Logistic Regression

Logistic Regression: The Model

- A model for doing *probabilistic* binary classification
- Predicts *label probabilities* rather than a hard value of the label

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\begin{aligned}
p(y_n = 1|\boldsymbol{x}_n, \boldsymbol{w}) &= \mu_n \\
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- The model's prediction is a probability defined using the sigmoid function

$$f(\boldsymbol{x}_n) = \mu_n = \sigma(\mathbf{w}^\top \mathbf{x}_n) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x}_n)} = \frac{\exp(\mathbf{w}^\top \mathbf{x}_n)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_n)}$$

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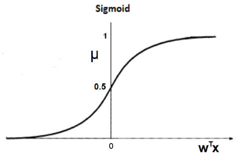
- The sigmoid first computes a real-valued "score" $\boldsymbol{w}^\top \boldsymbol{x} = \sum_{d=1}^{D} w_d x_d$ and "squashes" it between (0,1) to turn this score into a probability score



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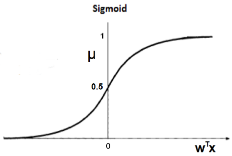

- Model parameter is the unknown $\boldsymbol{w}$. Need to learn it from training data.

Logistic Regression: An Interpretion

- Recall that the logistic regression model defines

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p(y=1|\boldsymbol{x},\boldsymbol{w}) &= \mu = \sigma(\boldsymbol{w}^\top \boldsymbol{x}) = \frac{1}{1+\exp(-\boldsymbol{w}^\top \boldsymbol{x})} = \frac{\exp(\boldsymbol{w}^\top \boldsymbol{x})}{1+\exp(\boldsymbol{w}^\top \boldsymbol{x})} \\
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- The log-odds of this model

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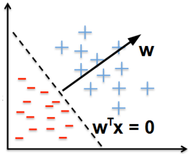
- Thus if $\boldsymbol{w}^\top\boldsymbol{x} > 0$ then the positive class is more probable
- A linear classification model. Separates the two classes via a hyperplane (similar to other linear classification models such as Perceptron and SVM)



Loss Function Optimization View for Logistic Regression

Logistic Regression: The Loss Function

- What loss function to use? One option is to use the squared loss

$$\ell(y_n, f(\boldsymbol{x}_n)) = (y_n - f(\boldsymbol{x}_n))^2 = (y_n - \mu_n)^2 = (y_n - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n))^2$$

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- This is a function of the unknown parameter $\boldsymbol{w}$ since $\mu_n = \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)$

Logistic Regression: The Loss Function

- The loss function over the entire training data

$$L(\boldsymbol{w}) = \sum_{n=1}^{N} \ell(y_n, f(\boldsymbol{x}_n)) = \sum_{n=1}^{N} [-y_n \log(\mu_n) - (1 - y_n) \log(1 - \mu_n)]$$

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- We can add a regularizer (e.g., squared ℓ_2 norm of $\boldsymbol{w}$) to prevent overfitting

$$\boxed{L(\boldsymbol{w}) = -\sum_{n=1}^{N} (y_n \boldsymbol{w}^\top \boldsymbol{x}_n - \log(1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n))) + \lambda||\boldsymbol{w}||^2}$$

Probabilstic Modeling View (MLE/MAP) for Logistic Regression

Logistic Regression: MLE Formulation

- Recall, each label y_n is binary with prob. μ_n. Assume Bernoulli likelihood:

$$p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \prod_{n=1}^{N} \mu_n^{y_n}(1-\mu_n)^{1-y_n}$$

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- Doing MLE would require maximizing the log likelihood w.r.t. $\boldsymbol{w}$

$$\log p(\mathbf{Y}|\mathbf{X}, \boldsymbol{w}) = \sum_{n=1}^{N} (y_n \log \mu_n + (1-y_n)\log(1-\mu_n))$$

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$$\log p(\mathbf{Y}|\mathbf{X}, \boldsymbol{w}) = \sum_{n=1}^{N}(y_n \log \mu_n + (1-y_n)\log(1-\mu_n))$$

- This is equivalent to minimizing the NLL. Plugging in $\mu_n = \frac{\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}{1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}$ we get

$$\boxed{\text{NLL}(\boldsymbol{w}) = -\sum_{n=1}^{N}(y_n \boldsymbol{w}^\top \boldsymbol{x}_n - \log(1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)))}$$

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- Not surprisingly, the NLL expression is the same as the loss function

Logisic Regression: MAP Formulation

- MLE estimate of $\boldsymbol{w}$ can lead to overfitting. Solution: use a prior on $\boldsymbol{w}$
- Just like the linear regression case, let's put a Gausian prior on $\boldsymbol{w}$

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- Ignoring the constants, we get the following objective for MAP estimation

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- Thus MAP estimation is equivalent to regularized logistic regression

Estimating the Weight Vector $\boldsymbol{w}$

- Loss function/NLL for logistic regression (ignoring the regularizer term)

$$L(\boldsymbol{w}) = -\sum_{n=1}^{N}(y_n \boldsymbol{w}^\top \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^\top \boldsymbol{x}_n)))$$

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- The gradient/derivative of $L(\boldsymbol{w})$ w.r.t. $\boldsymbol{w}$ (let's ignore the regularizer)

$$\mathbf{g} = \frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} \quad = \quad \frac{\partial}{\partial \boldsymbol{w}}[-\sum_{n=1}^{N}(y_n \boldsymbol{w}^\top \boldsymbol{x}_n - \log(1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)))]$$

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&= -\sum_{n=1}^{N}(y_n - \mu_n)\boldsymbol{x}_n = \mathbf{X}^\top(\boldsymbol{\mu} - \boldsymbol{y})
\end{aligned}$$

- Can't get a closed form solution for $\boldsymbol{w}$ by setting the derivative to zero
  - Need to use iterative methods (e.g., gradient descent) to solve for $\boldsymbol{w}$

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- Note that the updates give larger weights to those examples on which the current model makes larger mistakes, as measured by $(\mu_n^{(t)} - y_n)$
- **Note:** Computing the gradient in every iteration requires all the data. Thus GD can be expensive if N is very large. A cheaper alternative is to do GD using only a small randomly chosen minibatch of data. It is known as **Stochastic Gradient Descent** (SGD). Runs faster and converges faster.

More on Gradient Descent..

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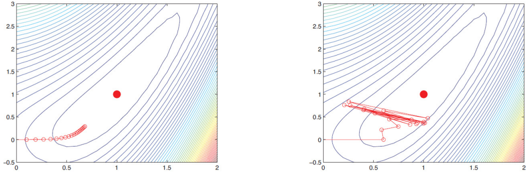

Figure: Left: small step sizes. Right: large step sizes

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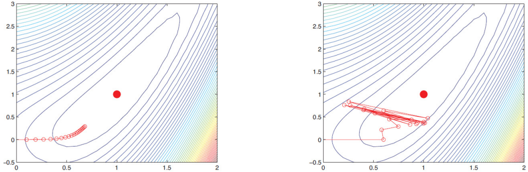

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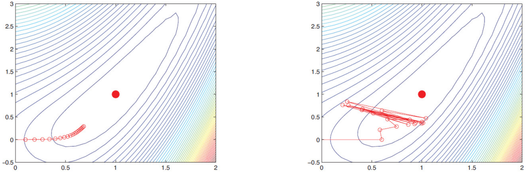

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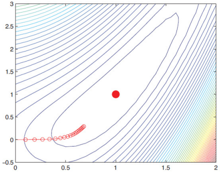

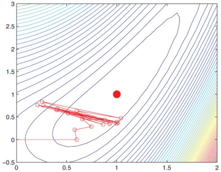

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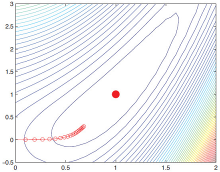

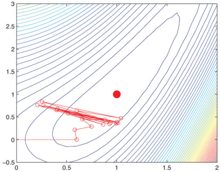

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  - Add a momentum term to the updates

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta_t \mathbf{g}^{(t)} + \alpha_t(\boldsymbol{w}^{(t)} - \boldsymbol{w}^{(t-1)})$$

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Multiclass Logistic (or "Softmax") Regression

- Logistic regression can be extended to handle $K > 2$ classes
- In this case, $y_n \in \{0, 1, 2, \ldots, K-1\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \mathbf{W}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^{K} \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk}$$

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- Can do MLE/MAP for $\mathbf{W}$ similar to the binary logistic regression case

Logistic Regression: Summary

- A probabilistic model for binary classification
- Simple objective, easy to optimize using gradient based methods
- Very widely used, very efficient solvers exist
- Can be extended for multiclass (softmax) classification
- Used as modules in more complex models (e.g, deep neural nets)