Statistical Machine Learning (BE4M33SSU)
Lecture 4: Support Vector Machines

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Linear classifier with minimal 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 $h\colon \mathcal{X} \to \mathcal{Y}$

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

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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

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

In this lecture we address the following issues:

1. The statistical consitency of the ERM for hypothesis space containing linear classifiers.

2. Algorithmic issues: in general, there is no known algorithm solving the task (1) in time polynomial in m.

Vapnik-Chervonenkis (VC) dimension

Definition 1. *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 2. *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 1. *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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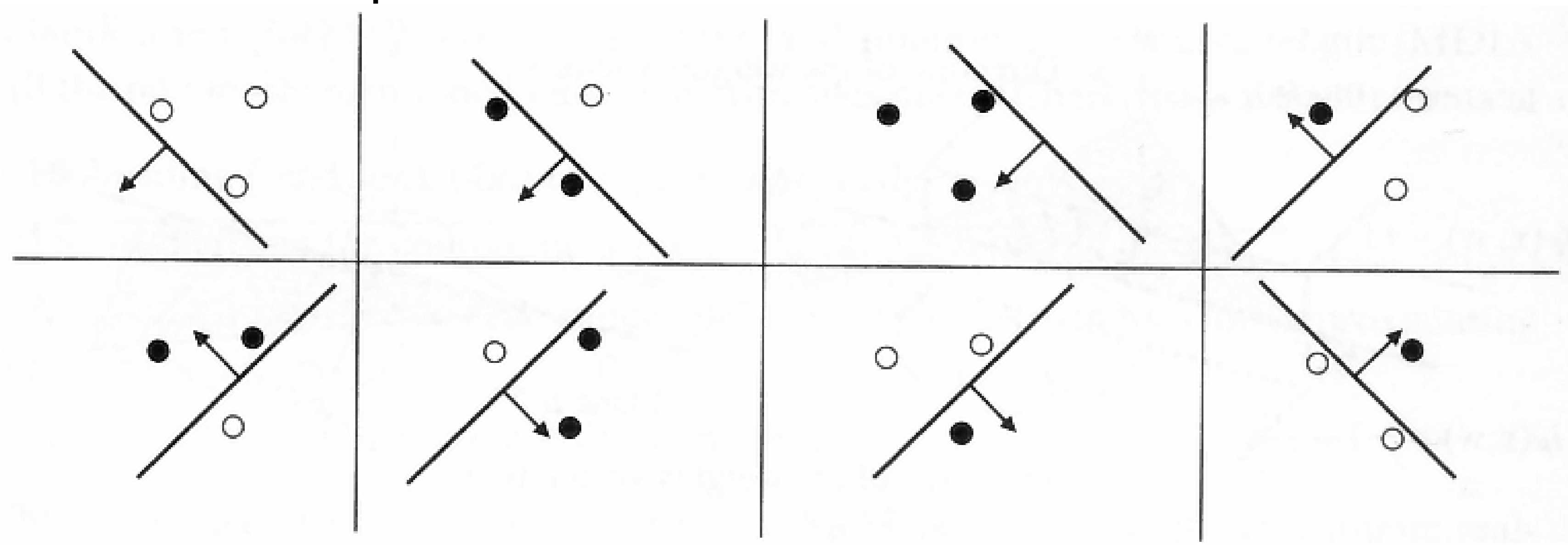
Example for $n = 2$-dimensional feature class



Consistency of prediction with two classes and $0/1$-loss

Theorem 2. *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*

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

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Corollary 1. *Let $\mathcal{H} \subseteq \{+1,-1\}^{\mathcal{X}}$ be a hypothesis class with VC dimension $d < \infty$. Then ULLN applies and hence ERM is statistically consistent in $\mathcal{H}$ w.r.t $\ell^{0/1}$ loss function.*

Training linear classifier from separable examples

Definition 3. *The examples* $\mathcal{T}^m = \{(x^i, y^i) \in (\mathcal{X} \times \mathcal{Y}) \mid i = 1, \ldots, m\}$ *are linearly separable w.r.t. feature map* $\boldsymbol{\phi} \colon \mathcal{X} \to \mathbb{R}^n$ *if there exists* $(\boldsymbol{w}, b) \in \mathbb{R}^{n+1}$ *such that*

$$y^i(\langle \boldsymbol{w}, \boldsymbol{\phi}(x^i) \rangle + b) > 0\,, \qquad i \in \{1, \ldots, m\} \tag{2}$$

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Perceptron algorithm:

Input: linearly separable examples $\mathcal{T}^m$

Output: linear classifier with $R^{0/1}_{\mathcal{T}^m}(h(\cdot; \boldsymbol{w}, b)) = 0$

step 1: $\boldsymbol{w} \leftarrow \mathbf{0}$, $b \leftarrow 0$

step 2: find $(\boldsymbol{x}^i, y^i)$ such that $y^i(\langle \boldsymbol{w}, \boldsymbol{\phi}(x^i)\rangle + b) \leq 0$.
If not found exit, the current $(\boldsymbol{w}, b)$ solves the problem.

step 3: $\boldsymbol{w} \leftarrow \boldsymbol{w} + y^i\, \boldsymbol{\phi}(x^i)$, $b \leftarrow b + y^i$ and goto to step 2.

Training linear classifier from NON-separable examples

- The intractable ERM problem we wish to solve

$$(\boldsymbol{w}^*, b^*) \in \operatorname*{Argmin}_{(\boldsymbol{w},b)\in(\mathbb{R}^n\times\mathbb{R})} \frac{1}{m}\sum_{i=1}^{m} \underbrace{[\![y^i \neq h(x^i;\boldsymbol{w},b)]\!]}_{\ell^{0/1}(y^i,h(x^i;\boldsymbol{w},b))}$$

where $h(x;\boldsymbol{w},b) = \mathrm{sign}(f(x;\boldsymbol{w},b))$ and $f(x;\boldsymbol{w},b) = \langle \boldsymbol{w}, \boldsymbol{\phi}(x)\rangle + b$.

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- The ERM problem is approximated by a tractable **convex problem**

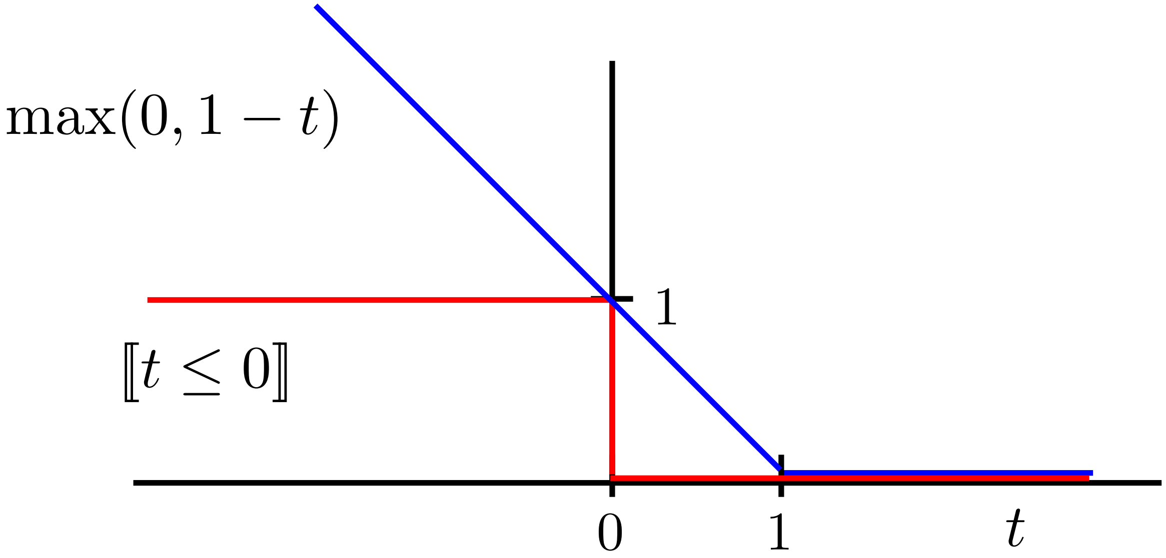
$$(\boldsymbol{w}^*, b^*) \in \operatorname*{Argmin}_{(\boldsymbol{w},b)\in(\mathbb{R}^n\times\mathbb{R})} \frac{1}{m}\sum_{i=1}^{m} \underbrace{\max\{0, 1 - y^i f(x^i;\boldsymbol{w},b)\}}_{\psi(y^i,f(x^i;\boldsymbol{w},b))}$$

where $\psi(y, f(x))$ is so called Hinge-loss.

The hinge-loss upper bounds the 0/1-loss

- The hinge-loss is an upper bound of the $0/1$-loss evaluated for the predictor $h(x) = \mathrm{sign}(f(x))$:

$$\underbrace{[\![\mathrm{sign}(f(x)) \neq y]\!]}_{\ell^{0/1}(y, f(x))} = [\![\, y\, f(x) \leq 0]\!] \leq \underbrace{\max\{0, 1 - y\ f(x)\}}_{\psi(y, f(x))}$$



Support Vector Machines

- Find linear classifier $h(x; \boldsymbol{w}, b) = \mathrm{sign}(\langle \boldsymbol{\phi}(x), \boldsymbol{w} \rangle + b)$ by solving

$$(\boldsymbol{w}^*, b^*) = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^n, b \in \mathbb{R}} \Bigg(\underbrace{\frac{1}{2} \|\boldsymbol{w}\|^2}_{\substack{\text{penalty}\\\text{term}}} + \underbrace{C \sum_{i=1}^{m} \max\{0, 1 - y^i(\langle \boldsymbol{w}, \boldsymbol{\phi}(x^i) \rangle + b)\}}_{\text{empirical error}} \Bigg)$$

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- The regularization constant $C \geq 0$ controls trade-off between estimation error and approximation error.
  - $C_1 < C_2$ implies $\|\boldsymbol{w}_1^*\| \leq \|\boldsymbol{w}_2^*\|$

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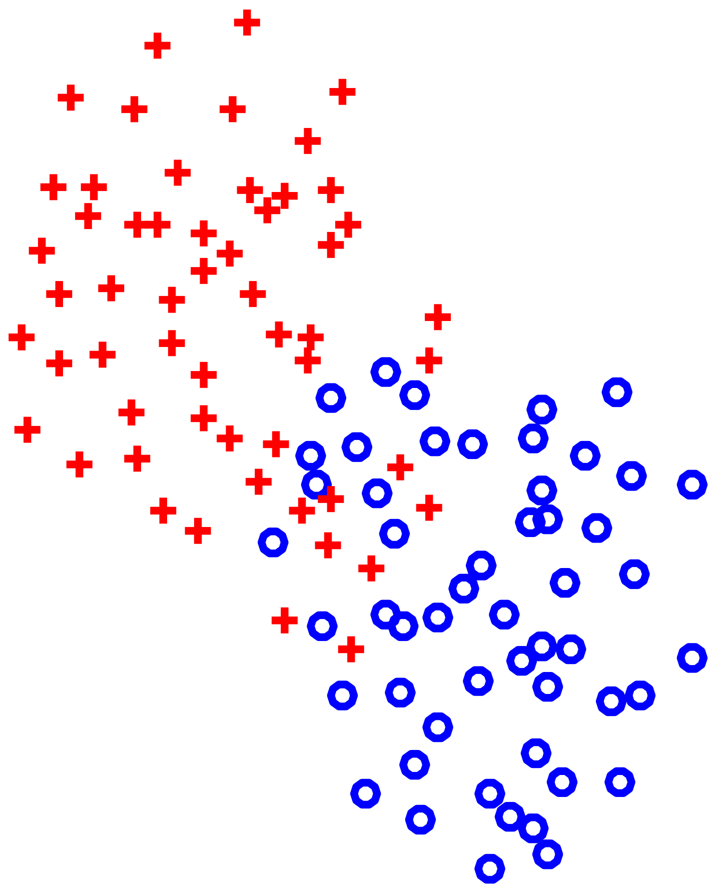
- Small $\|\boldsymbol{w}\|$ implies score $f(x; \boldsymbol{w}, b) = \langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b$ varies slowly.
  - Cauchy inequality:
    $(\langle \boldsymbol{\phi}(x), \boldsymbol{w} \rangle - \langle \boldsymbol{\phi}(x'), \boldsymbol{w} \rangle)^2 \leq \|\boldsymbol{\phi}(x) - \boldsymbol{\phi}(x')\|^2 \|\boldsymbol{w}\|^2$

Example: Primal SVM problem

$$(\boldsymbol{w}^*, b^*) = \operatorname*{argmin}_{\boldsymbol{w}\in\mathbb{R}^n, b\in\mathbb{R}} \Bigg(\underbrace{\frac{1}{2}\|\boldsymbol{w}\|^2}_{\text{penalty term}} + C \underbrace{\sum_{i=1}^{m} \max\{0, 1 - y^i(\langle \boldsymbol{w}, \boldsymbol{\phi}(x^i)\rangle + b)\}}_{\text{empirical error}} \Bigg)$$



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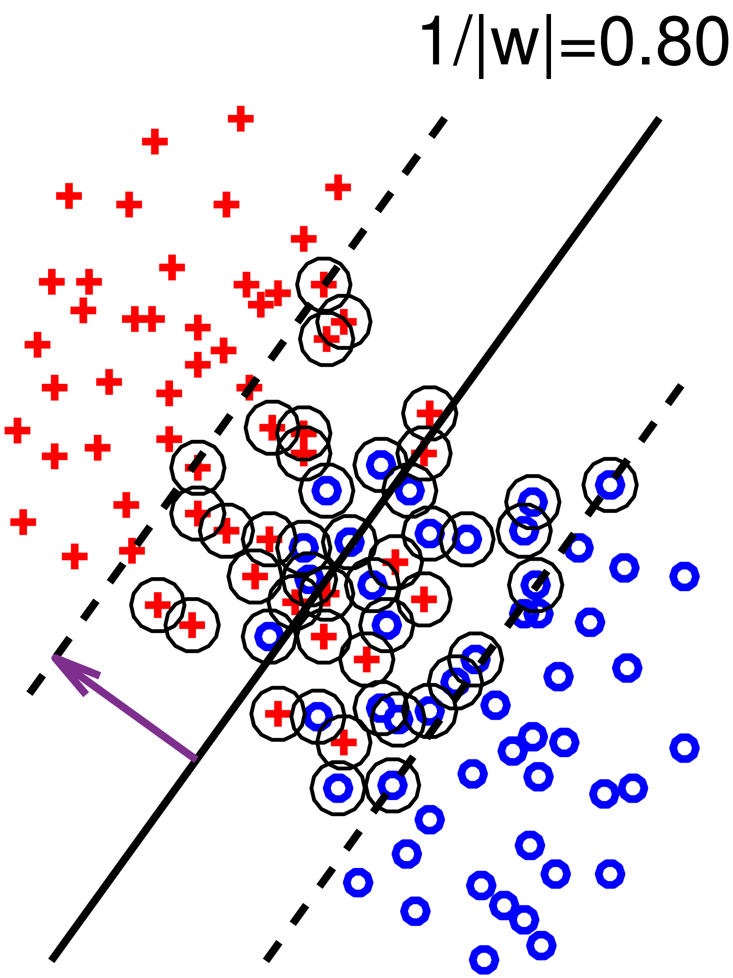

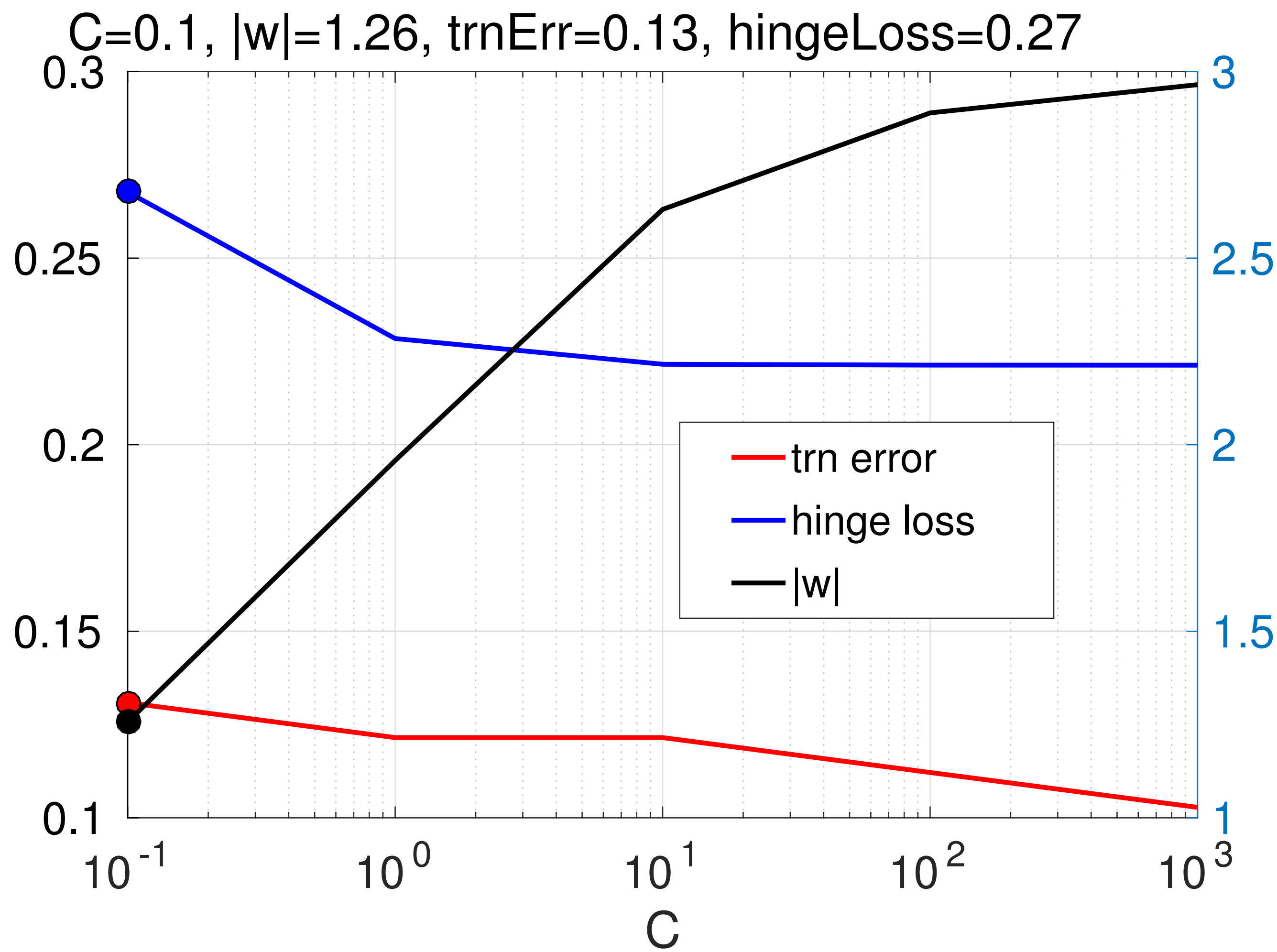

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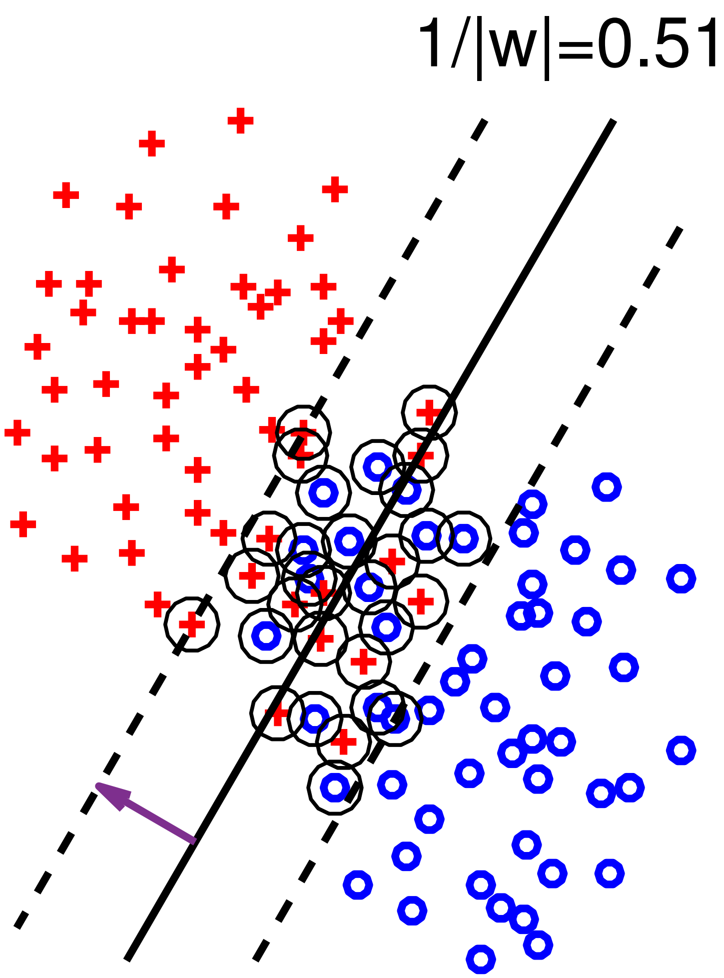

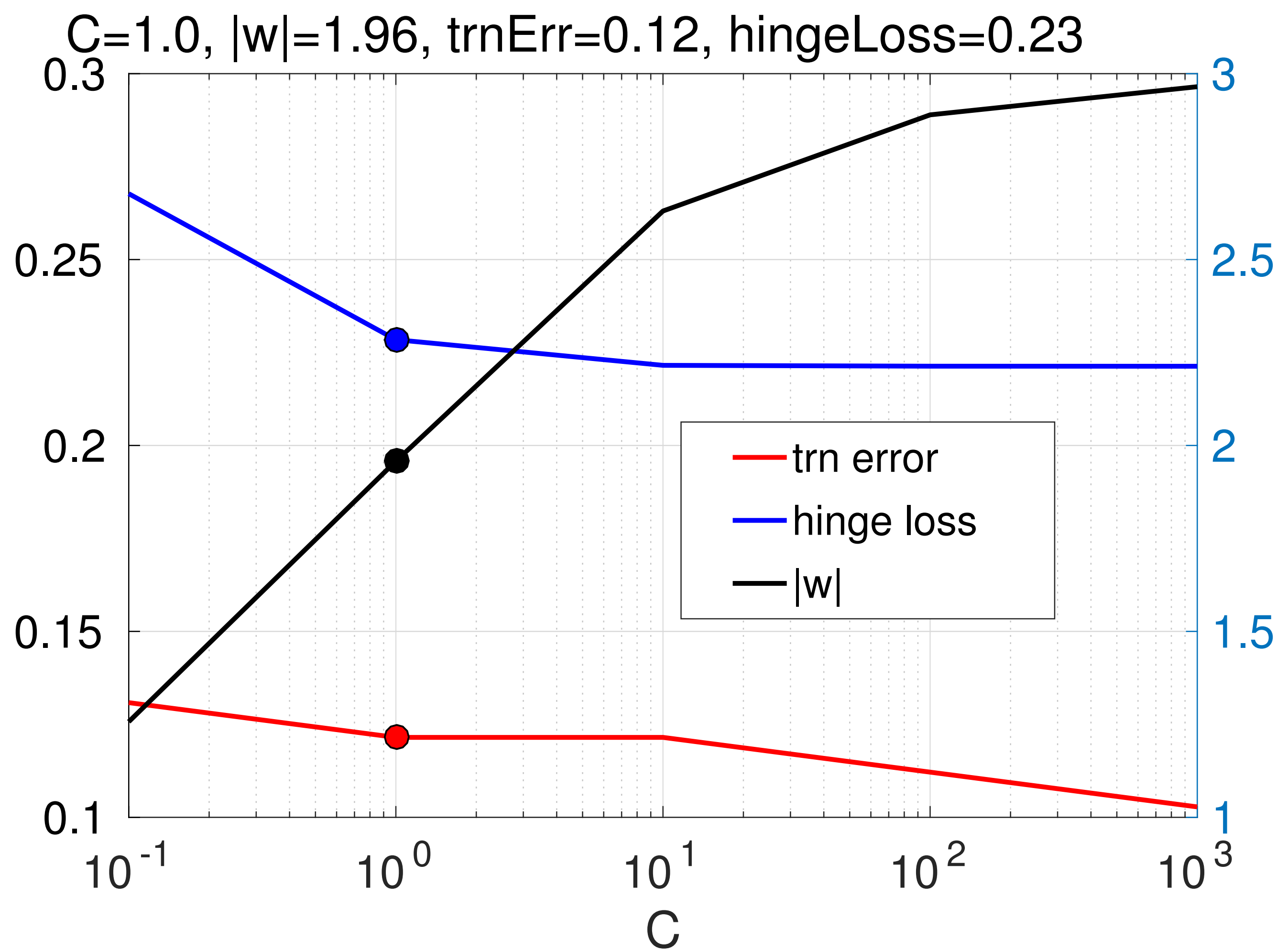

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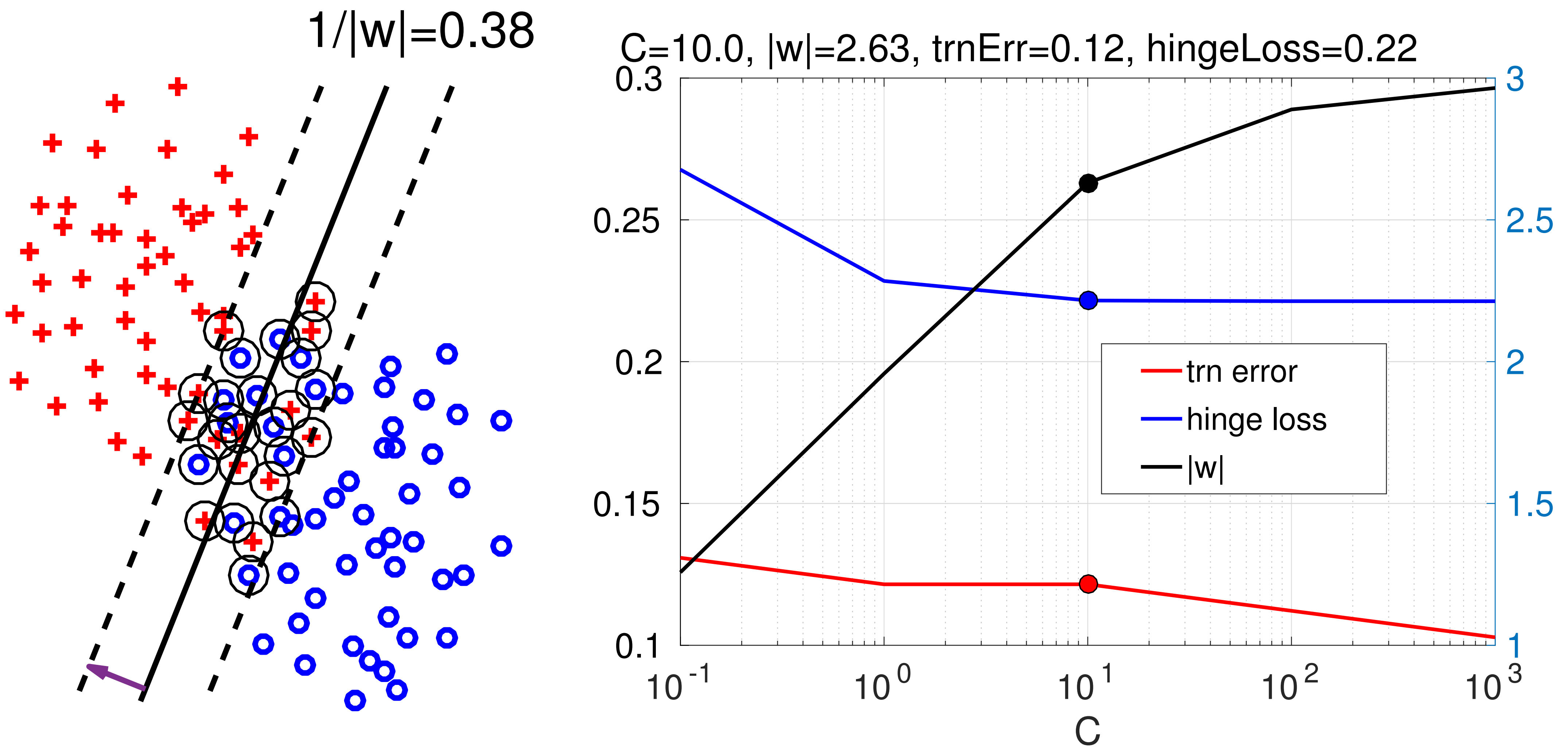

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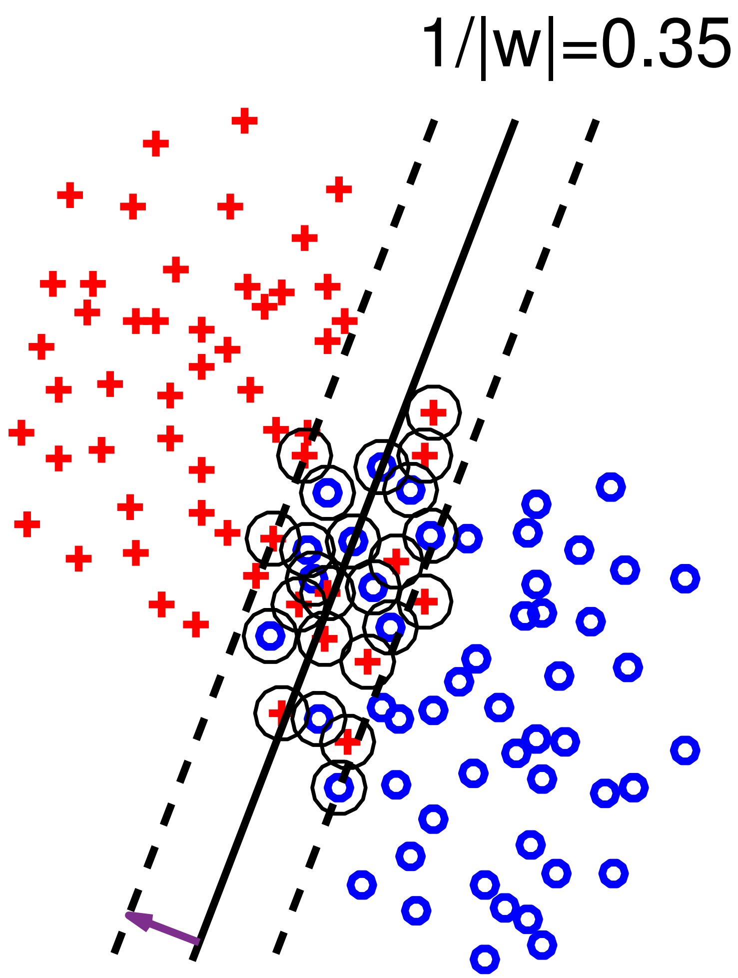

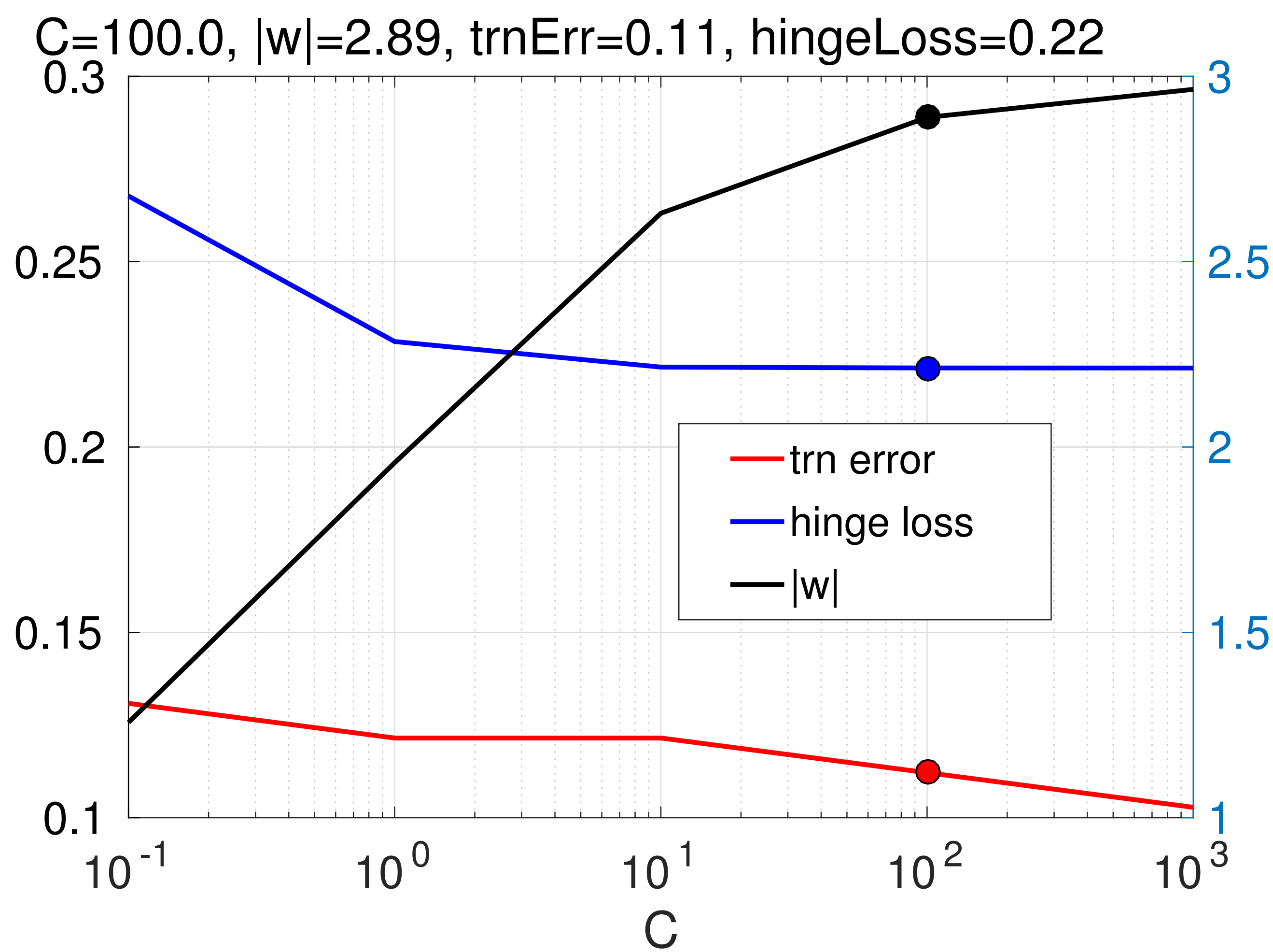

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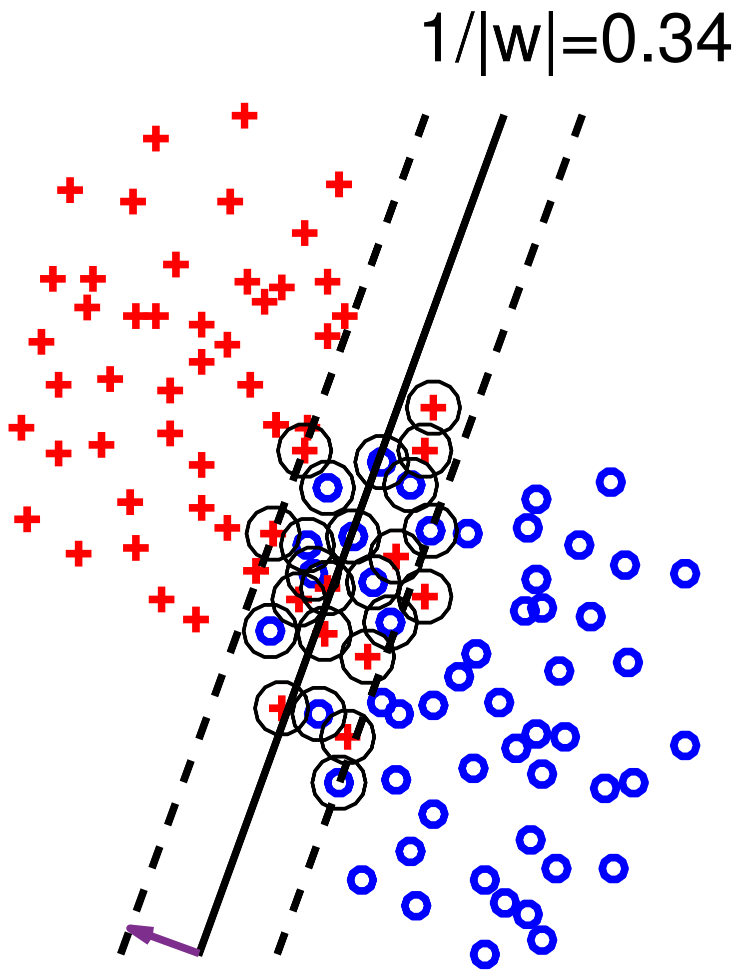

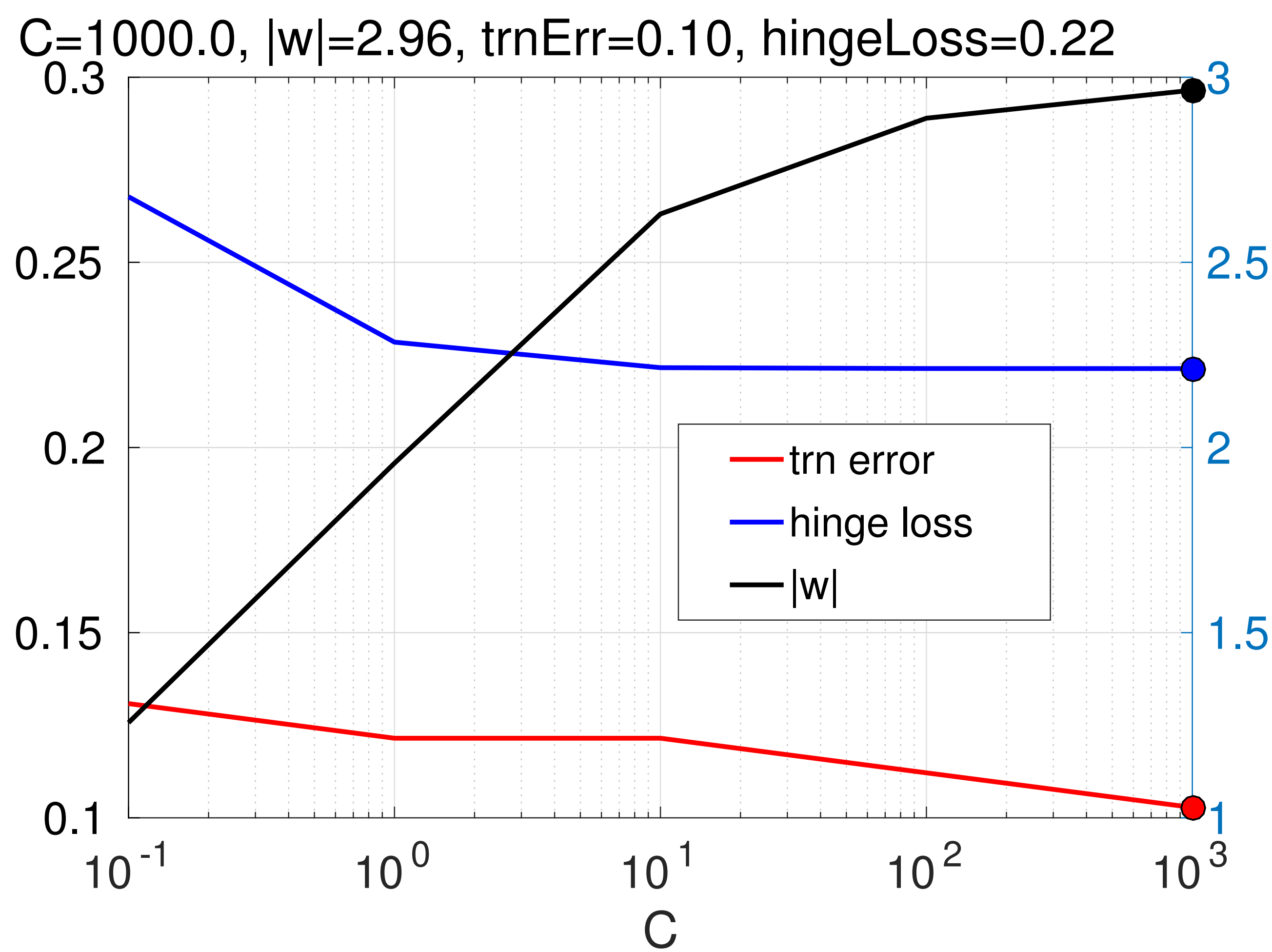

SVM as Quadratic Program

- Find linear classifier $h(x;\boldsymbol{w},b) = \mathrm{sign}(\langle \boldsymbol{\phi}(x), \boldsymbol{w}\rangle + b)$ by solving

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where $C > 0$ is the regularization constant.

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where $C > 0$ is the regularization constant.

- It can be re-formulated as a convex *quadratic program*

$$(\boldsymbol{w}^*, b^*, \boldsymbol{\xi}^*) = \operatorname*{argmin}_{\substack{(\boldsymbol{w}, b) \in \mathbb{R}^{n+1} \\ \boldsymbol{\xi} \in \mathbb{R}^m}} \left(\frac{1}{2} \|\boldsymbol{w}\|^2 + C \sum_{i=1}^{m} \xi_i \right)$$

subject to

$$\begin{aligned} \xi_i &\geq 1 - y^i(\langle \boldsymbol{w}, \boldsymbol{\phi}(x^i) \rangle + b) \,, & i \in \{1, \ldots, m\} \\ \xi_i &\geq 0 \,, & i \in \{1, \ldots, m\} \end{aligned}$$

From Primal SVM to Dual SVM problem

- Lagrangian of the primal SVM problem:

$$L(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \underbrace{\frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{m}\xi_i}_{\text{original objective}}$$

$$\underbrace{-\sum_{i=1}^{m}\alpha_i(y^i(\langle \boldsymbol{w}, \boldsymbol{\phi}(x^i)\rangle + b) - 1 + \xi_i) - \sum_{i=1}^{m}\mu_i\xi_i}_{\text{constraint violation penalty}}$$

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- Strong duality:

$$\underbrace{\min_{\substack{\boldsymbol{w}\in\mathbb{R}^n \\ b\in\mathbb{R} \\ \boldsymbol{\xi}\in\mathbb{R}^m}} \max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^m_+ \\ \boldsymbol{\mu}\in\mathbb{R}^m_+}} L(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\mu})}_{\text{primal problem}} = \underbrace{\max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^m_+ \\ \boldsymbol{\mu}\in\mathbb{R}^m_+}} \min_{\substack{\boldsymbol{w}\in\mathbb{R}^n \\ b\in\mathbb{R} \\ \boldsymbol{\xi}\in\mathbb{R}^m}} L(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\mu})}_{\text{dual problem}}$$

Dual SVM problem

- The dual SVM formulation is a convex quadratic program

$$\boldsymbol{\alpha}^* = \operatorname*{argmax}_{\boldsymbol{\alpha}\in\mathbb{R}^m} \left(\sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y^i y^j \langle \boldsymbol{\phi}(x^i), \boldsymbol{\phi}(x^j) \rangle \right)$$

$$\text{s.t.} \qquad \sum_{i=1}^m \alpha_i \, y^i = 0 \,, \quad 0 \le \alpha_i \le C \,, \quad i \in \{1, \ldots, m\}$$

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- The primal variables $(\boldsymbol{w}, b)$ are obtained from the dual variables $\boldsymbol{\alpha}$ by

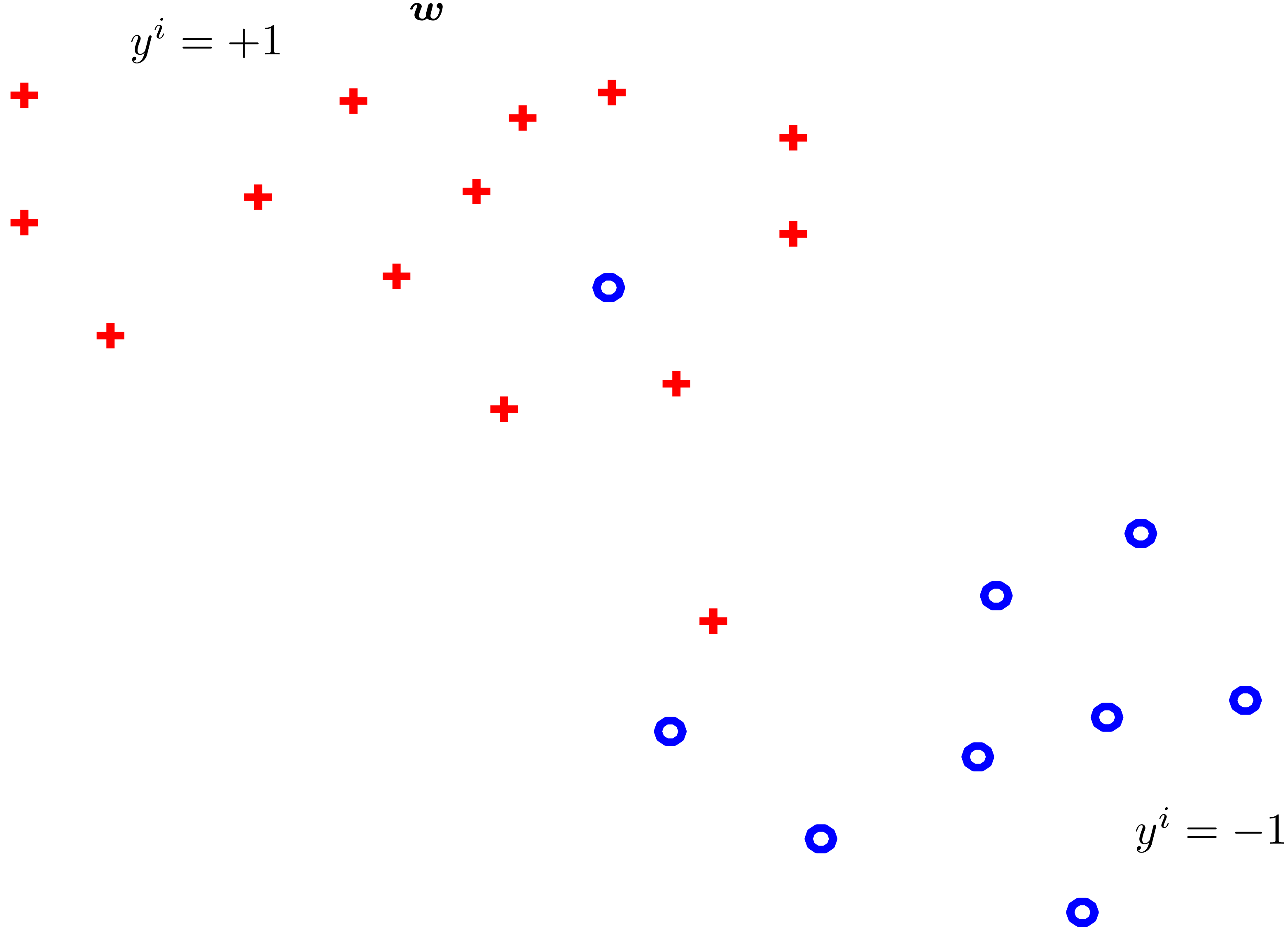
$$\boldsymbol{w} \;=\; \sum_{i=1}^m y^i \, \boldsymbol{\phi}(x^i) \, \alpha_i = \sum_{i\in\mathcal{I}_{\mathrm{SV}}} y^i \, \boldsymbol{\phi}(x^i) \, \alpha_i$$

$$b \;=\; y^i - \langle \boldsymbol{w}, \boldsymbol{\phi}(x^i)\rangle \,, \; \forall i \in \mathcal{I}_{\mathrm{sv}}^{\mathrm{b}} = \{ j \mid 0 < \alpha_j < C \}$$

- $\boldsymbol{\alpha}$ is sparse; $\boldsymbol{w}$ is lin. combination of Support Vectors $\mathcal{I}_{\mathrm{sv}} = \{ j \mid \alpha_j > 0 \}$

Example: SVM classifier

$$f(x) = \langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b = \langle \underbrace{\sum_{i=1}^{m} y^i \, \alpha_i \, \boldsymbol{\phi}(x^i)}_{\boldsymbol{w}}, \boldsymbol{\phi}(x) \rangle + b$$



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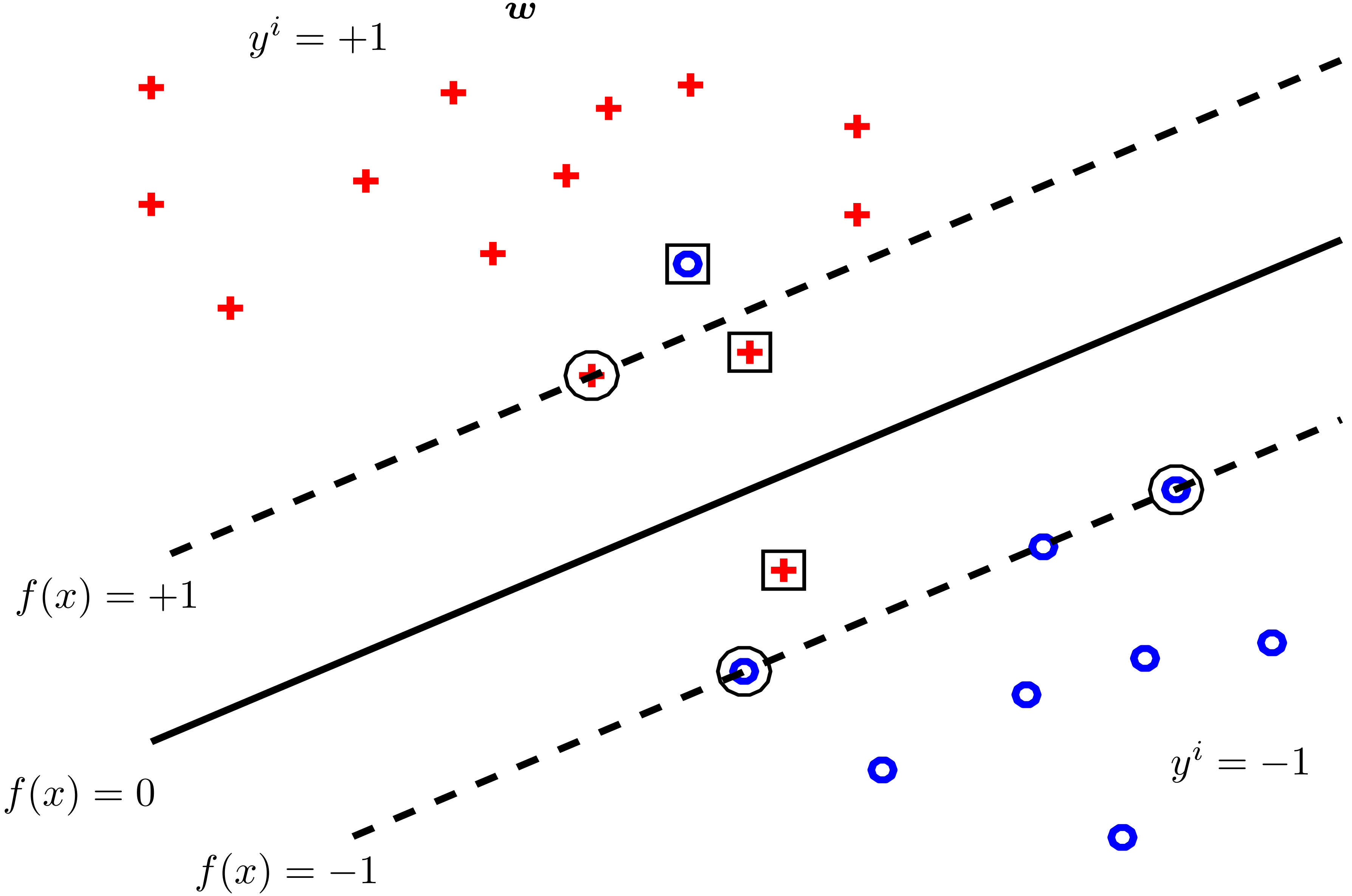

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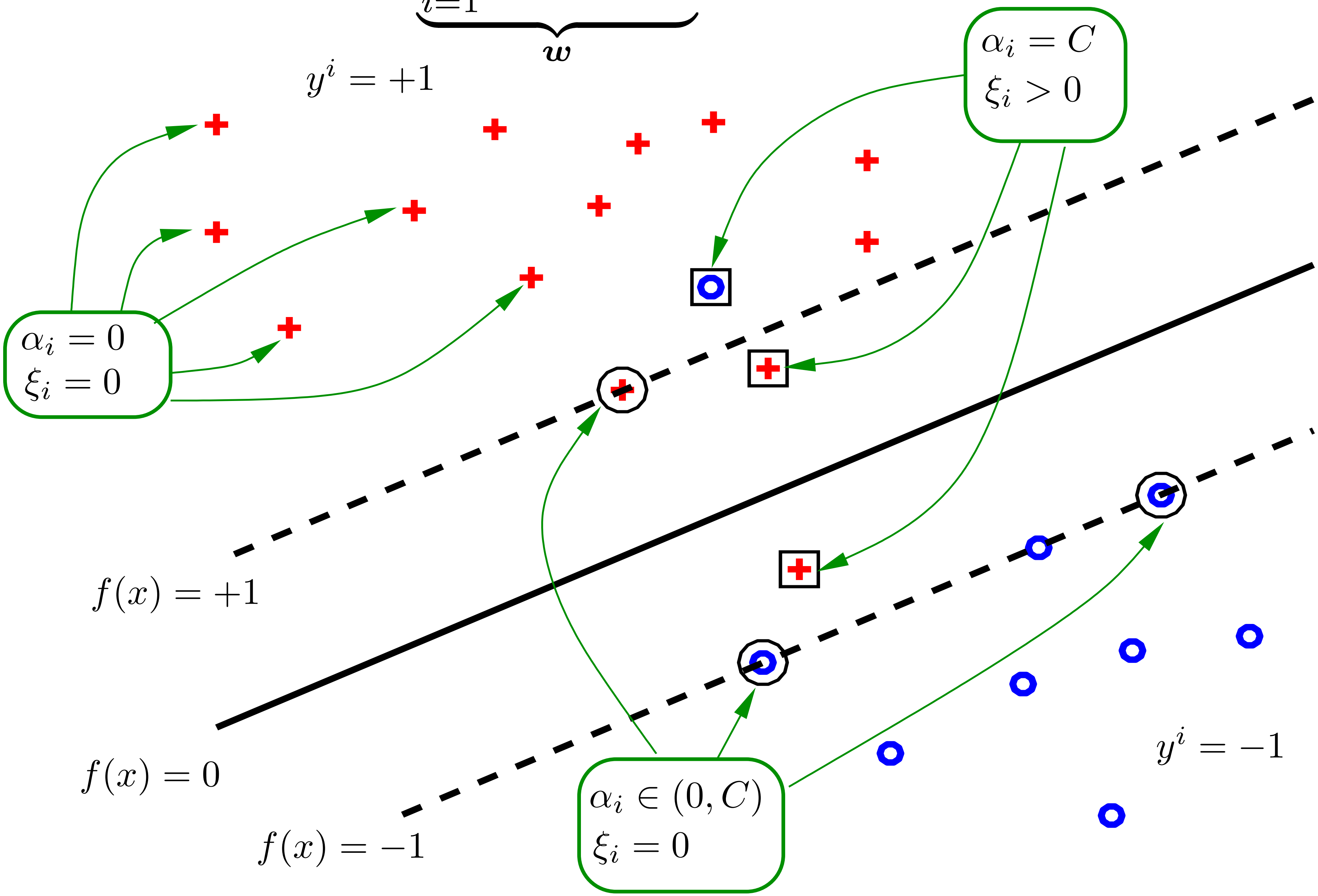
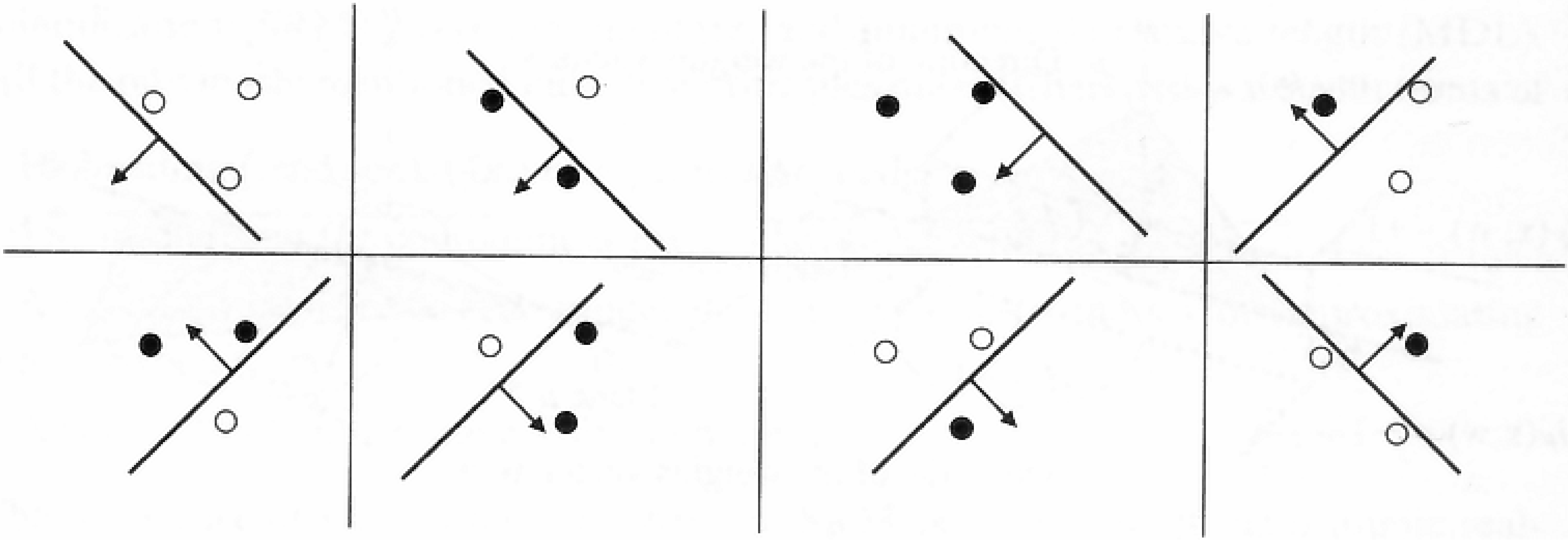
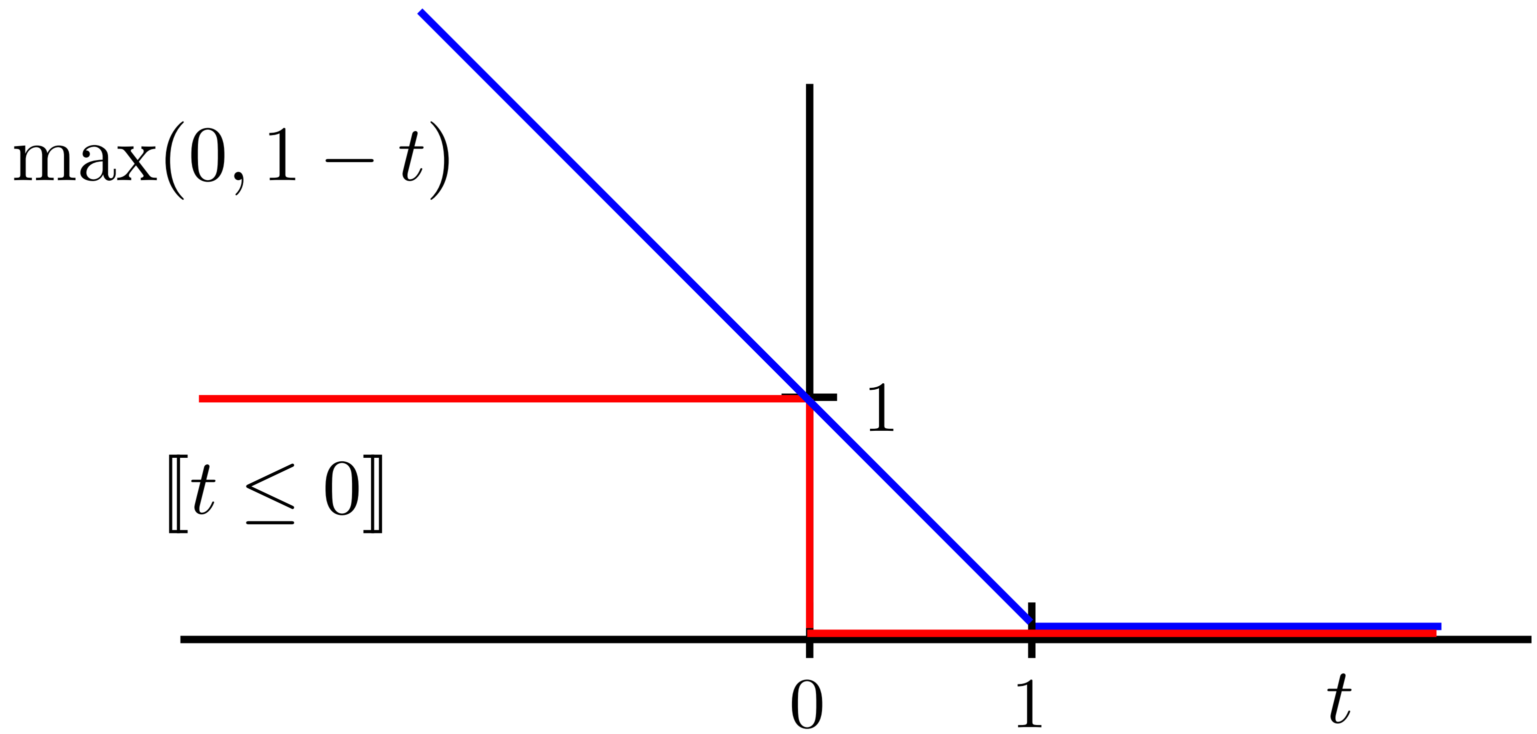
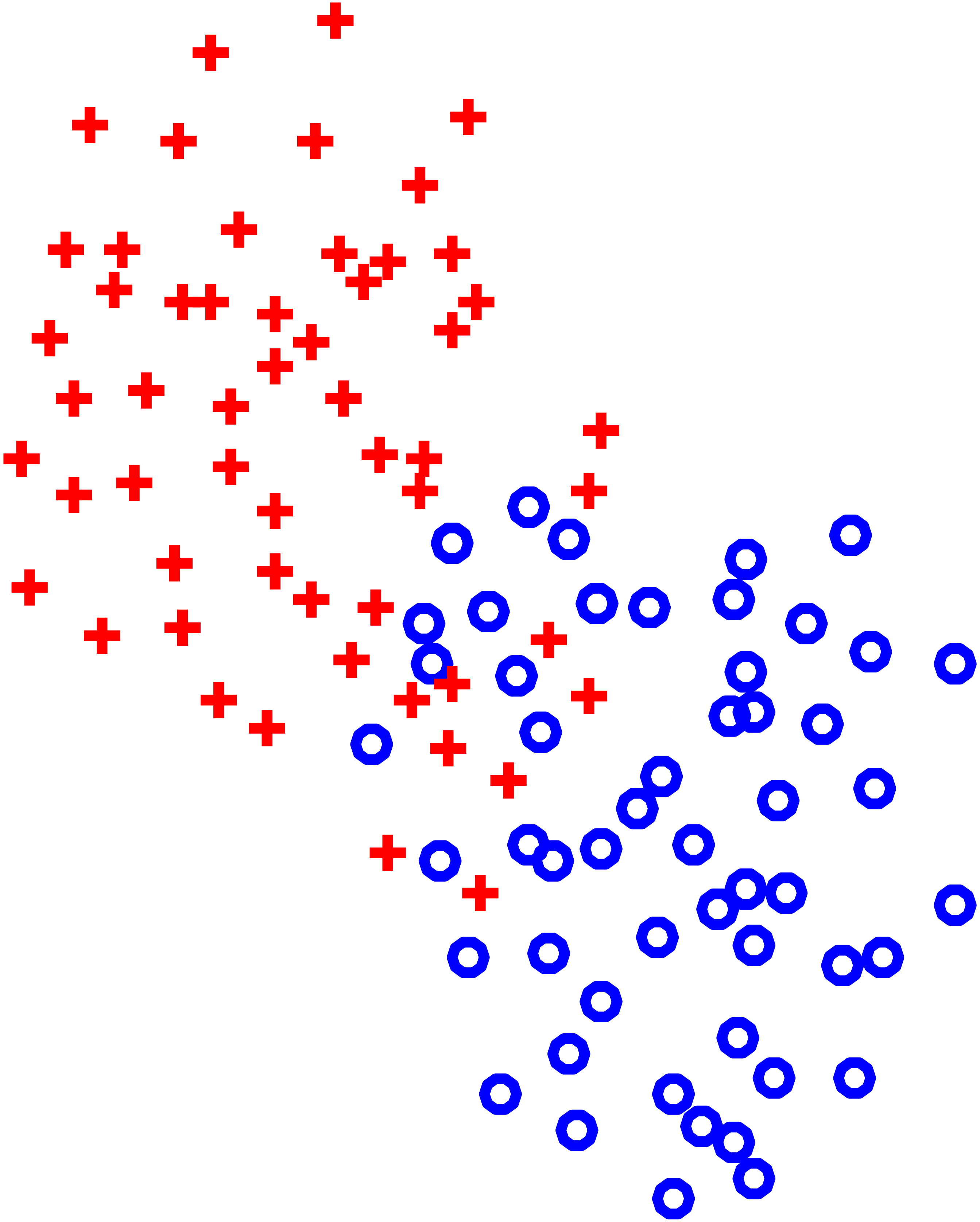
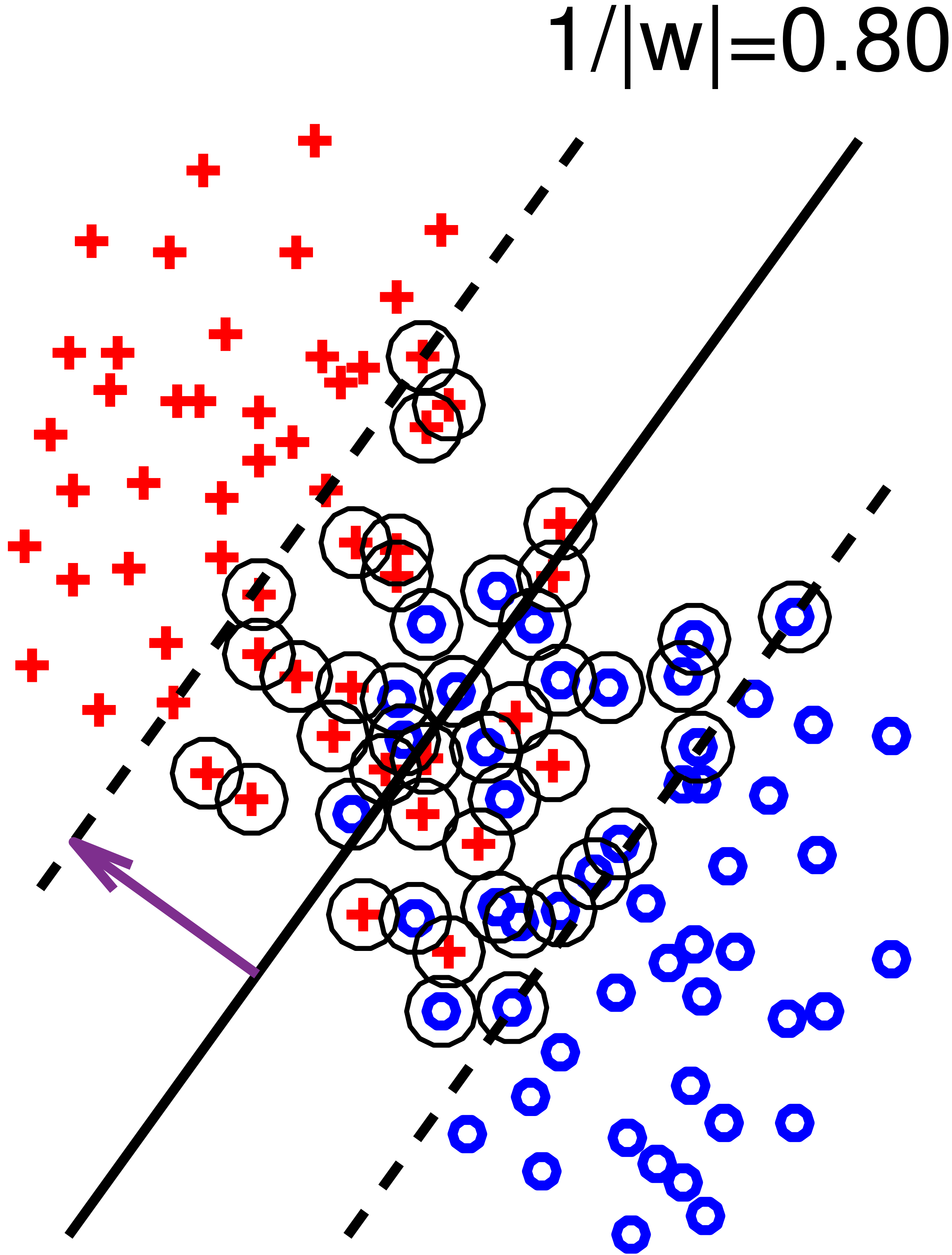


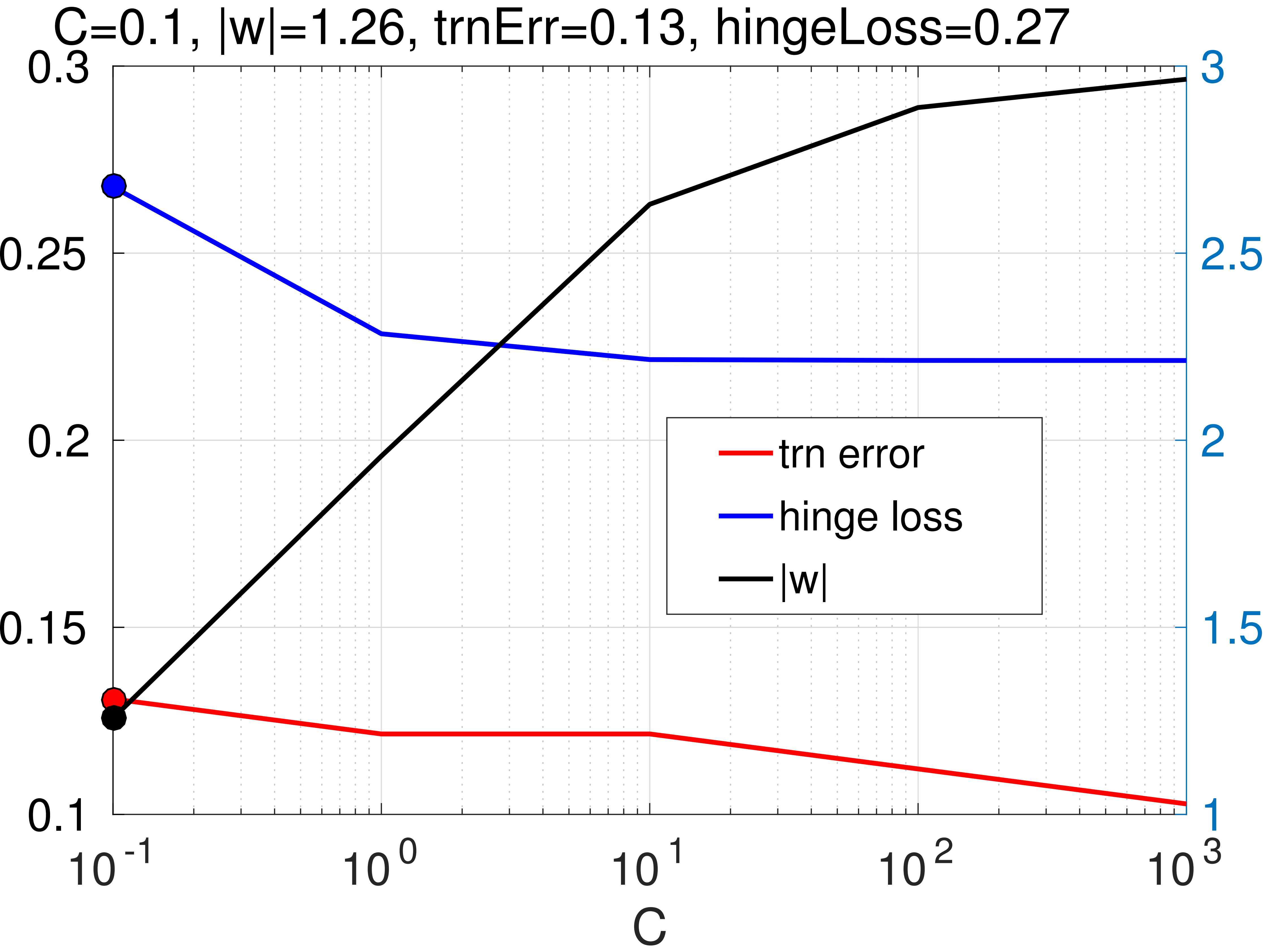




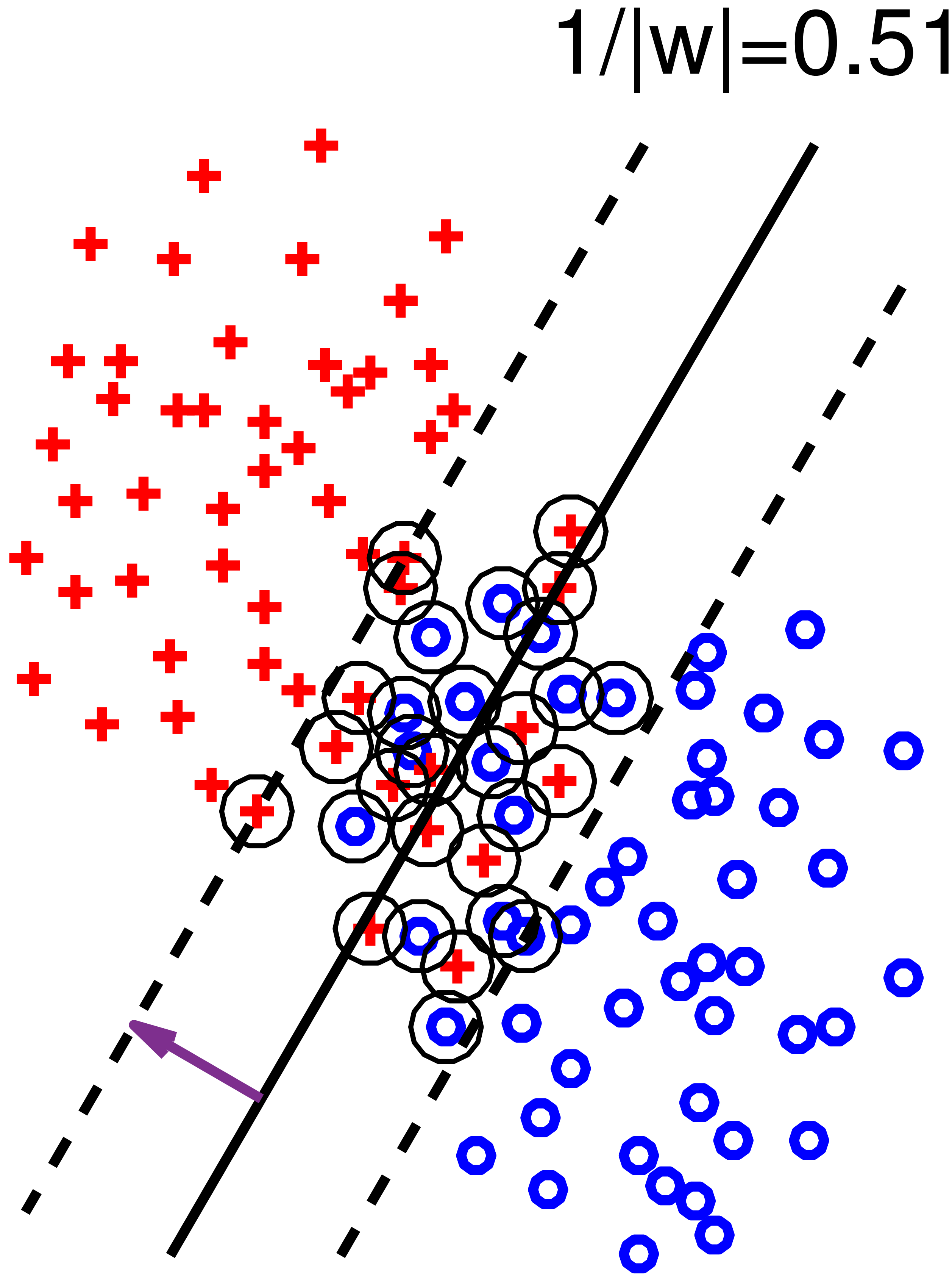
$\max(0, 1 - t)$
1
$[\![t \leq 0]\!]$
0
1
t

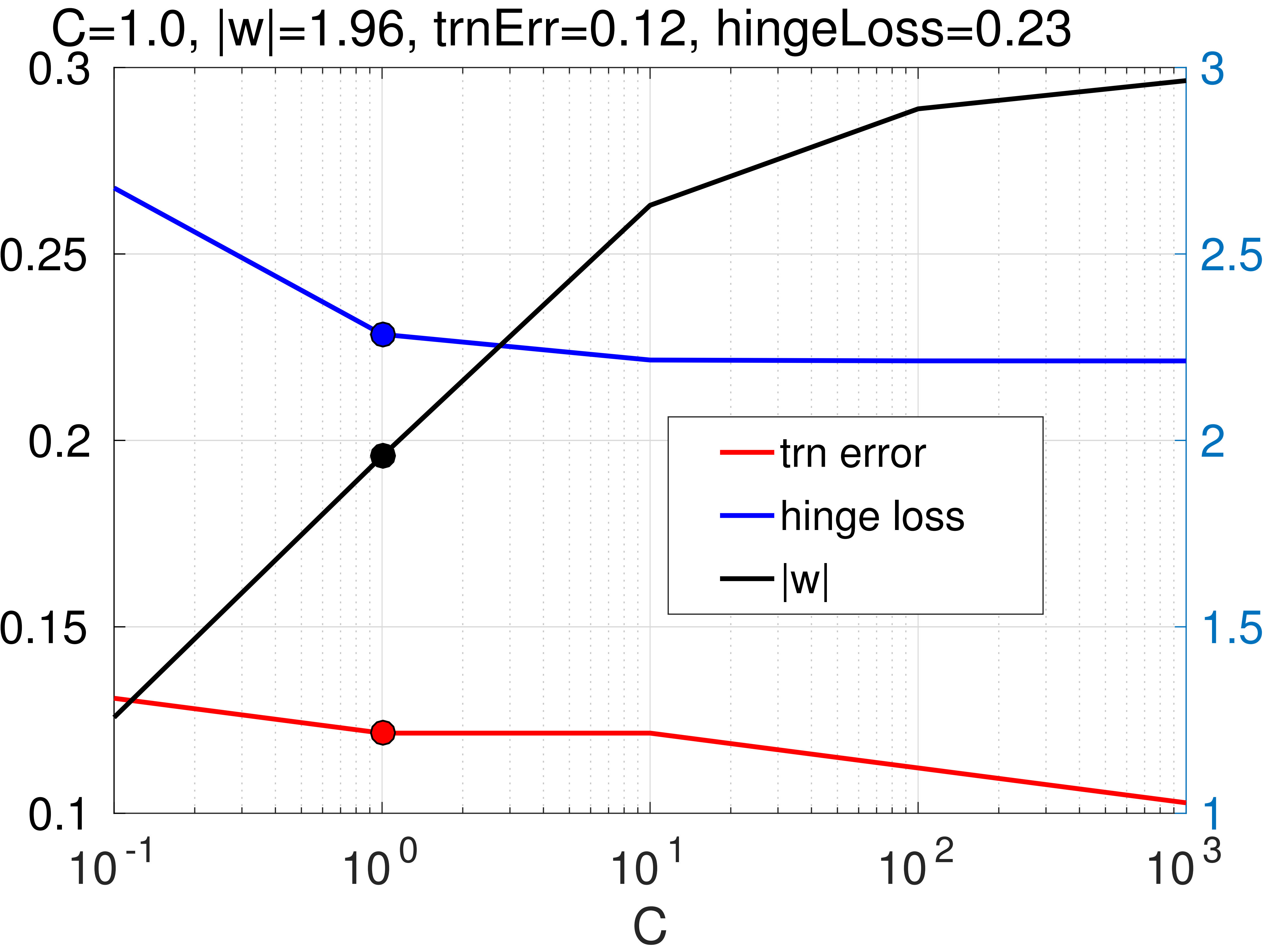



1/|w|=0.80



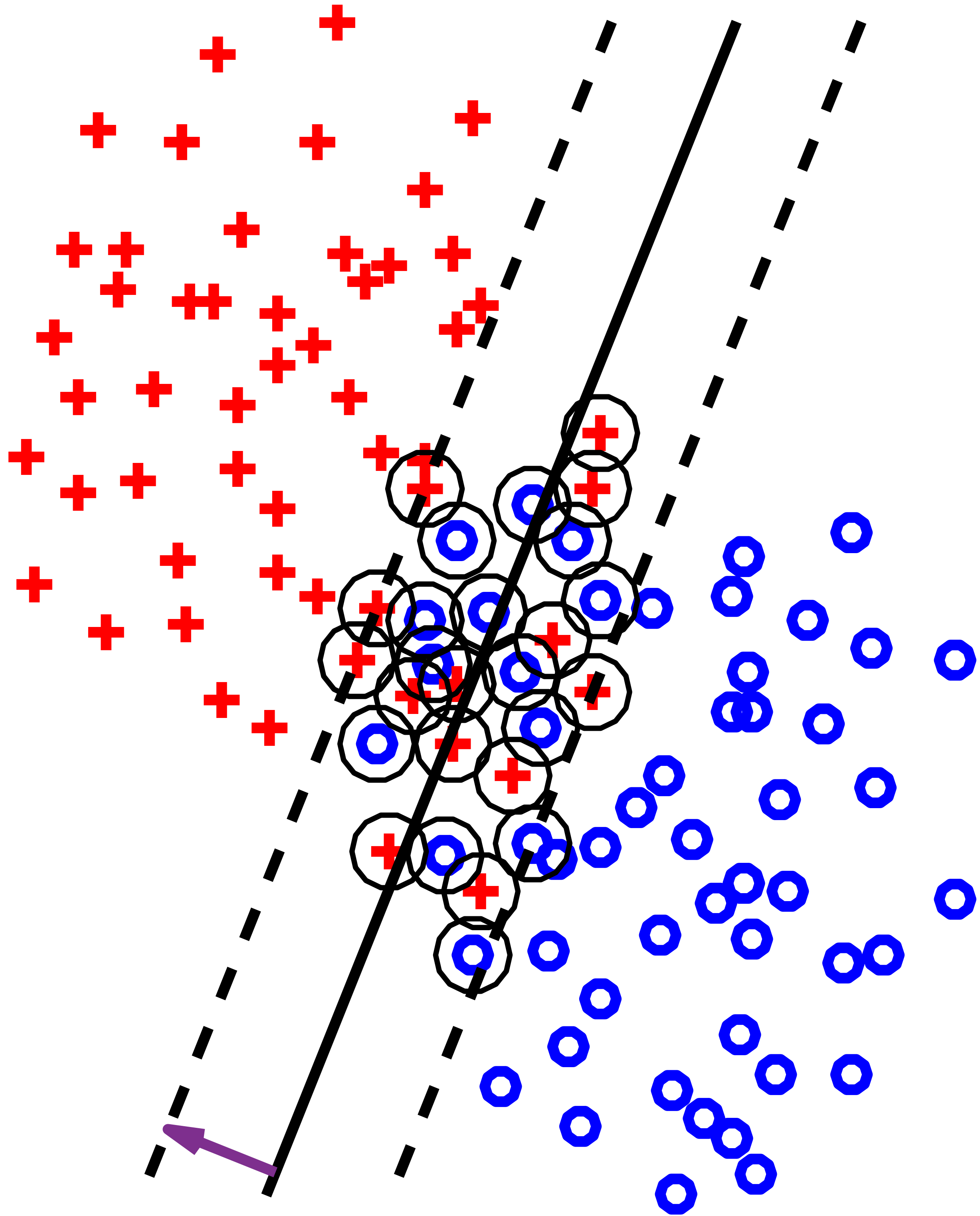
C=0.1, |w|=1.26, trnErr=0.13, hingeLoss=0.27
0.3
0.25
0.2
0.15
0.1
3
2.5
2
1.5
1
trn error
hinge loss
|w|
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
C

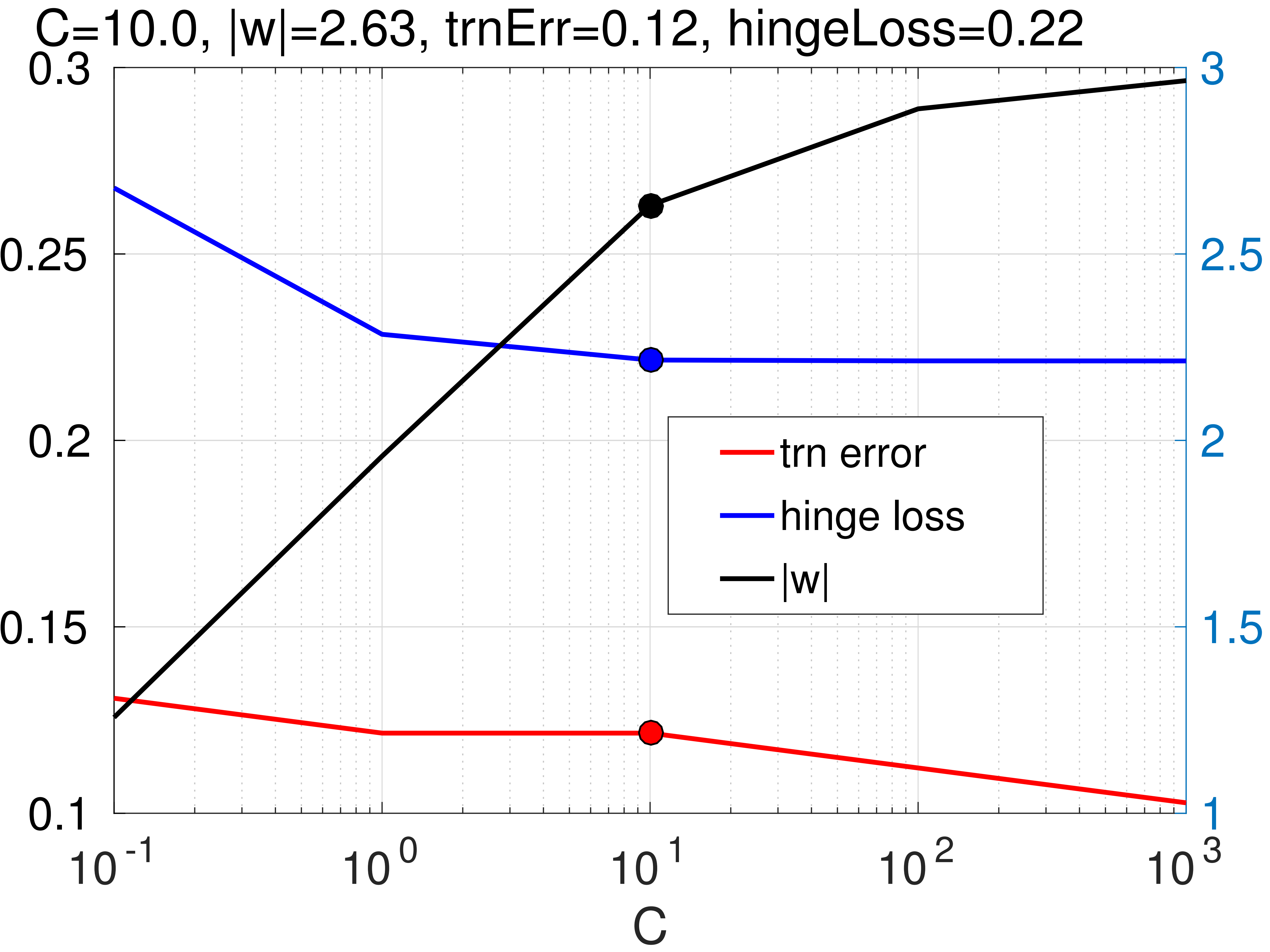

1/|w|=0.51

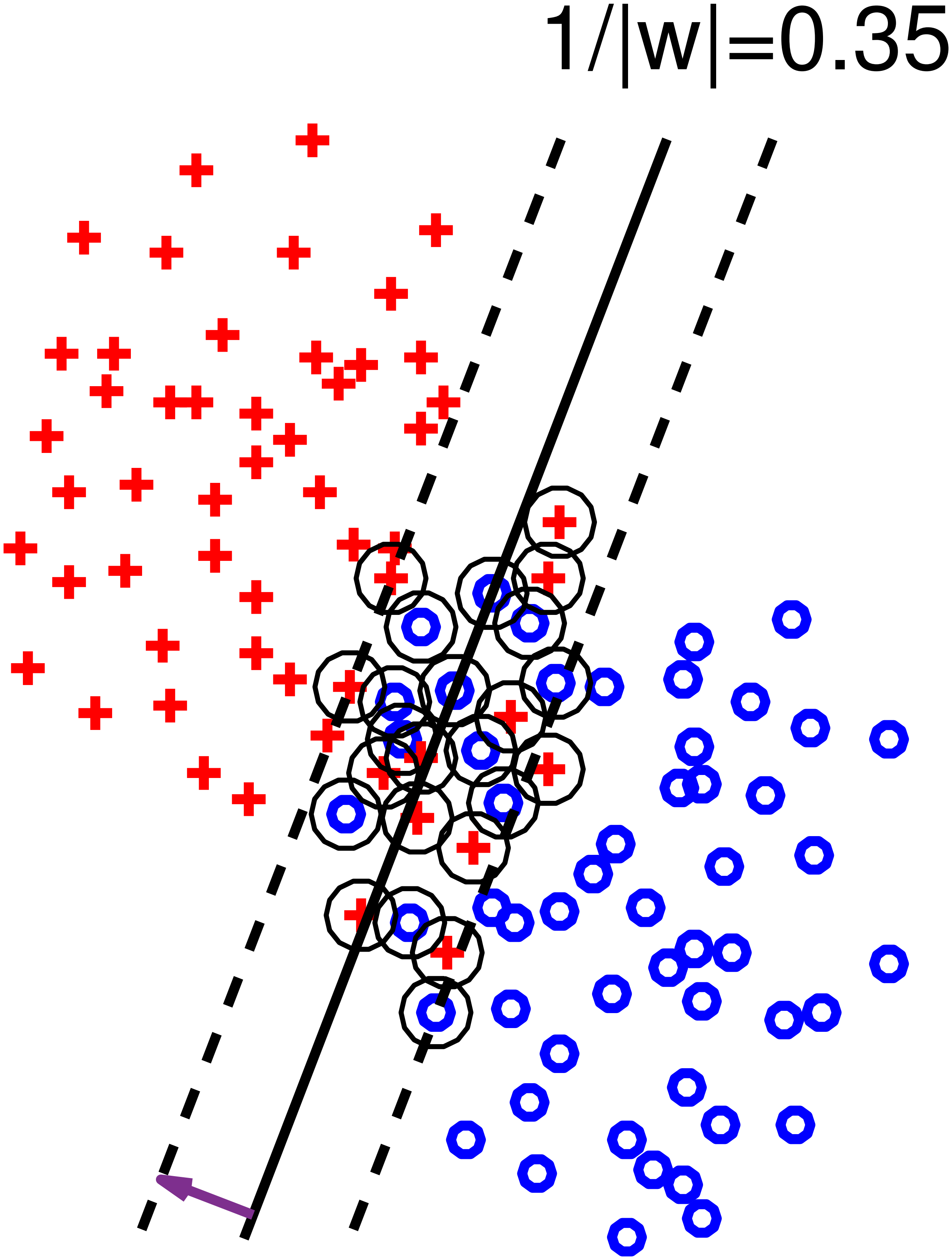


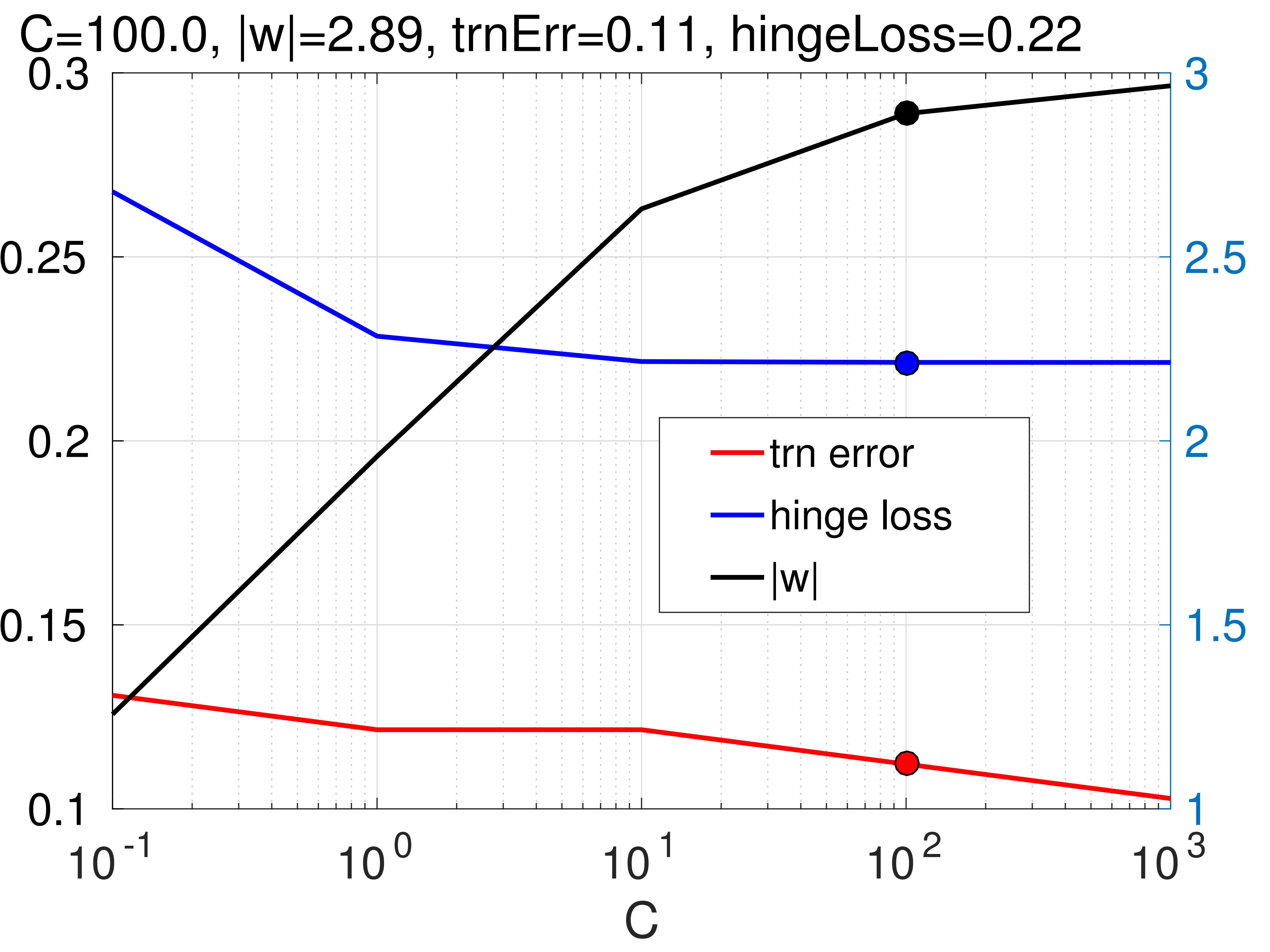
C=1.0, |w|=1.96, trnErr=0.12, hingeLoss=0.23
0.3
0.25
0.2
0.15
0.1
3
2.5
2
1.5
1
trn error
hinge loss
|w|
10^-1
10^0
10^1
10^2
10^3
C

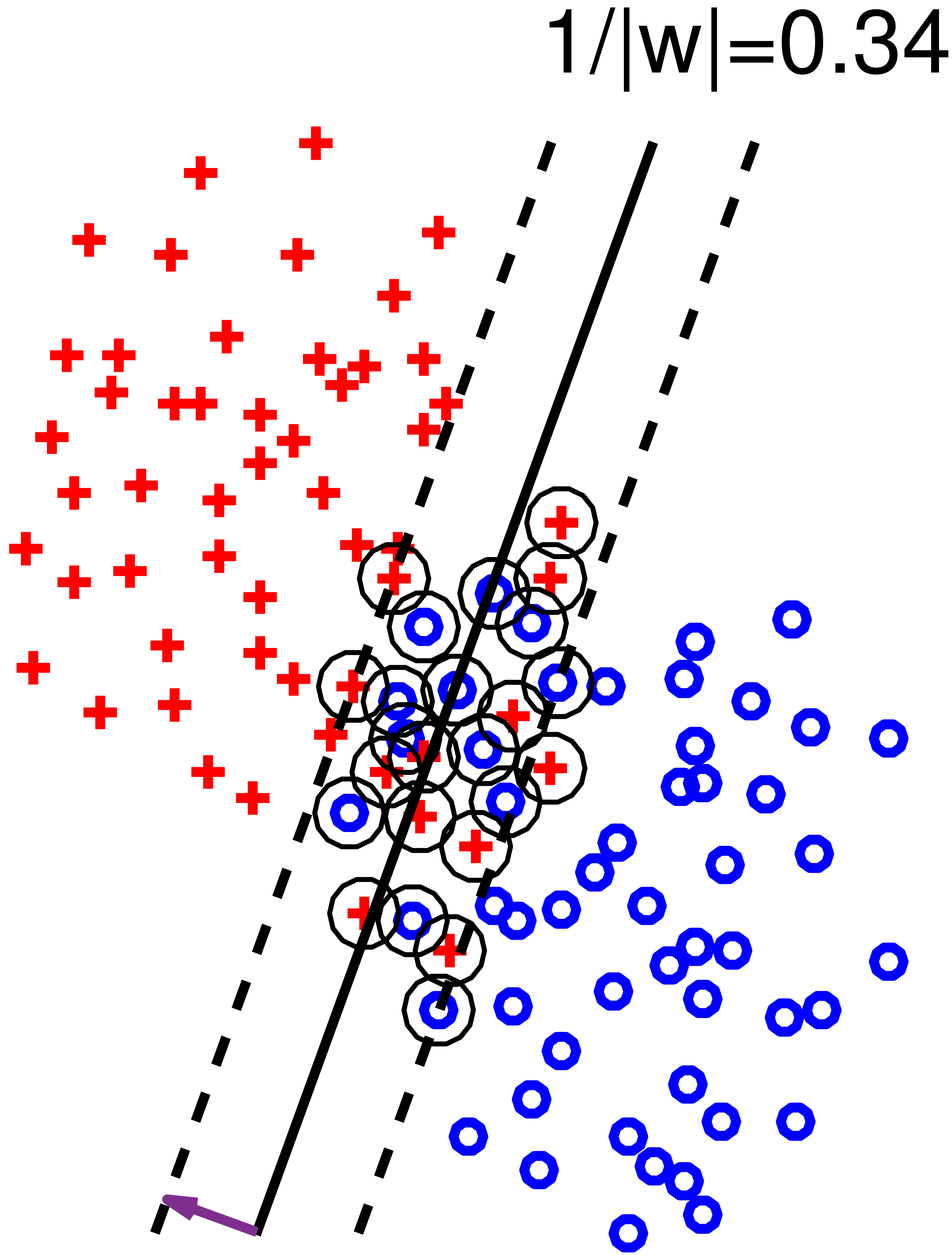
1/|w|=0.38



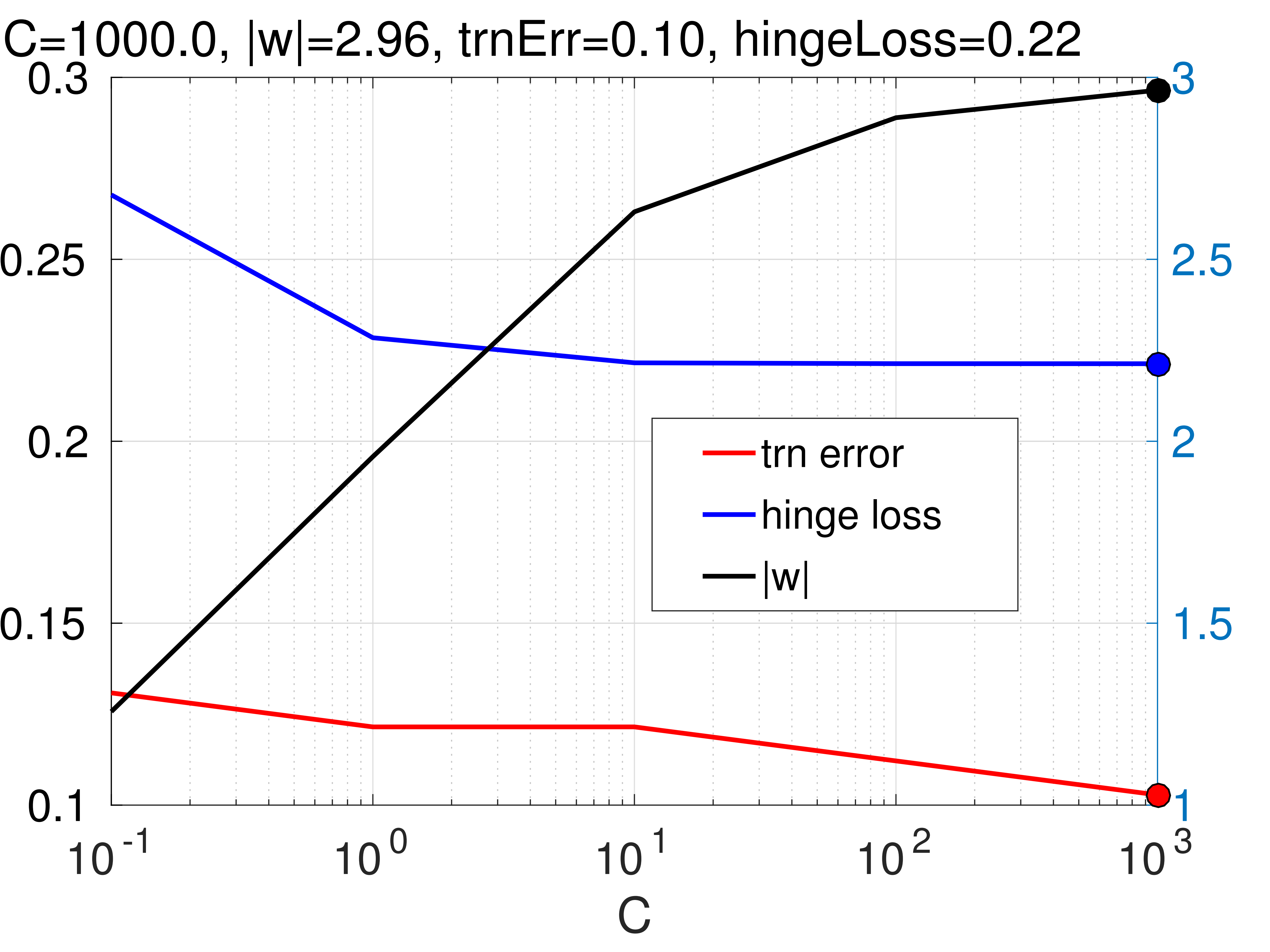

C=10.0, |w|=2.63, trnErr=0.12, hingeLoss=0.22
0.3
0.25
0.2
0.15
0.1
3
2.5
2
1.5
1
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
C
trn error
hinge loss
|w|

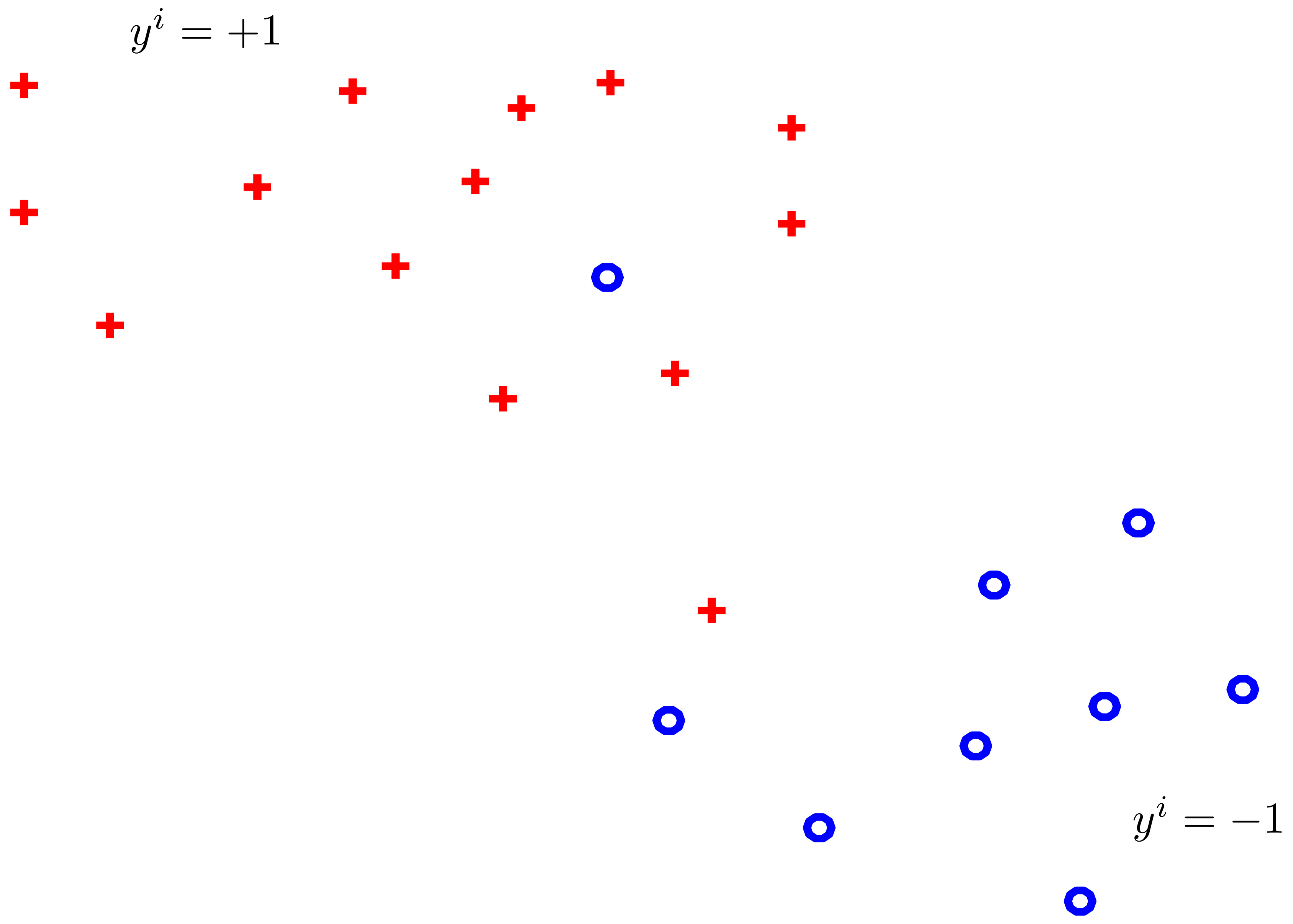

1/|w|=0.35


C=100.0, |w|=2.89, trnErr=0.11, hingeLoss=0.22
0.3
0.25
0.2
0.15
0.1
3
2.5
2
1.5
1
trn error
hinge loss
|w|
10^-1
10^0
10^1
10^2
10^3
C

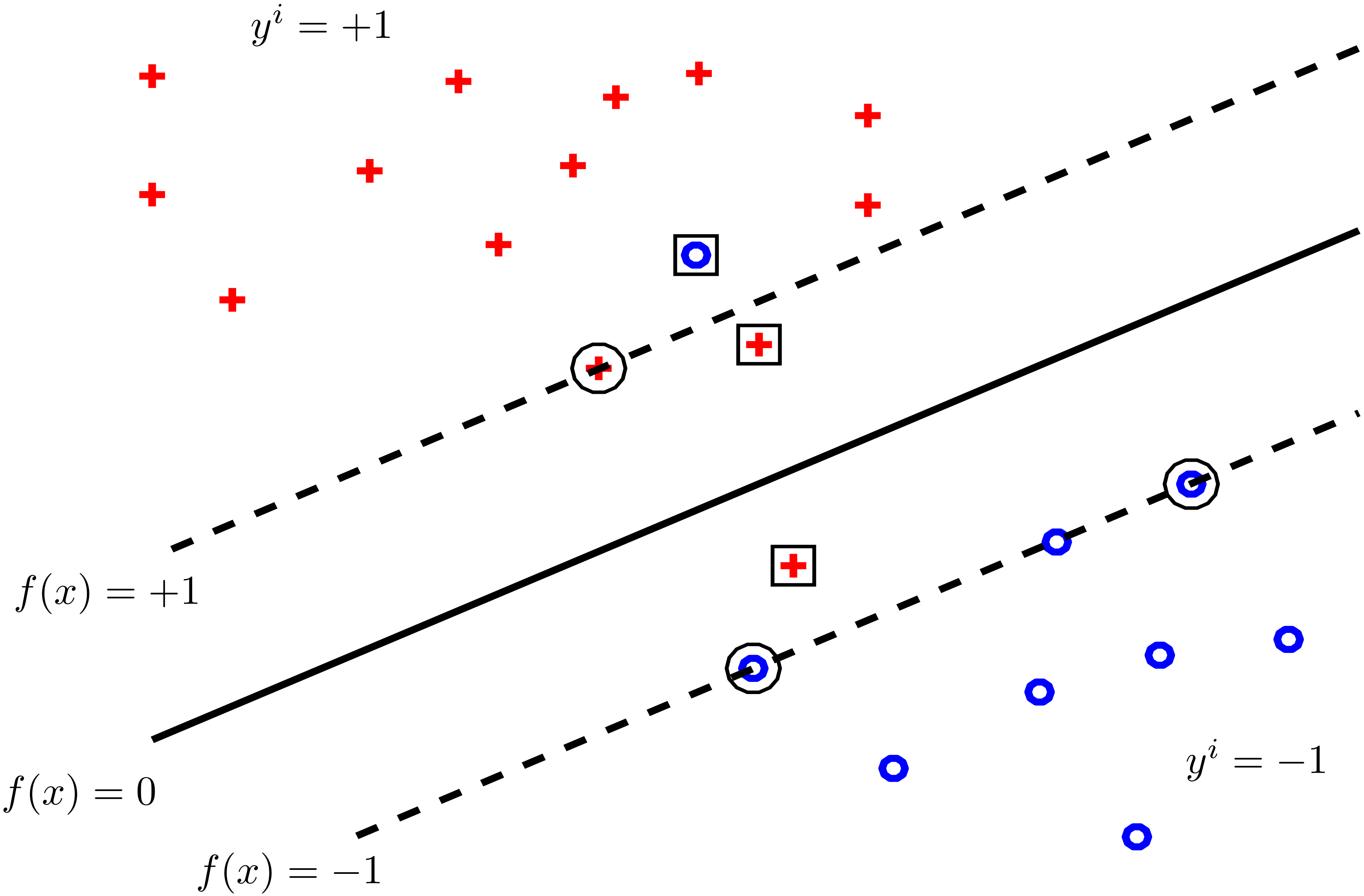


1/|w|=0.34

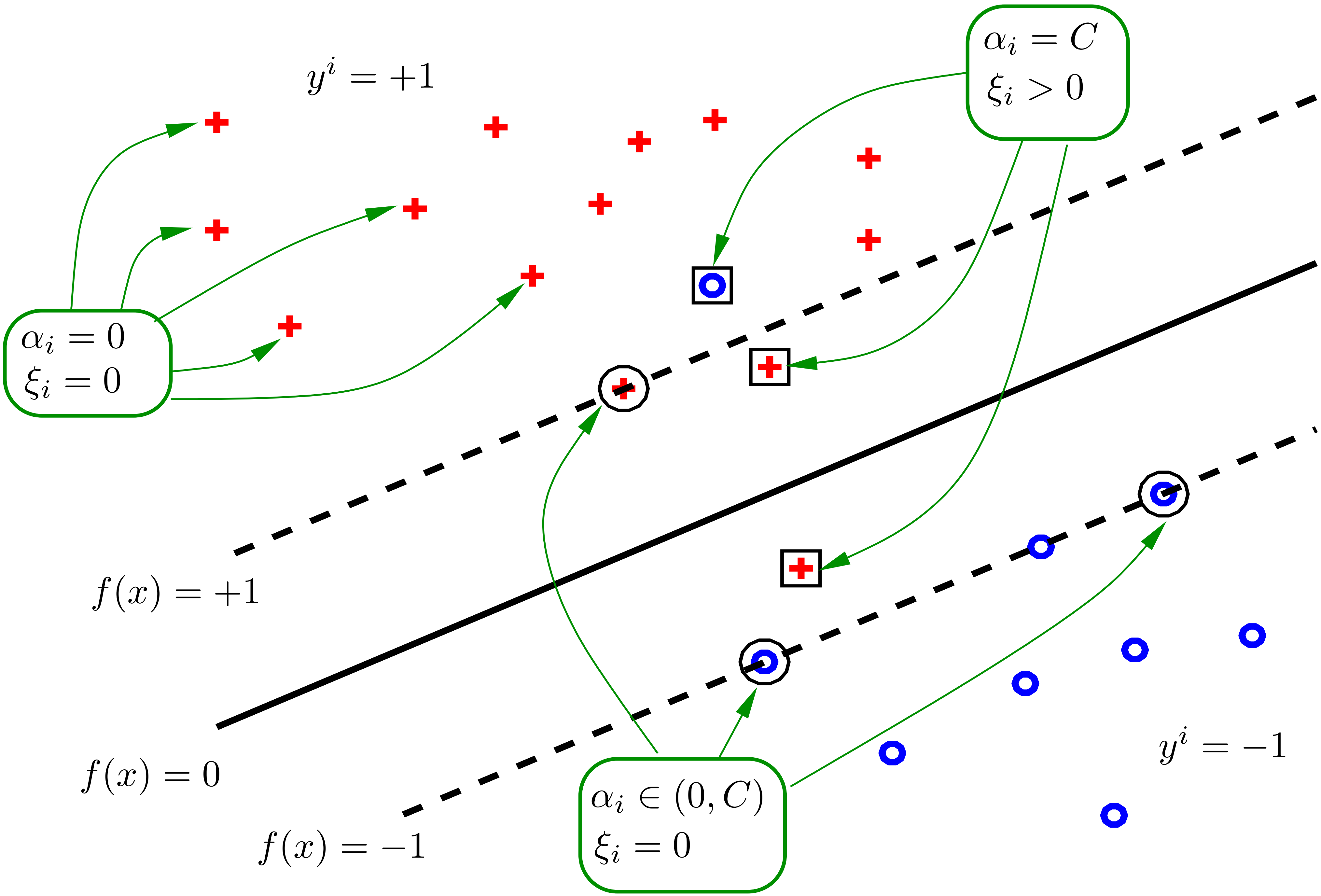

C=1000.0, |w|=2.96, trnErr=0.10, hingeLoss=0.22
0.3
0.25
0.2
0.15
0.1
3
2.5
2
1.5
1
trn error
hinge loss
|w|
10^-1
10^0
10^1
10^2
10^3
C



$y^i = +1$
$y^i = -1$



$y^i = +1$
$f(x) = +1$
$f(x) = 0$
$f(x) = -1$
$y^i = -1$



$y^i = +1$
$\alpha_i = C$
$\xi_i > 0$
$\alpha_i = 0$
$\xi_i = 0$
$f(x) = +1$
$f(x) = 0$
$f(x) = -1$
$\alpha_i \in (0, C)$
$\xi_i = 0$
$y^i = -1$