

# University of Pisa Department of Computer Science

Computational Mathematics
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Group 35

# Support Vector Machines

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#### 1 Track

- (M1.1) is a Support Vector Classifier (SVC) with the hinge loss.
  - (A1.1.1) is a momentum descent approach [1, 2, 3], an accelerated gradient method for solving the SVC in its primal formulation.
  - (A1.1.2) is the Sequential Minimal Optimization (SMO) algorithm [4, 5], an ad hoc active set method for training a SVC in its Wolfe dual formulation with linear, polynomial and gaussian kernels.
  - (A1.1.3) is the AdaGrad algorithm [6], a deflected subgradient method for solving the SVC in its Lagrangian dual formulation with linear, polynomial and gaussian kernels.
- (M1.2) is a Support Vector Classifier (SVC) with the squared hinge loss.
  - (A1.2.1) is a momentum descent approach [1, 2, 3], an accelerated gradient method for solving the SVC in its primal formulation.
  - (A1.2.2) is the AdaGrad algorithm [6], a deflected subgradient method for solving the SVC in its Lagrangian dual formulation with linear, polynomial and gaussian kernels.
- (M2.1) is a Support Vector Regression (SVR) with the epsilon-insensitive loss.
  - (A2.1.1) is a momentum descent approach [1, 2, 3], an accelerated gradient method for solving the SVR in its primal formulation.
  - (A2.1.2) is the Sequential Minimal Optimization (SMO) algorithm [7, 8], an ad hoc active set method for training a SVR in its Wolfe dual formulation with linear, polynomial and gaussian kernels.
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- (M2.2) is a Support Vector Regression (SVR) with the squared epsilon-insensitive loss.
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  - (A2.2.2) is the AdaGrad algorithm [6], a deflected subgradient method for solving the SVR in its Lagrangian dual formulation with linear, polynomial and gaussian kernels.

#### 2 Abstract

A Support Vector Machine is a learning model used both for classification and regression tasks whose goal is to construct a maximum margin separator, i.e., a decision boundary with the largest distance from the nearest training data points.

The aim of this report is to compare the *primal*, the Wolfe dual [9] and the Lagrangian dual formulations of this model in terms of numerical precision, accuracy and complexity.

Firstly, I will provide a detailed mathematical derivation of the model for all these formulations, then I will propose two algorithms to solve the optimization problem in case of *constrained* or *unconstrained* formulation of the problem, explaining their theoretical properties, i.e., *convergence* and *complexity*.

Finally, I will show some experiments for linearly and nonlinearly separable generated datasets to compare the performance of different kernels, also by comparing the custom results with sklearn SVM implementations, i.e., liblinear [10] and libsvm [11] implementations, and cvxopt [12] QP solver.

## 3 Linear Support Vector Classifier

Given n training points, where each input  $x_i$  has m attributes, i.e., is of dimensionality m, and is in one of two classes  $y_i = \pm 1$ , i.e., our training data is of the form:

$$\{(x_i, y_i), x_i \in \Re^m, y_i = \pm 1, i = 1, \dots, n\}$$
(1)

For simplicity we first assume that data are (not fully) linearly separable in the input space x, meaning that we can draw a line separating the two classes when m=2, a plane for m=3 and, more in general, a hyperplane for an arbitrary m.

Support vectors are the examples closest to the separating hyperplane and the aim of support vector machines is to orientate this hyperplane in such a way as to be as far as possible from the closest members of both classes, i.e., we need to maximize this margin.

This hyperplane is represented by the equation  $w^T x + b = 0$ . So, we need to find w and b so that our training data can be described by:

$$w^{T}x_{i} + b \ge +1 - \xi_{i}, \forall y_{i} = +1$$

$$w^{T}x_{i} + b \le -1 + \xi_{i}, \forall y_{i} = -1$$

$$\xi_{i} \ge 0 \ \forall_{i}$$

$$(2)$$

where the positive slack variables  $\xi_i$  are introduced to allow misclassified points. In this way data points on the incorrect side of the margin boundary will have a penalty that increases with the distance from it.

These two equations can be combined into:

$$y_i(w^T x_i + b) \ge 1 - \xi_i \ \forall_i$$
  
$$\xi_i \ge 0 \ \forall_i$$
 (3)

The margin is equal to  $\frac{1}{\|w\|}$  and maximizing it subject to the constraint in (3) while as we are trying to reduce the number of misclassifications is equivalent to finding:

$$\min_{\substack{w,b,\xi}} ||w|| + C \sum_{i=1}^{n} \xi_{i}$$
subject to 
$$y_{i}(w^{T}x_{i} + b) \ge 1 - \xi_{i} \,\forall_{i}$$

$$\xi_{i} \ge 0 \,\forall_{i}$$
(4)

Minimizing ||w|| is equivalent to minimizing  $\frac{1}{2}||w||^2$ , but in this form we will deal with a 1-strongly convex regularization term that has more desirable convergence properties. So we need to find:

$$\min_{\substack{w,b,\xi}} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i$$
subject to  $y_i(w^T x_i + b) \ge 1 - \xi_i \ \forall_i$ 

$$\xi_i \ge 0 \ \forall_i$$
(5)

where the parameter C controls the trade-off between the slack variable penalty and the size of the margin.



Figure 1: Linear SVC hyperplane

#### 3.1 Hinge loss

The *hinge* loss is defined as:

$$\mathcal{L}_1 = \max(0, 1 - y(w^T x + b)) \tag{6}$$

or, equivalently:

$$\mathcal{L}_1 = \begin{cases} 0 & \text{if } y(w^T x + b) \ge 1\\ 1 - y(w^T x + b) & \text{otherwise} \end{cases}$$
 (7)

and it is a nondifferentiable convex function due to its nonsmoothness in 1, but has a subgradient that is given by:

$$\partial_w \mathcal{L}_1 = \begin{cases} -yx & \text{if } y(w^T x + b) < 1\\ 0 & \text{otherwise} \end{cases}$$
 (8)

#### 3.1.1 Primal formulation

The general primal unconstrained formulation takes the form:

$$\min_{w,b} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \mathcal{L}(w,b;x_i,y_i)$$
(9)

where  $\frac{1}{2}||w||^2$  is the regularization term and  $\mathcal{L}(w, b; x_i, y_i)$  is the loss function associated with the observation  $(x_i, y_i)$  [13].

The quadratic optimization problem (5) can be equivalently formulated as:

$$\min_{w,b} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \max(0, 1 - y_i(w^T x_i + b))$$
(10)

where we make use of the hinge loss (6) or (7).

The above formulation penalizes slacks  $\xi$  linearly and is called  $\mathcal{L}_1$ -SVC.

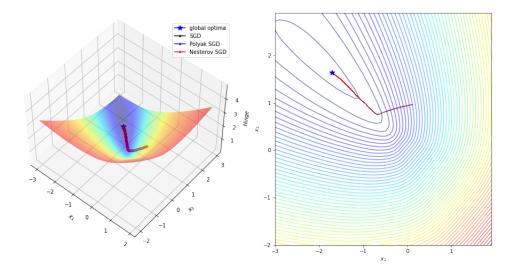


Figure 2: Hinge loss with different optimization steps

To simplify the notation and so also the design of the algorithms, the simplest approach to learn the bias term b is that of including that into the regularization term; so we can rewrite (9) as follows:

$$\min_{w,b} \frac{1}{2} (\|w\|^2 + b^2) + C \sum_{i=1}^{n} \mathcal{L}(w,b;x_i,y_i)$$
(11)

or, equivalently, by augmenting the weight vector w with the bias term b and each instance  $x_i$  with an additional dimension, i.e., with constant value equal to 1:

$$\min_{w} \quad \frac{1}{2} \|\hat{w}\|^{2} + C \sum_{i=1}^{n} \mathcal{L}(\hat{w}; \hat{x}_{i}, y_{i})$$
where  $\hat{w}^{T} = [w^{T}, b]$ 

$$\hat{x}_{i}^{T} = [x_{i}^{T}, 1]$$
(12)

with the advantages of having convex properties of the objective function useful for convergence analysis and the possibility to directly apply algorithms designed for models without the bias term.

In the specific case of the  $\mathcal{L}_1$ -SVC the objective (10) become:

$$\min_{w,b} \frac{1}{2} (\|w\|^2 + b^2) + C \sum_{i=1}^{n} \max(0, 1 - y_i(w^T x_i + b))$$
(13)

Note that in terms of numerical optimization the formulation (10) is not equivalent to (13) since in the first one the bias term b does not contribute to the regularization term, so the SVM formulation is based on an unregularized bias term b, as highlighted by the statistical learning theory. But, in machine learning sense, numerical experiments in [14] show that the accuracy does not vary much when the bias term b is embedded into the weight vector w.

(20)

#### 3.1.2 Wolfe Dual formulation

To reformulate the (5) as a Wolfe dual, we need to allocate the Lagrange multipliers  $\alpha_i, \mu_i \geq 0 \ \forall_i$ :

$$\max_{\alpha,\mu} \min_{w,b,\xi} \mathcal{W}(w,b,\xi,\alpha,\mu) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i (y_i(w^T x_i + b) - 1 + \xi_i) - \sum_{i=1}^n \mu_i \xi_i$$
(14)

We wish to find the w, b and  $\xi_i$  which minimizes, and the  $\alpha$  and  $\mu$  which maximizes  $\mathcal{W}$ , provided  $\alpha_i \geq 0$ ,  $\mu_i \geq 0 \,\forall_i$ . We can do this by differentiating  $\mathcal{W}$  wrt w and b and setting the derivatives to 0:

$$\frac{\partial \mathcal{W}}{\partial w} = w - \sum_{i=1}^{n} \alpha_i y_i x_i \Rightarrow w = \sum_{i=1}^{n} \alpha_i y_i x_i \tag{15}$$

$$\frac{\partial \mathcal{W}}{\partial b} = -\sum_{i=1}^{n} \alpha_i y_i \Rightarrow \sum_{i=1}^{n} \alpha_i y_i = 0$$
 (16)

$$\frac{\partial \mathcal{W}}{\partial \xi_i} = 0 \Rightarrow C = \alpha_i + \mu_i \tag{17}$$

Substituting (15) and (16) into (14) together with  $\mu_i \geq 0 \ \forall_i$ , which implies that  $\alpha \leq C$ , gives a new formulation being dependent on  $\alpha$ . We therefore need to find:

$$\max_{\alpha} \mathcal{W}(\alpha) = \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} \langle x_{i}, x_{j} \rangle$$

$$= \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} Q_{ij} \alpha_{j} \text{ where } Q_{ij} = y_{i} y_{j} \langle x_{i}, x_{j} \rangle$$

$$= \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \alpha^{T} Q \alpha \text{ subject to } 0 \leq \alpha_{i} \leq C \ \forall_{i}, \sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$(18)$$

or, equivalently:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} Q \alpha + q^{T} \alpha$$
subject to  $0 \le \alpha_{i} \le C \ \forall_{i}$ 

$$y^{T} \alpha = 0$$
(19)

where  $q^T = [1, ..., 1].$ 

By solving (19) we will know  $\alpha$  and, from (15), we will get w, so we need to calculate b. We know that any data point satisfying (16) which is a support vector  $x_s$  will have the form:

$$y_s(w^T x_s + b) = 1$$

and, by substituting in (15), we get:

$$y_s \left( \sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle + b \right) = 1 \tag{21}$$

where s denotes the set of indices of the support vectors and is determined by finding the indices i where  $\alpha_i > 0$ , i.e., nonzero Lagrange multipliers.

Multiplying through by  $y_s$  and then using  $y_s^2 = 1$  from (2):

$$y_s^2 \left( \sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle + b \right) = y_s \tag{22}$$

$$b = y_s - \sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle \tag{23}$$

Instead of using an arbitrary support vector  $x_s$ , it is better to take an average over all of the support vectors in S:

$$b = \frac{1}{N_s} \sum_{s \in S} y_s - \sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle \tag{24}$$

We now have the variables w and b that define our separating hyperplane's optimal orientation and hence our support vector machine. Each new point x' is classified by evaluating:

$$y' = \operatorname{sign}\left(\sum_{i=1}^{n} \alpha_i y_i \langle x_i, x' \rangle + b\right)$$
(25)

From (19) we can notice that the equality constraint  $y^T \alpha = 0$  arises form the stationarity condition  $\partial_b \mathcal{W} = 0$ . So, again, for simplicity, we can again consider the bias term b embedded into the weight vector. We report below the box-constrained dual formulation [14] that arises from the primal (11) or (12) where the bias term b is embedded into the weight vector w:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} (Q + yy^{T}) \alpha + q^{T} \alpha$$
subject to  $0 < \alpha_{i} < C \ \forall_{i}$  (26)

#### 3.1.3 Lagrangian Dual formulation

In order to relax the constraints in the Wolfe dual formulation (19) we define the problem as a Lagrangian dual relaxation by embedding them into objective function, so we need to allocate the Lagrange multipliers  $\mu$  and  $\lambda_+, \lambda_- \geq 0$ :

$$\max_{\mu,\lambda_{+},\lambda_{-}} \min_{\alpha} \mathcal{L}(\alpha,\mu,\lambda_{+},\lambda_{-}) = \frac{1}{2} \alpha^{T} Q \alpha + q^{T} \alpha - \mu^{T} (y^{T} \alpha) - \lambda_{+}^{T} (u - \alpha) - \lambda_{-}^{T} \alpha$$

$$= \frac{1}{2} \alpha^{T} Q \alpha + (q - \mu y + \lambda_{+} - \lambda_{-})^{T} \alpha - \lambda_{+}^{T} u$$
subject to  $\lambda_{+},\lambda_{-} \geq 0$ 

$$(27)$$

where the upper bound  $u^T = [C, \dots, C]$ .

Taking the derivative of the Lagrangian  $\mathcal{L}$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow Q\alpha + (q - \mu y + \lambda_{+} - \lambda_{-}) = 0 \tag{28}$$

With  $\alpha$  optimal solution of the linear system:

$$Q\alpha = -(q - \mu y + \lambda_+ - \lambda_-) \tag{29}$$

the gradient wrt  $\mu$ ,  $\lambda_{+}$  and  $\lambda_{-}$  are:

$$\frac{\partial \mathcal{L}}{\partial \mu} = -y\alpha \tag{30}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{+}} = \alpha - u \tag{31}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{-}} = -\alpha \tag{32}$$

From (19) we can notice that the equality constraint  $y^T \alpha = 0$  arises form the stationarity condition  $\partial_b \mathcal{W} = 0$ . So, again, for simplicity, we can again consider the bias term b embedded into the weight vector. In this way the dimensionality of (27) is reduced of 1/3 by removing the multipliers  $\mu$  which was allocated to control the equality constraint  $y^T \alpha = 0$ , so we will end up solving exactly the problem (26).

$$\max_{\lambda_{+},\lambda_{-}} \min_{\alpha} \mathcal{L}(\alpha,\lambda_{+},\lambda_{-}) = \frac{1}{2} \alpha^{T} (Q + yy^{T}) \alpha + q^{T} \alpha - \lambda_{+}^{T} (u - \alpha) - \lambda_{-}^{T} \alpha 
= \frac{1}{2} \alpha^{T} (Q + yy^{T}) \alpha + (q + \lambda_{+} - \lambda_{-})^{T} \alpha - \lambda_{+}^{T} u 
\text{subject to} \quad \lambda_{+},\lambda_{-} \ge 0$$
(33)

where, again, the upper bound  $u^T = [C, ..., C]$ .

Now, taking the derivative of the Lagrangian  $\mathcal{L}$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + yy^T)\alpha + (q + \lambda_+ - \lambda_-) = 0 \tag{34}$$

With  $\alpha$  optimal solution of the linear system:

$$(Q + yy^T)\alpha = -(q + \lambda_+ - \lambda_-)$$
(35)

the gradient wrt  $\lambda_{+}$  and  $\lambda_{-}$  are:

$$\frac{\partial \mathcal{L}}{\partial \lambda_{+}} = \alpha - u \tag{36}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{-}} = -\alpha \tag{37}$$

#### 3.2 Squared Hinge loss

The squared hinge loss is defined as:

$$\mathcal{L}_2 = \max(0, 1 - y(w^T x + b))^2 \tag{38}$$

or, equivalently:

$$\mathcal{L}_2 = \begin{cases} 0 & \text{if } y(w^T x + b) \ge 1\\ (1 - y(w^T x + b))^2 & \text{otherwise} \end{cases}$$
 (39)

It is a strictly convex function and its gradient is given by:

$$\nabla_w \mathcal{L}_2 = \begin{cases} -2yx & \text{if } y(w^T x + b) < 1\\ 0 & \text{otherwise} \end{cases}$$
 (40)

#### 3.2.1 Primal formulation

Since smoothed versions of objective functions may be preferred for optimization, we can reformulate (10) as:

$$\min_{w,b} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \max(0, 1 - y_i(w^T x_i + b))^2$$
(41)

where we make use of the squared hinge loss that quadratically penalized slacks  $\xi$  and is called  $\mathcal{L}_2$ -SVC. The  $\mathcal{L}_2$ -SVC objective (41) can be rewritten in form (11) or (12) as:

$$\min_{w,b} \frac{1}{2} (\|w\|^2 + b^2) + C \sum_{i=1}^{n} \max(0, 1 - y_i(w^T x_i + b))^2$$
(42)

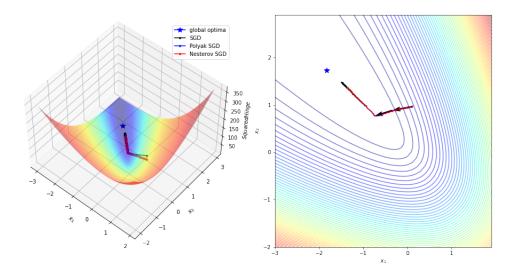


Figure 3: Squared Hinge loss with different optimization steps

#### 3.2.2 Wolfe Dual formulation

As done for the  $\mathcal{L}_1$ -SVC we can derive the Wolfe dual formulation of the  $\mathcal{L}_2$ -SVC by obtaining:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} (Q + D) \alpha + q^{T} \alpha$$
subject to  $\alpha_{i} \geq 0 \ \forall_{i}$ 

$$y^{T} \alpha = 0$$
(43)

or, alternatively, with the regularized bias term by obtaining:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} (Q + yy^{T} + D) \alpha + q^{T} \alpha$$
subject to  $\alpha_{i} \geq 0 \ \forall_{i}$  (44)

where the diagonal matrix  $D_{ii} = \frac{1}{2C} \,\forall_i$ .

#### 3.2.3 Lagrangian Dual formulation

In order to relax the constraints in the  $\mathcal{L}_2$ -SVC Wolfe dual formulation (43) we define the problem as a Lagrangian dual relaxation by embedding them into objective function, so we need to allocate the Lagrange multipliers  $\mu$  and  $\lambda \geq 0$ :

$$\max_{\mu,\lambda} \min_{\alpha} \mathcal{L}(\alpha, \mu, \lambda) = \frac{1}{2} \alpha^{T} (Q + D) \alpha + q^{T} \alpha - \mu^{T} (y^{T} \alpha) - \lambda^{T} \alpha$$

$$= \frac{1}{2} \alpha^{T} (Q + D) \alpha + (q - \mu y - \lambda)^{T} \alpha$$
subject to  $\lambda \geq 0$  (45)

Taking the derivative of the Lagrangian  $\mathcal{L}$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + D)\alpha + (q - \mu y - \lambda) = 0 \tag{46}$$

With  $\alpha$  optimal solution of the linear system:

$$(Q+D)\alpha = -(q-\mu y - \lambda) \tag{47}$$

the gradient wrt  $\mu$  and  $\lambda$  are:

$$\frac{\partial \mathcal{L}}{\partial \mu} = -y\alpha \tag{48}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = -\alpha \tag{49}$$

From (19) we can notice that the equality constraint  $y^T \alpha = 0$  arises form the stationarity condition  $\partial_b \mathcal{W} = 0$ . So, again, for simplicity, we can again consider the bias term b embedded into the weight vector. In this way the dimensionality of (45) is reduced of 1/3 by removing the multipliers  $\mu$  which was allocated to control the equality constraint  $y^T \alpha = 0$ , so we will end up solving exactly the problem (44).

$$\max_{\lambda} \min_{\alpha} \mathcal{L}(\alpha, \lambda) = \frac{1}{2} \alpha^{T} (Q + yy^{T} + D) \alpha + q^{T} \alpha - \lambda^{T} \alpha$$

$$= \frac{1}{2} \alpha^{T} (Q + yy^{T} + D) \alpha + (q - \lambda)^{T} \alpha$$
subject to  $\lambda \ge 0$  (50)

where, again, the upper bound  $u^T = [C, \dots, C]$ .

Now, taking the derivative of the Lagrangian  $\mathcal L$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + yy^T + D)\alpha + (q - \lambda) = 0$$
(51)

With  $\alpha$  optimal solution of the linear system:

$$(Q + yy^{T} + D)\alpha = -(q - \lambda)$$
(52)

the gradient wrt  $\lambda$  is:

$$\frac{\partial \mathcal{L}}{\partial \lambda} = -\alpha \tag{53}$$

## 4 Linear Support Vector Regression

In the case of regression the goal is to predict a real-valued output for y' so that our training data is of the form:

$$\{(x_i, y_i), x \in \Re^m, y_i \in \Re, i = 1, \dots, n\}$$
 (54)

The regression SVM use a loss function that not allocating a penalty if the predicted value  $y_i'$  is less than a distance  $\epsilon$  away from the actual value  $y_i$ , i.e., if  $|y_i - y_i'| \le \epsilon$ , where  $y_i' = w^T x_i + b$ . The region bound by  $y_i' \pm \epsilon \ \forall_i$  is called an  $\epsilon$ -insensitive tube. The output variables which are outside the tube are given one of two slack variable penalties depending on whether they lie above,  $\xi^+$ , or below,  $\xi^-$ , the tube, provided  $\xi^+ \ge 0$  and  $\xi^- \ge 0 \ \forall_i$ :

$$y_{i} \leq y'_{i} + \epsilon + \xi^{+} \forall_{i}$$

$$y_{i} \geq y'_{i} - \epsilon - \xi^{-} \forall_{i}$$

$$\xi_{i}^{+}, \xi_{i}^{-} \geq 0 \forall_{i}$$

$$(55)$$

The objective function for SVR can then be written as:

$$\min_{\substack{w,b,\xi^{+},\xi^{-} \\ w,b,\xi^{+},\xi^{-}}} \frac{1}{2} \|w\|^{2} + C \sum_{i=1}^{n} (\xi_{i}^{+} + \xi_{i}^{-})$$
subject to  $y_{i} - w^{T} x_{i} - b \leq \epsilon + \xi_{i}^{+} \ \forall_{i}$ 

$$w^{T} x_{i} + b - y_{i} \leq \epsilon + \xi_{i}^{-} \ \forall_{i}$$

$$\xi_{i}^{+}, \xi_{i}^{-} \geq 0 \ \forall_{i}$$
(56)



Figure 4: Linear SVR hyperplane

#### 4.1 Epsilon-insensitive loss

The *epsilon-insensitive* loss is defined as:

$$\mathcal{L}_{\epsilon}^{1} = \max(0, |y - (w^{T}x + b)| - \epsilon) \tag{57}$$

or, equivalently:

$$\mathcal{L}_{\epsilon}^{1} = \begin{cases} 0 & \text{if } |y - (w^{T}x + b)| \le \epsilon \\ |y - (w^{T}x + b)| - \epsilon & \text{otherwise} \end{cases}$$
 (58)

As the *hinge* loss, also the *epsilon-insensitive* loss is a nondifferentiable convex function due to its nonsmoothness in  $\pm \epsilon$ , but has a subgradient that is given by:

$$\partial_w \mathcal{L}_{\epsilon}^1 = \begin{cases} \frac{y - (w^T x + b)}{|y - (w^T x + b)|} x & \text{if } |y - (w^T x + b)| \ge \epsilon \\ 0 & \text{otherwise} \end{cases}$$
 (59)

#### 4.1.1 Primal formulation

The general primal unconstrained formulation takes the same form of (9).

The quadratic optimization problem (56) can be equivalently formulated as:

$$\min_{w,b} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \max(0, |y_i - (w^T x_i + b)| - \epsilon)$$
(60)

where we make use of the *epsilon-insensitive* loss (57) or (58).

The above formulation penalizes slacks  $\xi$  linearly and is called  $\mathcal{L}_1$ -SVR.

The  $\mathcal{L}_1$ -SVR objective (60) can be rewritten in form (11) or (12) as:

$$\min_{w,b} \frac{1}{2} (\|w\|^2 + b^2) + C \sum_{i=1}^{n} \max(0, |y_i - (w^T x_i + b)| - \epsilon)$$
(61)

#### 4.1.2 Wolfe Dual formulation

To reformulate the (56) as a Wolfe dual, we introduce the Lagrange multipliers  $\alpha_i^+, \alpha_i^-, \mu_i^+, \mu_i^- \geq 0 \ \forall i$ :

$$\max_{\alpha^{+},\alpha^{-},\mu^{+},\mu^{-}} \min_{w,b,\xi^{+},\xi^{-}} \mathcal{W}(w,b,\xi^{+},\xi^{-},\alpha^{+},\alpha^{-},\mu^{+},\mu^{-}) = \frac{1}{2} \|w\|^{2} + C \sum_{i=1}^{n} (\xi_{i}^{+} + \xi_{i}^{-}) - \sum_{i=1}^{n} (\mu_{i}^{+} \xi_{i}^{+} + \mu_{i}^{-} \xi_{i}^{-}) \\
- \sum_{i=1}^{n} \alpha_{i}^{+} (\epsilon + \xi_{i}^{+} + y_{i}' - y_{i}) - \sum_{i=1}^{n} \alpha_{i}^{-} (\epsilon + \xi_{i}^{-} - y_{i}' + y_{i})$$
(62)

Substituting for  $y_i$ , differentiating wrt  $w, b, \xi^+, \xi^-$  and setting the derivatives to 0 gives:

$$\frac{\partial \mathcal{W}}{\partial w} = w - \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) x_i \Rightarrow w = \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) x_i$$
 (63)

$$\frac{\partial \mathcal{W}}{\partial b} = -\sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) \Rightarrow \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) = 0$$
 (64)

$$\frac{\partial \mathcal{W}}{\partial \xi_i^+} = 0 \Rightarrow C = \alpha_i^+ + \mu_i^+ \tag{65}$$

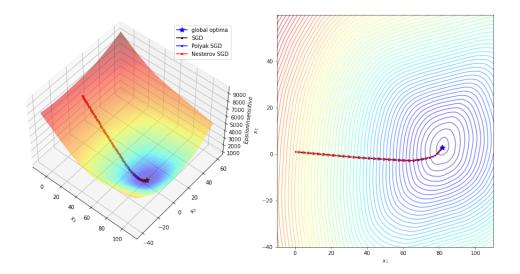


Figure 5: Epsilon-insensitive loss with different optimization steps

$$\frac{\partial \mathcal{W}}{\partial \xi_i^-} = 0 \Rightarrow C = \alpha_i^- + \mu_i^- \tag{66}$$

Substituting (63) and (64) in, we now need to maximize W wrt  $\alpha_i^+$  and  $\alpha_i^-$ , where  $\alpha_i^+ \ge 0$ ,  $\alpha_i^- \ge 0 \ \forall_i$ :

$$\max_{\alpha^{+},\alpha^{-}} \mathcal{W}(\alpha^{+},\alpha^{-}) = \sum_{i=1}^{n} y_{i}(\alpha_{i}^{+} - \alpha_{i}^{-}) - \epsilon \sum_{i=1}^{n} (\alpha_{i}^{+} + \alpha_{i}^{-}) - \frac{1}{2} \sum_{i,j} (\alpha_{i}^{+} - \alpha_{i}^{-}) \langle x_{i}, x_{j} \rangle (\alpha_{j}^{+} - \alpha_{j}^{-})$$
(67)

Using  $\mu_i^+ \ge 0$  and  $\mu_i^- \ge 0$  together with (63) and (64) means that  $\alpha_i^+ \le C$  and  $\alpha_i^- \le C$ . We therefore need to find:

$$\min_{\alpha^{+},\alpha^{-}} \frac{1}{2} (\alpha^{+} - \alpha^{-})^{T} K(\alpha^{+} - \alpha^{-}) + \epsilon e^{T} (\alpha^{+} + \alpha^{-}) - y^{T} (\alpha^{+} - \alpha^{-})$$
subject to  $0 \le \alpha_{i}^{+}, \alpha_{i}^{-} \le C \ \forall_{i}$ 

$$e^{T} (\alpha^{+} - \alpha^{-}) = 0$$
(68)

where  $e^T = [1, ..., 1].$ 

We can write the (68) in a standard quadratic form as:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^T Q \alpha - q^T \alpha$$
subject to  $0 \le \alpha_i \le C \ \forall_i$ 

$$e^T \alpha = 0$$
(69)

where the Hessian matrix  $Q = \begin{bmatrix} K & -K \\ -K & K \end{bmatrix}$ ,  $\alpha = \begin{bmatrix} \alpha^+ \\ \alpha^- \end{bmatrix}$ ,  $q = \begin{bmatrix} -y \\ y \end{bmatrix} + \epsilon$ , and  $e = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ . Each new predictions y' can be found using:

$$y' = \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) \langle x_i, x' \rangle + b$$
 (70)

A set S of support vectors  $x_s$  can be created by finding the indices i where  $0 \le \alpha \le C$  and  $\xi_i^+ = 0$  or  $\xi_i^- = 0$ . This gives us:

$$b = y_s - \epsilon - \sum_{m \in S} (\alpha_m^+ - \alpha_m^-) \langle x_m, x_s \rangle$$
 (71)

As before it is better to average over all the indices i in S:

$$b = \frac{1}{N_s} \sum_{s \in S} y_s - \epsilon - \sum_{m \in S} (\alpha_m^+ - \alpha_m^-) \langle x_m, x_s \rangle$$
 (72)

From (69) we can notice that the equality constraint  $e^T \alpha = 0$  arises form the stationarity condition  $\partial_b \mathcal{W} = 0$ . So, again, for simplicity, we can again consider the bias term b embedded into the weight vector. We report below the box-constrained dual formulation [14] that arises from the primal (11) or (12) where the bias term b is embedded into the weight vector w:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} (Q + ee^{T}) \alpha + q^{T} \alpha$$
subject to  $0 \le \alpha_{i} \le C \ \forall_{i}$  (73)

#### 4.1.3 Lagrangian Dual formulation

In order to relax the constraints in the Wolfe dual formulation (68) we define the problem as a Lagrangian dual relaxation by embedding them into objective function, so we need to allocate the Lagrange multipliers  $\mu$  and  $\lambda_+, \lambda_- \geq 0$ :

$$\max_{\mu,\lambda_{+},\lambda_{-}} \min_{\alpha} \mathcal{L}(\alpha,\mu,\lambda_{+},\lambda_{-}) = \frac{1}{2} \alpha^{T} Q \alpha + q^{T} \alpha - \mu^{T} (e^{T} \alpha) - \lambda_{+}^{T} (u - \alpha) - \lambda_{-}^{T} \alpha$$

$$= \frac{1}{2} \alpha^{T} Q \alpha + (q - \mu e + \lambda_{+} - \lambda_{-})^{T} \alpha - \lambda_{+}^{T} u$$
subject to  $\lambda_{+},\lambda_{-} \geq 0$  (74)

where the upper bound  $u^T = [C, \dots, C]$ .

Taking the derivative of the Lagrangian  $\mathcal{L}$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow Q\alpha + (q - \mu e + \lambda_{+} - \lambda_{-}) = 0 \tag{75}$$

With  $\alpha$  optimal solution of the linear system:

$$Q\alpha = -(q - \mu e + \lambda_+ - \lambda_-) \tag{76}$$

the gradient wrt  $\mu$ ,  $\lambda_{+}$  and  $\lambda_{-}$  are:

$$\frac{\partial \mathcal{L}}{\partial \mu} = -e\alpha \tag{77}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{+}} = \alpha - u \tag{78}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{-}} = -\alpha \tag{79}$$

From (69) we can notice that the equality constraint  $e^T \alpha = 0$  arises form the stationarity condition  $\partial_b \mathcal{W} = 0$ . So, again, for simplicity, we can again consider the bias term b embedded into the weight vector. In this way the dimensionality of (74) is reduced of 1/3 by removing the multipliers  $\mu$  which was allocated to control the equality constraint  $e^T \alpha = 0$ , so we will end up solving exactly the problem (73).

$$\max_{\lambda_{+},\lambda_{-}} \min_{\alpha} \mathcal{L}(\alpha,\lambda_{+},\lambda_{-}) = \frac{1}{2} \alpha^{T} (Q + ee^{T}) \alpha + q^{T} \alpha - \lambda_{+}^{T} (u - \alpha) - \lambda_{-}^{T} \alpha 
= \frac{1}{2} \alpha^{T} (Q + ee^{T}) \alpha + (q + \lambda_{+} - \lambda_{-})^{T} \alpha - \lambda_{+}^{T} u$$
subject to  $\lambda_{+},\lambda_{-} \geq 0$ 

$$(80)$$

where, again, the upper bound  $u^T = [C, \dots, C]$ .

Now, taking the derivative of the Lagrangian  $\hat{\mathcal{L}}$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + ee^T)\alpha + (q + \lambda_+ - \lambda_-) = 0$$
(81)

With  $\alpha$  optimal solution of the linear system:

$$(Q + ee^T)\alpha = -(q + \lambda_+ - \lambda_-) \tag{82}$$

the gradient wrt  $\lambda_+$  and  $\lambda_-$  are:

$$\frac{\partial \mathcal{L}}{\partial \lambda_{+}} = \alpha - u \tag{83}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{-}} = -\alpha \tag{84}$$

#### 4.2 Squared Epsilon-insensitive loss

The squared epsilon-insensitive loss is defined as:

$$\mathcal{L}_{\epsilon}^{2} = \max(0, |y - (w^{T}x + b)| - \epsilon)^{2} \tag{85}$$

or, equivalently:

$$\mathcal{L}_{\epsilon}^{2} = \begin{cases} 0 & \text{if } |y - (w^{T}x + b)| \le \epsilon \\ (|y - (w^{T}x + b)| - \epsilon)^{2} & \text{otherwise} \end{cases}$$
 (86)

As the *squared hinge* loss, also the *squared epsilon-insensitive* loss is a strictly convex function and its gradient is given by:

$$\nabla_w \mathcal{L}_{\epsilon}^2 = \begin{cases} 2\operatorname{sign}(y - (w^T x + b))(|y - (w^T x + b)| - \epsilon)x & \text{if } |y - (w^T x + b)| \ge \epsilon \\ 0 & \text{otherwise} \end{cases}$$
(87)

#### 4.2.1 Primal formulation

To provide a continuously differentiable function the optimization problem (60) can be formulated as:

$$\min_{w,b} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \max(0, |y_i - (w^T x_i + b)| - \epsilon)^2$$
(88)

where we make use of the squared epsilon-insensitive loss that quadratically penalized slacks  $\xi$  and is called  $\mathcal{L}_2$ -SVR.

The  $\mathcal{L}_2$ -SVR objective (88) can be rewritten in form (11) or (12) as:

$$\min_{w,b} \frac{1}{2} (\|w\|^2 + b^2) + C \sum_{i=1}^n \max(0, |y_i - (w^T x_i + b)| - \epsilon)^2$$
(89)

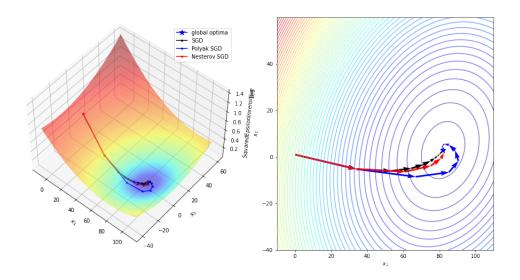


Figure 6: Squared Epsilon-insensitive loss with different optimization steps

#### 4.2.2 Wolfe Dual formulation

As done for the  $\mathcal{L}_1$ -SVR we can derive the Wolfe dual formulation of the  $\mathcal{L}_2$ -SVR by obtaining:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} (Q + D) \alpha + q^{T} \alpha$$
subject to  $\alpha_{i} \geq 0 \ \forall_{i}$ 

$$e^{T} \alpha = 0$$

$$(90)$$

or, alternatively, with the regularized bias term by obtaining:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} (Q + ee^{T} + D) \alpha + q^{T} \alpha$$
subject to  $\alpha_{i} \geq 0 \ \forall_{i}$  (91)

where the diagonal matrix  $D_{ii} = \frac{1}{2C} \,\forall_i$ .

#### 4.2.3 Lagrangian Dual formulation

In order to relax the constraints in the  $\mathcal{L}_2$ -SVR Wolfe dual formulation (90) we define the problem as a Lagrangian dual relaxation by embedding them into objective function, so we need to allocate the Lagrange multipliers  $\mu$  and  $\lambda \geq 0$ :

$$\max_{\mu,\lambda} \min_{\alpha} \mathcal{L}(\alpha, \mu, \lambda) = \frac{1}{2} \alpha^{T} (Q + D) \alpha + q^{T} \alpha - \mu^{T} (e^{T} \alpha) - \lambda^{T} \alpha$$

$$= \frac{1}{2} \alpha^{T} (Q + D) \alpha + (q - \mu e - \lambda)^{T} \alpha$$
subject to  $\lambda \geq 0$  (92)

Taking the derivative of the Lagrangian  $\mathcal{L}$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + D)\alpha + (q - \mu e - \lambda) = 0 \tag{93}$$

With  $\alpha$  optimal solution of the linear system:

$$(Q+D)\alpha = -(q-\mu e - \lambda) \tag{94}$$

the gradient wrt  $\mu$  and  $\lambda$  are:

$$\frac{\partial \mathcal{L}}{\partial \mu} = -e\alpha \tag{95}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = -\alpha \tag{96}$$

From (69) we can notice that the equality constraint  $e^T \alpha = 0$  arises form the stationarity condition  $\partial_b \mathcal{W} = 0$ . So, again, for simplicity, we can again consider the bias term b embedded into the weight vector. In this way the dimensionality of (92) is reduced of 1/3 by removing the multipliers  $\mu$  which was allocated to control the equality constraint  $e^T \alpha = 0$ , so we will end up solving exactly the problem (91).

$$\max_{\lambda} \min_{\alpha} \mathcal{L}(\alpha, \lambda) = \frac{1}{2} \alpha^{T} (Q + ee^{T} + D)\alpha + q^{T} \alpha - \lambda^{T} \alpha$$

$$= \frac{1}{2} \alpha^{T} (Q + ee^{T} + D)\alpha + (q - \lambda)^{T} \alpha$$
subject to  $\lambda \ge 0$  (97)

where, again, the upper bound  $u^T = [C, \dots, C]$ .

Now, taking the derivative of the Lagrangian  $\mathcal L$  wrt  $\alpha$  and settings it to 0 gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + ee^T + D)\alpha + (q - \lambda) = 0$$
(98)

With  $\alpha$  optimal solution of the linear system:

$$(Q + ee^T + D)\alpha = -(q - \lambda) \tag{99}$$

the gradient wrt  $\lambda$  is:

$$\frac{\partial \mathcal{L}}{\partial \lambda} = -\alpha \tag{100}$$

## 5 Nonlinear Support Vector Machines

When applying our SVC to linearly separable data in (18), we have started by creating a matrix Q from the dot product of our input variables:

$$Q_{ij} = y_i y_j k(x_i, x_j) \tag{101}$$

or, a matrix K from the dot product of our input variables in the SVR case (68):

$$K_{ij} = k(x_i, x_j) \tag{102}$$

where  $k(x_i, x_j)$  is an example of a family of functions called kernel functions and:

$$k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle = \phi(x_i)^T \phi(x_j)$$
(103)

where  $\phi(.)$  is the identity function, is known as *linear* kernel.

The reason that this *kernel trick* is useful is that there are many classification/regression problems that are nonlinearly separable/regressable in the *input space*, which might be in a higher dimensionality *feature space* given a suitable mapping  $x \to \phi(x)$ .

#### 5.1 Polynomial kernel

The *polynomial* kernel is defined as:

$$k(x_i, x_i) = (\gamma \langle x_i, x_i \rangle + r)^d \tag{104}$$

where  $\gamma$  define how far the influence of a single training example reaches (low values meaning 'far' and high values meaning 'close').

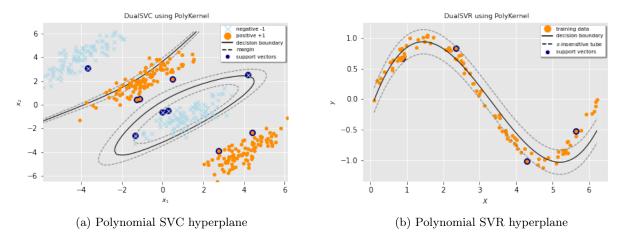


Figure 7: Polynomial SVM hyperplanes

#### 5.2 Gaussian RBF kernel

The gaussian kernel is defined as:

$$k(x_i, x_j) = \exp(-\frac{\|x_i - x_j\|^2}{2\sigma^2})$$
(105)

or, equivalently:

$$k(x_i, x_j) = \exp(-\gamma ||x_i - x_j||^2)$$
(106)

where  $\gamma = \frac{1}{2\sigma^2}$  define how far the influence of a single training example reaches (low values meaning 'far' and high values meaning 'close').

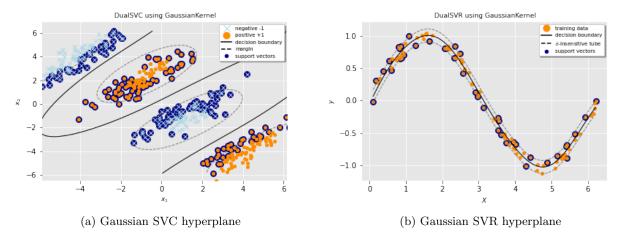


Figure 8: Gaussian SVM hyperplanes

## 6 Optimization Methods

In order to explain the *convergence rates* of the following optimization methods, we need to introduce some preliminary definitions about *convexity* and the *Lipschitz continuity* of a function [15].

**Definition 1** (Convexity).

(i) We say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is convex if:

$$(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y) \ \forall \ x, y \in \Re^m, \lambda \in [0, 1]$$

(ii) We say that a differentiable function  $f: \mathbb{R}^m \to \mathbb{R}$  is convex if:

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle \ \forall \ x, y \in \Re^m$$

(iii) We say that a twice differentiable function  $f: \Re^m \to \Re$  is convex iff:

$$\nabla^2 f(x) \succeq 0 \ \forall \ x \in \Re^m$$

i.e., the Hessian matix is positive semidefinite.

Definition 2 (Strict Convexity).

(i) We say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is strictly convex if:

$$(\lambda x + (1 - \lambda)y) < \lambda f(x) + (1 - \lambda)f(y) \ \forall \ x, y \in \Re^m, x \neq y, \lambda \in (0, 1)$$

(ii) We say that a differentiable function  $f: \mathbb{R}^m \to \mathbb{R}$  is strictly convex if:

$$f(y) > f(x) + \langle \nabla f(x), y - x \rangle \ \forall \ x, y \in \mathbb{R}^m, x \neq y$$

(iii) We say that a twice differentiable function  $f: \mathbb{R}^m \to \mathbb{R}$  is strictly convex iff:

$$\nabla^2 f(x) \succ 0 \ \forall \ x \in \Re^m$$

i.e., the Hessian matix is positive definite.

**Definition 3** (Strong Convexity). We say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is  $\mu$ -strongly convex if the function:

$$g(x) = f(x) - \frac{\mu}{2} ||x||^2$$

is convex for any  $\mu > 0$ . If f is differentiable this is also equivalent to:

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} ||y - x||^2 \,\forall \, x, y \in \Re^m$$

and, if f is a twice differentiable function then f is  $\mu$ -strongly convex iff:

$$\nabla^2 q(x) \succ 0 \ \forall \ x \in \Re^m$$

i.e., the Hessian matix is positive definite, which is:

$$\nabla^2 f(x) \succeq \mu I \ \forall \ x \in \Re^m$$

i.e., all the eigenvalues of the Hessian matrix are lower bounded by  $\mu I$ . **Definition 4** ( $L_f$ -Lipschitz continuity). We say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is  $L_f$ -Lipschitz continuous if:

$$|f(x) - f(y)| \le L_f ||x - y|| \ \forall \ x, y \in \Re^m$$

meaning that f is bounded above and below by a linear function.

Intuitively, L is a measure of how fast the function can change.

Finally, we say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is locally  $L_f$ -Lipschitz continuous if for every x in  $\mathbb{R}^m$  there exists a neighborhood U of x such that f restricted to U is  $L_f$ -Lipschitz continuous. Every convex function is locally  $L_f$ -Lipschitz continuous.

**Definition 5** (L-Lipschitz continuity). We say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is L-Lipschitz gradient continuous if f is differentiable and:

$$\|\nabla f(x) - \nabla f(y)\| \le L\|x - y\| \ \forall \ x, y \in \Re^m$$

that is equivalent to:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2 \,\forall \, x, y \in \Re^m$$

meaning that f is bounded above and below by a quadratic function.

Also, if f is a twice differentiable function this is equivalent to:

$$\nabla^2 f(x) \leq LI \ \forall \ x \in \Re^m$$

i.e., all the eigenvalues of the Hessian matrix are upperbounded by L.

Note that if f is a  $\mu$ -strongly convex function, we give the following Hessian bounds:

$$0 \prec \mu I \preceq \nabla^2 f(x) \preceq LI \ \forall \ x \in \Re^m$$

i.e., all the eigenvalues of the Hessian matrix are lowerbounded by  $\mu I$  and upperbounded by L.

Finally, we say that a function  $f: \mathbb{R}^m \to \mathbb{R}$  is locally L-Lipschitz gradient continuous if for every x in  $\mathbb{R}^m$  there exists a neighborhood U of x such that f restricted to U is L-Lipschitz gradient continuous.

**Definition 6** (Subgradient). Given a function  $f: \mathbb{R}^m \to \mathbb{R}$  and  $x \in \mathbb{R}^m$ , we define a subgradient  $g \in \mathbb{R}^m$  at x to be any point satisfying:

$$f(y) \ge f(x) + \langle g, y - x \rangle \ \forall \ y \in \Re^m$$

Subgradients always exist for convex function.

**Theorem 7** ( $L_f$ -Lipschitz continuity for convex functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a convex function and let K be a closed and bounded set contained in the relative interior of the domain of f, i.e.,  $K \subset \mathbb{R}^m$ . Then f is  $L_f$ -Lipschitz continuous on K, i.e.,:

$$|f(x) - f(y)| \le L_f ||x - y|| \ \forall \ x, y \in K$$

In particular, f is bounded on K.

*Proof.* Let x and y be any two points in the set K. Since  $\partial f(x)$  is nonempty, by using the subgradient inequality 6, it follows that:

$$f(y) \ge f(x) + \langle g, y - x \rangle \ \forall \ g \in \partial f(x)$$

implying that:

$$f(x) - f(y) \le ||g|| ||x - y|| \ \forall \ g \in \partial f(x)$$

By definition, the set  $\bigcup_{x \in K} \partial f(x)$  is nonempty and bounded, so that for some constant L > 0, we have:

$$||g|| \le L_f \quad \forall g \in \partial f(x) \quad \forall x \in K$$

and therefore:

$$f(x) - f(y) \le L_f ||x - y||$$

By exchanging the roles of x ad y, we similarly obtain:

$$f(y) - f(x) \le L_f ||x - y||$$

and by combining the preceding two relations, we see that:

$$|f(x) - f(y)| \le L_f ||x - y||$$

showing that f is  $L_f$ -Lipschitz continuous over K.

Note that this proof shows how to determine the Lipschitz constant  $L_f$ : it is the maximum subgradient norm, over all subgradients in  $\bigcup_{x \in K} \partial f(x)$ .

Strong convexity and L-Lipschitz continuity are related by Fenchel duality according to the following theorem, which proof is given in [16].

**Theorem 8** ( $\mu$ -strong convexity and L-Lipschitz continuity for convex functions). A function f and its Fenchel dual  $f^*$  satisfy the following assertions:

- (i) if f is  $\mu$ -strongly convex, then  $f^*$  is  $\frac{1}{\mu}$ -Lipschitz continuous.
- (ii) if f is convex and L-Lipschitz continuous, then  $f^*$  is  $\frac{1}{L}$ -strongly convex.

Note that since f is convex and its epigraph is a closed convex set,  $f^* = f$ , i.e., strong duality holds.

#### 6.1 Gradient Descent for Primal formulations

The Gradient Descent algorithm is the simplest *first-order optimization* method that exploits the orthogonality of the gradient wrt the level sets to take a descent direction. In particular, it performs the following iterations:

#### Algorithm 1 Gradient Descent

```
Require: Function f to minimize

Require: Learning rate or step size \alpha > 0

function Gradient Descent (f, \alpha)

Initialize weight vector x_0

t = 0

while not\_convergence do

x_{t+1} = x_t - \alpha \partial f(x_t)

t = t+1

end while

return x_t

end function
```

Gradient Descent is based on full gradients, since at each iteration we compute the average gradient on the whole dataset:

$$\partial f(x) = \frac{1}{n} \sum_{i=1}^{n} \partial f_i(x)$$

The downside is that every step is very computationally expensive,  $\mathcal{O}(nm)$  per iteration, where n is the number of samples in our dataset and m is the number of dimensions.

Since Gradient Descent becomes impractical when dealing with large datasets we introduce a stochastic version, called Stochastic Gradient Descent, which does not use the whole set of examples to compute the gradient at every step. By doing so, we can reduce computation all the way down to  $\mathcal{O}(m)$  per iteration.

#### Algorithm 2 Stochastic Gradient Descent

```
Require: Function f to minimize

Require: Learning rate or step size \alpha > 0

Require: Batch size k

function StochasticGradientDescent(f, \alpha, k)

Initialize weight vector x_0

t \leftarrow 0

while not\_convergence do

Sample (i_1, \ldots, i_k) \sim \mathcal{U}^k(1, \ldots, n)

x_{t+1} \leftarrow x_t - \alpha \frac{1}{k} \sum_{j=1}^k \partial f_{i_j}(x_t)

t \leftarrow t+1

end while

return x_t
end function
```

Note that in expectation, we converge like GD, since  $\mathbb{E}_{i \sim \mathcal{U}(1,...,n)}[\partial f_i(x_t)] = \partial f(x_t)$ , therefore, the expected iterate of SGD converges to the optimum.

Now, consider the SGD algorithm introduced previously but where each iteration is projected into the ball  $\mathcal{B}(0,R)$  with radius R>0 fixed. So, the following lower bounds on convergence rates are given.

**Theorem 9** (Stochastic Gradient Descent convergence for convex functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a L-Lipschitz continuous convex function and assume that exists b > 0 satisfying:

$$||f_i(x)|| \le b \ \forall \ x \in \mathcal{B}(0,R)$$

Besides, assume that all minima of f belong to  $\mathcal{B}(0,R)$ . Then the Stochastic Gradient Descent with step size  $\alpha = \frac{2R}{b\sqrt{k}}$  satisfies:

$$\mathbb{E}\left[f\left(\frac{1}{k}\sum_{t=1}^{k}x_{t}\right)\right] - f(x^{*}) \leq \frac{3Rb}{\sqrt{k}}$$

**Theorem 10** (Stochastic Gradient Descent convergence for strongly convex functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a L-Lipschitz continuous,  $\mu$ -strongly convex function and assume that exists b > 0 satisfying:

$$||f_i(x)|| \le b \ \forall \ x \in \mathcal{B}(0, R)$$

Besides, assume that all minima of f belong to  $\mathcal{B}(0,R)$ . Then the Stochastic Gradient Descent with step size  $\alpha = \frac{2}{\mu(k+1)}$  satisfies:

$$\mathbb{E}\left[f\left(\frac{2}{k(k+1)}\sum_{t=1}^{k}tx_{t-1}\right)\right] - f(x^*) \le \frac{2b^2}{\mu(k+1)}$$

SGD's convergence rate for L-Lipschitz continuous convex functions is  $\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$  and  $\mathcal{O}\left(\frac{1}{t}\right)$  for L-Lipschitz continuous and strongly convex functions. More iterations are needed to reach the same accuracy as GD, but the iterations are far cheaper.

#### 6.1.1 Nonsmooth

First, consider a nonsmooth, i.e., nondifferentiable, convex function. So, the following lower bounds on convergence rates are given.

**Theorem 11** (Subgradient Descent convergence for convex functions with Polyak's stepsize). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a  $L_f$ -Lipschitz continuous convex function. Then the Subgradient Descent with Polyak's step size  $\alpha_t = \frac{f(x_t) - f(x^*)}{\|g_t\|^2}$  satisfies:

$$f(x_t) - f(x^*) \le \frac{L||x_0 - x^*||^2}{\sqrt{t+1}}$$

Unfortunately, Polyak's stepsize rule requires knowledge of  $f(x^*)$ , which is often unknown a priori, so we might often need simpler rule for setting stepsizes.

**Theorem 12** (Subgradient Descent convergence for convex functions). Let  $f: \Re^m \to \Re$  be a  $L_f$ -Lipschitz continuous convex function. Then the Subgradient Descent with step size  $\alpha_t = \frac{1}{\sqrt{t}}$  satisfies:

$$f(x_t) - f(x^*) \le \frac{\|x_0 - x^*\|^2 + L^2 \log t}{\sqrt{t}}$$

**Theorem 13** (Subgradient Descent convergence for strongly convex functions). Let  $f: \Re^m \to \Re$  be a  $L_f$ -Lipschitz continuous and  $\mu$ -strongly convex function. Then the Subgradient Descent with step size  $\alpha_t = \frac{2}{\mu(t+1)}$  satisfies:

$$f(x_t) - f(x^*) \le \frac{2L^2}{\mu} \frac{1}{t+1}$$

In summary, the following convergence rates and iterations complexities are given:

Table 1: Subgradient Descent convergence rates and iterations complexities

|                                      | stepsize rule                 | convergence rate                             | iteration complexity                           |
|--------------------------------------|-------------------------------|--|--|
|                                      | 1                             | (1)  | (1)  |
| convex and $L_f$ -Lipschitz          | $\alpha = \frac{1}{\sqrt{t}}$ | $\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$ | $\mathcal{O}\left(\frac{1}{\epsilon^2}\right)$ |
| strongly convex and $L_f$ -Lipschitz | $\alpha = \frac{1}{t}$        | $\mathcal{O}\left(\frac{1}{t}\right)$        | $\mathcal{O}\left(\frac{1}{\epsilon}\right)$   |

Among algorithms that only use subgradient, these convergence rates cannot be futher improved.

#### 6.1.2 Smooth

Now, consider a smooth, i.e., differentiable, convex function. So, the following lower bounds on convergence rates are given.

**Theorem 14** (Gradient Descent convergence for convex functions). Let  $f: \Re^m \to \Re$  be a L-Lipschitz continuous convex function. Then the Gradient Descent with step size  $\alpha = 1/L$  satisfies:

$$f(x_t) - f(x^*) \le \frac{L||x_0 - x^*||^2}{2t}$$

**Theorem 15** (Gradient Descent convergence for strongly convex functions). Let  $f: \Re^m \to \Re$  be a L-Lipschitz continuous and  $\mu$ -strongly convex function. Then the Gradient Descent with step size  $\alpha = 1/L$  satisfies:

$$f(x_t) - f(x^*) \le \left(1 - \frac{\mu}{L}\right)^t ||f(x_0) - f(x^*)||^2$$
$$= \left(1 - \frac{1}{\kappa}\right)^t ||f(x_0) - f(x^*)||^2$$

where  $\kappa = L/\mu$ .

**Theorem 16** (Gradient Descent convergence for convex quadratic functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a L-Lipschitz continuous and  $\mu$ -strongly convex quadratic function. Then the Gradient Descent with step size  $\alpha = \frac{2}{L+\mu}$  and momentum  $\beta = \max\{|1 - \alpha\mu|, |1 - \alpha L|\}$  satisfies:

$$||x_t - x^*|| = \left(\frac{\kappa - 1}{\kappa + 1}\right)^t ||x_0 - x^*||$$

where  $\kappa = L/\mu$ .

In summary, the following convergence rates and iterations complexities are given:

Table 2: Gradient Descent convergence rates and iterations complexities

|                                 | stepsize rule          | convergence rate  | iteration complexity                                   |
|---------------------------------|------------------------|---|--|
| convex and L-Lipschitz          | $\alpha = \frac{1}{L}$ | $O\left(\frac{1}{4}\right)$                                 | $O\left(\frac{1}{-}\right)$                            |
| strongly convex and L-Lipschitz | $\alpha = \frac{1}{L}$ | $\mathcal{O}\left(\left(1-\frac{1}{\kappa}\right)^t\right)$ | $\mathcal{O}\left(\kappa\log\frac{1}{\epsilon}\right)$ |

#### 6.1.3 Momentum

To mitigate the pathological zig-zagging by speeding up the *convergence rate* of the SGD method, we introduce two accelerated methods [1] and [2, 3] that exploits information from the history, i.e., past iterates, to add some inertia, i.e., the momentum, to yield smoother trajectory.

In the Polyak's method [1] the velocity vector  $v_t$  is calculated by applying the  $\beta$  momentum to the previous  $v_{t-1}$  displacement, and subtracting the gradient step to  $x_t$ .

#### Polyak's Momentum



#### Nesterov's Momentum



Figure 9: Polyak's and Nesterov's Momentum

#### Algorithm 3 Polyak's Accelerated Gradient Descent or Polyak Heavy-Ball method

```
Require: Function f to minimize Require: Learning rate or step size \alpha>0 Require: Momentum \beta\in[0,1) function PolyakAcceleratedGradientDescent(f,\alpha,\beta) Initialize weight vector x_1\leftarrow x_0 and velocity vector v_0\leftarrow 0 t\leftarrow 1 while not\_convergence do v_t=\beta v_{t-1}+\alpha\nabla f(x_t) x_{t+1}=x_t-v_t t\leftarrow t+1 end while return x_t end function
```

**Theorem 17** (Polyak's Accelerated Gradient Descent convergence for convex quadratic functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a L-Lipschitz continuous and  $\mu$ -strongly convex quadratic function. Then the Polyak's Accelerated Gradient Descent with step size  $\alpha = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}$  and momentum  $\beta = \max\{|1 - \sqrt{\alpha\mu}|, |1 - \sqrt{\alpha L}|\}^2$  satisfies:

$$||x_t - x^*|| = \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^t ||x_0 - x^*||$$

where  $\kappa = L/\mu$ .

Leveraging the idea of momentum introduced by Polyak, Nesterov introduced a slightly altered update rule that has been shown to converge not only for quadratic functions, but for general convex functions. In the Nesterov's method [2], instead, the velocity vector  $v_t$  is calculated by applying the  $\beta$  momentum to the previous  $v_{t-1}$  displacement, and subtracting the gradient step to  $x_t + \beta v_{t-1}$ , which is the point where the momentum term leads from  $x_t$ .

#### Algorithm 4 Nesterov's Accelerated Gradient Descent or Nesterov Heavy-Ball method

```
Require: Function f to minimize Require: Learning rate \alpha>0 Require: Momentum \beta\in[0,1) function NesterovAcceleratedGradientDescent(f,\alpha,\beta) Initialize weight vector x_1\leftarrow x_0 and velocity vector v_0\leftarrow 0 t\leftarrow 1 while not\_convergence do  \hat{x}_t\leftarrow x_t+\beta v_{t-1} \\ v_t\leftarrow \beta v_{t-1}+\alpha \nabla f(\hat{x}_t) \\ x_{t+1}\leftarrow x_t-v_t \\ t\leftarrow t+1 \\ \text{end while} \\ \text{return } x_t \\ \text{end function}
```

Comparing the algorithm 3 with the algorithm 4, we can see that Polyak's method evaluates the gradient before adding momentum, whereas Nesterov's algorithm evaluates it after applying momentum, which intuitively brings us closer to the minimum  $x^*$ , as shown in figure 9.

**Theorem 18** (Nesterov's Accelerated Gradient Descent convergence for convex functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a L-Lipschitz continuous convex function. Then the Nesterov's Accelerated Gradient Descent with step size  $\alpha = 1/L$  and momentum  $\beta_{t+1} = t/(t+3)$  satisfies:

$$f(x_t) - f(x^*) \le \frac{2L||x_0 - x^*||^2}{(t+1)^2}$$

**Theorem 19** (Nesterov's Accelerated Gradient Descent convergence for strongly convex functions). Let  $f: \mathbb{R}^m \to \mathbb{R}$  be a L-Lipschitz continuous and  $\mu$ -strongly convex function. Then the Nesterov's Accelerated Gradient Descent with step size  $\alpha = 1/L$  and momentum  $\beta = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$  satisfies:

$$f(x_t) - f(x^*) \le \left(1 - \sqrt{\frac{\mu}{L}}\right)^t \left(f(x_0) - f(x^*) + \frac{\mu \|x_0 - x^*\|^2}{2}\right)$$
$$= \left(1 - \frac{1}{\sqrt{\kappa}}\right)^t \left(f(x_0) - f(x^*) + \frac{\mu \|x_0 - x^*\|^2}{2}\right)$$

where  $\kappa = L/\mu$ .

In summary, the following convergence rates and iterations complexities are given:

Table 3: Nesterov's Accelerated Gradient Descent convergence rates and iterations complexities

|                                 | stepsize rule          | convergence rate   | iteration complexity   |
|---------------------------------|------------------------|--|--|
| convex and L-Lipschitz          | $\alpha = \frac{1}{L}$ | $\mathcal{O}\!\left(\frac{1}{t^2}\right)$                            | $\mathcal{O}\left(\frac{1}{\sqrt{\epsilon}}\right)$            |
| strongly convex and L-Lipschitz | $\alpha = \frac{1}{L}$ | $\mathcal{O}\left(\left(1 - \frac{1}{\sqrt{\kappa}}\right)^t\right)$ | $\mathcal{O}\!\left(\sqrt{\kappa}\log rac{1}{\epsilon} ight)$ |

Note that in case of L-Lipschitz continuous and strongly convex functions, Nesterov's momentum gives the acceleration that we had with Polyak's momentum for quadratic functions. This is great because we get the guarantee for a more general class of functions, but these *convergence rates* cannot be futher improved only using first-order information.

# 6.2 Sequential Minimal Optimization for Wolfe Dual formulations

The Sequential Minimal Optimization (SMO) [4] method is the most popular approach for solving the SVM QP problem without any extra Q matrix storage required by common QP methods. The advantage of SMO lies in the fact that it performs a series of two-point optimizations since we deal with just one equality constraint, so the Lagrange multipliers can be solved analitically.

#### 6.2.1 Classification

At each iteration, SMO chooses two  $\alpha_i$  to jointly optimize, let  $\alpha_1$  and  $\alpha_2$ , finds the optimal values for these multipliers and update the SVM to reflect these new values. In order to solve for two Lagrange multipliers, SMO first computes the constraints over these and then solves for the constrained minimum. Since there are only two multipliers, the box-constraints cause the Lagrange multipliers to lie within a box, while the linear equality constraint causes the Lagrange multipliers to lie on a diagonal line inside the box. So, the constrained minimum must lie there as shown in 10.



Figure 10: SMO for two Lagrange multipliers

In case of classification the ends of the diagonal line segment, i.e., the lower and upper bounds, can be espressed as follow if the target  $y_1 \neq y_2$ :

$$L = max(0, \alpha_2 - \alpha_1)$$
  

$$H = min(C, C + \alpha_2 - \alpha_1)$$
(107)

or, alternatively, if the target  $y_1 = y_2$ :

$$L = max(0, \alpha_2 + \alpha_1 - C)$$
  

$$H = min(C, \alpha_2 + \alpha_1)$$
(108)

The second derivative of the objective quadratic function along the diagonl line can be expressed as:

$$\eta = K(x_1, x_1) + K(x_2, x_2) - 2K(x_1, x_2) \tag{109}$$

that will be grather than zero if the kernel matrix will be positive definite, so there will be a minimum along the linear equality constraints that will be:

$$\alpha_2^{new} = \alpha_2 + \frac{y_2(E_1 - E_2)}{\eta} \tag{110}$$

where  $E_i = y_i - y_i'$  is the error on the *i*-th training example and  $y_i'$  is the output of the SVC for the same. Then, the box-constrained minimum is found by clipping the unconstrained minimum to the ends of the line segment:

$$\alpha_2^{new,clipped} = \begin{cases} H & \text{if } \alpha_2^{new} \ge H\\ \alpha_2^{new} & \text{if } L < \alpha_2^{new} < H\\ L & \text{if } \alpha_2^{new} \le L \end{cases}$$
(111)

Finally, the value of  $\alpha_1$  is computed from the new clipped  $\alpha_2$  as:

$$\alpha_1^{new} = \alpha_1 + s(\alpha_2 - \alpha_2^{new, clipped}) \tag{112}$$

where  $s = y_1 y_2$ .

Since the *Karush-Kuhn-Tucker* conditions are necessary and sufficient conditions for optimality of a positive definite QP problem and the KKT conditions for the classification problem (19) are:

$$\alpha_{i} = 0 \Leftrightarrow y_{i}y'_{i} \geq 1$$

$$0 < \alpha_{i} < C \Leftrightarrow y_{i}y'_{i} = 1$$

$$\alpha_{i} = C \Leftrightarrow y_{i}y'_{i} \leq 1$$

$$(113)$$

the steps described above will be iterate as long as there will be an example that violates them.

After optimizing  $\alpha_1$  and  $\alpha_2$ , we select the threshold b such that the KKT conditions are satisfied for  $x_1$  and  $x_2$ . If, after optimization,  $\alpha_1$  is not at the bounds, i.e.,  $0 < \alpha_1 < C$ , then the following threshold  $b_{up}$  is valid, since it forces the SVC to output  $y_1$  when the input is  $x_1$ :

$$b_{up} = E_1 + y_1(\alpha_1^{new} - \alpha_1)K(x_1, x_1) + y_2(\alpha_2^{new, clipped} - \alpha_2)K(x_1, x_2) + b$$
(114)

similarly, the following threshold  $b_{low}$  is valid if  $0 < \alpha_2 < C$ :

$$b_{low} = E_2 + y_1(\alpha_1^{new} - \alpha_1)K(x_1, x_2) + y_2(\alpha_2^{new, clipped} - \alpha_2)K(x_2, x_2) + b$$
(115)

If, after optimization, both  $0 < \alpha_1 < C$  and  $0 < \alpha_2 < C$  then both these thresholds are valid, and they will be equal; else, if both  $\alpha_1$  and  $\alpha_2$  are at the bounds, i.e.,  $\alpha_1 = 0$  or  $\alpha_1 = C$  and  $\alpha_2 = 0$  or  $\alpha_2 = C$ , then all the thresholds between  $b_{up}$  and  $b_{low}$  satisfy the KKT conditions, so we choose the threshold to be halfway in between  $b_{up}$  and  $b_{low}$ . This gives the complete equation for b:

$$b = \begin{cases} b_{up} & \text{if } 0 < \alpha_1 < C \\ b_{low} & \text{if } 0 < \alpha_2 < C \\ \frac{b_{up} + b_{low}}{2} & \text{otherwise} \end{cases}$$
 (116)

#### Algorithm 5 Sequential Minimal Optimization for Classification

```
Require: Training examples matrix X \in \Re^{n \times m}
Require: Training target vector y \in \pm 1^n
Require: Kernel matrix K \in \Re^{n \times n}
Require: Regularization parameter C > 0
Require: Tolerance value tol for stopping criterion
  function SMOCLASSIFIER(X, y, K, C, tol)
      Initialize the Lagrange multipliers vector \alpha \in \Re^n, \alpha \leftarrow 0
      Initialize the empty set I0 \leftarrow \{i : 0 < \alpha_i < C\}
      Initialize the set I1 \leftarrow \{i: y_i = +1, \alpha_i = 0\} to contain all the indices of the training examples of class +1
      Initialize the empty set I2 \leftarrow \{i : y_i = -1, \alpha_i = C\}
      Initialize the empty set I3 \leftarrow \{i : y_i = +1, \alpha_i = C\}
      Initialize the set I4 \leftarrow \{i: y_i = -1, \alpha_i = 0\} to contain all the indices of the training examples of class -1
      Initialize b_{up} \leftarrow -1
      Initialize b_{low} \leftarrow +1
      Initialize the error cache vector errors \in \Re^n, errors \leftarrow 0
      while num\_changed > 0 or examine\_all = True do
          num\_changed \leftarrow 0
          examine\_all \leftarrow True
          if examine\_all = True then
              for i \leftarrow 0 to n do
                                                                                           ▷ loop over all training examples
                   num\_changed \leftarrow num\_changed + ExamineExample(i)
              end for
          else
              for i in I0 do
                                                        \triangleright loop over examples where \alpha_i are not already at their bounds
                  num\_changed \leftarrow num\_changed + ExamineExample(i)
                                                                                     \triangleright check if optimality on I0 is attained
                  if b_{up} > b_{low} - 2tol then
                      num\_changed \leftarrow 0
                      break
                  end if
              end for
          end if
          if examine\_all = True then
              examine\_all \leftarrow False
          else if num\_changed = 0 then
              examine\_all \leftarrow True
          end if
      end while
      Compute b by (116)
      return \alpha, b
  end function
```

```
Require: i2-th Lagrange multiplier
  function ExamineExample(i2)
      if i2 in I0 then
          E_2 \leftarrow errors_{i2}
      else
          Compute E_2
          errors_{i2} \leftarrow E_2
          Update (b_{low}, i_{low}) or (b_{up}, i_{up}) using (E_2, i2)
      if optimality is attained using current b_{low} and b_{up} then
          \mathbf{return}\ 0
      else
          Find an index i1 to do joint optimization with i2
          if TakeStep(i1, i2) = True then
              {\bf return}\ 1
          else
              {\bf return}\ 0
          end if
      end if
  end function
```

```
Require: i1-th Lagrange multiplier
Require: i2-th Lagrange multiplier
  function TakeStep(i1, i2)
       if i1 = i2 then
           return False
       end if
       Compute L and H using (107) or (108)
       if L = H then
           return False
       end if
       Compute \eta by (109)
                                                    \triangleright we assume that \eta > 0, i.e., the kernel matrix K is positive definite
       if \eta < 0 then
           Choose \alpha_2^{new,clipped} between L and H according to the largest value of the objective function at these
  points
       else
           Compute \alpha_2^{new} by (110)
Compute \alpha_2^{new,clipped} by (111)
       end if
       if changes in \alpha_2^{new,clipped} are larger than some eps then Compute \alpha_1^{new} by (112)

Update \alpha_2^{new,clipped} and \alpha_1^{new}
           for i in I0 do
               Update errors_i using new Lagrange multipliers
           end for
           Update \alpha using new Lagrange multipliers
           Update I0, I1, I2, I3 and I4
           Update errors_{i1} and errors_{i2}
           for i \text{ in } I0 \cup \{i1, i2\} \text{ do}
               Compute (i_{low}, b_{low}) by b_{low} = \max\{errors_i : i \in I0 \cup I3 \cup I4\}
               Compute (i_{up}, b_{up}) by b_{up} = \min\{errors_i : i \in I0 \cup I1 \cup I2\}
           end for
           return True
       else
           return False
       end if
  end function
```

#### 6.2.2 Regression

In case of regression the bounds and the new multipliers  $\alpha_1^{+,new}$  and  $\alpha_2^{+,new}$  can be expressed as follows if  $(\alpha_1^+ > 0 \text{ or } (\alpha_1^- = 0 \text{ and } E_1 - E_2 > 0))$  and  $(\alpha_2^+ > 0 \text{ or } (\alpha_2^- = 0 \text{ and } E_1 - E_2 < 0))$ :

$$L = max(0, \gamma - C)$$

$$H = min(C, \gamma)$$
(117)

$$\alpha_2^{+,new} = \alpha_2^+ - \frac{E_1 - E_2}{\eta} \tag{118}$$

$$\alpha_1^{+,new} = \alpha_1^+ - (\alpha_2^{+,new,clipped} - \alpha_2^+) \tag{119}$$

or, if  $(\alpha_1^+ > 0 \text{ or } (\alpha_1^- = 0 \text{ and } E_1 - E_2 > 2\epsilon))$  and  $(\alpha_2^- > 0 \text{ or } (\alpha_2^+ = 0 \text{ and } E_1 - E_2 > 2\epsilon))$ :

$$L = max(0, -\gamma)$$

$$H = min(C, -\gamma + C)$$
(120)

$$\alpha_2^{-,new} = \alpha_2^- + \frac{(E_1 - E_2) - 2\epsilon}{\eta} \tag{121}$$

$$\alpha_1^{+,new} = \alpha_1^+ + (\alpha_2^{-,new,clipped} - \alpha_2^-) \tag{122}$$

or, if  $(\alpha_1^- > 0 \text{ or } (\alpha_1^+ = 0 \text{ and } E_1 - E_2 < -2\epsilon))$  and  $(\alpha_2^+ > 0 \text{ or } (\alpha_2^- = 0 \text{ and } E_1 - E_2 < -2\epsilon))$ :

$$L = max(0, \gamma)$$

$$H = min(C, C + \gamma)$$
(123)

$$\alpha_2^{+,new} = \alpha_2^+ - \frac{(E_1 - E_2) + 2\epsilon}{\eta} \tag{124}$$

$$\alpha_1^{-,new} = \alpha_1^- + (\alpha_2^{+,new,clipped} - \alpha_2^+)$$

$$\tag{125}$$

or, finally, if  $(\alpha_1^- > 0 \text{ or } (\alpha_1^+ = 0 \text{ and } E_1 - E_2 < 0))$  and  $(\alpha_2^- > 0 \text{ or } (\alpha_2^+ = 0 \text{ and } E_1 - E_2 > 0))$ :

$$L = max(0, -\gamma - C)$$

$$H = min(C, -\gamma)$$
(126)

$$\alpha_2^{-,new} = \alpha_2^- + \frac{E_1 - E_2}{\eta} \tag{127}$$

$$\alpha_1^{-,new} = \alpha_1^- - (\alpha_2^{-,new,clipped} - \alpha_2^-)$$
(128)

where  $\gamma = \alpha_1^+ - \alpha_1^- + \alpha_2^+ - \alpha_2^-$ . Note that  $\eta$  and  $\alpha_2^{+,new,clipped}$  or  $\alpha_2^{-,new,clipped}$  are identical to (109) and (111) respectively.

The KKT conditions for the regression problem (68) are:

$$\alpha_i^+ - \alpha_i^- = 0 \Leftrightarrow |y_i - y_i'| < \epsilon$$

$$-C < \alpha_i^+ - \alpha_i^- < C \Leftrightarrow |y_i - y_i'| = \epsilon$$

$$\alpha_i^+ + \alpha_i^- = C \Leftrightarrow |y_i - y_i'| > \epsilon$$
(129)

so, the steps described above will be iterate as long as there will be an example that violates them. In case of regression we select the threshold b as follows:

$$b_{up} = E_1 + ((\alpha_1^+ - \alpha_1^-) - (\alpha_1^{+,new} - \alpha_1^{-,new}))K(x_1, x_1) + ((\alpha_2^+ - \alpha_2^-) - (\alpha_2^{+,new,clipped} - \alpha_2^{-,new,clipped}))K(x_1, x_2) + b$$

$$(130)$$

$$b_{low} = E_2 + ((\alpha_1^+ - \alpha_1^-) - (\alpha_1^{+,new} - \alpha_1^{-,new}))K(x_1, x_2) + ((\alpha_2^+ - \alpha_2^-) - (\alpha_2^{+,new,clipped} - \alpha_2^{-,new,clipped}))K(x_2, x_2) + b$$
(131)

$$b = \begin{cases} b_{up} & \text{if } 0 < \alpha_1^+, \alpha_1^- < C \\ b_{low} & \text{if } 0 < \alpha_2^+, \alpha_2^- < C \\ \frac{b_{up} + b_{low}}{2} & \text{otherwise} \end{cases}$$
 (132)

The improvements described in [5, 8] for classification and regression respectively are about the definition of subsets of multipliers to efficiently update them at each iteration by separating the multipliers at the bounds from those who can be further minimized.

#### Algorithm 6 Sequential Minimal Optimization for Regression

```
Require: Training examples matrix X \in \Re^{n \times m}
Require: Training target vector y \in \Re^n
Require: Kernel matrix K \in \Re^{n \times n}
Require: Regularization parameter C > 0
Require: Epsilon-tube value \epsilon > 0 within which no penalty is associated in the epsilon-insensitive loss function
Require: Tolerance value tol for stopping criterion
   function SMOREGRESSION(X, y, K, C, \epsilon, tol)
       Initialize the Lagrange multipliers vector \alpha^+ \in \Re^n, \alpha^+ \leftarrow 0
       Initialize the Lagrange multipliers vector \alpha^- \in \Re^n, \alpha^- \leftarrow 0
       Initialize the empty set I0 \leftarrow \{i : 0 < \alpha_i^+, \alpha_i^- < C\}
       Initialize the set I1 \leftarrow \{i: \alpha_i^+ = 0, \alpha_i^- = 0\} to contain all the indices of the training examples Initialize the empty set I2 \leftarrow \{i: \alpha_i^+ = 0, \alpha_i^- = C\} Initialize the empty set I3 \leftarrow \{i: \alpha_i^+ = C, \alpha_i^- = 0\}
       Initialize i_{up} \leftarrow 0
                                                                    \triangleright or any other target index i_{up} from the training examples
       Initialize i_{low} \leftarrow 0
                                                                   \triangleright or any other target index i_{low} from the training examples
       Initialize b_{up} \leftarrow y_{i_{up}} + \epsilon
       Initialize b_{low} \leftarrow y_{i_{low}} - \epsilon
       Initialize the error cache vector errors \in \mathbb{R}^n, errors \leftarrow 0
       while num\_changed > 0 or examine\_all = True do
            num\_changed \leftarrow 0
            examine\_all \leftarrow True
            if examine\_all = True then
                for i \leftarrow 0 to n do
                                                                                                       ▶ loop over all training examples
                     num\_changed \leftarrow num\_changed + ExamineExample(i)
                end for
            else
                for i in I0 do
                                                   \triangleright loop over examples where \alpha_i^+ and \alpha_i^- are not already at their bounds
                     num\_changed \leftarrow num\_changed + \text{ExamineExample}(i)
                     if b_{up} > b_{low} - 2tol then
                                                                                                \triangleright check if optimality on I0 is attained
                         num\_changed \leftarrow 0
                          break
                     end if
                end for
            end if
            if examine\_all = True then
                examine\_all \leftarrow False
            else if num\_changed = 0 then
                examine\_all \leftarrow True
            end if
       end while
       Compute b by (132)
       return \alpha^+, \alpha^-, b
   end function
```

```
Require: i1-th Lagrange multiplier
Require: i2-th Lagrange multiplier
   function TakeStep(i1, i2)
        if i1 = i2 then
            return False
        end if
        finished = False
        while not finished do
            Compute L and H using (117), (120), (123) or (126)
            if L < H then
                 Compute \eta by (109)
                                                          \triangleright we assume that \eta > 0, i.e., the kernel matrix K is positive definite
                 if \eta < 0 then
                      Choose \alpha_2^{+,new,clipped} or \alpha_2^{-,new,clipped} between L and H according to the largest value of the
   objective function at these points
                 else
                      Compute \alpha_2^{+,new} or \alpha_2^{-,new} using (118), (124) or (121), (127) respectively Compute \alpha_2^{+,new,clipped} or \alpha_2^{-,new,clipped} by (111)
                 Compute \alpha_1^{+,new} or \alpha_1^{-,new} using (119), (122) or (125), (128) respectively if changes in \alpha_2^{+,new,clipped}, \alpha_2^{-,new,clipped}, \alpha_1^{+,new} or \alpha_1^{-,new} are larger than some eps then Update \alpha_2^{+,new,clipped}, \alpha_2^{-,new,clipped}, \alpha_1^{+,new} or \alpha_1^{-,new}
                 end if
            else
                 finished = True
            end if
        end while
       if changes in \alpha_2^{+,new,clipped}, \alpha_2^{-,new,clipped}, \alpha_1^{+,new} or \alpha_1^{-,new} are larger than some eps then
            for i in I0 do
                 Update errors_i using new Lagrange multipliers
            Update \alpha^+ and \alpha^- using new Lagrange multipliers
            Update I0, I1, I2 and I3
            Update errors_{i1} and errors_{i2}
            for i in I0 \cup \{i1, i2\} do
                 Compute (i_{low}, b_{low}) by b_{low} = \max\{errors_i : i \in I0 \cup I1 \cup I2\}
                 Compute and (i_{up}, b_{up}) by b_{up} = \min\{errors_i : i \in I0 \cup I1 \cup I3\}
            end for
            return True
        else
            return False
        end if
   end function
```

# 6.3 AdaGrad for Lagrangian Dual formulations

Due to the sparsity of the weight vector of the Lagrangian dual, i.e., the Lagrange multipliers, we might end up in a situation where some components of the gradient are very small and others large. This, in terms of conditioning number, i.e.,  $\kappa = L/\mu \gg 1$ , means that the level sets of f are ellipsoid, i.e., we are dealing with an ill-conditioned problem. So, given a learning rate, a standard gradient descent approach might end up in a situation where it decreases too quickly the small weights or too slowly the large ones.

Another method, that is usually deprecated in ML applications due to its increased computational complexity, is Newton's method. Newton's method favors a much faster *convergence rate*, i.e., number of iterations, at the cost of being more expensive per iteration. For convex problems, the recursion is similar to the gradient descent algorithm:

$$x_{t+1} = x_t - \alpha H^{-1} \nabla f(x_t)$$

where  $\alpha$  is often close to one (damped-Newton) or one, and  $H^{-1}$  denotes the Hessian of f at the current point, i.e.,  $\nabla^2 f(x_t)$ .

The above suggest a general rule in optimization: find any preconditioner, in convex optimization it has to be positive semidefinite, that improves the performance of gradient descent in terms of iterations, but without wasting too much time to compute that precoditioner. The above result into:

$$x_{t+1} = x_t - \alpha P^{-1} \nabla f(x_t)$$

where P is the preconditioner. This idea is the basis of the BFGS quasi-Newton method.

The AdaGrad [6] algorithm is just a variant of preconditioned gradient descent, where P is selected to be a diagonal preconditioner matrix and is updated using the gradient information, in particular it is the diagonal approximation of the inverse of the square roots of gradient outer products, until the k-th iteration. The above lead to the algorithm:

```
Algorithm 7 AdaGrad
```

```
Require: Function f to minimize
Require: Learning rate or step size \alpha > 0
Require: Offset \epsilon > 0 to ensures not divide by 0
function ADAGRAD(f, \alpha, \epsilon)
Initialize weight vector x_0 and the squared accumulated gradients vector s_t \leftarrow 0
t = 1
while not\_convergence do
g_t \leftarrow \partial f(x_t) \qquad \qquad \triangleright \text{ if } f \text{ is differentiable then } \partial f(x_t) = \nabla f(x_t)
s_t \leftarrow s_{t-1} + g_t^2
x_{t+1} \leftarrow x_t - \alpha P_t^{-1} g_t = x_t - \frac{\alpha}{\sqrt{s_t + \epsilon}} \odot g_t \text{ where } P_t \leftarrow diag(s_t + \epsilon)^{1/2}
t \leftarrow t + 1
end while
\text{return } x_t
end function
```

In practical terms, AdaGrad addresses the problem of the sparse optimal by adaptively scaling the learning rate for each dimension with the magnitude of the gradients. Coordinates that routinely correspond to large gradients are scaled down significantly, whereas others with small gradients receive a much more gentle treatment.

### 6.4 Losses properties

Several losses and objectives have been presented in section 3 and 4. In our experiments, we will consider the following.

For what about the loss functions, two of them are nonsmooth convex functions, i.e., the *hinge* and the *epsilon-insensitive* losses for *classification* and *regression* tasks respectively, and linearly penalizes the misclassified points, i.e.,  $\mathcal{L}_1$ -SVM, meanwhile, their two *squared* versions are smooth, i.e.,  $\mathcal{L}_2$ -SVM, and quadratically penalizes the misclassified points.

Also, both the margin-based losses, i.e., the hinge and the squared hinge losses, are  $L_f$ -Lipschitz continuous; meanwhile, among the distance-based losses, the epsilon-insensitive loss is  $L_f$ -Lipschitz continuous but the squared epsilon-insensitive is not  $L_f$ -Lipschitz continuous, however it is convex and for this reason is locally  $L_f$ -Lipschitz continuous.

Also the regularization term, i.e.,  $\frac{1}{2}||w||^2$ , is not  $L_f$ -Lipschitz continuous since it becomes arbitrarily steep as w approaches infinity, but it is strictly convex and for this reason is locally  $L_f$ -Lipschitz continuous. Clearly, its gradient, i.e., w, is not bounded since, again, they go to infinity as w goes to infinity, so this function is not L-Lipschitz continuous.

Since for our purposes, we need to show that our  $\mathcal{L}_1$ -SVM objectives are  $L_f$ -Lipschitz continuous and the  $\mathcal{L}_2$ -SVM objectives are L-Lipschitz continuous for the applicability of the convergence theorems, we will use the theorem 7 and 8 respectively.

In general, if the objective function of a quadratic programming problem is strictly convex, i.e., the associated Hessian matrix is positive definite, the solution is unique. Meanwhile, if the objective function is convex, there may be cases where the solution is nonunique.

Assume that the hard margin SVM has a solution, i.e., the given problem is separable in the feature space. Then, since the objective function of the primal problem is  $\frac{1}{2}||w||^2$ , which is strongly convex, the primal problem has a unique solution for w and b.

Since the  $\mathcal{L}_1$ -SVM linearly penalizes the misclassified points, the primal objective function is convex. Likewise, the Hessian matrix of the dual objective function is positive semidefinite. Thus the primal and dual solutions may be nonunique. Meanwhile, the objective function of the primal problem for the  $\mathcal{L}_2$ -SVM is strictly convex, due to the quadratic penalization of the misclassified points. Therefore, w and b are uniquely determined if we solve the primal or dual problem.

In summary, the following properties for the SVM's objectives are given:

 $\mathcal{L}_2$ -SVR (89)

|                           | smooth | Lipschitz continuous | convexity |
|---------------------------|--------|----------------------|-----------|
| objective                 |        |                      |           |
| $\mathcal{L}_1$ -SVC (13) | no     | $L_f$ -Lipschitz     | convex    |
| $\mathcal{L}_2$ -SVC (42) | yes    | L-Lipschitz          | strongly  |
|                           |        |                      | convex    |
| C1-SVR (61)               | no     | LLinschitz           | convey    |

Table 4: SVM's objectives properties for primal formulations

And, according to the theoretical analysis, the following *convergence rates* are given for the primal and *Lagrangian dual* formulations respectively:

L-Lipschitz

strongly convex

yes

| objective                     | SGD convergence rate                         | Polyak SGD convergence rate                  | Nesterov SGD convergence rate                |
|-------------------------------|--|--|--|
| $\mathcal{L}_1$ -SVM (13, 61) | $\mathcal{O}\left(\frac{m}{\sqrt{t}}\right)$ | $\mathcal{O}\left(\frac{m}{\sqrt{t}}\right)$ | $\mathcal{O}\left(\frac{m}{\sqrt{t}}\right)$ |
| $\mathcal{L}_2$ -SVM (42, 89) | $\mathcal{O}\left(\frac{m}{t}\right)$        | $\mathcal{O}\left(\frac{m}{t}\right)$        | $\mathcal{O}\left(\frac{m}{t^2}\right)$      |

Table 5: SVM's objectives convergence rates for primal formulations

Table 6: SVM's objectives convergence rate for Lagrangian dual formulations

|  | AdaGrad convergence rate                        |
|--|---|
| objective  | (2000)  |
| $\mathcal{L}_1$ -SVM (27, 74) or (33, 80)                | $\mathcal{O}\!\left(\frac{nm}{\sqrt{t}}\right)$ |
| $\mathcal{L}_2\text{-SVM }(45, 92) \text{ or } (50, 97)$ | $\mathcal{O}\!\left(\frac{nm}{t}\right)$        |

To improve the practical convergence of all the *Lagrangian dual* formulations we adding a strictly convex augmentation term, so by considering a general quadratic optimization problem subject to linear constraints, i.e., equality and inequality constraints, defined as:

$$\min_{\alpha} \quad \frac{1}{2} \alpha^{T} Q \alpha + q^{T} \alpha$$
subject to  $A\alpha = b$ 

$$G\alpha \leq h$$

$$lb \leq \alpha \leq ub$$
(133)

or, equivalently:

with  $\rho > 0$ .

$$\min_{\alpha} \quad \frac{1}{2} \alpha^T Q \alpha + q^T \alpha$$
 subject to  $A\alpha = b$  
$$\hat{G}\alpha \leq \hat{h}$$
 (134)

where 
$$\hat{G} = \begin{bmatrix} G \\ -I \\ I \end{bmatrix}$$
 and  $\hat{h} = \begin{bmatrix} h & -lb & ub \end{bmatrix}$ ; we give the following augmented Lagrangian dual:
$$\max_{\substack{\mu,\lambda \quad \alpha \\ \mu}} \frac{1}{2} \alpha^T Q \alpha + q^T \alpha + \mu^T (A \alpha - b) + \lambda^T (\hat{G} \alpha - \hat{h}) + \frac{\rho}{2} ||A \alpha - b||^2 + \frac{\rho}{2} ||\hat{G} \alpha - \hat{h}||^2$$
subject to  $\lambda \geq 0$  (135)

# 7 Experiments

The following experiments refer to *linearly* and *nonlinearly* separable generated datasets of size 100. All the training times refer to running on a laptop with an Intel i7-6700HQ (8) @ 3.500GHz and 31.2 GB of memory. The Python source code is available at: github.com/dmeoli/optiml.

# 7.1 Support Vector Classifier

Below experiments are about the SVC for which I tested different values for the regularization hyperparameter C, i.e., from soft to  $hard\ margin$ , and in case of nonlinearly separable data also different  $kernel\ functions$  mentioned above.

The experiments about SVCs are available at: github.com/dmeoli/optiml/blob/master/notebooks/optimization/CM\_SVC\_report\_experiments.ipynb.

#### 7.1.1 Hinge loss

**Primal formulation** The experiments results shown in 7 referred to *Stochastic Gradient Descent* algorithm are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 0.02 and  $\beta$ , i.e., the *momentum*, equal to 0.5. Training is stopped if after 5 iterations the training loss is not lower than the best found so far within a tolerance of 1e-8.

|                      |          |      | $fit\_time$ | accuracy | $n\_iter$ | $n\_sv$ |
|----------------------|----------|------|-------------|----------|-----------|---------|
| solver               | momentum | С    |             |          |           |         |
| $\operatorname{sgd}$ | none     | 0.1  | 2.038373    | 0.975    | 7196      | 36      |
|                      |          | 1.0  | 1.168452    | 0.985    | 4092      | 15      |
|                      |          | 10.0 | 0.310208    | 0.980    | 947       | 10      |
|                      | polyak   | 0.1  | 1.041824    | 0.975    | 3589      | 37      |
|                      |          | 1.0  | 0.707970    | 0.985    | 2098      | 16      |
|                      |          | 10.0 | 0.190836    | 0.980    | 467       | 10      |
|                      | nesterov | 0.1  | 1.280432    | 0.975    | 4344      | 37      |
|                      |          | 1.0  | 0.690090    | 0.985    | 2115      | 16      |
|                      |          | 10.0 | 0.186116    | 0.980    | 472       | 10      |
| liblinear            | -        | 0.1  | 0.000979    | 0.980    | 31        | 37      |
|                      |          | 1.0  | 0.001046    | 0.985    | 332       | 16      |
|                      |          | 10.0 | 0.001936    | 0.985    | 1000      | 5       |

Table 7: Primal  $\mathcal{L}_1$ -SVC results

The results provided from the *custom* implementation, i.e., the SGD with different momentum settings, are strongly similar to those of *sklearn* implementation, i.e., *liblinear* [10] implementation, in terms of *accuracy* score. More training data points are selected as *support vectors* from the SGD solver but it always requires lower iterations, i.e., epochs, to achieve the same *numerical precision*. *Polyak* and *Nesterov* momentums always perform lower iterations as expected from the theoretical analysis of the convergence rate.

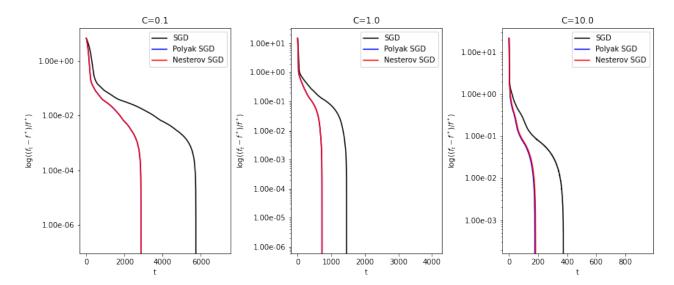


Figure 11: SGD Convergence for the Primal formulation of the  $\mathcal{L}_1$ -SVC

**Linear Dual formulations** The experiments results shown in 9 are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (19) and (26) respectively with  $\rho$  equals to 1.

|        |              | $fit\_time$ | accuracy | $n_{-iter}$ | $n_sv$ |
|--------|--------------|-------------|----------|-------------|--------|
| solver | $\mathbf{C}$ |             |          |             |        |
| smo    | 0.1          | 0.050194    | 0.985    | 33          | 38     |
|        | 1.0          | 0.035069    | 0.980    | 62          | 17     |
|        | 10.0         | 0.104582    | 0.980    | 295         | 10     |
| libsvm | 0.1          | 0.002047    | 0.985    | 37          | 38     |
|        | 1.0          | 0.002132    | 0.985    | 243         | 17     |
|        | 10.0         | 0.002683    | 0.985    | 194         | 10     |
| cvxopt | 0.1          | 0.028806    | 0.985    | 9           | 38     |
|        | 1.0          | 0.035333    | 0.980    | 10          | 17     |
|        | 10.0         | 0.039818    | 0.980    | 10          | 11     |

For what about the linear  $Wolfe\ dual$  formulation we can immediately notice as higher  $regularization\ hy-perparameter\ C$  makes the model harder, so the custom implementation of the SMO algorithm and also the sklearn implementation, i.e., libsvm [11] implementation, needs to perform more iterations to achieve the same  $numerical\ precision$ ; meanwhile the cvxopt [12] seems to be insensitive to the increasing complexity of the model. The results in terms of accuracy and number of  $support\ vectors$  are strongly similar to each others.

|               |              | $\operatorname{fit\_time}$ | accuracy | $n_{-iter}$ | $n\_sv$ |
|---------------|--------------|----------------------------|----------|-------------|---------|
| dual          | $\mathbf{C}$ |                            |          |             |         |
| reg_bias      | 0.1          | 15.485357                  | 0.985    | 10000       | 131     |
|               | 1.0          | 12.431954                  | 0.970    | 10000       | 94      |
|               | 10.0         | 17.027144                  | 0.970    | 10000       | 121     |
| $unreg\_bias$ | 0.1          | 16.659235                  | 0.975    | 10000       | 136     |
|               | 1.0          | 10.199121                  | 0.980    | 10000       | 126     |
|               | 10.0         | 12.724132                  | 0.965    | 10000       | 70      |

Table 9: Lagrangian Dual linear  $\mathcal{L}_1$ -SVC results

For what about the linear *Lagrangian dual* formulation we can see as it seems to be insensitive to the increasing complexity of the model in terms of number of *iterations* but it tends to select many training data points as *support vectors*.

Nonlinear Dual formulations The experiments results shown in 10 and 11 are obtained with d and r hyperparameters equal to 3 and 1 respectively for the *polynomial* kernel; gamma is setted to 'scale' for both polynomial and gaussian RBF kernels. The experiments results shown in 11 are obtained with  $\alpha$ , i.e., the learning rate or step size, setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (19) and (26) respectively with  $\rho$  equals to 1.

| Table | 10. | Wolfe | Dual | nonlinear | C1- | SVC | results |
|-------|-----|-------|------|-----------|-----|-----|---------|
|       |     |       |      |           |     |     |         |

|        |        |              | $\operatorname{fit\_time}$ | accuracy | $n_{iter}$ | $n_sv$ |
|--------|--------|--------------|----------------------------|----------|------------|--------|
| solver | kernel | $\mathbf{C}$ |                            |          |            |        |
| smo    | poly   | 0.1          | 0.475808                   | 0.8675   | 121        | 142    |
|        |        | 1.0          | 0.386903                   | 0.6825   | 143        | 30     |
|        |        | 10.0         | 0.204837                   | 0.9475   | 65         | 10     |
|        | rbf    | 0.1          | 0.392323                   | 1.0000   | 61         | 222    |
|        |        | 1.0          | 0.353054                   | 1.0000   | 66         | 51     |
|        |        | 10.0         | 0.203540                   | 1.0000   | 38         | 13     |
| libsvm | poly   | 0.1          | 0.005659                   | 1.0000   | 210        | 143    |
|        | - •    | 1.0          | 0.004032                   | 1.0000   | 233        | 30     |
|        |        | 10.0         | 0.002848                   | 1.0000   | 118        | 10     |
|        | rbf    | 0.1          | 0.006753                   | 1.0000   | 131        | 222    |
|        |        | 1.0          | 0.003834                   | 1.0000   | 252        | 50     |
|        |        | 10.0         | 0.002358                   | 1.0000   | 134        | 13     |
| cvxopt | poly   | 0.1          | 0.213058                   | 0.8575   | 10         | 143    |
| -      | 1 0    | 1.0          | 0.256055                   | 0.6775   | 10         | 31     |
|        |        | 10.0         | 0.231667                   | 0.9475   | 10         | 10     |
|        | rbf    | 0.1          | 0.172620                   | 1.0000   | 10         | 222    |
|        |        | 1.0          | 0.240220                   | 1.0000   | 10         | 49     |
|        |        | 10.0         | 0.239398                   | 1.0000   | 10         | 14     |

Table 11: Lagrangian Dual nonlinear  $\mathcal{L}_1\text{-SVC}$  results

|               |                |              | fit_time  | accuracy | n_iter | n_sv |
|---------------|----------------|--------------|-----------|----------|--------|------|
| dual          | kernel         | $\mathbf{C}$ |           |          |        |      |
| reg_bias      | poly           | 0.1          | 36.074888 | 0.790    | 10000  | 257  |
|               |                | 1.0          | 54.039554 | 0.875    | 10000  | 204  |
|               |                | 10.0         | 41.606979 | 0.790    | 10000  | 191  |
|               | rbf            | 0.1          | 63.063677 | 1.000    | 10000  | 310  |
|               |                | 1.0          | 44.399174 | 1.000    | 10000  | 213  |
|               |                | 10.0         | 37.221823 | 1.000    | 10000  | 182  |
| $unreg\_bias$ | poly           | 0.1          | 52.094757 | 0.845    | 10000  | 310  |
|               |                | 1.0          | 40.831654 | 0.750    | 10000  | 189  |
|               |                | 10.0         | 39.382344 | 0.780    | 10000  | 272  |
|               | $\mathrm{rbf}$ | 0.1          | 97.217501 | 1.000    | 10000  | 313  |
|               |                | 1.0          | 34.413624 | 1.000    | 10000  | 215  |
|               |                | 10.0         | 36.789399 | 1.000    | 10000  | 215  |

The same considerations made for the previous linear Wolfe dual and Lagrangian dual formulations are confirmed also in the nonlinearly separable case. In this setting the complexity of the model coming with higher C regularization values seems to be not paying a tradeoff in terms of the number of iterations of the algorithm and, moreover, the reg\_bias Lagrangian dual formulation seems to perform better wrt the unreg\_bias formulation, both tends to select even more training data points as support vectors.

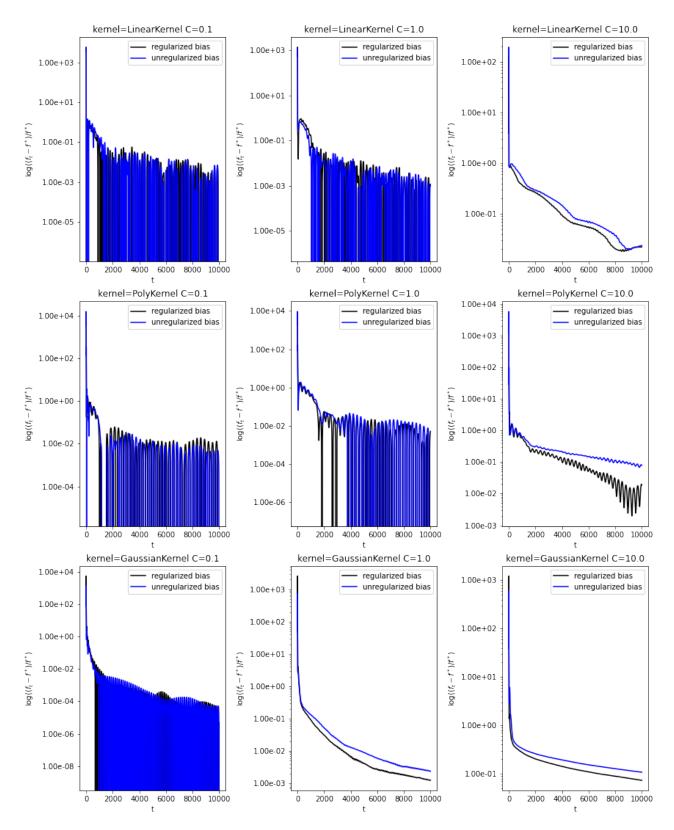


Figure 12: AdaGrad convergence for the Lagrangian Dual formulation of the nonlinear  $\mathcal{L}_1$ -SVC

#### 7.1.2 Squared Hinge loss

**Primal formulation** The experiments results shown in 12 referred to *Stochastic Gradient Descent* algorithm are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 0.02 and  $\beta$ , i.e., the *momentum*, equal to 0.5. Training is stopped if after 5 iterations the training loss is not lower than the best found so far within a tolerance of 1e-8.

|           |          |      | $\operatorname{fit\_time}$ | accuracy | $n\_iter$ | $n\_sv$ |
|-----------|----------|------|----------------------------|----------|-----------|---------|
| solver    | momentum | С    |                            |          |           |         |
| sgd       | none     | 0.1  | 0.173259                   | 0.975    | 488       | 49      |
|           |          | 1.0  | 0.196758                   | 0.980    | 433       | 24      |
|           |          | 10.0 | 0.041189                   | 0.985    | 57        | 21      |
|           | polyak   | 0.1  | 0.087903                   | 0.975    | 246       | 49      |
|           |          | 1.0  | 0.127343                   | 0.985    | 233       | 25      |
|           |          | 10.0 | 0.018536                   | 0.985    | 23        | 20      |
|           | nesterov | 0.1  | 0.097543                   | 0.975    | 247       | 49      |
|           |          | 1.0  | 0.134696                   | 0.985    | 234       | 23      |
|           |          | 10.0 | 0.023753                   | 0.985    | 30        | 18      |
| liblinear | -        | 0.1  | 0.001174                   | 0.980    | 52        | 46      |
|           |          | 1.0  | 0.001623                   | 0.980    | 563       | 25      |
|           |          | 10.0 | 0.002059                   | 0.980    | 1000      | 19      |

Table 12: Primal  $\mathcal{L}_2$ -SVC results

Again, the results provided from the *custom* implementation, i.e., the SGD with different momentum settings, are strongly similar to those of *sklearn* implementation, i.e., *liblinear* [10] implementation, in terms of *accuracy* score. More training data points are selected as *support vectors* from the SGD solver but it always requires even lower iterations, i.e., epochs, to achieve the same *numerical precision*. *Polyak* and *Nesterov* momentums always perform lower iterations as expected from the theoretical analysis of the convergence rate.

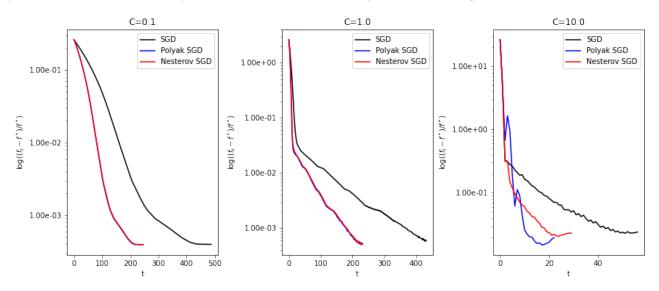


Figure 13: SGD convergence for the Primal formulation of the  $\mathcal{L}_2$ -SVC

**Linear Dual formulations** The experiments results shown in 13 are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (43) and (44) respectively with  $\rho$  equals to 1.

|               |      | $\operatorname{fit\_time}$ | accuracy | $_{\mathrm{n\_iter}}$ | $n\_sv$ |
|---------------|------|----------------------------|----------|-----------------------|---------|
| dual          | С    |                            |          |                       |         |
| reg_bias      | 0.1  | 11.991363                  | 0.980    | 10000                 | 46      |
|               | 1.0  | 13.825833                  | 0.985    | 10000                 | 139     |
|               | 10.0 | 13.258321                  | 0.945    | 10000                 | 101     |
| $unreg\_bias$ | 0.1  | 13.586800                  | 0.980    | 10000                 | 47      |
|               | 1.0  | 13.451519                  | 0.985    | 10000                 | 85      |
|               | 10.0 | 14.163535                  | 0.965    | 10000                 | 94      |

Table 13: Lagrangian Dual linear  $\mathcal{L}_2$ -SVC results

For what about the linear *Lagrangian dual* formulation we can see as it seems to be insensitive to the increasing complexity of the model in terms of number of *iterations* but it tends to select many training data points as *support vectors*.

Nonlinear Dual formulations The experiments results shown in 14 are obtained with d and r hyperparameters equal to 3 and 1 respectively for the polynomial kernel; gamma is setted to 'scale' for both polynomial and gaussian RBF kernels. The experiments results shown in 11 are obtained with  $\alpha$ , i.e., the learning rate or step size, setted to 1 for the AdaGrad algorithm. Note that the unreg\_bias and reg\_bias duals refers to the augmented dual formulations (135) of the problems (43) and (44) respectively with  $\rho$  equals to 1.

|              |        |              | $\operatorname{fit\_time}$ | accuracy | n_iter | n_sv |
|--------------|--------|--------------|----------------------------|----------|--------|------|
| dual         | kernel | $\mathbf{C}$ |                            |          |        |      |
| reg_bias     | poly   | 0.1          | 24.693942                  | 0.8675   | 10000  | 234  |
|              |        | 1.0          | 29.321871                  | 1.0000   | 10000  | 273  |
|              |        | 10.0         | 33.523163                  | 0.8225   | 10000  | 175  |
|              | rbf    | 0.1          | 5.595364                   | 1.0000   | 3419   | 345  |
|              |        | 1.0          | 27.956911                  | 1.0000   | 10000  | 130  |
|              |        | 10.0         | 33.733804                  | 1.0000   | 10000  | 215  |
| $unreg_bias$ | poly   | 0.1          | 21.976266                  | 0.8625   | 10000  | 234  |
|              | - •    | 1.0          | 32.952900                  | 1.0000   | 10000  | 196  |
|              |        | 10.0         | 34.304005                  | 0.7775   | 10000  | 289  |
|              | rbf    | 0.1          | 9.661301                   | 1.0000   | 5423   | 344  |
|              |        | 1.0          | 29.590797                  | 1.0000   | 10000  | 254  |
|              |        | 10.0         | 29.038893                  | 1.0000   | 10000  | 208  |

Table 14: Lagrangian Dual nonlinear  $\mathcal{L}_2$ -SVC results

The same considerations made for the previous linear Lagrangian dual formulations are confirmed also in the nonlinearly separable case. In this setting the complexity of the model coming with higher C regularization values seems to be not paying a tradeoff in terms of the number of iterations of the algorithm and, moreover, the reg\_bias Lagrangian dual formulation seems to perform better wrt the unreg\_bias formulation, both tends to select even more training data points as support vectors.

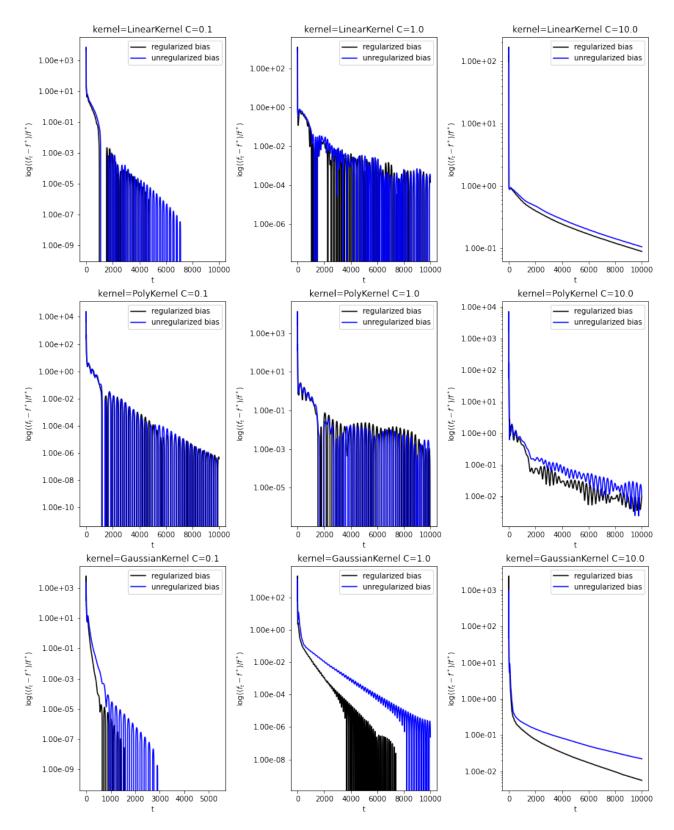


Figure 14: AdaGrad convergence for the Lagrangian Dual formulation of the nonlinear  $\mathcal{L}_2$ -SVC

# 7.2 Support Vector Regression

Below experiments are about the SVR for which I tested different values for regularization hyperparameter C, i.e., from soft to  $hard\ margin$ , the  $\epsilon$  penalty value and in case of nonlinearly separable data also different kernel functions mentioned above.

The experiments about SVRs are available at: github.com/dmeoli/optiml/blob/master/notebooks/optimization/CM\_SVR\_report\_experiments.ipynb.

### 7.2.1 Epsilon-insensitive loss

**Primal formulation** The experiments results shown in 15 referred to *Stochastic Gradient Descent* algorithm are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 0.02 and  $\beta$ , i.e., the *momentum*, equal to 0.4. Training is stopped if after 5 iterations the training loss is not lower than the best found so far within a tolerance of 1e-8.

Table 15: Primal  $\mathcal{L}_1$ -SVR results

|                                 |          |              |         | fit_time | r2       | n_iter | n_sv |
|---------------------------------|----------|--------------|---------|----------|----------|--------|------|
| solver                          | momentum | $\mathbf{C}$ | epsilon |          |          |        |      |
| $\overline{\operatorname{sgd}}$ | none     | 1            | 0.1     | 5.142108 | 0.954298 | 16161  | 100  |
| O                               |          |              | 0.2     | 3.760943 | 0.954544 | 12267  | 99   |
|                                 |          |              | 0.3     | 4.144172 | 0.955424 | 13665  | 99   |
|                                 |          | 10           | 0.1     | 0.279573 | 0.983893 | 806    | 98   |
|                                 |          |              | 0.2     | 0.305844 | 0.983891 | 884    | 98   |
|                                 |          |              | 0.3     | 0.325656 | 0.983884 | 958    | 97   |
|                                 |          | 100          | 0.1     | 0.052860 | 0.984034 | 85     | 97   |
|                                 |          |              | 0.2     | 0.061126 | 0.984047 | 96     | 98   |
|                                 |          |              | 0.3     | 0.068020 | 0.984056 | 109    | 98   |
|                                 | polyak   | 1            | 0.1     | 2.832931 | 0.954321 | 9874   | 100  |
|                                 |          |              | 0.2     | 2.156587 | 0.954549 | 7400   | 99   |
|                                 |          |              | 0.3     | 2.425077 | 0.955424 | 8200   | 99   |
|                                 |          | 10           | 0.1     | 0.192756 | 0.983893 | 487    | 97   |
|                                 |          |              | 0.2     | 0.204908 | 0.983891 | 535    | 98   |
|                                 |          |              | 0.3     | 0.216547 | 0.983885 | 569    | 98   |
|                                 |          | 100          | 0.1     | 0.030340 | 0.984030 | 48     | 98   |
|                                 |          |              | 0.2     | 0.035987 | 0.984046 | 56     | 98   |
|                                 |          |              | 0.3     | 0.039401 | 0.984055 | 61     | 97   |
|                                 | nesterov | 1            | 0.1     | 2.886144 | 0.954310 | 9785   | 100  |
|                                 |          |              | 0.2     | 2.263290 | 0.954546 | 7382   | 99   |
|                                 |          |              | 0.3     | 2.527795 | 0.955424 | 8198   | 99   |
|                                 |          | 10           | 0.1     | 0.209922 | 0.983892 | 489    | 97   |
|                                 |          |              | 0.2     | 0.212864 | 0.983890 | 533    | 97   |
|                                 |          |              | 0.3     | 0.228965 | 0.983884 | 579    | 98   |
|                                 |          | 100          | 0.1     | 0.038820 | 0.984031 | 61     | 98   |
|                                 |          |              | 0.2     | 0.036741 | 0.984047 | 58     | 98   |
|                                 |          |              | 0.3     | 0.039433 | 0.984057 | 62     | 98   |
| liblinear                       | -        | 1            | 0.1     | 0.001112 | 0.954684 | 12     | 100  |
|                                 |          |              | 0.2     | 0.001294 | 0.955112 | 10     | 99   |
|                                 |          |              | 0.3     | 0.001218 | 0.955415 | 10     | 97   |
|                                 |          | 10           | 0.1     | 0.001194 | 0.983893 | 57     | 99   |
|                                 |          |              | 0.2     | 0.001184 | 0.983890 | 69     | 98   |
|                                 |          |              | 0.3     | 0.000950 | 0.983906 | 142    | 97   |
|                                 |          | 100          | 0.1     | 0.001367 | 0.984023 | 980    | 97   |
|                                 |          |              | 0.2     | 0.001574 | 0.984029 | 1000   | 97   |
|                                 |          |              | 0.3     | 0.003733 | 0.984069 | 1000   | 97   |

The results provided from the custom implementation, i.e., the SGD with different momentum settings, are strongly similar to those of sklearn implementation, i.e., liblinear [10] implementation, in terms of r2 score, except in case of C regularization hyperparameter equals to 1 for which those of SGD are lower. Moreover, the SGD solver always requires lower iterations, i.e., epochs, for higher C regularization values, i.e., for C equals to 10 or 100, to achieve the same  $numerical\ precision$ . Again, Polyak and Nesterov momentums always perform lower iterations as expected from the theoretical analysis of the convergence rate. The results in terms of  $support\ vectors$  are strongly similar to each others.

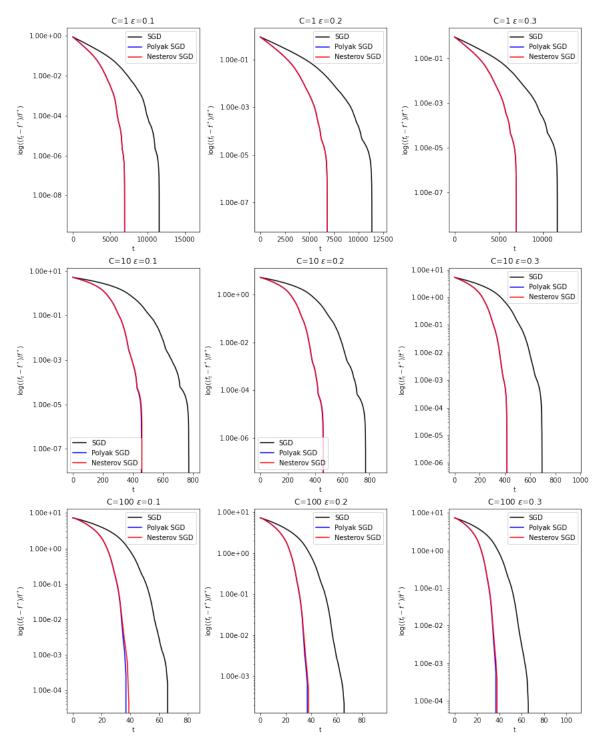


Figure 15: SGD convergence for the Primal formulation of the  $\mathcal{L}_1$ -SVR

**Linear Dual formulations** The experiments results shown in 17 are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (69) and (73) respectively with  $\rho$  equals to 1.

Table 16: Wolfe Dual linear  $\mathcal{L}_1$ -SVR results

|        |              |         | fit_time | r2       | n_iter | n_sv |
|--------|--------------|---------|----------|----------|--------|------|
| solver | $\mathbf{C}$ | epsilon |          |          |        |      |
| smo    | 1            | 0.1     | 0.073597 | 0.954396 | 10     | 100  |
|        |              | 0.2     | 0.030771 | 0.954546 | 15     | 100  |
|        |              | 0.3     | 0.061113 | 0.955429 | 13     | 99   |
|        | 10           | 0.1     | 0.263360 | 0.983893 | 44     | 99   |
|        |              | 0.2     | 0.167492 | 0.983893 | 48     | 99   |
|        |              | 0.3     | 0.139349 | 0.983893 | 41     | 99   |
|        | 100          | 0.1     | 0.847388 | 0.984071 | 623    | 98   |
|        |              | 0.2     | 0.442487 | 0.984088 | 157    | 98   |
|        |              | 0.3     | 0.609627 | 0.984103 | 334    | 98   |
| libsvm | 1            | 0.1     | 0.024892 | 0.954393 | 79     | 100  |
|        |              | 0.2     | 0.007021 | 0.954543 | 82     | 100  |
|        |              | 0.3     | 0.002929 | 0.955424 | 78     | 99   |
|        | 10           | 0.1     | 0.005642 | 0.983892 | 206    | 99   |
|        |              | 0.2     | 0.015230 | 0.983890 | 219    | 99   |
|        |              | 0.3     | 0.005720 | 0.983885 | 216    | 99   |
|        | 100          | 0.1     | 0.009251 | 0.984028 | 2239   | 98   |
|        |              | 0.2     | 0.003608 | 0.984041 | 1189   | 98   |
|        |              | 0.3     | 0.003550 | 0.984051 | 1366   | 98   |
| cvxopt | 1            | 0.1     | 0.117298 | 0.954685 | 9      | 100  |
|        |              | 0.2     | 0.088846 | 0.954849 | 9      | 100  |
|        |              | 0.3     | 0.199592 | 0.955429 | 10     | 100  |
|        | 10           | 0.1     | 0.118282 | 0.983893 | 9      | 100  |
|        |              | 0.2     | 0.156507 | 0.983893 | 8      | 100  |
|        |              | 0.3     | 0.081468 | 0.983893 | 8      | 100  |
|        | 100          | 0.1     | 0.094990 | 0.984071 | 9      | 100  |
|        |              | 0.2     | 0.065072 | 0.984088 | 9      | 100  |
|        |              | 0.3     | 0.087518 | 0.984103 | 8      | 100  |

For what about the linear Wolfe dual formulation we can immediately notice as higher regularization hyperparameter C and lower  $\epsilon$  values makes the model harder, so the custom implementation of the SMO algorithm and also the sklearn implementation, i.e., libsum [11] implementation, needs to perform more iterations to achieve the same numerical precision; meanwhile, again, the cuxopt [12] seems to be insensitive to the increasing complexity of the model. The results in terms of r2 and number of support vectors are strongly similar to each others.

Table 17: Lagrangian Dual linear  $\mathcal{L}_1$ -SVR results

|               |              |         | fit_time  | r2       | n_iter | n_sv |
|---------------|--------------|---------|-----------|----------|--------|------|
| dual          | $\mathbf{C}$ | epsilon |           |          |        |      |
| reg_bias      | 1            | 0.1     | 9.014390  | 0.954684 | 10000  | 100  |
|               |              | 0.2     | 9.522141  | 0.954846 | 10000  | 100  |
|               |              | 0.3     | 9.484683  | 0.955429 | 10000  | 100  |
|               | 10           | 0.1     | 9.553555  | 0.983899 | 10000  | 100  |
|               |              | 0.2     | 9.195415  | 0.983899 | 10000  | 100  |
|               |              | 0.3     | 9.738081  | 0.983891 | 10000  | 100  |
|               | 100          | 0.1     | 9.059696  | 0.984086 | 10000  | 100  |
|               |              | 0.2     | 9.252517  | 0.984088 | 10000  | 100  |
|               |              | 0.3     | 9.079562  | 0.984096 | 10000  | 100  |
| $unreg\_bias$ | 1            | 0.1     | 9.273358  | 0.954395 | 10000  | 100  |
|               |              | 0.2     | 9.031577  | 0.954535 | 10000  | 100  |
|               |              | 0.3     | 9.171732  | 0.955454 | 10000  | 99   |
|               | 10           | 0.1     | 9.490612  | 0.983892 | 10000  | 100  |
|               |              | 0.2     | 10.196379 | 0.983894 | 10000  | 100  |
|               |              | 0.3     | 9.208535  | 0.983890 | 10000  | 100  |
|               | 100          | 0.1     | 8.796887  | 0.983995 | 10000  | 100  |
|               |              | 0.2     | 9.366341  | 0.984055 | 10000  | 100  |
|               |              | 0.3     | 9.269228  | 0.984072 | 10000  | 100  |

For what about the linear  $Lagrangian\ dual$  formulation we can see as it seems to be insensitive to the increasing complexity of the model in terms of number of iterations and require many iterations wrt the  $Wolfe\ dual$  formulation.

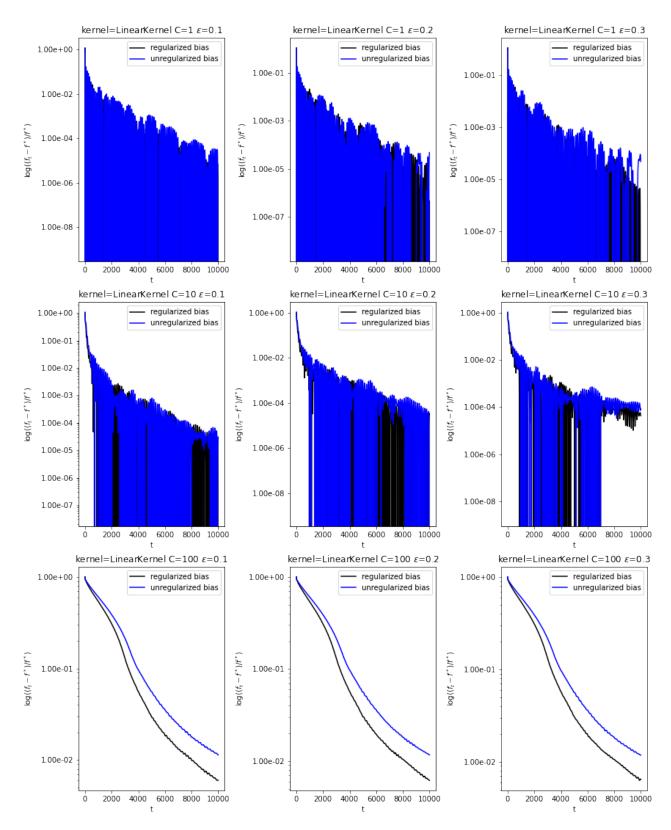


Figure 16: AdaGrad convergence for the Lagrangian Dual formulation of the linear  $\mathcal{L}_1$ -SVR

Nonlinear Dual formulations The experiments results shown in 18 and 19 are obtained with d and r hyperparameters both equal to 3 for the *polynomial* kernel; gamma is setted to 'scale' for both polynomial and  $gaussian\ RBF$  kernels. The experiments results shown in 11 are obtained with  $\alpha$ , i.e., the  $learning\ rate$  or  $step\ size$ , setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (69) and (73) respectively with  $\rho$  equals to 1.

Table 18: Wolfe Dual nonlinear  $\mathcal{L}_1\text{-SVR}$  formulation results

| solver | kernel               | C   | epsilon      | $\operatorname{fit\_time}$ | r2                  | n_iter   | n_sv |
|--------|----------------------|-----|--------------|----------------------------|---------------------|----------|------|
| smo    | poly                 | 1   | 0.1          | 68.392890                  | 0.810056            | 47694    | 36   |
|        | 1 0                  |     | 0.2          | 14.370649                  | 0.671256            | 8702     | 6    |
|        |                      |     | 0.3          | 5.386392                   | 0.302709            | 3654     | 4    |
|        |                      | 10  | 0.1          | 300.062039                 | 0.736098            | 256531   | 32   |
|        |                      |     | 0.2          | 41.746667                  | 0.923152            | 32629    | 4    |
|        |                      |     | 0.3          | 4.519509                   | 0.302709            | 3654     | 4    |
|        |                      | 100 | 0.1          | 1751.245163                | 0.635585            | 3294613  | 33   |
|        |                      | 100 | 0.2          | 39.353246                  | 0.923152            | 32629    | 4    |
|        |                      |     | $0.2 \\ 0.3$ | 4.833264                   | 0.302709            | 3654     | 4    |
|        | rbf                  | 1   | 0.1          | 0.058076                   | 0.988244            | 66       | 17   |
|        | 101                  | 1   | $0.1 \\ 0.2$ | 0.018418                   | 0.924292            | 20       | 7    |
|        |                      |     | $0.2 \\ 0.3$ | 0.015418 $0.015674$        | 0.924292 $0.883022$ | 17       | 5    |
|        |                      | 10  | $0.3 \\ 0.1$ | 0.463563                   | 0.883022 $0.989739$ | 389      | 18   |
|        |                      | 10  | $0.1 \\ 0.2$ | 0.403503 $0.014622$        | 0.989739 $0.924995$ | 25       | 6    |
|        |                      |     | $0.2 \\ 0.3$ | 0.014022 $0.012374$        | 0.924995 $0.882816$ | 23<br>11 | 5    |
|        |                      | 100 |              |                            |                     |          |      |
|        |                      | 100 | 0.1          | 3.754668                   | 0.974756            | 6664     | 19   |
|        |                      |     | 0.2          | 0.026766                   | 0.924995            | 25       | 6    |
| 1.1    | 1                    | -   | 0.3          | 0.014341                   | 0.882816            | 11       | 5    |
| libsvm | poly                 | 1   | 0.1          | 0.065797                   | 0.981438            | 155092   | 37   |
|        |                      |     | 0.2          | 0.009269                   | 0.976358            | 7326     | 6    |
|        |                      |     | 0.3          | 0.005210                   | 0.951282            | 3969     | 4    |
|        |                      | 10  | 0.1          | 0.168651                   | 0.981769            | 578347   | 32   |
|        |                      |     | 0.2          | 0.019524                   | 0.979414            | 28452    | 4    |
|        |                      |     | 0.3          | 0.004664                   | 0.951282            | 3969     | 4    |
|        |                      | 100 | 0.1          | 2.585694                   | 0.981844            | 13306191 | 35   |
|        |                      |     | 0.2          | 0.014572                   | 0.979414            | 28452    | 4    |
|        |                      |     | 0.3          | 0.016183                   | 0.951282            | 3969     | 4    |
|        | $\mathrm{rbf}$       | 1   | 0.1          | 0.004845                   | 0.990088            | 96       | 17   |
|        |                      |     | 0.2          | 0.008893                   | 0.977763            | 36       | 7    |
|        |                      |     | 0.3          | 0.001747                   | 0.945601            | 24       | 5    |
|        |                      | 10  | 0.1          | 0.002936                   | 0.990493            | 616      | 18   |
|        |                      |     | 0.2          | 0.009552                   | 0.980673            | 39       | 6    |
|        |                      |     | 0.3          | 0.001880                   | 0.945601            | 24       | 5    |
|        |                      | 100 | 0.1          | 0.022821                   | 0.990496            | 9854     | 18   |
|        |                      |     | 0.2          | 0.001701                   | 0.980673            | 39       | 6    |
|        |                      |     | 0.3          | 0.001951                   | 0.945601            | 24       | 5    |
| cvxopt | poly                 | 1   | 0.1          | 0.230761                   | 0.828482            | 10       | 37   |
| стлорт | poly                 | 1   | 0.2          | 0.132333                   | 0.666571            | 10       | 6    |
|        |                      |     | $0.2 \\ 0.3$ | 0.102333 $0.109379$        | 0.350876            | 9        | 4    |
|        |                      | 10  | 0.1          | 0.063353                   | 0.629433            | 10       | 33   |
|        |                      | 10  | $0.1 \\ 0.2$ | 0.062518                   | 0.023433 $0.928477$ | 10       | 4    |
|        |                      |     | $0.2 \\ 0.3$ | 0.002518 $0.133498$        | 0.320477 $0.350873$ | 10       |      |
|        |                      | 100 | $0.3 \\ 0.1$ |                            |                     |          | 4    |
|        |                      | 100 |              | 0.116879                   | 0.712681            | 10       | 36   |
|        |                      |     | 0.2          | 0.155555                   | 0.928478            | 10       | 4    |
|        | 1 C                  | -1  | 0.3          | 0.080267                   | 0.350876            | 10       | 4    |
|        | $\operatorname{rbf}$ | 1   | 0.1          | 0.056430                   | 0.988117            | 10       | 17   |
|        |                      |     | 0.2          | 0.037635                   | 0.924679            | 10       | 7    |
|        |                      | 10  | 0.3          | 0.031585                   | 0.883386            | 10       | 5    |
|        |                      | 10  | 0.1          | 0.033969                   | 0.989956            | 10       | 18   |
|        |                      |     | 0.2          | 0.034816                   | 0.925595            | 10       | 6    |
|        |                      |     | 0.3          | 0.039004                   | 0.883386            | 10       | 5    |
|        |                      | 100 | 0.1          | 0.026327                   | 0.990216            | 10       | 40   |
|        |                      |     | 0.2          | 0.036008                   | 0.925595            | 10       | 6    |
|        |                      |     | 0.3          | 0.030514                   | 0.883386            | 10       | 5    |

Table 19: Lagrangian Dual nonlinear  $\mathcal{L}_1\text{-SVR}$  results

|               |        |              |         | fit_time  | r2       | n_iter | n_sv |
|---------------|--------|--------------|---------|-----------|----------|--------|------|
| dual          | kernel | $\mathbf{C}$ | epsilon |           |          |        |      |
| reg_bias      | poly   | 1            | 0.1     | 8.753738  | 0.980649 | 10000  | 100  |
| O             | 1 0    |              | 0.2     | 8.196864  | 0.981475 | 10000  | 100  |
|               |        |              | 0.3     | 8.575808  | 0.980750 | 10000  | 100  |
|               |        | 10           | 0.1     | 9.458230  | 0.980042 | 10000  | 100  |
|               |        |              | 0.2     | 8.525160  | 0.980724 | 10000  | 100  |
|               |        |              | 0.3     | 8.916882  | 0.974359 | 10000  | 100  |
|               |        | 100          | 0.1     | 8.869521  | 0.981125 | 10000  | 100  |
|               |        |              | 0.2     | 8.441144  | 0.981479 | 10000  | 100  |
|               |        |              | 0.3     | 9.133370  | 0.978966 | 10000  | 99   |
|               | rbf    | 1            | 0.1     | 9.224121  | 0.990052 | 10000  | 81   |
|               |        |              | 0.2     | 10.106396 | 0.964400 | 10000  | 61   |
|               |        |              | 0.3     | 10.219767 | 0.952099 | 10000  | 54   |
|               |        | 10           | 0.1     | 9.175098  | 0.989754 | 10000  | 92   |
|               |        |              | 0.2     | 10.355982 | 0.983904 | 10000  | 43   |
|               |        |              | 0.3     | 10.386412 | 0.956593 | 10000  | 43   |
|               |        | 100          | 0.1     | 9.102558  | 0.989818 | 10000  | 86   |
|               |        |              | 0.2     | 10.319922 | 0.984017 | 10000  | 71   |
|               |        |              | 0.3     | 10.361556 | 0.937889 | 10000  | 70   |
| $unreg\_bias$ | poly   | 1            | 0.1     | 8.627309  | 0.981039 | 10000  | 100  |
|               |        |              | 0.2     | 8.490436  | 0.978000 | 10000  | 100  |
|               |        |              | 0.3     | 7.721025  | 0.977036 | 10000  | 99   |
|               |        | 10           | 0.1     | 9.866277  | 0.978251 | 10000  | 100  |
|               |        |              | 0.2     | 8.645740  | 0.981917 | 10000  | 99   |
|               |        |              | 0.3     | 7.725760  | 0.977723 | 10000  | 100  |
|               |        | 100          | 0.1     | 8.925465  | 0.978305 | 10000  | 100  |
|               |        |              | 0.2     | 10.440119 | 0.980187 | 10000  | 100  |
|               |        |              | 0.3     | 7.783286  | 0.965960 | 10000  | 100  |
|               | rbf    | 1            | 0.1     | 10.031470 | 0.989985 | 10000  | 90   |
|               |        |              | 0.2     | 9.228424  | 0.974585 | 10000  | 73   |
|               |        |              | 0.3     | 9.231140  | 0.937354 | 10000  | 75   |
|               |        | 10           | 0.1     | 9.533357  | 0.989713 | 10000  | 87   |
|               |        |              | 0.2     | 9.193305  | 0.974184 | 10000  | 75   |
|               |        |              | 0.3     | 9.457048  | 0.954241 | 10000  | 67   |
|               |        | 100          | 0.1     | 9.800612  | 0.989624 | 10000  | 93   |
|               |        |              | 0.2     | 9.465609  | 0.983461 | 10000  | 72   |
|               |        |              | 0.3     | 10.547809 | 0.942005 | 10000  | 82   |

The same considerations made for the previous linear Wolfe dual and Lagrangian dual formulations are confirmed also in the nonlinearly separable case. In this setting, the complexity of the model coming with higher C regularization hyperparameters and lower  $\epsilon$  values pays a larger tradeoff in terms of the number of iterations of the algorithm.

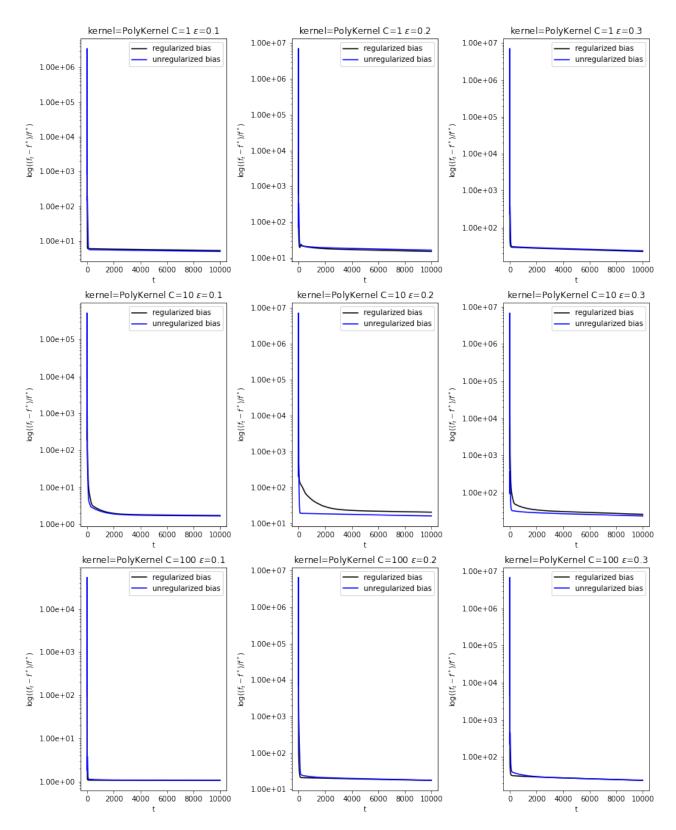


Figure 17: AdaGrad convergence for the Lagrangian Dual formulation of the Polynomial  $\mathcal{L}_1$ -SVR

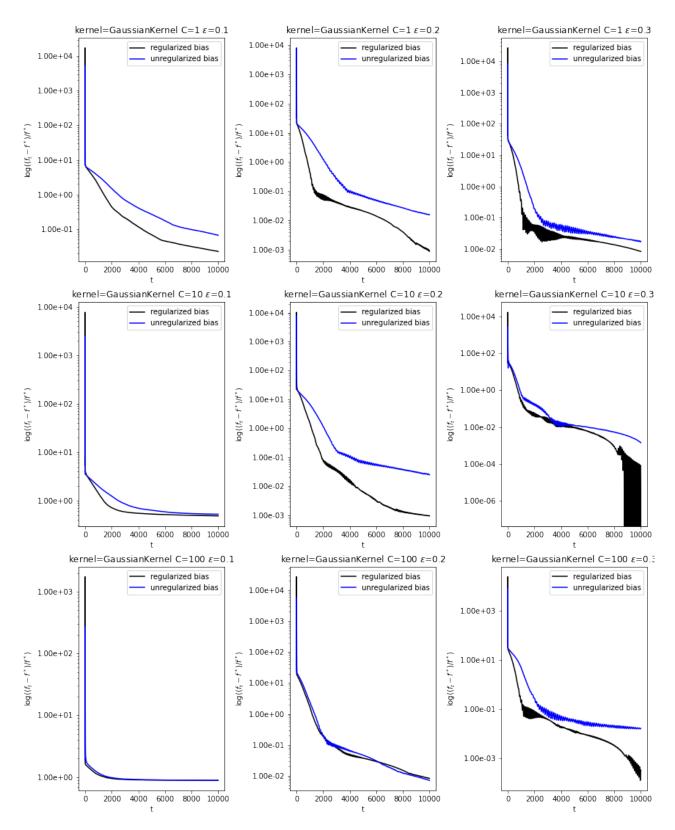


Figure 18: AdaGrad convergence for the Lagrangian Dual formulation of the Gaussian  $\mathcal{L}_1$ -SVR

### 7.2.2 Squared Epsilon-insensitive loss

**Primal formulation** The experiments results shown in 20 referred to *Stochastic Gradient Descent* algorithm are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 0.02 and  $\beta$ , i.e., the *momentum*, equal to 0.4. Training is stopped if after 5 iterations the training loss is not lower than the best found so far within a tolerance of 1e-8.

Table 20: Primal  $\mathcal{L}_2$ -SVR results

|           |          |              |         | $\operatorname{fit\_time}$ | r2       | n_iter | n_sv |
|-----------|----------|--------------|---------|----------------------------|----------|--------|------|
| solver    | momentum | $\mathbf{C}$ | epsilon |                            |          |        |      |
| sgd       | none     | 1            | 0.1     | 1.086567                   | 0.984109 | 3283   | 100  |
| O         |          |              | 0.2     | 1.088368                   | 0.984109 | 3294   | 100  |
|           |          |              | 0.3     | 1.101102                   | 0.984109 | 3321   | 98   |
|           |          | 10           | 0.1     | 0.165906                   | 0.984133 | 409    | 98   |
|           |          |              | 0.2     | 0.179832                   | 0.984133 | 410    | 98   |
|           |          |              | 0.3     | 0.178150                   | 0.984133 | 411    | 98   |
|           |          | 100          | 0.1     | 0.030447                   | 0.984133 | 47     | 98   |
|           |          |              | 0.2     | 0.030926                   | 0.984133 | 47     | 98   |
|           |          |              | 0.3     | 0.030644                   | 0.984133 | 47     | 98   |
|           | polyak   | 1            | 0.1     | 0.608905                   | 0.984109 | 2011   | 100  |
|           |          |              | 0.2     | 0.654603                   | 0.984109 | 2018   | 100  |
|           |          |              | 0.3     | 0.654698                   | 0.984109 | 2035   | 98   |
|           |          | 10           | 0.1     | 0.123878                   | 0.984133 | 241    | 98   |
|           |          |              | 0.2     | 0.125095                   | 0.984133 | 242    | 98   |
|           |          |              | 0.3     | 0.124025                   | 0.984133 | 243    | 98   |
|           |          | 100          | 0.1     | 0.026336                   | 0.984133 | 40     | 98   |
|           |          |              | 0.2     | 0.026389                   | 0.984133 | 40     | 98   |
|           |          |              | 0.3     | 0.026316                   | 0.984133 | 40     | 98   |
|           | nesterov | 1            | 0.1     | 0.644493                   | 0.984109 | 2015   | 100  |
|           |          |              | 0.2     | 0.652730                   | 0.984109 | 2022   | 100  |
|           |          |              | 0.3     | 0.656327                   | 0.984109 | 2039   | 98   |
|           |          | 10           | 0.1     | 0.125323                   | 0.984133 | 247    | 98   |
|           |          |              | 0.2     | 0.125930                   | 0.984133 | 248    | 98   |
|           |          |              | 0.3     | 0.126420                   | 0.984133 | 248    | 98   |
|           |          | 100          | 0.1     | 0.018405                   | 0.984133 | 27     | 98   |
|           |          |              | 0.2     | 0.018378                   | 0.984133 | 27     | 98   |
|           |          |              | 0.3     | 0.018410                   | 0.984133 | 27     | 98   |
| liblinear | -        | 1            | 0.1     | 0.001389                   | 0.984109 | 84     | 100  |
|           |          |              | 0.2     | 0.001621                   | 0.984109 | 84     | 100  |
|           |          |              | 0.3     | 0.001536                   | 0.984109 | 84     | 98   |
|           |          | 10           | 0.1     | 0.003507                   | 0.984133 | 778    | 98   |
|           |          |              | 0.2     | 0.003448                   | 0.984133 | 773    | 98   |
|           |          |              | 0.3     | 0.004677                   | 0.984133 | 773    | 98   |
|           |          | 100          | 0.1     | 0.004310                   | 0.984126 | 1000   | 100  |
|           |          |              | 0.2     | 0.004514                   | 0.984127 | 1000   | 98   |
|           |          |              | 0.3     | 0.005712                   | 0.984128 | 1000   | 98   |

Again, the results provided from the custom implementation, i.e., the SGD with different momentum settings, are strongly similar to those of sklearn implementation, i.e., liblinear [10] implementation, in terms of r2 score. SGD solver always requires even lower iterations, i.e., epochs, for higher C regularization values, i.e., for C equals to 10 or 100, to achieve the same  $numerical\ precision$ . Polyak and Nesterov momentums always perform

lower iterations as expected from the theoretical analysis of the convergence rate.

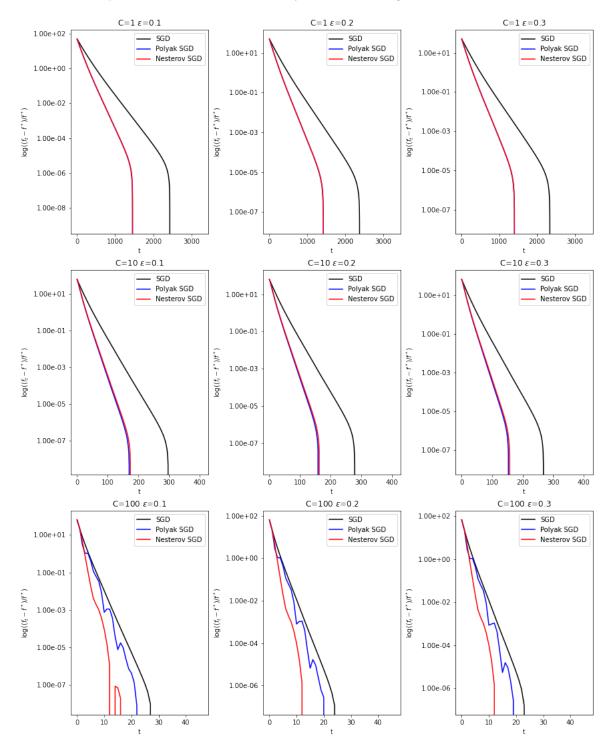


Figure 19: SGD convergence for the Primal formulation of the  $\mathcal{L}_2$ -SVR

**Linear Dual formulations** The experiments results shown in 21 are obtained with  $\alpha$ , i.e., the *learning rate* or *step size*, setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (90) and (91) respectively with  $\rho$  equals to 1.

Table 21: Lagrangian Dual linear  $\mathcal{L}_2\text{-SVR}$  results

|               |              |         | fit_time | r2       | n_iter | n_sv |
|---------------|--------------|---------|----------|----------|--------|------|
| dual          | $\mathbf{C}$ | epsilon |          |          |        |      |
| reg_bias      | 1            | 0.1     | 8.886250 | 0.984109 | 10000  | 100  |
|               |              | 0.2     | 8.447072 | 0.984109 | 10000  | 100  |
|               |              | 0.3     | 8.493953 | 0.984109 | 10000  | 98   |
|               | 10           | 0.1     | 8.203294 | 0.984133 | 10000  | 100  |
|               |              | 0.2     | 8.320815 | 0.984133 | 10000  | 100  |
|               |              | 0.3     | 8.490490 | 0.984133 | 10000  | 98   |
|               | 100          | 0.1     | 8.775280 | 0.984129 | 10000  | 100  |
|               |              | 0.2     | 9.019509 | 0.984130 | 10000  | 100  |
|               |              | 0.3     | 9.022733 | 0.984131 | 10000  | 100  |
| $unreg\_bias$ | 1            | 0.1     | 8.186003 | 0.984109 | 10000  | 100  |
|               |              | 0.2     | 9.028857 | 0.984109 | 10000  | 100  |
|               |              | 0.3     | 9.081488 | 0.984109 | 10000  | 98   |
|               | 10           | 0.1     | 9.138670 | 0.984133 | 10000  | 100  |
|               |              | 0.2     | 9.154195 | 0.984133 | 10000  | 100  |
|               |              | 0.3     | 9.228451 | 0.984133 | 10000  | 100  |
|               | 100          | 0.1     | 8.706512 | 0.984131 | 10000  | 100  |
|               |              | 0.2     | 8.119011 | 0.984132 | 10000  | 100  |
|               |              | 0.3     | 8.417662 | 0.984132 | 10000  | 100  |

For what about the linear  $Lagrangian\ dual$  formulation we can see as it seems to be insensitive to the increasing complexity of the model in terms of number of iterations and require many iterations wrt the  $Wolfe\ dual$  formulation.

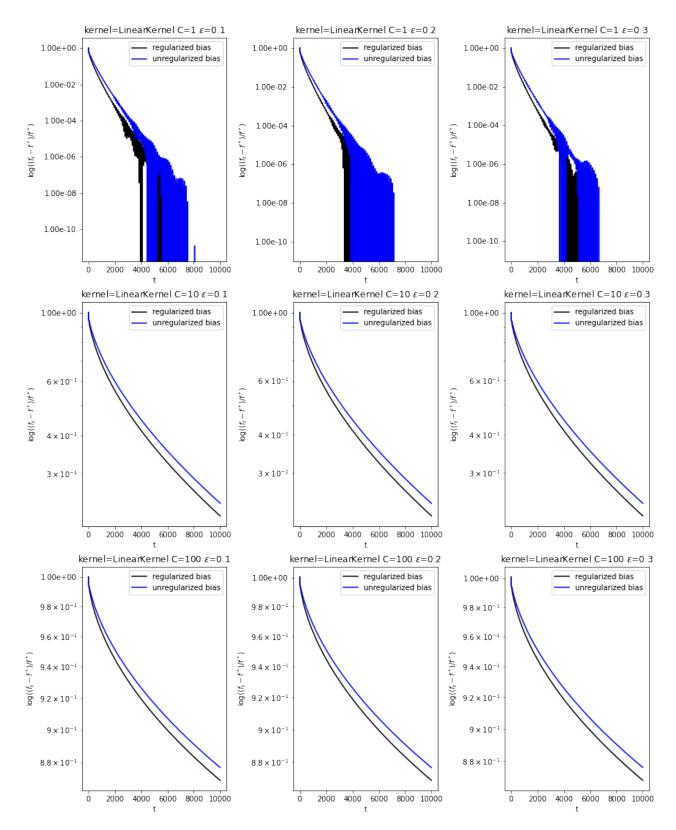


Figure 20: AdaGrad convergence for the Lagrangian Dual formulation of the linear  $\mathcal{L}_2$ -SVR

Nonlinear Dual formulations The experiments results shown in 22 are obtained with d and r hyperparameters both equal to 3 for the *polynomial* kernel; gamma is setted to 'scale' for both polynomial and gaussian RBF kernels. The experiments results shown in 22 are obtained with  $\alpha$ , i.e., the learning rate or step size, setted to 1 for the AdaGrad algorithm. Note that the  $unreg\_bias$  and  $reg\_bias$  duals refers to the augmented dual formulations (135) of the problems (90) and (91) respectively with  $\rho$  equals to 1.

Table 22: Lagrangian Dual nonlinear  $\mathcal{L}_2$ -SVR results

|               |        |              |         | fit_time  | r2       | n_iter | n_sv |
|---------------|--------|--------------|---------|-----------|----------|--------|------|
| dual          | kernel | $\mathbf{C}$ | epsilon |           |          |        |      |
| reg_bias      | poly   | 1            | 0.1     | 8.235232  | 0.978282 | 10000  | 100  |
|               |        |              | 0.2     | 8.716630  | 0.970738 | 10000  | 100  |
|               |        |              | 0.3     | 8.480382  | 0.963066 | 10000  | 98   |
|               |        | 10           | 0.1     | 8.115164  | 0.981600 | 10000  | 100  |
|               |        |              | 0.2     | 8.343646  | 0.978640 | 10000  | 100  |
|               |        |              | 0.3     | 8.470356  | 0.972543 | 10000  | 99   |
|               |        | 100          | 0.1     | 9.089824  | 0.979231 | 10000  | 100  |
|               |        |              | 0.2     | 8.650169  | 0.979959 | 10000  | 100  |
|               |        |              | 0.3     | 7.813888  | 0.968573 | 10000  | 98   |
|               | rbf    | 1            | 0.1     | 9.356709  | 0.971405 | 10000  | 35   |
|               |        |              | 0.2     | 10.505933 | 0.932771 | 10000  | 28   |
|               |        |              | 0.3     | 9.865885  | 0.897683 | 10000  | 16   |
|               |        | 10           | 0.1     | 9.698501  | 0.986052 | 10000  | 68   |
|               |        |              | 0.2     | 9.203216  | 0.979205 | 10000  | 35   |
|               |        |              | 0.3     | 9.812614  | 0.945504 | 10000  | 34   |
|               |        | 100          | 0.1     | 9.452740  | 0.989507 | 10000  | 77   |
|               |        |              | 0.2     | 9.319579  | 0.984410 | 10000  | 55   |
|               |        |              | 0.3     | 9.517304  | 0.948853 | 10000  | 53   |
| $unreg\_bias$ | poly   | 1            | 0.1     | 8.688517  | 0.971836 | 10000  | 100  |
|               |        |              | 0.2     | 7.715100  | 0.969615 | 10000  | 100  |
|               |        |              | 0.3     | 7.565595  | 0.979246 | 10000  | 100  |
|               |        | 10           | 0.1     | 8.340514  | 0.981361 | 10000  | 100  |
|               |        |              | 0.2     | 8.246735  | 0.977274 | 10000  | 100  |
|               |        |              | 0.3     | 7.812046  | 0.977763 | 10000  | 100  |
|               |        | 100          | 0.1     | 7.809393  | 0.978690 | 10000  | 100  |
|               |        |              | 0.2     | 8.281094  | 0.979153 | 10000  | 100  |
|               |        |              | 0.3     | 9.130430  | 0.976826 | 10000  | 100  |
|               | rbf    | 1            | 0.1     | 9.946135  | 0.971405 | 10000  | 35   |
|               |        |              | 0.2     | 9.118614  | 0.932774 | 10000  | 28   |
|               |        |              | 0.3     | 9.868906  | 0.907758 | 10000  | 44   |
|               |        | 10           | 0.1     | 9.417278  | 0.988111 | 10000  | 79   |
|               |        |              | 0.2     | 10.214749 | 0.965456 | 10000  | 63   |
|               |        |              | 0.3     | 9.133241  | 0.936584 | 10000  | 81   |
|               |        | 100          | 0.1     | 8.922632  | 0.989715 | 10000  | 86   |
|               |        |              | 0.2     | 9.714174  | 0.982249 | 10000  | 75   |
|               |        |              | 0.3     | 9.847793  | 0.942890 | 10000  | 75   |

The same considerations made for the previous linear Lagrangian dual formulations are confirmed also in the nonlinearly separable case. In this setting, the complexity of the model coming with higher C regularization hyperparameters and lower  $\epsilon$  values pays a larger tradeoff in terms of the number of iterations of the algorithm.

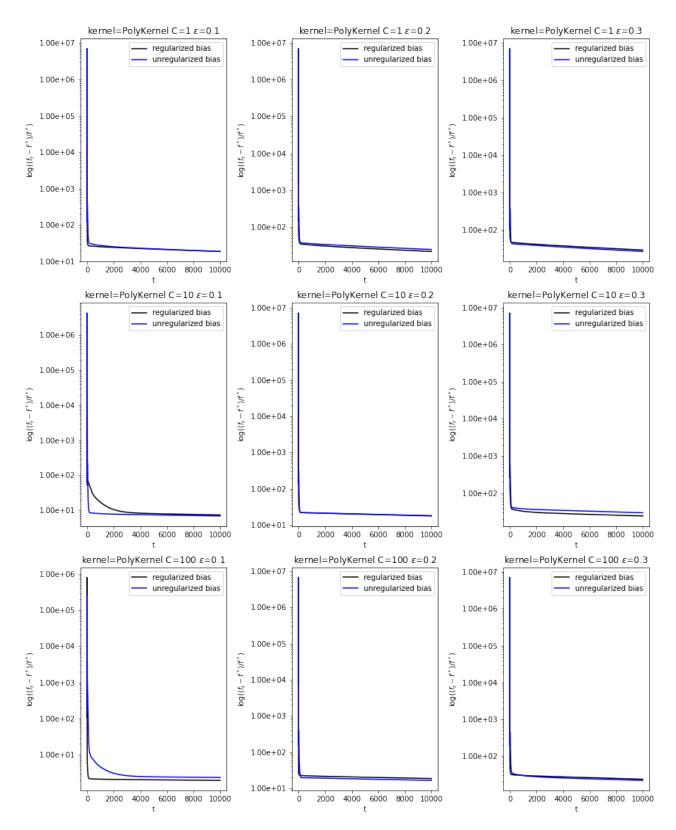


Figure 21: AdaGrad convergence for the Lagrangian Dual formulation of the Polynomial  $\mathcal{L}_2$ -SVR

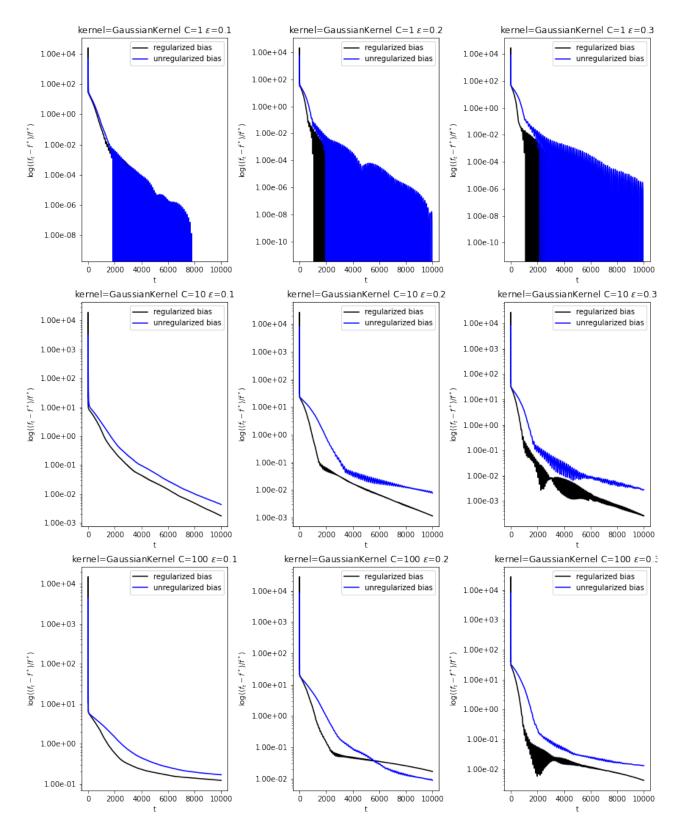


Figure 22: AdaGrad convergence for the Lagrangian Dual formulation of the Gaussian  $\mathcal{L}_2$ -SVR

## 8 Conclusions

For what about the SVM formulations, it is known, in general, that the *primal formulation*, is suitable for large linear training since the complexity of the model grows with the number of features or, more in general, when the number of examples n is much larger than the number of features m, i.e.,  $n \gg m$ ; meanwhile the dual formulation, is more suitable in case the number of examples n is less than the number of features m, i.e., n < m, since the complexity of the model is dominated by the number of examples, or more in general when the training data are not linearly separable in the input space.

From all these experiments we can see as all the *custom* implementations underperforms all the others, i.e., both *cvxopt* [12] and *sklearn* implementations, i.e., *liblinear* [10] and *libsvm* [11] implementations, in terms of *time* obviously due to the different core implementation languages, i.e., Python and C respectively.

In the *primal* formulations the *liblinear* [10] implementation uses an optimization method called *Coordinate* Gradient Descent which minimizes one coordinate at a time.

Meanwhile, for what about the Wolfe dual formulations we can notice as cvxopt [12] underperforms the sklearn implementation, i.e., libsvm [11] implementation, in terms of time since it is a general-purpose QP solver and it does not exploit the structure of the problem, as SMO does. An interesting consideration can be made about the number of iterations of custom SMO implementation wrt that in libsvm which seems to be always lower thanks to the improvements described in [5, 8] for classification and regression respectively.

Finally, in the *Lagrangian dual* formulations, we can see as fitting the intercept in an explicit way, i.e., by adding Lagrange multipliers to control the equality constraint always get lower scores wrt the *Lagrangian dual* of the same problem with the bias term embedded into the weight matrix.

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