Approximately optimal selection of regularization parameter

for L2 regularized convex loss minimization problems for supervised classifications

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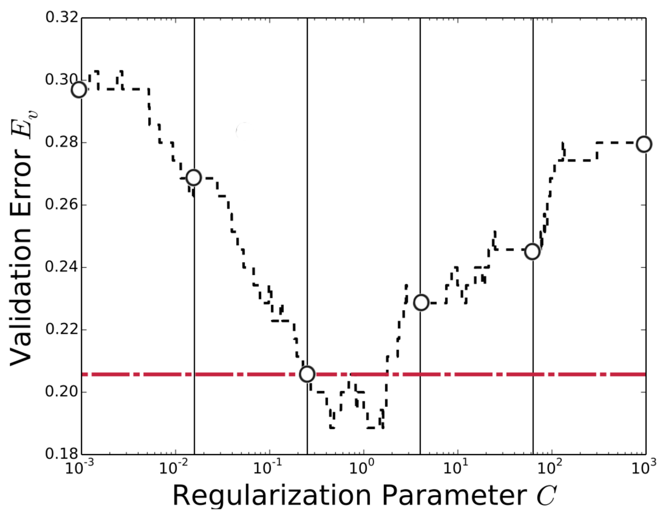
Abstract and problem formulation

Background : Grid search for model selection



- Can you find out about the difference in quality between exact optimal and a selected parameter ?
- If you use our algorithm, you can find out it in the sense that the validation error

Target problems: L2 regularized loss minimization problems (e.g. SVM)

- Training instances and labels : $\{(x_i, y_i) \in \mathbb{R}^d \times \{-1,1\}\}_{i\in[n]}$
- Validation instances and labels : $\{(x'_i, y'_i) \in \mathbb{R}^d \times \{-1,1\}\}_{i\in[n']}$

$$w^*_C := \arg\min_{w\in\mathbb{R}^d} \frac{1}{2}\|w\|^2 + C\sum_{i\in[n]} \ell(y_i, w^\top x_i) \quad (1)$$

Goal : Finding a theoretical approximation guarantee in the sense that the validation error for the regularization parameter is at most greater by $\varepsilon \in [0,1]$ than the smallest possible the validation error (2)

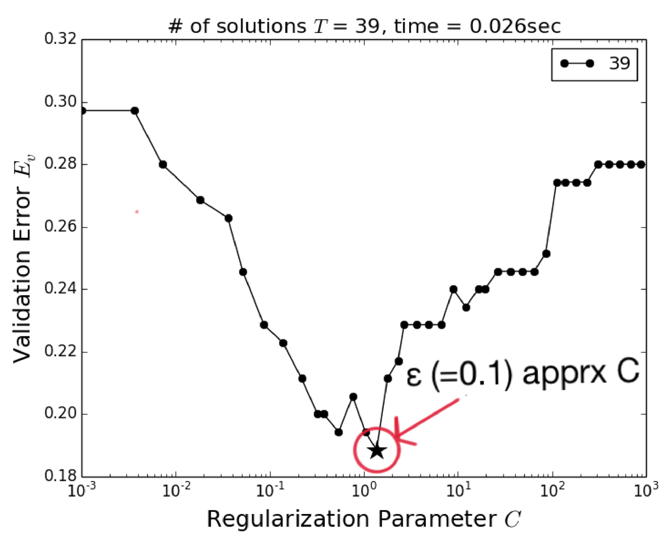
- Validation error : $E_v(w) := \frac{1}{n'}\sum_{i\in[n']} I(y'_i w^\top x'_i < 0)$
- ε-approximate regularization parameters ($\varepsilon \in [0,1]$) :

$$C(\varepsilon) := \left\{C \in [C_l, C_u] \,\middle|\, E_v(w^*_C) - (\text{the lowest } E_v \text{ in } [C_l, C_u]) \le \varepsilon\right\} \quad (2)$$

Contribution : The algorithm for finding an ε-approximate regularization parameter (input: ε, output: an ε-approximate regularization parameter)

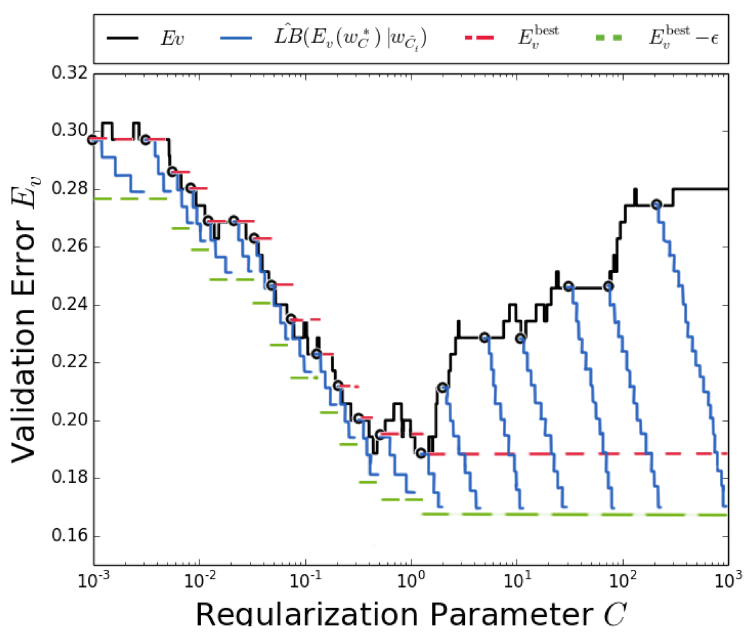
Approach : Computing the validation error lower bound as a function of the regularization parameter in the entire interval

Example : An illustration of the proposed algorithm (dataset : `ionosphere`)



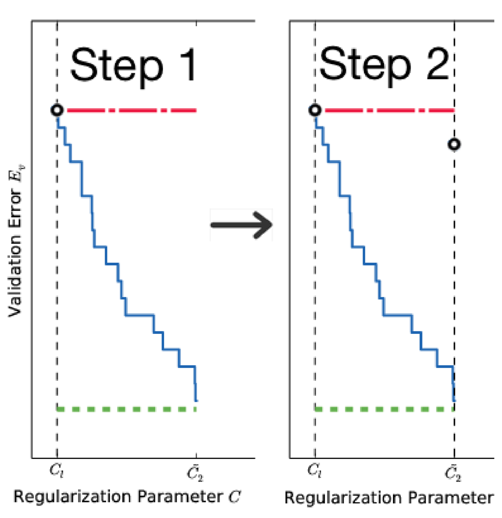
- The algorithm automatically selected 39 regularization parameter values in $[10^{-3}, 10^3]$
- And an upper bound of the validation error for each of the 39 regularization parameter values is obtained by solving an optimization problem (1)
- Among those 39 values, the one with the smallest validation error upper bound (indicated as ★ at $C = 1.368$) is guaranteed to be $\varepsilon(=0.1)$ *approximate regularization parameter* (2)

Details of approach : the behavior of the algorithm and the illustration



Our algorithm

- is built on novel technique for computing validation error lower bounds
- needs some solutions of (1) for computing validation error lower bound in the entire interval



Step0 Compute a solution $\hat{w}_{C_l}$ at the interval of the left end C_l

Step1 Compute validation error lower bound by using a solution we obtained at a previous step, and update the current best validation error upper bound

Step2 Find $\tilde{C}_{t+1}$ so that the best regularization parameter obtained is an ε-approximate regularization parameter in the interval $[C_l, \tilde{C}_{t+1}]$ and compute $\hat{w}_{\tilde{C}_{t+1}}$ at $C = \tilde{C}_{t+1}$

Step3 Continue Step1,2 until reach the interval of the right end C_u

Extensions : Cross-validation setup

- Proposed algorithm can be straightforwardly adapted to a cross-validation (CV) setup.

Theory : Validation error lower bounds $LB(E_v(w^*_C))$

$$LB(E_v(w^*_C)) = \frac{\text{\# validation instances that can be guaranteed to be mis-classified by using } w^*_C}{\text{\# validation instances}}$$

1. Compute lower and upper bound of inner product $w^{*\top}_C x'_i$
   - Construct existing ranges of optimal solutions (hypersphere) by using $\hat{w}_{\tilde{C}}$

1.1 Optimal condition : $(\underbrace{w^*_C + C\sum \xi_i(w^*_C)}_{\text{a subgradient of (1)}: g(w^*_C)})^\top (w^*_C - \hat{w}_{\tilde{C}}) \le 0$

$(\xi_i(w^*_C)$ is a subgradient of the loss function $\ell_i(w) := \ell(y_i, w^\top x_i))$

1.2 Definition of subgradient : $\ell_i(w^*_C) \ge \ell_i(\hat{w}_{\tilde{C}}) + \xi_i(\hat{w}_{\tilde{C}})^\top (w^*_C - \hat{w}_{\tilde{C}})$
$\ell_i(\hat{w}_{\tilde{C}}) \ge \ell_i(w^*_C) + \xi_i(w^*_C)^\top (\hat{w}_{\tilde{C}} - w^*_C)$

$$\Rightarrow \Big\|w^*_C - \underbrace{\frac{1}{2}\Big(\hat{w}_{\tilde{C}} - \frac{C}{\tilde{C}}(g(\hat{w}_{\tilde{C}}) - \hat{w}_{\tilde{C}})\Big)}_{\text{center}}\Big\|^2 \le \Big(\underbrace{\frac{1}{2}\Big\|\hat{w}_{\tilde{C}} + \frac{C}{\tilde{C}}(g(\hat{w}_{\tilde{C}}) - \hat{w}_{\tilde{C}})\Big\|}_{\text{radius}}\Big)^2 \quad (3)$$

- Solve following optimization problems :

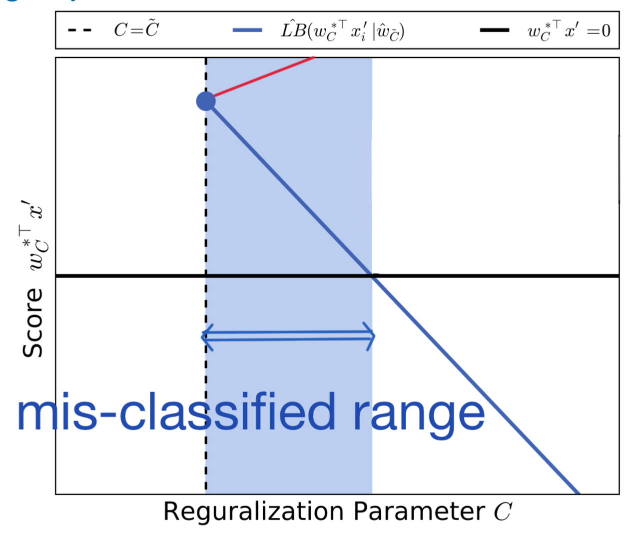
Lower bound : $w^{*\top}_C x'_i \ge \hat{LB}(w^{*\top}_C x'_i \mid \hat{w}_{\tilde{C}}) := \min_w w^\top x'_i$ s.t. (3)

Upper bound : $w^{*\top}_C x'_i \le \hat{UB}(w^{*\top}_C x'_i \mid \hat{w}_{\tilde{C}}) := \max_w w^\top x'_i$ s.t. (3)

   - have explicit solutions
   - are change linearly with a regularized parameter

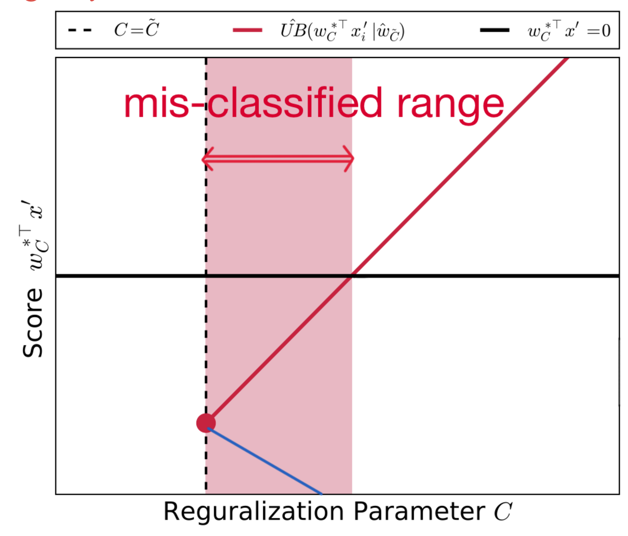
2. Identify the interval of C within which the validation instance is guaranteed to be mis-classified
   - similar to following two images (according to the sign of labels y'_i)

$\hat{LB}(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}})$:monotonic decrease ($C > \tilde{C}$)



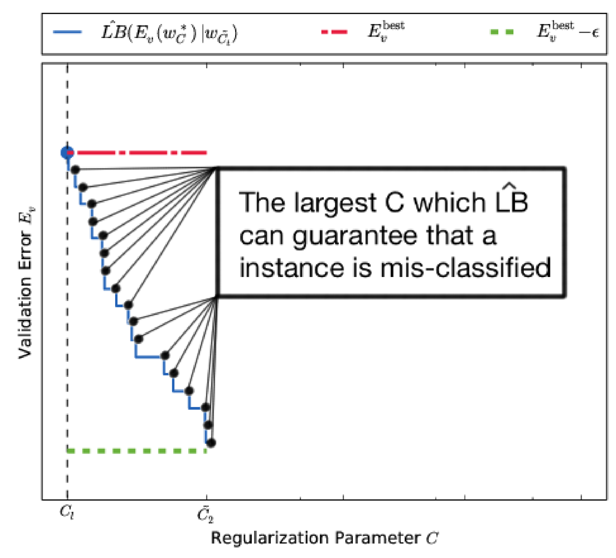
mis-classified case 1 ($y'_i = -1$) :
$0 < LB(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}}) \Rightarrow$
the interval between $\tilde{C}$ and C that $\hat{LB}(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}})$ becomes 0

$\hat{UB}(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}})$:monotonic increace ($C > \tilde{C}$)



mis-classified case2 ($y'_i = +1$) :
$UB(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}}) < 0 \Rightarrow$
the interval between $\tilde{C}$ and C that $\hat{UB}(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}})$ becomes 0

3. Compute validation error lower bound $\hat{LB}(E_v(w^*_C)|\hat{w}_{\tilde{C}})$

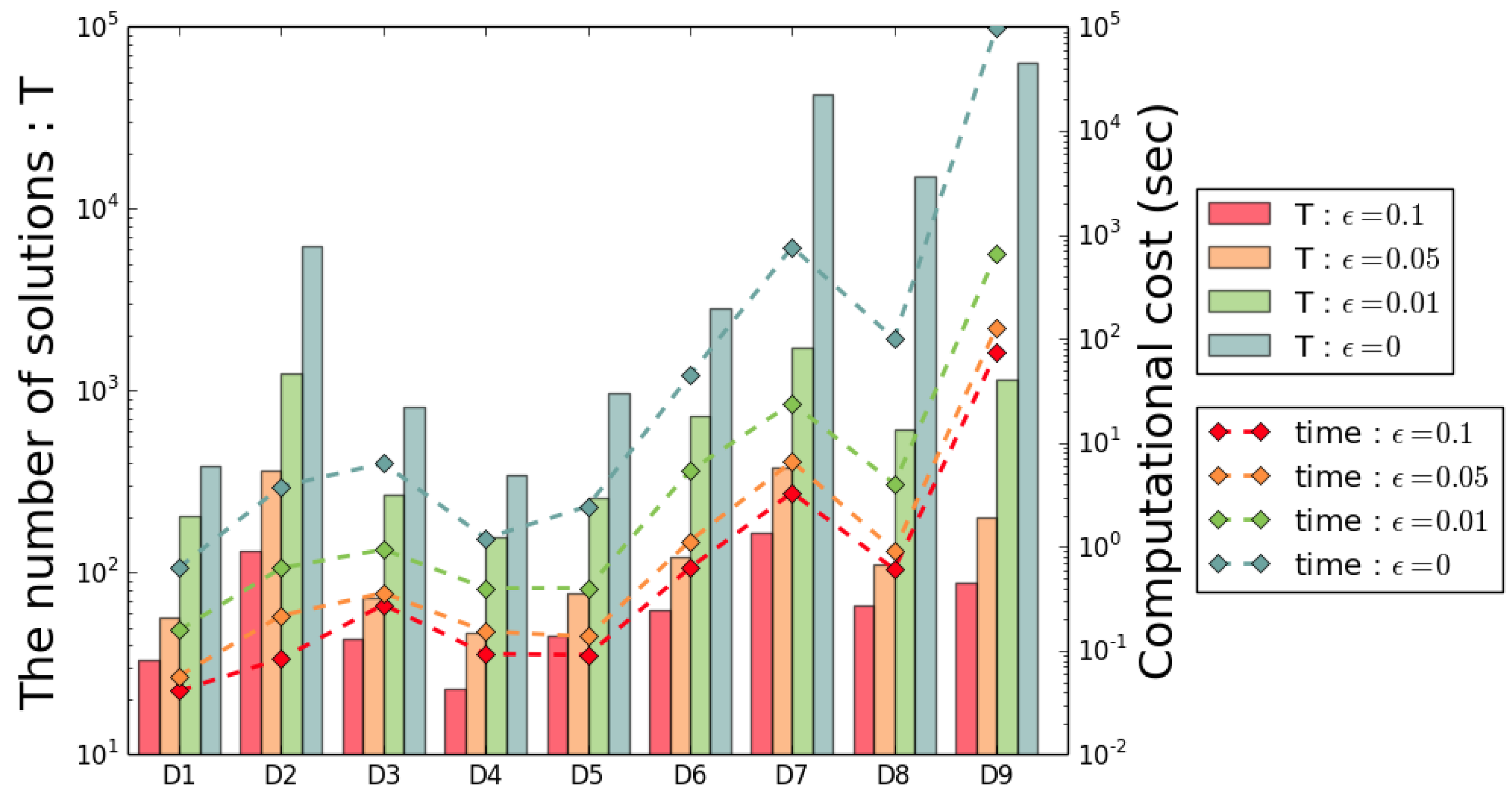


- When $\hat{LB}(w^{*\top}_C x'_i|\hat{w}_{\tilde{C}})$ cannot guarantee that a validation instance x'_i is mis-classified, the validation error lower bound decrease $1/n'$
- Therefore, the validation error lower bound is staircase function

Experiments : finding an ε-approximate regularization parameter

- Under 10-fold cross validation setup
- The entire interval of regularization parameter : $[10^{-3}, 10^3]$
- Loss function $\ell_i(w)$: smooth hinge-loss
- Input : $\varepsilon = \{0.1,\ 0.05,\ 0.01,\ 0\}$

	dataset name	sample size	input dimension		dataset name	sample size	input dimension
D1	`heart`	270	13	D6	`german.numer`	1000	24
D2	`liver-disorders`	345	6	D7	`svmguide3`	1284	21
D3	`ionosphere`	351	34	D8	`svmguide1`	7089	4
D4	`australian`	690	14	D9	`a1a`	32561	123
D5	`diabetes`	768	8				



Shibagaki et al. Regularization Path of Cross-Validation Error Lower Bounds. arXiv:1502.02344.