Learning via Probabilistic Modeling, Logistic and Softmax Regression

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Machine Learning (CS771A)

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Recap

Linear Regression: The Optimization View

- Define a loss function $\ell(y_n, f(\boldsymbol{x}_n)) = (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$ and solve the following loss minimization problem

$$\hat{\boldsymbol{w}} = \arg\min_{\mathbf{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

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- To avoid overfitting on training data, add a regularization $R(\boldsymbol{w}) = ||\boldsymbol{w}||^2$ on the weight vector and solve the regularized loss minimization problem

$$\hat{\boldsymbol{w}} = \arg\min_{\mathbf{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \lambda ||\boldsymbol{w}||^2$$

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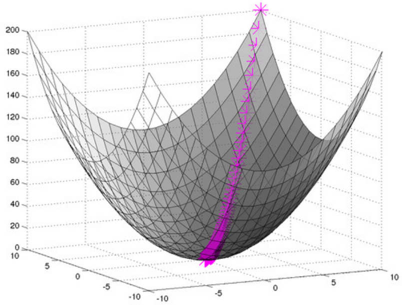
- Simple, convex loss functions in both cases. Closed-form solution for $\boldsymbol{w}$ can be found. Can also solve for $\boldsymbol{w}$ more efficiently using gradient based methods.

Linear Regression: Optimization View

A simple, quadratic in parameters, convex function



Pic source: Quora

Linear Regression: The Probabilistic View

- Under this viewpoint, we assume that the y_n's are drawn from a Gaussian $y_n \sim \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \sigma^2)$, which gives us a likelihood function

$$p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2}{2\sigma^2}\right\}$$

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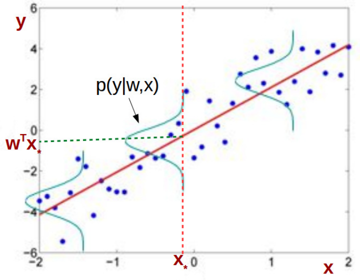

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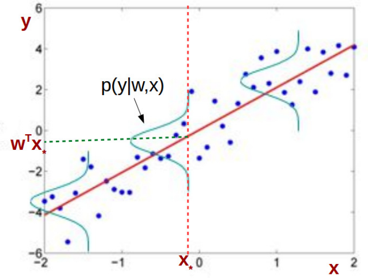

- The total likelihood (assuming i.i.d. responses) or *probability* of data:

$$p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{N}{2}} \exp\left\{-\sum_{n=1}^{N} \frac{(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2}{2\sigma^2}\right\}$$

Linear Regression: Probabilistic View

- Can solve for $\boldsymbol{w}$ using MLE, i.e., by maximizing the log likelihood. This is equivalent to minimizing the negative log likelihood (NLL) w.r.t. $\boldsymbol{w}$

$$NLL(\boldsymbol{w}) = -\log p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}) \propto \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

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- Can also combine the likelihood with a prior over $\boldsymbol{w}$, e.g., a multivariate Gaussian prior with zero mean: $p(\boldsymbol{w}) = \mathcal{N}(0, \rho^2\mathbf{I}_D) \propto \exp(-\boldsymbol{w}^\top\boldsymbol{w}/2\rho^2)$

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- The prior allows encoding our prior beliefs on $\boldsymbol{w}$, acts as a regularizer and, in this case, encourages the final solution to shrink towards the prior's mean
- Can now solve for $\boldsymbol{w}$ using MAP estimation, i.e., maximizing the log posterior or minimizing the negative of the log posterior w.r.t. $\boldsymbol{w}$

$$NLL(\boldsymbol{w}) - \log p(\boldsymbol{w}) \propto \sum_{n=1}^{N}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \frac{\sigma^2}{\rho^2}\boldsymbol{w}^\top\boldsymbol{w}$$

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- Optimization and probabilistic views led to same objective functions (though the probabilistic view also enables a full Bayesian treatment of the problem)

Today's Plan

- A binary classification model from optimization and probabilistic views
  - By minimizing a loss function and regularized loss function
  - By doing MLE and MAP estimation
- We will look at Logistic Regression as our example
- Note: The "regression" in logistic regression is a misnomer
- Will also look at its multiclass extension ("Softmax" Regression)

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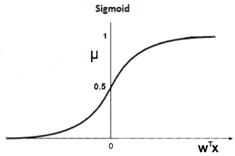
- The sigmoid first computes a real-valued "score" $\boldsymbol{w}^\top \boldsymbol{x} = \sum_{d=1}^{D} w_d x_d$ and "squashes" it between (0,1) to turn this score into a probability score



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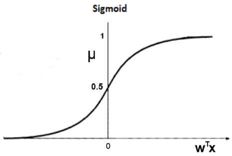

- Model parameter is the unknown $\boldsymbol{w}$. Need to learn it from training data.

Logistic Regression: An Interpretion

- Recall that the logistic regression model defines

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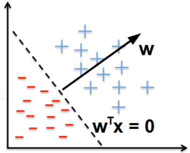
- Thus if $\boldsymbol{w}^\top\boldsymbol{x} > 0$ then the positive class is more probable
- A linear classification model. Separates the two classes via a hyperplane (similar to other linear classification models such as Perceptron and SVM)



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

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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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where $\mu_n = \frac{\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}{1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}$

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

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

Logistic Regression: MLE Formulation

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

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

where $\mu_n = \frac{\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}{1+\exp(\boldsymbol{w}^\top \boldsymbol{x}_n)}$

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

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

- 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 $\boldsymbol{w}$

$$p(\boldsymbol{w}) = \mathcal{N}(0, \lambda^{-1}\mathbf{I}_D) \propto \exp(-\lambda \boldsymbol{w}^\top \boldsymbol{w})$$

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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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- 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 $\boldsymbol{w}$

Gradient Descent for Logistic Regression

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$$\underbrace{\boldsymbol{w}^{(t+1)}}_{\text{new value}} = \underbrace{\boldsymbol{w}^{(t)}}_{\text{previous value}} - \eta \underbrace{\sum_{n=1}^{N}(\mu_n^{(t)} - y_n)\boldsymbol{x}_n}_{\text{gradient at previous value}}$$

where η is the learning rate and $\mu^{(t)} = \sigma(\boldsymbol{w}^{(t)^\top}\boldsymbol{x}_n)$ is the predicted label probability for $\boldsymbol{x}_n$ using $\boldsymbol{w} = \boldsymbol{w}^{(t)}$ from the previous iteration

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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 $(\mu_n^{(t)} - y_n)$

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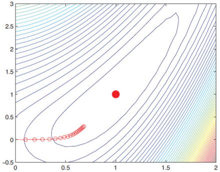
- **Note:** Computing the gradient in every iteration requires all the data. Thus GD can be expensive if N is very large. A cheaper alternative is to do GD using only a small randomly chosen minibatch of data. It is known as **Stochastic Gradient Descent** (SGD). Runs faster and converges faster.

More on Gradient Descent..

- GD can converge slowly and is also sensitive to the step size



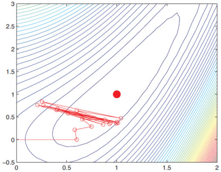


Figure: Left: small step sizes. Right: large step sizes

[1] Also see: "A comparison of numerical optimizers for logistic regression" by Tom Minka

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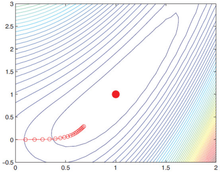

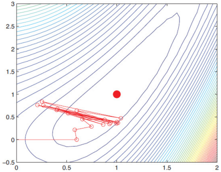

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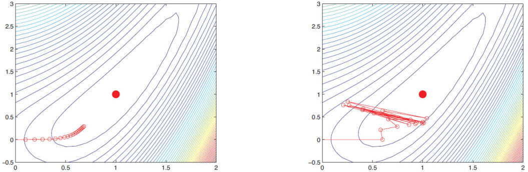

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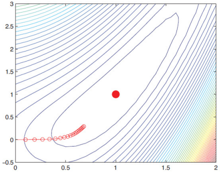

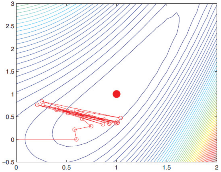

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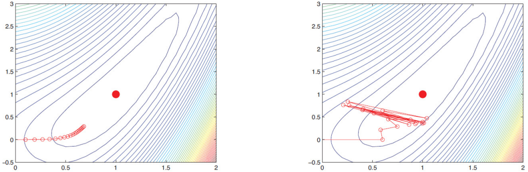

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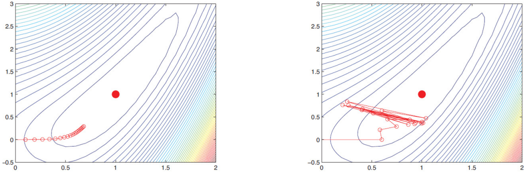

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  - Use second-order methods (e.g., **Newton's method**) to exploit the curvature of the loss function $L(\boldsymbol{w})$: Requires computing the Hessian matrix

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Newton's method for Logistic Regression

- Newton's method (a second order method) updates are as follows:

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  - It basically solves an Iteratively Reweighted Least Squares (IRLS) problem

$$\arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} S_n^{(t)}(\hat{y}_n^{(t)} - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

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  - The weight $S_n^{(t)}$ is the n^{th} diagonal element of $\mathbf{S}^{(t)}$
- Expensive in practice (requires matrix inversion). Can use Quasi-Newton (approximate the Hessian using gradients) or BFGS for better efficiency

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

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

- μ_{nk}: probability that example n belongs to class k. Also, $\sum_{\ell=1}^{K} \mu_{n\ell} = 1$
- $\mathbf{W} = [\boldsymbol{w}_1 \; \boldsymbol{w}_2 \; \ldots \; \boldsymbol{w}_K]$ is $D \times K$ weight matrix (column k for class k)

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- We can think of the y_n's as drawn from a multinomial distribution

$$p(\boldsymbol{y}|\mathbf{X}, \mathbf{W}) = \prod_{n=1}^N \prod_{\ell=1}^K \mu_{n\ell}^{y_{n\ell}} \qquad \text{(Likelihood function)}$$

where $y_{n\ell} = 1$ if true class of example n is ℓ and $y_{n\ell'} = 0$ for all other $\ell' \neq \ell$

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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)