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# Support Vector Machines

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# 2 Abstract

A *Support Vector Machine* is a learning model used both for *classification* and *regression* tasks whose goal is to constructs 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* [8] 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 performace of different *kernels*, also by comparing the *custom* results with *sklearn* SVM implementations, i.e., *liblinear* [9] and *libsvm* [10] implementations, and *cvxopt* [11] 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:

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

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:

$$\begin{aligned} & w^T x_i + b \geq +1 - \xi_i, \forall y_i = +1 \\ & w^T x_i + b \leq -1 + \xi_i, \forall y_i = -1 \\ & \xi_i \geq 0 \ \forall_i \end{aligned} \tag{2}$$

where the positive slack variables $\xi_i$ are introduced to allow missclassified 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:

$$\begin{aligned} & y_i(w^T x_i + b) \geq 1 - \xi_i \ \forall_i \\ & \xi_i \geq 0 \ \forall_i \end{aligned} \tag{3}$$

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

$$\begin{aligned} \min_{w,b,\xi} \quad & \|w\| + C \sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & y_i(w^T x_i + b) \geq 1 - \xi_i \ \forall_i \\ & \xi_i \geq 0 \ \forall_i \end{aligned} \tag{4}$$

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

$$\begin{aligned} \min_{w,b,\xi} \quad & \frac{1}{2}\|w\|^2 + C \sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & y_i(w^T x_i + b) \geq 1 - \xi_i \ \forall_i \\ & \xi_i \geq 0 \ \forall_i \end{aligned} \tag{5}$$

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

## 3.1 Hinge loss

The *hinge* loss is defined as:

$$\mathcal{L}_1 = \begin{cases} 0 & \text{if } y(w^T x + b) \geq 1 \\ 1 - y(w^T x + b) & \text{otherwise} \end{cases} \tag{6}$$

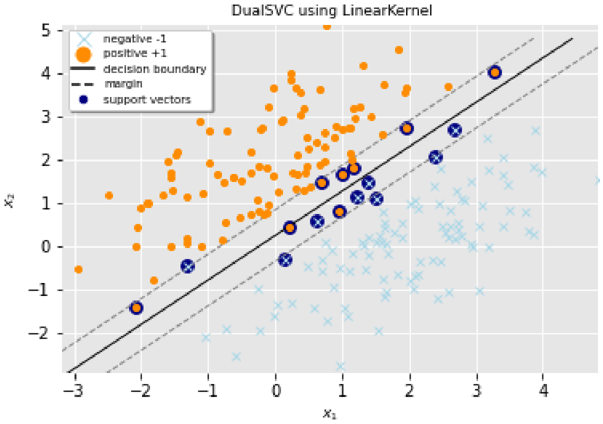


Figure 1: Linear SVC hyperplane

or, equivalently:

$$\mathcal{L}_1 = \max(0, 1 - y(w^T x + b)) \tag{7}$$

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

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

#### 3.1.1 Primal formulation

The general primal unconstrained formulation takes the form:

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

where $\mathcal{R}(w,b)$ is the *regularization term* and $\mathcal{L}(w,b;x_i,y_i)$ is the *loss function* associated with the observation $(x_i, y_i)$.

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

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

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.

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 (10) and (41) as follows:

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

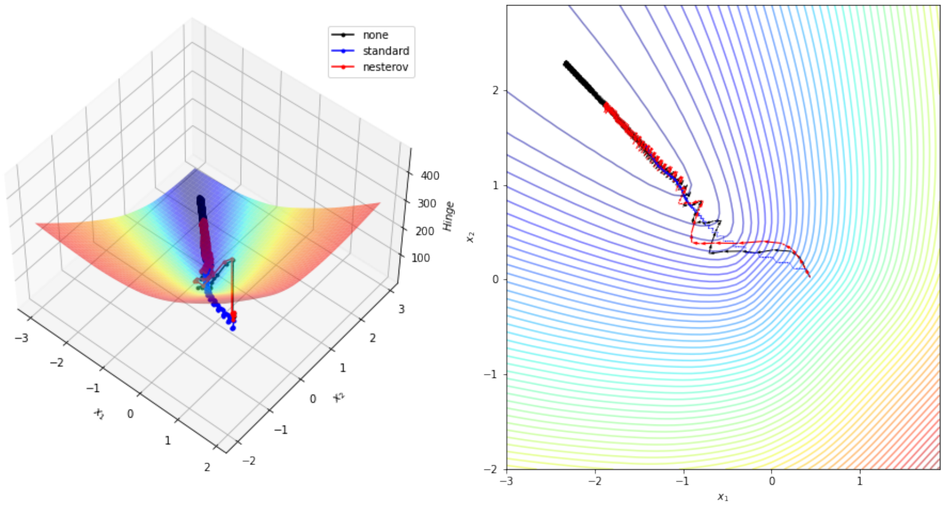


Figure 2: SVC Hinge loss with different optimization steps

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:

$$\begin{aligned} \min_{w} \quad & \frac{1}{2}\|\bar{w}\|^2 + C\sum_{i=1}^{n}\mathcal{L}(w;\bar{x}_i,y_i) \\ \text{where} \quad & \bar{w}^T = [w^T, b] \\ & \bar{x}_i^T = [x_i^T, 1] \end{aligned} \tag{12}$$

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.

Notice that in terms of numerical optimization the formulations (10) and (41) are not equivalent to (11) or (12) 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 [12] show that the accuracy does not vary much when the bias term $b$ is embedded into the weight vector $w$.

### 3.1.2 Wolfe Dual formulation

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

$$\max_{\alpha,\mu}\min_{w,b,\xi}\mathcal{W}(w,b,\xi,\alpha,\mu) = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i(y_i(w^Tx_i+b)-1+\xi_i) - \sum_{i=1}^{n}\mu_i\xi_i \tag{13}$$

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:

$$\frac{\partial\mathcal{W}}{\partial w} = w - \sum_{i=1}^{n}\alpha_i y_i x_i \Rightarrow w = \sum_{i=1}^{n}\alpha_i y_i x_i \tag{14}$$

$$\frac{\partial \mathcal{W}}{\partial b} = -\sum_{i=1}^{n} \alpha_i y_i \Rightarrow \sum_{i=1}^{n} \alpha_i y_i = 0 \tag{15}$$

$$\frac{\partial \mathcal{W}}{\partial \xi_i} = 0 \Rightarrow C = \alpha_i + \mu_i \tag{16}$$

Substituting (14) and (15) into (13) 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:

$$\begin{aligned} \max_{\alpha} \mathcal{W}(\alpha) &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \\ &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i Q_{ij} \alpha_j \text{ where } Q_{ij} = y_i y_j \langle x_i, x_j \rangle \\ &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\alpha^T Q \alpha \text{ subject to } 0 \leq \alpha_i \leq C \ \forall_i, \sum_{i=1}^{n} \alpha_i y_i = 0 \end{aligned} \tag{17}$$

or, equivalently:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2}\alpha^T Q \alpha + q^T \alpha \\ \text{subject to} \quad & 0 \leq \alpha_i \leq C \ \forall_i \\ & y^T \alpha = 0 \end{aligned} \tag{18}$$

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

By solving (18) we will know $\alpha$ and, from (14), we will get $w$, so we need to calculate $b$.

We know that any data point satisfying (15) which is a support vector $x_s$ will have the form:

$$y_s(w^T x_s + b) = 1 \tag{19}$$

and, by substituting in (14), we get:

$$y_s\big(\sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle + b\big) = 1 \tag{20}$$

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):

$$y_s^2\big(\sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle + b\big) = y_s \tag{21}$$

$$b = y_s - \sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle \tag{22}$$

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

$$b = \frac{1}{N_s}\sum_{s \in S} y_s - \sum_{m \in S} \alpha_m y_m \langle x_m, x_s \rangle \tag{23}$$

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:

$$y' = \operatorname{sgn}\big(\sum_{i=1}^{n} \alpha_i y_i \langle x_i, x' \rangle + b\big) \tag{24}$$

From (18) 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 [12] that arises from the primal (11) or (12) where the bias term $b$ is embedded into the weight vector $w$:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2}\alpha^T(Q + yy^T)\alpha + q^T\alpha \\ \text{subject to} \quad & 0 \leq \alpha_i \leq C \ \forall_i \end{aligned} \tag{25}$$

### 3.1.3 Lagrangian Dual formulation

In order to relax the constraints in the *Wolfe dual* formulation (18) we define the problem as a *Lagrangian dual* relaxation by embedding them into objective function, so we need to allocate the Lagrangian multipliers $\mu \geq 0, \lambda_+ \geq 0, \ \lambda_- \geq 0$:

$$\begin{aligned} \max_{\mu,\lambda_+,\lambda_-} \min_{\alpha} \mathcal{L}(\alpha,\mu,\lambda_+,\lambda_-) &= \frac{1}{2}\alpha^T Q\alpha + q^T\alpha - \mu^T(y^T\alpha) - \lambda_+^T(u-\alpha) - \lambda_-^T\alpha \\ &= \frac{1}{2}\alpha^T Q\alpha + (q - \mu y + \lambda_+ - \lambda_-)^T\alpha - \lambda_+^T u \end{aligned} \tag{26}$$

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:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow Q\alpha + (q - \mu y + \lambda_+ - \lambda_-) = 0 \tag{27}$$

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

$$Q\alpha = -(q - \mu y + \lambda_+ - \lambda_-) \tag{28}$$

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

$$\frac{\partial \mathcal{L}}{\partial \mu} = -y\alpha \tag{29}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_+} = \alpha - u \tag{30}$$

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

If the Hessian matrix Q is not positive definite, i.e., the Lagrangian function is not strictly convex since it will be linear along the eigenvectors correspondent to the null eigenvalues and so it will be unbounded below, the Lagrangian dual relaxation will be nondifferentiable, so it will have infinite solutions and for each of them it will have a different subgradient. In order to compute an approximation of the gradient, we will choose $\alpha$ in such a way as the one that minimizes the norm of the residual:

$$\begin{aligned} \min_{\alpha_n \in K_n(Q,b)} \quad & \|Q\alpha_n - b\| \\ \text{where} \quad & b = -(q - \mu y + \lambda_+ - \lambda_-) \end{aligned} \tag{32}$$

Since we are dealing with a symmetric but indefinite linear system we will choose a well-known Krylov method that performs the Lanczos iterate, i.e., symmetric Arnoldi iterate, called *minres*, i.e., symmetric *gmres*, to compute the vector $\alpha_n$ that minimizes the norm of the residual $r_n = Q\alpha_n - b$ among all vectors in $K_n(Q,b) = span(b, Qb, Q^2b, \dots, Q^{n-1}b)$.

From (18) 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 (26) 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 (25).

$$\begin{aligned} \max_{\lambda_+,\lambda_-} \min_{\alpha} \mathcal{L}(\alpha, \lambda_+, \lambda_-) &= \frac{1}{2}\alpha^T(Q + yy^T)\alpha + q^T\alpha - \lambda_+^T(u - \alpha) - \lambda_-^T\alpha \\ &= \frac{1}{2}\alpha^T(Q + yy^T)\alpha + (q + \lambda_+ - \lambda_-)^T\alpha - \lambda_+^T u \end{aligned} \tag{33}$$

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:

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

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

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

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:

$$\mathcal{L}_2 = \begin{cases} 0 & \text{if } y(w^Tx + b) \geq 1 \\ (1 - y(w^Tx + b))^2 & \text{otherwise} \end{cases} \tag{38}$$

or, equivalently:

$$\mathcal{L}_2 = \max(0, 1 - y(w^Tx + b))^2 \tag{39}$$

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

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

### 3.2.1 Primal formulation

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

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

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

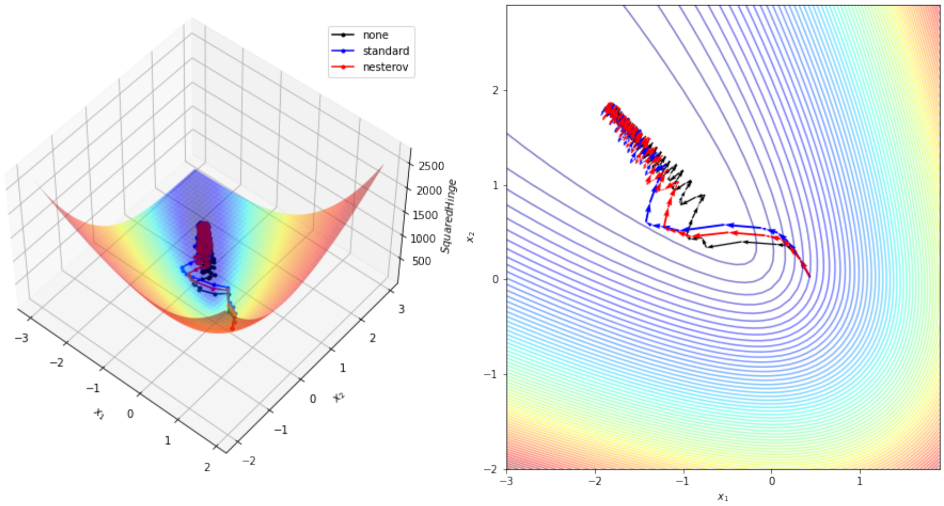


Figure 3: SVC Squared Hinge loss with different optimization steps

# 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:

$$\{(x_i, y_i), x \in \Re^m, y_i \in \Re, i = 1, \ldots, n\} \tag{42}$$

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 $|y_i - y'_i| \leq \epsilon$, 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 $\xi^+ \geq 0$ and $\xi^- \geq 0 \ \forall_i$:

$$\begin{aligned} & y_i \leq y'_i + \epsilon + \xi^+ \ \forall_i \\ & y_i \geq y'_i - \epsilon - \xi^- \ \forall_i \\ & \xi^+_i, \xi^-_i \geq 0 \ \forall_i \end{aligned} \tag{43}$$

The objective function for SVR can then be written as:

$$\begin{aligned} \min_{w,b,\xi^+,\xi^-} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi^+_i + \xi^-_i) \\ \text{subject to} \quad & y_i - w^T x_i - b \leq \epsilon + \xi^+_i \ \forall_i \\ & w^T x_i + b - y_i \leq \epsilon + \xi^-_i \ \forall_i \\ & \xi^+_i, \xi^-_i \geq 0 \ \forall_i \end{aligned} \tag{44}$$

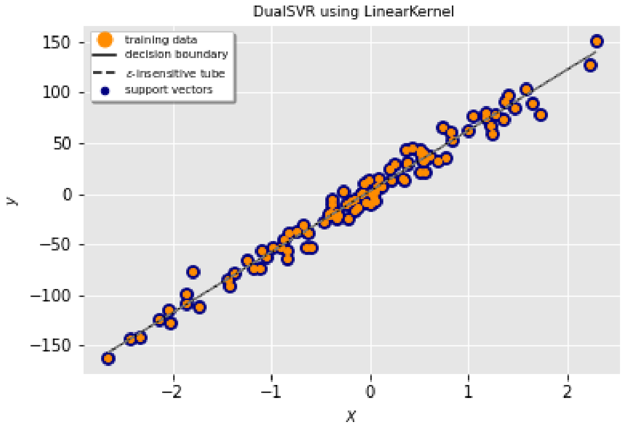


Figure 4: Linear SVR hyperplane

## 4.1 Epsilon-insensitive loss

The *epsilon-insensitive* loss is defined as:

$$\mathcal{L}_\epsilon = \begin{cases} 0 & \text{if } |y - (w^T x + b)| \leq \epsilon \\ |y - (w^T x + b)| - \epsilon & \text{otherwise} \end{cases} \tag{45}$$

or, equivalently:

$$\mathcal{L}_\epsilon = \max(0, |y - (w^T x + b)| - \epsilon) \tag{46}$$

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

$$\frac{\partial \mathcal{L}_\epsilon}{\partial w} = \begin{cases} (y - (w^T x + b))x & \text{if } |y - (w^T x + b)| > \epsilon \\ 0 & \text{otherwise} \end{cases} \tag{47}$$

### 4.1.1 Primal formulation

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

The quadratic optimization problem (44) can be equivalently formulated as:

$$\min_{w,b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \max(0, |y_i - (w^T x_i + b)| - \epsilon) \tag{48}$$

where we make use of the *epsilon-insensitive* loss (45) or (46).

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

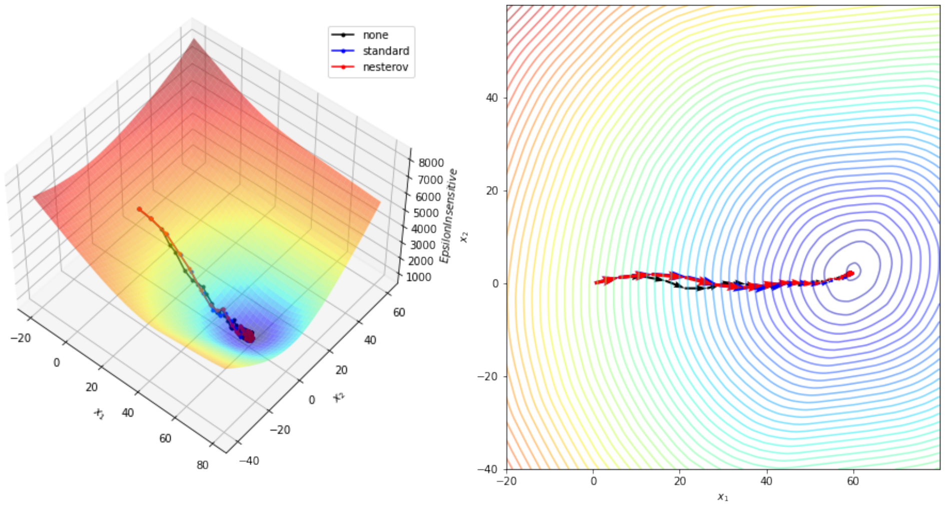


Figure 5: SVR Epsilon-insensitive loss with different optimization steps

#### 4.1.2 Wolfe Dual formulation

To reformulate the (44) as a *Wolfe dual*, we introduce the Lagrange multipliers $\alpha_i^+ \geq 0, \alpha_i^- \geq 0, \mu_i^+ \geq 0, \mu_i^- \geq 0 \; \forall_i$:

$$\begin{aligned} \max_{\alpha^+,\alpha^-,\mu^+,\mu^-} \min_{w,b,\xi^+,\xi^-} \mathcal{W}(w,b,\xi^+,\xi^-,\alpha^+,\alpha^-,\mu^+,\mu^-) = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi_i^+ + \xi_i^-) - \sum_{i=1}^{n}(\mu_i^+\xi_i^+ + \mu_i^-\xi_i^-) \\ - \sum_{i=1}^{n}\alpha_i^+(\epsilon + \xi_i^+ + y_i' - y_i) - \sum_{i=1}^{n}\alpha_i^-(\epsilon + \xi_i^- - y_i' + y_i) \end{aligned} \tag{49}$$

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

$$\frac{\partial \mathcal{W}}{\partial w} = w - \sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-)x_i \Rightarrow w = \sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-)x_i \tag{50}$$

$$\frac{\partial \mathcal{W}}{\partial b} = -\sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-) \Rightarrow \sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-) = 0 \tag{51}$$

$$\frac{\partial \mathcal{W}}{\partial \xi_i^+} = 0 \Rightarrow C = \alpha_i^+ + \mu_i^+ \tag{52}$$

$$\frac{\partial \mathcal{W}}{\partial \xi_i^-} = 0 \Rightarrow C = \alpha_i^- + \mu_i^- \tag{53}$$

Substituting (50) and (51) in, we now need to maximize $\mathcal{W}$ wrt $\alpha_i^+$ and $\alpha_i^-$, where $\alpha_i^+ \geq 0, \; \alpha_i^- \geq 0 \; \forall_i$:

$$\max_{\alpha^+,\alpha^-} \mathcal{W}(\alpha^+,\alpha^-) = \sum_{i=1}^{n} y_i(\alpha_i^+ - \alpha_i^-) - \epsilon\sum_{i=1}^{n}(\alpha_i^+ + \alpha_i^-) - \frac{1}{2}\sum_{i,j}(\alpha_i^+ - \alpha_i^-)\langle x_i, x_j\rangle(\alpha_j^+ - \alpha_j^-) \tag{54}$$

Using $\mu_i^+ \geq 0$ and $\mu_i^- \geq 0$ together with (50) and (51) means that $\alpha_i^+ \leq C$ and $\alpha_i^- \leq C$. We therefore need to find:

$$\begin{aligned} \min_{\alpha^+,\alpha^-} \quad & \frac{1}{2}(\alpha^+ - \alpha^-)^T K(\alpha^+ - \alpha^-) + \epsilon q^T(\alpha^+ + \alpha^-) - y^T(\alpha^+ - \alpha^-) \\ \text{subject to} \quad & 0 \leq \alpha_i^+, \alpha_i^- \leq C \ \forall_i \\ & q^T(\alpha^+ - \alpha^-) = 0 \end{aligned} \tag{55}$$

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

We can write the (55) in a standard quadratic form as:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2}\alpha^T Q\alpha - q^T\alpha \\ \text{subject to} \quad & 0 \leq \alpha_i \leq C \ \forall_i \\ & e^T\alpha = 0 \end{aligned} \tag{56}$$

where the Hessian matrix $Q$ is $\begin{bmatrix} K & -K \\ -K & K \end{bmatrix}$ , $q$ is $\begin{bmatrix} -y \\ y \end{bmatrix} + \epsilon$ , and $e$ is $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$.

Each new predictions $y'$ can be found using:

$$y' = \sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-)\langle x_i, x'\rangle + b \tag{57}$$

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

$$b = y_s - \epsilon - \sum_{m\in S}(\alpha_m^+ - \alpha_m^-)\langle x_m, x_s\rangle \tag{58}$$

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

$$b = \frac{1}{N_s}\sum_{s\in S} y_s - \epsilon - \sum_{m\in S}(\alpha_m^+ - \alpha_m^-)\langle x_m, x_s\rangle \tag{59}$$

From (56) 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 [12] that arises from the primal (11) or (12) where the bias term $b$ is embedded into the weight vector $w$:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2}\alpha^T(Q + ee^T)\alpha + q^T\alpha \\ \text{subject to} \quad & 0 \leq \alpha_i \leq C \ \forall_i \end{aligned} \tag{60}$$

### 4.1.3 Lagrangian Dual formulation

In order to relax the constraints in the *Wolfe dual* formulation (55) we define the problem as a *Lagrangian dual* relaxation by embedding them into objective function, so we need to allocate the Lagrangian multipliers $\mu \geq 0, \lambda_+ \geq 0, \lambda_- \geq 0$:

$$\begin{aligned} \max_{\mu,\lambda_+,\lambda_-} \min_{\alpha} \mathcal{L}(\alpha, \mu, \lambda_+, \lambda_-) &= \frac{1}{2}\alpha^T Q\alpha + q^T\alpha - \mu^T(e^T\alpha) - \lambda_+^T(u - \alpha) - \lambda_-^T\alpha \\ &= \frac{1}{2}\alpha^T Q\alpha + (q - \mu e + \lambda_+ - \lambda_-)^T\alpha - \lambda_+^T u \end{aligned} \tag{61}$$

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

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

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow Q\alpha + (q - \mu e + \lambda_+ - \lambda_-) = 0 \tag{62}$$

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

$$Q\alpha = -(q - \mu e + \lambda_+ - \lambda_-) \tag{63}$$

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

$$\frac{\partial \mathcal{L}}{\partial \mu} = -e\alpha \tag{64}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_+} = \alpha - u \tag{65}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_-} = -\alpha \tag{66}$$

If the Hessian matrix Q is not positive definite, i.e., the Lagrangian function is not strictly convex since it will be linear along the eigenvectors correspondent to the null eigenvalues and so it will be unbounded below, the Lagrangian dual relaxation will be nondifferentiable, so it will have infinite solutions and for each of them it will have a different subgradient. In order to compute an approximation of the gradient, we will choose $\alpha$ in such a way as the one that minimizes the norm of the residual:

$$\begin{aligned} \min_{\alpha_n \in K_n(Q,b)} \quad & \|Q\alpha_n - b\| \\ \text{where} \quad & b = -(q - \mu e + \lambda_+ - \lambda_-) \end{aligned} \tag{67}$$

Since we are dealing with a symmetric but indefinite linear system we will choose a well-known Krylov method that performs the Lanczos iterate, i.e., symmetric Arnoldi iterate, called *minres*, i.e., symmetric *gmres*, to compute the vector $\alpha_n$ that minimizes the norm of the residual $r_n = Q\alpha_n - b$ among all vectors in $K_n(Q, b) = span(b, Qb, Q^2b, \dots, Q^{n-1}b)$.

From (56) 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 (61) 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 (60).

$$\begin{aligned} \max_{\lambda_+,\lambda_-} \min_{\alpha} \mathcal{L}(\alpha, \lambda_+, \lambda_-) &= \frac{1}{2}\alpha^T(Q + ee^T)\alpha + q^T\alpha - \lambda_+^T(u - \alpha) - \lambda_-^T\alpha \\ &= \frac{1}{2}\alpha^T(Q + ee^T)\alpha + (q + \lambda_+ - \lambda_-)^T\alpha - \lambda_+^T u \end{aligned} \tag{68}$$

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:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow (Q + ee^T)\alpha + (q + \lambda_+ - \lambda_-) = 0 \tag{69}$$

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

$$(Q + ee^T)\alpha = -(q + \lambda_+ - \lambda_-) \tag{70}$$

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

$$\frac{\partial \mathcal{L}}{\partial \lambda_+} = \alpha - u \tag{71}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_-} = -\alpha \tag{72}$$

## 4.2 Squared Epsilon-insensitive loss

The *squared epsilon-insensitive* loss is defined as:

$$\mathcal{L}_\epsilon^2 = \begin{cases} 0 & \text{if } |y - (w^T x + b)| \leq \epsilon \\ (|y - (w^T x + b)| - \epsilon)^2 & \text{otherwise} \end{cases} \tag{73}$$

or, equivalently:

$$\mathcal{L}_\epsilon^2 = \max(0, |y - (w^T x + b)| - \epsilon)^2 \tag{74}$$

As the *squared hinge* loss, also the *squared epsilon-insensitive* loss is a strictly convex function and it has a gradient wrt $w$ that is given by:

$$\frac{\partial \mathcal{L}_\epsilon^2}{\partial w} = \begin{cases} 2((y - (w^T x + b))x) & \text{if } |y - (w^T x + b)| > \epsilon \\ 0 & \text{otherwise} \end{cases} \tag{75}$$

### 4.2.1 Primal formulation

To provide a continuously differentiable function the optimization problem (48) can be formulated as:

$$\min_{w,b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \max(0, |y_i - (w^T x_i + b)| - \epsilon)^2 \tag{76}$$

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

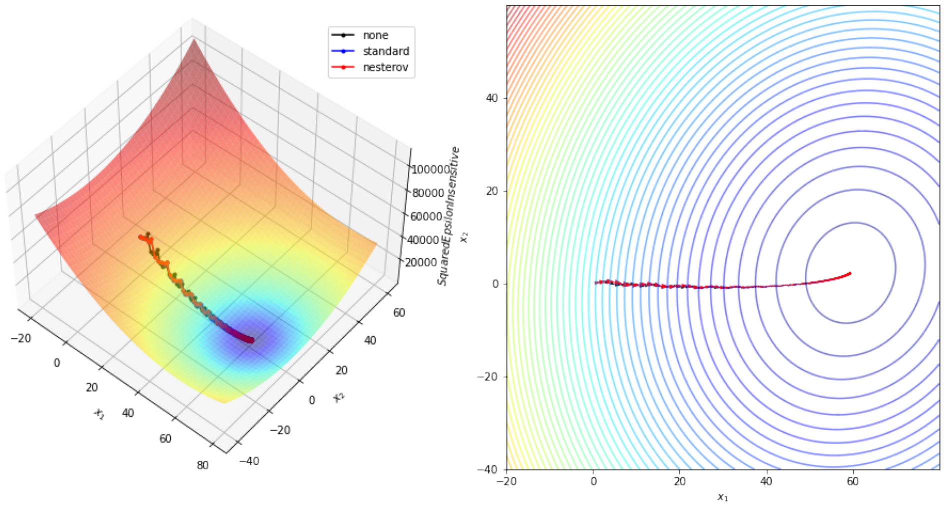


Figure 6: SVC Squared Epsilon-insensitive loss with different optimization steps

# 5 Nonlinear Support Vector Machines

When applying our SVC to *linearly separable* data in (17), we have started by creating a matrix $Q$ from the dot product of our input variables:

$$Q_{ij} = y_i y_j k(x_i, x_j) \tag{77}$$

or, a matrix $K$ from the dot product of our input variables in the SVR case (55):

$$K_{ij} = k(x_i, x_j) \tag{78}$$

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

$$k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle = \phi(x_i)^T \phi(x_j) \tag{79}$$

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

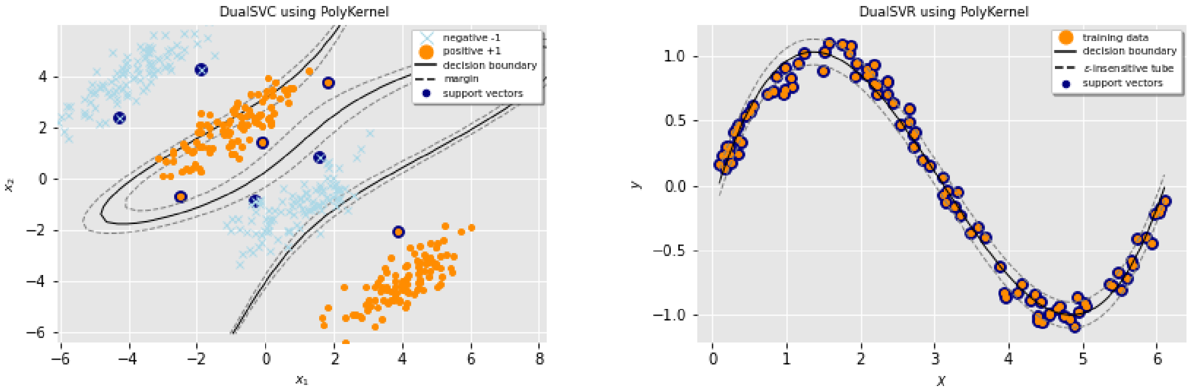
The reason that this *kernel trick* is useful is that there are many classification/regression problems that are nonlinearly separable/regressable in the *input space*, which might be in a higher dimensionality *feature space* given a suitable mapping $x \to \phi(x)$.

## 5.1 Polynomial kernel

The *polynomial* kernel is defined as:

$$k(x_i, x_j) = (\gamma \langle x_i, x_j \rangle + r)^d \tag{80}$$

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



(a) Polynomial SVC hyperplane

(b) Polynomial SVR hyperplane

Figure 7: Polynomial SVM hyperplanes

## 5.2 Gaussian RBF kernel

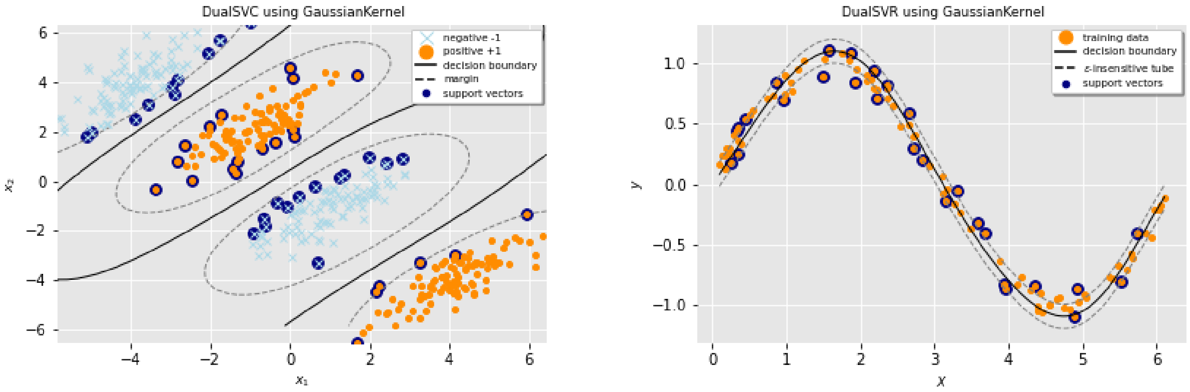
The *gaussian* kernel is defined as:

$$k(x_i, x_j) = \exp(-\frac{\|x_i - x_j\|^2}{2\sigma^2}) \tag{81}$$

or, equivalently:

$$k(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|^2) \tag{82}$$

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



(a) Gaussian SVC hyperplane

(b) Gaussian SVR hyperplane

Figure 8: Gaussian SVM hyperplanes

# 6 Optimization Methods

In order to explain the *convergence* and *efficiency* properties of the following optimization methods, we need to introduce some preliminary definitions about *convexity* and the *L-smoothness* of a function [13].

First of all, we give three different but equivalent definitions of convexity in terms of the function itself, the Jacobian and the Hessian.

**Definition 1** (Convexity)**.** We say that a function $f : \Re^m \to \Re$ is convex if:

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

**Definition 2** (Convexity - Jacobian)**.** We say that a differentiable function $f : \Re^m \to \Re$ is convex iff:

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

**Definition 3** (Convexity - Hessian)**.** We say that a twice differentiable function, i.e., the Hessian matrix is *symmetric*, $f : \Re^m \to \Re$ is convex iff:

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

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

The definitions of *strong convexity* and *L-smoothness* below will be useful for the theoretical convergence rate explanation of the further algorithms.

**Definition 4** (Strong Convexity)**.** We say that a function $f : \Re^m \to \Re$ is $\mu$-strongly convex if the function:

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

is convex for some $\mu > 0$. The latter, in terms of the Jacobian, is equivalent to:

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

and, in terms of the Hessian, is equivalent to:

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

which is:

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

**Definition 5** (L-smoothness)**.** We say that a function $f : \Re^m \to \Re$ is L-smooth, i.e., L-Lipschitz continuous, if it is differentiable and if:

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

## 6.1 Gradient Descent

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 GradientDescent($f, \alpha$)
      Initialize weight vector $x_0$
      $t = 0$
      while not_convergence do
          $x_{t+1} = x_t - \alpha \nabla f(x_t)$
          $t = t + 1$
      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:

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

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, instead of $\mathcal{O}(nm)$.

**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 $(i_1, \dots, i_k) \sim \mathcal{U}^k(1, \dots, n)$
          $x_{t+1} \leftarrow x_t - \alpha \frac{1}{k} \sum_{j=1}^{k} \nabla f_{i_j}(x_t)$
          $t \leftarrow t + 1$
      end while
      return $x_t$
  end function
```

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

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

### 6.1.1 Momentum

To mitigate the pathological zig-zagging of the SGD method we introduce two acellerated methods [1] and [2] 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 $x_t$.

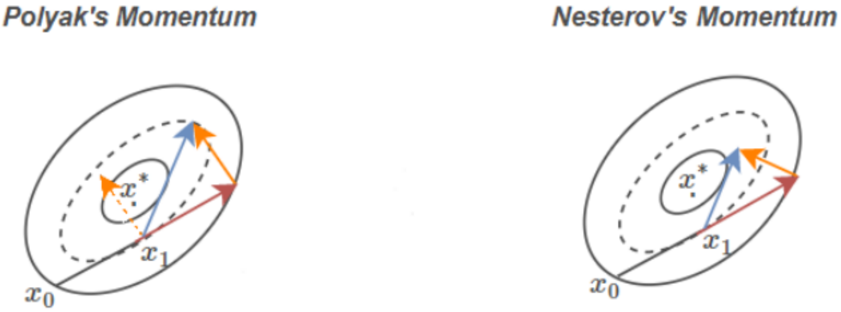


Figure 9: Polyak's and Nesterov's Momentum

**Algorithm 3** Polyak Accelerated Gradient Descent or or 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
```

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 Accelerated Gradient Descent

```
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
          $\hat{x}_t \leftarrow x_t + \beta v_{t-1}$
          $v_t \leftarrow \beta v_{t-1} + \alpha \nabla f(\hat{x}_t)$
          $x_{t+1} \leftarrow x_t - v_t$
          $t \leftarrow t + 1$
      end while
      return $x_t$
  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 showb in figure 9.

Nesterov momentum brings the rate of convergence from $\mathcal{O}\left(\frac{1}{t}\right)$ to $\mathcal{O}\left(\frac{1}{t^2}\right)$ and in the case of smooth and strongly convex functions 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.

We can write the iteration complexity of these methods, i.e., the smallest $t$ such that we're within $\epsilon$, for a L-smooth and $\mu$-strongly convex function as $\mathcal{O}\left(\kappa \log \frac{1}{\epsilon}\right)$ for the standard GD method, $\mathcal{O}\left(\sqrt{\kappa} \log \frac{1}{\epsilon}\right)$ for the Polyak's method and, finally, $\mathcal{O}\left(\frac{1}{\sqrt{\epsilon}}\right)$ for the NAG method to get $\epsilon$-close to global optimum and where $\kappa$, i.e., the *conditioning number*, is defined as $\kappa = L/\mu$ and where $L$ and $\mu$ are also equal to the smallest and the largest eigenvalues $\lambda_{min}$ and $\lambda_{max}$ respectively.

## 6.2 AdaGrad

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* [5] 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 5** 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
          $g_t \leftarrow \nabla f(x_t)$
          $s_t \leftarrow s_{t-1} + g_t^2$
          $x_{t+1} \leftarrow x_t - \alpha P^{-1} g_t = x_t - \frac{\alpha}{\sqrt{s_t + \epsilon}} \odot g_t$ where $P \leftarrow diag(s_t + \epsilon)^{1/2}$
          $t \leftarrow t + 1$
      end while
      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. *AdaGrad*'s convergence rate for L-smooth convex functions is $\mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big)$.

## 6.3 Sequential Minimal Optimization

The *Sequential Minimal Optimization (SMO)* [3] 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.

### 6.3.1 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.

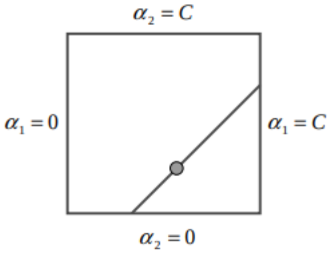


Figure 10: SMO for two Lagrange multipliers

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 $y_1 \neq y_2$:

$$\begin{aligned} L &= max(0, \alpha_2 - \alpha_1) \\ H &= min(C, C + \alpha_2 - \alpha_1) \end{aligned} \tag{83}$$

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

$$\begin{aligned} L &= max(0, \alpha_2 + \alpha_1 - C) \\ H &= min(C, \alpha_2 + \alpha_1) \end{aligned} \tag{84}$$

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

$$\eta = K(x_1, x_1) + K(x_2, x_2) - 2K(x_1, x_2) \tag{85}$$

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:

$$\alpha_2^{new} = \alpha_2 + \frac{y_2(E_1 - E_2)}{\eta} \tag{86}$$

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:

$$\alpha_2^{new,clipped} = \begin{cases} H & \text{if } \alpha_2^{new} \geq H \\ \alpha_2^{new} & \text{if } L < \alpha_2^{new} < H \\ L & \text{if } \alpha_2^{new} \leq L \end{cases} \tag{87}$$

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

$$\alpha_1^{new} = \alpha_1 + s(\alpha_2 - \alpha_2^{new,clipped}) \tag{88}$$

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 (18) are:

$$\begin{aligned} \alpha_i = 0 &\Leftrightarrow y_i y_i' \geq 1 \\ 0 < \alpha_i < C &\Leftrightarrow y_i y_i' = 1 \\ \alpha_i = C &\Leftrightarrow y_i y_i' \leq 1 \end{aligned} \tag{89}$$

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 $x_1$:

$$b_{up} = E_1 + y_1(\alpha_1^{new} - \alpha_1)K(x_1, x_1) + y_2(\alpha_2^{new,clipped} - \alpha_2)K(x_1, x_2) + b \tag{90}$$

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

$$b_{low} = E_2 + y_1(\alpha_1^{new} - \alpha_1)K(x_1, x_2) + y_2(\alpha_2^{new,clipped} - \alpha_2)K(x_2, x_2) + b \tag{91}$$

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 $b$:

$$b = \begin{cases} b_{up} & \text{if } 0 < \alpha_1 < C \\ b_{low} & \text{if } 0 < \alpha_2 < C \\ \dfrac{b_{up} + b_{low}}{2} & \text{otherwise} \end{cases} \tag{92}$$

**Algorithm 6** 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          ▷ loop over examples where $\alpha_i$ are not already at their bounds
          $num\_changed \leftarrow num\_changed +$ ExamineExample($i$)
          if $b_{up} > b_{low} - 2tol$ then                  ▷ 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 (92)
    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 $(E_2, i2)$
      end if
      if optimality is attained using current $b_{low}$ and $b_{up}$ then
          return 0
      else
          Find an index $i1$ to do joint optimization with $i2$
          if TakeStep($i1, i2$) = True then
              return 1
          else
              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 (83) or (84)
     if $L = H$ then
        return False
     end if
     Compute $\eta$ by (85)            ▷ 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 (86)
        Compute $\alpha_2^{new,clipped}$ by (87)
     end if
     if changes in $\alpha_2^{new,clipped}$ are larger than some eps then
        Compute $\alpha_1^{new}$ by (88)
        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 $i$ in $I0 \cup \{i1, i2\}$ 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
```

### 6.3.2 Regression

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

$$\begin{aligned} L &= max(0, \gamma - C) \\ H &= min(C, \gamma) \end{aligned} \tag{93}$$

$$\alpha_2^{+,new} = \alpha_2^+ - \frac{E_1 - E_2}{\eta} \tag{94}$$

$$\alpha_1^{+,new} = \alpha_1^+ - (\alpha_2^{+,new,clipped} - \alpha_2^+) \tag{95}$$

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

$$\begin{aligned} L &= max(0, -\gamma) \\ H &= min(C, -\gamma + C) \end{aligned} \tag{96}$$

$$\alpha_2^{-,new} = \alpha_2^- + \frac{(E_1 - E_2) - 2\epsilon}{\eta} \tag{97}$$

$$\alpha_1^{+,new} = \alpha_1^+ + (\alpha_2^{-,new,clipped} - \alpha_2^-) \tag{98}$$

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

$$\begin{aligned} L &= max(0, \gamma) \\ H &= min(C, C + \gamma) \end{aligned} \tag{99}$$

$$\alpha_2^{+,new} = \alpha_2^+ - \frac{(E_1 - E_2) + 2\epsilon}{\eta} \tag{100}$$

$$\alpha_1^{-,new} = \alpha_1^- + (\alpha_2^{+,new,clipped} - \alpha_2^+) \tag{101}$$

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

$$\begin{aligned} L &= max(0, -\gamma - C) \\ H &= min(C, -\gamma) \end{aligned} \tag{102}$$

$$\alpha_2^{-,new} = \alpha_2^- + \frac{E_1 - E_2}{\eta} \tag{103}$$

$$\alpha_1^{-,new} = \alpha_1^- - (\alpha_2^{-,new,clipped} - \alpha_2^-) \tag{104}$$

where $\gamma = \alpha_1^+ - \alpha_1^- + \alpha_2^+ - \alpha_2^-$. Notice that $\eta$ and $\alpha_2^{+,new,clipped}$ or $\alpha_2^{-,new,clipped}$ are identical to (85) and (87) respectively.

The KKT conditions for the regression problem (55) are:

$$\begin{aligned} \alpha_i^+ - \alpha_i^- = 0 &\Leftrightarrow |y_i - y_i'| < \epsilon \\ -C < \alpha_i^+ - \alpha_i^- < C &\Leftrightarrow |y_i - y_i'| = \epsilon \\ \alpha_i^+ + \alpha_i^- = C &\Leftrightarrow |y_i - y_i'| > \epsilon \end{aligned} \tag{105}$$

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:

$$b_{up} = E_1 + ((\alpha_1^+ - \alpha_1^-) - (\alpha_1^{+,new} - \alpha_1^{-,new}))K(x_1, x_1) + ((\alpha_2^+ - \alpha_2^-) - (\alpha_2^{+,new,clipped} - \alpha_2^{-,new,clipped}))K(x_1, x_2) + b \tag{106}$$

$$b_{low} = E_2+((\alpha_1^+-\alpha_1^-)-(\alpha_1^{+,new}-\alpha_1^{-,new}))K(x_1,x_2)+((\alpha_2^+-\alpha_2^-)-(\alpha_2^{+,new,clipped}-\alpha_2^{-,new,clipped}))K(x_2,x_2)+b \tag{107}$$

$$b = \begin{cases} b_{up} & \text{if } 0 < \alpha_1^+, \alpha_1^- < C \\ b_{low} & \text{if } 0 < \alpha_2^+, \alpha_2^- < C \\ \dfrac{b_{up}+b_{low}}{2} & \text{otherwise} \end{cases} \tag{108}$$

The improvements described in [4, 7] 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 7** 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 $\epsilon \geq 0$ 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 $i_{up} \leftarrow 0$                    ▷ or any other target index $i_{up}$ from the training examples
    Initialize $i_{low} \leftarrow 0$                   ▷ 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 $errors \in \Re^n, errors \leftarrow 0$
    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          ▷ loop over examples where $\alpha_i^+$ and $\alpha_i^-$ are not already at their bounds
          $num\_changed \leftarrow num\_changed +$ ExamineExample($i$)
          if $b_{up} > b_{low} - 2tol$ then                   ▷ 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 (108)
    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 (93), (96), (99) or (102)
          if $L < H$ then
              Compute $\eta$ by (85)        ▷ 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 (94), (100) or (97), (103) respectively
                  Compute $\alpha_2^{+,new,clipped}$ or $\alpha_2^{-,new,clipped}$ by (87)
              end if
              Compute $\alpha_1^{+,new}$ or $\alpha_1^{-,new}$ using (95), (98) or (101), (104) 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
          end for
          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
```

# 7 Experiments

The following experiments refer to 3-fold cross-validation over *linearly* and *nonlinearly* separable generated datasets of size 100, so the reported results are to considered as a mean over the 3 folds.

## 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.

### 7.1.1 Hinge loss

**Primal formulation** The experiments results shown in 1 referred to *Stochastic Gradient Descent* algorithm are obtained with $\alpha$, i.e., the *learning rate* or *step size*, setted to 0.001 and $\beta$, i.e., the *momentum*, equal to 0.4. The batch size is setted to 20. Training is stopped if after 5 iterations the training loss is not lower than the best found so far.

Table 1: SVC Primal formulation results with Hinge loss

| | | | fit_time | n_iter | train_accuracy | val_accuracy | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|
| solver | C | momentum | | | | | | |
| sgd | 1 | none | 0.794316 | 412 | 0.982494 | 0.979949 | 37 | 18 |
| | | standard | 0.526508 | 274 | 0.984981 | 0.984999 | 33 | 17 |
| | | nesterov | 0.506168 | 274 | 0.984981 | 0.984999 | 33 | 17 |
| | 10 | none | 0.848348 | 483 | 0.984981 | 0.984999 | 10 | 6 |
| | | standard | 0.652050 | 375 | 0.987487 | 0.989974 | 10 | 6 |
| | | nesterov | 0.485980 | 296 | 0.984981 | 0.984999 | 10 | 6 |
| | 100 | none | 0.449329 | 243 | 0.989994 | 0.989974 | 9 | 5 |
| | | standard | 0.348258 | 161 | 0.989994 | 0.989974 | 7 | 4 |
| | | nesterov | 0.134886 | 58 | 0.989994 | 0.989974 | 8 | 5 |
| liblinear | 1 | - | 0.001573 | 428 | 0.989994 | 0.989974 | 11 | 6 |
| | 10 | - | 0.001447 | 744 | 0.987487 | 0.984999 | 5 | 4 |
| | 100 | - | 0.001453 | 1000 | 0.985000 | 0.989974 | 7 | 2 |

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* [9] 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. Standard* or *Polyak* and *Nesterov* momentums always perform lower iterations as expected from the theoretical analysis of the convergence rate.

**Linear Dual formulations** The experiments results shown in 3 are obtained with $\alpha$, i.e., the *learning rate* or *step size*, setted to 0.5 for the *AdaGrad* algorithm. Notice that the *qp* dual refers to the formulation (26), while the *bcqp* dual refers to the formulation (33).

Table 2: Linear SVC Wolfe Dual formulation results with Hinge loss

| | | fit_time | n_iter | train_accuracy | val_accuracy | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|
| solver | C | | | | | | |
| smo | 1 | 0.076588 | 61 | 0.985000 | 0.989974 | 12 | 12 |
| | 10 | 0.076181 | 73 | 0.985000 | 0.979949 | 7 | 7 |
| | 100 | 0.373685 | 1196 | 0.985000 | 0.989974 | 6 | 6 |
| libsvm | 1 | 0.003042 | 99 | 0.987487 | 0.989974 | 12 | 12 |
| | 10 | 0.002565 | 90 | 0.987487 | 0.984999 | 7 | 7 |
| | 100 | 0.003477 | 2647 | 0.985000 | 0.984999 | 6 | 6 |
| cvxopt | 1 | 0.020731 | 10 | 0.985000 | 0.989974 | 12 | 12 |
| | 10 | 0.016735 | 10 | 0.985000 | 0.989974 | 7 | 7 |
| | 100 | 0.029245 | 10 | 0.985000 | 0.989974 | 8 | 8 |

For what about the linear *Wolfe dual* formulation we can immediately notice as the *regularization hyperparameter C* makes the model harder, so the *custom* implementation of the SMO algorithm and also the *sklearn* implementation, i.e., *libsvm* [10] implementation, needs to perform more iterations to achieve the same *numerical precision*; meanwhile the *cvxopt* [11] 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.

Table 3: Linear SVC Lagrangian Dual formulation results with Hinge loss

| | | fit_time | n_iter | train_accuracy | val_accuracy | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|
| dual | C | | | | | | |
| qp | 1 | 0.006492 | 1 | 0.985019 | 0.989974 | 131 | 131 |
| | 10 | 0.006105 | 1 | 0.985019 | 0.989974 | 131 | 131 |
| | 100 | 0.005686 | 1 | 0.985019 | 0.989974 | 131 | 131 |
| bcqp | 1 | 0.006973 | 1 | 0.985019 | 0.989974 | 130 | 130 |
| | 10 | 0.006043 | 1 | 0.985019 | 0.989974 | 130 | 130 |
| | 100 | 0.005027 | 1 | 0.985019 | 0.989974 | 130 | 130 |

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 4 and 5 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 5 are obtained with $\alpha$, i.e., the *learning rate* or *step size*, setted to 0.5 for the *AdaGrad* algorithm.

Table 4: Nonlinear SVC Wolfe Dual formulation results with Hinge loss

| | | | fit_time | n_iter | train_accuracy | val_accuracy | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|
| solver | kernel | C | | | | | | |
| smo | poly | 1 | 0.356696 | 88 | 0.851206 | 0.678412 | 28 | 28 |
| | | 10 | 0.270690 | 105 | 0.897426 | 0.660682 | 9 | 9 |
| | | 100 | 0.255688 | 198 | 0.916209 | 0.727921 | 8 | 8 |
| | rbf | 1 | 0.245166 | 49 | 1.000000 | 1.000000 | 41 | 41 |
| | | 10 | 0.204894 | 52 | 1.000000 | 1.000000 | 13 | 13 |
| | | 100 | 0.188844 | 64 | 1.000000 | 1.000000 | 11 | 11 |
| libsvm | poly | 1 | 0.005154 | 160 | 1.000000 | 0.992481 | 28 | 28 |
| | | 10 | 0.004598 | 436 | 1.000000 | 0.987469 | 10 | 10 |
| | | 100 | 0.006573 | 149 | 1.000000 | 0.987469 | 8 | 8 |
| | rbf | 1 | 0.004991 | 115 | 1.000000 | 1.000000 | 41 | 41 |
| | | 10 | 0.002472 | 164 | 1.000000 | 1.000000 | 13 | 13 |
| | | 100 | 0.003032 | 268 | 1.000000 | 1.000000 | 12 | 12 |
| cvxopt | poly | 1 | 0.105617 | 10 | 0.851206 | 0.678412 | 28 | 28 |
| | | 10 | 0.095708 | 10 | 0.911206 | 0.688026 | 10 | 10 |
| | | 100 | 0.072921 | 10 | 0.916209 | 0.722889 | 9 | 9 |
| | rbf | 1 | 0.093452 | 10 | 1.000000 | 1.000000 | 43 | 43 |
| | | 10 | 0.073576 | 10 | 1.000000 | 1.000000 | 14 | 14 |
| | | 100 | 0.069153 | 10 | 1.000000 | 1.000000 | 13 | 13 |

Table 5: Nonlinear SVC Lagrangian Dual formulation results with Hinge loss

| | | | fit_time | n_iter | train_accuracy | val_accuracy | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|
| dual | kernel | C | | | | | | |
| qp | poly | 1 | 1.315738 | 255 | 0.733773 | 0.513784 | 184 | 184 |
| | | 10 | 1.178677 | 255 | 0.733773 | 0.513784 | 184 | 184 |
| | | 100 | 1.203893 | 255 | 0.733773 | 0.513784 | 184 | 184 |
| | rbf | 1 | 1.241991 | 229 | 0.822618 | 0.727734 | 186 | 186 |
| | | 10 | 1.696262 | 376 | 0.751255 | 0.503741 | 153 | 153 |
| | | 100 | 1.312007 | 305 | 0.833652 | 0.586447 | 178 | 178 |
| bcqp | poly | 1 | 1.480641 | 337 | 0.783729 | 0.538810 | 199 | 199 |
| | | 10 | 1.266989 | 337 | 0.783729 | 0.538810 | 199 | 199 |
| | | 100 | 1.023042 | 337 | 0.783729 | 0.538810 | 199 | 199 |
| | rbf | 1 | 0.020001 | 1 | 0.998747 | 0.982568 | 240 | 240 |
| | | 10 | 0.021672 | 1 | 0.998747 | 0.982568 | 240 | 240 |
| | | 100 | 0.023396 | 1 | 0.998747 | 0.982568 | 240 | 240 |

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 *bcqp Lagrangian dual* formulation seems to perform better wrt the *qp* formulation, both tends to select even more training data points as *support vectors*.

### 7.1.2 Squared Hinge loss

**Primal formulation** The experiments results shown in 6 referred to *Stochastic Gradient Descent* algorithm are obtained with $\alpha$, i.e., the *learning rate* or *step size*, setted to 0.001 and $\beta$, i.e., the *momentum*, equal to 0.4. The batch size is setted to 20. Training is stopped if after 5 iterations the training loss is not lower than the best found so far.

Table 6: SVC Primal formulation results with Squared Hinge loss

| | | | fit_time | n_iter | train_accuracy | val_accuracy | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|
| solver | C | momentum | | | | | | |
| sgd | 1 | none | 0.354329 | 188 | 0.982494 | 0.979949 | 37 | 19 |
| | | standard | 0.241015 | 124 | 0.984981 | 0.979949 | 34 | 17 |
| | | nesterov | 0.227615 | 124 | 0.982494 | 0.979949 | 34 | 17 |
| | 10 | none | 0.149398 | 70 | 0.984981 | 0.980024 | 16 | 9 |
| | | standard | 0.109080 | 44 | 0.984981 | 0.980024 | 15 | 8 |
| | | nesterov | 0.103791 | 44 | 0.984981 | 0.980024 | 15 | 9 |
| | 100 | none | 0.082154 | 27 | 0.989994 | 0.989974 | 10 | 5 |
| | | standard | 0.066164 | 28 | 0.987487 | 0.989974 | 8 | 5 |
| | | nesterov | 0.069237 | 24 | 0.989994 | 0.989974 | 9 | 5 |
| liblinear | 1 | - | 0.001429 | 366 | 0.985000 | 0.989974 | 18 | 10 |
| | 10 | - | 0.002015 | 1000 | 0.985000 | 0.989974 | 14 | 8 |
| | 100 | - | 0.001806 | 1000 | 0.985000 | 0.980024 | 13 | 7 |

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* [9] 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*. *Standard* or *Polyak* and *Nesterov* momentums always perform lower iterations as expected from the theoretical analysis of the convergence rate.

## 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.

### 7.2.1 Epsilon-insensitive 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 0.001 and $\beta$, i.e., the *momentum*, equal to 0.4. The batch size is setted to 20. Training is stopped if after 5 iterations the training loss is not lower than the best found so far.

Table 7: SVR Primal formulation results with Epsilon-insensitive loss

| | | | | fit_time | n_iter | train_r2 | val_r2 | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|---|
| solver | C | momentum | epsilon | | | | | | |
| sgd | 1 | none | 0.1 | 0.099424 | 59 | 0.410998 | 0.402111 | 66 | 33 |
| | | | 0.2 | 0.125031 | 59 | 0.410998 | 0.402111 | 66 | 33 |
| | | | 0.3 | 0.116332 | 59 | 0.410998 | 0.402111 | 66 | 33 |
| | | standard | 0.1 | 0.085239 | 38 | 0.427455 | 0.418695 | 66 | 33 |
| | | | 0.2 | 0.095537 | 38 | 0.427455 | 0.418695 | 66 | 33 |
| | | | 0.3 | 0.126567 | 38 | 0.430658 | 0.421952 | 66 | 33 |
| | | nesterov | 0.1 | 0.082046 | 38 | 0.427207 | 0.418447 | 66 | 33 |
| | | | 0.2 | 0.081100 | 38 | 0.427207 | 0.418447 | 66 | 33 |
| | | | 0.3 | 0.083838 | 38 | 0.430409 | 0.421703 | 66 | 33 |
| | 10 | none | 0.1 | 0.150185 | 69 | 0.975885 | 0.971366 | 66 | 33 |
| | | | 0.2 | 0.116063 | 69 | 0.975752 | 0.971251 | 66 | 33 |
| | | | 0.3 | 0.129049 | 68 | 0.975685 | 0.971108 | 65 | 32 |
| | | standard | 0.1 | 0.106638 | 43 | 0.976441 | 0.971938 | 66 | 33 |
| | | | 0.2 | 0.101692 | 43 | 0.976441 | 0.971939 | 66 | 32 |
| | | | 0.3 | 0.096488 | 43 | 0.976363 | 0.971751 | 65 | 32 |
| | | nesterov | 0.1 | 0.065612 | 43 | 0.976374 | 0.971878 | 66 | 33 |
| | | | 0.2 | 0.068996 | 43 | 0.976374 | 0.971879 | 66 | 32 |
| | | | 0.3 | 0.066127 | 43 | 0.976347 | 0.971756 | 65 | 32 |
| | 100 | none | 0.1 | 0.061127 | 28 | 0.977986 | 0.973377 | 65 | 33 |
| | | | 0.2 | 0.047426 | 28 | 0.977986 | 0.973380 | 65 | 32 |
| | | | 0.3 | 0.044328 | 29 | 0.977986 | 0.973380 | 64 | 31 |
| | | standard | 0.1 | 0.055445 | 18 | 0.977997 | 0.973440 | 66 | 33 |
| | | | 0.2 | 0.033895 | 18 | 0.977997 | 0.973440 | 65 | 32 |
| | | | 0.3 | 0.030205 | 18 | 0.977997 | 0.973441 | 64 | 31 |
| | | nesterov | 0.1 | 0.027899 | 19 | 0.977995 | 0.973448 | 66 | 33 |
| | | | 0.2 | 0.026377 | 17 | 0.977994 | 0.973450 | 65 | 32 |
| | | | 0.3 | 0.030544 | 19 | 0.977995 | 0.973450 | 64 | 31 |
| liblinear | 1 | - | 0.1 | 0.000724 | 11 | 0.918768 | 0.916773 | 66 | 33 |
| | | | 0.2 | 0.000705 | 10 | 0.918763 | 0.916602 | 65 | 32 |
| | | | 0.3 | 0.000964 | 13 | 0.919296 | 0.917061 | 65 | 32 |
| | 10 | - | 0.1 | 0.001131 | 162 | 0.977849 | 0.972087 | 65 | 33 |
| | | | 0.2 | 0.000978 | 178 | 0.977852 | 0.972041 | 65 | 33 |
| | | | 0.3 | 0.000959 | 113 | 0.977871 | 0.972151 | 64 | 33 |
| | 100 | - | 0.1 | 0.001358 | 638 | 0.977725 | 0.974270 | 65 | 33 |
| | | | 0.2 | 0.001162 | 686 | 0.977664 | 0.974138 | 66 | 33 |
| | | | 0.3 | 0.001314 | 891 | 0.977653 | 0.974016 | 65 | 33 |

**Linear Dual formulations** The experiments results shown in 9 are obtained with $\alpha$, i.e., the *learning rate* or *step size*, setted to 0.5 for the *AdaGrad* algorithm. Notice that the *qp* dual refers to the formulation (61), while the *bcqp* dual refers to the formulation (68).

Table 8: Linear SVR Wolfe Dual formulation results with Epsilon-insensitive loss

| | | | fit_time | n_iter | train_r2 | val_r2 | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|
| solver | C | epsilon | | | | | | |
| smo | 1 | 0.1 | 0.017338 | 15 | 0.917773 | 0.914442 | 66 | 66 |
| | | 0.2 | 0.022597 | 13 | 0.918341 | 0.915019 | 66 | 66 |
| | | 0.3 | 0.039421 | 60 | 0.918942 | 0.915576 | 66 | 66 |
| | 10 | 0.1 | 0.053832 | 56 | 0.977920 | 0.972445 | 66 | 66 |
| | | 0.2 | 0.139534 | 219 | 0.977926 | 0.972457 | 65 | 65 |
| | | 0.3 | 0.053870 | 38 | 0.977953 | 0.972544 | 65 | 65 |
| | 100 | 0.1 | 0.524643 | 1508 | 0.977788 | 0.974139 | 66 | 66 |
| | | 0.2 | 0.266404 | 394 | 0.977742 | 0.974022 | 66 | 66 |
| | | 0.3 | 0.383196 | 900 | 0.977737 | 0.973939 | 66 | 66 |
| libsvm | 1 | 0.1 | 0.003532 | 63 | 0.917627 | 0.915448 | 66 | 66 |
| | | 0.2 | 0.003926 | 102 | 0.918194 | 0.915985 | 66 | 66 |
| | | 0.3 | 0.002088 | 54 | 0.918786 | 0.916554 | 66 | 66 |
| | 10 | 0.1 | 0.001896 | 282 | 0.977852 | 0.972051 | 66 | 66 |
| | | 0.2 | 0.001990 | 193 | 0.977851 | 0.972025 | 65 | 65 |
| | | 0.3 | 0.001814 | 593 | 0.977870 | 0.972135 | 65 | 65 |
| | 100 | 0.1 | 0.003821 | 2621 | 0.977723 | 0.974270 | 66 | 66 |
| | | 0.2 | 0.003551 | 2709 | 0.977673 | 0.974122 | 66 | 66 |
| | | 0.3 | 0.003090 | 4141 | 0.977655 | 0.974045 | 66 | 66 |
| cvxopt | 1 | 0.1 | 0.017656 | 9 | 0.917772 | 0.914479 | 67 | 67 |
| | | 0.2 | 0.017439 | 9 | 0.918341 | 0.915058 | 67 | 67 |
| | | 0.3 | 0.013357 | 10 | 0.918942 | 0.915614 | 66 | 66 |
| | 10 | 0.1 | 0.024514 | 9 | 0.977920 | 0.972466 | 67 | 67 |
| | | 0.2 | 0.018264 | 9 | 0.977926 | 0.972474 | 67 | 67 |
| | | 0.3 | 0.025372 | 10 | 0.977954 | 0.972562 | 66 | 66 |
| | 100 | 0.1 | 0.020310 | 9 | 0.977788 | 0.974150 | 67 | 67 |
| | | 0.2 | 0.024708 | 9 | 0.977742 | 0.974033 | 67 | 67 |
| | | 0.3 | 0.021550 | 9 | 0.977737 | 0.973956 | 67 | 67 |

Table 9: Linear SVR Lagrangian Dual formulation results with Epsilon-insensitive loss

| | | | fit_time | n_iter | train_r2 | val_r2 | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|
| dual | C | epsilon | | | | | | |
| qp | 1 | 0.1 | 0.711464 | 653 | 0.876534 | 0.870926 | 67 | 67 |
| | | 0.2 | 0.820021 | 653 | 0.876534 | 0.870927 | 67 | 67 |
| | | 0.3 | 0.648664 | 653 | 0.876534 | 0.870927 | 67 | 67 |
| | 10 | 0.1 | 0.510787 | 519 | 0.731825 | 0.722021 | 67 | 67 |
| | | 0.2 | 0.558384 | 524 | 0.731825 | 0.722021 | 67 | 67 |
| | | 0.3 | 0.519468 | 530 | 0.731825 | 0.722020 | 67 | 67 |
| | 100 | 0.1 | 0.631134 | 519 | 0.731825 | 0.722021 | 67 | 67 |
| | | 0.2 | 0.520121 | 524 | 0.731825 | 0.722021 | 67 | 67 |
| | | 0.3 | 0.539273 | 530 | 0.731825 | 0.722020 | 67 | 67 |
| bcqp | 1 | 0.1 | 0.630620 | 522 | 0.731073 | 0.721200 | 67 | 67 |
| | | 0.2 | 0.639167 | 524 | 0.731073 | 0.721199 | 67 | 67 |
| | | 0.3 | 0.630822 | 526 | 0.731073 | 0.721199 | 67 | 67 |
| | 10 | 0.1 | 0.610205 | 539 | 0.733638 | 0.723925 | 67 | 67 |
| | | 0.2 | 0.657547 | 541 | 0.733638 | 0.723924 | 67 | 67 |
| | | 0.3 | 0.637749 | 543 | 0.733638 | 0.723924 | 67 | 67 |
| | 100 | 0.1 | 0.635853 | 539 | 0.733638 | 0.723925 | 67 | 67 |
| | | 0.2 | 0.527298 | 541 | 0.733638 | 0.723924 | 67 | 67 |
| | | 0.3 | 0.494042 | 543 | 0.733638 | 0.723924 | 67 | 67 |

**Nonlinear Dual formulations** The experiments results shown in 10 and 11 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 5 are obtained with $\alpha$, i.e., the *learning rate* or *step size*, setted to 0.5 for the *AdaGrad* algorithm.

Table 10: Nonlinear SVR Wolfe Dual formulation results with Epsilon-insensitive loss

| | | | | fit_time | n_iter | train_r2 | val_r2 | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|---|
| solver | kernel | C | epsilon | | | | | | |
| smo | poly | 1 | 0.1 | 26.889628 | 38855 | 0.041472 | -20.235896 | 20 | 20 |
| | | | 0.2 | 2.366264 | 3607 | -5.523525 | -24.564063 | 5 | 5 |
| | | | 0.3 | 1.063623 | 1440 | 0.121370 | -48.392546 | 4 | 4 |
| | | 10 | 0.1 | 368.357509 | 939877 | 0.357291 | -11.310659 | 19 | 19 |
| | | | 0.2 | 2.833490 | 4317 | -4.173750 | -24.504696 | 4 | 4 |
| | | | 0.3 | 0.861725 | 1396 | 0.227988 | -48.232256 | 3 | 3 |
| | | 100 | 0.1 | 2431.854217 | 7053217 | 0.334627 | -12.438814 | 20 | 20 |
| | | | 0.2 | 2.970568 | 4317 | -4.173750 | -24.504696 | 4 | 4 |
| | | | 0.3 | 0.860159 | 1396 | 0.227988 | -48.232256 | 3 | 3 |
| | rbf | 1 | 0.1 | 0.070852 | 53 | 0.982232 | -0.107260 | 20 | 20 |
| | | | 0.2 | 0.015128 | 14 | 0.959560 | -1.732727 | 6 | 6 |
| | | | 0.3 | 0.011491 | 12 | 0.935447 | -2.495198 | 5 | 5 |
| | | 10 | 0.1 | 0.527717 | 398 | 0.981400 | 0.739074 | 18 | 18 |
| | | | 0.2 | 0.015757 | 16 | 0.951327 | -1.750890 | 5 | 5 |
| | | | 0.3 | 0.010530 | 12 | 0.929203 | -2.514675 | 4 | 4 |
| | | 100 | 0.1 | 1.742027 | 2574 | 0.979866 | 0.087491 | 17 | 17 |
| | | | 0.2 | 0.013848 | 16 | 0.951327 | -1.750890 | 5 | 5 |
| | | | 0.3 | 0.008658 | 12 | 0.929203 | -2.514675 | 4 | 4 |
| libsvm | poly | 1 | 0.1 | 0.019525 | 70279 | 0.978147 | -12.483928 | 20 | 20 |
| | | | 0.2 | 0.006174 | 3221 | 0.967412 | -40.598436 | 5 | 5 |
| | | | 0.3 | 0.011255 | 1293 | 0.917912 | -70.616835 | 4 | 4 |
| | | 10 | 0.1 | 0.797140 | 3301383 | 0.978557 | -11.345334 | 19 | 19 |
| | | | 0.2 | 0.010065 | 4829 | 0.969666 | -40.590296 | 4 | 4 |
| | | | 0.3 | 0.007448 | 1322 | 0.919258 | -70.610551 | 3 | 3 |
| | | 100 | 0.1 | 2.676930 | 16883444 | 0.978709 | -10.897898 | 23 | 23 |
| | | | 0.2 | 0.012942 | 4829 | 0.969666 | -40.590296 | 4 | 4 |
| | | | 0.3 | 0.001841 | 1322 | 0.919258 | -70.610551 | 3 | 3 |
| | rbf | 1 | 0.1 | 0.008771 | 88 | 0.982555 | -0.048065 | 20 | 20 |
| | | | 0.2 | 0.001233 | 21 | 0.961248 | -0.784327 | 6 | 6 |
| | | | 0.3 | 0.007089 | 24 | 0.911568 | -1.128042 | 5 | 5 |
| | | 10 | 0.1 | 0.016236 | 564 | 0.984309 | 0.794712 | 17 | 17 |
| | | | 0.2 | 0.014555 | 26 | 0.962020 | -0.784287 | 5 | 5 |
| | | | 0.3 | 0.008202 | 18 | 0.911949 | -1.126343 | 5 | 5 |
| | | 100 | 0.1 | 0.008616 | 3195 | 0.984358 | 0.339781 | 17 | 17 |
| | | | 0.2 | 0.002037 | 26 | 0.962020 | -0.784287 | 5 | 5 |
| | | | 0.3 | 0.004992 | 18 | 0.911949 | -1.126343 | 5 | 5 |
| cvxopt | poly | 1 | 0.1 | 0.017180 | 10 | 0.116876 | -16.797868 | 20 | 20 |
| | | | 0.2 | 0.017883 | 10 | -4.948070 | -13.077320 | 5 | 5 |
| | | | 0.3 | 0.012003 | 10 | 0.681960 | -44.133994 | 4 | 4 |
| | | 10 | 0.1 | 0.011285 | 10 | 0.953326 | -10.961264 | 22 | 22 |
| | | | 0.2 | 0.012770 | 10 | -3.642113 | -12.971183 | 4 | 4 |
| | | | 0.3 | 0.012743 | 10 | 0.783199 | -43.962270 | 3 | 3 |
| | | 100 | 0.1 | 0.011621 | 10 | 0.951861 | -9.443374 | 44 | 44 |
| | | | 0.2 | 0.013602 | 10 | -3.642117 | -12.971070 | 4 | 4 |
| | | | 0.3 | 0.013014 | 10 | 0.783091 | -43.966539 | 3 | 3 |
| | rbf | 1 | 0.1 | 0.016085 | 10 | 0.981573 | -0.007460 | 20 | 20 |
| | | | 0.2 | 0.019686 | 9 | 0.958544 | -1.311340 | 7 | 7 |
| | | | 0.3 | 0.015890 | 10 | 0.932149 | -2.681785 | 5 | 5 |
| | | 10 | 0.1 | 0.015052 | 10 | 0.981853 | 0.676330 | 20 | 20 |
| | | | 0.2 | 0.022038 | 10 | 0.950457 | -1.330465 | 6 | 6 |
| | | | 0.3 | 0.016398 | 10 | 0.925512 | -2.695479 | 5 | 5 |
| | | 100 | 0.1 | 0.021050 | 10 | 0.979321 | 0.229817 | 20 | 20 |
| | | | 0.2 | 0.016424 | 10 | 0.950458 | -1.330472 | 6 | 6 |
| | | | 0.3 | 0.015113 | 10 | 0.924244 | -2.228071 | 5 | 5 |

Table 11: Nonlinear SVR Lagrangian Dual formulation results with Epsilon-insensitive loss

| | | | | fit_time | n_iter | train_r2 | val_r2 | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|---|
| dual | kernel | C | epsilon | | | | | | |
| qp | poly | 1 | 0.1 | 0.013639 | 9 | 0.636530 | -16.889746 | 67 | 67 |
| | | | 0.2 | 0.032891 | 13 | 0.615075 | -12.838670 | 67 | 67 |
| | | | 0.3 | 0.026618 | 20 | 0.641814 | -12.639351 | 67 | 67 |
| | | 10 | 0.1 | 0.014575 | 9 | 0.636530 | -16.889746 | 67 | 67 |
| | | | 0.2 | 0.018876 | 13 | 0.615075 | -12.838670 | 67 | 67 |
| | | | 0.3 | 0.025337 | 20 | 0.641814 | -12.639351 | 67 | 67 |
| | | 100 | 0.1 | 0.012551 | 9 | 0.636530 | -16.889746 | 67 | 67 |
| | | | 0.2 | 0.020681 | 13 | 0.615075 | -12.838670 | 67 | 67 |
| | | | 0.3 | 0.026794 | 20 | 0.641814 | -12.639351 | 67 | 67 |
| | rbf | 1 | 0.1 | 0.326021 | 165 | 0.689146 | -4.135603 | 67 | 67 |
| | | | 0.2 | 0.362601 | 168 | 0.668805 | -4.085457 | 67 | 67 |
| | | | 0.3 | 0.502042 | 270 | 0.621731 | -4.407841 | 67 | 67 |
| | | 10 | 0.1 | 0.079275 | 40 | 0.712605 | -3.657736 | 67 | 67 |
| | | | 0.2 | 0.151516 | 84 | 0.704434 | -3.441384 | 67 | 67 |
| | | | 0.3 | 0.185606 | 113 | 0.614242 | -4.592174 | 67 | 67 |
| | | 100 | 0.1 | 0.074331 | 40 | 0.712605 | -3.657736 | 67 | 67 |
| | | | 0.2 | 0.164555 | 84 | 0.704434 | -3.441384 | 67 | 67 |
| | | | 0.3 | 0.190906 | 113 | 0.614242 | -4.592174 | 67 | 67 |
| bcqp | poly | 1 | 0.1 | 0.030819 | 11 | 0.636315 | -16.926529 | 67 | 67 |
| | | | 0.2 | 0.033619 | 15 | 0.612743 | -12.193272 | 67 | 67 |
| | | | 0.3 | 0.039668 | 30 | 0.636335 | -12.001298 | 67 | 67 |
| | | 10 | 0.1 | 0.014905 | 11 | 0.636315 | -16.926529 | 67 | 67 |
| | | | 0.2 | 0.021995 | 15 | 0.612743 | -12.193272 | 67 | 67 |
| | | | 0.3 | 0.048245 | 30 | 0.636335 | -12.001298 | 67 | 67 |
| | | 100 | 0.1 | 0.014796 | 11 | 0.636315 | -16.926529 | 67 | 67 |
| | | | 0.2 | 0.022666 | 15 | 0.612743 | -12.193272 | 67 | 67 |
| | | | 0.3 | 0.042290 | 30 | 0.636335 | -12.001298 | 67 | 67 |
| | rbf | 1 | 0.1 | 0.081437 | 47 | 0.736623 | -3.125274 | 67 | 67 |
| | | | 0.2 | 0.214357 | 125 | 0.678979 | -3.888105 | 67 | 67 |
| | | | 0.3 | 0.491642 | 327 | 0.582883 | -5.520437 | 67 | 67 |
| | | 10 | 0.1 | 0.079863 | 47 | 0.736623 | -3.125274 | 67 | 67 |
| | | | 0.2 | 0.204089 | 125 | 0.678979 | -3.888105 | 67 | 67 |
| | | | 0.3 | 0.355141 | 327 | 0.582883 | -5.520437 | 67 | 67 |
| | | 100 | 0.1 | 0.111757 | 47 | 0.736623 | -3.125274 | 67 | 67 |
| | | | 0.2 | 0.190357 | 125 | 0.678979 | -3.888105 | 67 | 67 |
| | | | 0.3 | 0.291476 | 327 | 0.582883 | -5.520437 | 67 | 67 |

### 7.2.2 Squared Epsilon-insensitive 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 0.001 and $\beta$, i.e., the *momentum*, equal to 0.4. The batch size is setted to 20. Training is stopped if after 5 iterations the training loss is not lower than the best found so far.

Table 12: SVR Primal formulation results with Squared Epsilon-insensitive loss

| | | | | fit_time | n_iter | train_r2 | val_r2 | train_n_sv | val_n_sv |
|---|---|---|---|---|---|---|---|---|---|
| solver | C | momentum | epsilon | | | | | | |
| sgd | 1 | none | 0.1 | 1.274976 | 825 | 0.977343 | 0.972962 | 66 | 33 |
| | | | 0.2 | 1.265650 | 814 | 0.977337 | 0.972946 | 65 | 33 |
| | | | 0.3 | 1.151264 | 803 | 0.977329 | 0.972927 | 65 | 33 |
| | | standard | 0.1 | 0.849939 | 534 | 0.977359 | 0.972998 | 66 | 33 |
| | | | 0.2 | 0.826579 | 525 | 0.977354 | 0.972985 | 65 | 33 |
| | | | 0.3 | 0.737108 | 516 | 0.977349 | 0.972969 | 65 | 33 |
| | | nesterov | 0.1 | 0.855992 | 534 | 0.977358 | 0.972997 | 66 | 33 |
| | | | 0.2 | 0.861291 | 526 | 0.977354 | 0.972985 | 65 | 33 |
| | | | 0.3 | 0.743692 | 515 | 0.977348 | 0.972967 | 65 | 33 |
| | 10 | none | 0.1 | 0.154300 | 99 | 0.978098 | 0.973423 | 66 | 33 |
| | | | 0.2 | 0.151321 | 100 | 0.978098 | 0.973424 | 65 | 32 |
| | | | 0.3 | 0.151889 | 100 | 0.978097 | 0.973420 | 64 | 32 |
| | | standard | 0.1 | 0.093561 | 61 | 0.978099 | 0.973502 | 66 | 33 |
| | | | 0.2 | 0.097428 | 62 | 0.978099 | 0.973503 | 65 | 32 |
| | | | 0.3 | 0.094527 | 62 | 0.978099 | 0.973505 | 65 | 32 |
| | | nesterov | 0.1 | 0.096757 | 62 | 0.978100 | 0.973491 | 66 | 33 |
| | | | 0.2 | 0.097347 | 62 | 0.978100 | 0.973493 | 65 | 32 |
| | | | 0.3 | 0.095362 | 63 | 0.978100 | 0.973495 | 65 | 32 |
| | 100 | none | 0.1 | 0.024512 | 15 | 0.977779 | 0.973078 | 65 | 33 |
| | | | 0.2 | 0.024470 | 15 | 0.977779 | 0.973078 | 65 | 32 |
| | | | 0.3 | 0.022335 | 15 | 0.977778 | 0.973084 | 64 | 32 |
| | | standard | 0.1 | 0.014060 | 8 | 0.977853 | 0.973014 | 66 | 32 |
| | | | 0.2 | 0.014139 | 8 | 0.977853 | 0.973017 | 64 | 32 |
| | | | 0.3 | 0.014335 | 10 | 0.977853 | 0.973014 | 64 | 31 |
| | | nesterov | 0.1 | 0.019476 | 10 | 0.977838 | 0.973043 | 66 | 32 |
| | | | 0.2 | 0.017619 | 10 | 0.977838 | 0.973042 | 64 | 32 |
| | | | 0.3 | 0.015698 | 10 | 0.977838 | 0.973045 | 64 | 31 |
| liblinear | 1 | - | 0.1 | 0.001004 | 84 | 0.978134 | 0.973997 | 67 | 32 |
| | | | 0.2 | 0.001132 | 84 | 0.978132 | 0.974006 | 66 | 32 |
| | | | 0.3 | 0.001113 | 83 | 0.978130 | 0.974011 | 66 | 32 |
| | 10 | - | 0.1 | 0.003276 | 768 | 0.978183 | 0.973959 | 66 | 33 |
| | | | 0.2 | 0.003045 | 765 | 0.978183 | 0.973965 | 66 | 33 |
| | | | 0.3 | 0.003119 | 765 | 0.978183 | 0.973970 | 66 | 32 |
| | 100 | - | 0.1 | 0.004366 | 1000 | 0.978025 | 0.973097 | 66 | 33 |
| | | | 0.2 | 0.004579 | 1000 | 0.978029 | 0.973107 | 66 | 33 |
| | | | 0.3 | 0.004397 | 1000 | 0.978033 | 0.973116 | 65 | 32 |

# 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 al the others, i.e., both *cvxopt* [11] and *sklearn* implementations, i.e., *liblinear* [9] and *libsvm* [10] implementations, in terms of *time* obviously due to the different core implementation languages, i.e., Python and C respectively. Moreover the *liblinear* [9] implementation uses an optimization method called *Coordinate Gradient Descent* which minimizes one coordinate at a time. An intresting

Meanwhile, for what about the *Wolfe dual* formulations we can notice as *cvxopt* [11] underperforms the *sklearn* implementation, i.e., *libsvm* [10] 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 intresting 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 [4, 7] for classification and regression respectively.

In the *Lagrangian dual* formulations the goodness of the solution in terms of *accuracy* or *r2* values depends by the residue in the solution of the *Lagrangian dual* at each step provided by *minres* algorithm. Finally, 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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