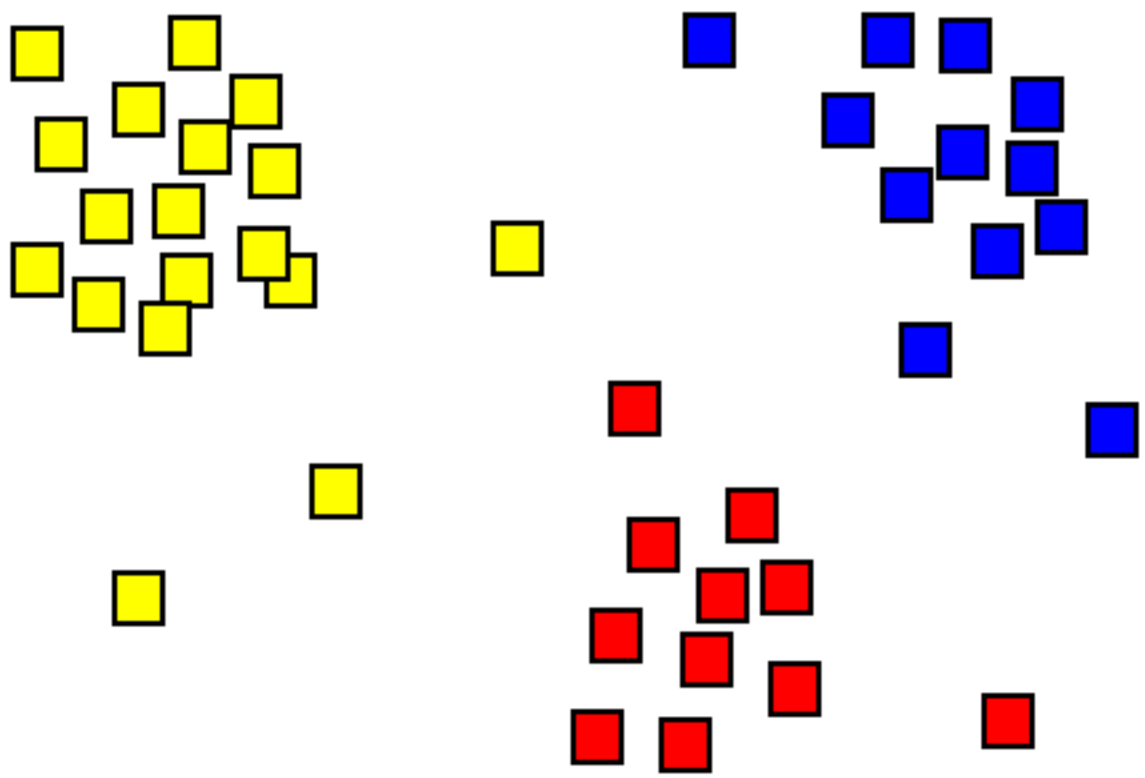
Multiclass classification



Multi-class and Multi-label

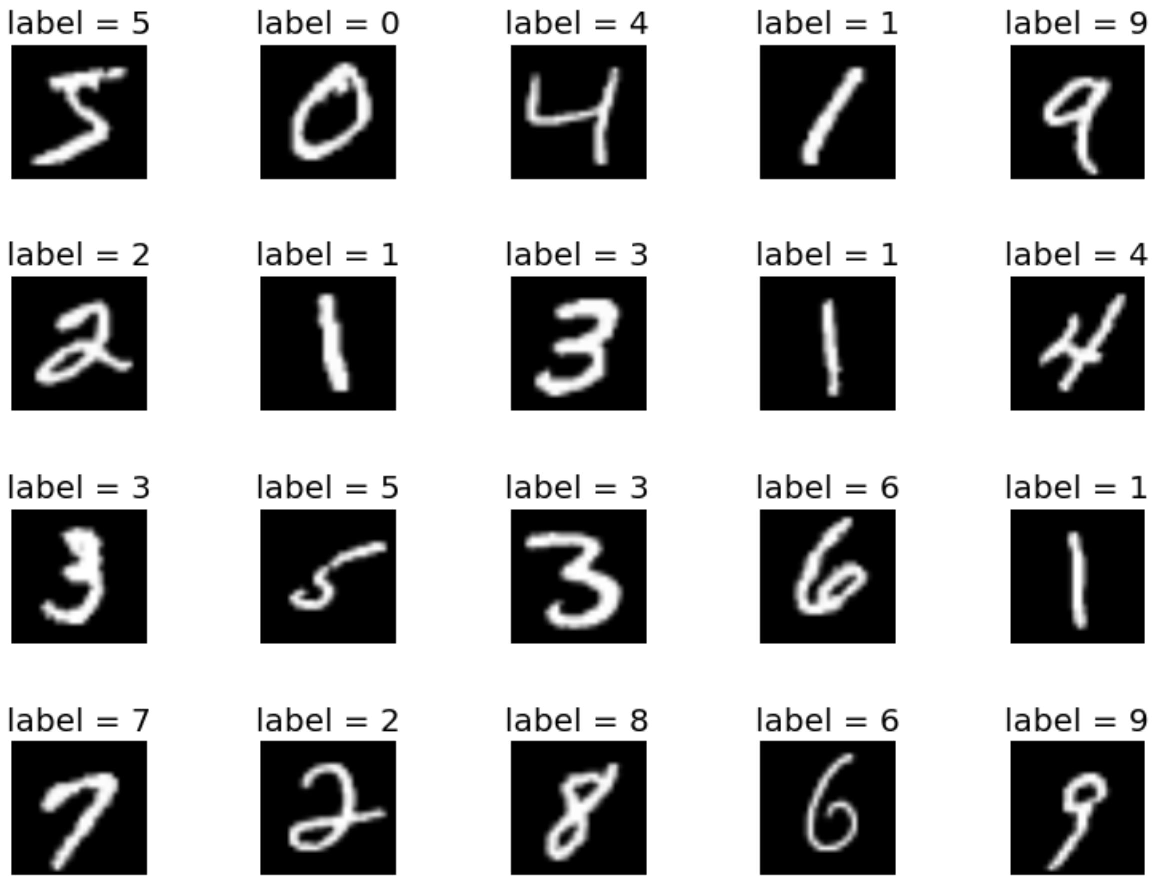
- Multi-class: have multiple classes, with each instance only in one class
  - e.g., a person can only have one blood type
- Multi-label: have multiple classes, where each instance can have multiple class labels
  - e.g., a newspaper article can be a sports article and medicine article

Exercise: problem representation for classification

- What if have many classes (e.g., image classification)?
  - Example: classify written digit (e.g., 7 or 3)
  - Example: classify images based on presence of an object (e.g., cat)
  - Is image classification multi-class or multi-label?

- What other settings can you imagine with many classes?

How can we learn this?



Exercise: problem representation for classification

- What if have many many classes (e.g., image classification)?
  - Example: classify written digit (e.g., 7 or 3)
  - Example: classify images based on presence of an object (e.g., cat)
  - Is image classification multi-class or multi-label?
- One approach for either multi-class or multi-label: learn one logistic regression model for each class separately
  - What are the issues here?
- What other techniques can we use for multi-class and multi-label?

One-vs-all

- Learn binary classifier for each class, w1, …, wk
  - i.e., weight vector w2 predict if the sample is either class 2 or its not
  - If training sample x is class 2, then weights w2 get label y = 1 and the weights wi for the other classes get a label of y = 0
- Once have wi, how do we predict on a new sample?
  - e.g., w1, w2 w3,
  - $p(y = 1 \mid x, w1) = 0.9$. $p(y = 1 \mid x, w2) = 0.6$. $p(y = 1 \mid x, w3) = 0.1$
- For multi-class, pick class such that $p(y = 1 \mid x, wi)$ is largest
  - In this example that is class 1
- For multi-label, pick classes such that $p(y = 1 \mid x, wi) > 0.5$
  - In this example that is class 1 and 2

One-vs-all for multi-class

- What are the issues with this approach for multi-class?
  - see many more negative samples
  - have to compare confidence p(y=1 | x) between different classes, but scale could be different

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One-vs-all for multi-label

- Called binary relevance for multi-label
- What are the issues with one-vs-rest for multi-label?
  - class independence assumption
  - Do not take advantage of relationships between classes

- Learn binary classifier for each class, w1, …, wk
  - i.e., weights w2 predict if the sample is either class 2 or its not
  - If training sample x is class 2, then weights w2 get label y = 1 and the weights wi for the other classes get a label of y = 0
- Once have wi, how do we predict on a new sample?
  - $p(y = 1 \mid x, w1) = 0.9$. $p(y = 1 \mid x, w2) = 0.6$. $p(y = 1 \mid x, w3) = 0.1$

One-vs-one for multi-class

- Learn k (k-1)/2 binary classifiers, with voting scheme: class with most positive predictions is outputted

- For k = 3 (three classes), train class 1 vs class 2 (p_12), class 1 vs 3 (p_13), class 2 vs 3 (p_23)

- Predict with

$$f(\mathbf{x}) = \arg \max_{i \in \{1,2,3\}} \sum_j p_{ij}(y = 1(\text{i.e., } y = i \text{ not } j)|\mathbf{x})$$

- Notice this uses p_{31}, but I didn't train that. Where does it come from?

Advantages to vs-all or vs-one

- Imagine you have a dataset with n samples, d features, k classes
- When might one-vs-all or one-vs-one be better?
  - Vs-one has to train about k^2 models, can be expensive!
  - But, gets to train k^2 models on a subset of the data (about 2 n / k if the data is balanced, i.e., equal number of each class)
- If n = 1 million and k = 10, which one might be better? Which learning methods might prefer one or the other?
  - If method scales poorly with sample size, vs-one might be better
  - If method can share part of solution across classes, vs-all might be better
  - If method suffers from class imbalance, vs-one might be better
  - If k is large, vs-all might be better
  - Easier to parallelize vs-one

Other approaches for multi-class

- naive Bayes (generative model)
- Instance-based approaches (e.g. k-NN)
  - keep a representative set of samples, compare to these points and what labels they had
- Hierarchical classification
- Multinomial logistic regression

Multinomial distributions

- Extend binary GLM (logistic regression) to multi-class, by moving from Bernoulli to Multinomial
- What does target y look like?
- y = [0 1 0 0] means that instance is in class 2 out of 4 classes
- What distribution matches such a target?
  - Clearly not Bernoulli, where its only zero or 1
  - Clearly not Gaussian…

Multinomial distributions

- Extend binary GLM (logistic regression) to multi-class, by moving from Bernoulli to Multinomial (here specifically Categorical dist)

- Multinomial distribution is probability of n successes in k Bernoulli trials

We have n = 1, e.g. y = [1 0 0 0]

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{y_1! \dots y_k!} p(y_1 = 1|\mathbf{x})^{y_1} \dots, p(y_k = 1|\mathbf{x})^{y_k}$$

Predictions

- Targets look like y = [0 1 0 0], meaning that instance is in class 2 out of 4 classes

- For a new sample, we predict
  [p(y=1 | x), p(y = 2| x), …, p(y = k | x)]

- Example: [0.1 0.2 0.6 0.1] suggests we should pick class y = 3, since it has the highest probability

- How do we generate such a vector of probabilities?

Multinomial logistic regression

(Categorical distribution)

- y = [0 1 0 0] means that instance is in class 2 out of 4 classes
- Let k be the number of classes, n = 1 for 1 success

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{y_1! \dots y_k!} p(y_1 = 1|\mathbf{x})^{y_1} \dots, p(y_k = 1|\mathbf{x})^{y_k}$$

- The transfer (inverse of link) is the softmax transfer

$$\begin{aligned} \mathrm{softmax}(\mathbf{x}^\top \mathbf{W}) &= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)}, \dots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)} \right] \\ &= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}, \dots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})} \right] \end{aligned}$$

$$\exp(\mathbf{x}^\top \mathbf{W}) = [\exp(\mathbf{x}^\top \mathbf{w}_1), \dots, \exp(\mathbf{x}^\top \mathbf{w}_k)] \qquad \mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_k] \in \mathbb{R}^{d \times k}$$

Softmax transfer

$$\mathrm{softmax}(\mathbf{x}^\top \mathbf{W}) = \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\sum_{j=1}^k \exp(\mathbf{x}^\top \mathbf{w}_j)}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\sum_{j=1}^k \exp(\mathbf{x}^\top \mathbf{w}_j)}\right]$$
$$= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}\right]$$

Normalization to ensure that get valid probabilities

Must set vector of weights w_k = 0 to make softmax an invertible transfer

Relation to logistic regression

- For k= 2, y = [0 1] or y = [1 0]

$$\mathrm{softmax}(\mathbf{x}^\top \mathbf{W}) = \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)} \right]$$

$$= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})} \right]$$

$$\mathbf{W} = [\mathbf{w},\ \mathbf{0}]$$

$$\begin{aligned} p(y = 0 | \mathbf{x}) &= \frac{\exp(\mathbf{x}^\top \mathbf{w})}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})} \\ &= \frac{\exp(\mathbf{x}^\top \mathbf{w})}{\exp(\mathbf{x}^\top \mathbf{w}) + \exp(\mathbf{x}^\top \mathbf{0})} \\ &= \frac{\exp(\mathbf{x}^\top \mathbf{w})}{\exp(\mathbf{x}^\top \mathbf{w}) + 1} \\ &= \sigma(\mathbf{x}^\top \mathbf{w}). \end{aligned}$$

Relation to logistic regression…

- In general, setting w_k to zero is a convention
  - could choose any of the classes, e.g., could learn p(y = 1 | x)

- Normalization enforces constraint on w_k (or on one of the classes), so can set w_k = 0
  - **Exercise**: show that setting w_k = 0 is also required to ensure that the softmax transfer is invertible

$$
\begin{aligned}
\operatorname{softmax}(\mathbf{x}^\top \mathbf{W}) &= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)} \right] \\
&= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})} \right]
\end{aligned}
$$

Summary of multinomial logistic regression

- p(y | x) is a multinomial distribution
- Corresponding transfer is the softmax transfer with w_k = 0
- Prediction on new x is
- softmax(xW) = [p(y=1 | x), p(y = 2| x), …, p(y = k | x)]

Learning strategy

- Using the minimization obtained for our generalized linear models, we can plug in the transfer to get

$$\min_{\mathbf{W}\in\mathbb{R}^{d\times k}:\mathbf{W}_{:k}=\mathbf{0}} \sum_{i=1}^{n} \log\left(\mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})\right) - \mathbf{x}_i^\top \mathbf{W}\mathbf{y}_i$$

with gradient

$$\nabla \sum_{i=1}^{n} \left(\log\left(\mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})\right) - \mathbf{x}_i^\top \mathbf{W}\mathbf{y}_i\right) = \sum_{i=1}^{n} \frac{\exp(\mathbf{x}_i^\top \mathbf{W})^\top \mathbf{x}_i^\top}{\mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})} - \mathbf{x}_i\mathbf{y}_i^\top.$$

How do we constrain w_k = 0?

$$(\mathrm{softmax}(\mathbf{x}_i^T \mathbf{w}) - y_i)\mathbf{x}_i$$

What is the algorithm?

Reminders: Oct. 24, 2019

- Assignment 2 due Friday
- Midterm in two weeks
- We will do a review class on Tuesday, with the midterm on Thursday
  - There is a practice midterm on eClass

Example: SGD for multinomial logistic regression

- For one stochastic update, with sample (xi, yi)

$$s = \mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})$$

$$\text{for } j = 1, \ldots, k-1$$

$$\mathbf{w}_j = \mathbf{w}_j - \eta \left[\frac{\exp(\mathbf{x}_i^\top \mathbf{w}_j)}{s} - \mathbf{y}_{ij} \right] \mathbf{x}_i$$

Exercise: nonlinear GLMs

- In linear regression, we used nonlinear expansions on the features to get nonlinear learning
  - e.g., convert x to polynomials
- Can we do the same for logistic regression or multinomial logistic regression?
- Why would we want to? Aren't GLMs already nonlinear?