A survey of some Machine Learning models

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Outline

Support Vector Machines

Neural Networks

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

$$\begin{aligned}
\nabla_{\mathbf{w}} L = 0 \quad &\Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i; \\
\nabla_b L = 0 \quad &\Rightarrow \quad \sum_{i=1}^{n} \alpha_i y_i = 0; \\
\alpha_i \left(y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 \right) = 0 \quad &\Rightarrow \quad \alpha_i = 0 \quad \text{OR} \quad y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1.
\end{aligned}$$

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 $C\mathrm{cost}_1(z_i)$. When $y_i = -1$ (and so $\tilde{y}_i = 0$) then the per-example loss is $C\mathrm{cost}_0(z_i) = C \max(1 + z_i, 0)$.

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

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

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Single Layer

Fix a dimension d and a function $\sigma : \mathbb{R} \longrightarrow \mathbb{R}$ (feel free to think of this as the logistic function, for now). For any $\omega = (\mathbf{w}, b) \in \mathbb{R}^{d+1}$, set $f_\omega(\mathbf{x}) = \sigma(\mathbf{w} \cdot \mathbf{x} + b)$.

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$f_\omega(\mathbf{x}) = \sigma(\mathbf{w} \cdot \mathbf{x} + b)$.
Given some collection $\omega_1 = (\mathbf{w}_1, b_1), \omega_2 = (\mathbf{w}_2, b_2), \ldots, \omega_m = (\mathbf{w}_m, b_m)$, define $F : \mathbb{R}^d \longrightarrow \mathbb{R}^m$ by setting

$$F(\mathbf{x}) = (f_{\omega_1}(\mathbf{x}), f_{\omega_2}(\mathbf{x}), \ldots, f_{\omega_m}(\mathbf{x})).$$

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If we use W to denote the $m \times d$ matrix with $\mathbf{w}_i$ as row i, and $\mathbf{b} = (b_1, \ldots, b_m)$, then we can write $F(\mathbf{x}) = \sigma(W\mathbf{x} + \mathbf{b})$ (*if we allow σ to be applied to a vector by applying the function to each component of the vector*).
W: called the "weight matrix" for the layer map; $\mathbf{b}$ is called the "bias vector."

Composing layers

A neural network is the result of composing some number of layer maps. That is, let $m_0, m_1, \ldots, m_L$ be positive integers and say that $F_1, F_2, \ldots, F_L$ are each layer maps (as in the previous slide), with $F_i : \mathbb{R}^{m_{i-1}} \longrightarrow \mathbb{R}^{m_i}$.

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The *fully connected* neural network, with activation function σ, associated to this collection of weight matrices and bias vectors is the parameterized function

$$f(\mathbf{x}) = F_L \circ F_{L-1} \circ \ldots \circ F_2 \circ F_1(\mathbf{x}).$$

The parameters for the function are $(W_1, \mathbf{b}_1, W_2, \mathbf{b}_2, \ldots, W_L, \mathbf{b}_L)$ (flattened out as a vector).

Example with Logistic model

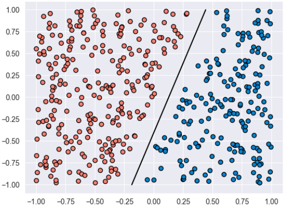
Given ± 1-labeled sample data $\mathcal{S} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, we found an expression for each partial derivative of $\mathcal{L}_\mathcal{S}$. In fact, if we call $w_{d+1} = b$ and $x_{i,d+1} = 1$ for every $1 \le i \le n$, then

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

for every $1 \le j \le d+1$.

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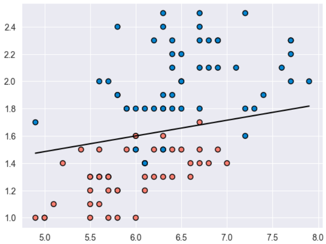
For visualization, I first show just the first and fourth coordinates, and the results for logistic model in 2D.



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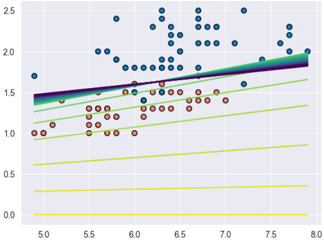

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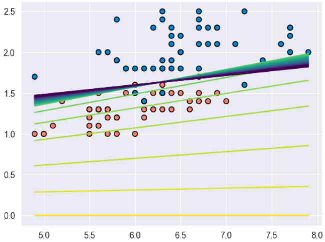

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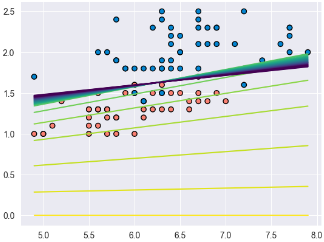

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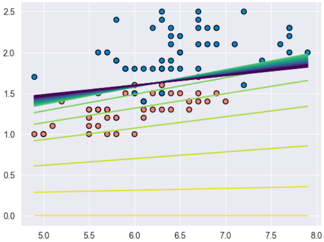
The model on the points in $\mathbb{R}^4$ took less updates (just under 3000). It had 97% accuracy on the data.



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