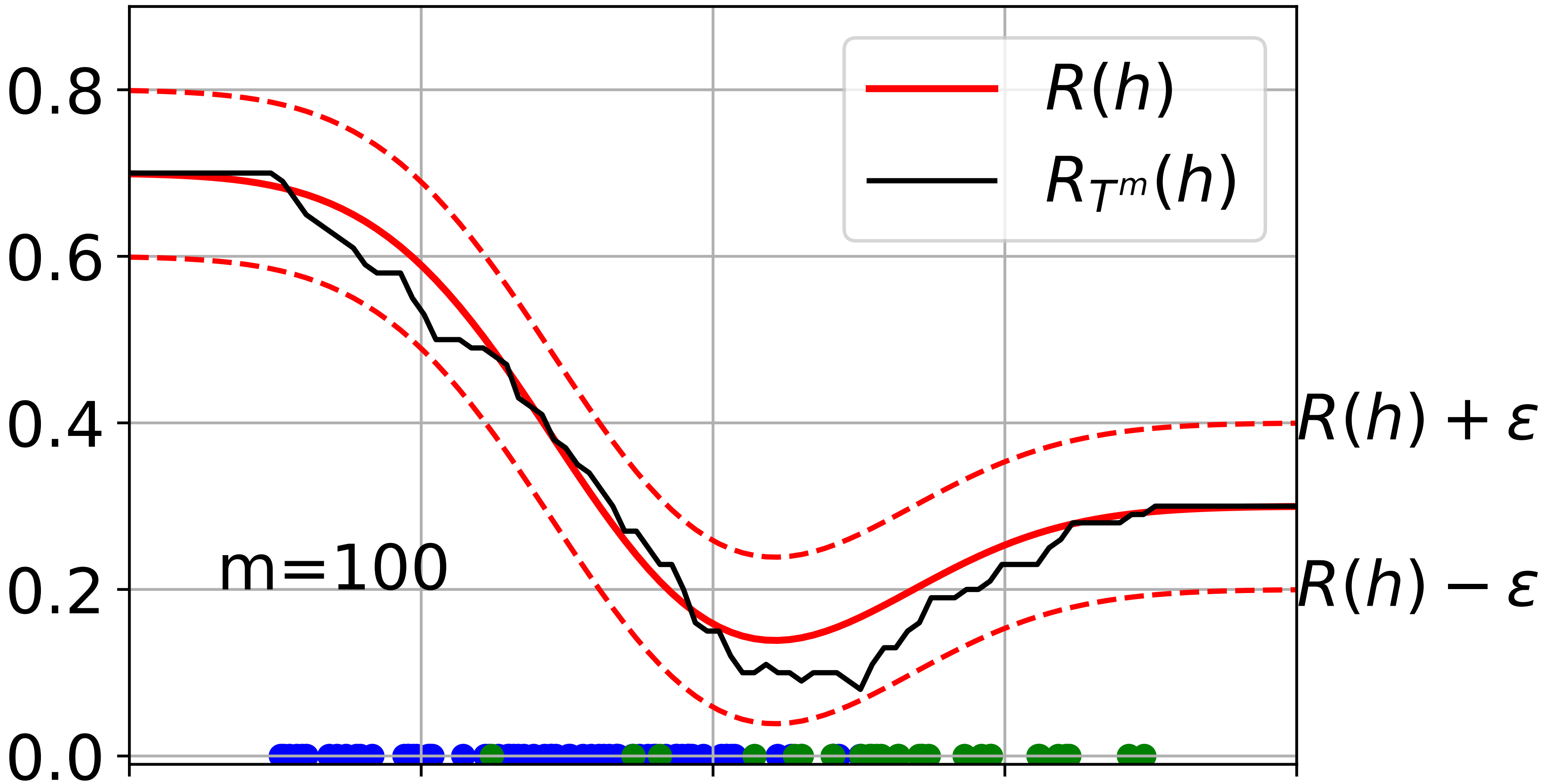

0.8
0.6
0.4
0.2
0.0
p(x,y=-1)
p(x,y=+1)


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

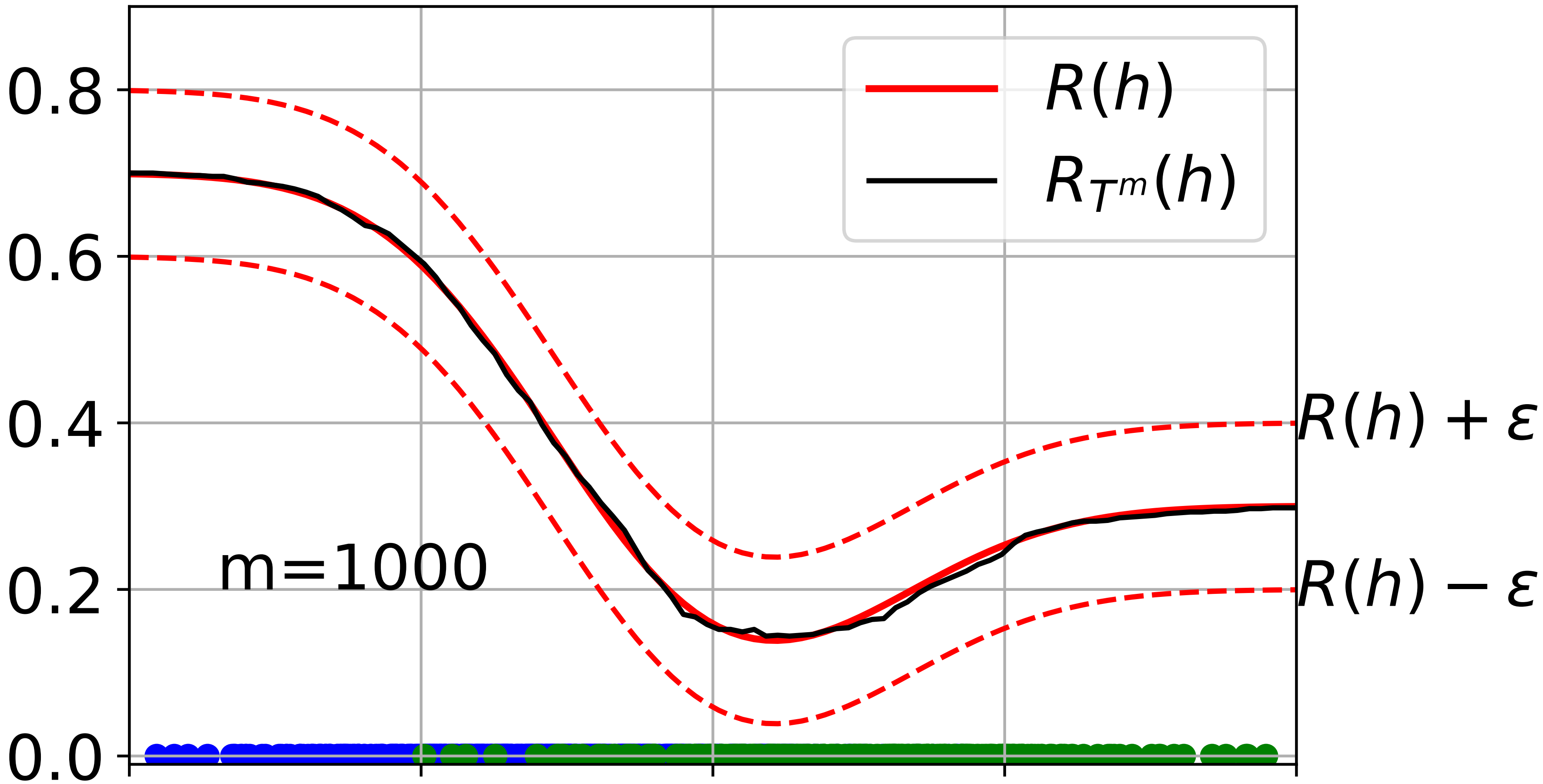

R(h)
R_{T^m}(h)
m=20
0.8
0.6
0.4
0.2
0.0



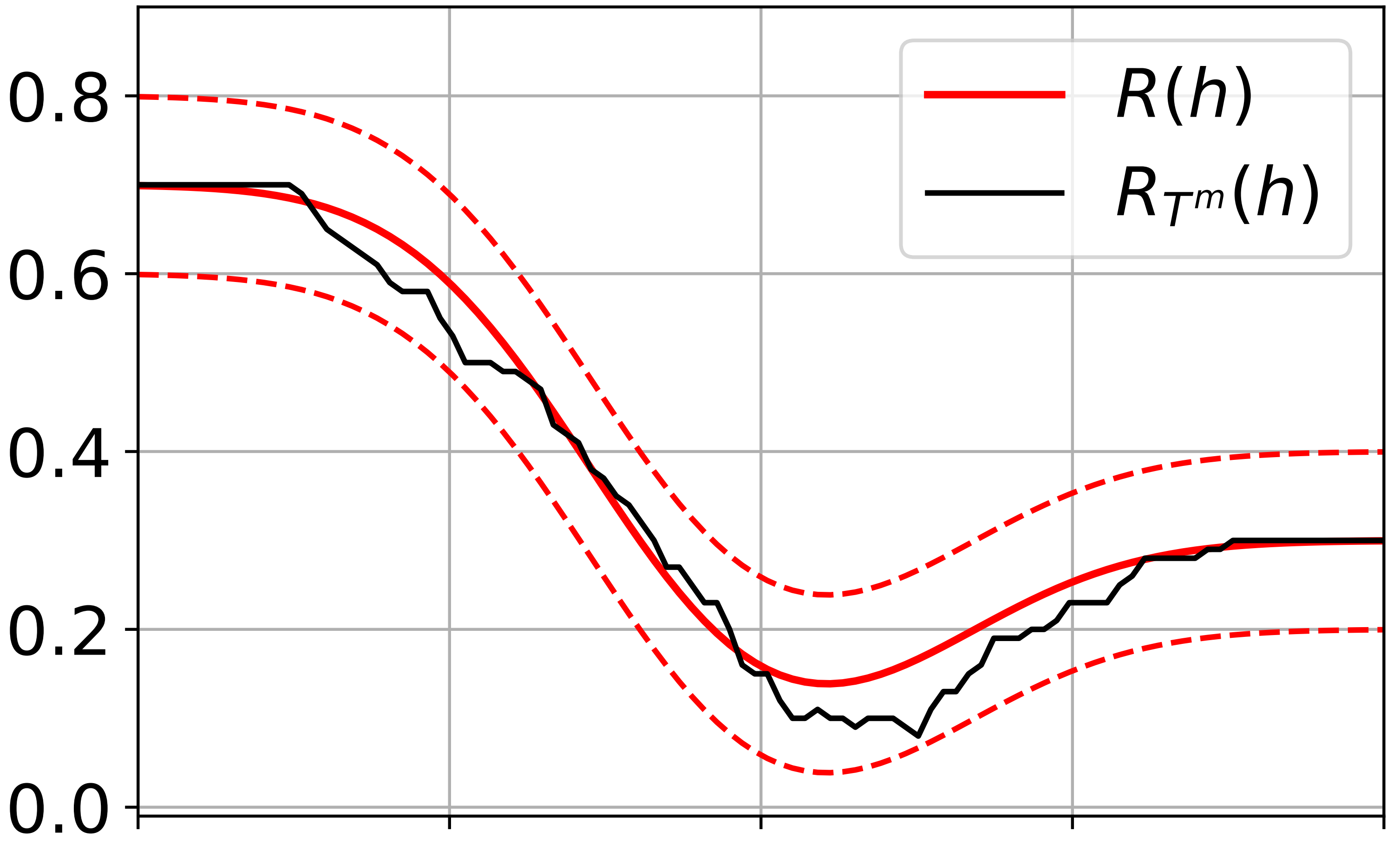
0.8
0.6
0.4
0.2
0.0
R(h)
$R_{T^m}(h)$
m=20
$R(h) + \varepsilon$
$R(h) - \varepsilon$



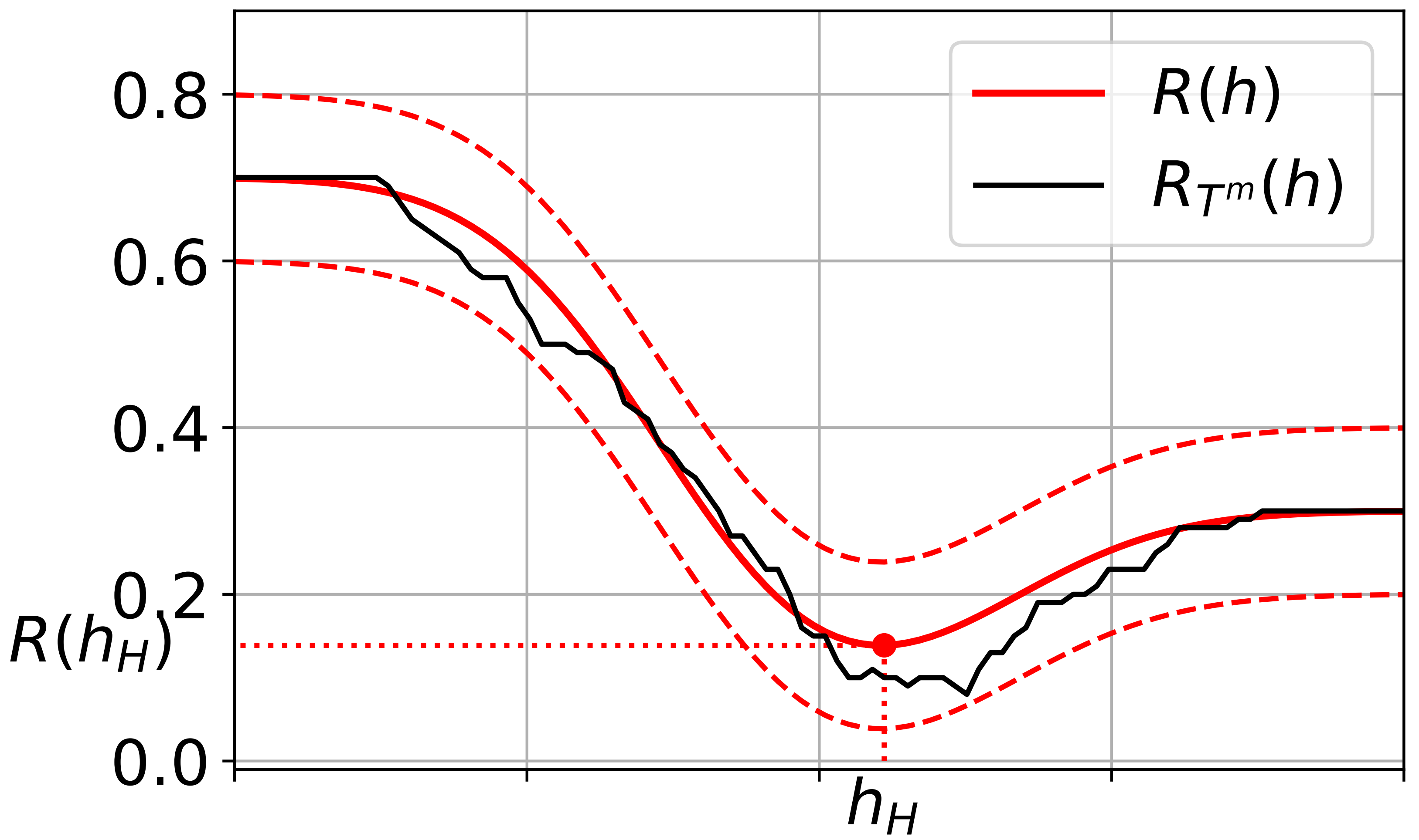
0.8
0.6
0.4
0.2
0.0
$R(h)$
$R_{T^m}(h)$
$R(h) + \varepsilon$
$R(h) - \varepsilon$
m=100



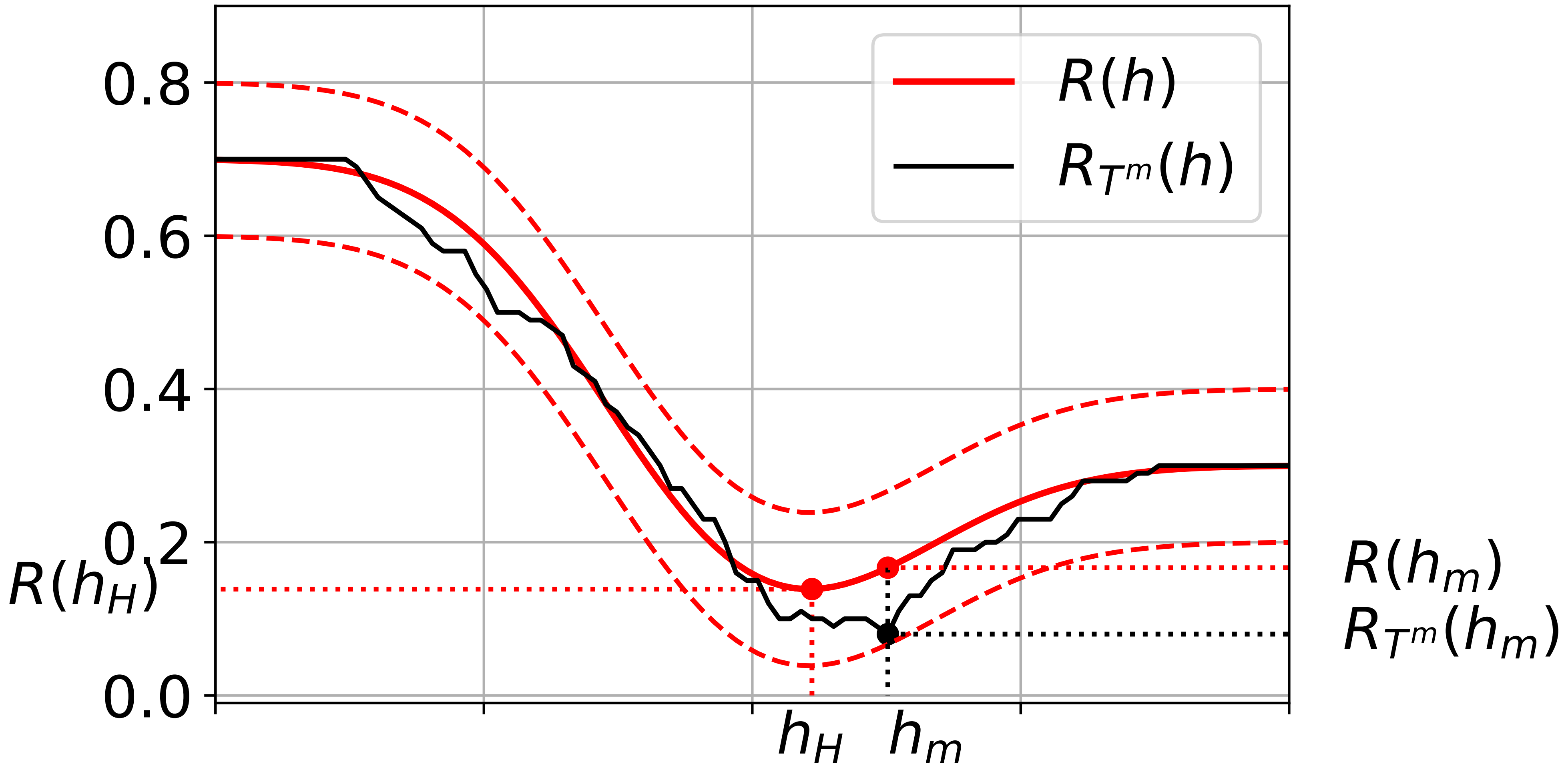
0.8
0.6
0.4
0.2
0.0
$R(h)$
$R_{T^m}(h)$
$R(h)+\varepsilon$
$R(h)-\varepsilon$
m=1000



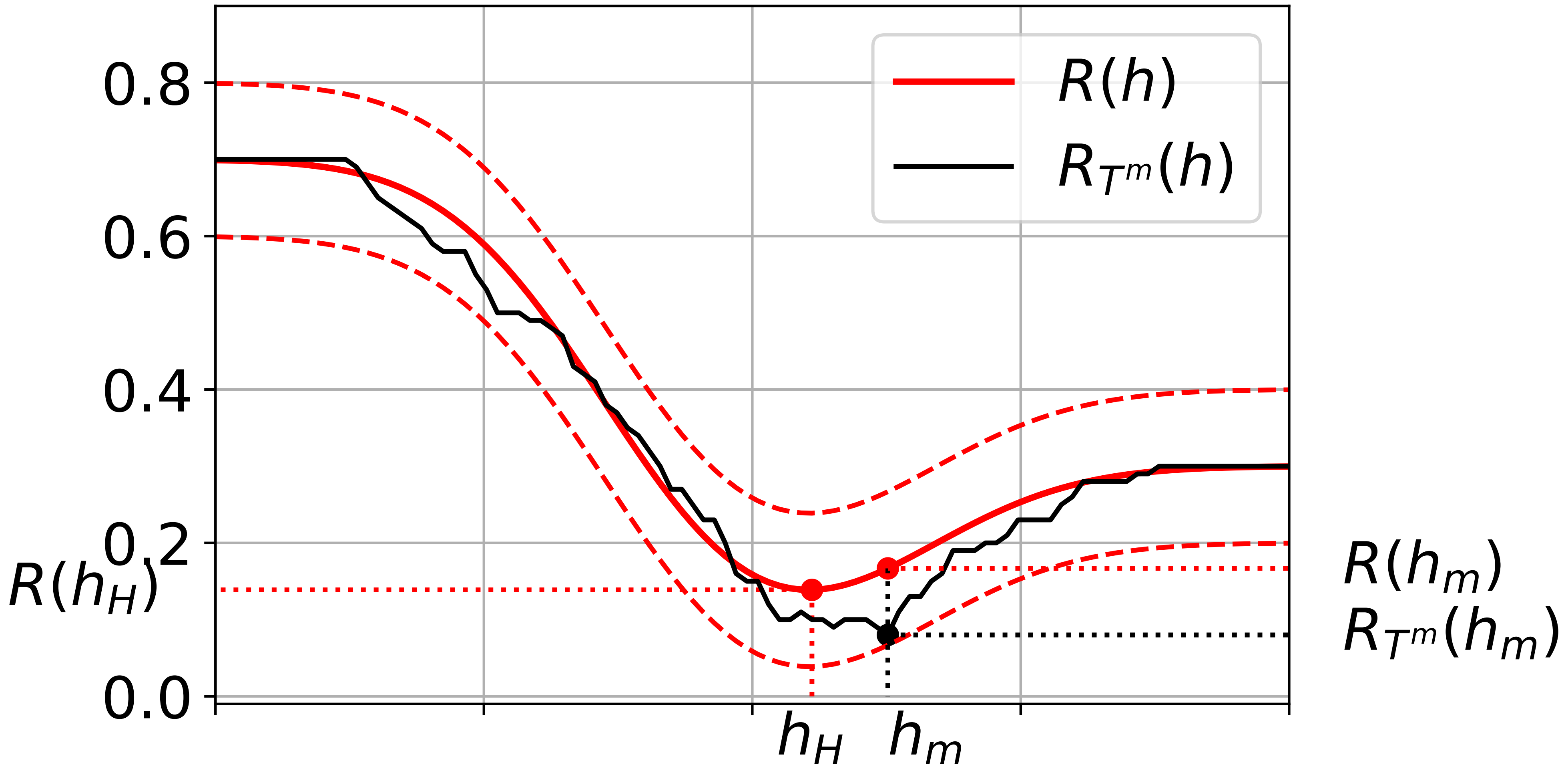
0.8
0.6
0.4
0.2
0.0
$R(h)$
$R_{T^m}(h)$

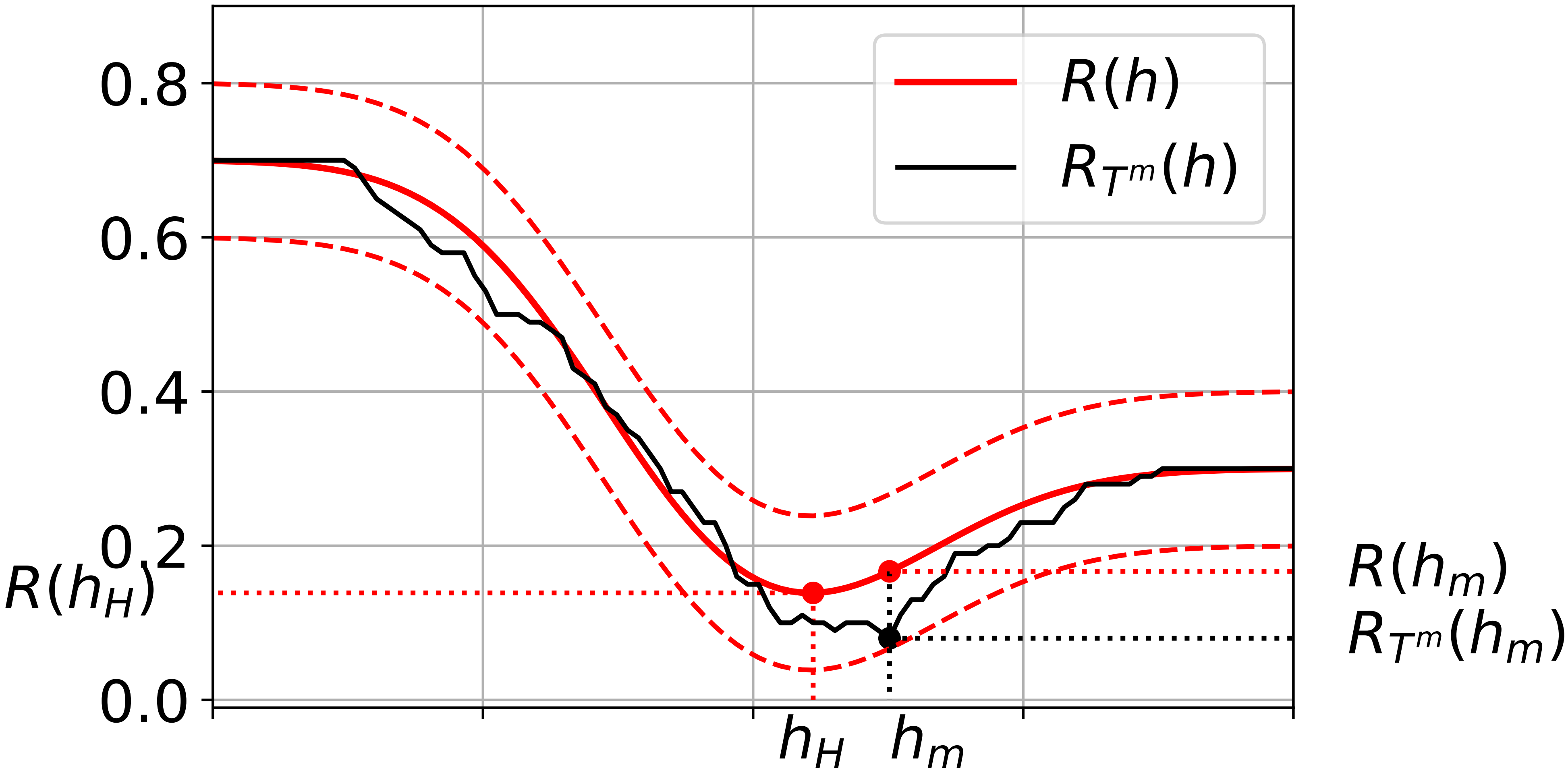


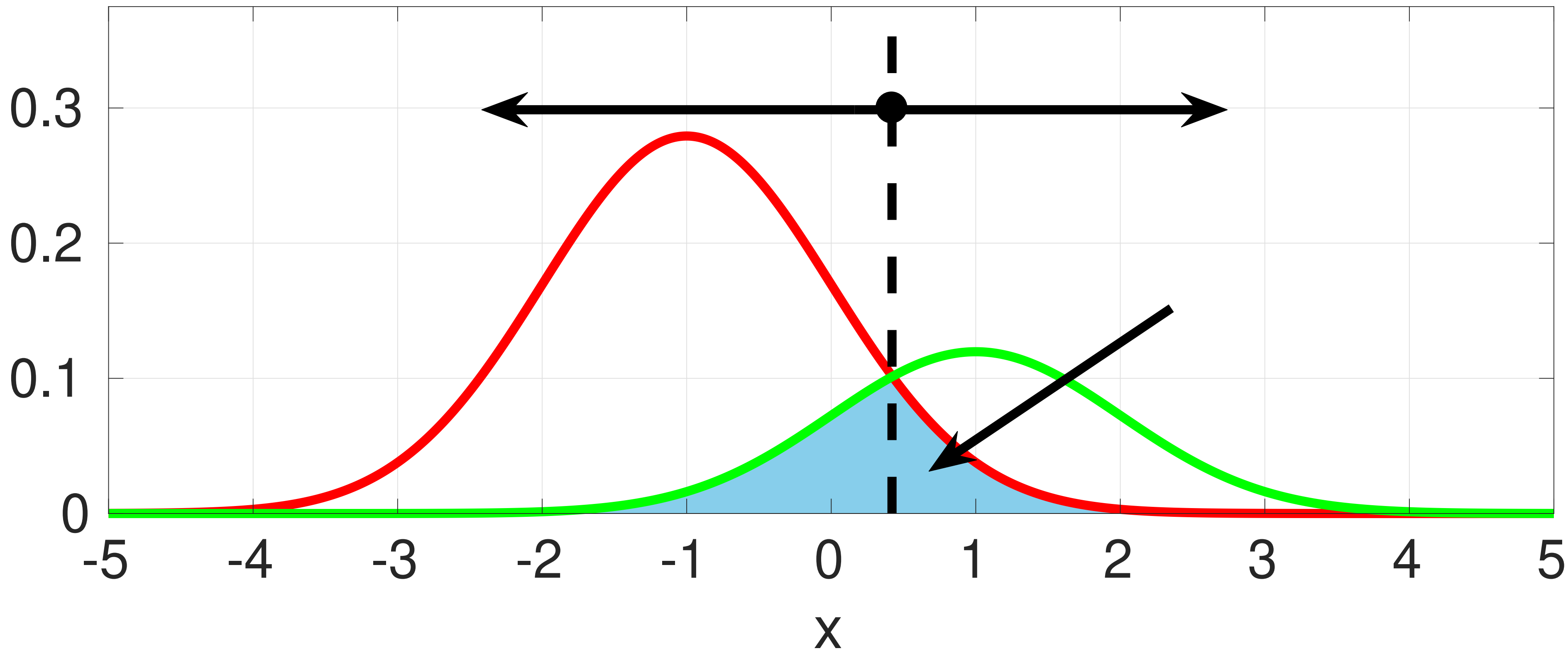
0.8
0.6
0.4
0.2
0.0
$R(h_H)$
h_H
$R(h)$
$R_{T^m}(h)$



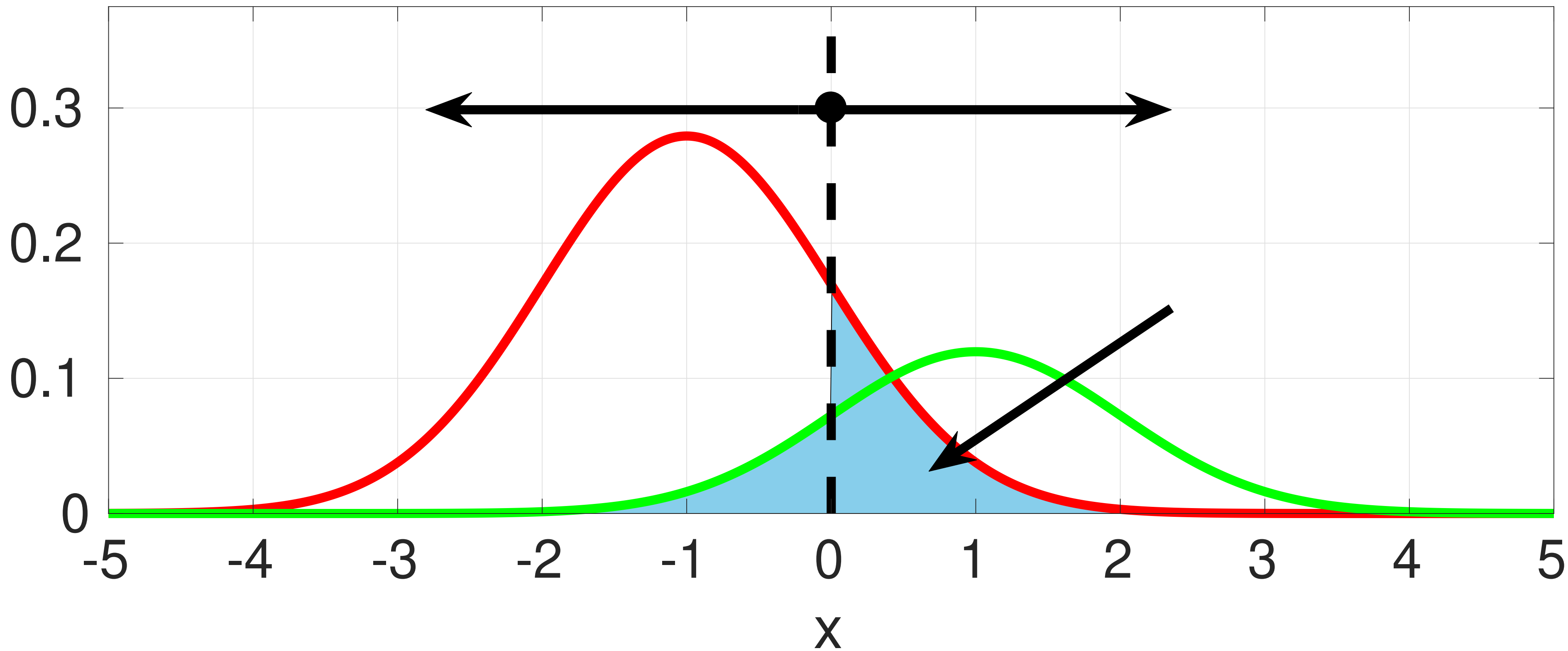
0.8
0.6
0.4
0.2
0.0
R(h)
$R_{T^m}(h)$
$R(h_H)$
$R(h_m)$
$R_{T^m}(h_m)$
h_H
h_m


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

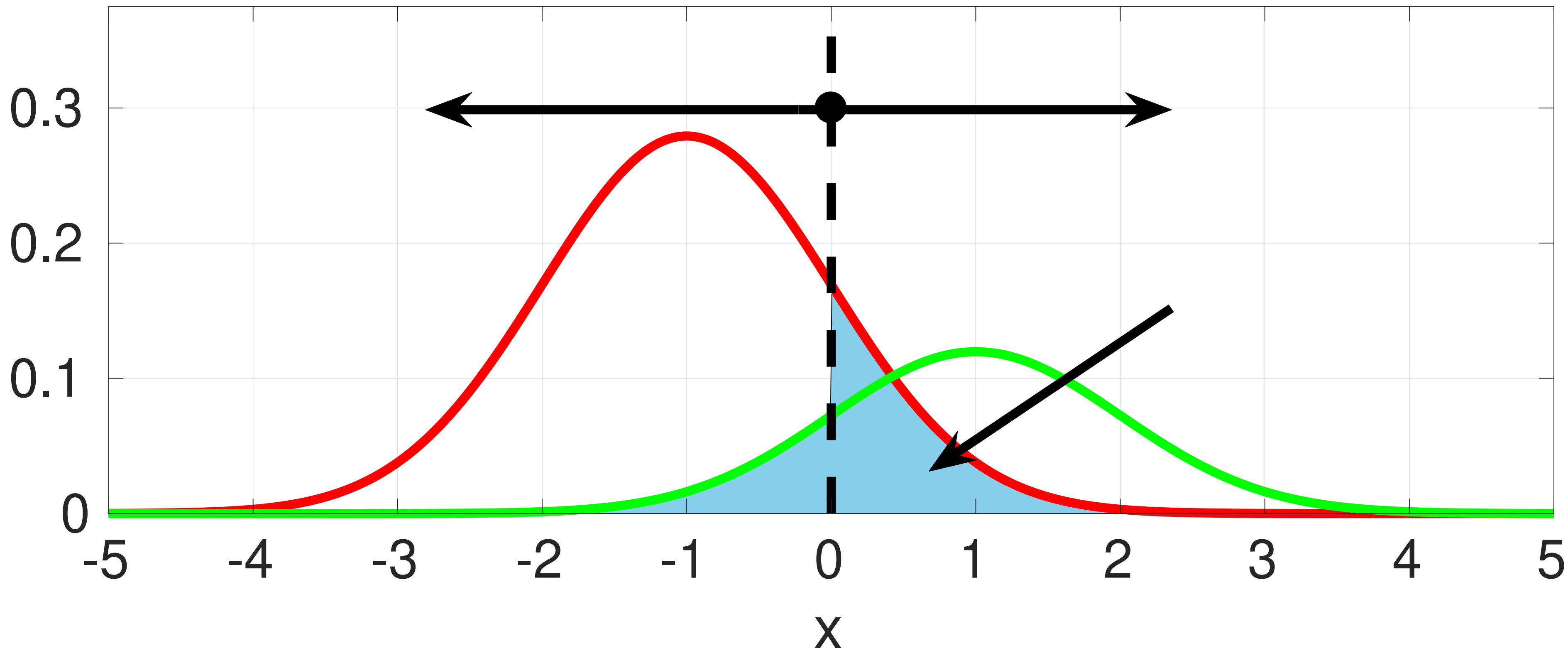

0.8
0.6
0.4
0.2
0.0
$R(h)$
$R_{T^m}(h)$
$R(h_H)$
$R(h_m)$
$R_{T^m}(h_m)$
h_H
h_m

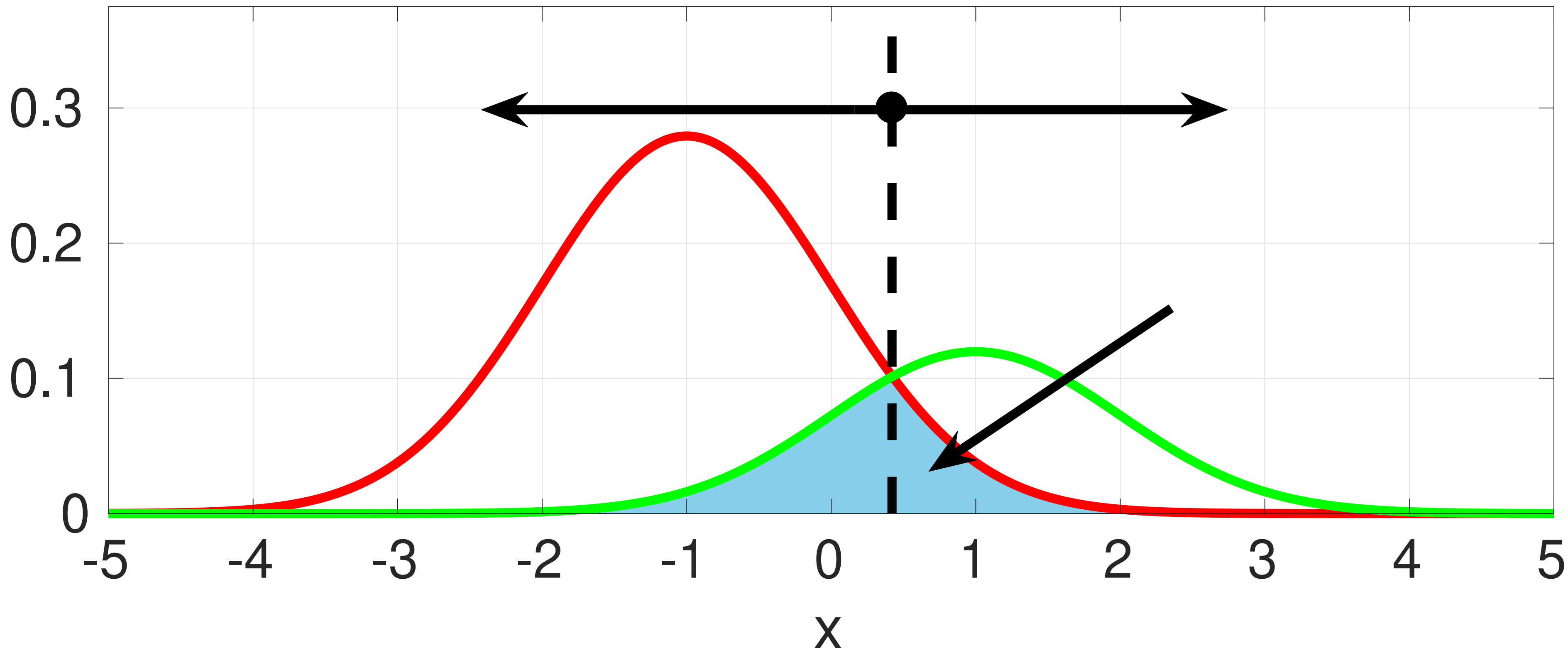


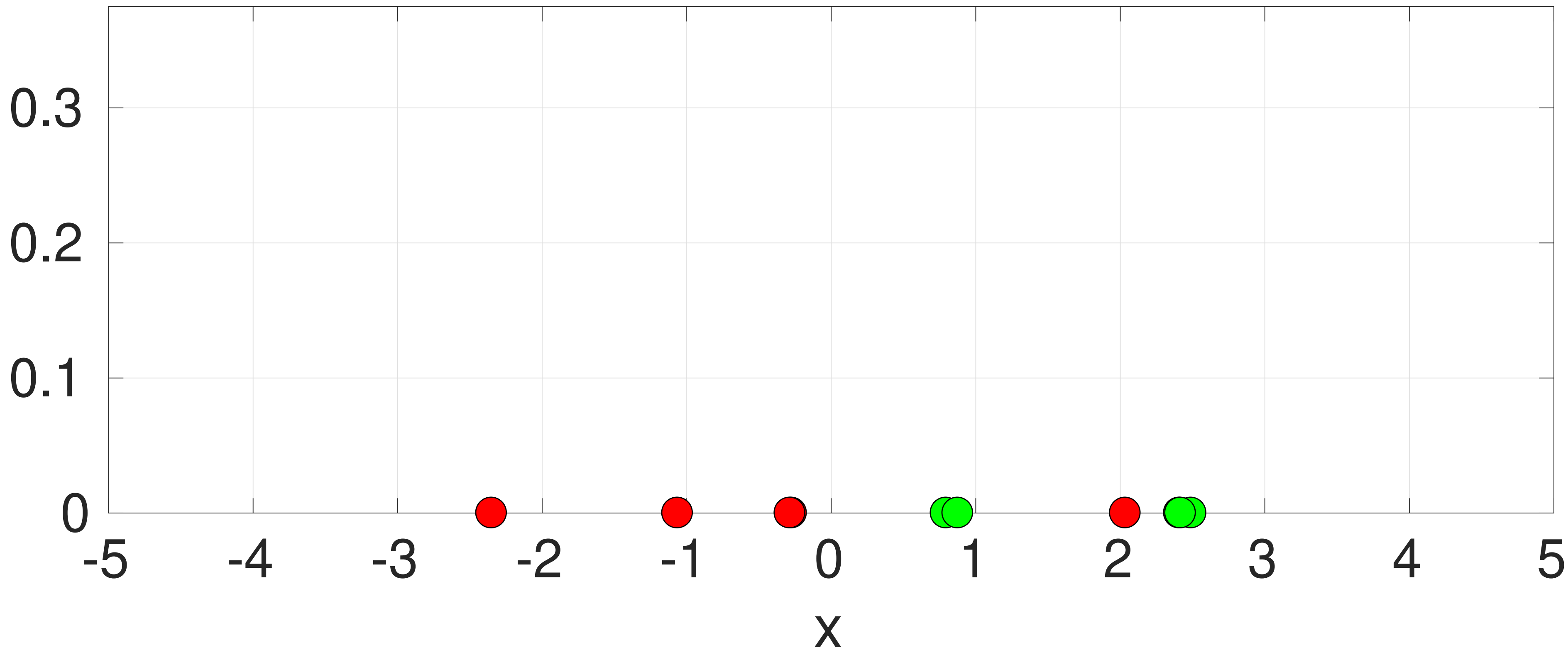
0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x

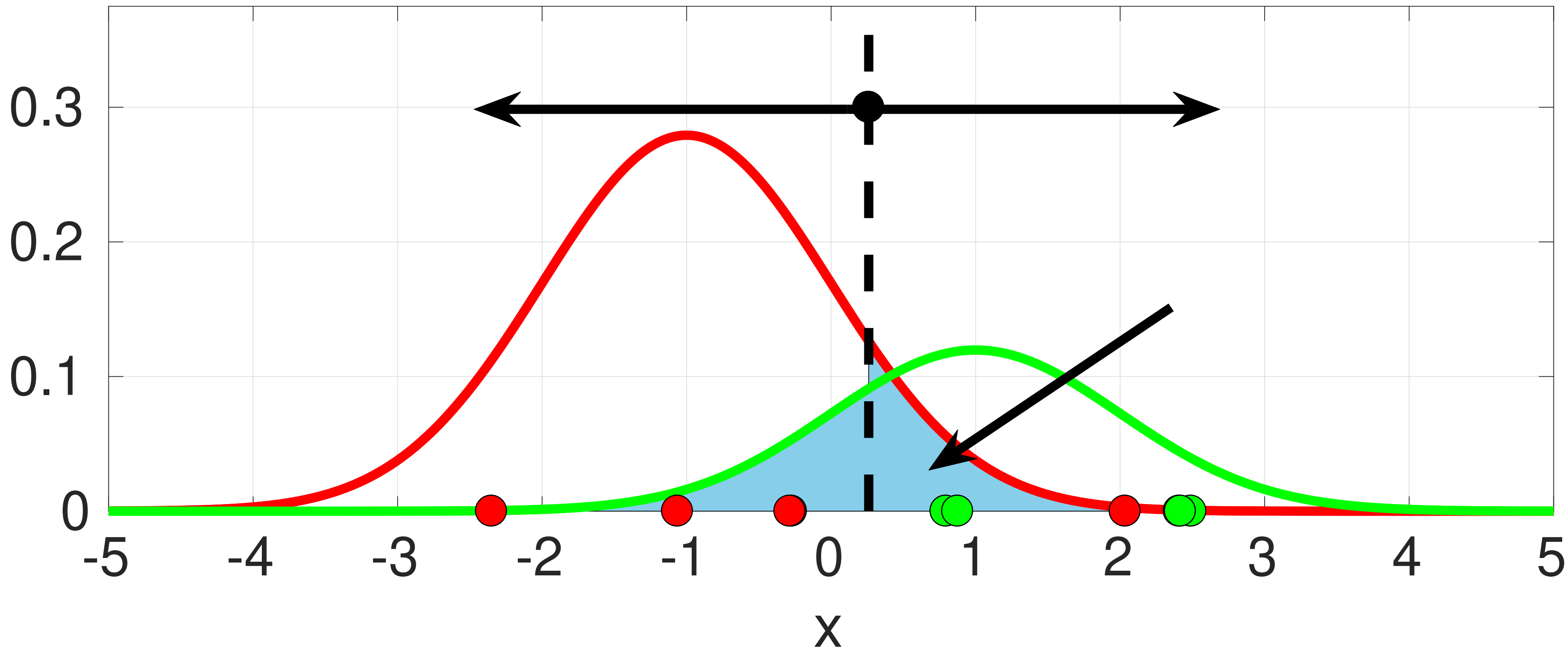


0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x

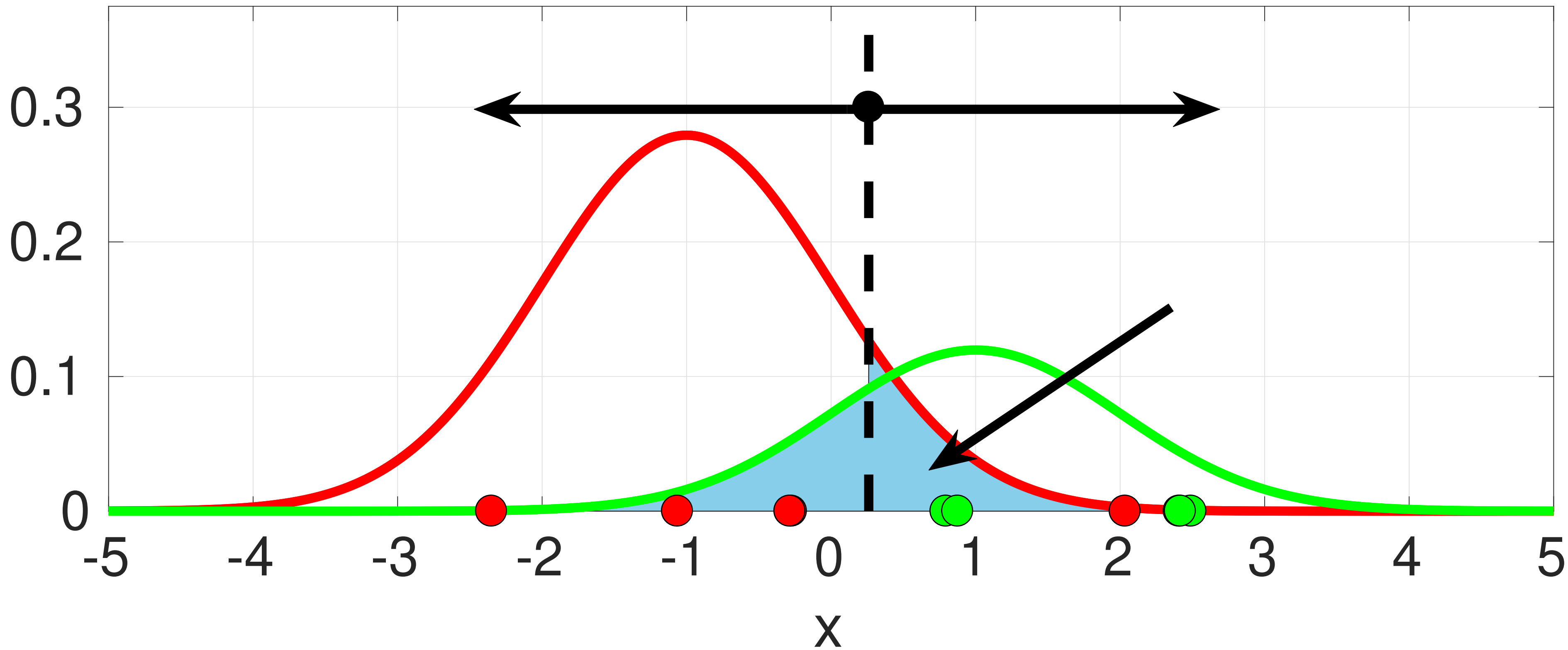

0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x


0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x


0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x



0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x


0.3
0.2
0.1
0
-5
-4
-3
-2
-1
0
1
2
3
4
5
x