> Fabio A. González Ph.D.

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Linear Classification Models

Fabio A. González Ph.D.

Depto. de Ing. de Sistemas e Industrial Universidad Nacional de Colombia, Bogotá

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Classification problems

• $predict(x) = \begin{cases} C_1, & y(x) \ge \text{threshold} \\ C_2, & y(x) < \text{threshold} \end{cases}$, with threshold = 0 or threshold = 0.5.

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Classification problems

- $predict(x) = \begin{cases} C_1, & y(x) \ge \text{threshold} \\ C_2, & y(x) < \text{threshold} \end{cases}$ with threshold = 0 or threshold = 0.5.
- Three ways to address the classification problem:

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Classification problems

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- Three ways to address the classification problem:
 - **1** Directly model the discrimination function: e.g $y(x) = w^T x + w_0$

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Classification problems

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- Three ways to address the classification problem:
 - ① Directly model the discrimination function: e.g $y(x) = w^T x + w_0$
 - 2 Generative model:

$$y(x) = P(C_k|x) = \frac{P(x|C_k)P(C_k)}{P(x)}$$

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Classification problems

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- Three ways to address the classification problem:
 - ① Directly model the discrimination function: e.g $y(x) = w^T x + w_0$
 - ② Generative model:

$$y(x) = P(C_k|x) = \frac{P(x|C_k)P(C_k)}{P(x)}$$

3 Discriminative model:

$$y(x) = P(C_k|x) = f(x),$$

with f an arbitrary function.

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Linear Models

$$y(x) = f(w^T x + w_0)$$

• $f(\cdot)$: activation function, may be non-linear

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Linear Models

$$y(x) = f(w^T x + w_0)$$

- $f(\cdot)$: activation function, may be non-linear
- Even if $f(\cdot)$ is non-linear, the decision boundary is linear

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$$y(x) = f(w^T x + w_0)$$

- $f(\cdot)$: activation function, may be non-linear
- Even if $f(\cdot)$ is non-linear, the decision boundary is linear
- Also called generalized linear models

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Linear Models

$$y(x) = f(w^T x + w_0)$$

- $f(\cdot)$: activation function, may be non-linear
- Even if $f(\cdot)$ is non-linear, the decision boundary is linear
- Also called generalized linear models
- Applicable if instead of x we use a vector of basis functions $\phi(x)$, corresponding to features in a feature space

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Using regression for classification

 We can use a regression model, such as least squares to fit a linear classification model with a linear activation function

$$\min_{w, w_o} \sum_{i=1}^{\ell} (t_i - w^T x_i + w_0)^2,$$

where $t_i \in \{-1,1\}$ is the label of the *i*-th training sample,

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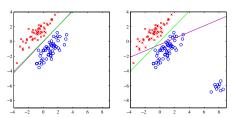
Using regression for classification

 We can use a regression model, such as least squares to fit a linear classification model with a linear activation function

$$\min_{w,w_o} \sum_{i=1}^{\ell} (t_i - w^T x_i + w_0)^2,$$

where $t_i \in \{-1, 1\}$ is the label of the *i*-th training sample,

but this strategy does not work well:



Logistic regression optimization

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Rosemblatt's perceptron



• Designed by Frank Rossemblat in 1957

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Rosemblatt's perceptron



- Designed by Frank Rossemblat in 1957
- A hardware implementation of the learning algorithm

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Rosemblatt's perceptron



- Designed by Frank Rossemblat in 1957
- A hardware implementation of the learning algorithm
- The precursor of neural networks

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Rosemblatt's perceptron



- Designed by Frank Rossemblat in 1957
- A hardware implementation of the learning algorithm
- The precursor of neural networks
- Criticized by Marvin Minsky, producing a decline in research funding

Logistic regression optimization

Perceptron learning

Activation function:

$$f(a) = \begin{cases} +1, & a \ge 0 \\ -1, & a < 0 \end{cases}$$

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Perceptron learning

Activation function:

$$f(a) = \begin{cases} +1, & a \ge 0 \\ -1, & a < 0 \end{cases}$$

• Loss function:

$$E_p(w) = -\sum_{n=1}^{\ell} w^T \phi_n t_n,$$

where $\phi_n = \phi(x_n)$.

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Perceptron learning

Activation function:

$$f(a) = \begin{cases} +1, & a \ge 0 \\ -1, & a < 0 \end{cases}$$

• Loss function:

$$E_p(w) = -\sum_{n=1}^{\ell} w^T \phi_n t_n,$$

where $\phi_n = \phi(x_n)$.

• Learning rule:

$$w^{(\tau+1)} = w^{(\tau)} + \eta \phi_n t_n$$

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Perceptron convergence

• If the training points are linearly separable, the perceptron algorithms converges (perceptron convergence theorem)

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Perceptron convergence

- If the training points are linearly separable, the perceptron algorithms converges (perceptron convergence theorem)
- It could converge to different solutions depending on the order of presentation of training sample

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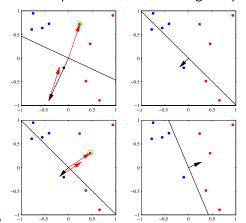
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Perceptron problems

• Non-probabilistic outputs

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Perceptron problems

- Non-probabilistic outputs
- Non-convex optimization problem

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Perceptron problems

- Non-probabilistic outputs
- Non-convex optimization problem
- No convergence guarantee if samples are not linearly separable

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Perceptron problems

- Non-probabilistic outputs
- Non-convex optimization problem
- No convergence guarantee if samples are not linearly separable
- Its power may be increased by stacking several perceptron layers (multilayer perceptrons) and using smooth activation functions

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Parametric discrimination

- These three conditions are equivalent:
 - $P(C_1|x) \ge 0.5$
 - $\bullet \ \frac{P(C_1|x)}{1 P(C_1|x)} \ge 1$
 - $logit(P(C_1|x)) = log \frac{P(C_1|x)}{1 P(C_1|x)} \ge 0$

Logistic regression optimization

Parametric discrimination

- These three conditions are equivalent:
 - $P(C_1|x) \ge 0.5$
 - $\frac{P(C_1|x)}{1-P(C_1|x)} \ge 1$
 - $\operatorname{logit}(P(C_1|x)) = \log \frac{P(C_1|x)}{1 P(C_1|x)} \ge 0$
- If we assume that $P(x|C_1)$ and $P(x|C_2)$ are normally distributed sharing the same covariance matrix:

$$logit(P(C_1|x)) = log \frac{P(C_1|x)}{P(C_2|x)} = w^T x + w_0,$$

where

$$w = \Sigma^{-1}(\mu_1 + \mu_2)$$

$$w_0 = -\frac{1}{2}(\mu_1 + \mu_2)^T \Sigma^{-1}(\mu_1 + \mu_2) + \log \frac{P(C_1)}{P(C_2)}$$

Logistic regression optimizatio

Logistic function

• The logit function:

$$logit(P(C_1|x)) = log \frac{P(C_1|x)}{1 - P(C_1|x)} = w^T x + w_0$$

Logistic regression optimization

Logistic function

• The logit function:

$$logit(P(C_1|x)) = log \frac{P(C_1|x)}{1 - P(C_1|x)} = w^T x + w_0$$

• The inverse-logit:

$$P(C_1|x) = \sigma(w^T x + w_0) = \frac{1}{1 + e^{-(w^T x + w_0)}}$$

Logistic regression optimization

Logistic function

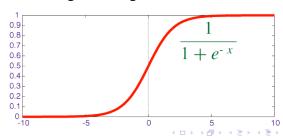
• The logit function:

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• The inverse-logit:

$$P(C_1|x) = \sigma(w^T x + w_0) = \frac{1}{1 + e^{-(w^T x + w_0)}}$$

• σ is called the logistic or sigmoid function.



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Logistic regression

$$y(x) = P(C_1|x) = \sigma(w^T x)$$

$$y(x) = P(C_1|x) = \sigma(w^T x)$$

Find w using maximum likelihood estimation:

$$p(\mathbf{t}|w) = \prod_{n=1}^{\ell} y_n^{t_n} (1 - y_n)^{1 - t_n},$$

where
$$\mathbf{t} = \{t_1, \dots, t_\ell\}$$
 and $y_n = y(x_n)$.

Logistic regression

$$y(x) = P(C_1|x) = \sigma(w^T x)$$

• Find w using maximum likelihood estimation:

$$p(\mathbf{t}|w) = \prod_{n=1}^{\ell} y_n^{t_n} (1 - y_n)^{1 - t_n},$$

where $\mathbf{t} = \{t_1, \dots, t_\ell\}$ and $y_n = y(x_n)$.

• Cross-entropy error:

$$E(w) = -\ln p(\mathbf{t}|w) = -\sum_{n=0}^{\ell} [t_n \ln y_n + (1 - t_n) \ln(1 - y_n)]$$

Multiclass logistic regression

$$y_k(x) = P(C_k|x) = \frac{e^{w_k^T x}}{\sum_j e^{w_j^T x}}$$

Multiclass logistic regression

 $y_k(x) = P(C_k|x) = \frac{e^{w_k^T x}}{\sum_{i} e^{w_j^T x}}$

Likelihood:

$$p(\mathbf{T}|w_1 \dots w_K) = \prod_{n=1}^{\ell} \prod_{k=1}^{K} y_{nk}^{t_{nk}},$$

where $y_{nk} = y_k(x_n)$ and $\mathbf{T} \in \mathbb{R}^{\ell \times K}$ is a matrix of target variables with elements t_{nk} .

Multiclass logistic regression

•

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Likelihood:

$$p(\mathbf{T}|w_1 \dots w_K) = \prod_{n=1}^{\ell} \prod_{k=1}^{K} y_{nk}^{t_{nk}},$$

where $y_{nk} = y_k(x_n)$ and $\mathbf{T} \in \mathbb{R}^{\ell \times K}$ is a matrix of target variables with elements t_{nk} .

• Multiclass cross-entropy error:

$$E(w_1, \dots, w_K) = -\ln p(\mathbf{T}|w_1 \dots w_K) = -\sum_{n=1}^{\ell} \sum_{k=1}^{K} t_{nk} \ln y_{nk}$$

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Logistic regression optimization

Optimization problem

$$\min_{w} E(w) = \min_{w} - \sum_{n=1}^{\ell} \left[t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right]$$

Optimization problem

$$\min_{w} E(w) = \min_{w} - \sum_{n=1}^{\ell} \left[t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right]$$

$$\nabla E(w) = \sum_{n=1}^{\ell} (y_n - t_n) \phi_n$$

Optimization problem

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$$\nabla E(w) = \sum_{n=1}^{\ell} (y_n - t_n) \phi_n$$

$$w^{(\tau+1)} = w^{(\tau)} - \eta \sum_{n=1}^{\ell} (y_n - t_n) \phi_n$$

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Newton-Raphson

$$w^{(\tau+1)} = w^{(\tau)} - H^{-1} \nabla E(w)$$

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Newton-Raphson

$$w^{(\tau+1)} = w^{(\tau)} - H^{-1} \nabla E(w)$$

$$\nabla E(w) = \Phi^T(\mathbf{y} - \mathbf{t})$$

Logistic regression optimization

Newton-Raphson

$$w^{(\tau+1)} = w^{(\tau)} - H^{-1} \nabla E(w)$$

$$\nabla E(w) = \Phi^{T}(\mathbf{y} - \mathbf{t})$$

$$\mathbf{H} = \nabla \nabla E(w) = \Phi^T \mathbf{R} \Phi,$$

with \mathbf{R} a diagonal matrix with $R_{nn} = y_n(1 - y_n)$.

Logistic regression optimization

Newton-Raphson

$$w^{(\tau+1)} = w^{(\tau)} - H^{-1} \nabla E(w)$$

$$\nabla E(w) = \Phi^{T}(\mathbf{y} - \mathbf{t})$$

$$\mathbf{H} = \nabla \nabla E(w) = \Phi^T \mathbf{R} \Phi,$$

with \mathbf{R} a diagonal matrix with $R_{nn} = y_n(1 - y_n)$.

• The resulting algorithm is called *iterative reweighted least* squares.

Regularization

$$\min_{w} -C \sum_{n=1}^{\ell} \left[t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right] + \|w\|^2$$

Regularization

•

$$\min_{w} -C \sum_{n=1}^{\ell} \left[t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right] + \|w\|^2$$

• Prevents overfitting.

Regularization

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$$\min_{w} -C \sum_{n=1}^{\ell} \left[t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right] + \|w\|^2$$

- Prevents overfitting.
- Equivalent to the inclusion of a prior and finding a MAP solution for W.

Stochastic gradient descent

$$\min_{w} Q(w) = \min_{w} \sum_{i=1}^{n} Q_i(w)$$

Stochastic gradient descent

•

$$\min_{w} Q(w) = \min_{w} \sum_{i=1}^{n} Q_i(w)$$

Batch gradient descent:

$$w^{(\tau+1)} = w^{(\tau)} - \alpha \nabla Q(w) = w^{(\tau)} - \alpha \sum_{i=1}^{n} \nabla Q_i(w)$$

Stochastic gradient descent

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$$\min_{w} Q(w) = \min_{w} \sum_{i=1}^{n} Q_i(w)$$

Batch gradient descent:

$$w^{(\tau+1)} = w^{(\tau)} - \alpha \nabla Q(w) = w^{(\tau)} - \alpha \sum_{i=1}^{n} \nabla Q_i(w)$$

• on-line gradient descent:

$$w^{(\tau+1)} = w^{(\tau)} - \alpha \nabla Q_i(w)$$

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Russell, S and Norvig, P. 2010 Artificial Intelligence: a Modern Approach, 3rd Ed, Prentice-Hall (Sect 18.6)