A survey of some Machine Learning models

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Outline

Setup

Similar to a logistic model, a **support vector machine** is a model for binary classification, using a hyperplane, of the form $\{\mathbf{x} \in \mathbb{R}^d \mid \mathbf{w} \cdot \mathbf{x} + b = 0\}$, as decision boundary.

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However, the optimization goal is different.

Given sample data $\mathcal{S} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, the goal is to minimize the value of $\frac{1}{2}|\mathbf{w}|^2$, the vector norm[1], subject to the condition that for all $1 \leq i \leq n$, $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$ is satisfied.[2]

To work with a data set that is not linearly separable, one introduces so-called "slack variables" $\xi_i \geq 0$, $i = 1, \ldots, n$ into the inequalities. They change to $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i$.

The reason for wanting to minimize $\frac{1}{2}|\mathbf{w}|^2$?

- Supposing no $\mathbf{x}_i$ passes through hyperplane with parameters $\mathbf{w}, b$, we can scale both the normal vector and b so that $\min_i |\mathbf{w} \cdot \mathbf{x}_i + b| = 1$.
- The distance from any $\mathbf{x} \in \mathbb{R}^d$ to the hyperplane is $\frac{|\mathbf{w} \cdot \mathbf{x} + b|}{|\mathbf{w}|}$. So, if $\mathbf{x}_i \in \mathcal{S}$ is such that $|\mathbf{w} \cdot \mathbf{x}_i + b| = 1$, then its distance to decision boundary is $\rho = \frac{1}{|\mathbf{w}|}$.
- Want to maximize distance to decision boundary, so want to minimize $|\mathbf{w}|$.

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Constrained minimization and SVM

We can understand minimizing $\frac{1}{2}|\mathbf{w}|^2$ subject to $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$ with a Lagrangian. (Method of Lagrange multipliers; see Section 7.2 in the Mathematics for Machine Learning book.)
For $\underline{\alpha} = (\alpha_1, \ldots, \alpha_n)$, with $\alpha_i \in \mathbb{R}$, Lagrangian is

$$L(\mathbf{w}, b, \underline{\alpha}) = \frac{1}{2}|\mathbf{w}|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 \right).$$

It is minimized when

$$\nabla_{\mathbf{w}} L = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i;$$

$$\nabla_b L = 0 \quad \Rightarrow \quad \sum_{i=1}^{n} \alpha_i y_i = 0;$$

$$\alpha_i \left(y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 \right) = 0 \quad \Rightarrow \quad \alpha_i = 0 \quad \text{OR} \quad y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1.$$

Support vectors are those $\mathbf{x}_i$ for which $\alpha_i \neq 0$, and so $\mathbf{w} \cdot \mathbf{x}_i + b = \pm 1$.

Lagrangian Duality

Something interesting happens when we convert the previous Lagrangian optimization problem into its "Lagrangian dual problem." This means that we take the minimum solution for $\mathbf{w}$, put it into $L(\mathbf{w}, b, \underline{\alpha})$ and want multipliers $\alpha_i \geq 0$ that *maximize* the value of this. That is, maximize

$$\frac{1}{2}\left|\sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i\right|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j \right) \cdot \mathbf{x}_i + y_i b - 1 \right).$$

Rearranged, you can rewrite it:

$$\max_{\underline{\alpha}} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

subject to $\alpha_i \geq 0$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$.
This optimization problem only depends on knowing $\mathbf{x}_i \cdot \mathbf{x}_j$ for each (i, j), and this leads to what are called **kernel methods** that are very computationally efficient and allow one to use SVM models that have non-linear decision boundaries.

SVMs via Gradient Descent

An alternative for optimizing an SVM classifier is to do so with a loss function. The loss function has a fair amount of similarity to the log-loss function we used in logistic regression; however, the per-example losses use a piecewise linear function.

When $y_i = 1$ then, writing $z_i = \mathbf{w} \cdot \mathbf{x}_i + b$, the per-example loss is $C \max(1 - z_i, 0)$ for some constant C. Call this $C\text{cost}_1(z_i)$. When $y_i = -1$ (and so $\tilde{y}_i = 0$) then the per-example loss is $C\text{cost}_0(z_i) = C \max(1 + z_i, 0)$.

However, we also include the norm of $\mathbf{w}$ in the loss:

$$\mathcal{L}_{\mathcal{S}}(\mathbf{w}, b) = \frac{1}{2}|\mathbf{w}|^2 + \frac{1}{n}\sum_{i=1}^{n} C\left(\tilde{y}_i \text{cost}_1(\mathbf{w} \cdot \mathbf{x}_i + b) + (1 - \tilde{y}_i)\text{cost}_0(\mathbf{w} \cdot \mathbf{x}_i + b)\right).$$

Similarity to Perceptron algorithm updates

Consider the **per-example loss**: given one $(\mathbf{x}_i, y_i) \in \mathcal{S}$, have the term $-\tilde{y}_i \log(f_\omega(\mathbf{x}_i)) - (1 - \tilde{y}_i) \log(1 - f_\omega(\mathbf{x}))$.
Its partial w.r.t. w_j is

$$-\tilde{y}_i x_{i,j} * (1 - f_\omega(\mathbf{x}_i)) + (1 - \tilde{y}_i) x_{i,j} f_\omega(\mathbf{x}_i).$$

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If $\tilde{y}_i = 1$, but $f_\omega(\mathbf{x}_i)$ is close to 0, then this is *almost* $-x_{i,j} = -y_i x_{i,j}$. Were we to do an update with $\eta = 1$ then we would have $w_j^{(t)} \approx w_j^{(t-1)} + y_i x_{i,j}$. (The Perceptron update in the j^{th} coordinate.)

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Likewise, if $\tilde{y}_i = 0$, but $f_\omega(\mathbf{x}_i)$ is close to 1, then the partial is approximately $x_{i,j}$; so, using $\eta = 1$, we would get $w_j^{(t)} \approx w_j^{(t-1)} - x_{i,j} = w_j^{(t-1)} + y_i x_{i,j}$. (Like the Perceptron algorithm update again.)

Example with Logistic model

Given ± 1-labeled sample data $\mathcal{S} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, we found an expression for each partial derivative of $\mathcal{L}_\mathcal{S}$. In fact, if we call $w_{d+1} = b$ and $x_{i,d+1} = 1$ for every $1 \leq i \leq n$, then

$$\frac{\partial}{\partial w_j}\mathcal{L}_\mathcal{S} = \frac{1}{n}\sum_{i=1}^{n} -\tilde{y}_i x_{i,j}(1 - f_\omega(\mathbf{x}_i)) + (1-\tilde{y}_i)x_{i,j}f_\omega(\mathbf{x}_i)$$

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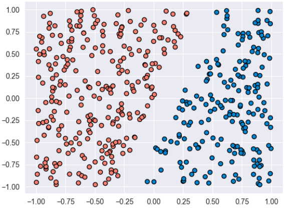
Example: consider simulated sample data below, drawn uniformly from a subset of $[-1,1]^2$, consisting of points at least a fixed distance from $H = \{(x_1, x_2) \in \mathbb{R}^2 \mid 2x_1 - \frac{2}{3}x_2 - \frac{1}{5} = 0\}$. Positively labeled points are in blue.



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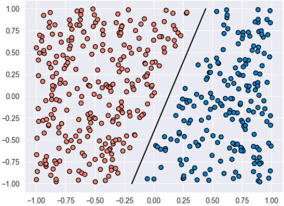
Example (cont'd): Batch gradient descent, with learning rate 0.5, stopping with threshhold 0.0005, gives (approximately) parameters for:

$$\hat{H} = \{(x_1, x_2) \in \mathbb{R}^2 \mid 2.01x_1 - 0.63x_2 - 0.26 = 0\}.$$



Logistic regression on the Iris data

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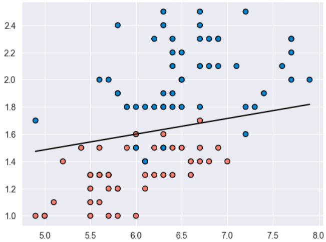
For visualization, I first show just the first and fourth coordinates, and the results for logistic model in 2D.



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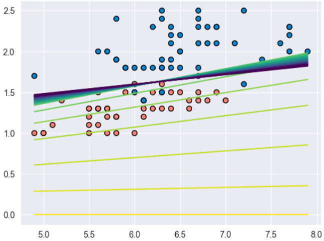
Pictured below are selected lines found during the batch gradient descent.



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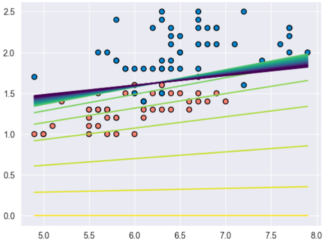
Pictured below are selected lines found during the batch gradient descent. As before, yellow-to-purple is progression through the procedure. Consecutive lines that are shown have 200 updates between them; ≈ 4000 updates in total.



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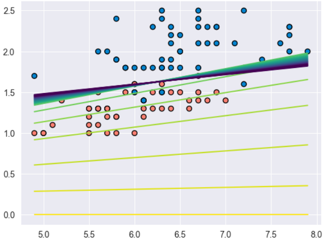

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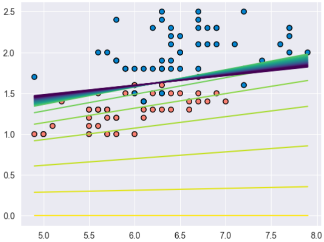
The model on the points in $\mathbb{R}^4$ took less updates (just under 3000). It had 97% accuracy on the data.



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