Multi-Class Classification

Shusen Wang

Multi-Class Classification

Tasks

Methods

Algorithms

Multi-Class Classification

Example 1: face recognition.

- #classes = #people

Multi-Class Classification

Example 2: hand-written digit recognition.

- #classes = 10

Softmax Classifier: Preliminaries

One-Hot Encoding

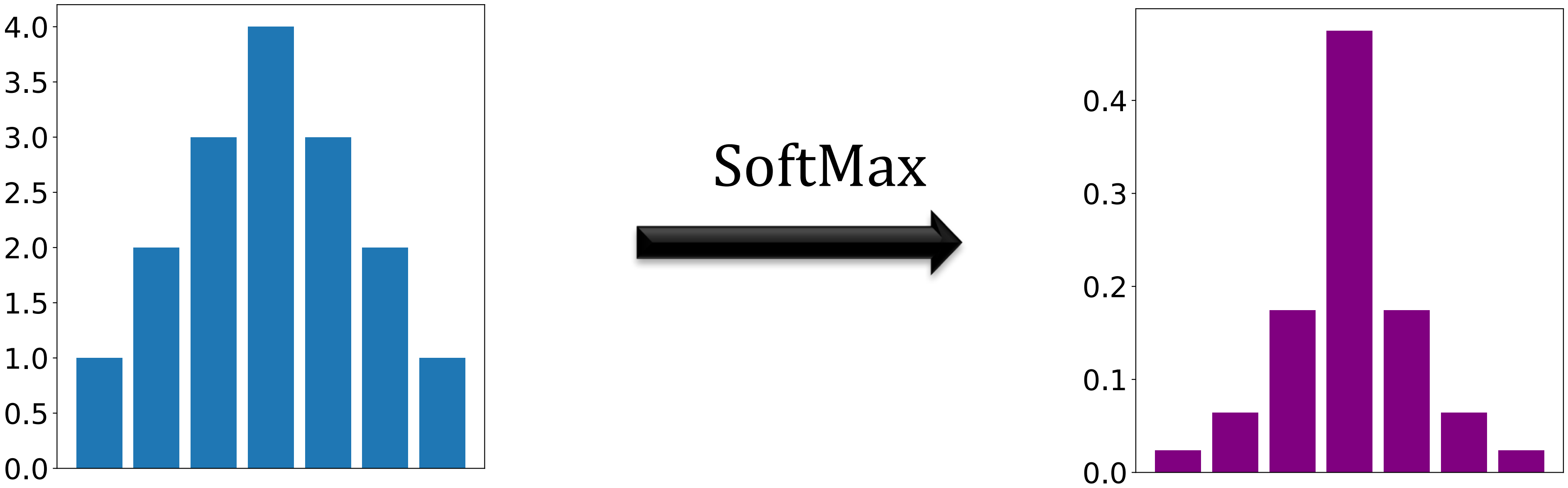
- #Class = 10 (e.g., in digit recognition).
- One-hot encode of $y = 3$:

$$\mathbf{y} \; = \; [0, 0, 0, 1, 0, 0, 0, 0, 0, 0]^T \; \in \; \{1,0\}^{10}$$

Softmax Function

- $\boldsymbol{\phi} \in \mathbb{R}^K$
- $\mathbf{p} = \text{SoftMax}(\boldsymbol{\phi}) \in \mathbb{R}^K$; its entries are

$$p_k = \frac{\exp(\phi_k)}{\sum_{j=1}^{K} \exp(\phi_j)}, \text{ for } k = 1, \cdots, K.$$



Cross-Entropy

- The vectors $\mathbf{y}$ and $\mathbf{p}$ are both K-dim.

$$y_1 + \cdots + y_K = 1 \quad \text{and} \quad p_1 + \cdots + p_K = 1.$$

- Cross-entropy between $\mathbf{y}$ and $\mathbf{p}$:

$$H(\mathbf{y}, \mathbf{p}) = -\sum_{l=1}^{K} y_l \log p_l \ .$$

Cross-Entropy

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$$H(\mathbf{y}, \mathbf{p}) = -\sum_{l=1}^{K} y_l \, \log p_l \, .$$

- Cross-entropy measures the dissimilarity between $\mathbf{y}$ and $\mathbf{p}$.
- When used as loss function, $H(\mathbf{y}, \mathbf{p})$ can be replaced by

$$||\mathbf{y} - \mathbf{p}||_2^2 \quad \text{or} \quad ||\mathbf{y} - \mathbf{p}||_1.$$

Softmax Classifier

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Softmax Classifier

Input: feature vectors $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ and labels $\mathbf{y}_1, \cdots, \mathbf{y}_n \in \mathbb{R}^K$.

n: #samples d: #features K: #classes

Remark: If the given labels are scalars $y_1, \cdots, y_n \in \{0, 1, \cdots, K-1\}$, turn them to K-dim vectors $\mathbf{y}_1, \cdots, \mathbf{y}_n \in \{0,1\}^K$ using one-hot encoding.

Example: One-hot encode of $y_i = 3$ (where K=10):

$$\mathbf{y}_i = [0, 0, 0, 1, 0, 0, 0, 0, 0, 0]^T \in \{1,0\}^{10}$$

Softmax Classifier

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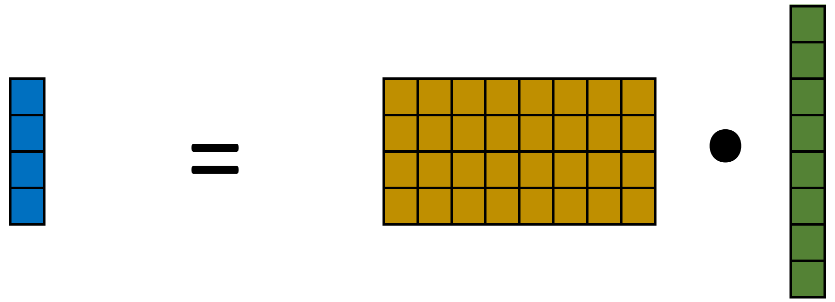
n: #samples d: #features K: #classes

- $\boldsymbol{\phi}_i = \mathbf{W}\mathbf{x}_i \in \mathbb{R}^K$
- $\phi_{i,k}$ (the k-th entry of $\boldsymbol{\phi}_i$) indicates how likely $\mathbf{x}_i$ is in the k-th class.



$\boldsymbol{\phi}$ $\mathbf{W}$ $\mathbf{x}$

$K\times 1$ $K\times d$ $d\times 1$

Softmax Classifier

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- $\phi_{i,k}$ (the k-th entry of $\boldsymbol{\phi}_i$) indicates how likely $\mathbf{x}_i$ is in the k-th class.
- Softmax function: $p_{i,k} = \dfrac{\exp(\phi_{i,k})}{\sum_{j=1}^{K} \exp(\phi_{i,j})}$.

- $p_{i,1} + \cdots + p_{i,K} = 1$.
- Thus $\mathbf{p}_i = [p_{i,1}, \cdots, p_{i,K}] \in \mathbb{R}^K$ is a distribution.

Softmax Classifier

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- $\phi_{i,k}$ (the k-th entry of $\boldsymbol{\phi}_i$) indicates how likely $\mathbf{x}_i$ is in the k-th class.
- Softmax function: $p_{i,k} = \frac{\exp(\phi_{i,k})}{\sum_{j=1}^K \exp(\phi_{i,j})}$.
- Cross-entropy loss: $H(\mathbf{y}_i, \mathbf{p}_i) = -\sum_{k=1}^K y_{i,k} \log p_{i,k}$.

Softmax Classifier

Input: feature vectors $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ and labels $\mathbf{y}_1, \cdots, \mathbf{y}_n \in \mathbb{R}^K$.

- Softmax classifier: $\min_{\mathbf{W}} \sum_{i=1}^{n} H(\mathbf{y}_i, \mathbf{p}_i)$

$$\boldsymbol{\phi}_i = \mathbf{W}\mathbf{x}_i \in \mathbb{R}^K, \quad \underbrace{\mathbf{p}_i = \mathrm{SoftMax}(\boldsymbol{\phi}_i)}_{\text{Softmax function}}, \quad \text{and} \quad \underbrace{H(\mathbf{y}_i, \mathbf{p}_i) = -\sum_{k=1}^{K} y_{i,k} \log\left(p_{i,k}\right)}_{\text{Cross-entropy loss}}.$$

Softmax Classifier

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$$\boldsymbol{\phi}_i = \mathbf{W}\mathbf{x}_i \in \mathbb{R}^K, \quad \mathbf{p}_i = \mathrm{SoftMax}(\boldsymbol{\phi}_i), \quad \text{and} \quad H(\mathbf{y}_i, \mathbf{p}_i) = -\sum_{k=1}^{K} y_{i,k} \log(p_{i,k}).$$

- The role of minimizing $H(\mathbf{y}_i, \mathbf{p}_i)$ is making $\mathbf{p}_i$ similar to $\mathbf{y}_i$.
- $H(\mathbf{y}_i, \mathbf{p}_i)$ can be replaced by $||\mathbf{y}_i - \mathbf{p}_i||_2^2$.
- In practice, cross-entropy works better.

Softmax Classifier

Input: feature vectors $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ and labels $\mathbf{y}_1, \cdots, \mathbf{y}_n \in \mathbb{R}^K$.

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Tasks	Methods	Algorithms
Binary Classification	Softmax	Gradient Descent (GD)
Multi-Class Classification	KNN	Accelerated GD
	Neural Networks	Stochastic GD

Gradient of the Objective Function

$\boldsymbol{\phi} = \mathbf{W}\mathbf{x} \in \mathbb{R}^K$, $\quad p_q = \frac{e^{\phi_q}}{\sum_{k=1}^{K} e^{\phi_k}}$, $\quad$ and $\quad H(\mathbf{y}, \mathbf{p}) = -\sum_{k=1}^{K} y_k \log(p_k)$.

- Leave out the subscript i (which indexes a sample.)

Gradient of the Objective Function

$\boldsymbol{\phi} = \mathbf{W}\mathbf{x} \in \mathbb{R}^K$, $\boxed{p_q = \frac{e^{\phi_q}}{\sum_{k=1}^{K} e^{\phi_k}},}$ and $H(\mathbf{y}, \mathbf{p}) = -\sum_{k=1}^{K} y_k \log\boxed{(p_k)}.$

- $H(\mathbf{y}, \mathbf{p}) = -\sum_{k=1}^{K} y_k \phi_k + \log\left(\sum_{j=1}^{K} e^{\phi_j}\right) \cdot \sum_{k=1}^{K} y_k.$

Gradient of the Objective Function

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- $\frac{\partial H}{\partial \phi_k} = -y_k + \frac{1}{\sum_{j=1}^{K} e^{\phi_j}} \cdot e^{\phi_k} \cdot \sum_{k=1}^{K} y_k$

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- $\frac{\partial H}{\partial \phi_k} = -y_k + \underbrace{\boxed{\frac{1}{\sum_{j=1}^{K} e^{\phi_j}} \cdot e^{\phi_k}}}_{= p_k} \cdot \underbrace{\boxed{\sum_{k=1}^{K} y_k}}_{= 1} = -y_k + p_k.$

Gradient of the Objective Function

$\boldsymbol{\phi} = \mathbf{W}\mathbf{x} \in \mathbb{R}^K$ and $H(\mathbf{y}, \mathbf{p}) = -\sum_{k=1}^{K} y_k \phi_k + \log\left(\sum_{j=1}^{K} e^{\phi_j}\right) \cdot \sum_{k=1}^{K} y_k.$

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- $\frac{\partial \phi_k}{\partial \mathbf{w}_{j:}} = \frac{\partial \mathbf{w}_{k:}^T \mathbf{x}}{\partial \mathbf{w}_{j:}} = \begin{cases} \mathbf{x}, & \text{if } k = j; \\ \mathbf{0}, & \text{otherwise.} \end{cases}$ (Here $\mathbf{w}_{j:}$ is the j-th row of $\mathbf{W}$.)
- ➔ $\frac{\partial H}{\partial \mathbf{w}_{j:}} = \sum_{k=1}^{K} \frac{\partial \phi_k}{\partial \mathbf{w}_{j:}} \cdot \frac{\partial H}{\partial \phi_k}$

Gradient of the Objective Function

$\boldsymbol{\phi} = \mathbf{W}\mathbf{x} \in \mathbb{R}^K$ and $H(\mathbf{y}, \mathbf{p}) = -\sum_{k=1}^{K} y_k \phi_k + \log\left(\sum_{j=1}^{K} e^{\phi_j}\right) \cdot \sum_{k=1}^{K} y_k$.

- $\boxed{\frac{\partial H}{\partial \phi_k}} = -y_k + \frac{1}{\sum_{j=1}^{K} e^{\phi_j}} \cdot e^{\phi_k} \cdot \sum_{k=1}^{K} y_k = -y_k + p_k$.
- $\boxed{\frac{\partial \phi_k}{\partial \mathbf{w}_{j:}}} = \frac{\partial \mathbf{w}_{k:}^T \mathbf{x}}{\partial \mathbf{w}_{j:}} = \begin{cases} \mathbf{x}, & \text{if } k = j; \\ \mathbf{0}, & \text{otherwise.} \end{cases}$ (Here $\mathbf{w}_{j:}$ is the j-th row of $\mathbf{W}$.)
- $\rightarrow$ $\frac{\partial H}{\partial \mathbf{w}_{j:}} = \sum_{k=1}^{K} \boxed{\frac{\partial \phi_k}{\partial \mathbf{w}_{j:}}} \cdot \boxed{\frac{\partial H}{\partial \phi_k}} = \left(p_j - y_j\right) \mathbf{x} \in \mathbb{R}^d$.
- $\rightarrow$ $\frac{\partial H}{\partial \mathbf{W}} = (\mathbf{p} - \mathbf{y}) \cdot \mathbf{x}^T \in \mathbb{R}^{K \times d}$.

Softmax Classifier

Input: feature vectors $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ and labels $\mathbf{y}_1, \cdots, \mathbf{y}_n \in \mathbb{R}^K$.

- Softmax classifier: $\min_{\mathbf{W}} \sum_{i=1}^{n} H(\mathbf{y}_i, \mathbf{p}_i)$

  $\boldsymbol{\phi}_i = \mathbf{W}\mathbf{x}_i \in \mathbb{R}^K$, $\mathbf{p}_i = \mathrm{SoftMax}(\boldsymbol{\phi}_i)$, and $H(\mathbf{y}_i, \mathbf{p}_i) = -\sum_{k=1}^{K} y_{i,k} \log\left(p_{i,k}\right)$.

- A stochastic gradient is $\frac{\partial H(\mathbf{y}_i, \mathbf{p}_i)}{\partial \, \mathbf{W}} = (\mathbf{p}_i - \mathbf{y}_i) \cdot \mathbf{x}_i^T \in \mathbb{R}^{K \times d}$.

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Algorithm: Iteratively update $\mathbf{W}$ using the (stochastic) gradient.

Softmax Classifier: Train and Test

- Train (given feature vectors $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ and labels $\mathbf{y}_1, \cdots, \mathbf{y}_n \in \mathbb{R}^K$)
  - Compute $\mathbf{W}^\star = \underset{\mathbf{W}}{\operatorname{argmin}} \sum_{i=1}^{n} -H(\mathbf{y}_i, \mathbf{p}_i)$ by some algorithm, e.g., AGD, SGD, etc.
- Test (for a sample $\mathbf{x}' \in \mathbb{R}^d$)
  - $\boldsymbol{\phi}' = \mathbf{W}^\star \mathbf{x}' \in \mathbb{R}^K$.
  - Return the index of the largest entry of $\boldsymbol{\phi}'$.

Limitations of Softmax Classifier

#Parameter v.s. #Classes

- Suppose $\#\text{features} = 1K$.
- Suppose $\#\text{classes} = 10$ (e.g., digit recognition).
  - $1K \times 10 = 10K$ parameters.
- Suppose $\#\text{classes} = 1K$ (e.g., ImageNet image recognition).
  - $1K \times 1K = 1M$ parameters.
- Suppose $\#\text{classes} = 1M$ (e.g., face recognition).
  - $1K \times 1M = 1G$ parameters ➔ Heavy computation and memory costs.

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  - $1K \times 1K = 1M$ parameters.
- Suppose $\#\text{classes} = 1M$ (e.g., face recognition).
  - $1K \times 1M = 1G$ parameters ➔ Heavy computation and memory costs.
- What if $\#\text{classes} = 1G$? (E.g., face recognition for all the Chinese citizens.)