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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* 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* and *libsvm* implementations, and *cvxopt* 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 ξ_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 $\dfrac{1}{2}\|w\|^2$, 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:

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

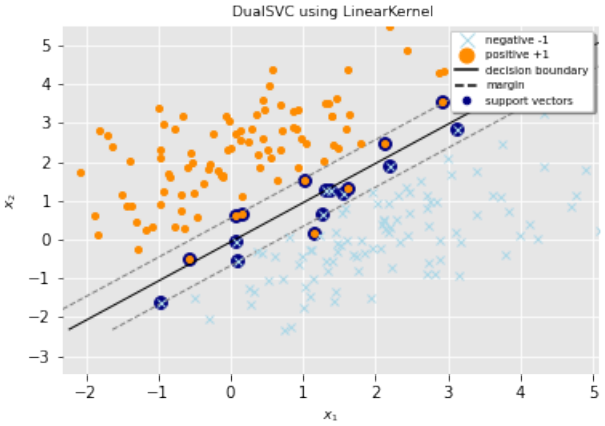


Figure 1: Linear SVC hyperplane

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 ξ 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:

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

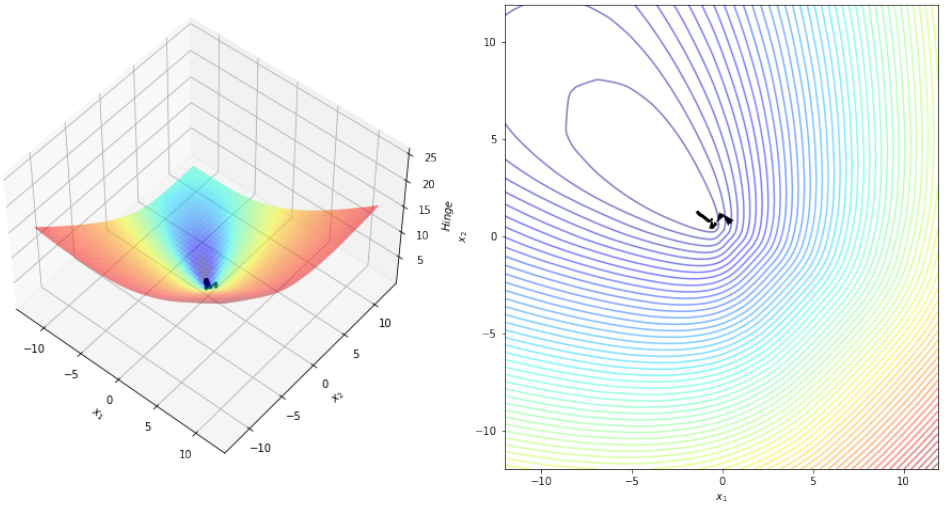


Figure 2: SVC Hinge loss with optimization steps

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 [6] 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 $\alpha_i \geq 0, \mu_i \geq 0\ \forall_i$:

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

We wish to find the w, b and ξ_i which minimizes, and the α and μ 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 α. 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 α 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:

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

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 [6] 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 $u^T = [C, \ldots, C]$.
Taking the derivative of the Lagrangian $\mathcal{L}$ wrt α 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 α optimal solution of the linear system:

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

the gradient wrt μ, λ_+ and λ_- 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 indefinite, i.e., the Lagrangian function is not strictly convex since it will be linear along the eigenvectors correspondent to the null eigenvalues, 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 the gradient, we will choose α in such a way as the one that minimizes the residue, i.e. the least-squares solution:

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

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*, which computes the vector α that minimizes $\|Q\alpha - b\|$ among all vectors in $K_n(Q, b) = span(b, Qb, Q^2b, \ldots, Q^{n-1}b)$.

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 μ 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 α 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 α optimal solution of the linear system:

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

the gradient wrt λ_+ and λ_- 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 ξ and is called $\mathcal{L}_2$-SVC.

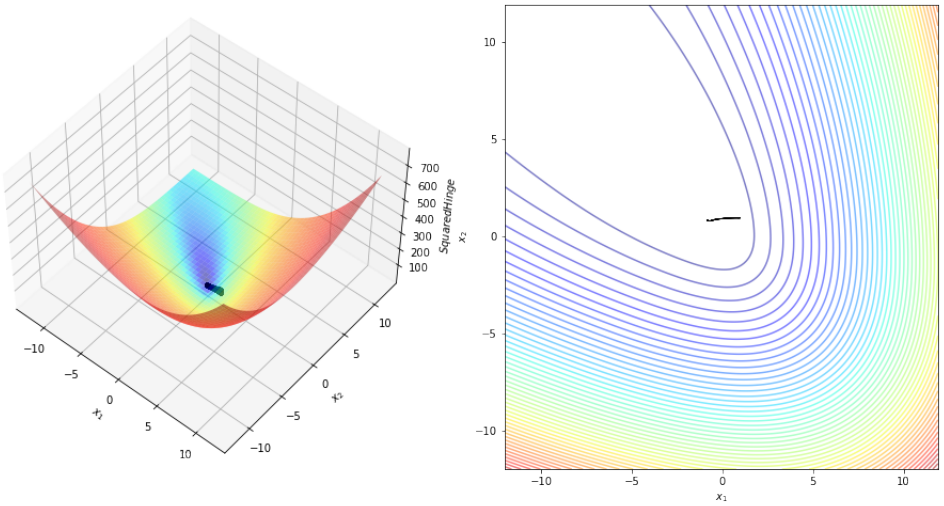


Figure 3: SVC Squared Hinge loss with optimization steps

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 ϵ 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 ϵ-insensitive tube. The output variables which are outside the tube are given one of two slack variable penalties depending on whether they lie above, ξ^+, or below, ξ^-, 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:

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

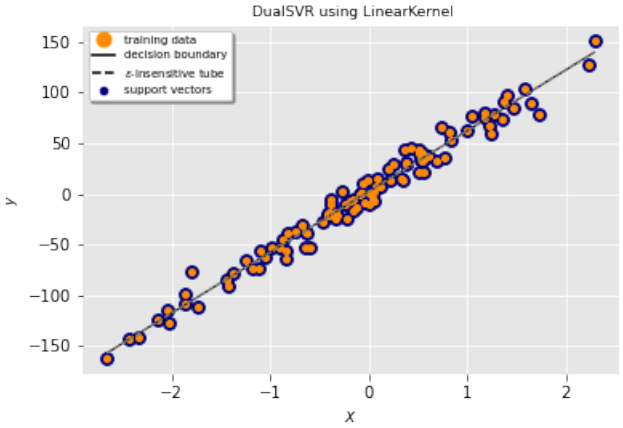


Figure 4: Linear SVR hyperplane

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 $\pm\epsilon$, 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 ξ linearly and is called $\mathcal{L}_1$-SVR.

4.1.2 Wolfe Dual formulation

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

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

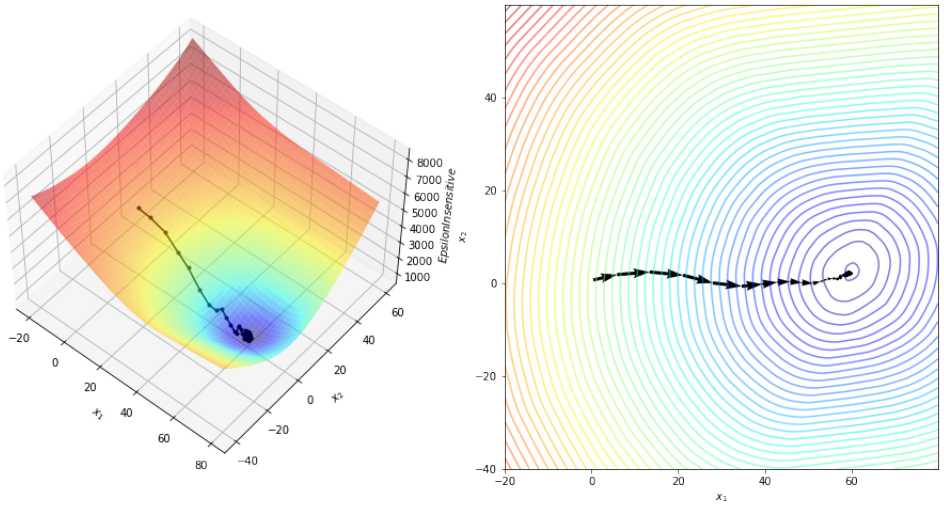


Figure 5: SVR Epsilon-insensitive loss with optimization steps

Substituting for y_i, differentiating wrt w, b, ξ^+, ξ^- 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 α_i^+ and α_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 [6] 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 α 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 α optimal solution of the linear system:

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

the gradient wrt μ, λ_+ and λ_- 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 indefinite, i.e., the Lagrangian function is not strictly convex since it will be linear along the eigenvectors correspondent to the null eigenvalues, 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 the gradient, we will choose α in such a way as the one that minimizes the residue, i.e. the least-squares solution:

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

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*, which computes the vector α that minimizes $\|Q\alpha - b\|$ among all vectors in $K_n(Q, b) = span(b, Qb, Q^2b, \ldots, Q^{n-1}b)$.

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 μ 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 $u^T = [C, \ldots, C]$.
Now, taking the derivative of the Lagrangian $\mathcal{L}$ wrt α 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 α optimal solution of the linear system:

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

the gradient wrt λ_+ and λ_- 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 ξ and is called $\mathcal{L}_2$-SVR.

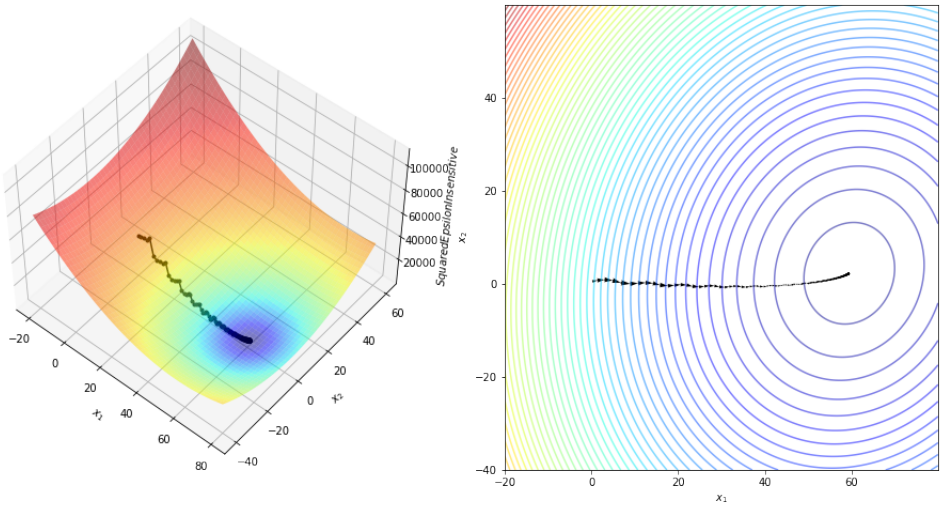


Figure 6: SVC Squared Epsilon-insensitive loss with optimization steps

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.

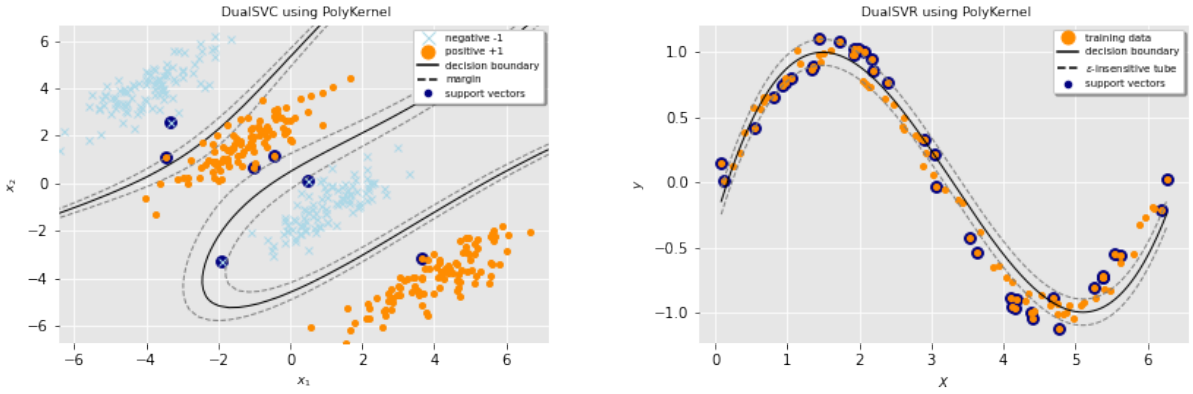
The reason that this *kernel trick* is useful is that there are many classification/regression problems that are nonlinearly separable/regressable in the *input space*, which might be in a higher dimensionality *feature space* given a suitable mapping $x \rightarrow \phi(x)$.

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 γ 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

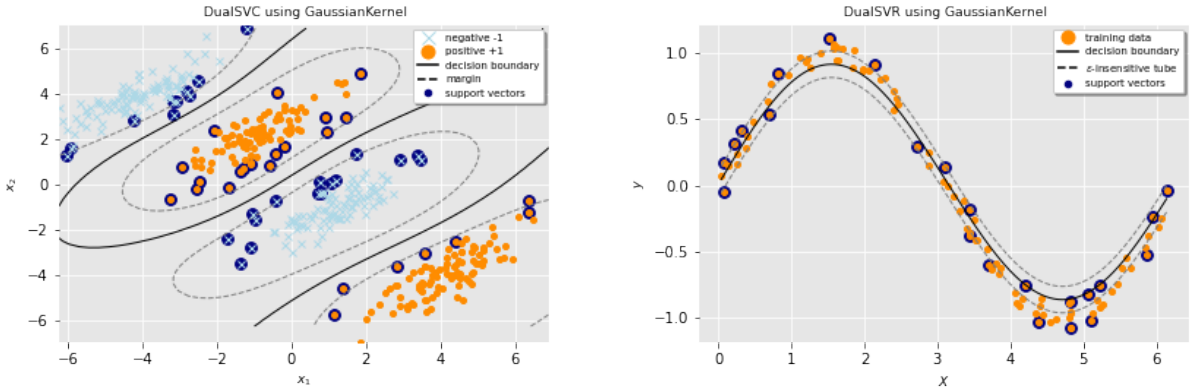
The *gaussian* kernel is defined as:

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

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 Numerical & Optimization Methods

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

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 $\mathcal{L} : \Re^m \to \Re$ is convex if:

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

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

$$\mathcal{L}(x) \geq \mathcal{L}(y) + \langle \nabla\mathcal{L}(y), x - y\rangle \ \forall \ x, y \in \Re^m$$

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

$$\nabla^2\mathcal{L}(x) \succeq 0 \ \forall \ x \in \Re^m$$

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

The definitions of *strong convexity* and *L-smoothness* below will be useful.

Definition 4 (Strong Convexity)**.** We say that a function $\mathcal{L} : \Re^m \to \Re$ is μ-strongly convex if:

$$\mathcal{G}(x) = \mathcal{L}(x) - \frac{\mu}{2}\|x\|^2$$

is convex. The latter, in terms of the Jacobian, is equivalent to:

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

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

$$\nabla^2\mathcal{G}(x) \succ 0 \ \forall \ x \in \Re^m$$

which is:

$$\nabla^2\mathcal{L}(x) \succeq \mu \ \forall \ x \in \Re^m$$

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

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

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 $\mathcal{L}$ to minimize
Require: Learning rate or step size $\alpha > 0$
  function GRADIENT DESCENT($\mathcal{L}, \alpha$)
    Initialize weight vector w_0
    $k = 0$
    while *not_convergence* **do**
      $w_{k+1} = w_k - \alpha\nabla\mathcal{L}(w_k)$
      $k = k + 1$
    end while
    return w_k
  end function

Theorem 6 (Gradient Descent convergence for convex functions)**.** *Let $\mathcal{L} : \Re^m \to \Re$ be a L-smooth convex function. Let w_* be the minimum of $\mathcal{L}$ on $\Re^m$. Then the Gradient Descent with step size $\alpha \leq 1/L$ satisfies:*

$$\mathcal{L}(w_k) - \mathcal{L}(w_*) \leq \frac{\|w_0 - w_*\|^2}{2\alpha k}$$

In particular, for $\alpha = 1/L$:

$$\frac{L\|w_0 - w_*\|^2}{2k}$$

Theorem 7 (Gradient Descent convergence for strictly convex functions)**.** *Let $\mathcal{L} : \Re^m \to \Re$ be a L-smooth, μ strictly convex function. Let w_* be the minimum of $\mathcal{L}$ on $\Re^m$. Then the Gradient Descent with step size $\alpha \leq 1/L$ satisfies:*

$$\mathcal{L}(w_k) - \mathcal{L}(w_*) \leq (1 - \alpha\mu)^k \|w_0 - w_*\|^2$$

In particular, for $\alpha = 1/L$:

$$(1 - \frac{\mu}{L})^k \|w_0 - w_*\|^2$$

We say that this method is based on full gradient, since at each iteration we need to compute:

$$\nabla\mathcal{L}(w) = \frac{1}{n}\sum_{i=1} n\nabla\mathcal{L}_i(w)$$

which depends on the whole dataset.

6.1.1 Momentum

Polyak etc.

Algorithm 2 Polyak or Heavy-Ball Momentum Accelerated Gradient Descent

Require: Function $\mathcal{L}$ to minimize
Require: Learning rate or step size $\alpha > 0$
Require: Momentum $\beta \in [0, 1]$
  function ACCELERATED GRADIENT DESCENT($\mathcal{L}, \alpha, \beta$)
    Initialize weight vector $w_1 = w_0$ and velocity vector $v_0 = 0$
    $k = 1$
    while *not_convergence* **do**
      $v_k = \beta v_{k-1} + \alpha\nabla\mathcal{L}(w_k)$
      $w_{k+1} = w_k - v_k$
      $k = k + 1$
    end while
    return w_k
  end function

Nesterov etc.

Algorithm 3 Nesterov Momentum Accelerated Gradient Descent

Require: Function $\mathcal{L}$ to minimize
Require: Learning rate $\alpha > 0$
Require: Momentum $\beta \in [0, 1]$
  function NESTEROV ACCELERATED GRADIENT DESCENT($\mathcal{L}, \alpha, \beta$)
    Initialize weight vector $w_1 = w_0$ and velocity vector $v_0 = 0$
    $k = 1$
    while *not_convergence* **do**
      $\hat{w}_k = w_k + \beta v_{k-1}$
      $v_k = \beta v_{k-1} + \alpha \nabla \mathcal{L}(\hat{w}_k)$
      $w_{k+1} = w_k - v_k$
      $k = k + 1$
    end while
    return w_k
  end function

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., $\kappa = L/\mu >> 1$, means that the level sets of $\mathcal{L}$ 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:

$$w_{k+1} = w_k - \alpha H^{-1} \nabla \mathcal{L}(w_k)$$

where α is often close to one (damped-Newton) or one, and H^{-1} denotes the Hessian of $\mathcal{L}$ at the current point.

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:

$$w_{k+1} = w_k - \alpha P^{-1} \nabla \mathcal{L}(w_k)$$

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

The *AdaGrad* [3] 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 4 AdaGrad

Require: Function $\mathcal{L}$ to minimize
Require: Learning rate or step size $\alpha > 0$
Require: Offset $\epsilon > 0$ to ensures not divide by 0
function AdaGrad($\mathcal{L}, \alpha, \epsilon$)
Initialize weight vector w_0 and the squared accumulated gradients vector $s_k = 0$
$k = 1$
while *not_convergence* **do**
$g_k = \nabla\mathcal{L}(w_k)$
$s_k = s_{k-1} + g_k^2$
$w_{k+1} = w_k - \alpha P_k^{-1} g_k = w_k - \frac{\alpha}{\sqrt{s_k + \epsilon}} g_k$ where $P_k = diag(s_k + \epsilon)^{1/2}$
$k = k + 1$
end while
return w_k
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.

6.3 Sequential Minimal Optimization

The *Sequential Minimal Optimization (SMO)* [1] 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, i.e., $y^T\alpha = 0$, so the Lagrange multipliers can be solved analitically.

At each iteration, SMO chooses two α_i to jointly optimize, let α_1 and α_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 bound 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.

6.3.1 Classification

The ends of the diagonal line segment in terms of α_2 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 $E_i = u_i - y_i$ is the error on the i-th training example and u_i is the output of the SVM 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 α_1 is computed from the new clipped α_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 problem 18 are:

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

the steps described above will be iterate as long as there will be an example that violates these KKT conditions.

6.3.2 Regression

6.4 MINRES

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 α, i.e., the *learning rate* or *step size*, setted to 0.001 and β, 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

solver	C	momentum	fit_time	n_iter	train_accuracy	val_accuracy	train_n_sv	val_n_sv
sgd	1	none	0.614727	2222	0.987525	0.985075	38	21
		standard	0.386092	1417	0.987525	0.985075	36	20
		nesterov	0.396583	1368	0.985019	0.980100	34	20
	10	none	1.435118	4602	0.990012	0.980100	13	7
		standard	1.195032	4068	0.987506	0.985075	12	7
		nesterov	1.120775	3940	0.992500	0.985075	12	7
	100	none	0.505901	1919	0.990012	0.985075	5	3
		standard	0.292062	911	0.990012	0.985075	6	4
		nesterov	0.286854	1060	0.990012	0.985075	5	3
liblinear	1	-	0.001517	146	0.979969	0.979798	11	5
	10	-	0.001479	397	0.982475	0.984848	7	5
	100	-	0.002547	1000	0.979950	0.984924	6	4

Linear Dual formulations The experiments results shown in 3 are obtained with α, i.e., the *learning rate* or *step size*, setted to 0.5 for the *AdaGrad* algorithm.

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

solver	C	fit_time	n_iter	train_accuracy	val_accuracy	train_n_sv	val_n_sv
cvxopt	1	0.022609	10	0.987525	0.974974	12	12
	10	0.017216	10	0.987525	0.974974	9	9
	100	0.031388	10	0.982512	0.974974	7	7
smo	1	0.094136	105	0.987525	0.974974	12	12
	10	0.121012	144	0.987525	0.974974	8	8
	100	0.660060	2050	0.982512	0.974974	7	7
libsvm	1	0.002635	257	0.982512	0.970074	14	14
	10	0.004053	522	0.982512	0.965099	9	9
	100	0.003277	3866	0.985019	0.955073	7	7

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

dual	C	fit_time	n_iter	train_accuracy	val_accuracy	train_n_sv	val_n_sv
bcqp	1	0.006318	1	0.980006	0.970074	129	129
	10	0.006567	1	0.980006	0.970074	129	129
	100	0.005008	1	0.980006	0.970074	129	129
qp	1	0.007371	1	0.982494	0.970074	131	131
	10	0.005883	1	0.982494	0.970074	131	131
	100	0.005801	1	0.982494	0.970074	131	131

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. Moreover, the experiments results shown in 5 are obtained with α, 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

solver	kernel	C	fit_time	n_iter	train_accuracy	val_accuracy	train_n_sv	val_n_sv
cvxopt	poly	1	0.092079	10	0.832507	0.675831	32	32
		10	0.111197	10	0.956159	0.830734	11	11
		100	0.097903	10	0.993734	0.985056	8	8
	rbf	1	0.072104	10	0.998747	1.000000	48	48
		10	0.069883	10	1.000000	0.997494	16	16
		100	0.077572	10	1.000000	0.997494	12	12
libsvm	poly	1	0.002903	382	0.997498	0.992481	30	30
		10	0.005636	344	0.998752	0.992481	11	11
		100	0.002283	285	1.000000	0.989975	7	7
	rbf	1	0.003181	99	0.998752	1.000000	44	44
		10	0.003128	238	1.000000	1.000000	15	15
		100	0.002410	234	1.000000	0.995006	9	9
smo	poly	1	0.391564	137	0.831259	0.675831	32	32
		10	0.311969	141	0.948640	0.810852	11	11
		100	0.293261	241	0.993734	0.987562	8	8
	rbf	1	0.253831	38	0.998747	1.000000	44	44
		10	0.234757	39	1.000000	0.997494	15	15
		100	0.164737	47	1.000000	0.997494	11	11

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

dual	kernel	C	fit_time	n_iter	train_accuracy	val_accuracy	train_n_sv	val_n_sv
bcqp	poly	1	1.300455	347	0.781213	0.531328	206	206
		10	1.221536	347	0.781213	0.531328	206	206
		100	1.109463	347	0.781213	0.531328	206	206
	rbf	1	0.023433	1	1.000000	1.000000	235	235
		10	0.021801	1	1.000000	1.000000	235	235
		100	0.020279	1	1.000000	1.000000	235	235
qp	poly	1	0.708087	153	0.773723	0.518797	179	179
		10	0.744719	153	0.773723	0.518797	179	179
		100	0.743838	153	0.773723	0.518797	179	179
	rbf	1	1.063100	180	0.772526	0.543560	190	190
		10	0.805252	144	0.837515	0.663300	198	198
		100	2.084545	679	0.782584	0.615681	151	151

7.1.2 Squared Hinge loss

Primal formulation The experiments results shown in 6 referred to *Stochastic Gradient Descent* algorithm are obtained with α, i.e., the *learning rate* or *step size*, setted to 0.001 and β, 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

solver	C	momentum	fit_time	n_iter	train_accuracy	val_accuracy	train_n_sv	val_n_sv
sgd	1	none	0.311301	738	0.944937	0.949796	41	23
		standard	0.212955	575	0.949968	0.949872	31	16
		nesterov	0.347608	647	0.952456	0.944821	36	19
	10	none	0.119227	311	0.949950	0.949796	22	12
		standard	0.084966	183	0.952437	0.949796	22	12
		nesterov	0.091229	192	0.952456	0.949796	22	12
	100	none	0.094943	167	0.952437	0.944821	16	9
		standard	0.047192	99	0.952437	0.949796	14	8
		nesterov	0.045644	111	0.957450	0.944821	15	7
liblinear	1	-	0.004304	483	0.954925	0.949796	25	14
	10	-	0.006314	1000	0.957412	0.954772	24	13
	100	-	0.008837	1000	0.949968	0.939997	33	22

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 ϵ 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 α, i.e., the *learning rate* or *step size*, setted to 0.001 and β, 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

solver	C	momentum	epsilon	fit_time	n_iter	train_r2	val_r2	train_n_sv	val_n_sv
sgd	1	none	0.1	0.106166	237	0.411391	0.401611	67	33
			0.2	0.106419	238	0.412166	0.403340	67	33
			0.3	0.091189	236	0.410766	0.402880	66	33
		standard	0.1	0.074834	153	0.432297	0.423067	67	33
			0.2	0.061122	152	0.429879	0.421839	67	33
			0.3	0.061095	153	0.431896	0.422854	66	33
		nesterov	0.1	0.103907	153	0.431737	0.422469	67	33
			0.2	0.076444	150	0.433204	0.424880	66	33
			0.3	0.102051	149	0.430432	0.422459	67	33
	10	none	0.1	0.098588	278	0.975931	0.971440	66	33
			0.2	0.105382	277	0.975854	0.971280	66	33
			0.3	0.143399	274	0.975728	0.971152	65	32
		standard	0.1	0.098547	174	0.976466	0.971978	66	33
			0.2	0.066722	173	0.976360	0.971758	66	32
			0.3	0.072765	173	0.976365	0.971780	65	32
		nesterov	0.1	0.066162	174	0.976402	0.971913	66	33
			0.2	0.087989	174	0.976385	0.971874	66	32
			0.3	0.067238	173	0.976321	0.971723	65	32
	100	none	0.1	0.043171	113	0.977985	0.973378	65	33
			0.2	0.038699	113	0.977986	0.973381	65	32
			0.3	0.047013	118	0.977986	0.973380	64	31
		standard	0.1	0.044742	72	0.977997	0.973440	66	33
			0.2	0.025275	72	0.977997	0.973440	65	32
			0.3	0.023395	73	0.977997	0.973441	64	31
		nesterov	0.1	0.026245	78	0.977995	0.973448	66	33
			0.2	0.035033	69	0.977994	0.973450	65	32
			0.3	0.025729	77	0.977995	0.973450	64	31
liblinear	1	-	0.1	0.001592	12	0.918771	0.916780	65	33
			0.2	0.001386	10	0.918678	0.916518	65	32
			0.3	0.001457	14	0.919337	0.917112	64	32
	10	-	0.1	0.001766	69	0.977852	0.972056	65	33
			0.2	0.002331	183	0.977852	0.972041	64	33
			0.3	0.001727	89	0.977870	0.972127	64	33
	100	-	0.1	0.002813	675	0.977723	0.974270	66	33
			0.2	0.002606	771	0.977673	0.974124	66	33
			0.3	0.003231	820	0.977638	0.973863	65	33

Linear Dual formulations The experiments results shown in 9 are obtained with α, i.e., the *learning rate* or *step size*, setted to 0.5 for the *AdaGrad* algorithm.

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

solver	C	epsilon	fit_time	n_iter	train_r2	val_r2	train_n_sv	val_n_sv
cvxopt	1	0.1	0.021536	9	0.917772	0.914479	67	67
		0.2	0.022979	9	0.918341	0.915058	67	67
		0.3	0.019355	10	0.918942	0.915614	66	66
	10	0.1	0.021882	9	0.977920	0.972466	67	67
		0.2	0.013598	9	0.977926	0.972474	67	67
		0.3	0.012306	10	0.977954	0.972562	66	66
	100	0.1	0.012041	9	0.977788	0.974150	67	67
		0.2	0.027912	9	0.977742	0.974033	67	67
		0.3	0.009634	9	0.977737	0.973956	67	67
smo	1	0.1	0.014631	15	0.917773	0.914442	66	66
		0.2	0.014218	13	0.918341	0.915019	66	66
		0.3	0.040505	60	0.918942	0.915576	66	66
	10	0.1	0.063922	56	0.977920	0.972445	66	66
		0.2	0.146936	219	0.977926	0.972457	65	65
		0.3	0.053513	38	0.977953	0.972544	65	65
	100	0.1	0.595028	1508	0.977788	0.974139	66	66
		0.2	0.327064	394	0.977742	0.974022	66	66
		0.3	0.515121	900	0.977737	0.973939	66	66
libsvm	1	0.1	0.002211	63	0.917627	0.915448	66	66
		0.2	0.002491	102	0.918194	0.915985	66	66
		0.3	0.002069	54	0.918786	0.916554	66	66
	10	0.1	0.001865	282	0.977852	0.972051	66	66
		0.2	0.002066	193	0.977851	0.972025	65	65
		0.3	0.002003	593	0.977870	0.972135	65	65
	100	0.1	0.003146	2621	0.977723	0.974270	66	66
		0.2	0.003566	2709	0.977673	0.974122	66	66
		0.3	0.003817	4141	0.977655	0.974045	66	66

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

dual	C	epsilon	fit_time	n_iter	train_r2	val_r2	train_n_sv	val_n_sv
bcqp	1	0.1	0.656280	522	0.731073	0.721200	67	67
		0.2	0.658018	524	0.731073	0.721199	67	67
		0.3	0.602584	526	0.731073	0.721199	67	67
	10	0.1	0.614027	539	0.733638	0.723925	67	67
		0.2	0.668057	541	0.733638	0.723924	67	67
		0.3	0.637837	543	0.733638	0.723924	67	67
	100	0.1	0.733603	539	0.733638	0.723925	67	67
		0.2	0.627369	541	0.733638	0.723924	67	67
		0.3	0.409460	543	0.733638	0.723924	67	67
qp	1	0.1	0.674449	653	0.876534	0.870926	67	67
		0.2	0.678396	653	0.876534	0.870927	67	67
		0.3	0.722974	653	0.876534	0.870927	67	67
	10	0.1	0.498502	519	0.731825	0.722021	67	67
		0.2	0.563454	524	0.731825	0.722021	67	67
		0.3	0.537692	530	0.731825	0.722020	67	67
	100	0.1	0.652838	519	0.731825	0.722021	67	67
		0.2	0.604621	524	0.731825	0.722021	67	67
		0.3	0.550931	530	0.731825	0.722020	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. Moreover, the experiments results shown in 5 are obtained with α, 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

solver	kernel	C	epsilon	fit_time	n_iter	train_r2	val_r2	train_n_sv	val_n_sv
cvxopt	poly	1	0.1	0.015057	10	0.848547	-5.090164	23	23
			0.2	0.017265	10	-3.609617	-8.632746	6	6
			0.3	0.011037	10	-0.786399	-8.517434	4	4
		10	0.1	0.010415	10	0.968145	-5.331473	25	25
			0.2	0.022692	10	-3.609013	-8.638973	4	4
			0.3	0.011880	10	-0.780783	-8.483884	4	4
		100	0.1	0.012144	10	0.945501	-5.188429	27	27
			0.2	0.014013	10	-3.608986	-8.638995	4	4
			0.3	0.012482	10	-0.780887	-8.484199	4	4
	rbf	1	0.1	0.014662	10	0.979933	0.327020	14	14
			0.2	0.021198	10	0.961792	-0.943080	6	6
			0.3	0.017357	9	0.890164	-1.687411	5	5
		10	0.1	0.014854	10	0.977704	0.640986	14	14
			0.2	0.016555	10	0.952051	-0.963789	6	6
			0.3	0.014812	10	0.882145	-1.696148	4	4
		100	0.1	0.015500	10	0.974118	0.715636	15	15
			0.2	0.018510	10	0.965122	-0.935738	7	7
			0.3	0.018584	10	0.882145	-1.696145	4	4
smo	poly	1	0.1	80.259683	175472	0.850381	-6.479953	23	23
			0.2	4.845339	6682	-5.669765	-15.026022	6	6
			0.3	0.531903	909	-2.663418	-16.100682	4	4
		10	0.1	660.696393	1352666	0.958635	-6.309580	23	23
			0.2	3.283288	5413	-5.659396	-15.048805	4	4
			0.3	4.703530	7008	-2.652290	-16.086707	4	4
		100	0.1	3838.989156	9325434	0.956258	-6.351469	23	23
			0.2	3.581371	5413	-5.659396	-15.048805	4	4
			0.3	2.518382	7008	-2.652290	-16.086707	4	4
	rbf	1	0.1	0.035963	30	0.979269	0.337883	14	14
			0.2	0.014002	14	0.953442	-0.706423	6	6
			0.3	0.009471	9	0.880480	-1.956576	5	5
		10	0.1	0.294246	198	0.979879	0.614804	14	14
			0.2	0.018293	20	0.943679	-0.729439	5	5
			0.3	0.010107	11	0.872418	-1.965274	4	4
		100	0.1	0.869753	1199	0.976323	0.735233	14	14
			0.2	0.019184	20	0.943679	-0.729439	5	5
			0.3	0.008680	11	0.872418	-1.965274	4	4
libsvm	poly	1	0.1	0.065331	202636	0.981648	-29.427063	20	20
			0.2	0.008808	5634	0.971457	-44.854253	5	5
			0.3	0.012103	1133	0.921669	-67.995416	4	4
		10	0.1	0.577278	2329808	0.981723	-28.867737	18	18
			0.2	0.012278	4967	0.972091	-44.851795	4	4
			0.3	0.001801	925	0.922233	-67.994190	3	3
		100	0.1	1.439916	6416597	0.980670	-14.594558	24	24
			0.2	0.009960	4967	0.972091	-44.851795	4	4
			0.3	0.021700	925	0.922233	-67.994190	3	3
	rbf	1	0.1	0.015557	71	0.986549	-2.969459	16	16
			0.2	0.018801	33	0.964555	-4.149278	5	5
			0.3	0.002971	8	0.912691	-4.815179	4	4
		10	0.1	0.004562	474	0.987401	-2.477526	15	15
			0.2	0.011069	34	0.964563	-4.149231	5	5
			0.3	0.001300	8	0.913367	-4.813685	4	4
		100	0.1	0.006711	2712	0.987693	-1.428809	13	13
			0.2	0.002964	34	0.964563	-4.149231	5	5
			0.3	0.002766	8	0.913367	-4.813685	4	4

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

dual	kernel	C	epsilon	fit_time	n_iter	train_r2	val_r2	train_n_sv	val_n_sv
bcqp	poly	1	0.1	0.482641	345	0.643482	-10.313337	67	67
			0.2	0.507596	348	0.632323	-8.680716	67	67
			0.3	0.980019	669	0.623699	-7.643487	67	67
		10	0.1	0.517057	345	0.643482	-10.313337	67	67
			0.2	0.458200	348	0.632323	-8.680716	67	67
			0.3	0.920299	669	0.623699	-7.643487	67	67
		100	0.1	0.557809	345	0.643482	-10.313337	67	67
			0.2	0.492806	348	0.632323	-8.680716	67	67
			0.3	0.654942	669	0.623699	-7.643487	67	67
	rbf	1	0.1	0.043660	19	0.740194	-1.880483	67	67
			0.2	0.192294	92	0.740177	-1.882909	67	67
			0.3	0.290547	164	0.603015	-3.956481	67	67
		10	0.1	0.037314	19	0.740194	-1.880483	67	67
			0.2	0.150209	92	0.740177	-1.882909	67	67
			0.3	0.290903	164	0.603015	-3.956481	67	67
		100	0.1	0.044858	19	0.740194	-1.880483	67	67
			0.2	0.180130	92	0.740177	-1.882909	67	67
			0.3	0.264654	164	0.603015	-3.956481	67	67
qp	poly	1	0.1	0.471979	347	0.641413	-10.283007	67	67
			0.2	0.667717	348	0.633767	-8.692657	67	67
			0.3	0.634864	349	0.626387	-7.655867	67	67
		10	0.1	0.421276	347	0.641413	-10.283007	67	67
			0.2	0.454034	348	0.633767	-8.692657	67	67
			0.3	0.492867	349	0.626387	-7.655867	67	67
		100	0.1	0.474953	347	0.641413	-10.283007	67	67
			0.2	0.574175	348	0.633767	-8.692657	67	67
			0.3	0.406300	349	0.626387	-7.655867	67	67
	rbf	1	0.1	0.191649	102	0.721454	-2.320027	67	67
			0.2	0.407150	157	0.675573	-2.863975	67	67
			0.3	0.479133	213	0.627853	-3.010361	67	67
		10	0.1	0.128122	42	0.723816	-2.306795	67	67
			0.2	0.227605	95	0.675184	-2.866411	67	67
			0.3	0.292192	163	0.614802	-3.217847	67	67
		100	0.1	0.080129	42	0.723816	-2.306795	67	67
			0.2	0.244637	95	0.675184	-2.866411	67	67
			0.3	0.393030	163	0.614802	-3.217847	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 α, i.e., the *learning rate* or *step size*, setted to 0.001 and β, 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

solver	C	momentum	epsilon	fit_time	n_iter	train_r2	val_r2	train_n_sv	val_n_sv
sgd	1	none	0.1	1.682880	3276	0.977341	0.972958	66	33
			0.2	1.638918	3249	0.977336	0.972944	65	33
			0.3	1.704772	3166	0.977322	0.972912	65	32
		standard	0.1	1.083981	2112	0.977357	0.972994	66	33
			0.2	0.949405	2037	0.977347	0.972969	65	33
			0.3	1.152253	1993	0.977336	0.972941	65	33
		nesterov	0.1	1.133447	2112	0.977357	0.972994	66	33
			0.2	1.065994	2040	0.977348	0.972970	65	33
			0.3	1.092851	2057	0.977348	0.972968	65	33
	10	none	0.1	0.278023	396	0.978098	0.973424	66	33
			0.2	0.359594	398	0.978098	0.973423	65	32
			0.3	0.265300	398	0.978098	0.973424	65	32
		standard	0.1	0.129566	244	0.978100	0.973504	66	33
			0.2	0.137887	246	0.978100	0.973479	65	32
			0.3	0.151681	248	0.978100	0.973508	65	32
		nesterov	0.1	0.172341	248	0.978100	0.973488	66	33
			0.2	0.157168	249	0.978100	0.973487	65	32
			0.3	0.115858	250	0.978100	0.973489	65	32
	100	none	0.1	0.029804	62	0.977779	0.973078	65	33
			0.2	0.035275	62	0.977779	0.973079	65	32
			0.3	0.024690	61	0.977778	0.973084	64	32
		standard	0.1	0.016081	34	0.977853	0.973014	66	32
			0.2	0.016552	40	0.977853	0.973017	64	32
			0.3	0.015752	40	0.977853	0.973014	64	31
		nesterov	0.1	0.025452	41	0.977838	0.973043	66	32
			0.2	0.024878	41	0.977838	0.973042	64	32
			0.3	0.015031	41	0.977838	0.973045	64	31
liblinear	1	-	0.1	0.000833	88	0.978134	0.973998	67	32
			0.2	0.000823	88	0.978132	0.974007	66	32
			0.3	0.000989	88	0.978130	0.974014	66	32
	10	-	0.1	0.002979	759	0.978184	0.973972	66	33
			0.2	0.003070	754	0.978183	0.973978	66	33
			0.3	0.002643	764	0.978183	0.973982	66	32
	100	-	0.1	0.004287	1000	0.977992	0.974905	66	33
			0.2	0.004157	1000	0.978139	0.973717	66	33
			0.3	0.003960	1000	0.978111	0.973347	66	31

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, $n >> m$; meanwhile the *dual formulation*, is more suitable in case the number of examples n is less than the number of features m, $n < m$, since the complexity of the model is dominated by the number of examples.

From all these experiments we can see as, for what about the *primal* formulations, the results provided from the *custom* implementations are strongly similar to those of *sklearn* implementations, i.e., *liblinear* implementations, with a slight exception about the time gap obviously due to the different core implementation languages, Python and C respectively.

Meanwhile, for what about the *dual* formulations we can notice as *cvxopt* underperforms the *sklearn* implementations, i.e., *libsvm* implementations, 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. Despite this, the *custom* implementations does not overperform the *cvxopt* probably due to the gap generated from the different core implementation languages, again Python and C respectively. For these reasons, *sklearn* provides better results in terms of time wrt the other implementations since it is designed to work in a large-scale context and its core is implemented in C. Furthermore, in the SVC example with the polynomial kernel of degree 5, we can see that the time gap is significatively, properly two different orders of magnitude ($\simeq$ 29min vs. $\simeq$ 19ms), and this could not depend just only by the different implementation languages; it's probable that *liblinear* adopts some heuristics, i.e., low rank approssimations of the kernel matrix, to deal with the polynomial kernel in case of high degree.

Important consideration involves the number of support vector machines: the *Lagrangian dual* formulation tends to select all the data points as support vectors, so it makes the model complex and it tends to give low scores wrt the equivalent *Wolfe dual* formulation. In particular, the *Lagrangian relaxation* resulting from the *Wolfe dual* always gives rise to a nonsmooth optimization with an exception for the SVC with a Gaussian kernel where the two formulations solve exactly the same problem. In all the other cases the goodness of the solution depends on the residue in the solution of the *Lagrangian dual* at each step; one of the wrost results certainly concerns the SVC with the polynomial kernel of degree 3, where the residue is in the order of $+02/03$ and so the approssimation is horrible. 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 relaxation* of the same problem with the bias term embedded into the weight matrix.

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