Machine Learning
ITCS 4156

Logistic Regression

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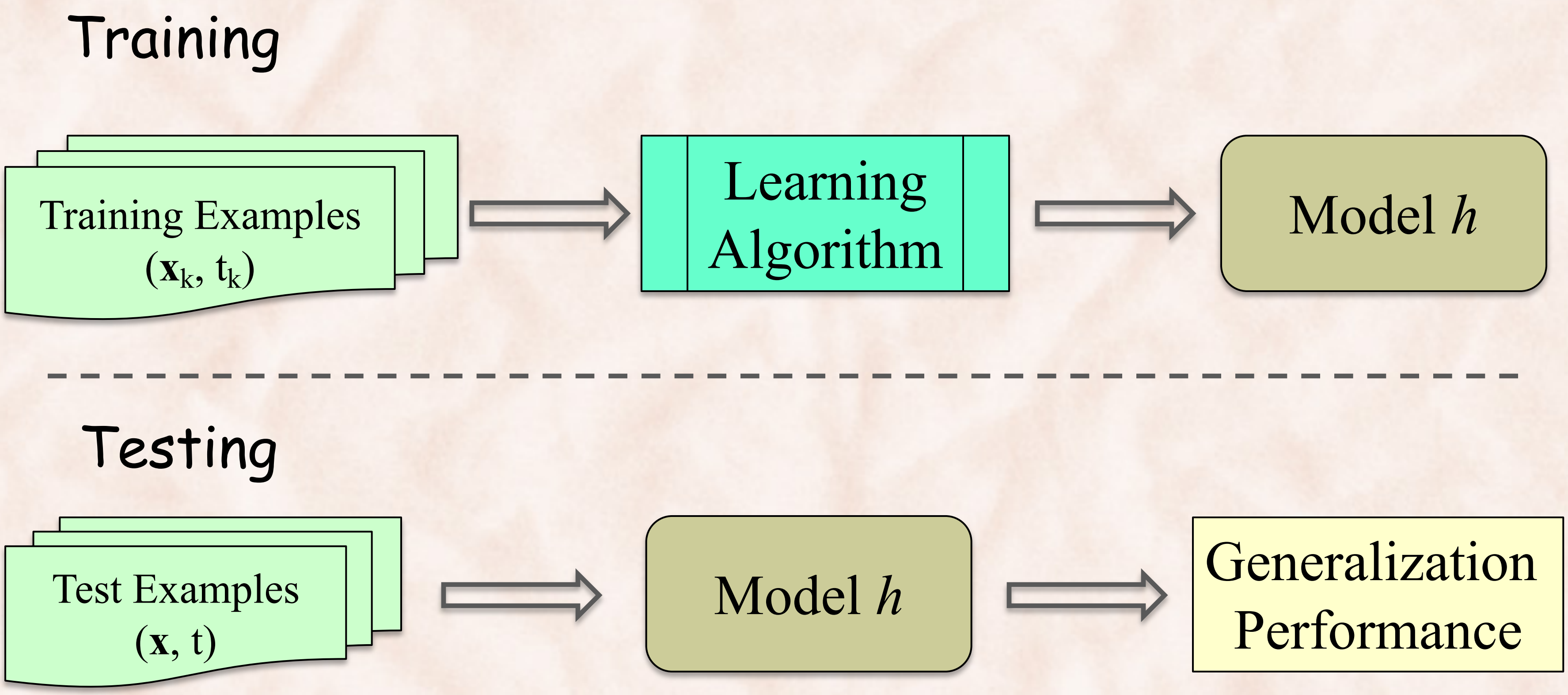
Supervised Learning



Supervised Learning

- **Task** = learn an (unkown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - **Classification**:
    - The output $t(\mathbf{x}) \in T$ is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t(\mathbf{x}) \in T$ is continuous, or has a continuous component.

- Target function $t(\mathbf{x})$ is known (only) through (noisy) set of training examples:

  $(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$

Parametric Approaches to Supervised Learning

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:

    => h is able to fit data that it has seen.
  - h also matches t well on test data:

    => h is able to **generalize to unseen data**.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters **w**:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

Three Parametric Approaches to Classification

1) Discriminant Functions: construct $f : X \rightarrow T$ that directly assigns a vector $\mathbf{x}$ to a specific class C_k.
   - Inference and decision combined into a single learning problem.
   - *Linear Discriminant*: the decision surface is a hyperplane in X:
     - Perceptron
     - Support Vector Machines
     - Fisher 's Linear Discriminant

Three Parametric Approaches to Classification

2) Probabilistic Discriminative Models: directly model the posterior class probabilities $p(C_k \mid \mathbf{x})$.
   - Inference and decision are separate.
   - Less data needed to estimate $p(C_k \mid \mathbf{x})$ than $p(\mathbf{x} \mid C_k)$.
   - Can accommodate many overlapping features.
     - Logistic Regression
     - Conditional Random Fields

Three Parametric Approaches to Classification

3) Probabilistic Generative Models:
   - Model class-conditional $p(\mathbf{x} \mid C_k)$ as well as the priors $p(C_k)$, then use Bayes's theorem to find $p(C_k \mid \mathbf{x})$.
     - or model $p(\mathbf{x}, C_k)$ directly, then marginalize to obtain the posterior probabilities $p(C_k \mid \mathbf{x})$.
   - Inference and decision are separate.
   - Can use $p(\mathbf{x})$ for *outlier* or *novelty detection*.
   - Need to model dependencies between features.
     - Naïve Bayes.
     - Hidden Markov Models.

Generative and Discriminative Classifiers

Suppose we're distinguishing cat from dog images

ImageNet

ImageNet

Generative Classifier:

- Build a model of what's in a cat image
  - Knows about whiskers, ears, eyes
  - Assigns a probability to any image:
    - how cat-y is this image?

Also build a model for dog images

Given a new image:

Run both models and see which one fits better.

Discriminative Classifier

Just try to distinguish dogs from cats

Oh look, dogs have collars!

Let's ignore everything else.

Finding the correct class c from a document d in Generative vs Discriminative Classifiers

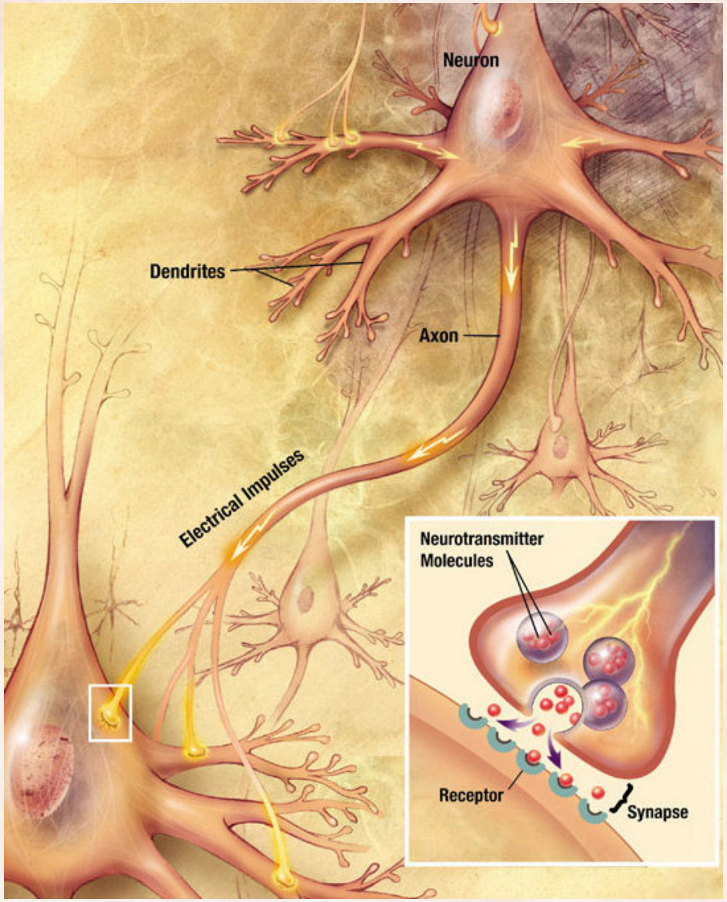
- Naive Bayes

$$\hat{c} = \operatorname*{argmax}_{c \in C} \overbrace{P(d|c)}^{\text{likelihood}} \overbrace{P(c)}^{\text{prior}}$$

- Logistic Regression

$$\hat{c} = \operatorname*{argmax}_{c \in C} \overset{\text{posterior}}{P(c|d)}$$

Neurons



Soma is the central part of the neuron:

- *where the input signals are combined.*

Dendrites are cellular extensions:

- *where majority of the input occurs.*

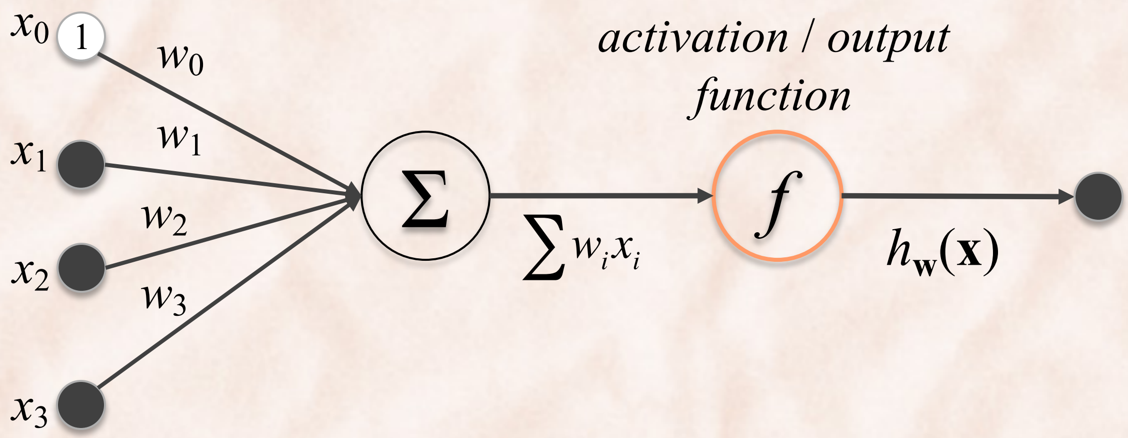
Axon is a fine, long projection:

- *carries nerve signals to other neurons.*

Synapses are molecular structures between axon terminals and other neurons:

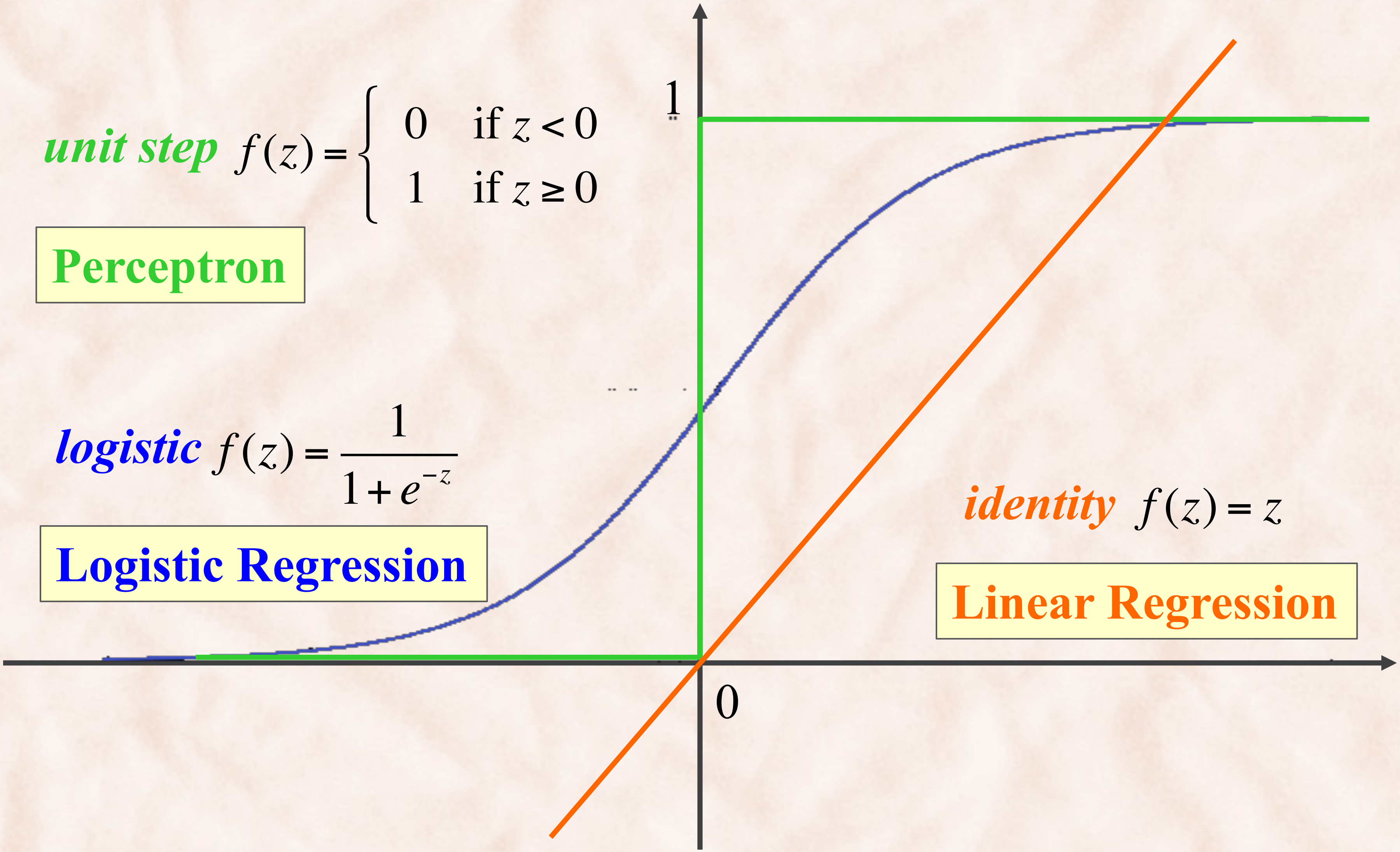
- *where the communication takes place.*

McCulloch-Pitts Neuron Function

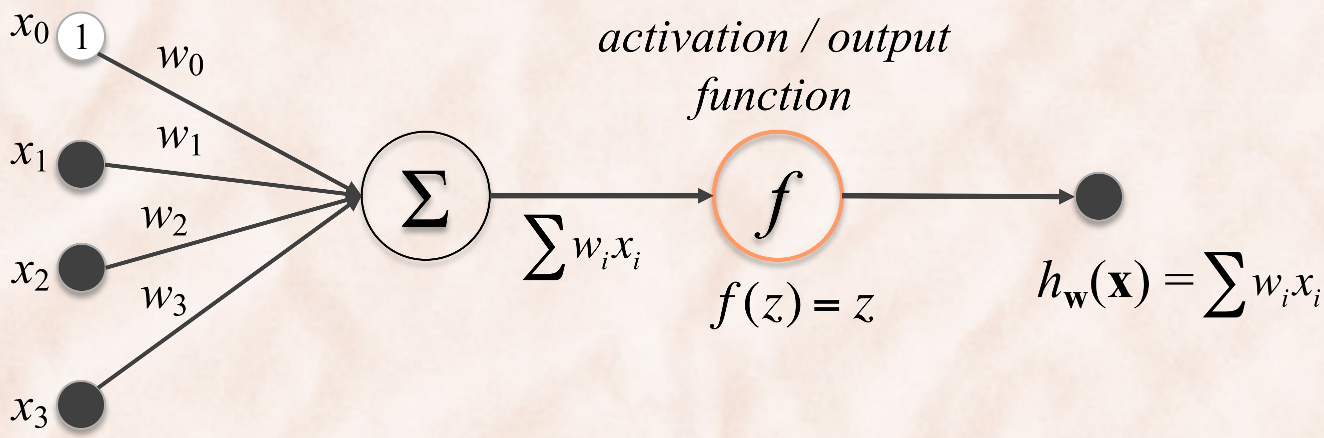


- Algebraic interpretation:
  - The output of the neuron is a **linear combination** of inputs from other neurons, **rescaled by** the synaptic **weights**.
    - weights w_i correspond to the synaptic weights (activating or inhibiting).
    - summation corresponds to combination of signals in the soma.
  - It is often transformed through an **activation / output function**.

Activation Functions



Linear Regression

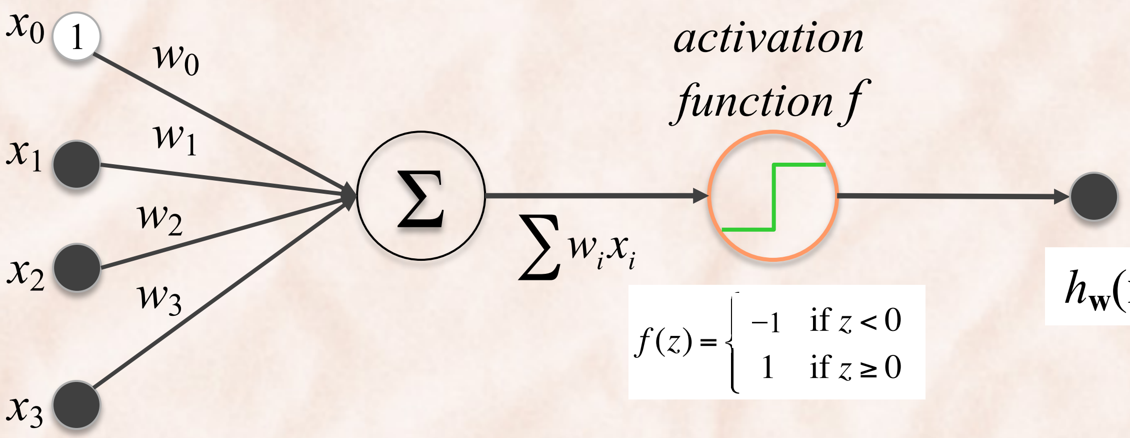


- Polynomial curve fitting is Linear Regression:

  $\mathbf{x} = \varphi(x) = [1, x, x^2, \ldots, x^M]^T$

  $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$

Perceptron



$$f(z) = \begin{cases} -1 & \text{if } z < 0 \\ 1 & \text{if } z \geq 0 \end{cases}$$

$$h_{\mathbf{w}}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w}^T\mathbf{x} > 0 \\ -1 & \text{otherwise} \end{cases}$$

- Assume classes $T = \{c_1, c_2\} = \{1, -1\}$.
- Training set is $(\mathbf{x}_1, t_1), (\mathbf{x}_2, t_2), \ldots (\mathbf{x}_n, t_n)$.

  $\mathbf{x} = [1, x_1, x_2, ..., x_k]^T$

  $h(\mathbf{x}) = sgn(\mathbf{w}^T\mathbf{x}) = sgn(w_0 + w_1\, x_1 + \ldots + w_k\, x_k)$

a linear discriminant function

Linear Discriminant Functions

- Use a linear function of the input vector:

$$h(\mathbf{x}) = \underbrace{\mathbf{w}^T}_{\textit{weight vector}} \varphi(\mathbf{x}) + \underbrace{w_0}_{\textit{bias} = -\textit{threshold}}$$

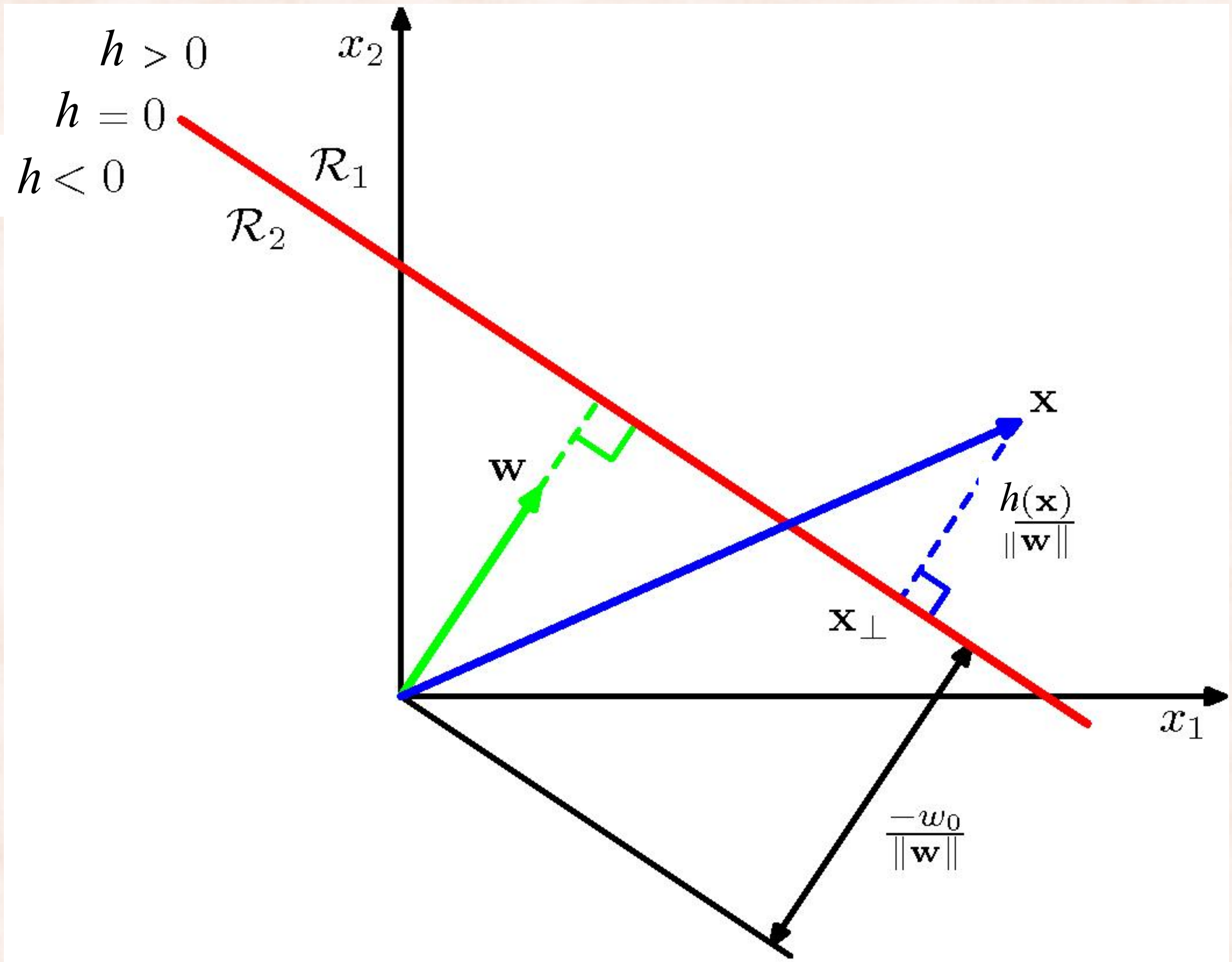
- Decision:

$\mathbf{x} \in C_1$ if $h(\mathbf{x}) \geq 0$, otherwise $\mathbf{x} \in C_2$.

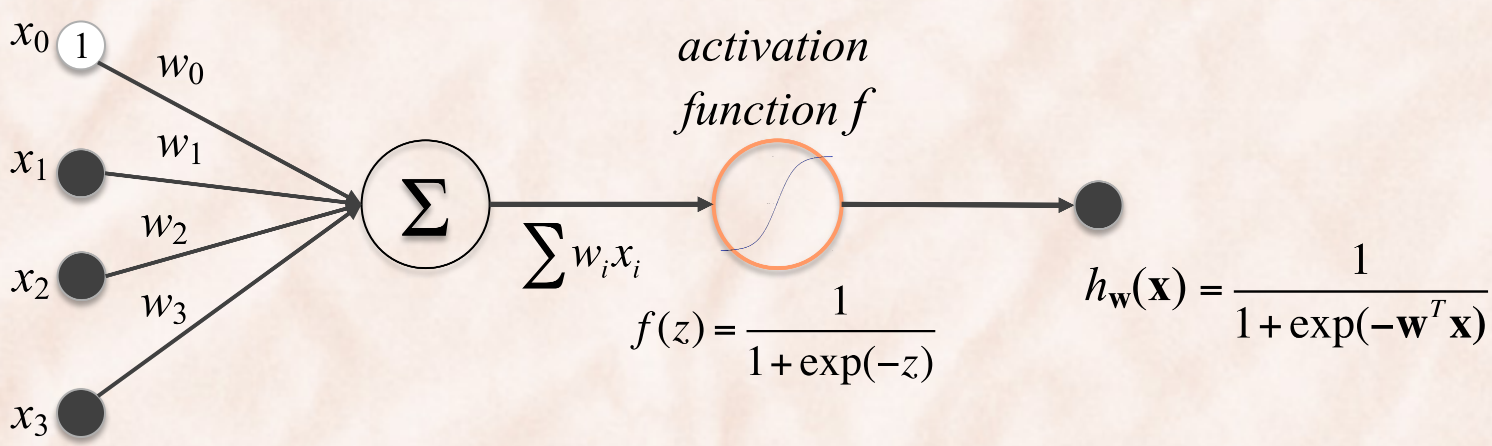
$\Rightarrow$ decision boundary is hyperplane $h(\mathbf{x}) = 0$.

- Properties:
  - $\mathbf{w}$ is orthogonal to vectors lying within the decision surface.
  - w_0 controls the location of the decision hyperplane.

Geometric Interpretation



Logistic Regression



- Training set is $(\mathbf{x}_1,t_1)$, $(\mathbf{x}_2,t_2)$, … $(\mathbf{x}_n,t_n)$.

  $\mathbf{x} = [1, x_1, x_2, ..., x_k]^T$

  $h(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x})$

- Can be used for both classification and regression:
  - Classification: $T = \{C_1, C_2\} = \{1, 0\}$.
  - Regression: $T = [0, 1]$ (i.e. output needs to be normalized).

Logistic Regression for Binary Classification

- Model output can be interpreted as **posterior class probabilities**:

$$p(C_1 | \mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}))}$$

$$p(C_2 | \mathbf{x}) = 1 - \sigma(\mathbf{w}^T \mathbf{x}) = \frac{\exp(-\mathbf{w}^T \mathbf{x})}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$

- How do we train a logistic regression model?
  - What **error/cost function** to minimize?

Example: LR for Sentiment Classification

Logistic Regression Learning

- Learning = finding the "right" parameters $\mathbf{w}^T = [w_0, w_1, \dots, w_k]$
  - Find $\mathbf{w}$ that minimizes an *error function* $E(\mathbf{w})$ which measures the misfit between $h(\mathbf{x}_n, \mathbf{w})$ and t_n.
  - Expect that $h(\mathbf{x},\mathbf{w})$ performing well on training examples $\mathbf{x}_n \Rightarrow$ $h(\mathbf{x},\mathbf{w})$ will perform well on arbitrary test examples $\mathbf{x} \in X$.

- **Least Squares** error function?

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{h(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

  - Differentiable => can use gradient descent ✓
  - Non-convex => not guaranteed to find the global optimum ✗

Maximum Likelihood

Training set is D = $\{\langle \mathbf{x}_n, t_n\rangle \mid t_n \in \{0,1\}, n \in 1\ldots\mathrm{N}\}$

Let $h_n = p(C_1 \mid \mathbf{x}_n) \Leftrightarrow h_n = p(t_n = 1 \mid \mathbf{x}_n) = \sigma(\mathbf{w}^T \mathbf{x}_n)$

Maximum Likelihood (ML) principle: find parameters that maximize the likelihood of the labels.

- The likelihood function is $p(\mathbf{t} \mid \mathbf{w}) = \prod_{n=1}^{N} h_n^{t_n}(1-h_n)^{(1-t_n)}$
- The negative log-likelihood (cross entropy) error function:

$$E(\mathbf{w}) = -\ln p(\mathbf{t} \mid \mathbf{x}) = -\sum_{n=1}^{N}\{t_n \ln h_n + (1-t_n)\ln(1-h_n)\} \times \frac{1}{N}$$

we also average

Maximum Likelihood Learning for Logistic Regression

- The ML solution is:

convex in **w**

$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} p(\mathbf{t} \mid \mathbf{w}) = \arg\min_{\mathbf{w}} \boxed{E(\mathbf{w})}$$

- ML solution is given by $\nabla E(\mathbf{w}) = 0$.
  - Cannot solve analytically => solve numerically with gradient based methods: (stochastic) gradient descent, conjugate gradient, L-BFGS, etc.
  - Gradient is (prove it):

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T \times \frac{1}{N}$$

Regularized Logistic Regression

- Use a Gaussian prior over the parameters:

$$\mathbf{w} = [w_0, w_1, \dots, w_M]^{\mathrm{T}}$$

$$p(\mathbf{w}) = N(\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

- Bayes' Theorem:

$$p(\mathbf{w} \mid \mathbf{t}) = \frac{p(\mathbf{t} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathbf{t})} \propto p(\mathbf{t} \mid \mathbf{w})\, p(\mathbf{w})$$

- MAP solution:

$$\mathbf{w}_{MAP} = \arg\max_{\mathbf{w}} p(\mathbf{w} \mid \mathbf{t})$$

Regularized Logistic Regression

- MAP solution:

$$\mathbf{w}_{MAP} = \arg\max_{\mathbf{w}} p(\mathbf{w} \mid \mathbf{t}) \quad = \arg\max_{\mathbf{w}} p(\mathbf{t} \mid \mathbf{w}) p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} - \ln p(\mathbf{t} \mid \mathbf{w}) p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} - \ln p(\mathbf{t} \mid \mathbf{w}) - \ln p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} E_D(\mathbf{w}) - \ln p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} E_D(\mathbf{w}) + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} \qquad \boxed{= \arg\min_{\mathbf{w}} E_D(\mathbf{w}) + E_{\mathbf{w}}(\mathbf{w})}$$

$$E_D(\mathbf{w}) = -\sum_{n=1}^{N} \{ t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \} \times \frac{1}{N} \dashrightarrow \boxed{\textit{data term}}$$

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} \dashrightarrow \boxed{\textit{regularization term}}$$

Regularized Logistic Regression

- MAP solution:

$$\mathbf{w}_{MAP} = \arg\min_{\mathbf{w}} \boxed{E_D(\mathbf{w}) + E_{\mathbf{w}}(\mathbf{w})}$$

still convex in **w**

- ML solution is given by $\nabla E(\mathbf{w}) = 0$.

α is also called ***decay***

$$\nabla E(\mathbf{w}) = \nabla E_D(\mathbf{w}) + \nabla E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(h_n - t_n)\mathbf{x}_n^T + \alpha \mathbf{w}^T$$

where $h_n = \sigma(\mathbf{w}^T \mathbf{x}_n)$

- Cannot solve analytically => solve numerically:
  - (stochastic) gradient descent [PRML 3.1.3], Newton Raphson iterative optimization [PRML 4.3.3], conjugate gradient, LBFGS.

Implementation: Vectorization of LR

- **Version 1**: Compute gradient component-wise.

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T \times \frac{1}{N}$$

  – Assume example $\mathbf{x}_n$ is stored in column X[:,n] in data matrix X.

```
grad = np.zeros(K)
for n in range(N):
    h = sigmoid(w.dot(X[:,n]))
    temp = h − t[n]
    for k in range(K):
        grad[k] = grad[k] + temp * X[k,n] / N
```

```
def sigmoid(x):
    return 1 / (1 + np.exp(−x))
```

Implementation: Vectorization of LR

- **Version 2**: Compute gradient, partially vectorized.

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T \times \frac{1}{N}$$

```
grad = np.zeros(K)
for n in range(N):
    grad = grad + (sigmoid(w.dot(X[:,n])) − t[n]) * X[:,n] / N
```

```
def sigmoid(x):
    return 1 / (1 + np.exp(−x))
```

Implementation: Vectorization of LR

- **Version 3**: Compute gradient, vectorized.

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T \times \frac{1}{N}$$

grad = X.dot(sigmoid(**w**.dot(X)) − **t**) / N

```
def sigmoid(x):
    return 1 / (1 + np.exp(−x))
```

Vectorization of LR with Separate Bias

- Separate the bias b from the weight vector $\mathbf{w}$.
- Compute gradient separately with respect to $\mathbf{w}$ and b:
  - Gradient with respect to $\mathbf{w}$ is:

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T \times \frac{1}{N}$$

$$h_n = \sigma(\mathbf{w}^T \mathbf{x}_n + b)$$

grad = X.dot(sigmoid(**w**.dot(X) + *b*) − **t**) / N

  - Gradient with respect to bias b is:

$$\Delta b = -\frac{1}{N} \sum_{n=1}^{N} (h_n - t_n)$$

```
def sigmoid(x):
   return 1 / (1 + np.exp(−x))
```

Vectorization of LR with Regularization

- Only the gradient with respect to **w** changes:
  - never use L2 regularization on bias.

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T \times \frac{1}{N} + \alpha \mathbf{w}$$

grad = X.dot(sigmoid(**w**.dot(X) + *b*) − **t**) / N + *α***w**

Softmax Regression = Logistic Regression for Multiclass Classification

- Multiclass classification:

  $T = \{C_1, C_2, ..., C_K\} = \{1, 2, ..., K\}$.

- Training set is $(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \dots (\mathbf{x}_n,t_n)$.

  $\mathbf{x} = [1, x_1, x_2, ..., x_M]$

  $t_1, t_2, \dots t_n \in \{1, 2, ..., K\}$

- One weight vector per class [PRML 4.3.4]:

$$p(C_k \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_k^T \mathbf{x}))}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x})}$$

bias parameter inside each $\mathbf{w}_j$

$$p(C_k|\mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T \mathbf{x}_n + b_k)}{\sum_{j=1..K} \exp(\mathbf{w}_j^T \mathbf{x}_n + b_j)}$$

separate bias parameter b_j

Softmax Regression (K ≥ 2)

- Inference:

$$C_* = \arg\max_{C_k} p(C_k \mid \mathbf{x})$$

$$= \arg\max_{C_k} \frac{\exp(\mathbf{w}_k^T \mathbf{x})}{\boxed{\sum_j \exp(\mathbf{w}_j^T \mathbf{x})}}$$

$Z(\mathbf{x})$ a normalization constant

$$= \arg\max_{C_k} \exp(\mathbf{w}_k^T \mathbf{x})$$

$$= \arg\max_{C_k} \mathbf{w}_k^T \mathbf{x}$$

- Training using:
  - Maximum Likelihood (ML)
  - Maximum A Posteriori (MAP) with a Gaussian prior on **w**.

Softmax Regression

- The **negative log-likelihood** error function is:

$$E_D(\mathbf{w}) = -\frac{1}{N}\ln\prod_{n=1}^{N} p(t_n \mid \mathbf{x}_n) = \boxed{-\frac{1}{N}\sum_{n=1}^{N}\ln\frac{\exp(\mathbf{w}_{t_n}^T\mathbf{x}_n)}{Z(\mathbf{x}_n)}}$$

convex in $\mathbf{w}$

- The Maximum Likelihood solution is:

$$\mathbf{w}_{ML} = \arg\min_{\mathbf{w}} E_D(\mathbf{w})$$

- The **gradient** is (prove it):

$$\nabla_{\mathbf{w}_k} E_D(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N}\big(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\big)\mathbf{x}_n$$

where $\delta_t(x) = \begin{cases} 1 & x = t \\ 0 & x \neq t \end{cases}$ is the *Kronecker delta* function.

Regularized Softmax Regression

- The new **cost** function is:

$$E(\mathbf{w}) = E_D(\mathbf{w}) + E_{\mathbf{w}}(\mathbf{w})$$

$$= -\frac{1}{N}\sum_{n=1}^{N} \ln \frac{\exp\left(\mathbf{w}_{t_n}^T \mathbf{x}_n\right)}{Z(\mathbf{x}_n)} + \frac{\alpha}{2}\|\mathbf{w}\|^2$$

- The new **gradient** is (prove it):

$$\boldsymbol{grad}_k = \nabla_{\mathbf{w}_k} E(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha \mathbf{w}_k^T$$

Softmax Regression

- ML solution is given by $\nabla E_D(\mathbf{w}) = 0$.
  - Cannot solve analytically.
  - Solve numerically, by pluging [*cost*, *gradient*] = [$E(\mathbf{w})$, $\nabla E(\mathbf{w})$] values into general convex solvers:
    - L-BFGS
    - Newton methods
    - conjugate gradient
    - (stochastic / minibatch) gradient-based methods.
      - gradient descent (with / without momentum).
      - AdaGrad, AdaDelta
      - RMSProp
      - ADAM, ...

Implementation

- Need to compute [*cost*, ***grad***]:
  - *cost* $= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\delta_k(t_n)\ln p(C_k \mid \mathbf{x}_n) + \frac{\alpha}{2}\sum_{k=1}^{K}\mathbf{w}_k^T\mathbf{w}_k$
  - ***grad***$_k$ $= -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha\mathbf{w}_k^T$

=> need to compute, for k = 1, ..., K:

- *output* $p(C_k \mid \mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n))}{\sum_j \exp(\mathbf{w}_j^T\mathbf{x}_n)}$

Overflow when $\mathbf{w}_k{}^T\mathbf{x}_n$ are too large.

Implementation: Preventing Overflows

- Subtract from each product $\mathbf{w}_k{}^{\mathrm{T}}\mathbf{x}_n$ the maximum product:

$$c_n = \max_{1 \le k \le K} \mathbf{w}_k^T \mathbf{x}_n$$

$$p(C_k \mid \mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T \mathbf{x}_n - c_n))}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x}_n - c_n)}$$

- When using separate bias b_k, replace $\mathbf{w}_k^T \mathbf{x}_n$ everywhere with $\mathbf{w}_k^T \mathbf{x}_n + b_k$.

Vectorization of Softmax with Separate Bias

- Separate the bias b_k from the weight vector $\mathbf{w}_k$.
- Compute gradient separately with respect to $\mathbf{w}_k$ and b_k :
  - Gradient with respect to $\mathbf{w}_k$ is:

$$\mathbf{grad}_k = -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha \mathbf{w}_k^T$$

Gradient matrix is $[\mathbf{grad}_1 \mid \mathbf{grad}_2 \mid \ldots \mid \mathbf{grad}_K]$

- Gradient with respect to b_k is:

$$\Delta b_k = -\frac{1}{N}\sum_{n=1}^{N}(\delta_k(t_n) - p(C_k|\mathbf{x}_n))$$

Gradient vector is $\Delta \mathrm{b} = [\Delta b_1 \mid \Delta b_2 \mid \ldots \mid \Delta b_K]$

$$p(C_k|\mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n + b_k)}{\sum_{j=1..K}\exp(\mathbf{w}_j^T\mathbf{x}_n + b_j)}$$

$$\delta_k(t_n) = \begin{cases} 1\,, if\ t_n = k \\ 0\,, if\ t_n \neq k \end{cases}$$

Vectorization of Softmax

- Need to compute [*cost*, ***grad***, Δb]:

$$p(C_k|\mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n + b_k)}{\sum_{j=1..K}\exp(\mathbf{w}_j^T\mathbf{x}_n + b_j)}$$

  - *cost* $= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\delta_k(t_n)\ln p(C_k \mid \mathbf{x}_n) + \frac{\alpha}{2}\sum_{k=1}^{K}\mathbf{w}_k^T\mathbf{w}_k$
  - ***grad***$_k$ $= -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha\mathbf{w}_k^T$

=> compute ground truth matrix G such that G[k,n] = $\delta_k(t_n)$

$$\delta_k(t_n) = \begin{cases} 1, \text{if } t_n = k \\ 0, \text{if } t_n \neq k \end{cases}$$

```
from scipy.sparse import coo_matrix
groundTruth = coo_matrix((np.ones(N, dtype = np.uint8),
                          (labels, np.arange(N)))).toarray()
```

Vectorization of Softmax

- Compute $cost = -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\delta_k(t_n)\ln p(C_k \mid \mathbf{x}_n) + \frac{\alpha}{2}\sum_{k=1}^{K}\mathbf{w}_k^T\mathbf{w}_k$
  - Compute matrix of $\mathbf{w}_k^T\mathbf{x}_n + b_k$.
  - Compute matrix of $\mathbf{w}_k^T\mathbf{x}_n + b_k - c_n$.
  - Compute matrix of $\exp(\mathbf{w}_k^T\mathbf{x}_n + b_k - c_n)$.
  - Compute matrix of $\ln p(C_k|\mathbf{x}_n)$.
  - Compute log-likelihood cost using all the above.

$$p(C_k|\mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n + b_k)}{\sum_{j=1..K}\exp(\mathbf{w}_j^T\mathbf{x}_n + b_j)}$$

$$\delta_k(t_n) = \begin{cases} 1, if\ t_n = k \\ 0, if\ t_n \neq k \end{cases}$$

$$c_n = \max_{1\le k\le K} \mathbf{w}_k^T\mathbf{x}_n + b_k$$

Vectorization of Softmax

- Compute $\mathbf{grad}_k = -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha \mathbf{w}_k^T$
  - **Gradient matrix** = [**grad**$_1$ | **grad**$_2$ | … | **grad**$_K$]
    - Compute matrix of $p(C_k|\mathbf{x}_n)$.
    - Compute matrix of gradient of data term.
    - Compute matrix of gradient of regularization term.

$$p(C_k|\mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n + b_k)}{\sum_{j=1..K}\exp(\mathbf{w}_j^T\mathbf{x}_n + b_j)}$$

$$\delta_k(t_n) = \begin{cases} 1, if\ t_n = k \\ 0, if\ t_n \neq k \end{cases}$$

Vectorization of Softmax

- Useful Numpy functions:
  - np.dot()
  - np.amax()
  - np.argmax()
  - np.exp()
  - np.sum()
  - np.log()
  - np.mean()

Implementation: Gradient Checking

- Want to minimize $J(\theta)$, where θ is a scalar.

- Mathematical definition of derivative:

$$\frac{d}{d\theta}J(\theta) = \lim_{\varepsilon \to 0} \frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}$$

- Numerical approximation of derivative:

$$\frac{d}{d\theta}J(\theta) \approx \frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon} \qquad \text{where } \varepsilon = 0.0001$$

Implementation: Gradient Checking

- If $\boldsymbol{\theta}$ is a vector of parameters $\boldsymbol{\theta}_i$,
  - Compute numerical derivative with respect to each $\boldsymbol{\theta}_i$.
    - Create a vector $\mathbf{v}$ that is ε in position i and 0 everywhere else:
      - *How do you do this without a for loop in NumPy?*
    - Compute $G_{\text{num}}(\boldsymbol{\theta}_i) = (J(\boldsymbol{\theta} + \mathbf{v}) - J(\boldsymbol{\theta} - \mathbf{v})) / 2\varepsilon$
  - Aggregate all derivatives into numerical gradient $G_{\text{num}}(\boldsymbol{\theta})$.

- Compare numerical gradient $G_{\text{num}}(\boldsymbol{\theta})$ with implementation of gradient $G_{\text{imp}}(\boldsymbol{\theta})$:

$$\frac{\left\| G_{num}(\boldsymbol{\theta}) - G_{imp}(\boldsymbol{\theta}) \right\|}{\left\| G_{num}(\boldsymbol{\theta}) + G_{imp}(\boldsymbol{\theta}) \right\|} \leq 10^{-6}$$