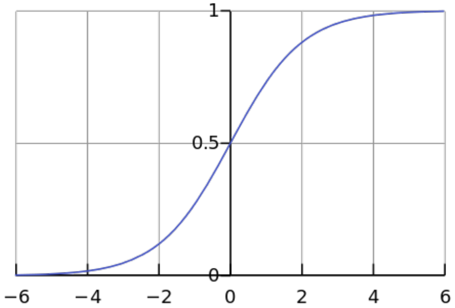
Lecture 17: Logistic Regression contd.

Instructor: Prof. Ganesh Ramakrishnan

Sigmoidal (perceptron) Classifier

1. **(Binary) Logistic Regression**, abbreviated as **LR** is a single node perceptron-like classifier, but with....
   - $sign\left((\mathbf{w}^*)^T\phi(\mathbf{x})\right)$ replaced by $g\left((\mathbf{w}^*)^T\phi(\mathbf{x})\right)$ where $g(s)$ is sigmoid function: $g(s) = \frac{1}{1+e^{-s}}$
2. $f_{\mathbf{w}}(\mathbf{x}) = g\left((\mathbf{w}^*)^T\phi(\mathbf{x})\right) = \frac{1}{1+e^{-(\mathbf{w}^*)^T\phi(\mathbf{x})}} \in [0,1]$ can be interpreted as $Pr(y=1|\mathbf{x})$
   - Then $Pr(y=0|x) = 1 - f_{\mathbf{w}}(\mathbf{x})$



Logistic Regression: The Sigmoidal (perceptron) Classifier

1. Estimator $\widehat{\mathbf{w}}$ is a function of the dataset $\mathcal{D} = \left\{(\phi(\mathbf{x}^{(1)}, y^{(1)}), (\phi(\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\phi(\mathbf{x}^{(m)}, y^{(m)}))\right\}$
   - Estimator $\widehat{\mathbf{w}}$ is meant to approximate the parameter $\mathbf{w}$.
2. Maximum Likelihood Estimator: Estimator $\widehat{\mathbf{w}}$ that maximizes the likelihood $L(\mathcal{D}; \mathbf{w})$ of the data $\mathcal{D}$.
   - Assumes that all the instances $(\phi(\mathbf{x}^{(1)}, y^{(1)}), (\phi(\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\phi(\mathbf{x}^{(m)}, y^{(m)}))$ in $\mathcal{D}$ are all independent and identically distributed (iid)
   - Thus, Likelihood is the probability of $\mathcal{D}$ under iid assumption: $\hat{\mathbf{w}} = \max_{\mathbf{w}} L(\mathcal{D}, \mathbf{w}) =$

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   - Thus, Likelihood is the probability of $\mathcal{D}$ under iid assumption: $\hat{\mathbf{w}} = \max_{\mathbf{w}} L(\mathcal{D}, \mathbf{w}) =$ $\text{argmax}_{\mathbf{w}} \prod_{i=1}^{m} p(y^{(i)}|\phi(\mathbf{x}^{(i)})) = \text{argmax}_{\mathbf{w}} \prod_{i=1}^{m} \left(\frac{1}{1+e^{-(\mathbf{w})^T\phi(\mathbf{x}^{(i)})}}\right)^{y^{(i)}} \left(\frac{e^{-(\mathbf{w})^T\phi(\mathbf{x}^{(i)})}}{1+e^{-(\mathbf{w})^T\phi(\mathbf{x}^{(i)})}}\right)^{1-y^{(i)}}$

Training LR

1. Thus, Maximum Likelihood Estimator for $\mathbf{w}$ is

$$\hat{\mathbf{w}} = \operatorname*{argmax}_{\mathbf{w}} \; L(\mathcal{D}, w) = \operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{m} p(y^{(i)}|\phi(\mathbf{x}^{(i)}))$$

$$= \operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{m} \left(\frac{1}{1 + e^{-\mathbf{w}^T\phi(\mathbf{x}^{(i)})}} \right)^{y^{(i)}} \left(\frac{e^{-\mathbf{w}^T\phi(\mathbf{x}^{(i)})}}{1 + e^{-\mathbf{w}^T\phi(\mathbf{x}^{(i)})}} \right)^{1-y^{(i)}}$$

$$= \operatorname*{argmax}_{\mathbf{w}} \; \prod_{i=1}^{m} \left(f_{\mathbf{w}} \left(\mathbf{x}^{(i)} \right) \right)^{y^{(i)}} \left(1 - f_{\mathbf{w}} \left(\mathbf{x}^{(i)} \right) \right)^{1-y^{(i)}}$$

2. Maximizing the likelihood $\Pr(\mathcal{D}; \mathbf{w})$ w.r.t $\mathbf{w}$, is the same as minimizing the negative log-likelihood $E(\mathbf{w}) = -\frac{1}{m} \log \Pr(\mathcal{D}; \mathbf{w})$ w.r.t $\mathbf{w}$.
   - Derive the expression for $E(\mathbf{w})$.
   - $E(\mathbf{w})$ is called the cross-entropy loss function

Minimizing negative Log-likelihood for LR

1. The Cross-entropy Loss function:

[1] https://en.wikipedia.org/wiki/Cross_entropy

Minimizing negative Log-likelihood for LR

1. The Cross-entropy Loss function:

$$E(\mathbf{w}) = -\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)}\log f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) + \left(1-y^{(i)}\right)\log\left(1-f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)\right)\right] \quad (1)$$

or with some simplification,

$$E(\mathbf{w}) = -\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)}\mathbf{w}^{T}\phi(\mathbf{x}^{(i)}) - \log\left(1+exp\left(\mathbf{w}^{T}\mathbf{x}^{(i)}\right)\right)\right)\right] \quad (2)$$

2. Cross-entropy[1] is the average number of bits needed to identify an event (example $\mathbf{x}$) drawn from the (data) set $\mathcal{D}$, if a coding scheme is used that is optimized for a modeled probability distribution $\Pr\left(y|\mathbf{w},\phi(.)\right)$, rather than the 'true' distribution $\Pr(y|\mathcal{D})$.

$$E(\mathbf{w}) = \mathbf{E}_{\Pr(y|\mathcal{D})}\left[-\log\Pr\left(y|\mathbf{w},\phi(.)\right)\right] \quad (3)$$

[1] https://en.wikipedia.org/wiki/Cross_entropy

Gradient descent for LR

1. No closed form solution to the cross-entropy loss

$$\widehat{\mathbf{w}}^{MLE} = \underset{\mathbf{w}}{\operatorname{argmin}} - \left[\frac{1}{m} \sum_{i=1}^{m} \left(y^{(i)} \log f_{\mathbf{w}} \left(\mathbf{x}^{(i)} \right) + \left(1 - y^{(i)} \right) \log \left(1 - f_{\mathbf{w}} \left(\mathbf{x}^{(i)} \right) \right) \right) \right] \tag{4}$$

2. Apply gradient descent with $\mathbf{w}^{(k+1)} = \mathbf{w}^k - \eta \nabla E \left(\mathbf{w}^k \right)$

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3. The descent update

$$-\eta \nabla E(\mathbf{w}) = -\eta \left[\frac{1}{m} \sum_{i=1}^{m} \left(y^{(i)} \nabla \log f_{\mathbf{w}} \left(\mathbf{x}^{(i)} \right) + \left(1 - y^{(i)} \right) \nabla \log \left(1 - f_{\mathbf{w}} \left(\mathbf{x}^{(i)} \right) \right) \right) \right] \quad (5)$$

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4. $\nabla f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) = \phi(\mathbf{x}^{(i)}) \left(\frac{e^{-(\mathbf{w})^{T}\phi(\mathbf{x}^{(i)})}}{1+e^{-(\mathbf{w})^{T}\phi(\mathbf{x}^{(i)})}} \right)$
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   $\Rightarrow$
5. $\nabla \log f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) = \phi(\mathbf{x}^{(i)}) e^{-(\mathbf{w})^T \phi(\mathbf{x}^{(i)})} \left(\frac{1}{1+e^{-(\mathbf{w})^T \phi(\mathbf{x}^{(i)})}} \right)^2$ and

   $\nabla \log\left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right) = -\phi(\mathbf{x}^{(i)}) \left(\frac{1}{1+e^{-(\mathbf{w})^T \phi(\mathbf{x}^{(i)})}} \right)^2$

Descent update for LR

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2. $\Rightarrow$ The final descent update is

Descent update for LR

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1. $\nabla \log f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) = \phi(\mathbf{x}^{(i)}) e^{-(\mathbf{w})^T \phi(\mathbf{x}^{(i)})} \left(\frac{1}{1+e^{-(\mathbf{w})^T \phi(\mathbf{x}^{(i)})}}\right)^2$ and
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2. $\Rightarrow$ The final descent update is

$$-\eta \nabla E(\mathbf{w}) = \eta \left[\frac{1}{m} \sum_{i=1}^{m} \left(y^{(i)} - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right) \phi(\mathbf{x}^{(i)}) \right] \quad (7)$$

Gradient descent for LR

1. The final descent update

$$-\eta\nabla E(\mathbf{w}) = \eta\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)\phi(\mathbf{x}^{(i)})\right] \tag{8}$$

2. The iterative update rule:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{k} + \eta\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - f_{\mathbf{w}^k}\left(\mathbf{x}^{(i)}\right)\right)\phi(\mathbf{x}^{(i)})\right] \tag{9}$$

3. Stochastic version of the same:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{k} + \eta\left(y^{(i)} - f_{\mathbf{w}^k}\left(\mathbf{x}^{(i)}\right)\right)\phi(\mathbf{x}^{(i)}) \tag{10}$$

4. How would you contrast the updates with sigmoid (LR) against those with the step function (perceptron)?

Sigmoid (LR) vs. step function (perceptron)

1. Stochastic update for step fn (perceptron) with $y^{(i)} \in \{-1, 1\}$: Pick any example $\left(\mathbf{x}^{(i)}, y^{(i)}\right)$, for which $sign\left(\left(\mathbf{w}^{(k)}\right)^{T} \phi\left(\mathbf{x}^{(i)}\right)\right) \neq y^{(i)}$.
$$\mathbf{w}^{(k+1)} = \mathbf{w}^{k} + \eta y^{(i)} \phi(\mathbf{x}^{(i)}) \tag{11}$$

2. Stochastic update for sigmoid fn (LR) with $y^{(i)} \in \{0, 1\}$:
Pick any example $\left(\mathbf{x}^{(i)}, y^{(i)}\right)$, for which $|f_{\mathbf{w}^k}\left(\mathbf{x}^{(i)}\right) - y^{(i)}| > 0.5$.
$$\mathbf{w}^{(k+1)} = \mathbf{w}^{k} + \eta\left(y^{(i)} - f_{\mathbf{w}^k}\left(\mathbf{x}^{(i)}\right)\right) \phi(\mathbf{x}^{(i)}) \tag{12}$$

3. Recall: (12) is also the stochastic update for linear regression! (12) is a characteristic update for **generalized linear models**[2] of which perceptron, linear regression and logistic are special cases.

[2] https://en.wikipedia.org/wiki/Generalized_linear_model

Regularized LR and its Probabilistic Interpretation

1. The Regularized (Logistic) Cross-Entropy Loss function:

$$E(\mathbf{w}) = -\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)}\log f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) + \left(1 - y^{(i)}\right)\log\left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)\right)\right] + \frac{\lambda}{2m}\|\mathbf{w}\|_2^2 \quad (13)$$

2. Motivations: Avoiding overfitting by discouraging large values of w_j for every j.
3. Probabilistic Explanation?

Regularized LR and its Probabilistic Interpretation

1. The Regularized (Logistic) Cross-Entropy Loss function:

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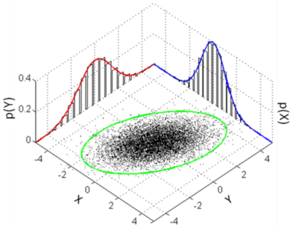
2. Motivations: Avoiding overfitting by discouraging large values of w_j for every j.
3. Probabilistic Explanation? A Bayesian Posterior probabilistic explanation to regularized LR (next)
4. We will reinvoke Bayesian (Parameter) Estimation

Bayesian Inference For Logistic Regression

MAP Estimation and regularized LR

1. Recall the multivariate Gaussian (Normal) Distribution:
   $\mathcal{N}(\mathbf{w};\mu,\Sigma) = \frac{1}{(2\pi)^{\frac{m}{2}}|\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(\mathbf{w}-\mu)^T\Sigma^{-1}(\mathbf{w}-\mu)}$ when $\Sigma \in \Re^{m\times m}$ is positive-definite and
   

   $\mu \in \Re^m$
2. Suppose we want each $|w_i|$ to be bounded roughly by $\pm\frac{3}{\lambda}$
3. Then by the $3-\sigma$ rule we let $\mathbf{w} \sim \mathcal{N}(\mathbf{w}; 0, \frac{1}{\lambda}I)$ where I is an $m \times m$ identity matrix
4. $\Rightarrow \Pr(\mathbf{w}) = \frac{1}{\left(\frac{2\pi}{\lambda}\right)^{\frac{m}{2}}} e^{-\frac{\lambda}{2}\|\mathbf{w}\|_2^2}$

MAP estimation and regularized LR

1. $\Pr(\mathbf{w}) = \frac{1}{(\frac{2\pi}{\lambda})^{\frac{m}{2}}} e^{-\frac{\lambda}{2}\|\mathbf{w}\|_2^2}$
2. Recall the MLE for LR: $\hat{\mathbf{w}} = \operatorname*{argmax}_{\mathbf{w}} L(\mathcal{D}; \mathbf{w})$

$$= \operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{m} \left(f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{y^{(i)}} \left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{1-y^{(i)}}$$

3. Now the MAP for LR: $\tilde{\mathbf{w}} = \operatorname*{argmax}_{\mathbf{w}} \Pr(\mathbf{w}) L(\mathcal{D}; \mathbf{w}) =$

MAP estimation and regularized LR

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   $$= \operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{m} \left(f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{y^{(i)}} \left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{1-y^{(i)}}$$
3. Now the MAP for LR: $\tilde{\mathbf{w}} = \operatorname{argmax}_{\mathbf{w}} \Pr(\mathbf{w}) L(\mathcal{D}; \mathbf{w}) =$
   $$\operatorname*{argmax}_{\mathbf{w}} \frac{1}{\left(\frac{2\pi}{\lambda}\right)^{\frac{m}{2}}} e^{-\frac{\lambda}{2}\|\mathbf{w}\|_2^2} \prod_{i=1}^{m} \left(f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{y^{(i)}} \left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{(1-y^{(i)})}$$

MAP estimation and regularized LR

1. **FROM** MAP for LR: $\tilde{\mathbf{w}} = \underset{\mathbf{w}}{\mathrm{argmax}}\, \Pr(\mathbf{w}) L(\mathcal{D}, \mathbf{w})$

$$= \underset{\mathbf{w}}{\mathrm{argmax}} \frac{1}{\left(\frac{2\pi}{\lambda}\right)^{\frac{m}{2}}} e^{-\frac{\lambda}{2}\|\mathbf{w}\|_2^2} \prod_{i=1}^{m} \left(f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{y^{(i)}} \left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)^{1-y^{(i)}}$$

.....Taking $-\frac{1}{m}\log(.)$ transformation,

2. **TO** Min of the Regularized Logistic (Cross-Entropy) Loss function:

$$\tilde{\mathbf{w}} = \underset{\mathbf{w}}{\mathrm{argmin}} - \left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)}\log f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) + \left(1 - y^{(i)}\right)\log\left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)\right)\right] + \frac{\lambda}{2}\|\mathbf{w}\|_2^2 \qquad (14)$$

where we have ignored $-\frac{1}{m}\log\left(\left(\frac{2\pi}{\lambda}\right)^{\frac{m}{2}}\right)$ since this term is independent of $\mathbf{w}$.

.....Thus, MAP $\tilde{\mathbf{w}}$ can be found by minimizing the *Regularized Cross Entropy Error*

Gradient descent for Regularized LR

Gradient descent for Regularized LR

1. The final descent update

$$-\eta\nabla E(\mathbf{w}) = \eta\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)\phi(\mathbf{x}^{(i)}) - \lambda\mathbf{w}\right] \tag{15}$$

2. The iterative update rule:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{k} + \eta\left[\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - f_{\mathbf{w}^k}\left(\mathbf{x}^{(i)}\right)\right)\phi(\mathbf{x}^{(i)}) - \lambda\mathbf{w}^{k}\right] \tag{16}$$

3. Stochastic version of the same:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{k} + \eta\left(y^{(i)} - f_{\mathbf{w}^k}\left(\mathbf{x}^{(i)}\right)\right)\phi(\mathbf{x}^{(i)}) - \eta\lambda\mathbf{w}^{k} \tag{17}$$

Extension to multi-class logistic

1. Each class $c = 1, 2, \ldots, K-1$ can have a different weight vector $[\mathbf{w}_{c,1}, \mathbf{w}_{c,2}, \ldots, \mathbf{w}_{c,k}, \ldots, \mathbf{w}_{c,K-1}]$ and

$$p(Y = c|\phi(\mathbf{x})) = \frac{e^{-(\mathbf{w}_c)^T\phi(\mathbf{x})}}{1 + \sum_{k=1}^{K-1} e^{-(\mathbf{w}_k)^T\phi(\mathbf{x})}}$$

for $c = 1, \ldots, K-1$ so that

$$p(Y = K|\phi(\mathbf{x})) = \frac{1}{1 + \sum_{k=1}^{K-1} e^{-(\mathbf{w}_k)^T\phi(\mathbf{x})}}$$

Alternative (equivalent) extension to multi-class logistic

1. Each class $c = 1, 2, \ldots, K$ can have a different weight vector $[\mathbf{w}_{c,1}, \mathbf{w}_{c,2} \ldots \mathbf{w}_{c,p}]$ and

$$p(Y = c|\phi(\mathbf{x})) = \frac{e^{-(\mathbf{w}_c)^T\phi(\mathbf{x})}}{\sum_{k=1}^{K} e^{-(\mathbf{w}_k)^T\phi(\mathbf{x})}}$$

for $c = 1, \ldots, K$.