Introduction to Machine Learning

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1 Lecture 1

linear function

$$y = f_{\mathbf{W}}(\mathbf{X}) = f(\mathbf{X}, \mathbf{W}) = \mathbf{W}^{\mathrm{T}}\mathbf{X}$$

linear classifier (perception model)

$$\mathbf{x}_i \cdot \mathbf{w} + b \geq 0$$

$$\mathbf{x}_i \cdot \mathbf{w} + b < 0$$

linear regression in 1 dimension

$$y^i = \mathbf{W}^{\mathrm{T}}\mathbf{X}^i + \epsilon^i$$

where ϵ is the noise(loss).

Loss function: sum of squared errors

$$L(\mathbf{W}) = \sum_{i=1}^{N} (\epsilon^i)^2$$

$$L(w_0, w_1) = \sum_{i=1}^{N}$$

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} \frac{\partial [y^i - (w_0 x_0^i + w_1 x_1^i)]^2}{\partial w_0} = -2 \sum_{i=1}^{N} (y^i - (w_0 x_0^i + w_1 x_1^i)) x_0^i = 0$$

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

as follow, the partial gradient of w_1 would be

$$\sum_{i=1}^{N} y^i x_1^i = w_0 \sum_{i=1}^{N} x_0^i x_1^i + w_1 \sum_{i=1}^{N} x_1^i x_1^i$$

Therefore

$$\begin{bmatrix} \sum_{i=1}^{N} y^i x_0^i \\ \sum_{i=1}^{N} y^i x_1^i \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} x_0^i x_0^i & \sum_{i=1}^{N} x_0^i x_1^i \\ \sum_{i=1}^{N} x_0^i x_1^i & \sum_{i=1}^{N} x_1^i x_1^i \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \tag{1}$$

Formally, it could conclude that

$$\mathbf{X}^{\mathrm{T}}\mathbf{y} = \mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{w}$$

$$\mathbf{w} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

Here still need to add the trace version(more generalized version):

$$\begin{aligned}
\hat{\mathbf{Y}} &= \mathbf{Xw} \\
Loss &= (\mathbf{Y} - \mathbf{Xw})^{\mathbf{2}} \\
&= (\mathbf{Y} - \mathbf{Xw})^{\mathbf{T}}(\mathbf{Y} - \mathbf{Xw}) \\
&= \mathbf{Y^TY} - \mathbf{w^TX^TY} - \mathbf{Y^TXw} + \mathbf{w^TX^TXw} \\
Tr[\frac{\partial}{\partial \mathbf{w}} Loss] &= -\mathbf{X^TY} - \mathbf{X^TY} + \mathbf{X^TXw} + \mathbf{X^TXw} \\
&= 0 \\
\mathbf{w} &= (X^TX)^{-1}X^TY
\end{aligned}$$

Due to the matrix derivatives:

$$\begin{aligned}
\mathrm{Tr[ABC]} &= \mathrm{Tr[CAB]} \\
\frac{\partial}{\partial \mathrm{A}} \mathrm{Tr[A^TB]} &= B \\
\frac{\partial}{\partial \mathrm{A}} \mathrm{Tr[A^TBAC]} &= BAC + B^T A C^T
\end{aligned}$$

Least squares solution, vector form

$$\begin{aligned}
L(\mathbf{w}) &= (\mathbf{y} - \mathbf{Xw})^t(\mathbf{y} - \mathbf{Xw}) \\
1 &= 2
\end{aligned}$$

Why the gradient could be equal to 0

Hessian matrix is a square matrix of second-order partial derivatives of scalar-valued function, or scalar field.

$$\mathbf{H}(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \tag{2}$$

$$\mathbf{H} = \begin{vmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial x^2} \end{vmatrix}$$

In the 2 dimension, when $\mathbf{H} > 0$: if $\frac{\partial^2 f}{\partial x^2} > 0$, then point$(x_0, y_0)$ is the local min point. If $\frac{\partial^2 f}{\partial x^2} < 0$, then point$(x_0, y_0)$ is the local max point.
when $\mathbf{H} < 0$, then point(x_0, y_0) is the stationary point.
when $\mathbf{H} = 0$, second order cannot decide the point property, then consider it in higher order Taylor's Expansion.
In the example,$\mathbf{H} = 4(x_0^i)^2(x_1^i)^2 - 4(x_1^i x_0^i)(x_0^i x_1^i) = 0$, and $\frac{\partial^2 f}{\partial x^2} = 4(x_0^i)^2(x_1^i)^2 > 0$. Therefore, it is a local min point for the loss function.
In higher dimension space (multi-variables), $\mathbf{H}(f)$ should be a positive definite matrix($(\nabla \mathbf{x})^{\mathrm{T}} \mathbf{H}(f) \nabla \mathbf{x} \geq 0$ for any $\nabla \mathbf{x}$).
The more detail of Hessian matrix could look up Taylor expansion.

Generalized linear regression

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^{\mathrm{T}} \phi(\mathrm{x}^i))^{\mathrm{T}}$$

where $\phi(\mathbf{x}^i)$ is a polynomial function for $\mathbf{x}^i$

normalization

L2 norm(euclidean) norm:

$$||\mathbf{w}||_2 = \sqrt{\sum_{d=1}^{D} w_d^2} = \sqrt{< \mathbf{w}, \mathbf{w} >}$$

L1 norm(manhattan) norm:

$$||\mathbf{w}||_1 = \sum_{d=1}^{D} |w_d|$$

Lp norm, $p > 1$:

$$||\mathbf{w}||_p = (\sum_{d=1}^{D} w_d^p)^{\frac{1}{p}}$$

Ridge regression: L2-regularized linear regression

$$\begin{aligned} L(\mathbf{w}) &= \epsilon^{\mathrm{T}}\epsilon + \lambda\mathbf{w}^{\mathrm{T}}\mathbf{w} = \mathbf{y}^{\mathrm{T}}\mathbf{y} - 2\mathbf{y}^{\mathrm{T}}\mathbf{X}\mathbf{w} + \mathbf{w}^{\mathrm{T}}(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \lambda\mathbf{I})\mathbf{w} \\ \nabla L(\mathbf{w}^*) &= 0 \\ \mathbf{w}^* &= (\mathbf{X}^{\mathrm{T}}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y} \end{aligned}$$

In some case, the matrix cannot be inversed, then add $\lambda\mathbf{I}$ to make it invertible..

invertible matrix

Lasso regression: L1-regularized linear regression

suitable for small sample, large dimension.

It could shrink some coefficient into 0, helpful for feature selection.

The optimization would be gradient descent, LARS, PGD.

Logistic regression

sigmoid function:

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

Given training set:$\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}, \mathbf{x} \in \mathbb{R}^D, y \in \{0,1\}$ The ML function would be:

$$
\begin{aligned}
p(y^1, \ldots, y^n | \mathbf{x}^1, \ldots, \mathbf{x}^N) &= \prod_{i=1}^{N} P(y^i|\mathbf{x}^i) \\
&= \prod_{i=1}^{N} \sigma(\mathbf{w}^T\mathbf{x}^i)^{y^i}(1-\sigma(\mathbf{w}^T\mathbf{x}^i))^{1-y^i} \\
logP(\mathbf{y}|\mathbf{X};\mathbf{w}) &= \sum_{i=1}^{N} y^i log\sigma(\mathbf{w}^T\mathbf{x}^i) + (1-y^i)log(1-\sigma(\mathbf{w}^T\mathbf{x}^i))
\end{aligned}
$$

quadratic loss is trying to close the distance, while logistic is trying to close the classification.

multiple classes

Softmax function:

$$P(y=c|\mathbf{x};\mathbf{W}) = \frac{\exp(\mathbf{w}_c^T\mathbf{x})}{\sum_{c'=1}^{C}\exp(\mathbf{w}_{c'}^T\mathbf{x})} = g_c(\mathbf{x}, \mathbf{W})$$

Likelihood function of training sample: $(\mathbf{y}^i, \mathbf{x}^i)$

$$P(\mathbf{y}^i|\mathbf{x}^i;\mathbf{w}) = \prod_{c=1}^{C}(g_c(\mathbf{x},\mathbf{W}))^{\mathbf{y}_c^i}$$

Optimization criterion:

$$L(\mathbf{W}) = -\sum_{i=1}^{N}\sum_{c=1}^{C}\mathbf{y}_c^i \log(g_c(\mathbf{x},\mathbf{W}))$$

Mapping data to higher-dimensional space

while the data cannot be linear detected, the method is mapping the data to higher-dimensional space.

$$L(\mathbf{W}') = -\sum_{i=1}^{N}\sum_{c=1}^{C}\mathbf{y}_c^i \log(g_c(\phi(\mathbf{x}),\mathbf{W}))$$

Optimization to loss function

Gradient-based optimization

$$
\begin{aligned}
\frac{\partial L(\mathbf{w})}{\partial w_k} &= -\sum_{i=1}^{N}\left[y^i \frac{1}{g(\mathbf{w}^T\mathbf{x}^i)}\frac{\partial g(\mathbf{w}^T\mathbf{x}^i)}{\partial w_k} + (1-y^i)\frac{1}{1-g(\mathbf{w}^T\mathbf{x}^i)}(-\frac{\partial g(\mathbf{w}^T\mathbf{x}^i)}{\partial w_k})\right] \\
&= -\sum_{i=1}^{N}[y^i - g(\mathbf{w}^T\mathbf{x}^i)]\mathbf{x}_k^i
\end{aligned}
$$

This is for the non-linear system of binary classification.

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$
$$Initial : \mathbf{x_0}$$
$$Update : \mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x_i})$$

It always works for **convex function**. But it is hard to set α. second-order methods (newton method) First order Taylor series approximation:

$$f(x) \approx f(a) + (x-a)f'(a) + e(x)$$

Second order Taylor series approximation:

$$\begin{aligned} f(x) &= f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a) + e(x) \\ q'(x) &= f'(x_i) + (x - x_i)f''(x_i) = 0 \\ x_{i+1} &= x_i - \frac{f'(x_i)}{f''(x_i)} \end{aligned}$$

For the higher dimension

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)\nabla f(\mathbf{x}_i) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_i)^T \mathbf{H}(\mathbf{x} - \mathbf{x}_i) \\ \mathbf{H_{i,j}} &= \frac{\partial^2 f}{\partial x_i \partial x_j} \\ \nabla q(\mathbf{x}) &= 0 \\ \nabla f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)^T \mathbf{H}(\mathbf{x_i}) &= 0 \\ \mathbf{x}_{i+1} &= \mathbf{x}_i - (\mathbf{H}(\mathbf{x_i}))^{-1} \nabla f(\mathbf{x}_i) \end{aligned}$$

Here is the hessian matrix for logistic loss function:

$$\begin{aligned} \frac{\partial^2 L(\mathbf{w})}{\partial_{w_k} \partial_{w_j}} &= \frac{\partial(-\sum_{i=1}^N [y^i - g(\mathbf{w}^T \mathbf{x}^i)]\mathbf{x}_k^i)}{\partial w_j} \\ &= \sum_{i=1}^N \mathbf{x}_k^i \frac{\partial g(\mathbf{w}^T \mathbf{x}^i)}{\partial w_j} \\ &= \sum_{i=1}^N \mathbf{x}_k^i g(\mathbf{w}^T \mathbf{x}^i)(1 - g(\mathbf{w}^T \mathbf{x}^i))\mathbf{x}_j^i \end{aligned}$$

Perception

Given $f(x) = sign(wx + b)$ as perception which is a discriminant. The distance between any point x_0 and the boundary is $\frac{|w \cdot x_0 + b|}{||w||}$.
For the wrong classified data (x_i, y_i): $-y_i(w \cdot x_i + b) > 0$. Therefore, the distance between wrong classified data (x_i, y_i) and the boundary is $-\frac{y_i(w \cdot x_i + b)}{||w||}$.
Then the loss function would be

$$L(w, b) = -\sum_{x_i \in M} y_i(w \cdot x_i + b)$$

Where the $\frac{1}{||w||}$ is ignored. The reasons: 1) $||w||$ is only a scalar, which does not influence the vector w direction 2)The perception training end condition is that loss $L(w, b) = 0$, so the $||w||$ does not influence that.
For the training, the update would be:

$$w \leftarrow w + \eta y_i x_i$$

$$b \leftarrow b + \eta y_i$$

Dual Property

For fast calculation.

$$w = \sum_{i=1}^{N} \alpha_i y_i x_i$$

$$b = \sum_{i=1}^{N} \alpha_i y_i$$

to be continued.

SVM

Given the Discriminant: $y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$

Functional Margins

$$\begin{aligned} \mathbf{w}^T\mathbf{x}^i &\gg 0, if y^i = 1 \\ \mathbf{w}^T\mathbf{x}^i &\ll 0, if y^i = -1 \\ y^i(\mathbf{w}^T\mathbf{x}^i) &\gg 0 \end{aligned}$$

According to that $\mathbf{w}$ **is vertical to the boundary**(Due to $\mathbf{w} \cdot \mathbf{x} = -b \quad \forall \mathbf{x}$) and $\mathbf{x} = \mathbf{x}_\perp + \gamma\frac{\mathbf{w}}{|\mathbf{w}|}$, the distance between the point and the boundary would be $\gamma = \frac{\mathbf{w^T x} + b}{|\mathbf{w}|}$

Support Vector

The vectors (cases) that define the hyperplane are the support vectors.
Here we define that, for the positive support vector, $\mathbf{w}^T\mathbf{x}_{+}+b = +1$ and $\mathbf{w}^T\mathbf{x}_{-}+b = -1$
In that way, the margin could be given as follow

$$\frac{\mathbf{w}^T(\mathbf{x}_{+} - \mathbf{x}_{-})}{||\mathbf{w}||} = \frac{2}{||\mathbf{w}||}$$

Then we needs to maximum the margin.

$$\max_{\mathbf{w}} \frac{2}{||\mathbf{w}||} \rightarrow \min_{\mathbf{w}} ||\mathbf{w}||^2$$
$$\texttt{s.t.} \quad y^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1 \quad \forall i$$

Dual

$$\min \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha^i \alpha^j y^i y^j < \mathbf{x}^i, \mathbf{x}^j >$$
$$\texttt{s.t.} \quad y^i \left(\sum_{j=1}^{N} \alpha^j y^j < \mathbf{x}^i, \mathbf{x}^j > +b \right) \geq 1 \quad \forall i$$